



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 06:09 PM EST

PDB ID : 4GW9
Title : Structure of a bacteriophytochrome and light-stimulated protomer swapping with a gene repressor
Authors : Bellini, D.; Papiz, M.Z.
Deposited on : 2012-09-01
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

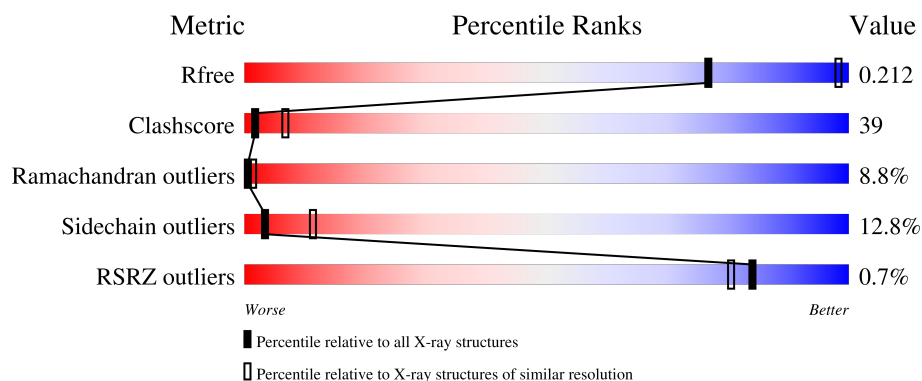
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	 41% 37% 16% • 5%
1	B	655	 46% 36% 11% • 5%
1	C	655	 44% 39% 11% • 5%
1	D	655	 45% 34% 14% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BLA	A	900	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called bacteriophytochrome.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	Se	0	4	0
			4902	3085	883	910	8	16			
1	B	621	Total	C	N	O	S	Se	0	0	0
			4823	3032	870	900	8	13			
1	C	622	Total	C	N	O	S	Se	0	1	0
			4839	3042	875	901	8	13			
1	D	615	Total	C	N	O	S	Se	0	1	0
			4785	3005	865	894	8	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP B3Q7C0
A	-18	GLY	-	expression tag	UNP B3Q7C0
A	-17	SER	-	expression tag	UNP B3Q7C0
A	-16	SER	-	expression tag	UNP B3Q7C0
A	-15	HIS	-	expression tag	UNP B3Q7C0
A	-14	HIS	-	expression tag	UNP B3Q7C0
A	-13	HIS	-	expression tag	UNP B3Q7C0
A	-12	HIS	-	expression tag	UNP B3Q7C0
A	-11	HIS	-	expression tag	UNP B3Q7C0
A	-10	HIS	-	expression tag	UNP B3Q7C0
A	-9	SER	-	expression tag	UNP B3Q7C0
A	-8	SER	-	expression tag	UNP B3Q7C0
A	-7	GLY	-	expression tag	UNP B3Q7C0
A	-6	LEU	-	expression tag	UNP B3Q7C0
A	-5	VAL	-	expression tag	UNP B3Q7C0
A	-4	PRO	-	expression tag	UNP B3Q7C0
A	-3	ARG	-	expression tag	UNP B3Q7C0
A	-2	GLY	-	expression tag	UNP B3Q7C0
A	-1	SER	-	expression tag	UNP B3Q7C0
A	0	HIS	-	expression tag	UNP B3Q7C0
A	2	VAL	-	SEE REMARK 999	UNP B3Q7C0

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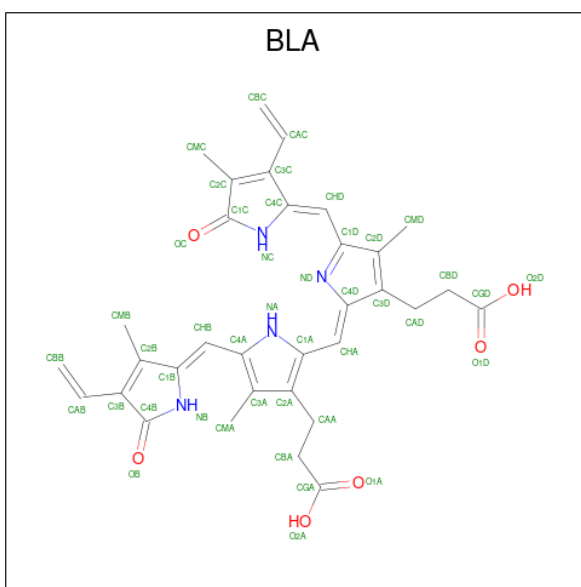
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
A	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
B	-19	MSE	-	expression tag	UNP B3Q7C0
B	-18	GLY	-	expression tag	UNP B3Q7C0
B	-17	SER	-	expression tag	UNP B3Q7C0
B	-16	SER	-	expression tag	UNP B3Q7C0
B	-15	HIS	-	expression tag	UNP B3Q7C0
B	-14	HIS	-	expression tag	UNP B3Q7C0
B	-13	HIS	-	expression tag	UNP B3Q7C0
B	-12	HIS	-	expression tag	UNP B3Q7C0
B	-11	HIS	-	expression tag	UNP B3Q7C0
B	-10	HIS	-	expression tag	UNP B3Q7C0
B	-9	SER	-	expression tag	UNP B3Q7C0
B	-8	SER	-	expression tag	UNP B3Q7C0
B	-7	GLY	-	expression tag	UNP B3Q7C0
B	-6	LEU	-	expression tag	UNP B3Q7C0
B	-5	VAL	-	expression tag	UNP B3Q7C0
B	-4	PRO	-	expression tag	UNP B3Q7C0
B	-3	ARG	-	expression tag	UNP B3Q7C0
B	-2	GLY	-	expression tag	UNP B3Q7C0
B	-1	SER	-	expression tag	UNP B3Q7C0
B	0	HIS	-	expression tag	UNP B3Q7C0
B	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
B	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
B	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
C	-19	MSE	-	expression tag	UNP B3Q7C0
C	-18	GLY	-	expression tag	UNP B3Q7C0
C	-17	SER	-	expression tag	UNP B3Q7C0
C	-16	SER	-	expression tag	UNP B3Q7C0
C	-15	HIS	-	expression tag	UNP B3Q7C0
C	-14	HIS	-	expression tag	UNP B3Q7C0
C	-13	HIS	-	expression tag	UNP B3Q7C0
C	-12	HIS	-	expression tag	UNP B3Q7C0
C	-11	HIS	-	expression tag	UNP B3Q7C0
C	-10	HIS	-	expression tag	UNP B3Q7C0
C	-9	SER	-	expression tag	UNP B3Q7C0
C	-8	SER	-	expression tag	UNP B3Q7C0
C	-7	GLY	-	expression tag	UNP B3Q7C0
C	-6	LEU	-	expression tag	UNP B3Q7C0
C	-5	VAL	-	expression tag	UNP B3Q7C0
C	-4	PRO	-	expression tag	UNP B3Q7C0
C	-3	ARG	-	expression tag	UNP B3Q7C0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP B3Q7C0
C	-1	SER	-	expression tag	UNP B3Q7C0
C	0	HIS	-	expression tag	UNP B3Q7C0
C	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
C	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
C	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
D	-19	MSE	-	expression tag	UNP B3Q7C0
D	-18	GLY	-	expression tag	UNP B3Q7C0
D	-17	SER	-	expression tag	UNP B3Q7C0
D	-16	SER	-	expression tag	UNP B3Q7C0
D	-15	HIS	-	expression tag	UNP B3Q7C0
D	-14	HIS	-	expression tag	UNP B3Q7C0
D	-13	HIS	-	expression tag	UNP B3Q7C0
D	-12	HIS	-	expression tag	UNP B3Q7C0
D	-11	HIS	-	expression tag	UNP B3Q7C0
D	-10	HIS	-	expression tag	UNP B3Q7C0
D	-9	SER	-	expression tag	UNP B3Q7C0
D	-8	SER	-	expression tag	UNP B3Q7C0
D	-7	GLY	-	expression tag	UNP B3Q7C0
D	-6	LEU	-	expression tag	UNP B3Q7C0
D	-5	VAL	-	expression tag	UNP B3Q7C0
D	-4	PRO	-	expression tag	UNP B3Q7C0
D	-3	ARG	-	expression tag	UNP B3Q7C0
D	-2	GLY	-	expression tag	UNP B3Q7C0
D	-1	SER	-	expression tag	UNP B3Q7C0
D	0	HIS	-	expression tag	UNP B3Q7C0
D	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
D	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
D	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0
2	C	1	Total 43	C 33	N 4	O 6	0	0
2	D	1	Total 43	C 33	N 4	O 6	0	0

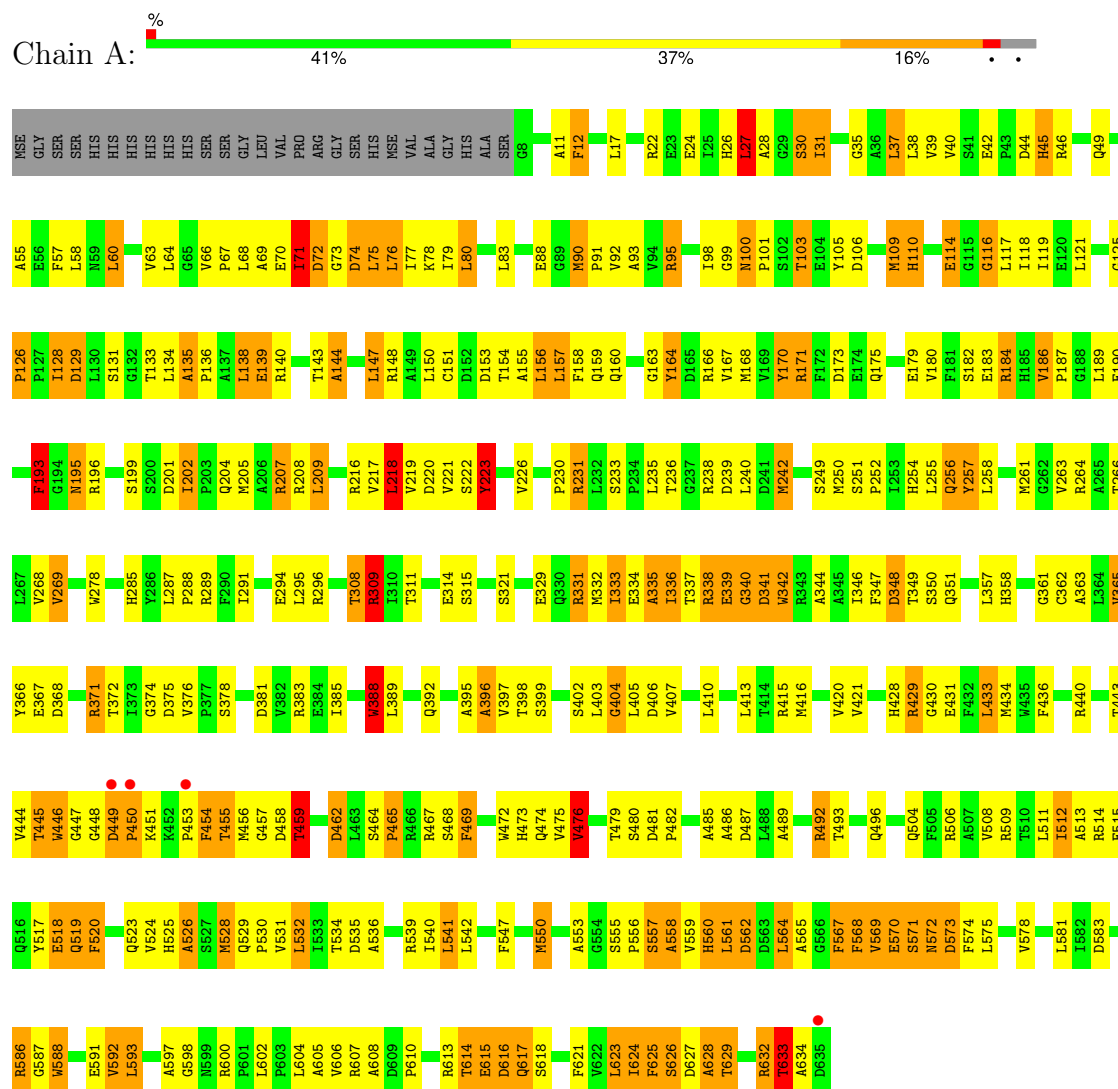
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0
3	B	69	Total O 69 69	0	0
3	C	92	Total O 92 92	0	0
3	D	77	Total O 77 77	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: bacteriophytochrome



• Molecule 1: bacteriophytochrome



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.94Å 146.87Å 139.55Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.90) 97.0 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.200 , 0.243 0.208 , 0.212	Depositor DCC
R_{free} test set	4392 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19838	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	3/5009 (0.1%)	1.19	19/6787 (0.3%)
1	B	0.78	5/4915 (0.1%)	1.15	27/6663 (0.4%)
1	C	0.88	4/4934 (0.1%)	1.16	17/6686 (0.3%)
1	D	0.78	1/4875 (0.0%)	1.08	9/6607 (0.1%)
All	All	0.84	13/19733 (0.1%)	1.15	72/26743 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	TRP	CD2-CE2	8.14	1.51	1.41
1	C	20	CYS	CB-SG	-6.85	1.70	1.82
1	A	446	TRP	CD2-CE2	6.21	1.48	1.41
1	B	388	TRP	CD2-CE2	6.08	1.48	1.41
1	C	266	THR	CB-CG2	5.99	1.72	1.52
1	B	230	PRO	N-CA	-5.47	1.38	1.47
1	D	388	TRP	CD2-CE2	5.43	1.47	1.41
1	C	446	TRP	CD2-CE2	5.25	1.47	1.41
1	A	588	TRP	CD2-CE2	5.23	1.47	1.41
1	B	472	TRP	CD2-CE2	5.14	1.47	1.41
1	C	588	TRP	CD2-CE2	5.09	1.47	1.41
1	B	90	MSE	CG-SE	-5.07	1.78	1.95
1	B	446	TRP	CD2-CE2	5.02	1.47	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	C-N-CD	-19.55	77.59	120.60
1	B	229	GLU	C-N-CA	13.09	176.96	122.00
1	B	242	MSE	CG-SE-CE	-7.85	81.63	98.90
1	A	506	ARG	NE-CZ-NH1	7.74	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	GLY	N-CA-C	7.38	131.55	113.10
1	D	437	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	230	PRO	CA-N-CD	-7.28	101.31	111.50
1	A	404	GLY	N-CA-C	-7.25	94.96	113.10
1	B	466	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	625	PHE	CB-CA-C	7.03	124.46	110.40
1	A	331	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	519	GLN	N-CA-C	-6.67	93.00	111.00
1	A	487	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	B	280	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	C	229	GLU	C-N-CD	6.47	142.00	128.40
1	C	338	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	232	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	337	THR	N-CA-C	-6.41	93.69	111.00
1	C	118	ILE	CB-CA-C	-6.40	98.80	111.60
1	A	518	GLU	N-CA-C	-6.31	93.96	111.00
1	C	231	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	27	LEU	CA-CB-CG	6.22	129.61	115.30
1	C	302	LEU	CA-CB-CG	6.21	129.59	115.30
1	D	214	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	61	GLY	N-CA-C	-6.08	97.90	113.10
1	B	205	MSE	CG-SE-CE	-6.06	85.57	98.90
1	B	389	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	116	GLY	N-CA-C	5.94	127.96	113.10
1	C	123	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	564	LEU	CA-CB-CG	5.90	128.88	115.30
1	C	207	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	170	TYR	CA-CB-CG	5.67	124.17	113.40
1	A	309	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	43	PRO	CA-N-CD	-5.65	103.59	111.50
1	B	404	GLY	N-CA-C	-5.61	99.07	113.10
1	D	349	THR	N-CA-CB	5.61	120.95	110.30
1	D	142	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	117	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	B	506	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	125	GLY	N-CA-C	5.54	126.94	113.10
1	C	165	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	B	338	ARG	N-CA-C	-5.50	96.16	111.00
1	A	341	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	49	GLN	N-CA-C	5.49	125.82	111.00
1	C	248	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	518	GLU	N-CA-C	-5.46	96.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	338	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	331	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	475	VAL	N-CA-C	-5.38	96.48	111.00
1	B	48	ILE	N-CA-C	-5.34	96.58	111.00
1	B	309	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	117	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	340	GLY	N-CA-C	5.28	126.30	113.10
1	A	218	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	C	205	MSE	CG-SE-CE	-5.23	87.40	98.90
1	B	28	ALA	N-CA-C	-5.20	96.95	111.00
1	A	129	ASP	N-CA-C	5.19	125.01	111.00
1	C	230	PRO	N-CA-C	-5.18	98.62	112.10
1	C	509	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	470	ALA	N-CA-C	-5.15	97.11	111.00
1	B	432	PHE	CB-CA-C	-5.11	100.18	110.40
1	A	462	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	583	ASP	CB-CG-OD1	5.09	122.89	118.30
1	B	97	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	97	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	378	SER	N-CA-CB	5.07	118.11	110.50
1	D	575	LEU	N-CA-C	-5.06	97.34	111.00
1	B	44	ASP	N-CA-C	5.05	124.64	111.00
1	A	207	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	207	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	218	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4902	0	4861	428	0
1	B	4823	0	4770	373	0
1	C	4839	0	4794	338	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4785	0	4727	367	0
2	A	43	0	31	24	0
2	B	43	0	31	19	0
2	C	43	0	31	10	0
2	D	43	0	30	7	0
3	A	79	0	0	16	0
3	B	69	0	0	14	0
3	C	92	0	0	10	0
3	D	77	0	0	7	0
All	All	19838	0	19275	1527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1527) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:BLA:HMB3	2:B:900:BLA:CMA	1.52	1.40
2:C:900:BLA:CMA	2:C:900:BLA:HMB3	1.50	1.37
1:A:336:ILE:HG21	1:A:342:TRP:CA	1.55	1.35
1:A:336:ILE:CG2	1:A:342:TRP:HA	1.59	1.32
1:A:624:ILE:O	1:A:624:ILE:HD13	1.36	1.22
1:D:519:GLN:O	1:D:521:SER:N	1.71	1.20
1:A:591:GLU:HA	3:A:1019:HOH:O	1.47	1.14
1:B:336:ILE:CG2	1:B:342:TRP:HA	1.77	1.14
2:B:900:BLA:HBC1	2:B:900:BLA:HMC1	1.29	1.14
1:C:218:LEU:HD22	1:C:250:MSE:SE	1.99	1.13
1:D:257:TYR:HD2	1:D:261:MSE:HE2	1.11	1.12
1:C:332:MSE:HE1	1:C:498:VAL:HG22	1.21	1.11
1:D:336:ILE:HG21	1:D:342:TRP:CA	1.79	1.11
1:D:336:ILE:CG2	1:D:342:TRP:HA	1.80	1.10
1:B:331:ARG:HG2	1:B:351:GLN:NE2	1.65	1.09
1:A:336:ILE:CD1	1:A:344:ALA:HB2	1.81	1.09
1:D:385:ILE:HG21	1:D:434:MSE:HE1	1.32	1.09
1:A:336:ILE:HD13	1:A:344:ALA:CB	1.82	1.08
2:C:900:BLA:HMB3	2:C:900:BLA:HMA1	1.34	1.08
1:C:534:THR:HG23	3:C:1047:HOH:O	1.52	1.08
1:A:218:LEU:HD23	1:A:250:MSE:SE	2.03	1.08
1:B:611:VAL:O	1:B:612:THR:HG22	1.50	1.08
1:D:534:THR:HG21	1:D:561:LEU:HD21	1.16	1.08
1:C:90:MSE:HE3	1:C:109:MSE:HE3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:900:BLA:HMB3	2:C:900:BLA:HMA2	1.14	1.06
1:D:413:LEU:HB2	1:D:416:MSE:HE1	1.37	1.06
1:A:385:ILE:HG21	1:A:434:MSE:HE1	1.13	1.06
1:A:337:THR:O	1:A:338:ARG:HG3	1.53	1.06
1:B:385:ILE:HG21	1:B:434:MSE:HE1	1.36	1.05
1:B:331:ARG:HG2	1:B:351:GLN:HE22	1.17	1.05
2:A:900:BLA:HMB3	2:A:900:BLA:HMA2	1.07	1.05
1:D:551:LEU:O	1:D:553:ALA:N	1.90	1.05
1:C:258:LEU:HD23	1:C:261:MSE:CE	1.87	1.05
2:A:900:BLA:HMB3	2:A:900:BLA:CMA	1.85	1.04
1:B:90:MSE:HE2	1:B:110:HIS:HA	1.36	1.04
1:A:218:LEU:CD2	1:A:250:MSE:SE	2.55	1.03
1:B:550:MSE:CE	1:B:604:LEU:HD11	1.87	1.03
2:C:900:BLA:CMA	2:C:900:BLA:CMB	2.37	1.03
1:A:453:PRO:HA	1:A:454:PHE:HB2	1.38	1.02
1:D:257:TYR:CD2	1:D:261:MSE:HE2	1.95	1.01
1:B:611:VAL:HG21	1:C:511:LEU:HD23	1.42	1.00
1:B:336:ILE:HG23	1:B:342:TRP:HA	1.37	0.99
2:B:900:BLA:CMA	2:B:900:BLA:CMB	2.40	0.99
1:B:77:ILE:O	1:B:78:LYS:HB2	1.57	0.99
1:A:150:LEU:O	1:A:154:THR:HG23	1.62	0.99
1:A:335:ALA:O	1:A:336:ILE:HB	1.59	0.99
2:B:900:BLA:HMB3	2:B:900:BLA:HMA2	1.00	0.99
1:C:608:ALA:HB2	1:C:623:LEU:HD13	1.44	0.99
1:D:26:HIS:CD2	1:D:205:MSE:HE3	1.96	0.98
1:A:42:GLU:OE2	1:A:117:LEU:HD13	1.62	0.98
1:B:26:HIS:CD2	1:B:27:LEU:HD13	1.99	0.98
1:D:168:MSE:HE3	1:D:170:TYR:CE1	1.99	0.98
2:A:900:BLA:HMA2	2:A:900:BLA:CMB	1.93	0.98
2:A:900:BLA:HMC1	2:A:900:BLA:HBC1	1.47	0.96
2:B:900:BLA:CMB	2:B:900:BLA:HMA2	1.94	0.96
1:D:292[A]:HIS:H	1:D:292[A]:HIS:CD2	1.71	0.96
1:A:128:ILE:HD12	3:A:1072:HOH:O	1.66	0.95
1:A:625:PHE:HB3	1:A:626:SER:HA	1.48	0.95
1:D:107:GLY:C	1:D:108:LEU:HD12	1.86	0.95
1:A:434:MSE:HE2	1:A:436:PHE:HE1	1.29	0.95
1:B:476:VAL:N	3:B:1009:HOH:O	1.92	0.95
1:A:336:ILE:HD13	1:A:344:ALA:HB2	0.97	0.94
1:D:518:GLU:O	1:D:519:GLN:CB	2.16	0.94
1:A:625:PHE:HB2	1:A:626:SER:CB	1.97	0.94
1:A:385:ILE:CG2	1:A:434:MSE:HE1	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:PHE:HB2	1:A:626:SER:OG	1.69	0.93
1:B:605:ALA:HB3	1:B:627:ASP:HB2	1.47	0.93
1:C:130:LEU:HD22	1:C:134:LEU:HD13	1.50	0.93
2:C:900:BLA:HMA2	2:C:900:BLA:CMB	1.99	0.92
1:B:550:MSE:HE1	1:B:604:LEU:HD11	1.49	0.92
1:C:258:LEU:HD23	1:C:261:MSE:HE3	1.51	0.92
1:B:100:ASN:HD22	1:B:101:PRO:CD	1.83	0.92
1:C:327[A]:ARG:NH1	1:C:351:GLN:OE1	2.03	0.91
2:C:900:BLA:HBB1	2:C:900:BLA:HMB1	1.48	0.91
1:B:100:ASN:HD22	1:B:101:PRO:HD2	1.32	0.90
1:A:235:LEU:HD13	1:A:235:LEU:O	1.72	0.90
1:A:434:MSE:HE2	1:A:436:PHE:CE1	2.08	0.89
1:D:534:THR:HG21	1:D:561:LEU:CD2	2.01	0.89
1:C:475:VAL:O	1:C:476:VAL:HG22	1.72	0.89
1:A:568:PHE:CE2	1:A:592:VAL:HG11	2.09	0.88
1:B:257:TYR:CE2	1:B:261:MSE:HE3	2.08	0.88
1:B:336:ILE:HG21	1:B:342:TRP:HA	1.53	0.88
1:D:168:MSE:HE1	2:D:900:BLA:HAB	1.55	0.88
1:A:114:GLU:OE1	1:A:236:THR:HG21	1.74	0.88
1:C:291:ILE:HD11	1:C:295:LEU:HD22	1.55	0.88
1:A:155:ALA:O	1:A:167:VAL:HG21	1.72	0.87
1:A:518:GLU:OE2	3:A:1038:HOH:O	1.92	0.87
1:C:370:ILE:HD12	1:C:379:THR:HG23	1.54	0.87
1:C:629:THR:HB	1:C:630:ASP:HB3	1.54	0.87
1:A:605:ALA:HA	3:A:1019:HOH:O	1.75	0.87
1:B:26:HIS:CD2	1:B:27:LEU:CD1	2.57	0.87
1:A:258:LEU:HB3	1:A:263:VAL:CG2	2.04	0.87
1:A:332:MSE:HE2	1:A:342:TRP:CE3	2.09	0.86
1:B:59:ASN:HB3	1:B:100:ASN:HD21	1.40	0.86
1:B:59:ASN:HB3	1:B:100:ASN:ND2	1.89	0.86
2:B:900:BLA:HMB3	2:B:900:BLA:HMA1	1.57	0.86
1:D:348:ASP:C	1:D:350:SER:H	1.75	0.86
1:A:258:LEU:HD23	1:A:261:MSE:HE3	1.56	0.86
1:A:453:PRO:HA	1:A:454:PHE:CB	2.04	0.86
2:A:900:BLA:HMA1	2:A:900:BLA:C1B	2.04	0.86
1:A:624:ILE:O	1:A:624:ILE:CD1	2.23	0.86
1:D:168:MSE:HE3	1:D:170:TYR:HE1	1.37	0.86
1:D:534:THR:CG2	1:D:561:LEU:HD21	2.04	0.85
1:D:250:MSE:HE2	1:D:255:LEU:HD23	1.57	0.85
1:C:370:ILE:HD13	1:C:370:ILE:O	1.76	0.85
1:A:257:TYR:CD2	1:A:261:MSE:HE2	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:CE2	1:A:261:MSE:HE2	2.11	0.84
1:C:541:LEU:HD23	3:C:1082:HOH:O	1.76	0.84
1:A:339:GLU:O	3:A:1017:HOH:O	1.94	0.84
1:A:475:VAL:O	1:A:476:VAL:HG12	1.77	0.83
1:A:550:MSE:HE1	1:A:604:LEU:HD11	1.59	0.83
1:C:434:MSE:HE2	1:C:436:PHE:CZ	2.12	0.83
1:A:73:GLY:O	1:A:75:LEU:N	2.11	0.83
1:A:335:ALA:O	1:A:336:ILE:CB	2.25	0.83
1:B:77:ILE:O	1:B:78:LYS:CB	2.27	0.83
1:A:518:GLU:O	1:A:519:GLN:HB2	1.77	0.83
1:A:334:GLU:O	1:A:336:ILE:N	2.12	0.83
1:A:567:PHE:O	1:A:568:PHE:HB2	1.78	0.83
1:B:90:MSE:HE2	1:B:110:HIS:CA	2.09	0.83
1:B:142:ARG:N	3:B:1041:HOH:O	2.11	0.83
1:D:132:GLY:O	1:D:134:LEU:N	2.12	0.83
1:D:144:ALA:O	1:D:309:ARG:NH1	2.11	0.82
1:B:26:HIS:ND1	1:B:205:MSE:HE3	1.94	0.82
1:A:338:ARG:O	1:A:339:GLU:HG2	1.79	0.82
1:A:518:GLU:O	1:A:519:GLN:CB	2.28	0.82
1:D:389:LEU:HD21	1:D:422:ALA:CB	2.09	0.82
1:A:410:LEU:HB3	1:A:413:LEU:HD12	1.62	0.81
1:A:100:ASN:OD1	1:A:101:PRO:HD2	1.80	0.81
1:A:332:MSE:C	1:A:335:ALA:HB3	2.00	0.81
1:A:336:ILE:HG23	1:A:341:ASP:O	1.80	0.81
1:A:509:ARG:HD2	1:D:520:PHE:CE1	2.16	0.81
1:D:365:VAL:HG12	1:D:370:ILE:HG13	1.61	0.81
1:B:166:ARG:HD2	1:B:168:MSE:HE2	1.63	0.81
2:A:900:BLA:CMA	2:A:900:BLA:CMB	2.57	0.81
1:B:365:VAL:HG22	1:B:430:GLY:O	1.81	0.80
1:C:37:LEU:HD23	1:C:38:LEU:N	1.96	0.80
1:A:458:ASP:O	1:A:459:THR:HG23	1.80	0.80
1:B:63:VAL:O	1:B:66:VAL:HG13	1.81	0.80
1:C:144:ALA:O	1:C:309:ARG:NH1	2.14	0.80
2:C:900:BLA:HBC1	2:C:900:BLA:HMC1	1.64	0.80
1:C:357:LEU:HD21	1:C:491:ALA:HB2	1.64	0.79
1:D:332:MSE:HE1	1:D:498:VAL:HA	1.64	0.79
1:A:291:ILE:CG1	1:A:295:LEU:HD12	2.11	0.79
1:B:335:ALA:O	1:B:336:ILE:HG22	1.83	0.79
1:B:594:LEU:HD23	1:B:602:LEU:HD13	1.64	0.79
1:C:42:GLU:HB3	1:C:43:PRO:HD2	1.65	0.79
1:C:457:GLY:N	3:C:1089:HOH:O	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TRP:O	1:A:476:VAL:HG12	1.82	0.78
1:B:409:GLU:OE1	1:B:410:LEU:HD12	1.84	0.78
1:B:420:VAL:CG2	1:B:434:MSE:CE	2.61	0.78
1:B:471:LYS:O	1:B:475:VAL:HG12	1.84	0.78
1:C:542:LEU:HD12	1:C:543:MSE:N	1.98	0.78
1:C:555:SER:HB3	1:C:556:PRO:C	2.04	0.78
1:D:336:ILE:HG23	1:D:337:THR:N	1.96	0.78
1:D:394:ARG:O	1:D:395:ALA:CB	2.31	0.78
1:D:229:GLU:O	1:D:231:ARG:N	2.17	0.78
1:C:608:ALA:CB	1:C:623:LEU:HD13	2.15	0.77
1:D:623:LEU:N	1:D:623:LEU:HD23	1.98	0.77
1:B:553:ALA:C	3:B:1003:HOH:O	2.22	0.77
1:D:151:CYS:HA	1:D:154:THR:HG23	1.66	0.77
1:D:71:ILE:N	1:D:71:ILE:HD12	1.99	0.77
1:B:336:ILE:HD13	1:B:342:TRP:N	1.99	0.77
1:A:71:ILE:O	1:A:72:ASP:CB	2.33	0.77
1:C:63:VAL:O	1:C:66:VAL:HG23	1.84	0.77
1:C:90:MSE:HE3	1:C:109:MSE:CE	2.13	0.77
1:C:42:GLU:O	1:C:43:PRO:C	2.22	0.77
1:B:611:VAL:O	1:B:612:THR:CG2	2.31	0.76
1:C:173:ASP:OD2	1:C:440:ARG:NH2	2.18	0.76
1:B:157:LEU:O	1:B:157:LEU:HD12	1.84	0.76
1:A:291:ILE:O	1:A:296:ARG:NH1	2.18	0.76
1:C:42:GLU:O	1:C:44:ASP:N	2.18	0.76
1:A:395:ALA:O	1:A:396:ALA:C	2.24	0.76
1:D:396:ALA:O	1:D:397:VAL:HG23	1.85	0.76
1:A:44:ASP:O	1:A:45[A]:HIS:CD2	2.39	0.76
1:D:292[A]:HIS:CD2	1:D:292[A]:HIS:N	2.53	0.76
1:A:250:MSE:HE2	2:A:900:BLA:O2D	1.84	0.76
1:A:572:ASN:HB2	1:A:575:LEU:HD12	1.66	0.76
1:D:83:LEU:HD13	1:D:90:MSE:HE1	1.67	0.76
1:B:257:TYR:CD2	1:B:261:MSE:HE3	2.22	0.75
1:A:541:LEU:N	1:A:541:LEU:HD12	2.01	0.75
1:D:550:MSE:HE1	1:D:604:LEU:HD11	1.69	0.75
1:B:420:VAL:HG21	1:B:434:MSE:CE	2.16	0.75
1:C:37:LEU:HD23	1:C:37:LEU:C	2.07	0.75
1:A:541:LEU:N	1:A:541:LEU:CD1	2.50	0.75
1:A:625:PHE:CB	1:A:626:SER:CA	2.64	0.75
1:B:77:ILE:HD12	1:B:77:ILE:H	1.51	0.75
1:D:518:GLU:O	1:D:519:GLN:HB2	1.84	0.75
1:D:298:ILE:O	1:D:302:LEU:HD22	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ILE:CG2	1:B:434:MSE:HE1	2.15	0.74
1:C:291:ILE:CD1	1:C:295:LEU:HD22	2.16	0.74
1:C:561:LEU:HD22	1:C:578:VAL:HG13	1.69	0.74
2:A:900:BLA:HBC1	2:A:900:BLA:CMC	2.17	0.74
1:B:475:VAL:HA	3:B:1009:HOH:O	1.85	0.74
1:B:443:THR:HG23	1:B:443:THR:O	1.87	0.74
1:A:336:ILE:HG12	1:A:342:TRP:N	2.02	0.74
1:B:100:ASN:ND2	1:B:101:PRO:HD2	2.03	0.74
1:B:484:THR:HG22	1:B:486:ALA:H	1.53	0.74
1:B:336:ILE:HD12	1:B:344:ALA:H	1.53	0.73
1:C:90:MSE:HE2	1:C:109:MSE:C	2.08	0.73
1:A:218:LEU:HD22	1:A:250:MSE:SE	2.37	0.73
1:A:258:LEU:HB3	1:A:263:VAL:HG23	1.70	0.73
1:A:331:ARG:HE	1:A:351:GLN:HE22	1.36	0.73
1:A:337:THR:O	1:A:338:ARG:CG	2.34	0.73
2:A:900:BLA:CMA	2:A:900:BLA:C2B	2.66	0.73
1:A:625:PHE:CB	1:A:626:SER:HA	2.18	0.73
1:B:128:ILE:HD11	1:B:130:LEU:CD2	2.18	0.73
2:C:900:BLA:HMA1	2:C:900:BLA:CMB	2.07	0.73
1:B:544:ASN:HD22	1:B:544:ASN:H	1.35	0.73
1:D:258:LEU:HA	1:D:261:MSE:HE3	1.69	0.73
1:A:625:PHE:CB	1:A:626:SER:CB	2.67	0.73
1:B:524:VAL:CG1	1:B:531:VAL:HG21	2.18	0.73
1:D:291:ILE:HD12	1:D:295:LEU:HD23	1.71	0.73
1:B:59:ASN:CB	1:B:100:ASN:HD21	2.02	0.73
1:A:201:ASP:HB3	2:A:900:BLA:HHB	1.71	0.73
1:C:233:SER:HB3	1:C:236:THR:HG22	1.70	0.72
1:B:169:VAL:HG13	1:B:182:SER:HB3	1.70	0.72
1:C:233:SER:CB	1:C:236:THR:HG22	2.20	0.72
1:D:316:PHE:O	1:D:319:SER:HB3	1.89	0.72
1:B:114:GLU:HG3	1:B:236:THR:HG21	1.72	0.72
1:D:75:LEU:N	3:D:1067:HOH:O	2.22	0.72
1:D:625:PHE:HB3	1:D:626:SER:HA	1.70	0.72
1:A:39:VAL:HB	1:A:49:GLN:HB2	1.72	0.72
1:A:428:HIS:O	1:A:429:ARG:HB2	1.90	0.72
1:B:109:MSE:SE	1:B:117:LEU:HD12	2.40	0.72
1:C:95:ARG:NH1	1:C:106:ASP:OD1	2.23	0.72
1:D:544:ASN:C	1:D:544:ASN:HD22	1.93	0.72
1:A:395:ALA:O	1:A:396:ALA:O	2.06	0.71
1:A:385:ILE:HG21	1:A:434:MSE:CE	2.07	0.71
1:B:420:VAL:CG2	1:B:434:MSE:HE3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ASP:C	1:D:350:SER:N	2.42	0.71
1:D:519:GLN:O	1:D:520:PHE:C	2.26	0.71
1:B:336:ILE:HD13	1:B:341:ASP:C	2.10	0.71
1:D:328:LEU:O	1:D:332:MSE:HG3	1.89	0.71
1:A:26:HIS:NE2	1:A:27:LEU:HD22	2.05	0.71
1:C:591:GLU:O	1:C:592:VAL:HG13	1.90	0.71
1:D:268:VAL:HG21	2:D:900:BLA:HBA2	1.71	0.71
1:C:613:ARG:NH1	1:C:617:GLN:OE1	2.24	0.71
1:A:625:PHE:HB3	1:A:626:SER:CA	2.21	0.71
1:B:162:THR:HG23	1:B:164:TYR:CD2	2.26	0.71
1:B:336:ILE:HG23	1:B:341:ASP:O	1.90	0.71
1:B:268:VAL:CG1	1:B:280:LEU:HD13	2.21	0.71
1:B:469:PHE:O	1:B:470:ALA:HB2	1.91	0.71
1:D:336:ILE:CG2	1:D:341:ASP:O	2.39	0.71
1:B:514:ARG:NH1	1:B:518:GLU:OE1	2.24	0.70
1:C:568:PHE:HB2	1:C:594:LEU:HD12	1.72	0.70
1:A:26:HIS:CE1	1:A:27:LEU:HD22	2.26	0.70
1:B:434:MSE:HE2	1:B:436:PHE:CE1	2.27	0.70
1:A:443:THR:HG22	1:A:444:VAL:H	1.56	0.70
1:A:569:VAL:O	1:A:571:SER:N	2.24	0.70
1:B:581:LEU:HD13	1:B:587:GLY:HA2	1.74	0.70
1:C:42:GLU:CD	1:C:111:ARG:HH12	1.94	0.70
1:A:291:ILE:HG12	1:A:295:LEU:HD12	1.73	0.70
1:A:550:MSE:HE1	1:A:604:LEU:CD1	2.21	0.70
1:B:606:VAL:HG22	1:B:625:PHE:HE1	1.57	0.70
1:A:26:HIS:CD2	1:A:27:LEU:HD13	2.26	0.70
1:A:581:LEU:HD13	1:A:587:GLY:HA2	1.74	0.70
1:B:611:VAL:HG21	1:C:511:LEU:CD2	2.20	0.70
1:C:565:ALA:CB	1:C:575:LEU:HD22	2.22	0.70
1:C:205:MSE:HE1	1:C:208:ARG:NE	2.06	0.70
1:A:332:MSE:HE3	1:A:346:ILE:HD11	1.73	0.69
1:D:39:VAL:HG13	1:D:49:GLN:HB3	1.74	0.69
1:A:458:ASP:O	1:A:459:THR:CG2	2.40	0.69
1:B:134:LEU:O	1:B:138:LEU:HD23	1.92	0.69
1:C:561:LEU:HD22	1:C:578:VAL:CG1	2.22	0.69
2:B:900:BLA:HBC1	2:B:900:BLA:CMC	2.14	0.69
1:B:336:ILE:HG21	1:B:342:TRP:CA	2.21	0.69
1:A:473:HIS:O	1:A:475:VAL:O	2.11	0.69
2:A:900:BLA:HMC1	2:A:900:BLA:CBC	2.22	0.69
2:A:900:BLA:HMA1	2:A:900:BLA:C2B	2.22	0.69
1:C:58:LEU:HB2	1:C:60:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:N	1:C:60:LEU:HD22	2.06	0.69
1:A:365:VAL:HG22	1:A:430:GLY:O	1.92	0.69
1:A:348:ASP:O	1:A:349:THR:HG22	1.92	0.69
1:D:518:GLU:O	1:D:519:GLN:HB3	1.92	0.69
1:D:232:LEU:HD13	1:D:232:LEU:H	1.57	0.68
1:B:594:LEU:CD2	1:B:602:LEU:HD13	2.23	0.68
1:A:332:MSE:CA	1:A:335:ALA:HB3	2.22	0.68
1:A:44:ASP:O	1:A:45[A]:HIS:HD2	1.77	0.68
1:D:550:MSE:CE	1:D:604:LEU:HD11	2.23	0.68
1:D:250:MSE:HE3	1:D:254:HIS:CD2	2.29	0.68
1:D:470:ALA:O	1:D:471:LYS:CB	2.42	0.68
1:D:568:PHE:O	1:D:569:VAL:C	2.31	0.68
1:C:90:MSE:HE3	1:C:109:MSE:HB3	1.74	0.68
1:C:612:THR:CG2	3:C:1084:HOH:O	2.41	0.68
1:D:83:LEU:CD1	1:D:90:MSE:HE1	2.24	0.68
1:B:158:PHE:O	1:B:162:THR:HB	1.94	0.68
1:C:258:LEU:HD23	1:C:261:MSE:HE1	1.74	0.68
1:D:545:ASP:O	1:D:546:SER:C	2.30	0.68
1:A:31:ILE:HD11	1:A:37:LEU:HD23	1.75	0.68
1:A:336:ILE:HG12	1:A:341:ASP:C	2.14	0.68
1:B:26:HIS:CG	1:B:27:LEU:HD13	2.28	0.68
1:B:258:LEU:HB3	1:B:263:VAL:HG22	1.74	0.68
1:C:48:ILE:HD12	1:C:235:LEU:HD21	1.74	0.68
1:A:606:VAL:HA	1:A:625:PHE:HA	1.74	0.68
1:C:565:ALA:HB1	1:C:575:LEU:HD22	1.76	0.68
1:A:336:ILE:HG13	1:A:341:ASP:H	1.59	0.67
1:B:268:VAL:HG13	1:B:280:LEU:HD13	1.75	0.67
1:B:475:VAL:CA	3:B:1009:HOH:O	2.41	0.67
2:B:900:BLA:HBB1	2:B:900:BLA:HMB1	1.75	0.67
1:D:336:ILE:CG1	1:D:341:ASP:O	2.43	0.67
1:A:71:ILE:O	1:A:72:ASP:HB3	1.95	0.67
1:A:550:MSE:CE	1:A:604:LEU:HD11	2.25	0.67
1:B:82:HIS:CD2	1:B:92:VAL:HG21	2.28	0.67
1:A:348:ASP:O	1:A:349:THR:CG2	2.43	0.67
1:D:338:ARG:O	1:D:339:GLU:HG3	1.94	0.67
1:D:442:HIS:O	1:D:443:THR:HG23	1.94	0.67
1:A:540:ILE:C	1:A:541:LEU:HD12	2.15	0.67
1:C:407:VAL:O	1:C:410:LEU:N	2.27	0.67
1:A:71:ILE:HG22	1:A:72:ASP:N	2.09	0.67
1:A:291:ILE:HG13	1:A:295:LEU:HD12	1.76	0.67
1:D:537:GLU:OE1	1:D:539:ARG:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:LEU:HD13	1:D:587:GLY:HA2	1.75	0.67
1:D:214:ARG:CG	1:D:214:ARG:HH11	2.07	0.67
1:A:519:GLN:O	1:A:520:PHE:HB2	1.93	0.66
1:C:612:THR:HG22	3:C:1084:HOH:O	1.95	0.66
1:D:475:VAL:O	1:D:476:VAL:HG22	1.94	0.66
1:C:542:LEU:HD12	1:C:542:LEU:C	2.15	0.66
1:D:327:ARG:O	1:D:331:ARG:HB2	1.94	0.66
1:B:428:HIS:O	1:B:429:ARG:HB2	1.96	0.66
1:B:467:ARG:O	1:B:470:ALA:HB3	1.94	0.66
1:B:90:MSE:HE3	1:B:109:MSE:HG2	1.76	0.66
1:D:19:ASN:HD22	1:D:19:ASN:N	1.93	0.66
1:D:242:MSE:HE2	1:D:248:ARG:HG3	1.76	0.66
1:C:421:VAL:HG12	1:C:483:TRP:CZ2	2.30	0.66
1:C:532:LEU:HD22	1:C:540:ILE:HD11	1.77	0.66
1:D:68:LEU:HA	1:D:71:ILE:HD13	1.78	0.66
1:D:517:TYR:C	1:D:517:TYR:CD1	2.68	0.66
1:D:544:ASN:ND2	1:D:547:PHE:H	1.92	0.66
2:A:900:BLA:CMA	2:A:900:BLA:C1B	2.72	0.66
1:B:40:VAL:HG13	1:B:45:HIS:HA	1.76	0.66
1:B:141:ILE:HD13	1:B:306:ILE:HG13	1.78	0.66
1:D:471:LYS:O	1:D:475:VAL:HG12	1.95	0.66
1:D:559:VAL:HG22	1:D:563:ASP:OD1	1.95	0.66
1:D:625:PHE:CA	1:D:626:SER:OG	2.44	0.66
1:B:520:PHE:O	1:C:510:THR:HG23	1.96	0.66
1:C:40:VAL:HG12	1:C:45:HIS:HA	1.78	0.66
1:C:166:ARG:HD2	1:C:168:MSE:HE2	1.77	0.66
1:A:509:ARG:HD2	1:D:520:PHE:CZ	2.30	0.66
1:B:128:ILE:HD11	1:B:130:LEU:HD21	1.77	0.66
1:B:218:LEU:HB2	1:B:250:MSE:HE1	1.77	0.66
1:C:135:ALA:HB3	1:C:136:PRO:HD3	1.78	0.66
1:C:205:MSE:HE1	1:C:208:ARG:CZ	2.25	0.66
1:C:434:MSE:HE2	1:C:436:PHE:HZ	1.57	0.66
1:D:71:ILE:HD12	1:D:71:ILE:H	1.59	0.66
1:D:122:GLU:OE1	1:D:296:ARG:NH2	2.28	0.66
1:A:332:MSE:HE2	1:A:342:TRP:HE3	1.60	0.66
1:B:519:GLN:O	1:B:520:PHE:HB2	1.94	0.66
1:D:531:VAL:HG12	1:D:544:ASN:OD1	1.95	0.66
1:A:338:ARG:O	1:A:339:GLU:CG	2.43	0.66
1:C:202:ILE:HG22	1:C:207:ARG:HG2	1.78	0.66
1:D:250:MSE:HE2	1:D:255:LEU:CD2	2.25	0.66
1:A:160:GLN:NE2	3:A:1035:HOH:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ALA:O	1:A:629:THR:HG23	1.96	0.65
1:B:517:TYR:O	1:B:521:SER:OG	2.10	0.65
1:C:443:THR:HG22	1:C:444:VAL:H	1.60	0.65
1:C:424:PRO:HA	1:C:432:PHE:HB3	1.77	0.65
1:B:469:PHE:O	1:B:470:ALA:CB	2.45	0.65
1:C:629:THR:CB	1:C:630:ASP:HB3	2.27	0.65
1:D:238:ARG:O	1:D:239:ASP:C	2.34	0.65
1:C:417:ALA:HB1	1:C:420:VAL:HG12	1.79	0.65
1:D:424:PRO:HA	1:D:432:PHE:HB3	1.78	0.65
1:A:334:GLU:HG3	1:A:335:ALA:H	1.61	0.65
1:B:544:ASN:HD22	1:B:544:ASN:N	1.92	0.65
1:D:392:GLN:O	1:D:394:ARG:NH2	2.29	0.65
1:D:496:GLN:HA	1:D:496:GLN:NE2	2.12	0.65
1:A:449:ASP:HB2	1:A:473:HIS:CD2	2.32	0.65
1:D:42:GLU:HB3	1:D:43:PRO:HD2	1.78	0.65
1:B:466:ARG:HG2	1:B:466:ARG:HH11	1.62	0.65
1:C:48:ILE:HD12	1:C:235:LEU:CD2	2.27	0.65
1:C:180:VAL:O	1:C:193:PHE:O	2.14	0.65
1:D:578:VAL:HG12	1:D:582:ILE:HD12	1.78	0.65
1:A:135:ALA:HB3	1:A:136:PRO:HD3	1.79	0.65
1:C:155:ALA:HB1	1:C:184:ARG:HB2	1.79	0.65
1:D:421:VAL:HG13	1:D:435:TRP:HB2	1.79	0.65
1:A:158:PHE:HE1	1:A:269:VAL:HG11	1.62	0.65
1:C:564:LEU:HA	1:C:567:PHE:HB2	1.80	0.64
1:D:428:HIS:O	1:D:429:ARG:HB2	1.96	0.64
1:B:60:LEU:HD21	1:B:98:ILE:HG21	1.80	0.64
1:D:337:THR:O	1:D:338:ARG:NE	2.28	0.64
1:B:608:ALA:CB	1:B:623:LEU:HD23	2.27	0.64
1:C:28:ALA:C	1:C:242:MSE:HE3	2.18	0.64
1:B:579:ALA:N	3:B:1036:HOH:O	2.29	0.64
1:D:519:GLN:O	1:D:521:SER:CA	2.46	0.64
1:C:421:VAL:HG13	1:C:435:TRP:HB2	1.79	0.64
1:D:393:PRO:O	1:D:394:ARG:CB	2.45	0.64
1:A:233:SER:OG	1:A:236:THR:OG1	2.15	0.64
1:A:45[A]:HIS:CE1	1:A:69:ALA:N	2.66	0.64
1:A:565:ALA:HB2	1:A:574:PHE:HD2	1.62	0.64
1:C:134:LEU:O	1:C:138:LEU:HG	1.97	0.64
1:C:444:VAL:O	1:C:445:THR:HG22	1.98	0.64
1:C:501:ILE:C	1:C:501:ILE:HD12	2.18	0.64
1:A:332:MSE:CE	1:A:342:TRP:CE3	2.80	0.64
1:A:519:GLN:O	1:A:520:PHE:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:CG1	1:C:45:HIS:HA	2.27	0.64
1:C:484:THR:HG1	1:C:487:ASP:H	1.44	0.64
1:D:558:ALA:CB	1:D:564:LEU:HD11	2.27	0.64
2:A:900:BLA:ND	2:A:900:BLA:NA	2.46	0.64
1:B:89:GLY:O	1:B:90:MSE:CG	2.46	0.64
1:B:568:PHE:CD2	1:B:592:VAL:HG21	2.32	0.64
1:D:168:MSE:HE3	1:D:170:TYR:CZ	2.32	0.63
1:C:385:ILE:HG21	1:C:434:MSE:HE1	1.79	0.63
1:C:593:LEU:HD23	1:C:603:PRO:HA	1.80	0.63
1:D:129:ASP:O	1:D:130:LEU:HB2	1.98	0.63
1:D:606:VAL:HG23	1:D:625:PHE:CE2	2.33	0.63
1:A:233:SER:HG	1:A:236:THR:HG1	1.39	0.63
1:A:453:PRO:CA	1:A:454:PHE:CB	2.76	0.63
1:B:568:PHE:HA	1:B:594:LEU:HA	1.79	0.63
1:A:557:SER:O	1:A:558:ALA:HB2	1.98	0.63
1:A:171:ARG:NH1	1:A:179:GLU:OE1	2.31	0.63
1:B:90:MSE:CE	1:B:110:HIS:CA	2.76	0.63
1:C:337:THR:O	1:C:338:ARG:HB3	1.98	0.63
1:C:476:VAL:HG23	1:C:476:VAL:O	1.98	0.63
1:D:100:ASN:HB3	1:D:101:PRO:HD3	1.81	0.63
1:D:258:LEU:HD23	1:D:261:MSE:HE1	1.80	0.63
1:D:334:GLU:O	1:D:336:ILE:O	2.16	0.63
1:A:556:PRO:O	1:A:557:SER:C	2.37	0.63
1:B:11:ALA:O	1:B:14:THR:HB	1.98	0.63
1:B:629:THR:HB	3:B:1043:HOH:O	1.99	0.63
1:C:90:MSE:HE2	1:C:110:HIS:N	2.14	0.63
1:D:64:LEU:HD11	1:D:230:PRO:HD3	1.79	0.63
1:B:37:LEU:HD23	1:B:37:LEU:C	2.19	0.62
1:D:85:PRO:HA	3:D:1062:HOH:O	1.99	0.62
1:D:555:SER:HB3	1:D:556:PRO:HA	1.79	0.62
1:D:291:ILE:HG23	1:D:295:LEU:HB3	1.81	0.62
1:B:553:ALA:O	1:B:554:GLY:C	2.38	0.62
1:C:615:GLU:N	3:C:1001:HOH:O	2.33	0.62
1:A:79:ILE:HB	1:A:109:MSE:HE1	1.82	0.62
1:B:257:TYR:HE2	1:B:261:MSE:HE3	1.61	0.62
1:C:90:MSE:HE2	1:C:110:HIS:HA	1.81	0.62
1:D:302:LEU:HD13	1:D:302:LEU:N	2.14	0.62
1:B:127:PRO:O	1:B:128:ILE:HG22	2.00	0.62
1:D:394:ARG:O	1:D:395:ALA:HB2	1.98	0.62
1:D:389:LEU:HD21	1:D:422:ALA:HB1	1.82	0.62
1:A:336:ILE:HG21	1:A:342:TRP:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:CB	1:C:60:LEU:HD23	2.30	0.62
1:C:472:TRP:O	1:C:475:VAL:O	2.17	0.62
1:D:336:ILE:HG12	1:D:341:ASP:O	2.00	0.62
1:A:30:SER:O	1:A:31:ILE:HD12	2.00	0.61
1:D:156:LEU:O	1:D:160:GLN:HG3	1.99	0.61
1:D:393:PRO:O	1:D:394:ARG:HB2	2.00	0.61
1:D:545:ASP:O	1:D:547:PHE:N	2.32	0.61
1:D:600:ARG:O	1:D:601:PRO:O	2.17	0.61
1:C:254:HIS:NE2	1:C:258:LEU:HD11	2.15	0.61
1:C:583:ASP:O	1:C:584:HIS:C	2.39	0.61
1:B:279:GLY:O	1:B:280:LEU:HD23	2.00	0.61
1:C:205:MSE:CE	1:C:208:ARG:HE	2.13	0.61
1:D:416:MSE:HE2	1:D:417:ALA:CB	2.30	0.61
2:D:900:BLA:ND	3:D:1077:HOH:O	2.31	0.61
1:A:90:MSE:HE1	1:A:117:LEU:HD11	1.82	0.61
1:A:557:SER:O	1:A:558:ALA:CB	2.48	0.61
1:C:58:LEU:O	1:C:60:LEU:CD2	2.48	0.61
1:C:59:ASN:C	1:C:60:LEU:HD22	2.21	0.61
1:C:569:VAL:HA	1:C:593:LEU:O	2.01	0.61
1:D:100:ASN:HD22	1:D:101:PRO:HD3	1.64	0.61
1:B:231:ARG:NH1	1:B:239:ASP:OD2	2.34	0.61
1:D:558:ALA:CB	1:D:564:LEU:CD1	2.78	0.61
1:B:139:GLU:C	3:B:1041:HOH:O	2.38	0.61
1:B:297:ALA:O	1:B:301:LEU:HD22	2.00	0.61
1:A:444:VAL:CG2	1:A:445:THR:N	2.64	0.61
1:B:135:ALA:HB3	1:B:136:PRO:CD	2.31	0.61
1:A:58:LEU:O	1:A:60:LEU:HD13	2.01	0.61
1:A:128:ILE:HG22	1:A:128:ILE:O	2.01	0.61
1:C:28:ALA:HB3	1:C:242:MSE:HE3	1.82	0.61
1:A:125:GLY:N	1:A:126:PRO:HD3	2.15	0.60
1:A:251:SER:O	1:A:255:LEU:HG	2.00	0.60
1:B:99:GLY:O	1:B:100:ASN:ND2	2.33	0.60
1:B:484:THR:HB	1:B:487:ASP:H	1.64	0.60
2:D:900:BLA:HMA2	2:D:900:BLA:O2A	2.01	0.60
1:B:103:THR:HG23	1:B:105:TYR:CE2	2.36	0.60
1:B:404:GLY:O	1:B:405:LEU:HB2	2.01	0.60
2:B:900:BLA:HMC1	2:B:900:BLA:CBC	2.18	0.60
1:B:347:PHE:CZ	1:B:371:ARG:HG2	2.36	0.60
1:C:476:VAL:HA	1:C:479:THR:OG1	2.00	0.60
1:C:529:GLN:NE2	1:C:626:SER:O	2.34	0.60
1:D:39:VAL:HG13	1:D:49:GLN:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HG2	1:A:184:ARG:N	2.16	0.60
1:B:562:ASP:HA	1:B:575:LEU:CD1	2.31	0.60
1:B:581:LEU:HD13	1:B:587:GLY:CA	2.32	0.60
1:A:180:VAL:HB	1:A:193:PHE:O	2.01	0.60
2:C:900:BLA:HMA1	2:C:900:BLA:C2B	2.30	0.60
1:B:128:ILE:HD11	1:B:130:LEU:HD23	1.84	0.60
1:B:532:LEU:HD11	1:B:547:PHE:CZ	2.37	0.60
1:B:331:ARG:CG	1:B:351:GLN:HE22	2.05	0.60
1:B:388:TRP:CZ3	1:B:407:VAL:HG21	2.37	0.60
1:A:37:LEU:HD13	1:A:118:ILE:HG23	1.83	0.60
1:A:266:THR:HG23	1:A:268:VAL:HG23	1.84	0.60
1:A:617:GLN:HA	1:A:617:GLN:HE21	1.67	0.60
1:D:416:MSE:HE2	1:D:417:ALA:HB3	1.82	0.60
1:C:162:THR:HB	1:C:164:TYR:HD2	1.67	0.59
1:B:293:PHE:O	1:B:294:GLU:C	2.39	0.59
1:C:90:MSE:HE2	1:C:110:HIS:CA	2.32	0.59
1:D:156:LEU:HG	1:D:160:GLN:HE21	1.66	0.59
1:A:168:MSE:HE3	1:A:170:TYR:CE1	2.37	0.59
1:B:257:TYR:CE2	1:B:261:MSE:CE	2.84	0.59
1:B:626:SER:O	1:B:626:SER:OG	2.11	0.59
1:D:250:MSE:HE3	1:D:254:HIS:HD2	1.67	0.59
1:D:336:ILE:HG21	1:D:342:TRP:HA	0.84	0.59
1:A:357:LEU:O	1:A:358:HIS:C	2.41	0.59
1:A:381:ASP:HB3	1:A:413:LEU:HD21	1.85	0.59
1:B:600:ARG:O	1:B:602:LEU:N	2.35	0.59
1:D:392:GLN:O	1:D:393:PRO:O	2.20	0.59
1:A:476:VAL:HG23	1:A:479:THR:HG21	1.84	0.59
1:D:100:ASN:HB3	1:D:101:PRO:CD	2.33	0.59
1:B:550:MSE:HE2	1:B:604:LEU:HD11	1.79	0.59
1:D:19:ASN:N	1:D:19:ASN:ND2	2.50	0.59
1:D:141:ILE:HG12	1:D:306:ILE:HD12	1.84	0.59
1:D:608:ALA:HB2	1:D:623:LEU:HB3	1.83	0.59
1:A:486:ALA:O	1:A:489:ALA:HB3	2.02	0.59
1:B:268:VAL:HG21	2:B:900:BLA:HBA2	1.85	0.59
1:C:47:ILE:HG21	1:C:63:VAL:HG23	1.82	0.59
1:C:446:TRP:CG	1:C:447:GLY:N	2.71	0.59
1:C:540:ILE:HG23	1:C:540:ILE:O	2.03	0.59
1:A:100:ASN:OD1	1:A:101:PRO:CD	2.50	0.59
1:A:428:HIS:O	1:A:429:ARG:CB	2.50	0.59
1:B:172:PHE:CE2	1:B:279:GLY:HA2	2.38	0.59
1:B:351:GLN:O	1:B:351:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ALA:O	1:B:397:VAL:N	2.35	0.59
1:C:42:GLU:OE1	1:C:111:ARG:NH1	2.36	0.59
1:B:520:PHE:O	1:C:510:THR:CG2	2.50	0.59
1:C:74:ASP:O	1:C:76:LEU:N	2.36	0.58
1:D:252:PRO:HA	1:D:255:LEU:HB2	1.85	0.58
1:D:377:PRO:HG3	1:D:416:MSE:HE3	1.84	0.58
1:A:258:LEU:HB3	1:A:263:VAL:HG22	1.81	0.58
1:B:74:ASP:O	1:B:75:LEU:CB	2.50	0.58
1:B:90:MSE:CE	1:B:110:HIS:HA	2.22	0.58
1:C:449:ASP:CB	1:C:450:PRO:HD3	2.33	0.58
1:D:168:MSE:CE	1:D:170:TYR:OH	2.51	0.58
1:D:515:GLU:O	1:D:518:GLU:O	2.21	0.58
1:D:550:MSE:HE1	1:D:604:LEU:CD1	2.31	0.58
1:B:420:VAL:HG22	1:B:434:MSE:HE3	1.84	0.58
1:B:476:VAL:HG23	1:B:476:VAL:O	2.04	0.58
1:D:531:VAL:CG1	1:D:544:ASN:OD1	2.51	0.58
1:C:118:ILE:HG22	1:C:119:ILE:N	2.19	0.58
1:B:63:VAL:HG12	1:B:64:LEU:N	2.18	0.58
1:D:550:MSE:HE1	1:D:604:LEU:HD21	1.85	0.58
1:A:201:ASP:OD2	1:A:468:SER:OG	2.21	0.58
1:B:26:HIS:CD2	1:B:27:LEU:HD11	2.36	0.58
1:B:27:LEU:C	1:B:28:ALA:O	2.38	0.58
1:A:158:PHE:CE1	1:A:269:VAL:HG11	2.38	0.58
1:B:336:ILE:HG13	3:B:1014:HOH:O	2.04	0.58
1:B:348:ASP:C	1:B:350:SER:H	2.07	0.58
1:C:90:MSE:CE	1:C:109:MSE:HE3	2.22	0.58
1:C:259:LYS:NZ	3:C:1026:HOH:O	2.37	0.58
1:D:365:VAL:HG23	1:D:430:GLY:O	2.03	0.58
1:A:139:GLU:HA	1:A:139:GLU:OE1	2.04	0.58
1:B:49:GLN:HE22	1:B:233:SER:HA	1.68	0.58
1:C:74:ASP:O	1:C:75:LEU:C	2.41	0.58
1:D:336:ILE:HD13	1:D:341:ASP:O	2.04	0.58
1:D:229:GLU:O	1:D:230:PRO:C	2.41	0.57
1:D:569:VAL:O	1:D:571:SER:N	2.35	0.57
1:B:66:VAL:HG21	1:B:71:ILE:HD13	1.86	0.57
1:C:463:LEU:O	1:C:464:SER:HB3	2.04	0.57
1:D:285:HIS:CD2	1:D:289:ARG:HD2	2.40	0.57
1:D:331:ARG:O	1:D:335:ALA:HB3	2.04	0.57
1:B:100:ASN:ND2	1:B:101:PRO:CD	2.60	0.57
1:A:150:LEU:HD13	1:A:309:ARG:HG3	1.85	0.57
1:B:230:PRO:O	1:B:231:ARG:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:MSE:HE3	1:C:528:MSE:HA	1.85	0.57
1:A:134:LEU:O	1:A:135:ALA:CB	2.52	0.57
1:A:255:LEU:C	1:A:257:TYR:H	2.07	0.57
1:B:445:THR:HG22	1:B:446:TRP:N	2.18	0.57
2:B:900:BLA:HMA1	2:B:900:BLA:C2B	2.35	0.57
1:C:460:PRO:HA	1:C:463:LEU:HG	1.86	0.57
1:C:627:ASP:OD1	1:C:627:ASP:N	2.38	0.57
1:D:108:LEU:HD12	1:D:108:LEU:N	2.18	0.57
1:B:511:LEU:HD23	1:C:611:VAL:HG21	1.87	0.57
1:C:205:MSE:CE	1:C:208:ARG:NE	2.67	0.57
1:C:218:LEU:CD2	1:C:250:MSE:SE	2.90	0.57
1:C:446:TRP:CD2	1:C:447:GLY:N	2.72	0.57
1:D:71:ILE:O	1:D:72:ASP:C	2.42	0.57
1:D:330:GLN:HE21	1:D:330:GLN:C	2.07	0.57
1:D:496:GLN:HA	1:D:496:GLN:HE21	1.69	0.57
1:B:89:GLY:O	1:B:90:MSE:SE	2.72	0.57
1:C:74:ASP:HB3	1:C:78:LYS:HG2	1.85	0.57
1:C:498:VAL:O	1:C:499:ALA:C	2.39	0.57
1:D:517:TYR:C	1:D:517:TYR:HD1	2.07	0.57
1:A:164:TYR:CD2	1:A:289:ARG:HD2	2.40	0.57
1:C:349:THR:C	1:C:351:GLN:H	2.08	0.57
1:D:107:GLY:O	1:D:108:LEU:HD12	2.04	0.57
1:D:544:ASN:HD21	1:D:547:PHE:H	1.53	0.57
1:A:136:PRO:HD2	3:A:1020:HOH:O	2.05	0.56
1:B:201:ASP:HB3	2:B:900:BLA:HBB	1.87	0.56
1:A:92:VAL:HG22	1:A:93:ALA:N	2.20	0.56
1:A:144:ALA:O	1:A:309:ARG:NH1	2.37	0.56
1:B:49:GLN:NE2	1:B:233:SER:HA	2.20	0.56
1:A:536:ALA:HB2	1:A:618:SER:O	2.06	0.56
1:C:370:ILE:HD13	1:C:370:ILE:C	2.26	0.56
1:D:238:ARG:HD2	1:D:238:ARG:N	2.20	0.56
1:A:365:VAL:CG2	1:A:430:GLY:O	2.53	0.56
1:A:624:ILE:O	1:A:625:PHE:C	2.43	0.56
1:B:128:ILE:HG13	1:B:294:GLU:OE2	2.04	0.56
1:B:504:GLN:HB2	1:C:624:ILE:HD11	1.87	0.56
1:B:611:VAL:CG2	1:C:511:LEU:HD23	2.26	0.56
1:C:42:GLU:HB3	1:C:43:PRO:CD	2.32	0.56
1:D:336:ILE:HG23	1:D:341:ASP:O	2.05	0.56
1:A:347:PHE:CZ	1:A:371:ARG:HG2	2.40	0.56
1:A:464:SER:OG	1:A:465:PRO:N	2.37	0.56
1:B:475:VAL:O	1:B:476:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:HD11	1:B:547:PHE:CE1	2.40	0.56
1:B:537:GLU:O	1:B:582:ILE:HD13	2.05	0.56
1:C:233:SER:HB3	1:C:236:THR:CG2	2.36	0.56
1:D:134:LEU:O	1:D:138:LEU:HB2	2.05	0.56
1:D:241:ASP:OD2	1:D:243:SER:OG	2.13	0.56
1:A:532:LEU:HD12	1:A:623:LEU:HB2	1.87	0.56
1:B:524:VAL:HG12	1:B:531:VAL:HG21	1.86	0.56
1:A:252:PRO:HA	1:A:255:LEU:HB2	1.88	0.56
1:B:325:VAL:HG11	1:B:493:THR:HG22	1.87	0.56
1:B:336:ILE:HD11	1:B:341:ASP:HB3	1.86	0.56
1:A:155:ALA:C	1:A:167:VAL:HG21	2.26	0.56
1:B:472:TRP:O	1:B:475:VAL:O	2.24	0.56
1:C:331:ARG:HD2	1:C:349:THR:HG21	1.87	0.56
1:B:624:ILE:HD13	1:C:503:LEU:HG	1.87	0.56
1:C:127:PRO:CB	1:C:128:ILE:HA	2.36	0.56
1:A:71:ILE:CG2	1:A:72:ASP:N	2.69	0.55
1:B:71:ILE:O	1:B:72:ASP:HB2	2.05	0.55
1:B:258:LEU:HD22	1:B:263:VAL:HG21	1.88	0.55
1:C:60:LEU:N	1:C:60:LEU:CD2	2.69	0.55
1:C:354:LEU:HD11	1:C:373:ILE:HG23	1.87	0.55
1:C:385:ILE:HG21	1:C:434:MSE:CE	2.36	0.55
1:A:46:ARG:HA	1:A:67:PRO:HA	1.88	0.55
1:B:218:LEU:HB2	1:B:250:MSE:CE	2.36	0.55
2:B:900:BLA:CMB	2:B:900:BLA:HMA1	2.26	0.55
1:B:539:ARG:HA	1:B:560:HIS:HA	1.88	0.55
1:C:273:VAL:HG21	1:C:310:ILE:HG21	1.87	0.55
1:A:26:HIS:NE2	1:A:27:LEU:CD2	2.70	0.55
1:B:169:VAL:CG1	1:B:182:SER:HB3	2.36	0.55
1:B:625:PHE:O	1:B:627:ASP:N	2.39	0.55
1:A:166:ARG:HD3	1:A:168:MSE:SE	2.57	0.55
1:B:89:GLY:O	1:B:90:MSE:HG3	2.06	0.55
1:B:66:VAL:HG21	1:B:71:ILE:CD1	2.37	0.55
1:C:183:GLU:OE1	1:C:191:SER:HB3	2.05	0.55
1:C:434:MSE:HE2	1:C:436:PHE:CE1	2.40	0.55
1:D:338:ARG:H	1:D:340:GLY:H	1.54	0.55
1:A:30:SER:HB2	1:A:249:SER:OG	2.06	0.55
1:A:464:SER:OG	1:A:465:PRO:HD2	2.06	0.55
1:B:561:LEU:HD11	1:B:623:LEU:HD11	1.88	0.55
1:C:233:SER:OG	1:C:236:THR:HG22	2.07	0.55
1:D:599:ASN:O	1:D:600:ARG:C	2.45	0.55
1:D:547:PHE:O	1:D:550:MSE:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:O	1:A:71:ILE:HB	2.06	0.55
1:A:395:ALA:C	1:A:396:ALA:O	2.43	0.55
1:A:508:VAL:HG12	1:A:512:ILE:CD1	2.36	0.55
1:B:336:ILE:HG21	1:B:342:TRP:C	2.27	0.55
1:D:346:ILE:HG22	1:D:347:PHE:CG	2.41	0.55
1:A:218:LEU:HD11	1:A:221:VAL:HA	1.88	0.55
1:A:347:PHE:O	1:A:349:THR:HG22	2.07	0.55
1:A:362:CYS:SG	1:A:363:ALA:N	2.79	0.55
1:B:388:TRP:CE3	1:B:407:VAL:HG21	2.42	0.55
1:C:27:LEU:C	1:C:28:ALA:O	2.43	0.55
1:C:593:LEU:CD2	1:C:603:PRO:HA	2.37	0.55
1:D:336:ILE:HD13	1:D:341:ASP:C	2.27	0.55
1:A:76:LEU:CD2	1:A:80:LEU:CD1	2.85	0.54
1:B:444:VAL:HG12	1:B:444:VAL:O	2.07	0.54
1:C:110:HIS:NE2	1:C:118:ILE:HD12	2.21	0.54
1:C:472:TRP:O	1:C:476:VAL:HG22	2.08	0.54
1:A:366:TYR:O	1:A:367:GLU:C	2.44	0.54
1:B:562:ASP:HB3	1:B:575:LEU:HD11	1.88	0.54
1:C:30:SER:N	1:C:242:MSE:HE1	2.22	0.54
1:C:218:LEU:HD21	1:C:255:LEU:HD23	1.88	0.54
1:D:519:GLN:O	1:D:522:SER:N	2.39	0.54
1:A:472:TRP:O	1:A:476:VAL:CG1	2.53	0.54
1:B:127:PRO:O	1:B:128:ILE:CG2	2.55	0.54
1:D:230:PRO:O	1:D:232:LEU:HD22	2.07	0.54
1:A:268:VAL:HG21	2:A:900:BLA:HBA2	1.90	0.54
1:D:393:PRO:O	1:D:394:ARG:NE	2.40	0.54
1:A:66:VAL:HG23	1:A:67:PRO:O	2.07	0.54
1:A:289:ARG:NH2	3:A:1037:HOH:O	2.40	0.54
1:A:496:GLN:HA	1:A:496:GLN:NE2	2.21	0.54
1:A:514:ARG:HD2	1:D:517:TYR:HE2	1.72	0.54
1:B:147:LEU:HD11	1:B:278:TRP:CZ2	2.43	0.54
1:B:349:THR:O	1:B:350:SER:OG	2.19	0.54
1:B:428:HIS:O	1:B:429:ARG:CB	2.54	0.54
1:C:522:SER:O	1:C:525:HIS:N	2.41	0.54
1:D:170:TYR:CE2	2:D:900:BLA:HMA3	2.42	0.54
1:D:257:TYR:HD2	1:D:261:MSE:CE	2.01	0.54
1:D:389:LEU:HD21	1:D:422:ALA:HB3	1.86	0.54
1:D:550:MSE:SE	1:D:604:LEU:HD11	2.58	0.54
1:A:361:GLY:HA3	1:A:375:ASP:O	2.07	0.54
1:B:156:LEU:HD22	1:B:160:GLN:HE21	1.72	0.54
1:B:172:PHE:CD2	1:B:279:GLY:HA2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:O	1:C:310:ILE:C	2.45	0.54
1:A:625:PHE:CB	1:A:626:SER:OG	2.51	0.54
1:C:175:GLN:HB2	1:C:177:HIS:HD2	1.73	0.54
1:A:76:LEU:HD22	1:A:80:LEU:CD1	2.37	0.54
1:A:472:TRP:O	1:A:475:VAL:O	2.26	0.54
1:C:127:PRO:HD2	1:C:128:ILE:HG23	1.89	0.54
1:D:17:LEU:HD21	1:D:467:ARG:HH22	1.72	0.54
1:D:230:PRO:O	1:D:232:LEU:O	2.26	0.54
1:D:266:THR:HG23	1:D:268:VAL:HG23	1.90	0.54
1:D:291:ILE:HD12	1:D:295:LEU:CD2	2.37	0.54
1:B:26:HIS:CE1	1:B:205:MSE:HE3	2.43	0.54
1:C:378:SER:O	1:C:382:VAL:N	2.35	0.54
1:D:100:ASN:CB	1:D:101:PRO:HD3	2.38	0.54
1:D:112:PRO:HD2	1:D:116:GLY:O	2.07	0.54
1:A:336:ILE:HD12	3:A:1017:HOH:O	2.08	0.53
1:A:444:VAL:HG23	1:A:446:TRP:H	1.73	0.53
1:A:469:PHE:O	1:A:472:TRP:HB3	2.08	0.53
1:A:561:LEU:O	1:A:562:ASP:C	2.46	0.53
1:B:126:PRO:O	1:B:128:ILE:N	2.41	0.53
1:B:180:VAL:HG11	1:B:192:TYR:O	2.08	0.53
1:D:250:MSE:HE1	1:D:258:LEU:CD1	2.38	0.53
1:A:119:ILE:HG22	1:A:121:LEU:HD22	1.90	0.53
1:A:445:THR:HG22	1:A:445:THR:O	2.08	0.53
1:B:484:THR:HG22	1:B:485:ALA:N	2.23	0.53
1:D:119:ILE:HG22	1:D:121:LEU:CD1	2.39	0.53
1:D:538:GLY:O	1:D:561:LEU:CD2	2.56	0.53
1:A:308:THR:O	1:A:309:ARG:C	2.47	0.53
1:A:347:PHE:O	1:A:348:ASP:C	2.46	0.53
1:A:347:PHE:CE2	1:A:371:ARG:HG2	2.43	0.53
1:B:531:VAL:H	1:B:544:ASN:HD21	1.57	0.53
1:D:333:ILE:HG23	1:D:338:ARG:HH22	1.72	0.53
1:A:35:GLY:HA2	1:A:57:PHE:CZ	2.44	0.53
1:B:126:PRO:N	1:B:127:PRO:HD2	2.24	0.53
1:C:475:VAL:HG22	1:C:476:VAL:HG13	1.90	0.53
1:D:61:GLY:O	1:D:63:VAL:HG23	2.08	0.53
1:D:168:MSE:HE3	1:D:170:TYR:OH	2.08	0.53
1:D:625:PHE:HB2	1:D:626:SER:OG	2.09	0.53
1:A:134:LEU:HD13	1:A:138:LEU:HD22	1.90	0.53
1:A:625:PHE:HB2	1:A:626:SER:HB2	1.86	0.53
1:B:409:GLU:OE1	1:B:410:LEU:CD1	2.56	0.53
1:B:619:LEU:HD21	1:C:515:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LYS:HG3	1:C:474:GLN:HE22	1.73	0.53
1:D:524:VAL:CG1	1:D:531:VAL:HG11	2.38	0.53
1:A:74:ASP:OD2	1:A:78:LYS:NZ	2.41	0.53
1:A:591:GLU:O	1:A:592:VAL:HG23	2.08	0.53
1:C:388:TRP:CE2	1:C:392:GLN:NE2	2.76	0.53
1:D:235:LEU:O	1:D:237:GLY:N	2.42	0.53
1:A:37:LEU:HD12	1:A:38:LEU:N	2.22	0.53
1:A:332:MSE:O	1:A:335:ALA:HB3	2.09	0.53
1:A:515:GLU:O	1:A:518:GLU:O	2.27	0.53
1:C:558:ALA:HB1	1:C:563:ASP:HB2	1.90	0.53
1:B:135:ALA:HB3	1:B:136:PRO:HD3	1.90	0.53
1:C:42:GLU:CD	1:C:111:ARG:NH1	2.61	0.53
1:D:357:LEU:HD23	1:D:421:VAL:HG11	1.90	0.53
1:D:544:ASN:C	1:D:544:ASN:ND2	2.61	0.53
1:A:173:ASP:C	1:A:173:ASP:OD1	2.48	0.53
1:A:443:THR:O	1:A:445:THR:N	2.39	0.53
1:A:632:ARG:HA	1:A:633:THR:OG1	2.09	0.53
1:C:258:LEU:HA	1:C:261:MSE:HE3	1.91	0.53
1:D:580:GLU:O	1:D:583:ASP:O	2.27	0.53
1:A:223:TYR:CD1	1:A:223:TYR:C	2.82	0.52
1:A:336:ILE:HG13	1:A:341:ASP:N	2.24	0.52
1:B:534:THR:OG1	1:B:535:ASP:N	2.41	0.52
1:D:459:THR:OG1	1:D:460:PRO:HD2	2.09	0.52
1:D:460:PRO:O	1:D:463:LEU:HD11	2.09	0.52
1:A:458:ASP:OD1	1:A:459:THR:N	2.39	0.52
1:C:591:GLU:O	1:C:592:VAL:CG1	2.56	0.52
1:D:218:LEU:HB3	1:D:266:THR:HB	1.91	0.52
1:D:434:MSE:HE2	1:D:436:PHE:CE1	2.45	0.52
1:A:512:ILE:HG22	1:A:513:ALA:N	2.24	0.52
1:B:111:ARG:O	1:B:111:ARG:HG2	2.10	0.52
1:B:576:ARG:C	3:B:1036:HOH:O	2.47	0.52
1:C:90:MSE:HB3	1:C:91:PRO:HA	1.91	0.52
1:C:205:MSE:SE	1:C:208:ARG:HH21	2.42	0.52
1:A:368:ASP:O	1:A:383:ARG:NH2	2.41	0.52
1:B:66:VAL:CG2	1:B:71:ILE:CD1	2.88	0.52
1:C:443:THR:O	1:C:445:THR:N	2.42	0.52
1:C:516:GLN:O	1:C:519:GLN:O	2.28	0.52
1:D:291:ILE:CD1	1:D:295:LEU:HD23	2.37	0.52
1:A:329:GLU:O	1:A:333:ILE:HG12	2.09	0.52
1:A:625:PHE:HB2	1:A:626:SER:HG	1.71	0.52
1:B:162:THR:CG2	1:B:164:TYR:CD2	2.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ILE:N	1:B:540:ILE:HD12	2.24	0.52
1:B:559:VAL:O	1:B:559:VAL:HG23	2.10	0.52
1:C:555:SER:CB	1:C:556:PRO:CA	2.87	0.52
1:D:77:ILE:HD12	1:D:77:ILE:O	2.09	0.52
1:D:299:CYS:HA	1:D:302:LEU:HD23	1.92	0.52
1:D:538:GLY:O	1:D:561:LEU:HD22	2.10	0.52
1:A:336:ILE:HG21	1:A:342:TRP:HA	0.67	0.52
1:A:464:SER:OG	1:A:465:PRO:CD	2.58	0.52
1:B:17:LEU:HD13	1:B:460:PRO:HD3	1.92	0.52
1:B:516:GLN:O	1:B:517:TYR:HB2	2.10	0.52
1:B:606:VAL:HG22	1:B:625:PHE:CE1	2.40	0.52
1:D:385:ILE:HG21	1:D:434:MSE:CE	2.23	0.52
1:A:220:ASP:O	1:A:223:TYR:HB3	2.09	0.52
1:C:127:PRO:CG	1:C:128:ILE:HA	2.40	0.52
1:D:71:ILE:N	1:D:71:ILE:CD1	2.69	0.52
1:C:519:GLN:O	1:C:520:PHE:CB	2.58	0.52
1:A:254:HIS:CD2	2:A:900:BLA:HBD2	2.44	0.52
1:B:568:PHE:CD2	1:B:592:VAL:CG2	2.93	0.52
1:C:162:THR:HB	1:C:164:TYR:CD2	2.45	0.52
1:C:475:VAL:O	1:C:476:VAL:CG2	2.52	0.52
1:D:39:VAL:CG1	1:D:49:GLN:HB3	2.40	0.52
1:D:568:PHE:O	1:D:570:GLU:N	2.43	0.52
1:D:593:LEU:O	1:D:594:LEU:CB	2.57	0.52
1:D:622:VAL:O	1:D:622:VAL:HG23	2.10	0.52
1:A:37:LEU:HD12	1:A:37:LEU:C	2.29	0.51
1:A:336:ILE:CG2	1:A:341:ASP:O	2.56	0.51
1:A:366:TYR:HA	1:A:431:GLU:HG2	1.92	0.51
1:A:398:THR:HG22	1:A:399:SER:N	2.25	0.51
1:A:444:VAL:HG22	1:A:445:THR:N	2.25	0.51
1:A:508:VAL:HG12	1:A:512:ILE:HD13	1.90	0.51
1:A:567:PHE:O	1:A:568:PHE:CB	2.54	0.51
1:B:45:HIS:CD2	1:B:76:LEU:HD11	2.45	0.51
1:B:348:ASP:OD1	1:B:350:SER:N	2.42	0.51
1:C:211:GLU:O	1:C:214:ARG:HD2	2.10	0.51
1:D:148:ARG:NH2	1:D:181:PHE:O	2.40	0.51
1:D:547:PHE:O	1:D:550:MSE:CG	2.59	0.51
1:B:562:ASP:CB	1:B:575:LEU:HD11	2.39	0.51
1:A:114:GLU:OE1	1:A:236:THR:CG2	2.55	0.51
1:A:397:VAL:HG23	1:A:492:ARG:HG2	1.91	0.51
1:A:570:GLU:O	1:A:571:SER:C	2.49	0.51
1:D:218:LEU:HD22	1:D:250:MSE:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:CD1	1:A:118:ILE:HG23	2.39	0.51
1:A:222:SER:O	1:A:223:TYR:O	2.29	0.51
1:A:508:VAL:CG1	1:A:512:ILE:CD1	2.88	0.51
1:C:90:MSE:CE	1:C:109:MSE:HB3	2.40	0.51
1:C:403:LEU:HD23	1:C:413:LEU:CD1	2.41	0.51
1:D:74:ASP:C	3:D:1067:HOH:O	2.48	0.51
1:D:80:LEU:HA	1:D:83:LEU:HD23	1.92	0.51
1:B:466:ARG:H	1:B:466:ARG:HD3	1.76	0.51
1:C:266:THR:HG23	1:C:268:VAL:HG23	1.91	0.51
1:C:332:MSE:HE2	1:C:342:TRP:CE3	2.45	0.51
1:B:336:ILE:CG2	1:B:341:ASP:O	2.58	0.51
1:B:437:ARG:NH2	1:B:483:TRP:CE3	2.79	0.51
1:B:466:ARG:HH11	1:B:466:ARG:CG	2.24	0.51
1:C:171:ARG:HD3	1:C:278:TRP:CH2	2.45	0.51
1:D:336:ILE:CD1	1:D:341:ASP:O	2.59	0.51
2:D:900:BLA:NC	3:D:1077:HOH:O	2.24	0.51
1:A:420:VAL:HG22	1:A:436:PHE:HD1	1.76	0.51
1:A:31:ILE:CD1	1:A:37:LEU:HD23	2.41	0.51
1:A:523:GLN:O	1:A:526:ALA:HB3	2.09	0.51
1:A:568:PHE:CE2	1:A:592:VAL:CG1	2.89	0.51
1:B:90:MSE:CE	1:B:109:MSE:HG2	2.40	0.51
1:B:347:PHE:O	1:B:349:THR:HG22	2.10	0.51
1:B:443:THR:O	1:B:443:THR:CG2	2.58	0.51
1:B:612:THR:HG23	1:B:612:THR:O	2.11	0.51
1:D:97:ARG:NH1	1:D:104:GLU:OE2	2.44	0.51
1:D:128:ILE:HG23	1:D:129:ASP:N	2.25	0.51
1:D:157:LEU:HD13	1:D:157:LEU:C	2.31	0.51
1:A:183:GLU:CG	1:A:184:ARG:N	2.73	0.51
1:A:332:MSE:HE3	1:A:346:ILE:CD1	2.39	0.51
1:A:610:PRO:HA	1:A:621:PHE:HD1	1.76	0.51
1:C:133:THR:CG2	1:C:161:CYS:SG	2.99	0.51
1:C:385:ILE:CD1	1:C:434:MSE:HE1	2.41	0.51
1:C:565:ALA:HB2	1:C:575:LEU:HD22	1.93	0.51
1:D:214:ARG:HH11	1:D:214:ARG:HG2	1.73	0.51
1:A:569:VAL:O	1:A:569:VAL:HG23	2.11	0.51
1:B:54:ALA:HB1	1:B:63:VAL:HG21	1.93	0.51
1:D:37:LEU:HD22	1:D:120:GLU:HG2	1.93	0.51
1:D:394:ARG:O	1:D:395:ALA:HB3	2.10	0.51
1:A:76:LEU:CD2	1:A:80:LEU:HD11	2.41	0.50
1:B:261:MSE:HE2	1:B:465:PRO:HG3	1.92	0.50
1:D:470:ALA:O	1:D:471:LYS:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LEU:HD21	1:D:620:GLY:HA3	1.92	0.50
1:A:592:VAL:CG1	1:A:593:LEU:N	2.74	0.50
1:A:617:GLN:HE21	1:A:617:GLN:CA	2.24	0.50
1:B:54:ALA:CB	1:B:63:VAL:HG21	2.41	0.50
1:C:18:SER:OG	1:C:19:ASN:N	2.43	0.50
1:C:236:THR:HG23	1:C:238:ARG:N	2.26	0.50
1:B:608:ALA:HB1	1:B:623:LEU:HD23	1.93	0.50
1:D:338:ARG:O	1:D:339:GLU:CG	2.60	0.50
2:A:900:BLA:HMB3	2:A:900:BLA:C3A	2.39	0.50
1:B:420:VAL:CG2	1:B:434:MSE:HE2	2.42	0.50
1:A:17:LEU:HD22	1:A:458:ASP:OD1	2.12	0.50
1:A:348:ASP:CG	1:A:350:SER:H	2.14	0.50
1:A:348:ASP:OD1	1:A:350:SER:N	2.42	0.50
1:A:561:LEU:O	1:A:564:LEU:HB3	2.12	0.50
1:B:394:ARG:HG2	1:B:398:THR:OG1	2.10	0.50
1:B:530:PRO:HD2	1:B:626:SER:H	1.75	0.50
1:C:229:GLU:HA	1:C:229:GLU:OE1	2.11	0.50
1:C:298:ILE:HG23	1:C:302:LEU:CD2	2.41	0.50
1:C:393:PRO:O	1:C:394:ARG:CZ	2.60	0.50
1:C:393:PRO:O	1:C:394:ARG:HB2	2.12	0.50
1:D:100:ASN:CB	1:D:101:PRO:CD	2.90	0.50
1:D:586:ARG:NE	1:D:586:ARG:HA	2.27	0.50
1:B:607:ARG:HH22	1:B:634:ALA:HB2	1.76	0.50
1:C:60:LEU:HD21	1:C:98:ILE:HG22	1.94	0.50
1:C:130:LEU:HD22	1:C:134:LEU:CD1	2.33	0.50
1:C:205:MSE:HE1	1:C:208:ARG:NH2	2.26	0.50
1:D:332:MSE:O	1:D:336:ILE:HG22	2.12	0.50
1:D:346:ILE:HG22	1:D:347:PHE:CD1	2.47	0.50
1:A:615:GLU:O	1:A:616:ASP:OD1	2.30	0.50
1:C:126:PRO:HG2	1:C:294:GLU:HB2	1.94	0.50
1:B:16:ASP:C	1:B:16:ASP:OD1	2.51	0.50
1:B:348:ASP:O	1:B:349:THR:CG2	2.60	0.50
1:B:404:GLY:O	1:B:405:LEU:CB	2.59	0.50
1:C:218:LEU:HD21	1:C:255:LEU:CD2	2.41	0.50
1:D:173:ASP:OD1	1:D:175:GLN:HB2	2.11	0.50
1:D:298:ILE:CG2	1:D:302:LEU:HD21	2.42	0.50
1:A:193:PHE:C	1:A:193:PHE:HD2	2.15	0.49
1:B:30:SER:HG	1:B:249:SER:HG	1.56	0.49
1:B:466:ARG:O	1:B:469:PHE:O	2.30	0.49
1:C:555:SER:HB3	1:C:556:PRO:CA	2.42	0.49
1:D:625:PHE:CB	1:D:626:SER:OG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416[B]:MSE:SE	1:A:416[B]:MSE:H	2.45	0.49
1:A:440:ARG:CD	1:A:479:THR:HG22	2.43	0.49
1:A:446:TRP:O	1:A:448:GLY:N	2.45	0.49
1:A:534:THR:HG21	1:A:561:LEU:HD21	1.94	0.49
1:B:257:TYR:HE2	1:B:261:MSE:CE	2.21	0.49
1:D:334:GLU:HG2	1:D:335:ALA:N	2.27	0.49
1:A:74:ASP:HA	1:A:77:ILE:HG12	1.94	0.49
1:A:570:GLU:O	1:A:572:ASN:N	2.44	0.49
1:A:615:GLU:O	1:A:615:GLU:HG2	2.13	0.49
1:B:45:HIS:HD2	1:B:76:LEU:HD11	1.77	0.49
1:B:66:VAL:CG2	1:B:71:ILE:HD11	2.42	0.49
1:C:118:ILE:CG2	1:C:119:ILE:N	2.74	0.49
1:D:459:THR:HG23	1:D:461:ALA:H	1.78	0.49
1:A:30:SER:HA	1:A:226:VAL:O	2.13	0.49
1:A:266:THR:CG2	1:A:268:VAL:HG23	2.41	0.49
1:B:47:ILE:C	1:B:48:ILE:O	2.46	0.49
1:B:518:GLU:O	1:B:519:GLN:CG	2.61	0.49
1:C:112:PRO:O	1:C:113:PRO:C	2.50	0.49
1:A:163:GLY:O	1:A:164:TYR:O	2.31	0.49
1:A:440:ARG:HD3	1:A:476:VAL:CG2	2.43	0.49
1:D:42:GLU:HA	1:D:42:GLU:OE1	2.13	0.49
1:D:348:ASP:OD1	1:D:349:THR:C	2.51	0.49
1:A:24:GLU:HG2	3:A:1013:HOH:O	2.13	0.49
1:A:193:PHE:C	1:A:193:PHE:CD2	2.86	0.49
1:A:403:LEU:C	1:A:404:GLY:O	2.48	0.49
1:A:444:VAL:HG22	1:A:445:THR:H	1.77	0.49
1:A:454:PHE:CE2	1:A:467:ARG:HG3	2.48	0.49
1:A:586:ARG:HA	1:A:586:ARG:NE	2.26	0.49
1:B:336:ILE:CG1	1:B:341:ASP:O	2.60	0.49
1:D:610:PRO:HA	1:D:621:PHE:HD1	1.78	0.49
1:B:562:ASP:CA	1:B:575:LEU:HD11	2.42	0.49
1:C:37:LEU:C	1:C:37:LEU:CD2	2.80	0.49
1:C:47:ILE:HG21	1:C:63:VAL:CG2	2.42	0.49
1:C:346:ILE:HG22	1:C:347:PHE:CD1	2.48	0.49
1:C:606:VAL:HG11	1:C:625:PHE:CE1	2.47	0.49
1:A:118:ILE:CD1	1:A:240:LEU:HD21	2.43	0.49
1:B:336:ILE:HG12	1:B:341:ASP:O	2.13	0.49
1:C:47:ILE:HD13	1:C:63:VAL:HG23	1.94	0.49
1:D:407:VAL:CG2	1:D:410:LEU:HD12	2.43	0.49
1:A:76:LEU:HD22	1:A:80:LEU:HD13	1.93	0.49
1:A:164:TYR:CE2	1:A:289:ARG:CD	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TRP:CH2	1:A:407:VAL:HG21	2.48	0.49
1:B:80:LEU:N	1:B:81:PRO:HD2	2.27	0.49
1:B:562:ASP:HA	1:B:575:LEU:HD12	1.94	0.49
1:B:606:VAL:HG12	1:B:607:ARG:N	2.28	0.49
1:C:146:SER:HA	1:C:313:LEU:HD22	1.93	0.49
1:A:39:VAL:HG22	1:A:118:ILE:HD13	1.95	0.49
1:A:60:LEU:CD1	1:A:99:GLY:HA2	2.42	0.49
1:A:109:MSE:O	1:A:118:ILE:O	2.31	0.49
1:A:332:MSE:CA	1:A:335:ALA:CB	2.86	0.49
1:B:48:ILE:O	1:B:49:GLN:O	2.30	0.49
1:B:156:LEU:HD22	1:B:160:GLN:NE2	2.27	0.49
1:B:516:GLN:O	1:B:517:TYR:CB	2.59	0.49
1:C:270:SER:HA	1:C:280:LEU:HD23	1.94	0.49
1:D:246:PHE:CE1	1:D:296:ARG:NH1	2.80	0.49
1:D:439:GLU:HG2	1:D:441:VAL:HG12	1.94	0.49
1:D:393:PRO:O	1:D:394:ARG:CG	2.62	0.48
1:D:569:VAL:HA	1:D:595:ARG:HD2	1.95	0.48
1:A:236:THR:C	1:A:238:ARG:H	2.17	0.48
1:B:232:LEU:HD22	1:B:237:GLY:O	2.14	0.48
1:A:204:GLN:HA	1:A:207:ARG:HG3	1.95	0.48
1:A:476:VAL:HG22	1:A:476:VAL:O	2.13	0.48
1:B:233:SER:C	1:B:235:LEU:H	2.16	0.48
1:B:613:ARG:O	1:B:614:THR:HG23	2.13	0.48
1:D:416:MSE:CE	1:D:417:ALA:HB3	2.44	0.48
1:A:205:MSE:HE2	1:A:208:ARG:HH12	1.79	0.48
1:A:258:LEU:CB	1:A:263:VAL:CG2	2.86	0.48
1:A:529:GLN:HB3	1:A:626:SER:HB3	1.95	0.48
1:B:366:TYR:HA	1:B:431:GLU:HG2	1.95	0.48
1:B:394:ARG:HD3	1:B:398:THR:HG21	1.95	0.48
1:B:579:ALA:HB1	3:B:1018:HOH:O	2.12	0.48
1:C:434:MSE:CE	1:C:436:PHE:CZ	2.93	0.48
1:D:120:GLU:HB3	1:D:247:LEU:HD12	1.94	0.48
1:D:463:LEU:H	1:D:463:LEU:HD12	1.79	0.48
1:D:550:MSE:HE1	1:D:604:LEU:CD2	2.43	0.48
1:A:374:GLY:O	1:A:376:VAL:HG22	2.14	0.48
1:B:95:ARG:NH2	1:B:104:GLU:OE1	2.47	0.48
1:B:181:PHE:CG	1:B:181:PHE:O	2.66	0.48
1:B:561:LEU:CD1	1:B:623:LEU:HD11	2.44	0.48
1:A:398:THR:CG2	1:A:399:SER:N	2.76	0.48
1:C:449:ASP:HB2	1:C:450:PRO:HD3	1.95	0.48
1:C:566:GLY:C	1:C:568:PHE:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:O	1:A:187:PRO:C	2.52	0.48
1:A:571:SER:O	1:A:573:ASP:N	2.47	0.48
1:A:615:GLU:O	1:A:616:ASP:CG	2.52	0.48
1:C:186:VAL:HG22	1:C:189:LEU:HD12	1.96	0.48
1:C:201:ASP:HB3	2:C:900:BLA:HHB	1.95	0.48
1:D:70:GLU:O	1:D:71:ILE:C	2.52	0.48
1:D:108:LEU:N	1:D:108:LEU:CD1	2.77	0.48
1:D:250:MSE:HE1	1:D:258:LEU:HD12	1.96	0.48
1:D:396:ALA:O	1:D:397:VAL:CG2	2.59	0.48
1:A:168:MSE:HE3	1:A:170:TYR:HE1	1.78	0.48
1:B:520:PHE:O	1:C:510:THR:OG1	2.23	0.48
1:C:446:TRP:CE3	1:C:473:HIS:CE1	3.01	0.48
1:A:76:LEU:CD2	1:A:80:LEU:HD13	2.44	0.48
1:A:235:LEU:O	1:A:235:LEU:CD1	2.54	0.48
1:B:35:GLY:HA2	1:B:57:PHE:CZ	2.49	0.48
1:B:40:VAL:CG1	1:B:45:HIS:HA	2.44	0.48
1:B:279:GLY:C	1:B:280:LEU:HD23	2.34	0.48
1:C:29:GLY:C	1:C:242:MSE:HE1	2.34	0.48
1:C:258:LEU:HA	1:C:261:MSE:CE	2.44	0.48
1:A:71:ILE:O	1:A:72:ASP:HB2	2.11	0.48
1:A:336:ILE:HG23	1:A:337:THR:N	2.29	0.48
1:A:569:VAL:CG1	1:A:600:ARG:HB3	2.44	0.48
1:B:66:VAL:HG22	1:B:71:ILE:HD11	1.95	0.48
1:B:173:ASP:C	1:B:173:ASP:OD1	2.51	0.48
1:B:336:ILE:CD1	1:B:341:ASP:C	2.81	0.48
1:B:338:ARG:O	1:B:339:GLU:HG3	2.14	0.48
1:A:45[A]:HIS:ND1	1:A:68:LEU:HB3	2.29	0.47
1:A:118:ILE:HD11	1:A:240:LEU:HD21	1.95	0.47
1:A:509:ARG:O	1:A:513:ALA:CB	2.62	0.47
1:C:110:HIS:CE1	1:C:118:ILE:HD12	2.49	0.47
1:C:416:MSE:H	1:C:416:MSE:SE	2.48	0.47
1:D:260:ASN:N	1:D:260:ASN:HD22	2.11	0.47
1:D:332:MSE:HE3	1:D:501:ILE:HG12	1.94	0.47
1:A:593:LEU:N	1:A:593:LEU:HD12	2.28	0.47
1:B:34:HIS:CE1	1:B:219:VAL:HG21	2.49	0.47
1:B:273:VAL:HG21	1:B:310:ILE:HG21	1.96	0.47
1:B:544:ASN:H	1:B:544:ASN:ND2	2.07	0.47
1:B:572:ASN:ND2	1:B:572:ASN:H	2.11	0.47
1:C:133:THR:HG21	1:C:161:CYS:SG	2.54	0.47
1:C:540:ILE:O	1:C:540:ILE:CG2	2.61	0.47
1:D:31:ILE:HG13	1:D:226:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:PHE:O	1:D:348:ASP:C	2.52	0.47
1:B:547:PHE:O	1:B:550:MSE:HB3	2.14	0.47
1:B:605:ALA:HB3	1:B:627:ASP:CB	2.32	0.47
1:C:63:VAL:HG22	1:C:64:LEU:N	2.29	0.47
1:C:336:ILE:HA	1:C:340:GLY:O	2.14	0.47
1:A:220:ASP:OD1	1:A:220:ASP:C	2.53	0.47
1:A:574:PHE:O	1:A:578:VAL:HG23	2.13	0.47
1:B:572:ASN:O	1:B:575:LEU:N	2.46	0.47
1:C:32:GLN:HE22	1:C:218:LEU:HA	1.80	0.47
1:C:449:ASP:CB	1:C:450:PRO:CD	2.92	0.47
1:C:559:VAL:O	1:C:560:HIS:HB2	2.14	0.47
1:B:550:MSE:HE1	1:B:604:LEU:CD1	2.33	0.47
1:C:612:THR:HG23	3:C:1084:HOH:O	2.10	0.47
1:D:413:LEU:HD13	1:D:413:LEU:O	2.14	0.47
1:D:533:ILE:HG23	1:D:622:VAL:HG12	1.97	0.47
1:A:258:LEU:CB	1:A:263:VAL:HG22	2.43	0.47
1:B:231:ARG:O	1:B:232:LEU:CB	2.62	0.47
1:D:383:ARG:O	1:D:386:ALA:HB3	2.14	0.47
1:A:258:LEU:CA	1:A:263:VAL:HG22	2.45	0.47
1:A:388:TRP:CZ3	1:A:407:VAL:HG21	2.50	0.47
1:A:525:HIS:NE2	1:A:542:LEU:HD11	2.30	0.47
1:A:559:VAL:O	1:A:560:HIS:O	2.31	0.47
1:A:614:THR:HG22	1:A:615:GLU:N	2.30	0.47
1:B:21:GLU:HG3	1:B:21:GLU:O	2.14	0.47
1:B:148:ARG:NH2	1:B:181:PHE:O	2.48	0.47
1:B:291:ILE:HD12	1:B:295:LEU:HD12	1.96	0.47
1:B:349:THR:HG23	1:B:351:GLN:HG2	1.97	0.47
1:B:351:GLN:O	1:B:351:GLN:CG	2.62	0.47
1:B:370:ILE:HD12	1:B:371:ARG:N	2.30	0.47
1:B:594:LEU:CG	1:B:602:LEU:HD13	2.45	0.47
2:B:900:BLA:HMA2	2:B:900:BLA:O2A	2.15	0.47
1:C:346:ILE:CG2	1:C:346:ILE:O	2.62	0.47
1:C:532:LEU:HB2	1:C:623:LEU:HB2	1.97	0.47
1:D:138:LEU:HD11	1:D:305:ALA:HB2	1.97	0.47
1:D:242:MSE:O	1:D:243:SER:C	2.52	0.47
1:D:299:CYS:HA	1:D:302:LEU:CD2	2.45	0.47
1:A:534:THR:HA	1:A:541:LEU:HD13	1.95	0.47
1:A:555:SER:O	1:A:557:SER:N	2.48	0.47
1:B:30:SER:OG	1:B:249:SER:OG	2.29	0.47
1:B:397:VAL:HG12	1:B:397:VAL:O	2.13	0.47
1:B:530:PRO:HD3	1:B:626:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASN:ND2	1:D:101:PRO:HD3	2.29	0.47
1:A:258:LEU:HA	1:A:263:VAL:HG22	1.97	0.47
1:B:169:VAL:HG22	1:B:169:VAL:O	2.13	0.47
1:C:586:ARG:HD3	1:C:587:GLY:H	1.80	0.47
1:D:625:PHE:CB	1:D:626:SER:HA	2.40	0.47
1:A:155:ALA:HB1	1:A:167:VAL:HG23	1.96	0.47
1:B:325:VAL:HG11	1:B:493:THR:CG2	2.45	0.47
1:C:365:VAL:O	1:C:431:GLU:HA	2.15	0.47
1:C:622:VAL:HG22	1:C:624:ILE:HG13	1.97	0.47
1:D:397:VAL:HG21	1:D:492:ARG:HA	1.97	0.47
1:D:558:ALA:HB1	1:D:564:LEU:CD1	2.44	0.47
1:A:332:MSE:HA	1:A:335:ALA:CB	2.45	0.46
1:A:504:GLN:HA	1:D:624:ILE:HD11	1.96	0.46
1:B:370:ILE:HD12	1:B:370:ILE:C	2.36	0.46
1:B:553:ALA:O	1:B:555:SER:N	2.49	0.46
1:D:37:LEU:HD13	1:D:38:LEU:N	2.30	0.46
1:D:75:LEU:O	1:D:79:ILE:HG23	2.15	0.46
1:D:337:THR:O	1:D:338:ARG:CB	2.62	0.46
1:A:171:ARG:HG2	1:A:278:TRP:CH2	2.50	0.46
1:B:348:ASP:O	1:B:349:THR:HG22	2.15	0.46
1:B:529:GLN:HB2	1:B:530:PRO:CD	2.45	0.46
1:C:166:ARG:NH1	1:C:183:GLU:OE2	2.49	0.46
1:C:540:ILE:HG22	1:C:559:VAL:HA	1.96	0.46
1:B:611:VAL:O	1:B:612:THR:CB	2.64	0.46
1:C:50:ALA:O	1:C:51:SER:C	2.52	0.46
1:C:74:ASP:O	1:C:77:ILE:N	2.45	0.46
1:D:552:PRO:O	1:D:553:ALA:O	2.34	0.46
1:A:95:ARG:NH1	1:A:106:ASP:OD1	2.47	0.46
1:A:164:TYR:CE2	1:A:289:ARG:HD3	2.50	0.46
1:A:166:ARG:NH2	1:A:190:GLU:O	2.49	0.46
1:A:528:MSE:HA	1:A:528:MSE:CE	2.46	0.46
1:B:254:HIS:CE1	2:B:900:BLA:C1A	2.98	0.46
1:C:285:HIS:CD2	1:C:289:ARG:HD2	2.51	0.46
1:C:564:LEU:HD13	1:C:564:LEU:N	2.31	0.46
1:C:568:PHE:CE1	1:C:592:VAL:HB	2.50	0.46
1:A:219:VAL:O	1:A:288:PRO:HB3	2.16	0.46
1:B:600:ARG:H	1:B:601:PRO:CD	2.28	0.46
1:C:258:LEU:CD2	1:C:261:MSE:CE	2.78	0.46
1:C:410:LEU:HA	1:C:412:HIS:CE1	2.51	0.46
1:C:611:VAL:O	1:C:619:LEU:N	2.47	0.46
1:D:472:TRP:O	1:D:475:VAL:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PRO:HD2	1:C:116:GLY:O	2.15	0.46
1:C:327[B]:ARG:HA	1:C:327[B]:ARG:HD3	1.62	0.46
1:A:58:LEU:HG	1:A:98:ILE:HG21	1.96	0.46
1:A:250:MSE:O	1:A:251:SER:C	2.55	0.46
1:D:232:LEU:H	1:D:232:LEU:CD1	2.23	0.46
1:D:333:ILE:HG23	1:D:338:ARG:NH2	2.30	0.46
1:A:90:MSE:HA	1:A:91:PRO:C	2.35	0.46
1:B:562:ASP:HA	1:B:575:LEU:HD11	1.98	0.46
1:B:575:LEU:O	1:B:578:VAL:HG13	2.16	0.46
1:C:8:GLY:N	3:C:1005:HOH:O	2.48	0.46
1:D:246:PHE:CZ	1:D:296:ARG:NH1	2.84	0.46
1:D:286:TYR:O	1:D:287:LEU:HG	2.15	0.46
1:D:298:ILE:HG22	1:D:302:LEU:HD21	1.97	0.46
1:D:404:GLY:O	1:D:408:PRO:HA	2.16	0.46
1:D:628:ALA:O	1:D:629:THR:HB	2.14	0.46
1:A:514:ARG:CZ	1:D:541:LEU:HD13	2.46	0.46
2:A:900:BLA:CMB	2:A:900:BLA:C3A	2.94	0.46
1:B:13:GLY:HA2	1:B:252:PRO:HG2	1.98	0.46
1:B:166:ARG:CD	1:B:168:MSE:HE2	2.41	0.46
1:B:484:THR:HG22	1:B:486:ALA:N	2.27	0.46
1:A:250:MSE:HE2	2:A:900:BLA:CGD	2.46	0.46
1:B:26:HIS:CE1	1:B:205:MSE:CE	2.99	0.46
1:B:388:TRP:CZ3	1:B:407:VAL:CG2	2.99	0.46
1:B:561:LEU:O	1:B:562:ASP:C	2.53	0.46
1:C:58:LEU:O	1:C:60:LEU:HD22	2.14	0.46
1:C:569:VAL:CA	1:C:593:LEU:O	2.63	0.46
1:D:291:ILE:HD13	1:D:291:ILE:HA	1.79	0.46
1:D:625:PHE:CB	1:D:626:SER:CA	2.94	0.46
1:A:336:ILE:CG2	1:A:341:ASP:C	2.84	0.45
1:B:468:SER:O	1:B:472:TRP:N	2.33	0.45
1:C:235:LEU:N	1:C:235:LEU:HD22	2.31	0.45
1:C:417:ALA:C	1:C:419:GLY:N	2.68	0.45
1:D:238:ARG:O	1:D:239:ASP:O	2.33	0.45
1:A:173:ASP:OD1	1:A:175:GLN:N	2.49	0.45
1:A:363:ALA:HB3	1:A:434:MSE:HG2	1.98	0.45
1:C:127:PRO:HB2	1:C:128:ILE:HA	1.97	0.45
1:C:288:PRO:O	1:C:289:ARG:HB2	2.16	0.45
1:A:480:SER:O	1:A:481:ASP:C	2.54	0.45
1:B:459:THR:HB	1:B:460:PRO:HD2	1.97	0.45
1:B:553:ALA:O	1:B:555:SER:OG	2.29	0.45
1:C:92:VAL:HG22	1:C:93:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:HD12	1:D:77:ILE:C	2.37	0.45
1:A:381:ASP:CG	1:A:413:LEU:HD21	2.37	0.45
1:C:393:PRO:O	1:C:394:ARG:NE	2.48	0.45
1:C:535:ASP:OD1	1:C:539:ARG:N	2.49	0.45
1:D:578:VAL:HG12	1:D:582:ILE:CD1	2.46	0.45
1:A:476:VAL:O	1:A:476:VAL:HG13	2.17	0.45
1:A:565:ALA:O	3:A:1040:HOH:O	2.21	0.45
1:B:141:ILE:HD13	1:B:306:ILE:CG1	2.44	0.45
1:B:338:ARG:O	1:B:339:GLU:CB	2.65	0.45
1:D:420:VAL:HG12	1:D:436:PHE:HD1	1.81	0.45
1:B:328:LEU:HG	1:B:332:MSE:HE2	1.99	0.45
1:B:349:THR:CG2	1:B:351:GLN:HG2	2.47	0.45
1:B:401:ALA:HB1	1:B:480:SER:OG	2.17	0.45
1:B:540:ILE:N	1:B:540:ILE:CD1	2.80	0.45
1:D:64:LEU:HD11	1:D:230:PRO:CD	2.43	0.45
1:D:484:THR:HG23	1:D:487:ASP:OD2	2.16	0.45
1:D:537:GLU:O	1:D:560:HIS:HE1	2.00	0.45
1:A:381:ASP:CB	1:A:413:LEU:HD21	2.46	0.45
1:B:11:ALA:O	1:B:12:PHE:C	2.55	0.45
1:C:140:ARG:NH1	1:C:153:ASP:OD1	2.50	0.45
1:D:238:ARG:N	1:D:238:ARG:CD	2.80	0.45
1:D:397:VAL:CG2	1:D:492:ARG:HA	2.47	0.45
1:D:524:VAL:HG13	1:D:531:VAL:HG11	1.97	0.45
1:A:555:SER:HA	3:A:1025:HOH:O	2.16	0.45
1:C:40:VAL:CG1	1:C:45:HIS:CA	2.95	0.45
1:C:267:LEU:HD12	1:C:268:VAL:N	2.32	0.45
1:C:519:GLN:O	1:C:520:PHE:HB2	2.17	0.45
1:D:337:THR:O	1:D:338:ARG:HB2	2.16	0.45
1:A:402:SER:O	1:A:406:ASP:HB2	2.17	0.45
1:B:130:LEU:HB2	1:B:131:SER:HA	1.99	0.45
1:C:421:VAL:HG12	1:C:483:TRP:CE2	2.52	0.45
1:C:519:GLN:O	1:C:520:PHE:CG	2.70	0.45
1:D:214:ARG:CG	1:D:214:ARG:NH1	2.75	0.45
1:A:258:LEU:HD22	1:A:263:VAL:HG21	1.99	0.45
1:A:291:ILE:HD12	1:A:291:ILE:HA	1.80	0.45
1:A:366:TYR:C	1:A:368:ASP:N	2.66	0.45
1:A:629:THR:HG22	1:A:632:ARG:HD2	1.99	0.45
1:B:126:PRO:O	1:B:127:PRO:C	2.55	0.45
1:C:68:LEU:HD22	1:C:75:LEU:HD13	1.98	0.45
1:C:559:VAL:O	1:C:560:HIS:CB	2.65	0.45
1:D:90:MSE:SE	1:D:109:MSE:HE3	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:C	1:A:257:TYR:N	2.70	0.44
1:B:146:SER:C	1:B:148:ARG:N	2.70	0.44
1:B:569:VAL:HG12	1:B:570:GLU:H	1.82	0.44
1:D:628:ALA:O	1:D:629:THR:CB	2.64	0.44
1:C:215:VAL:HG21	1:C:296:ARG:HD2	1.99	0.44
1:C:569:VAL:N	1:C:595:ARG:HG3	2.32	0.44
1:D:578:VAL:CG1	1:D:582:ILE:CD1	2.95	0.44
1:A:348:ASP:C	1:A:349:THR:HG22	2.37	0.44
1:A:457:GLY:HA3	1:A:458:ASP:HA	1.74	0.44
1:A:608:ALA:HB2	1:A:623:LEU:HD13	1.99	0.44
1:B:278:TRP:CE2	1:B:310:ILE:HD13	2.53	0.44
1:B:519:GLN:C	1:B:521:SER:N	2.70	0.44
1:C:133:THR:HG23	1:C:161:CYS:SG	2.58	0.44
1:C:175:GLN:HB2	1:C:177:HIS:CD2	2.52	0.44
1:D:141:ILE:HG22	1:D:309:ARG:HG3	1.99	0.44
1:D:148:ARG:HG3	1:D:152:ASP:OD1	2.17	0.44
1:A:308:THR:O	1:A:311:THR:N	2.50	0.44
2:B:900:BLA:CMB	2:B:900:BLA:C3A	2.93	0.44
1:C:83:LEU:HD21	1:C:109:MSE:SE	2.68	0.44
1:D:39:VAL:HG13	1:D:49:GLN:CB	2.44	0.44
1:D:214:ARG:CZ	1:D:272:VAL:HG11	2.47	0.44
1:D:357:LEU:HD21	1:D:491:ALA:HB2	1.98	0.44
1:D:551:LEU:C	1:D:553:ALA:H	2.14	0.44
1:D:606:VAL:HG23	1:D:625:PHE:CD2	2.53	0.44
1:A:230:PRO:O	1:A:231:ARG:CB	2.64	0.44
1:A:560:HIS:HD2	1:A:562:ASP:HB2	1.82	0.44
1:A:613:ARG:O	1:A:617:GLN:O	2.35	0.44
1:B:37:LEU:HD23	1:B:38:LEU:N	2.32	0.44
1:B:162:THR:HG22	1:B:164:TYR:HB2	1.99	0.44
1:C:599:ASN:O	1:C:601:PRO:N	2.50	0.44
1:D:307:ALA:O	1:D:308:THR:C	2.55	0.44
1:D:378:SER:O	1:D:382:VAL:HG23	2.17	0.44
1:A:171:ARG:CG	1:A:278:TRP:CH2	3.01	0.44
1:A:223:TYR:CD1	1:A:223:TYR:O	2.71	0.44
1:B:518:GLU:O	1:B:519:GLN:CB	2.64	0.44
1:C:73:GLY:HA3	1:C:97:ARG:O	2.17	0.44
1:C:120:GLU:HG2	1:C:247:LEU:HD12	2.00	0.44
1:D:79:ILE:O	1:D:83:LEU:HD22	2.17	0.44
1:A:40:VAL:HG13	1:A:45[B]:HIS:HA	1.99	0.44
1:A:144:ALA:HB3	1:A:309:ARG:HD2	1.99	0.44
1:A:285:HIS:HD2	1:A:287:LEU:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASP:C	1:A:459:THR:CG2	2.86	0.44
1:B:28:ALA:O	1:B:242:MSE:HE1	2.18	0.44
1:B:230:PRO:O	1:B:231:ARG:HB3	2.17	0.44
1:C:338:ARG:O	1:C:340:GLY:N	2.51	0.44
1:D:134:LEU:HD11	1:D:301:LEU:HD12	2.00	0.44
1:D:622:VAL:O	1:D:622:VAL:CG2	2.66	0.44
1:A:95:ARG:NH2	1:A:128:ILE:HD11	2.33	0.44
1:B:521:SER:HA	1:B:524:VAL:HG23	2.00	0.44
1:B:605:ALA:CB	1:B:627:ASP:HB2	2.33	0.44
1:A:458:ASP:O	1:A:462:ASP:HB2	2.18	0.44
1:A:515:GLU:C	1:A:517:TYR:H	2.21	0.44
1:A:568:PHE:CZ	1:A:592:VAL:HG11	2.50	0.44
1:C:452:LYS:O	1:C:452:LYS:NZ	2.35	0.44
1:D:147:LEU:N	1:D:313:LEU:HD13	2.33	0.44
1:B:233:SER:C	1:B:235:LEU:N	2.70	0.43
1:C:221:VAL:HG12	1:C:264:ARG:HA	2.00	0.43
1:C:346:ILE:HG22	1:C:347:PHE:CE1	2.53	0.43
1:D:25:ILE:HD11	1:D:206:ALA:HA	2.00	0.43
1:A:164:TYR:CE2	1:A:289:ARG:HD2	2.53	0.43
1:B:336:ILE:HD13	1:B:342:TRP:CA	2.48	0.43
1:B:578:VAL:O	1:B:581:LEU:HB3	2.18	0.43
1:C:27:LEU:O	1:C:28:ALA:O	2.34	0.43
1:C:291:ILE:O	1:C:296:ARG:NH1	2.51	0.43
1:C:432:PHE:HE1	1:C:434:MSE:SE	2.52	0.43
1:B:553:ALA:N	3:B:1003:HOH:O	2.51	0.43
1:C:60:LEU:HD11	1:C:71:ILE:HG22	2.00	0.43
1:C:63:VAL:C	1:C:66:VAL:HG23	2.38	0.43
1:D:76:LEU:O	1:D:80:LEU:HB2	2.19	0.43
1:D:129:ASP:O	1:D:130:LEU:CB	2.65	0.43
1:D:151:CYS:CA	1:D:154:THR:HG23	2.43	0.43
1:D:331:ARG:NH1	3:D:1036:HOH:O	2.51	0.43
1:D:623:LEU:N	1:D:623:LEU:CD2	2.73	0.43
1:A:613:ARG:O	1:A:615:GLU:N	2.51	0.43
1:B:71:ILE:O	1:B:72:ASP:CB	2.67	0.43
1:C:133:THR:O	1:C:135:ALA:N	2.52	0.43
1:C:413:LEU:CD1	1:C:413:LEU:O	2.67	0.43
1:C:542:LEU:C	1:C:542:LEU:CD1	2.85	0.43
1:D:34:HIS:CE1	1:D:219:VAL:HG23	2.52	0.43
1:D:588:TRP:NE1	1:D:606:VAL:HG11	2.34	0.43
1:A:28:ALA:O	1:A:242:MSE:HE1	2.19	0.43
1:A:204:GLN:O	1:A:205:MSE:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD12	1:B:63:VAL:CG2	2.49	0.43
1:C:199:SER:O	1:C:201:ASP:N	2.51	0.43
1:C:202:ILE:CG2	1:C:207:ARG:HG2	2.47	0.43
1:C:440:ARG:HG2	1:C:481:ASP:N	2.34	0.43
1:D:385:ILE:CG2	1:D:434:MSE:HE1	2.24	0.43
1:A:163:GLY:O	1:A:164:TYR:C	2.57	0.43
1:A:539:ARG:O	1:A:541:LEU:CD1	2.67	0.43
1:B:103:THR:CG2	1:B:105:TYR:OH	2.66	0.43
1:C:76:LEU:HD12	1:C:80:LEU:HD13	2.01	0.43
1:D:626:SER:O	1:D:627:ASP:C	2.56	0.43
1:A:205:MSE:O	1:A:209:LEU:HD22	2.18	0.43
1:A:336:ILE:O	1:A:340:GLY:N	2.52	0.43
1:A:455:THR:C	1:A:457:GLY:H	2.22	0.43
1:C:236:THR:HG23	1:C:238:ARG:H	1.83	0.43
1:D:323:LEU:HD11	1:D:327:ARG:NE	2.34	0.43
1:D:357:LEU:O	1:D:437:ARG:NH2	2.51	0.43
1:D:470:ALA:O	1:D:471:LYS:HB2	2.19	0.43
1:A:180:VAL:O	1:A:180:VAL:HG12	2.18	0.43
1:A:509:ARG:O	1:A:513:ALA:HB3	2.19	0.43
1:B:147:LEU:N	1:B:313:LEU:HD13	2.34	0.43
1:B:149:ALA:O	1:B:153:ASP:HB2	2.18	0.43
1:B:168:MSE:HE1	1:B:284:HIS:CE1	2.53	0.43
1:B:276:LYS:HE2	3:B:1046:HOH:O	2.19	0.43
1:C:357:LEU:O	1:C:358:HIS:C	2.57	0.43
1:C:446:TRP:CD2	1:C:473:HIS:CE1	3.06	0.43
1:C:525:HIS:HE1	1:C:542:LEU:HD13	1.84	0.43
1:D:229:GLU:C	1:D:231:ARG:N	2.70	0.43
1:D:392:GLN:O	1:D:394:ARG:NE	2.51	0.43
1:D:464:SER:OG	1:D:467:ARG:HB3	2.18	0.43
2:D:900:BLA:HMC1	2:D:900:BLA:CBC	2.48	0.43
1:A:314:GLU:O	1:A:315:SER:C	2.57	0.43
1:A:604:LEU:HA	1:A:627:ASP:O	2.18	0.43
1:B:84:ASP:OD1	1:B:84:ASP:C	2.57	0.43
1:B:252:PRO:HA	1:B:255:LEU:HB2	2.00	0.43
1:B:393:PRO:O	1:B:394:ARG:CB	2.65	0.43
1:C:130:LEU:C	1:C:130:LEU:HD12	2.39	0.43
1:C:195:ASN:ND2	3:C:1010:HOH:O	2.51	0.43
1:D:246:PHE:CZ	1:D:296:ARG:CZ	3.01	0.43
1:D:336:ILE:HG23	1:D:337:THR:H	1.80	0.43
1:D:497:THR:O	1:D:501:ILE:HG23	2.19	0.43
1:D:532:LEU:HD11	1:D:547:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:HA	1:A:252:PRO:HD3	1.88	0.43
2:B:900:BLA:NC	3:B:1069:HOH:O	2.31	0.43
1:C:204:GLN:O	1:C:208:ARG:HB2	2.19	0.43
1:C:518:GLU:O	1:C:521:SER:HB3	2.19	0.43
1:D:625:PHE:C	1:D:626:SER:OG	2.56	0.43
1:A:83:LEU:HD12	1:A:83:LEU:N	2.34	0.42
1:A:92:VAL:CG2	1:A:93:ALA:N	2.81	0.42
1:A:151:CYS:HB3	1:A:182:SER:OG	2.19	0.42
1:A:201:ASP:OD2	1:A:468:SER:CB	2.66	0.42
1:A:381:ASP:HB3	1:A:413:LEU:CD2	2.49	0.42
1:A:535:ASP:OD2	1:A:539:ARG:HB2	2.19	0.42
1:B:420:VAL:O	1:B:420:VAL:CG1	2.67	0.42
1:B:420:VAL:O	1:B:420:VAL:HG13	2.19	0.42
1:B:520:PHE:CD2	1:C:509:ARG:HB3	2.54	0.42
1:B:544:ASN:N	1:B:544:ASN:ND2	2.64	0.42
1:C:147:LEU:HD12	1:C:147:LEU:HA	1.74	0.42
1:C:561:LEU:HD23	1:C:561:LEU:O	2.18	0.42
1:D:168:MSE:HE2	1:D:170:TYR:OH	2.19	0.42
1:D:235:LEU:C	1:D:237:GLY:H	2.22	0.42
1:D:257:TYR:CD2	1:D:261:MSE:CE	2.84	0.42
1:D:377:PRO:CG	1:D:416:MSE:HE3	2.49	0.42
1:A:88:GLU:O	1:A:88:GLU:HG2	2.19	0.42
1:A:184:ARG:HE	1:A:184:ARG:HB2	1.60	0.42
1:A:201:ASP:O	2:A:900:BLA:NC	2.52	0.42
1:A:222:SER:OG	1:A:264[B]:ARG:NH1	2.50	0.42
1:A:454:PHE:HE2	1:A:467:ARG:HG3	1.83	0.42
1:B:103:THR:HG23	1:B:105:TYR:OH	2.19	0.42
1:B:233:SER:OG	1:B:236:THR:HG23	2.18	0.42
1:B:594:LEU:HG	1:B:602:LEU:HD13	2.01	0.42
1:C:298:ILE:CG2	1:C:302:LEU:CD2	2.97	0.42
1:C:403:LEU:CD2	1:C:413:LEU:HD11	2.49	0.42
1:D:148:ARG:NH1	1:D:181:PHE:CZ	2.88	0.42
1:D:416:MSE:HE2	1:D:417:ALA:N	2.34	0.42
1:A:156:LEU:HD22	1:A:160:GLN:OE1	2.19	0.42
1:A:235:LEU:HD12	3:A:1032:HOH:O	2.19	0.42
1:A:257:TYR:CD2	1:A:261:MSE:CE	2.95	0.42
1:C:202:ILE:O	1:C:203:PRO:C	2.55	0.42
1:C:449:ASP:HB3	1:C:450:PRO:HD3	1.99	0.42
1:D:79:ILE:HD12	1:D:109:MSE:SE	2.69	0.42
1:D:141:ILE:O	1:D:309:ARG:HG3	2.19	0.42
1:D:198:PRO:HG2	1:D:471:LYS:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ASP:OD1	1:D:350:SER:N	2.52	0.42
1:D:517:TYR:HD1	1:D:518:GLU:N	2.17	0.42
1:A:440:ARG:NH1	1:A:482:PRO:HD3	2.34	0.42
1:A:561:LEU:O	1:A:564:LEU:N	2.52	0.42
1:B:42:GLU:CD	1:B:117:LEU:HD23	2.40	0.42
1:B:348:ASP:C	1:B:350:SER:N	2.71	0.42
1:B:365:VAL:CG2	1:B:430:GLY:O	2.60	0.42
1:B:504:GLN:HB2	1:C:624:ILE:CD1	2.49	0.42
1:B:532:LEU:HD21	1:B:547:PHE:CD2	2.54	0.42
1:C:188:GLY:O	1:C:189:LEU:HG	2.20	0.42
1:C:337:THR:O	1:C:338:ARG:CB	2.64	0.42
1:D:74:ASP:O	1:D:96:CYS:HB2	2.19	0.42
1:A:368:ASP:OD1	1:A:383:ARG:NH2	2.52	0.42
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.86	0.42
1:B:82:HIS:CG	1:B:92:VAL:HG21	2.53	0.42
1:B:291:ILE:HD12	1:B:295:LEU:CD1	2.49	0.42
1:B:532:LEU:HD21	1:B:547:PHE:CG	2.55	0.42
1:C:273:VAL:HG23	1:C:278:TRP:HB2	2.02	0.42
1:C:324:PHE:CD2	1:C:324:PHE:C	2.93	0.42
1:D:439:GLU:OE2	1:D:441:VAL:HG11	2.20	0.42
1:B:71:ILE:HD13	1:B:71:ILE:HA	1.78	0.42
1:B:376:VAL:HB	1:B:377:PRO:HD2	2.02	0.42
1:B:574:PHE:O	1:B:578:VAL:HG12	2.19	0.42
1:B:593:LEU:HD12	1:B:593:LEU:N	2.34	0.42
1:C:12:PHE:CG	1:C:28:ALA:HA	2.55	0.42
1:C:60:LEU:CD1	1:C:71:ILE:HG22	2.50	0.42
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.71	0.42
1:C:421:VAL:HG12	1:C:483:TRP:CH2	2.53	0.42
1:D:407:VAL:HG21	1:D:410:LEU:HD12	2.02	0.42
1:A:455:THR:OG1	1:A:474:GLN:NE2	2.52	0.42
1:B:246:PHE:CE1	1:B:296:ARG:NH1	2.88	0.42
1:C:31:ILE:HB	1:C:247:LEU:HB3	2.01	0.42
1:C:72:ASP:O	1:C:98:ILE:HA	2.20	0.42
1:C:146:SER:O	1:C:149:ALA:N	2.53	0.42
1:C:496:GLN:O	1:C:497:THR:C	2.58	0.42
1:D:46:ARG:HA	1:D:67:PRO:HA	2.01	0.42
1:D:336:ILE:HD12	1:D:344:ALA:H	1.84	0.42
1:D:498:VAL:O	1:D:502:VAL:HG23	2.19	0.42
1:A:449:ASP:O	1:A:450:PRO:C	2.57	0.42
1:A:597:ALA:HA	1:A:598:GLY:HA2	1.74	0.42
1:B:157:LEU:HD12	1:B:157:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ARG:HB3	1:D:102:SER:OG	2.19	0.42
1:D:566:GLY:O	1:D:595:ARG:NH1	2.53	0.42
1:A:485:ALA:O	1:A:489:ALA:HB2	2.20	0.42
1:A:530:PRO:HB3	1:A:547:PHE:HA	2.02	0.42
1:B:125:GLY:C	1:B:127:PRO:HD2	2.40	0.42
1:B:506:ARG:HD2	1:C:523:GLN:OE1	2.19	0.42
1:C:346:ILE:HG22	1:C:346:ILE:O	2.19	0.42
1:A:103:THR:HB	1:A:105:TYR:CE1	2.55	0.42
1:A:131:SER:O	3:A:1008:HOH:O	2.22	0.42
1:A:140:ARG:O	1:A:143:THR:HB	2.19	0.42
1:A:586:ARG:HA	1:A:586:ARG:CZ	2.50	0.42
1:C:258:LEU:HD22	1:C:263:VAL:CG1	2.49	0.42
1:C:302:LEU:O	1:C:306:ILE:HD12	2.20	0.42
1:D:258:LEU:HD23	1:D:261:MSE:CE	2.47	0.42
1:A:202:ILE:HG12	2:A:900:BLA:C4A	2.50	0.41
1:C:559:VAL:O	1:C:559:VAL:HG23	2.20	0.41
1:D:28:ALA:O	1:D:242:MSE:SE	2.88	0.41
1:D:402:SER:O	1:D:403:LEU:C	2.58	0.41
1:D:551:LEU:C	1:D:553:ALA:N	2.69	0.41
1:A:40:VAL:HG13	1:A:45[A]:HIS:HA	2.02	0.41
1:A:170:TYR:OH	2:A:900:BLA:O2A	2.37	0.41
1:A:216:ARG:NE	2:A:900:BLA:O2D	2.52	0.41
1:A:569:VAL:HG23	1:A:571:SER:OG	2.19	0.41
1:A:617:GLN:HA	1:A:617:GLN:NE2	2.35	0.41
1:B:100:ASN:HD22	1:B:101:PRO:N	2.15	0.41
1:B:103:THR:HG23	1:B:105:TYR:CZ	2.55	0.41
1:B:164:TYR:CD1	1:B:285:HIS:HB2	2.54	0.41
1:D:139:GLU:HB2	1:D:142:ARG:NH1	2.36	0.41
1:D:139:GLU:HG3	3:D:1070:HOH:O	2.20	0.41
1:A:153:ASP:O	1:A:154:THR:C	2.58	0.41
1:B:170:TYR:CE2	2:B:900:BLA:HMA3	2.55	0.41
1:C:298:ILE:HG22	1:C:302:LEU:HD23	2.01	0.41
1:C:566:GLY:C	1:C:568:PHE:N	2.73	0.41
1:D:31:ILE:CG1	1:D:226:VAL:HG13	2.51	0.41
1:D:128:ILE:HG13	1:D:130:LEU:HD13	2.03	0.41
1:D:407:VAL:HG23	1:D:407:VAL:O	2.20	0.41
1:D:628:ALA:O	1:D:629:THR:HG22	2.20	0.41
1:A:22:ARG:NH2	3:A:1063:HOH:O	2.52	0.41
1:A:40:VAL:HG21	1:A:68:LEU:HD22	2.02	0.41
1:A:230:PRO:O	1:A:231:ARG:HB3	2.19	0.41
1:A:289:ARG:HG2	3:A:1023:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLN:O	1:A:520:PHE:CG	2.72	0.41
1:B:90:MSE:HE3	1:B:109:MSE:CG	2.49	0.41
1:B:613:ARG:C	1:B:614:THR:HG23	2.40	0.41
1:D:32:GLN:HE22	1:D:218:LEU:HA	1.85	0.41
1:D:177:HIS:HD2	1:D:199:SER:HB2	1.85	0.41
1:D:351:GLN:O	1:D:351:GLN:HG3	2.20	0.41
1:A:11:ALA:O	1:A:12:PHE:C	2.59	0.41
1:A:147:LEU:HA	1:A:147:LEU:HD13	1.82	0.41
1:A:164:TYR:CD2	1:A:289:ARG:CD	3.04	0.41
1:A:520:PHE:O	1:A:524:VAL:HG23	2.20	0.41
1:A:568:PHE:HA	1:A:593:LEU:O	2.21	0.41
1:B:626:SER:O	1:B:628:ALA:N	2.52	0.41
1:C:58:LEU:C	1:C:60:LEU:CD2	2.89	0.41
1:C:109:MSE:HG3	1:C:119:ILE:HG12	2.02	0.41
1:D:169:VAL:HA	1:D:280:LEU:O	2.20	0.41
1:B:336:ILE:HB	1:B:344:ALA:HB3	2.02	0.41
1:C:40:VAL:HG21	1:C:68:LEU:HD11	2.02	0.41
1:C:407:VAL:O	1:C:408:PRO:C	2.59	0.41
1:D:157:LEU:O	1:D:157:LEU:HD22	2.20	0.41
1:D:355:GLN:HB2	1:D:356:PRO:HD3	2.03	0.41
1:B:90:MSE:HG2	1:B:109:MSE:HE3	2.02	0.41
1:B:156:LEU:CD2	1:B:160:GLN:NE2	2.84	0.41
1:B:253:ILE:HG21	2:B:900:BLA:CAC	2.51	0.41
1:B:416:MSE:HA	1:B:416:MSE:HE3	2.03	0.41
1:D:346:ILE:HD13	1:D:346:ILE:HA	1.84	0.41
1:A:336:ILE:CG2	1:A:337:THR:N	2.84	0.41
1:B:59:ASN:CB	1:B:100:ASN:ND2	2.67	0.41
1:B:84:ASP:HB3	1:B:87:ALA:HB3	2.03	0.41
1:C:135:ALA:HB3	1:C:136:PRO:CD	2.46	0.41
1:C:221:VAL:HG23	1:C:255:LEU:HD22	2.03	0.41
1:C:530:PRO:HD2	1:C:625:PHE:O	2.21	0.41
1:D:118:ILE:HD13	1:D:245:CYS:SG	2.60	0.41
1:D:204:GLN:O	1:D:205:MSE:C	2.58	0.41
1:D:270:SER:HA	1:D:280:LEU:HD23	2.03	0.41
1:A:223:TYR:O	1:A:223:TYR:CG	2.74	0.41
1:A:336:ILE:CG2	1:A:342:TRP:CA	2.48	0.41
1:B:37:LEU:C	1:B:37:LEU:CD2	2.87	0.41
1:B:135:ALA:N	1:B:136:PRO:HD2	2.36	0.41
1:B:357:LEU:HD12	1:B:357:LEU:N	2.35	0.41
1:C:298:ILE:CG2	1:C:302:LEU:HD23	2.51	0.41
1:C:522:SER:O	1:C:523:GLN:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:HD11	1:D:230:PRO:HG3	2.03	0.41
1:D:119:ILE:HG22	1:D:121:LEU:HD13	2.02	0.41
1:D:323:LEU:HD11	1:D:327:ARG:CZ	2.51	0.41
1:A:45[A]:HIS:CE1	1:A:69:ALA:HB2	2.56	0.41
1:A:76:LEU:HD21	1:A:80:LEU:HD11	2.03	0.41
1:A:568:PHE:O	1:A:569:VAL:C	2.59	0.41
1:B:130:LEU:CB	1:B:131:SER:HA	2.51	0.41
1:C:133:THR:O	1:C:134:LEU:C	2.60	0.41
1:C:387:GLY:O	1:C:388:TRP:C	2.58	0.41
1:C:449:ASP:HB2	1:C:450:PRO:CD	2.50	0.41
1:D:203:PRO:O	1:D:207:ARG:HG3	2.21	0.41
1:D:358:HIS:HB2	1:D:437:ARG:HH21	1.85	0.41
1:A:202:ILE:HG23	2:A:900:BLA:C1A	2.51	0.40
1:A:217:VAL:HG12	1:A:218:LEU:N	2.35	0.40
1:B:560:HIS:O	1:B:563:ASP:HB3	2.21	0.40
1:D:59:ASN:CG	1:D:59:ASN:O	2.60	0.40
1:D:265:ALA:HB3	1:D:285:HIS:HB3	2.03	0.40
1:D:410:LEU:O	1:D:413:LEU:HD12	2.21	0.40
1:D:569:VAL:HG13	1:D:571:SER:OG	2.21	0.40
1:A:63:VAL:O	1:A:66:VAL:HG13	2.21	0.40
1:A:195:ASN:O	1:A:196:ARG:HD3	2.21	0.40
1:A:366:TYR:O	1:A:368:ASP:N	2.55	0.40
1:B:231:ARG:O	1:B:232:LEU:HB2	2.21	0.40
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.84	0.40
1:B:356:PRO:C	1:B:357:LEU:HD12	2.41	0.40
1:C:126:PRO:CG	1:C:294:GLU:HB2	2.51	0.40
1:C:218:LEU:HB3	1:C:266:THR:HB	2.03	0.40
1:C:378:SER:O	1:C:379:THR:C	2.59	0.40
1:C:514:ARG:O	1:C:518:GLU:HG2	2.22	0.40
1:D:370:ILE:HD12	1:D:370:ILE:N	2.35	0.40
1:D:397:VAL:HG21	1:D:492:ARG:CA	2.51	0.40
1:B:62:SER:O	1:B:66:VAL:HG11	2.21	0.40
1:B:334:GLU:CG	1:B:335:ALA:H	2.35	0.40
1:B:366:TYR:CE1	1:B:506:ARG:NH1	2.90	0.40
1:B:520:PHE:O	1:C:510:THR:CB	2.69	0.40
1:C:25:ILE:O	1:C:248:ARG:HD2	2.21	0.40
1:C:90:MSE:HE2	1:C:109:MSE:O	2.22	0.40
1:C:184:ARG:HH11	1:C:184:ARG:HG3	1.86	0.40
1:C:349:THR:C	1:C:351:GLN:N	2.75	0.40
1:C:407:VAL:O	1:C:409:GLU:N	2.54	0.40
1:D:90:MSE:HB2	1:D:91:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:ALA:HB2	1:D:564:LEU:CD1	2.50	0.40
1:A:40:VAL:CG1	1:A:45[A]:HIS:HA	2.51	0.40
1:A:98:ILE:HG22	1:A:99:GLY:N	2.35	0.40
1:A:362:CYS:SG	1:A:433:LEU:HD11	2.60	0.40
1:A:372:THR:HB	1:A:376:VAL:HG21	2.03	0.40
1:A:511:LEU:O	1:A:512:ILE:C	2.60	0.40
1:B:66:VAL:CG2	1:B:71:ILE:HD13	2.51	0.40
1:B:194:GLY:O	1:B:195:ASN:O	2.40	0.40
1:C:74:ASP:CB	1:C:78:LYS:HG2	2.49	0.40
1:C:75:LEU:CD2	1:C:79:ILE:HD13	2.52	0.40
1:C:166:ARG:CD	1:C:168:MSE:HE2	2.49	0.40
1:C:216:ARG:NH2	1:C:250:MSE:HE2	2.36	0.40
1:C:420:VAL:HA	1:C:435:TRP:O	2.21	0.40
1:D:143:THR:O	1:D:143:THR:HG22	2.21	0.40
1:D:347:PHE:CG	1:D:373:ILE:HD13	2.57	0.40
1:D:348:ASP:HB2	1:D:352:SER:HA	2.04	0.40
1:D:578:VAL:CG1	1:D:582:ILE:HD12	2.47	0.40
1:A:37:LEU:HD13	1:A:118:ILE:CG2	2.51	0.40
1:A:157:LEU:HD22	1:A:157:LEU:O	2.21	0.40
1:A:606:VAL:HG23	1:A:625:PHE:CD1	2.56	0.40
1:C:46:ARG:HA	1:C:67:PRO:HA	2.02	0.40
1:C:382:VAL:O	1:C:383:ARG:C	2.59	0.40
1:C:530:PRO:HB3	1:C:547:PHE:HA	2.03	0.40
1:D:469:PHE:O	1:D:472:TRP:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	630/655 (96%)	479 (76%)	89 (14%)	62 (10%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	617/655 (94%)	473 (77%)	88 (14%)	56 (9%)	0	1
1	C	619/655 (94%)	482 (78%)	94 (15%)	43 (7%)	1	2
1	D	612/655 (93%)	480 (78%)	76 (12%)	56 (9%)	0	1
All	All	2478/2620 (95%)	1914 (77%)	347 (14%)	217 (9%)	0	1

All (217) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	55	ALA
1	A	72	ASP
1	A	74	ASP
1	A	110	HIS
1	A	128	ILE
1	A	129	ASP
1	A	135	ALA
1	A	164	TYR
1	A	193	PHE
1	A	223	TYR
1	A	335	ALA
1	A	336	ILE
1	A	338	ARG
1	A	339	GLU
1	A	348	ASP
1	A	396	ALA
1	A	450	PRO
1	A	454	PHE
1	A	526	ALA
1	A	553	ALA
1	A	557	SER
1	A	558	ALA
1	A	560	HIS
1	A	568	PHE
1	A	570	GLU
1	A	571	SER
1	A	615	GLU
1	A	616	ASP
1	A	625	PHE
1	A	633	THR
1	B	49	GLN
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	89	GLY
1	B	90	MSE
1	B	100	ASN
1	B	127	PRO
1	B	130	LEU
1	B	195	ASN
1	B	230	PRO
1	B	232	LEU
1	B	340	GLY
1	B	348	ASP
1	B	396	ALA
1	B	405	LEU
1	B	519	GLN
1	B	564	LEU
1	B	569	VAL
1	B	601	PRO
1	B	626	SER
1	C	42	GLU
1	C	43	PRO
1	C	72	ASP
1	C	75	LEU
1	C	87	ALA
1	C	127	PRO
1	C	134	LEU
1	C	341	ASP
1	C	348	ASP
1	C	351	GLN
1	C	378	SER
1	C	444	VAL
1	C	520	PHE
1	C	555	SER
1	C	560	HIS
1	C	630	ASP
1	D	43	PRO
1	D	71	ILE
1	D	114	GLU
1	D	130	LEU
1	D	229	GLU
1	D	230	PRO
1	D	236	THR
1	D	338	ARG
1	D	339	GLU

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Mol	Chain	Res	Type
1	D	340	GLY
1	D	348	ASP
1	D	393	PRO
1	D	394	ARG
1	D	395	ALA
1	D	397	VAL
1	D	471	LYS
1	D	519	GLN
1	D	520	PHE
1	D	552	PRO
1	D	553	ALA
1	D	556	PRO
1	D	557	SER
1	D	570	GLU
1	D	571	SER
1	D	601	PRO
1	D	627	ASP
1	D	629	THR
1	A	71	ILE
1	A	100	ASN
1	A	116	GLY
1	A	126	PRO
1	A	256	GLN
1	A	429	ARG
1	A	445	THR
1	A	447	GLY
1	A	451	LYS
1	A	519	GLN
1	A	520	PHE
1	A	562	ASP
1	A	572	ASN
1	A	628	ALA
1	B	62	SER
1	B	74	ASP
1	B	78	LYS
1	B	99	GLY
1	B	336	ILE
1	B	339	GLU
1	B	341	ASP
1	B	378	SER
1	B	429	ARG
1	B	470	ALA

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Mol	Chain	Res	Type
1	B	517	TYR
1	B	552	PRO
1	B	553	ALA
1	B	554	GLY
1	B	557	SER
1	B	597	ALA
1	B	599	ASN
1	B	612	THR
1	B	631	ARG
1	C	28	ALA
1	C	89	GLY
1	C	200	SER
1	C	393	PRO
1	C	394	ARG
1	C	445	THR
1	C	449	ASP
1	C	553	ALA
1	C	569	VAL
1	C	584	HIS
1	C	598	GLY
1	C	626	SER
1	D	127	PRO
1	D	132	GLY
1	D	133	THR
1	D	239	ASP
1	D	411	ALA
1	D	429	ARG
1	D	441	VAL
1	D	477	GLU
1	D	546	SER
1	D	576	ARG
1	D	596	GLY
1	D	616	ASP
1	D	633	THR
1	A	342	TRP
1	A	614	THR
1	B	128	ILE
1	B	349	THR
1	B	450	PRO
1	B	477	GLU
1	B	563	ASP
1	B	615	GLU

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Mol	Chain	Res	Type
1	B	630	ASP
1	C	147	LEU
1	C	377	PRO
1	C	429	ARG
1	C	484	THR
1	D	378	SER
1	D	476	VAL
1	D	554	GLY
1	D	594	LEU
1	D	626	SER
1	A	114	GLU
1	A	309	ARG
1	A	455	THR
1	A	459	THR
1	A	561	LEU
1	A	634	ALA
1	B	72	ASP
1	B	133	THR
1	B	161	CYS
1	B	402	SER
1	B	443	THR
1	B	449	ASP
1	B	521	SER
1	B	558	ALA
1	B	600	ARG
1	C	131	SER
1	C	380	GLN
1	C	531	VAL
1	C	600	ARG
1	D	70	GLU
1	D	231	ARG
1	D	335	ALA
1	D	341	ASP
1	D	600	ARG
1	A	308	THR
1	A	415	ARG
1	A	476	VAL
1	C	128	ILE
1	C	615	GLU
1	D	19	ASN
1	D	74	ASP
1	D	195	ASN

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Mol	Chain	Res	Type
1	D	377	PRO
1	A	144	ALA
1	A	449	ASP
1	A	465	PRO
1	A	632	ARG
1	C	428	HIS
1	C	450	PRO
1	D	555	SER
1	A	569	VAL
1	C	408	PRO
1	C	464	SER
1	C	476	VAL
1	D	569	VAL
1	A	333	ILE
1	B	355	GLN
1	B	476	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/526 (100%)	443 (84%)	82 (16%)	2	7
1	B	515/526 (98%)	457 (89%)	58 (11%)	4	15
1	C	517/526 (98%)	453 (88%)	64 (12%)	4	12
1	D	511/526 (97%)	448 (88%)	63 (12%)	4	12
All	All	2068/2104 (98%)	1801 (87%)	267 (13%)	3	11

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	30	SER
1	A	31	ILE
1	A	37	LEU
1	A	45[A]	HIS

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Mol	Chain	Res	Type
1	A	45[B]	HIS
1	A	60	LEU
1	A	64	LEU
1	A	70	GLU
1	A	71	ILE
1	A	75	LEU
1	A	76	LEU
1	A	80	LEU
1	A	90	MSE
1	A	95	ARG
1	A	103	THR
1	A	109	MSE
1	A	110	HIS
1	A	133	THR
1	A	138	LEU
1	A	139	GLU
1	A	147	LEU
1	A	148	ARG
1	A	156	LEU
1	A	157	LEU
1	A	159	GLN
1	A	171	ARG
1	A	184	ARG
1	A	186	VAL
1	A	189	LEU
1	A	193	PHE
1	A	195	ASN
1	A	199	SER
1	A	202	ILE
1	A	209	LEU
1	A	218	LEU
1	A	223	TYR
1	A	231	ARG
1	A	239	ASP
1	A	242	MSE
1	A	256	GLN
1	A	257	TYR
1	A	269	VAL
1	A	294	GLU
1	A	309	ARG
1	A	321	SER
1	A	365	VAL

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Mol	Chain	Res	Type
1	A	371	ARG
1	A	378	SER
1	A	388	TRP
1	A	389	LEU
1	A	392	GLN
1	A	405	LEU
1	A	421	VAL
1	A	433	LEU
1	A	456[A]	MSE
1	A	456[B]	MSE
1	A	459	THR
1	A	469	PHE
1	A	476	VAL
1	A	492	ARG
1	A	493	THR
1	A	512	ILE
1	A	528	MSE
1	A	531	VAL
1	A	532	LEU
1	A	541	LEU
1	A	550	MSE
1	A	567	PHE
1	A	573	ASP
1	A	586	ARG
1	A	588	TRP
1	A	592	VAL
1	A	593	LEU
1	A	602	LEU
1	A	607	ARG
1	A	617	GLN
1	A	623	LEU
1	A	624	ILE
1	A	626	SER
1	A	629	THR
1	A	633	THR
1	B	27	LEU
1	B	66	VAL
1	B	100	ASN
1	B	103	THR
1	B	114	GLU
1	B	117	LEU
1	B	123	ARG

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Mol	Chain	Res	Type
1	B	139	GLU
1	B	153	ASP
1	B	157	LEU
1	B	159	GLN
1	B	161	CYS
1	B	169	VAL
1	B	208	ARG
1	B	230	PRO
1	B	236	THR
1	B	238	ARG
1	B	293	PHE
1	B	301	LEU
1	B	308	THR
1	B	309	ARG
1	B	310	ILE
1	B	311	THR
1	B	318	GLN
1	B	327	ARG
1	B	331	ARG
1	B	336	ILE
1	B	351	GLN
1	B	354	LEU
1	B	365	VAL
1	B	370	ILE
1	B	379	THR
1	B	388	TRP
1	B	390	ASP
1	B	393	PRO
1	B	405	LEU
1	B	409	GLU
1	B	416	MSE
1	B	446	TRP
1	B	466	ARG
1	B	476	VAL
1	B	479	THR
1	B	492	ARG
1	B	502	VAL
1	B	504	GLN
1	B	512	ILE
1	B	528	MSE
1	B	531	VAL
1	B	534	THR

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	564	LEU
1	B	572	ASN
1	B	577	ASN
1	B	578	VAL
1	B	589	ARG
1	B	600	ARG
1	B	615	GLU
1	B	619	LEU
1	C	22	ARG
1	C	63	VAL
1	C	80	LEU
1	C	86	THR
1	C	95	ARG
1	C	102	SER
1	C	103	THR
1	C	108	LEU
1	C	109	MSE
1	C	128	ILE
1	C	129	ASP
1	C	130	LEU
1	C	140	ARG
1	C	159	GLN
1	C	184	ARG
1	C	205	MSE
1	C	212	ARG
1	C	215	VAL
1	C	233	SER
1	C	238	ARG
1	C	256	GLN
1	C	276	LYS
1	C	288	PRO
1	C	291	ILE
1	C	295	LEU
1	C	301	LEU
1	C	304	GLU
1	C	309	ARG
1	C	318	GLN
1	C	323	LEU
1	C	349	THR
1	C	351	GLN
1	C	355	GLN

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Mol	Chain	Res	Type
1	C	370	ILE
1	C	378	SER
1	C	379	THR
1	C	413	LEU
1	C	414	THR
1	C	415	ARG
1	C	416	MSE
1	C	420	VAL
1	C	421	VAL
1	C	429	ARG
1	C	434	MSE
1	C	440	ARG
1	C	445	THR
1	C	446	TRP
1	C	452	LYS
1	C	466	ARG
1	C	469	PHE
1	C	475	VAL
1	C	493	THR
1	C	501	ILE
1	C	502	VAL
1	C	531	VAL
1	C	534	THR
1	C	542	LEU
1	C	564	LEU
1	C	574	PHE
1	C	586	ARG
1	C	600	ARG
1	C	623	LEU
1	C	625	PHE
1	C	627	ASP
1	D	19	ASN
1	D	37	LEU
1	D	39	VAL
1	D	43	PRO
1	D	44	ASP
1	D	64	LEU
1	D	74	ASP
1	D	77	ILE
1	D	88	GLU
1	D	121	LEU
1	D	122	GLU

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Mol	Chain	Res	Type
1	D	139	GLU
1	D	147	LEU
1	D	148	ARG
1	D	154	THR
1	D	159	GLN
1	D	167	VAL
1	D	169	VAL
1	D	195	ASN
1	D	214	ARG
1	D	226	VAL
1	D	228	LEU
1	D	232	LEU
1	D	238	ARG
1	D	242	MSE
1	D	266	THR
1	D	270	SER
1	D	272	VAL
1	D	291	ILE
1	D	292[A]	HIS
1	D	292[B]	HIS
1	D	302	LEU
1	D	304	GLU
1	D	309	ARG
1	D	330	GLN
1	D	337	THR
1	D	346	ILE
1	D	406	ASP
1	D	413	LEU
1	D	414	THR
1	D	415	ARG
1	D	416	MSE
1	D	421	VAL
1	D	432	PHE
1	D	442	HIS
1	D	443	THR
1	D	459	THR
1	D	463	LEU
1	D	466	ARG
1	D	467	ARG
1	D	469	PHE
1	D	484	THR
1	D	501	ILE

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Mol	Chain	Res	Type
1	D	517	TYR
1	D	518	GLU
1	D	531	VAL
1	D	544	ASN
1	D	564	LEU
1	D	576	ARG
1	D	586	ARG
1	D	588	TRP
1	D	623	LEU
1	D	632	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	34	HIS
1	A	177	HIS
1	A	224	GLN
1	A	254	HIS
1	A	351	GLN
1	A	355	GLN
1	A	473	HIS
1	A	474	GLN
1	A	496	GLN
1	A	519	GLN
1	A	529	GLN
1	A	560	HIS
1	A	577	ASN
1	A	617	GLN
1	B	34	HIS
1	B	45	HIS
1	B	49	GLN
1	B	82	HIS
1	B	100	ASN
1	B	160	GLN
1	B	177	HIS
1	B	195	ASN
1	B	260	ASN
1	B	351	GLN
1	B	380	GLN
1	B	516	GLN
1	B	544	ASN

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Mol	Chain	Res	Type
1	B	572	ASN
1	B	577	ASN
1	B	617	GLN
1	C	32	GLN
1	C	177	HIS
1	C	195	ASN
1	C	256	GLN
1	C	260	ASN
1	C	392	GLN
1	C	428	HIS
1	C	496	GLN
1	C	525	HIS
1	C	599	ASN
1	D	19	ASN
1	D	26	HIS
1	D	32	GLN
1	D	100	ASN
1	D	160	GLN
1	D	177	HIS
1	D	254	HIS
1	D	260	ASN
1	D	326	GLN
1	D	330	GLN
1	D	380	GLN
1	D	496	GLN
1	D	529	GLN
1	D	544	ASN
1	D	560	HIS
1	D	577	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BLA	D	900	1	42,46,46	2.88	11 (26%)	54,67,67	2.49	27 (50%)
2	BLA	A	900	1	42,46,46	3.15	13 (30%)	54,67,67	3.16	26 (48%)
2	BLA	B	900	1	42,46,46	3.00	14 (33%)	54,67,67	2.85	21 (38%)
2	BLA	C	900	1	42,46,46	3.17	11 (26%)	54,67,67	2.81	25 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	D	900	1	-	6/26/74/74	0/4/4/4
2	BLA	A	900	1	-	8/26/74/74	0/4/4/4
2	BLA	B	900	1	-	4/26/74/74	0/4/4/4
2	BLA	C	900	1	-	4/26/74/74	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	CHA-C4D	14.51	1.49	1.35
2	A	900	BLA	CHA-C4D	12.99	1.47	1.35
2	B	900	BLA	CHA-C4D	11.50	1.46	1.35
2	D	900	BLA	CHA-C4D	11.47	1.46	1.35
2	A	900	BLA	CHB-C1B	7.85	1.50	1.34
2	B	900	BLA	CHB-C1B	7.73	1.50	1.34
2	D	900	BLA	CHB-C1B	7.56	1.50	1.34
2	A	900	BLA	C3B-C2B	6.72	1.50	1.37
2	C	900	BLA	CHB-C1B	6.16	1.47	1.34
2	B	900	BLA	C3B-C2B	6.10	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	C3D-C2D	5.76	1.49	1.36
2	B	900	BLA	C3D-C2D	5.40	1.48	1.36
2	D	900	BLA	C3B-C2B	5.31	1.48	1.37
2	D	900	BLA	C3C-C2C	5.11	1.47	1.37
2	D	900	BLA	C3D-C2D	5.03	1.47	1.36
2	C	900	BLA	C3C-C2C	4.94	1.47	1.37
2	C	900	BLA	C3B-C2B	4.62	1.46	1.37
2	A	900	BLA	CHD-C4C	4.58	1.48	1.37
2	B	900	BLA	C3C-C2C	4.39	1.46	1.37
2	D	900	BLA	CHD-C4C	4.38	1.48	1.37
2	A	900	BLA	C3D-C2D	4.24	1.45	1.36
2	B	900	BLA	CHD-C4C	4.15	1.47	1.37
2	A	900	BLA	C4B-NB	-3.89	1.29	1.38
2	C	900	BLA	CHD-C4C	3.81	1.47	1.37
2	B	900	BLA	CHD-C1D	3.77	1.49	1.40
2	A	900	BLA	C3C-C2C	3.59	1.44	1.37
2	C	900	BLA	CHD-C1D	3.49	1.48	1.40
2	D	900	BLA	CHD-C1D	3.43	1.48	1.40
2	C	900	BLA	OB-C4B	3.43	1.30	1.23
2	A	900	BLA	OB-C4B	3.35	1.29	1.23
2	A	900	BLA	CHD-C1D	3.33	1.48	1.40
2	C	900	BLA	C2A-C3A	3.30	1.47	1.37
2	B	900	BLA	OC-C1C	3.18	1.29	1.23
2	B	900	BLA	OB-C4B	3.12	1.29	1.23
2	A	900	BLA	O1A-CGA	3.07	1.32	1.22
2	B	900	BLA	C2A-C3A	3.03	1.46	1.37
2	D	900	BLA	C2A-C3A	2.92	1.46	1.37
2	C	900	BLA	OC-C1C	2.88	1.29	1.23
2	A	900	BLA	C2A-C3A	2.58	1.45	1.37
2	B	900	BLA	C1B-C2B	2.53	1.49	1.45
2	A	900	BLA	C4C-NC	-2.53	1.33	1.37
2	D	900	BLA	OC-C1C	2.50	1.28	1.23
2	C	900	BLA	C4D-C3D	2.47	1.49	1.45
2	B	900	BLA	C4C-NC	-2.45	1.33	1.37
2	D	900	BLA	OB-C4B	2.31	1.28	1.23
2	B	900	BLA	C4A-CHB	2.28	1.50	1.41
2	B	900	BLA	C4B-NB	-2.13	1.33	1.38
2	A	900	BLA	C1B-C2B	2.09	1.48	1.45
2	D	900	BLA	C4A-CHB	2.01	1.49	1.41

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C1A-CHA-C4D	-9.20	116.41	128.73
2	A	900	BLA	C3B-C2B-C1B	-6.95	100.18	107.92
2	A	900	BLA	CHB-C1B-NB	-6.65	106.85	130.33
2	B	900	BLA	C3B-C2B-C1B	-6.37	100.82	107.92
2	A	900	BLA	CHB-C1B-C2B	6.31	139.53	126.99
2	B	900	BLA	CMC-C2C-C1C	6.05	133.87	121.21
2	C	900	BLA	CHB-C1B-NB	-5.71	110.17	130.33
2	B	900	BLA	CHB-C1B-NB	-5.65	110.40	130.33
2	C	900	BLA	C3B-C4B-NB	5.59	113.16	106.13
2	C	900	BLA	C4C-NC-C1C	-5.56	103.83	110.66
2	A	900	BLA	CMC-C2C-C1C	5.55	132.81	121.21
2	B	900	BLA	C3B-C4B-NB	5.34	112.84	106.13
2	C	900	BLA	CMB-C2B-C1B	5.32	130.63	124.16
2	D	900	BLA	C3B-C4B-NB	5.32	112.82	106.13
2	C	900	BLA	C3B-C2B-C1B	-5.25	102.08	107.92
2	B	900	BLA	C4D-C3D-C2D	-5.21	101.09	106.73
2	A	900	BLA	CMB-C2B-C1B	5.11	130.38	124.16
2	B	900	BLA	CHA-C4D-ND	-5.09	121.84	128.76
2	A	900	BLA	C2C-C1C-NC	4.91	117.55	106.55
2	B	900	BLA	C3D-C4D-ND	4.84	116.90	110.04
2	C	900	BLA	CHB-C1B-C2B	4.83	136.58	126.99
2	B	900	BLA	C2B-C1B-NB	4.73	113.86	106.97
2	A	900	BLA	C4C-NC-C1C	-4.72	104.86	110.66
2	D	900	BLA	C4C-NC-C1C	-4.70	104.89	110.66
2	D	900	BLA	C2C-C1C-NC	4.64	116.93	106.55
2	D	900	BLA	CMB-C2B-C1B	4.58	129.73	124.16
2	D	900	BLA	CHA-C4D-ND	-4.58	122.55	128.76
2	A	900	BLA	C2B-C1B-NB	4.51	113.54	106.97
2	C	900	BLA	CHA-C4D-ND	-4.45	122.72	128.76
2	C	900	BLA	C2C-C1C-NC	4.43	116.47	106.55
2	A	900	BLA	OB-C4B-NB	-4.41	114.75	125.08
2	B	900	BLA	CHB-C1B-C2B	4.37	135.68	126.99
2	B	900	BLA	C2C-C1C-NC	4.36	116.30	106.55
2	C	900	BLA	C2B-C1B-NB	4.25	113.17	106.97
2	B	900	BLA	CMB-C2B-C1B	4.24	129.31	124.16
2	B	900	BLA	C1A-CHA-C4D	-4.16	123.16	128.73
2	C	900	BLA	CBA-CAA-C2A	4.13	119.48	112.54
2	A	900	BLA	CAD-C3D-C4D	4.13	132.27	125.02
2	A	900	BLA	C3B-C4B-NB	4.11	111.29	106.13
2	D	900	BLA	C4D-C3D-C2D	-4.06	102.33	106.73
2	C	900	BLA	C3C-C4C-NC	4.00	113.17	106.64
2	B	900	BLA	C4C-NC-C1C	-3.93	105.84	110.66
2	D	900	BLA	C3D-C4D-ND	3.93	115.60	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	CHB-C1B-NB	-3.79	116.95	130.33
2	D	900	BLA	C3B-C2B-C1B	-3.77	103.72	107.92
2	C	900	BLA	OB-C4B-C3B	-3.77	120.60	129.71
2	D	900	BLA	OB-C4B-C3B	-3.68	120.81	129.71
2	A	900	BLA	CAD-CBD-CGD	-3.67	103.94	113.67
2	C	900	BLA	OC-C1C-C2C	-3.62	114.07	128.04
2	C	900	BLA	C1B-NB-C4B	-3.61	106.23	110.66
2	C	900	BLA	CHD-C1D-ND	-3.57	117.24	124.95
2	A	900	BLA	CHA-C4D-ND	-3.47	124.05	128.76
2	A	900	BLA	O2A-CGA-O1A	3.32	131.86	123.33
2	C	900	BLA	C4D-C3D-C2D	-3.27	103.18	106.73
2	B	900	BLA	C1B-NB-C4B	-3.24	106.69	110.66
2	C	900	BLA	C1D-C2D-C3D	-3.23	102.81	106.48
2	B	900	BLA	O1A-CGA-CBA	-3.20	112.96	123.09
2	D	900	BLA	C3C-C4C-NC	3.15	111.78	106.64
2	C	900	BLA	O1A-CGA-CBA	-3.10	113.25	123.09
2	D	900	BLA	CMC-C2C-C1C	3.06	127.62	121.21
2	A	900	BLA	O1A-CGA-CBA	-3.01	113.55	123.09
2	A	900	BLA	CBD-CAD-C3D	2.88	120.51	112.53
2	D	900	BLA	C2B-C1B-NB	2.84	111.10	106.97
2	C	900	BLA	C3D-C4D-ND	2.83	114.05	110.04
2	C	900	BLA	O2A-CGA-CBA	2.82	122.90	114.00
2	D	900	BLA	CBA-CAA-C2A	2.82	117.27	112.54
2	C	900	BLA	CHD-C4C-C3C	-2.80	119.94	127.94
2	D	900	BLA	C1A-CHA-C4D	-2.77	125.02	128.73
2	B	900	BLA	CAD-CBD-CGD	-2.76	106.35	113.67
2	B	900	BLA	C3C-C4C-NC	2.74	111.11	106.64
2	D	900	BLA	O1A-CGA-CBA	-2.73	114.45	123.09
2	A	900	BLA	C3C-C4C-NC	2.71	111.06	106.64
2	D	900	BLA	CMD-C2D-C1D	2.62	129.17	125.10
2	D	900	BLA	C1B-NB-C4B	-2.55	107.53	110.66
2	A	900	BLA	CBC-CAC-C3C	-2.52	114.95	127.53
2	A	900	BLA	CAA-C2A-C3A	-2.47	120.16	127.25
2	D	900	BLA	CHB-C1B-C2B	2.46	131.87	126.99
2	B	900	BLA	O2A-CGA-CBA	2.45	121.76	114.00
2	D	900	BLA	OC-C1C-C2C	-2.43	118.68	128.04
2	A	900	BLA	CAD-C3D-C2D	-2.41	123.34	127.87
2	D	900	BLA	C4B-C3B-C2B	-2.40	104.84	107.92
2	D	900	BLA	CHD-C1D-ND	-2.37	119.84	124.95
2	D	900	BLA	C1D-C2D-C3D	-2.36	103.79	106.48
2	B	900	BLA	OB-C4B-C3B	-2.36	124.02	129.71
2	C	900	BLA	CAD-C3D-C2D	2.35	132.28	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	O1D-CGD-CBD	-2.35	115.64	123.09
2	A	900	BLA	CHD-C1D-C2D	-2.25	119.10	124.87
2	C	900	BLA	CMC-C2C-C1C	2.18	125.77	121.21
2	D	900	BLA	CAD-CBD-CGD	-2.17	107.90	113.67
2	B	900	BLA	CBD-CAD-C3D	2.17	118.54	112.53
2	A	900	BLA	C4D-C3D-C2D	-2.17	104.38	106.73
2	C	900	BLA	CMD-C2D-C3D	2.14	131.95	126.15
2	B	900	BLA	CAA-CBA-CGA	-2.09	108.21	113.83
2	C	900	BLA	CMC-C2C-C3C	2.08	133.46	128.43
2	D	900	BLA	CAD-C3D-C4D	2.07	128.66	125.02
2	A	900	BLA	CBB-CAB-C3B	-2.06	117.25	127.53
2	D	900	BLA	O2D-CGD-CBD	2.04	120.45	114.00
2	A	900	BLA	C4B-C3B-C2B	-2.01	105.35	107.92
2	A	900	BLA	O2D-CGD-O1D	2.01	128.49	123.33

There are no chirality outliers.

All (22) torsion outliers are listed below:

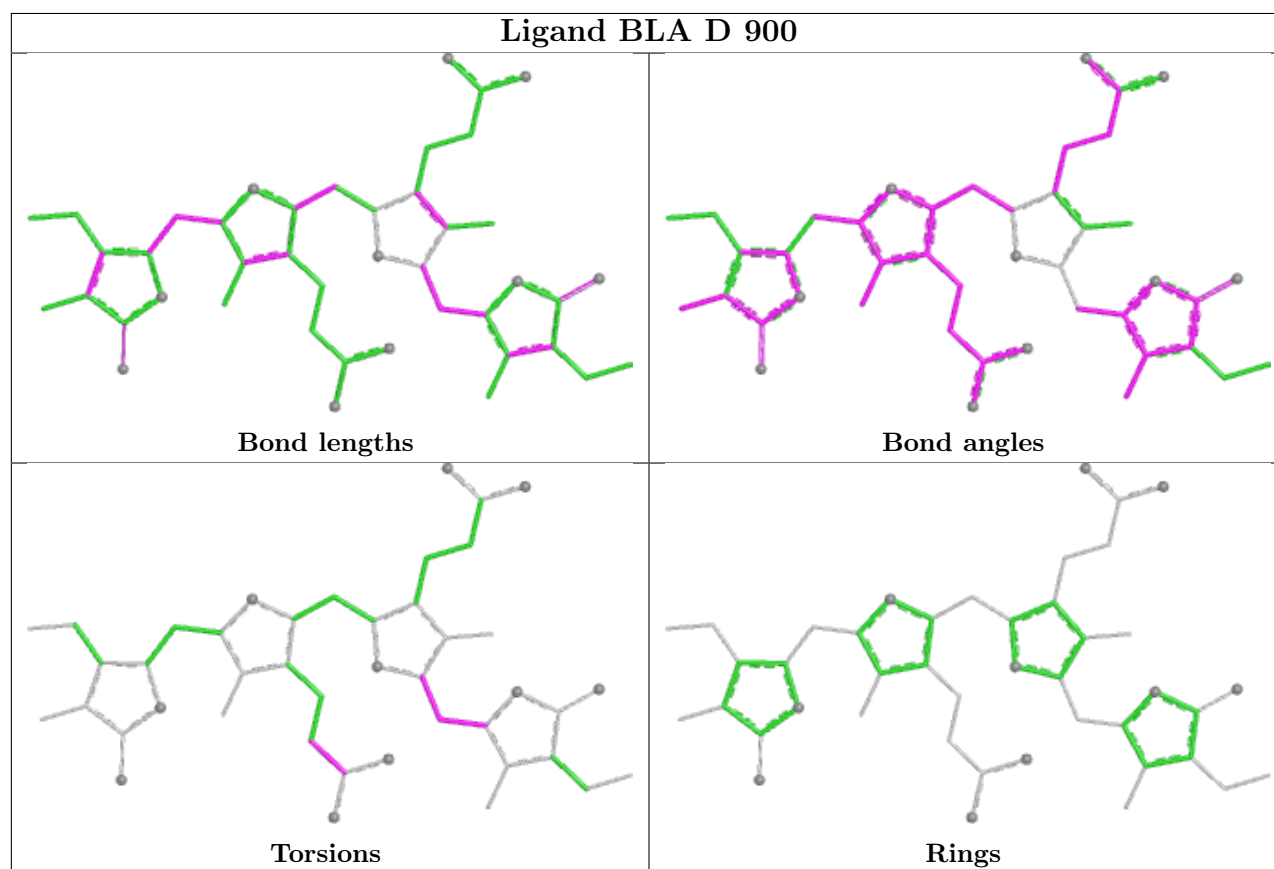
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	C1A-C2A-CAA-CBA
2	A	900	BLA	C3A-C2A-CAA-CBA
2	D	900	BLA	NA-C4A-CHB-C1B
2	D	900	BLA	C3A-C4A-CHB-C1B
2	A	900	BLA	C4D-C3D-CAD-CBD
2	A	900	BLA	C2D-C3D-CAD-CBD
2	A	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	NB-C1B-CHB-C4A
2	C	900	BLA	NB-C1B-CHB-C4A
2	D	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D
2	D	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	CAD-CBD-CGD-O1D
2	D	900	BLA	CAD-CBD-CGD-O1D
2	A	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	C2B-C1B-CHB-C4A
2	D	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O2D

There are no ring outliers.

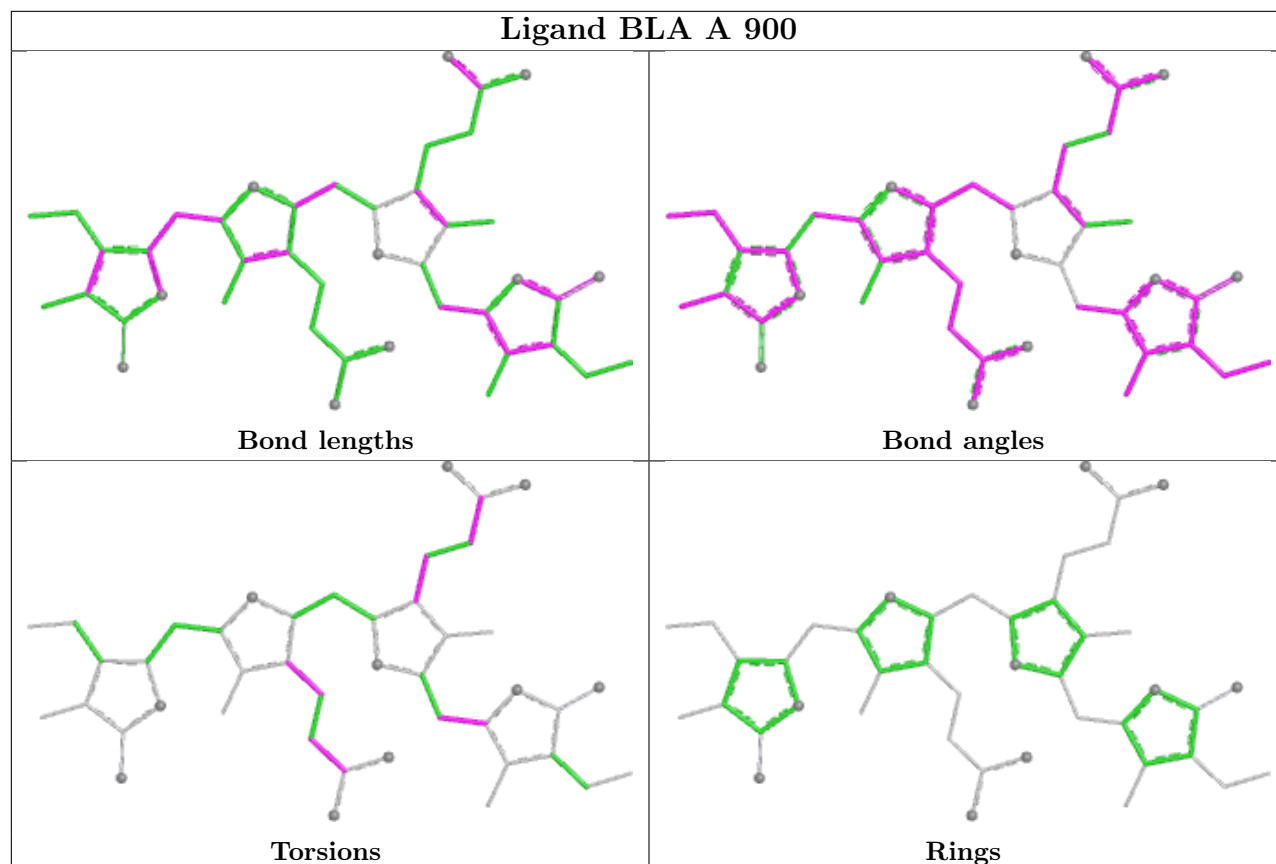
4 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	BLA	7	0
2	A	900	BLA	24	0
2	B	900	BLA	19	0
2	C	900	BLA	10	0

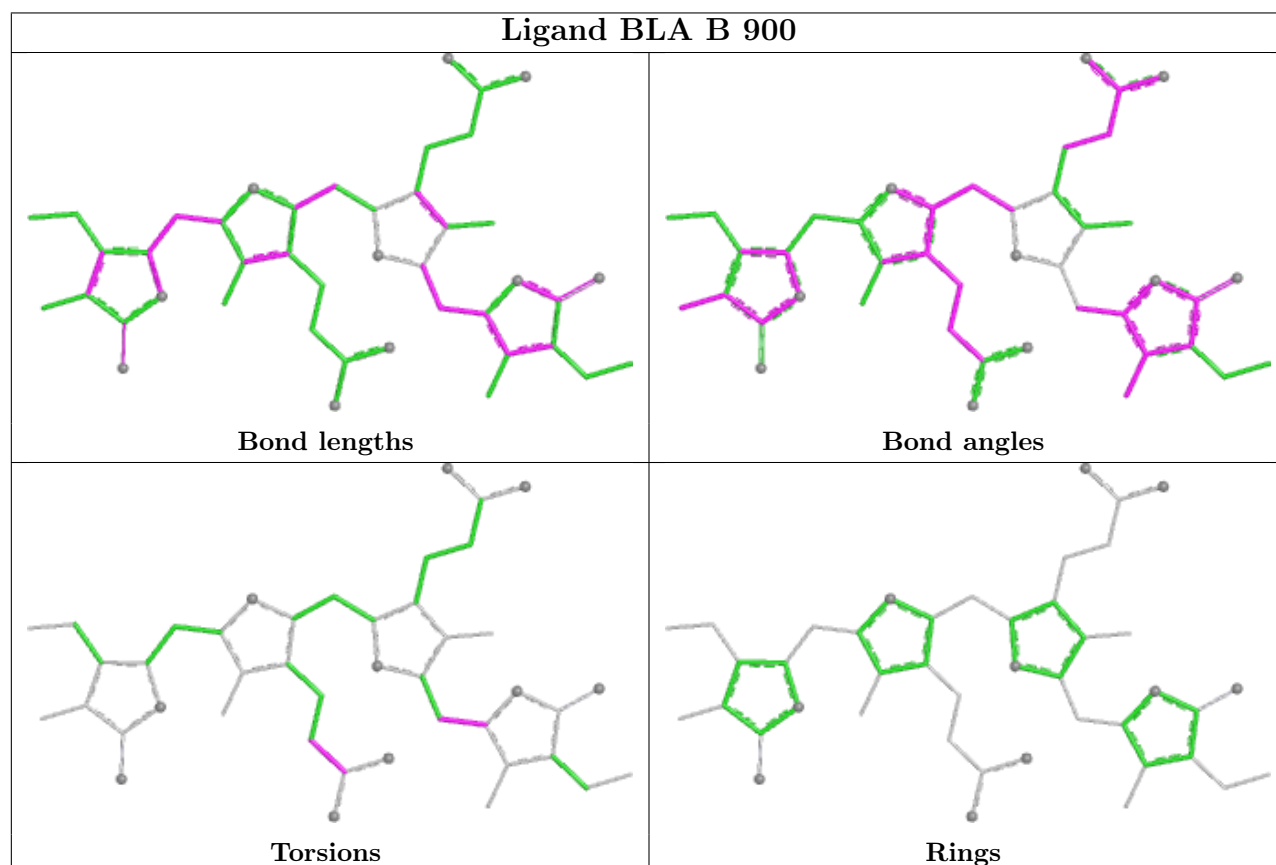
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

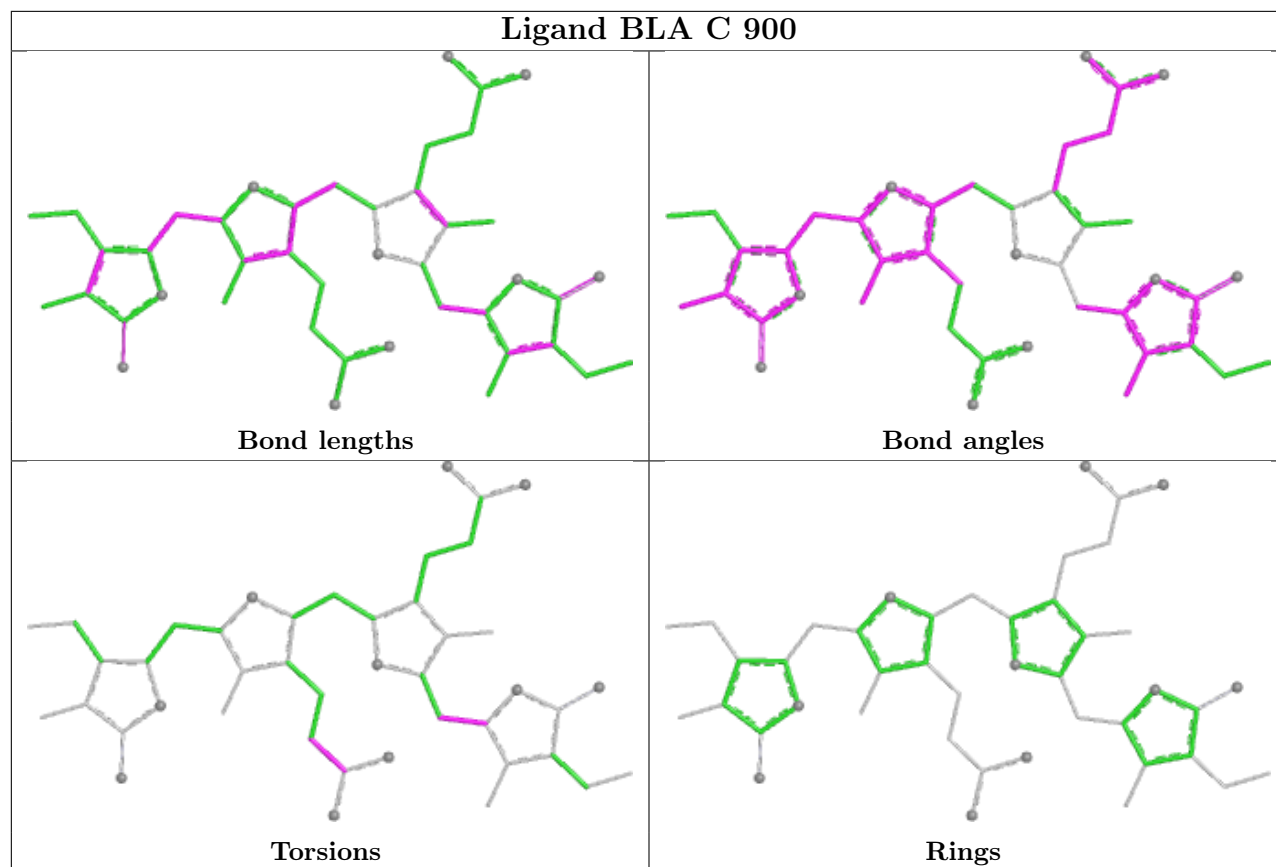


Ligand BLA A 900



Ligand BLA B 900





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	614/655 (93%)	-0.65	4 (0%) 84 80	28, 65, 128, 180	2 (0%)
1	B	608/655 (92%)	-0.55	6 (0%) 79 74	43, 72, 145, 176	0
1	C	609/655 (92%)	-0.62	3 (0%) 87 84	35, 64, 147, 168	1 (0%)
1	D	602/655 (91%)	-0.60	5 (0%) 82 78	33, 70, 124, 175	1 (0%)
All	All	2433/2620 (92%)	-0.60	18 (0%) 84 80	28, 68, 138, 180	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ALA	6.4
1	D	335	ALA	5.0
1	C	450	PRO	3.9
1	A	449	ASP	2.8
1	A	450	PRO	2.7
1	B	569	VAL	2.7
1	D	292[A]	HIS	2.7
1	D	553	ALA	2.5
1	D	336	ILE	2.4
1	C	627	ASP	2.4
1	B	634	ALA	2.3
1	D	391	ARG	2.3
1	B	89	GLY	2.2
1	C	633	THR	2.2
1	A	453	PRO	2.1
1	A	635	ASP	2.1
1	B	130	LEU	2.0
1	B	450	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

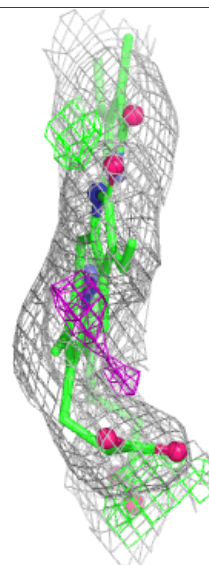
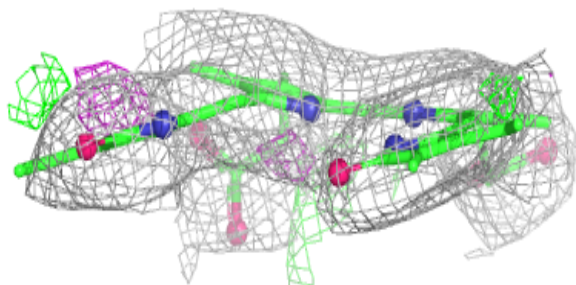
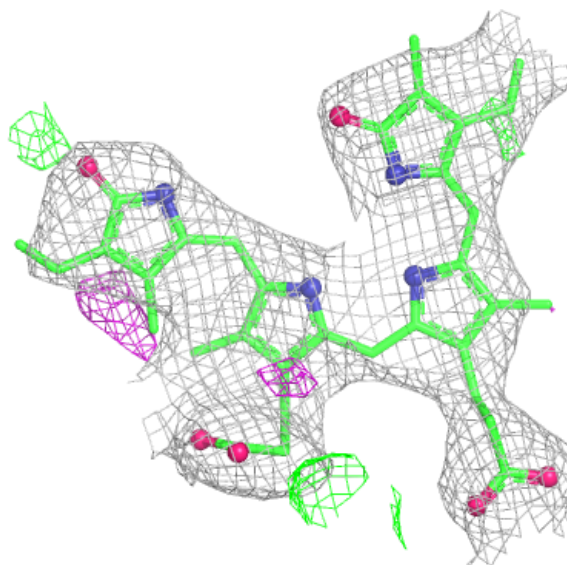
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BLA	D	900	43/43	0.92	0.09	59,64,71,73	0
2	BLA	B	900	43/43	0.93	0.09	54,63,71,75	0
2	BLA	C	900	43/43	0.95	0.08	44,51,58,61	0
2	BLA	A	900	43/43	0.96	0.07	37,41,55,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

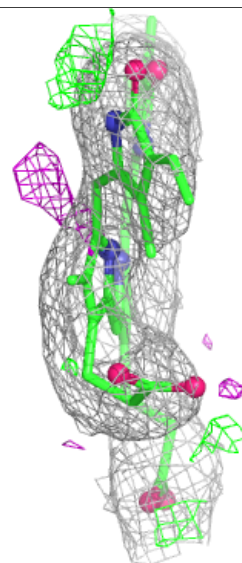
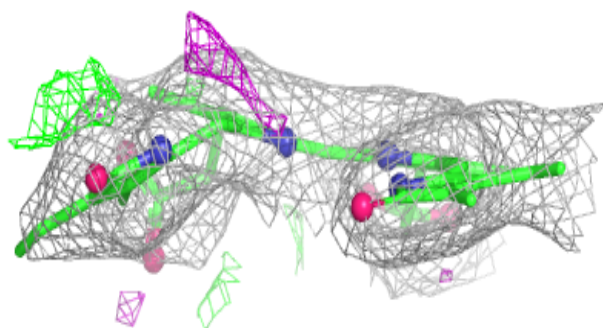
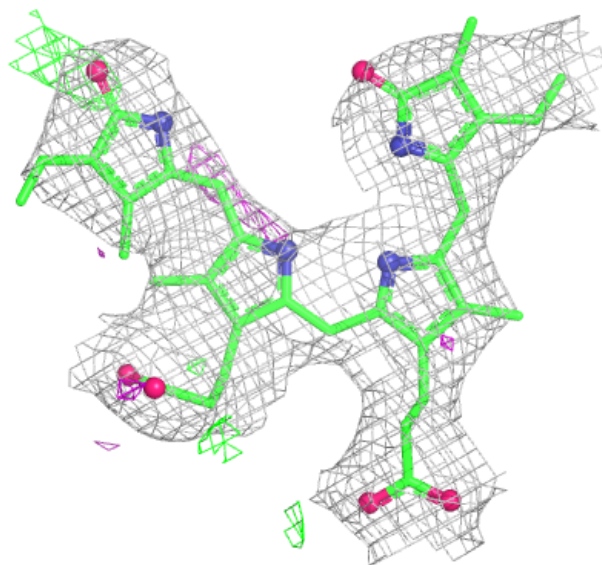
Electron density around BLA D 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



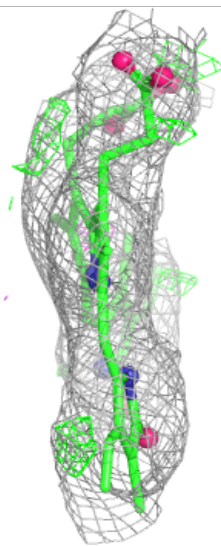
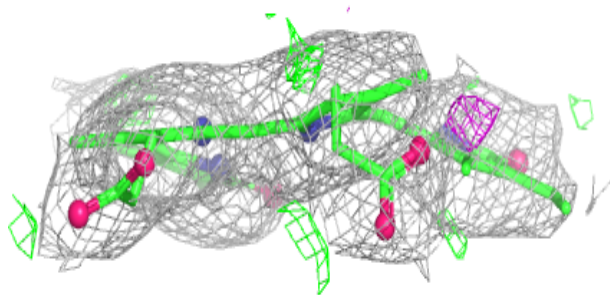
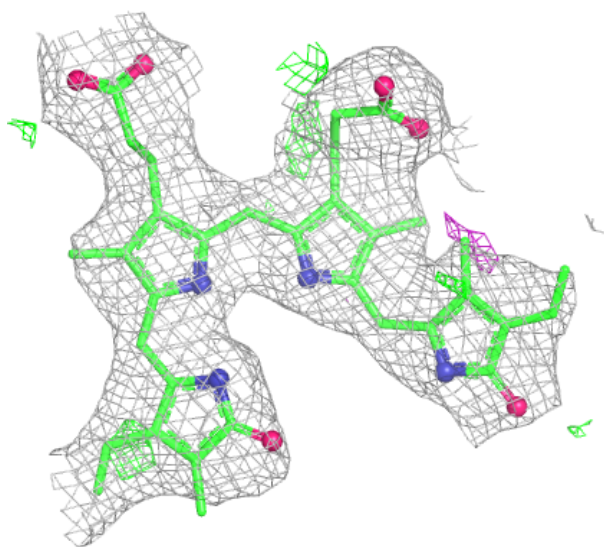
Electron density around BLA B 900:

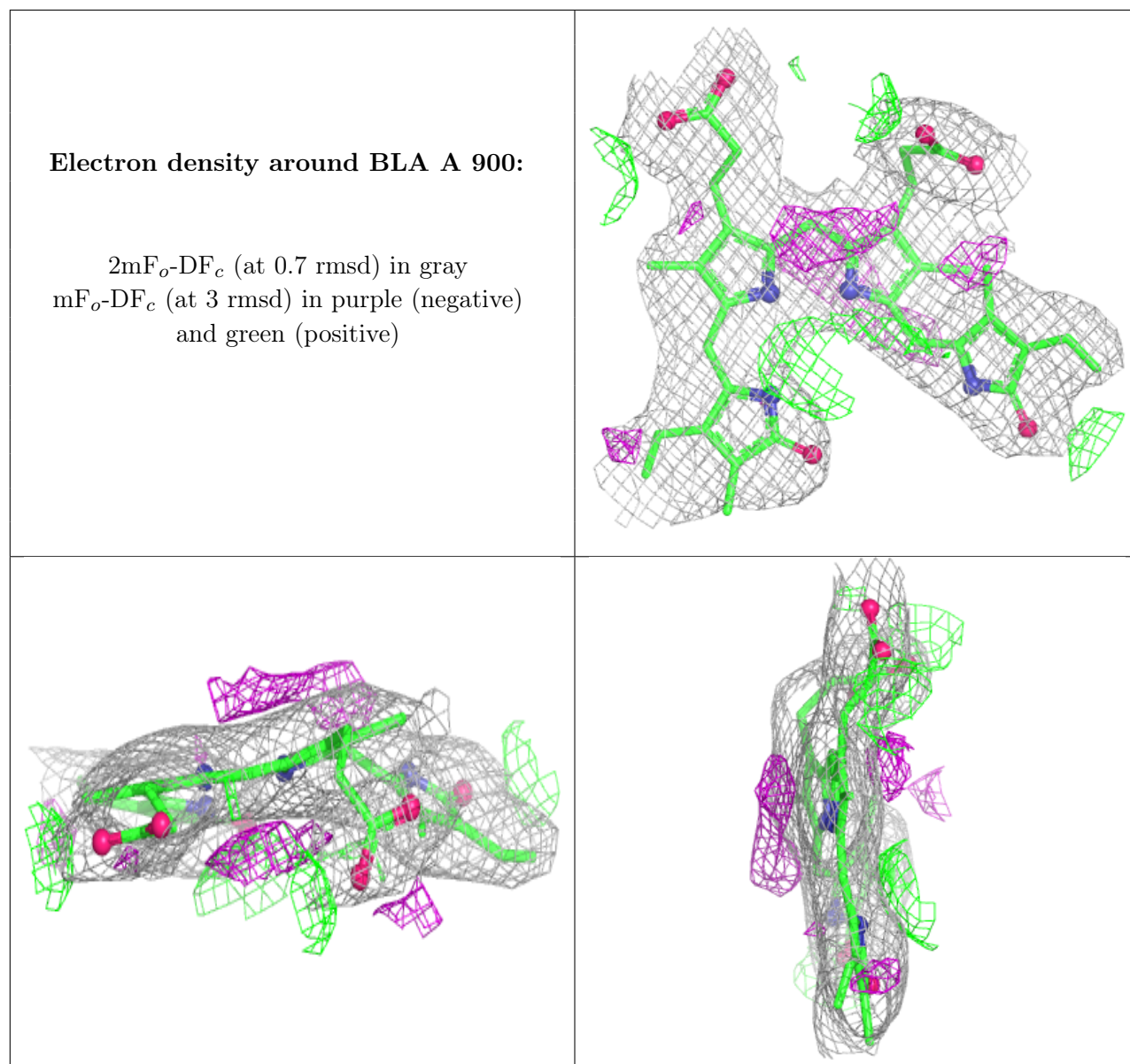
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA C 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.