



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 02:42 PM EDT

PDB ID : 5B00
Title : Structure of the prenyltransferase MoeN5 in complex with geranyl pyrophosphate
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2015-10-27
Resolution : 2.95 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

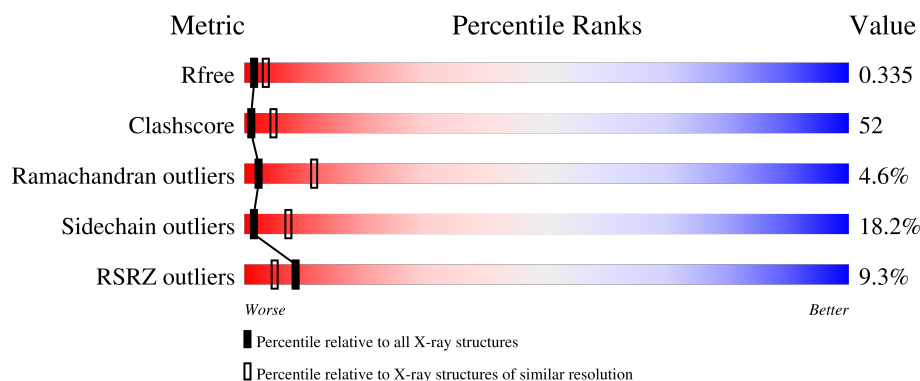
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	294	<div> <div>5%</div> <div>32%</div> <div>47%</div> <div>10%</div> <div>11%</div> </div>
1	B	294	<div> <div>6%</div> <div>35%</div> <div>42%</div> <div>12%</div> <div>11%</div> </div>
1	C	294	<div> <div>14%</div> <div>24%</div> <div>49%</div> <div>14%</div> <div>11%</div> </div>

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	GPP	C	500	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6233 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 MoeN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 1995	C 1236	N 371	O 377	S 11	0	0	0
1	B	261	Total 1995	C 1236	N 371	O 377	S 11	0	0	0
1	C	261	Total 1995	C 1236	N 371	O 377	S 11	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP A0A010
A	-32	ALA	-	expression tag	UNP A0A010
A	-31	HIS	-	expression tag	UNP A0A010
A	-30	HIS	-	expression tag	UNP A0A010
A	-29	HIS	-	expression tag	UNP A0A010
A	-28	HIS	-	expression tag	UNP A0A010
A	-27	HIS	-	expression tag	UNP A0A010
A	-26	HIS	-	expression tag	UNP A0A010
A	-25	VAL	-	expression tag	UNP A0A010
A	-24	ASP	-	expression tag	UNP A0A010
A	-23	ASP	-	expression tag	UNP A0A010
A	-22	ASP	-	expression tag	UNP A0A010
A	-21	ASP	-	expression tag	UNP A0A010
A	-20	LYS	-	expression tag	UNP A0A010
A	-19	ALA	-	expression tag	UNP A0A010
A	-18	ALA	-	expression tag	UNP A0A010
A	-17	SER	-	expression tag	UNP A0A010
A	-16	TRP	-	expression tag	UNP A0A010
A	-15	SER	-	expression tag	UNP A0A010
A	-14	HIS	-	expression tag	UNP A0A010
A	-13	PRO	-	expression tag	UNP A0A010
A	-12	GLN	-	expression tag	UNP A0A010
A	-11	PHE	-	expression tag	UNP A0A010

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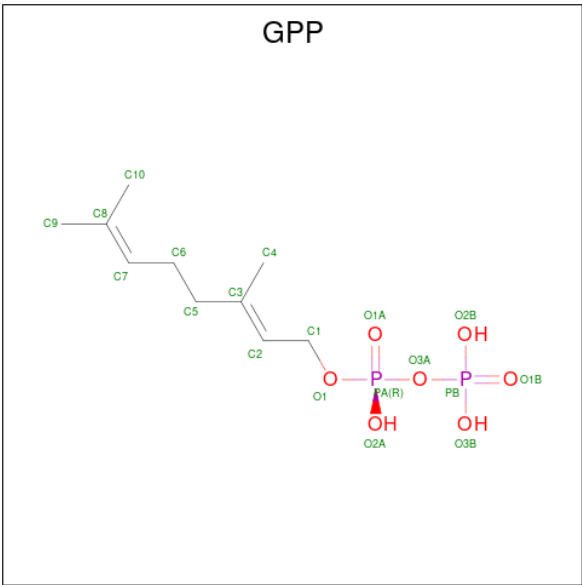
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLU	-	expression tag	UNP A0A010
A	-9	LYS	-	expression tag	UNP A0A010
A	-8	GLY	-	expression tag	UNP A0A010
A	-7	ALA	-	expression tag	UNP A0A010
A	-6	GLU	-	expression tag	UNP A0A010
A	-5	ASN	-	expression tag	UNP A0A010
A	-4	LEU	-	expression tag	UNP A0A010
A	-3	TYR	-	expression tag	UNP A0A010
A	-2	PHE	-	expression tag	UNP A0A010
A	-1	GLN	-	expression tag	UNP A0A010
A	0	SER	-	expression tag	UNP A0A010
B	-33	MET	-	expression tag	UNP A0A010
B	-32	ALA	-	expression tag	UNP A0A010
B	-31	HIS	-	expression tag	UNP A0A010
B	-30	HIS	-	expression tag	UNP A0A010
B	-29	HIS	-	expression tag	UNP A0A010
B	-28	HIS	-	expression tag	UNP A0A010
B	-27	HIS	-	expression tag	UNP A0A010
B	-26	HIS	-	expression tag	UNP A0A010
B	-25	VAL	-	expression tag	UNP A0A010
B	-24	ASP	-	expression tag	UNP A0A010
B	-23	ASP	-	expression tag	UNP A0A010
B	-22	ASP	-	expression tag	UNP A0A010
B	-21	ASP	-	expression tag	UNP A0A010
B	-20	LYS	-	expression tag	UNP A0A010
B	-19	ALA	-	expression tag	UNP A0A010
B	-18	ALA	-	expression tag	UNP A0A010
B	-17	SER	-	expression tag	UNP A0A010
B	-16	TRP	-	expression tag	UNP A0A010
B	-15	SER	-	expression tag	UNP A0A010
B	-14	HIS	-	expression tag	UNP A0A010
B	-13	PRO	-	expression tag	UNP A0A010
B	-12	GLN	-	expression tag	UNP A0A010
B	-11	PHE	-	expression tag	UNP A0A010
B	-10	GLU	-	expression tag	UNP A0A010
B	-9	LYS	-	expression tag	UNP A0A010
B	-8	GLY	-	expression tag	UNP A0A010
B	-7	ALA	-	expression tag	UNP A0A010
B	-6	GLU	-	expression tag	UNP A0A010
B	-5	ASN	-	expression tag	UNP A0A010
B	-4	LEU	-	expression tag	UNP A0A010
B	-3	TYR	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PHE	-	expression tag	UNP A0A010
B	-1	GLN	-	expression tag	UNP A0A010
B	0	SER	-	expression tag	UNP A0A010
C	-33	MET	-	expression tag	UNP A0A010
C	-32	ALA	-	expression tag	UNP A0A010
C	-31	HIS	-	expression tag	UNP A0A010
C	-30	HIS	-	expression tag	UNP A0A010
C	-29	HIS	-	expression tag	UNP A0A010
C	-28	HIS	-	expression tag	UNP A0A010
C	-27	HIS	-	expression tag	UNP A0A010
C	-26	HIS	-	expression tag	UNP A0A010
C	-25	VAL	-	expression tag	UNP A0A010
C	-24	ASP	-	expression tag	UNP A0A010
C	-23	ASP	-	expression tag	UNP A0A010
C	-22	ASP	-	expression tag	UNP A0A010
C	-21	ASP	-	expression tag	UNP A0A010
C	-20	LYS	-	expression tag	UNP A0A010
C	-19	ALA	-	expression tag	UNP A0A010
C	-18	ALA	-	expression tag	UNP A0A010
C	-17	SER	-	expression tag	UNP A0A010
C	-16	TRP	-	expression tag	UNP A0A010
C	-15	SER	-	expression tag	UNP A0A010
C	-14	HIS	-	expression tag	UNP A0A010
C	-13	PRO	-	expression tag	UNP A0A010
C	-12	GLN	-	expression tag	UNP A0A010
C	-11	PHE	-	expression tag	UNP A0A010
C	-10	GLU	-	expression tag	UNP A0A010
C	-9	LYS	-	expression tag	UNP A0A010
C	-8	GLY	-	expression tag	UNP A0A010
C	-7	ALA	-	expression tag	UNP A0A010
C	-6	GLU	-	expression tag	UNP A0A010
C	-5	ASN	-	expression tag	UNP A0A010
C	-4	LEU	-	expression tag	UNP A0A010
C	-3	TYR	-	expression tag	UNP A0A010
C	-2	PHE	-	expression tag	UNP A0A010
C	-1	GLN	-	expression tag	UNP A0A010
C	0	SER	-	expression tag	UNP A0A010

- Molecule 2 is GERANYL DIPHOSPHATE (three-letter code: GPP) (formula: C₁₀H₂₀O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			19	10	7	2		
2	B	1	Total	C	O	P	0	0
			19	10	7	2		
2	C	1	Total	C	O	P	0	0
			19	10	7	2		

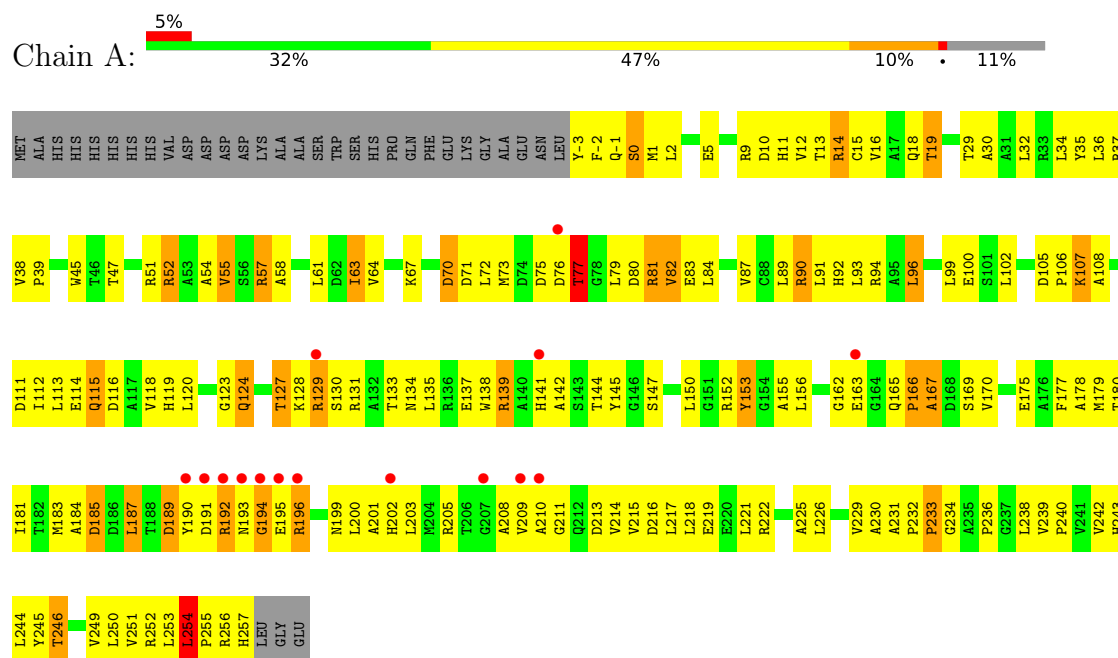
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	54	Total	O	0	0
			54	54		
3	C	58	Total	O	0	0
			58	58		

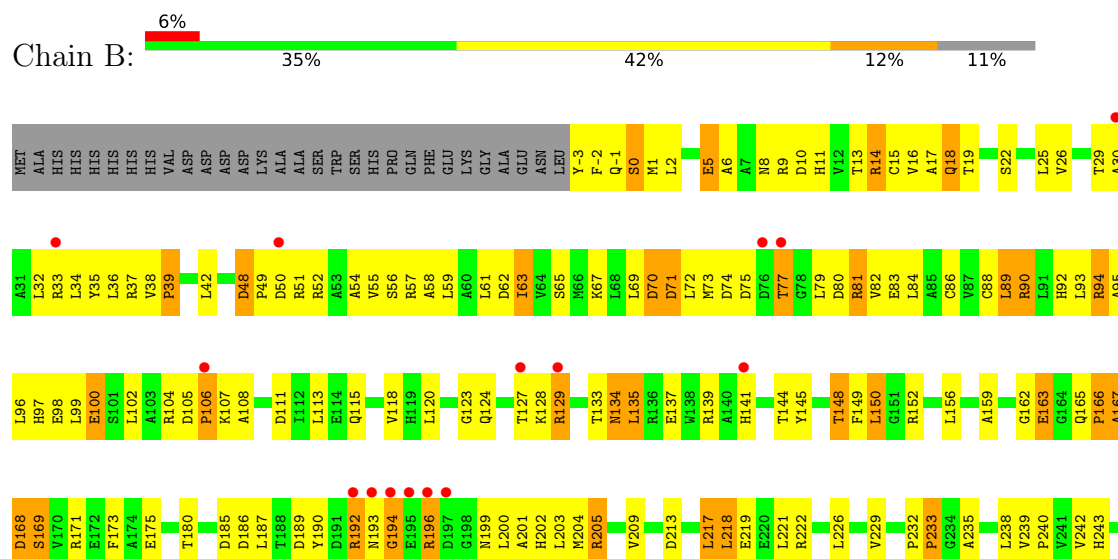
3 Residue-property plots

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: MoeN5

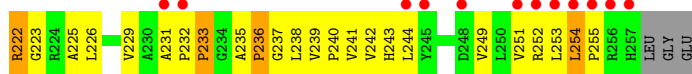
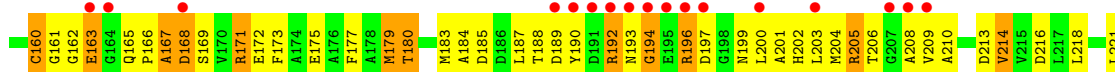
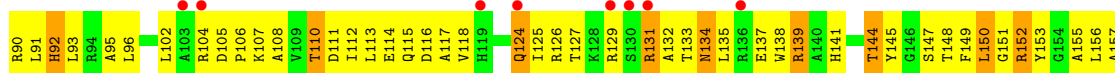
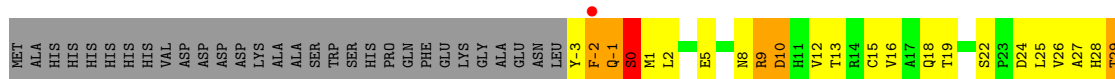


• Molecule 1: MoeN5





● Molecule 1: MoeN5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.85Å 58.55Å 92.68Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.95 24.75 – 2.94	Depositor EDS
% Data completeness (in resolution range)	90.8 (25.00-2.95) 90.0 (24.75-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 2.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.287 , 0.337 0.279 , 0.335	Depositor DCC
R_{free} test set	1056 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	1.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% 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: GPP

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	0.69	0/2029	0.86	2/2758 (0.1%)
1	B	0.66	0/2029	0.87	1/2758 (0.0%)
1	C	0.66	1/2029 (0.0%)	0.87	2/2758 (0.1%)
All	All	0.67	1/6087 (0.0%)	0.87	5/8274 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	TRP	CB-CG	6.14	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-2	PHE	N-CA-C	-6.42	93.67	111.00
1	C	72	LEU	CA-CB-CG	6.35	129.91	115.30
1	C	84	LEU	CA-CB-CG	-5.48	102.70	115.30
1	A	254	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	89	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain

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	1995	0	1978	187	0
1	B	1995	0	1978	218	0
1	C	1995	0	1978	242	0
2	A	19	0	17	1	0
2	B	19	0	17	2	0
2	C	19	0	17	7	0
3	A	79	0	0	0	0
3	B	54	0	0	1	0
3	C	58	0	0	3	0
All	All	6233	0	5985	630	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 52.

All (630) 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)
1:B:79:LEU:HD23	1:B:80:ASP:N	1.58	1.18
1:B:79:LEU:HD23	1:B:80:ASP:H	0.94	1.09
1:B:104:ARG:NH1	1:B:159:ALA:HA	1.69	1.07
1:A:249:VAL:HA	1:A:253:LEU:HD12	1.08	1.06
1:B:6:ALA:HA	1:B:9:ARG:HH22	1.23	1.04
1:C:151:GLY:HA3	1:C:171:ARG:HH21	1.19	1.04
1:C:132:ALA:HB2	1:C:141:HIS:HD2	1.23	1.02
1:A:249:VAL:HA	1:A:253:LEU:CD1	1.89	1.01
1:B:83:GLU:HG2	1:C:129:ARG:HH21	1.26	0.98
1:A:249:VAL:CA	1:A:253:LEU:HD12	1.94	0.97
1:B:25:LEU:HB2	1:B:79:LEU:HD11	1.47	0.96
1:B:81:ARG:HD3	1:C:73:MET:O	1.67	0.95
1:B:-3:TYR:HD2	1:B:-1:GLN:HB2	1.30	0.94
1:B:42:LEU:HD11	1:B:150:LEU:HD21	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.33	0.94
1:C:132:ALA:HB2	1:C:141:HIS:CD2	2.02	0.94
1:C:153:TYR:HA	1:C:156:LEU:HD12	1.46	0.93
1:C:59:LEU:O	1:C:63:ILE:HG13	1.70	0.92
1:B:-3:TYR:CD2	1:B:-1:GLN:HB2	2.06	0.91
1:B:222:ARG:HG2	1:B:226:LEU:HD12	1.54	0.90
1:B:6:ALA:HA	1:B:9:ARG:NH2	1.89	0.88
1:A:1:MET:HE2	1:A:37:ARG:HD3	1.52	0.88
1:C:42:LEU:HD11	1:C:150:LEU:HD23	1.58	0.85
1:A:183:MET:O	1:A:187:LEU:HD23	1.77	0.85
1:A:5:GLU:OE1	1:A:9:ARG:NH1	2.08	0.84
1:C:104:ARG:HD3	1:C:163:GLU:HG3	1.57	0.84
1:C:139:ARG:HH11	1:C:179:MET:CE	1.90	0.84
1:B:-3:TYR:HD2	1:B:-1:GLN:CB	1.90	0.84
1:B:253:LEU:C	1:B:255:PRO:HD2	1.98	0.83
1:B:79:LEU:CD2	1:B:80:ASP:H	1.87	0.83
1:A:70:ASP:O	1:A:72:LEU:N	2.12	0.83
1:B:229:VAL:HG13	1:B:235:ALA:HB3	1.59	0.83
1:C:66:MET:HG3	1:C:153:TYR:OH	1.79	0.83
1:C:183:MET:O	1:C:187:LEU:HG	1.79	0.82
1:A:29:THR:HA	1:A:32:LEU:HD12	1.61	0.81
1:C:139:ARG:HH11	1:C:179:MET:HE1	1.44	0.80
1:B:222:ARG:HG2	1:B:226:LEU:CD1	2.12	0.80
1:C:42:LEU:HD11	1:C:150:LEU:CD2	2.11	0.80
1:B:218:LEU:HD11	1:B:249:VAL:HG11	1.62	0.80
1:B:61:LEU:CD1	1:B:94:ARG:HG3	2.11	0.79
1:C:54:ALA:HB1	1:C:102:LEU:HD11	1.63	0.79
1:C:5:GLU:HG3	1:C:37:ARG:HB3	1.65	0.79
1:B:252:ARG:HH11	1:B:253:LEU:HD21	1.46	0.79
1:A:51:ARG:O	1:A:55:VAL:HG23	1.84	0.78
1:A:238:LEU:O	1:A:242:VAL:HG23	1.83	0.78
1:A:185:ASP:O	1:A:189:ASP:HB2	1.82	0.78
1:A:70:ASP:O	1:A:73:MET:N	2.17	0.77
1:C:12:VAL:O	1:C:16:VAL:HG23	1.84	0.77
1:B:22:SER:O	1:B:26:VAL:HG23	1.85	0.77
1:B:61:LEU:HD13	1:B:94:ARG:HG3	1.66	0.77
1:C:225:ALA:O	1:C:229:VAL:HG13	1.84	0.76
1:A:135:LEU:HB2	1:A:209:VAL:HG22	1.65	0.76
1:A:203:LEU:HD23	1:A:203:LEU:N	2.00	0.76
1:B:9:ARG:NH2	1:B:9:ARG:HB3	2.00	0.76
1:B:127:THR:HA	1:B:141:HIS:ND1	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ALA:HA	1:C:111:ASP:OD2	1.85	0.76
1:B:81:ARG:HB3	1:B:81:ARG:CZ	2.16	0.76
1:C:60:ALA:O	1:C:64:VAL:HG23	1.86	0.76
1:A:81:ARG:HH11	1:A:81:ARG:CG	1.99	0.75
1:B:83:GLU:HG2	1:C:129:ARG:NH2	1.99	0.75
1:C:124:GLN:HE21	2:C:500:GPP:H93	1.52	0.75
1:B:79:LEU:CD2	1:B:80:ASP:N	2.45	0.75
1:C:70:ASP:HB2	1:C:71:ASP:OD1	1.85	0.75
1:C:70:ASP:O	1:C:72:LEU:N	2.19	0.75
1:B:16:VAL:HG12	1:B:26:VAL:HG22	1.68	0.75
1:B:70:ASP:O	1:B:72:LEU:N	2.20	0.74
1:A:210:ALA:HB3	1:A:213:ASP:OD2	1.87	0.74
1:C:185:ASP:O	1:C:189:ASP:HB2	1.87	0.74
1:C:238:LEU:O	1:C:242:VAL:HG23	1.88	0.74
1:B:217:LEU:HD12	1:B:217:LEU:O	1.88	0.74
1:B:16:VAL:HG11	1:B:26:VAL:HA	1.69	0.73
1:C:131:ARG:CZ	1:C:133:THR:HG22	2.19	0.73
1:B:135:LEU:HB2	1:B:209:VAL:HG13	1.70	0.73
1:B:171:ARG:O	1:B:175:GLU:HG3	1.89	0.73
1:B:219:GLU:OE1	1:B:222:ARG:NH2	2.22	0.72
1:C:249:VAL:HG22	1:C:253:LEU:HD12	1.71	0.72
1:A:214:VAL:HG11	1:A:254:LEU:HD21	1.71	0.72
1:B:80:ASP:O	1:B:84:LEU:HG	1.89	0.72
1:A:166:PRO:HB2	1:A:169:SER:HB2	1.72	0.71
1:B:34:LEU:O	1:B:38:VAL:HG23	1.90	0.71
1:C:226:LEU:O	1:C:229:VAL:HG22	1.90	0.71
1:B:48:ASP:OD2	1:B:51:ARG:HB2	1.90	0.71
1:B:9:ARG:HB3	1:B:9:ARG:HH21	1.51	0.71
1:B:79:LEU:HD13	1:B:84:LEU:HD21	1.72	0.70
1:B:82:VAL:HB	1:C:129:ARG:HH22	1.56	0.70
1:C:54:ALA:HA	1:C:57:ARG:CZ	2.22	0.70
1:C:40:HIS:CE1	1:C:52:ARG:NH2	2.60	0.70
1:A:152:ARG:O	1:A:156:LEU:HG	1.92	0.69
1:B:104:ARG:HH11	1:B:159:ALA:HA	1.56	0.69
1:C:25:LEU:O	1:C:29:THR:HG23	1.93	0.69
1:B:29:THR:HA	1:B:32:LEU:HD12	1.74	0.69
1:C:252:ARG:HH12	1:C:253:LEU:HD23	1.57	0.69
1:B:92:HIS:NE2	1:B:96:LEU:HD11	2.07	0.69
1:C:252:ARG:HH12	1:C:253:LEU:CD2	2.04	0.69
1:C:135:LEU:HB2	1:C:209:VAL:HG22	1.75	0.69
1:C:156:LEU:O	1:C:160:CYS:SG	2.47	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG21	1:A:30:ALA:HB2	1.73	0.69
1:B:75:ASP:OD1	1:B:81:ARG:NH2	2.26	0.69
1:C:151:GLY:HA3	1:C:171:ARG:NH2	2.01	0.69
1:A:252:ARG:O	1:A:256:ARG:NH1	2.26	0.68
1:C:151:GLY:CA	1:C:171:ARG:HH21	2.04	0.68
1:B:217:LEU:HD12	1:B:217:LEU:C	2.14	0.68
1:A:232:PRO:HA	1:A:233:PRO:C	2.12	0.68
1:A:45:TRP:HB2	1:A:165:GLN:HE21	1.58	0.68
1:B:-3:TYR:C	1:B:-1:GLN:H	1.96	0.68
1:C:249:VAL:HG13	1:C:253:LEU:HD12	1.74	0.68
1:B:104:ARG:NH1	1:B:159:ALA:CA	2.54	0.68
1:A:128:LYS:C	1:A:129:ARG:HH11	1.98	0.68
1:A:177:PHE:O	1:A:181:ILE:HG12	1.93	0.67
1:B:9:ARG:O	1:B:9:ARG:HG2	1.95	0.67
1:B:16:VAL:CG1	1:B:26:VAL:HG22	2.25	0.67
1:B:232:PRO:HA	1:B:233:PRO:C	2.14	0.67
1:A:201:ALA:HB1	1:A:257:HIS:CE1	2.29	0.67
1:B:185:ASP:O	1:B:189:ASP:HB2	1.94	0.67
1:B:252:ARG:NH1	1:B:253:LEU:HD21	2.10	0.67
1:A:249:VAL:HG22	1:A:253:LEU:HD12	1.77	0.67
1:C:254:LEU:HD13	1:C:254:LEU:O	1.94	0.67
1:B:16:VAL:HG21	1:B:29:THR:HG21	1.76	0.67
1:C:29:THR:HA	1:C:32:LEU:HD12	1.75	0.67
1:C:9:ARG:HB2	1:C:36:LEU:HD13	1.78	0.66
1:C:77:THR:HG23	1:C:78:GLY:H	1.61	0.66
1:C:236:PRO:HG2	3:C:608:HOH:O	1.95	0.66
1:A:128:LYS:C	1:A:129:ARG:NH1	2.49	0.66
1:C:251:VAL:HG21	3:C:612:HOH:O	1.95	0.66
1:A:124:GLN:HG3	1:A:124:GLN:O	1.95	0.65
1:C:51:ARG:NH2	1:C:160:CYS:O	2.30	0.65
1:C:149:PHE:O	1:C:152:ARG:HG2	1.96	0.65
1:A:123:GLY:O	1:A:127:THR:HB	1.96	0.65
1:B:113:LEU:HB3	1:C:93:LEU:HD22	1.79	0.65
1:B:199:ASN:O	1:B:203:LEU:HG	1.97	0.65
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.32	0.65
1:C:204:MET:SD	1:C:214:VAL:HG21	2.37	0.65
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.79	0.65
1:A:9:ARG:HB2	1:A:36:LEU:HD13	1.78	0.64
1:B:13:THR:HG21	1:B:30:ALA:HB2	1.78	0.64
1:A:153:TYR:HA	1:A:156:LEU:HD12	1.78	0.64
1:C:92:HIS:CD2	1:C:96:LEU:HD13	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HE1	1:A:218:LEU:HG	1.80	0.64
1:A:201:ALA:HB1	1:A:257:HIS:HE1	1.63	0.64
1:C:59:LEU:HD22	1:C:153:TYR:HB3	1.79	0.64
1:C:200:LEU:O	1:C:204:MET:HG3	1.97	0.64
1:C:70:ASP:O	1:C:73:MET:N	2.23	0.63
1:B:144:THR:OG1	1:B:145:TYR:N	2.30	0.63
1:B:218:LEU:HD22	1:B:246:THR:HG23	1.79	0.63
1:A:11:HIS:CG	1:A:57:ARG:HD3	2.32	0.63
1:C:187:LEU:HB2	1:C:253:LEU:HD13	1.81	0.63
1:A:226:LEU:HD21	1:A:242:VAL:HB	1.79	0.63
1:B:70:ASP:O	1:B:73:MET:N	2.26	0.63
1:B:84:LEU:O	1:B:88:CYS:HB2	1.98	0.63
1:C:62:ASP:O	1:C:66:MET:HG2	1.98	0.63
1:A:219:GLU:OE2	1:A:250:LEU:HD11	1.98	0.63
1:C:180:THR:HG22	1:C:218:LEU:CD2	2.28	0.63
1:A:199:ASN:O	1:A:203:LEU:HG	1.99	0.63
1:A:16:VAL:HG21	1:A:29:THR:HG21	1.79	0.62
1:B:127:THR:HA	1:B:141:HIS:CE1	2.33	0.62
1:C:1:MET:HG2	1:C:2:LEU:N	2.13	0.62
1:C:104:ARG:HD3	1:C:163:GLU:CG	2.27	0.62
1:A:34:LEU:O	1:A:38:VAL:HG23	2.00	0.62
1:A:105:ASP:HB3	1:A:108:ALA:HB2	1.81	0.62
1:C:70:ASP:O	1:C:73:MET:HG2	1.99	0.62
1:C:165:GLN:O	1:C:167:ALA:N	2.28	0.62
1:A:183:MET:CE	1:A:218:LEU:HG	2.29	0.62
1:A:190:TYR:CD2	1:A:201:ALA:HB3	2.34	0.62
1:B:218:LEU:CD2	1:B:246:THR:HG23	2.30	0.62
1:A:12:VAL:HG22	1:A:61:LEU:HD23	1.81	0.62
1:C:252:ARG:O	1:C:252:ARG:HG2	2.00	0.62
1:B:165:GLN:O	1:B:167:ALA:N	2.32	0.61
1:B:104:ARG:HH12	1:B:159:ALA:HA	1.62	0.61
1:C:8:ASN:OD1	1:C:57:ARG:HA	1.99	0.61
1:B:25:LEU:O	1:B:29:THR:HG23	2.01	0.61
1:B:96:LEU:O	1:B:100:GLU:HB2	2.00	0.61
1:B:218:LEU:HD11	1:B:249:VAL:CG1	2.30	0.61
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.81	0.61
1:C:104:ARG:NH1	1:C:162:GLY:H	1.99	0.61
1:C:190:TYR:HB2	1:C:199:ASN:OD1	2.01	0.60
1:C:226:LEU:HD11	1:C:243:HIS:CE1	2.36	0.60
1:A:226:LEU:O	1:A:229:VAL:HG22	2.01	0.60
1:B:55:VAL:O	1:B:59:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ARG:HH11	1:C:162:GLY:H	1.49	0.60
1:C:180:THR:HG22	1:C:218:LEU:HD23	1.83	0.60
1:B:238:LEU:O	1:B:242:VAL:HG23	2.01	0.60
1:C:200:LEU:O	1:C:200:LEU:HD12	2.02	0.60
1:A:134:ASN:ND2	1:A:137:GLU:OE1	2.35	0.60
1:B:83:GLU:CG	1:C:129:ARG:HH21	2.08	0.60
1:B:89:LEU:HD22	1:C:69:LEU:HD21	1.84	0.59
1:A:190:TYR:HE2	1:A:202:HIS:HB2	1.66	0.59
1:B:251:VAL:CG1	1:B:252:ARG:N	2.65	0.59
1:C:251:VAL:O	1:C:255:PRO:HG2	2.01	0.59
1:A:29:THR:HA	1:A:32:LEU:CD1	2.32	0.59
1:C:124:GLN:O	1:C:124:GLN:HG3	2.01	0.59
1:C:80:ASP:OD1	1:C:81:ARG:N	2.36	0.59
1:B:80:ASP:HB3	1:B:83:GLU:HG3	1.83	0.59
1:B:100:GLU:HA	1:B:100:GLU:OE1	2.03	0.59
1:A:63:ILE:HD12	1:A:153:TYR:CD1	2.38	0.59
1:B:42:LEU:HD11	1:B:150:LEU:CD2	2.27	0.59
1:A:256:ARG:HB2	1:A:257:HIS:HD2	1.68	0.58
1:B:69:LEU:HD12	1:B:69:LEU:O	2.03	0.58
1:B:81:ARG:NH1	1:B:81:ARG:CB	2.66	0.58
1:B:200:LEU:O	1:B:200:LEU:HG	2.03	0.58
1:C:5:GLU:O	1:C:9:ARG:HB3	2.03	0.58
1:C:44:GLU:HG2	1:C:235:ALA:HB1	1.85	0.58
1:A:61:LEU:HD22	1:A:91:LEU:HD22	1.84	0.58
1:B:9:ARG:NH2	1:B:9:ARG:CB	2.64	0.58
1:C:45:TRP:CD1	1:C:166:PRO:HG3	2.38	0.58
1:A:129:ARG:HH11	1:A:129:ARG:N	2.02	0.58
1:B:35:TYR:HD1	1:B:63:ILE:HG23	1.67	0.58
1:B:251:VAL:HG13	1:B:252:ARG:N	2.17	0.58
1:B:81:ARG:CZ	1:B:81:ARG:CB	2.82	0.58
1:B:89:LEU:HD22	1:C:69:LEU:CD2	2.34	0.58
1:A:81:ARG:CG	1:A:81:ARG:NH1	2.63	0.58
1:A:67:LYS:HD2	1:A:67:LYS:O	2.04	0.58
1:C:51:ARG:HD3	1:C:161:GLY:O	2.03	0.58
1:C:139:ARG:HH11	1:C:179:MET:HE3	1.69	0.58
1:C:237:GLY:O	1:C:240:PRO:HD2	2.04	0.57
1:B:58:ALA:HB1	1:B:99:LEU:HG	1.86	0.57
1:C:54:ALA:HA	1:C:57:ARG:NH2	2.19	0.57
1:C:105:ASP:HB3	1:C:108:ALA:HB2	1.86	0.57
1:B:14:ARG:HG3	1:B:15:CYS:N	2.16	0.57
1:B:61:LEU:HD13	1:B:94:ARG:CG	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ARG:NH1	1:C:253:LEU:HD23	2.20	0.57
1:C:37:ARG:C	1:C:39:PRO:HD2	2.25	0.57
1:A:92:HIS:O	1:A:93:LEU:C	2.43	0.57
1:A:249:VAL:CG2	1:A:253:LEU:HD12	2.34	0.57
1:B:5:GLU:CG	1:B:9:ARG:HH12	2.17	0.57
1:B:124:GLN:O	1:B:127:THR:HG22	2.05	0.57
1:C:104:ARG:CD	1:C:163:GLU:HG3	2.33	0.57
1:B:55:VAL:CG2	1:B:102:LEU:HD13	2.35	0.57
1:C:131:ARG:NH1	1:C:133:THR:HG22	2.20	0.57
1:A:249:VAL:HG22	1:A:253:LEU:CD1	2.35	0.56
1:B:81:ARG:NH1	1:B:81:ARG:HB2	2.19	0.56
1:B:123:GLY:O	1:B:127:THR:HB	2.04	0.56
1:C:206:THR:HG23	1:C:206:THR:O	2.05	0.56
1:A:200:LEU:HG	1:A:200:LEU:O	2.06	0.56
1:A:222:ARG:NE	1:A:246:THR:HG21	2.20	0.56
1:A:139:ARG:HH21	1:A:139:ARG:HG3	1.71	0.56
1:B:152:ARG:O	1:B:156:LEU:HG	2.05	0.56
1:A:19:THR:CG2	1:A:87:VAL:HG22	2.35	0.55
1:B:134:ASN:ND2	1:B:137:GLU:HB2	2.21	0.55
1:A:116:ASP:OD1	1:A:116:ASP:N	2.36	0.55
1:A:251:VAL:O	1:A:255:PRO:HG2	2.06	0.55
1:A:35:TYR:O	1:A:39:PRO:HD3	2.06	0.55
1:B:1:MET:HE2	1:B:2:LEU:HG	1.87	0.55
1:B:67:LYS:O	1:B:67:LYS:HD3	2.06	0.55
1:C:22:SER:HB3	1:C:83:GLU:OE2	2.05	0.55
1:B:199:ASN:OD1	1:B:201:ALA:HB3	2.07	0.55
1:C:66:MET:O	1:C:69:LEU:HB3	2.07	0.55
1:A:177:PHE:CE2	1:A:181:ILE:HD11	2.42	0.55
1:B:79:LEU:HD13	1:B:84:LEU:CD2	2.36	0.55
1:A:138:TRP:CE2	1:A:200:LEU:HB2	2.42	0.55
1:A:150:LEU:HD23	1:A:178:ALA:HB2	1.89	0.55
1:C:139:ARG:NH1	1:C:179:MET:CE	2.65	0.55
1:C:232:PRO:HA	1:C:233:PRO:C	2.26	0.55
1:B:222:ARG:HD3	1:B:243:HIS:ND1	2.22	0.54
1:C:200:LEU:HD11	1:C:214:VAL:CG2	2.37	0.54
1:C:131:ARG:NH2	1:C:133:THR:HG22	2.22	0.54
1:A:51:ARG:O	1:A:54:ALA:HB3	2.07	0.54
1:B:54:ALA:O	1:B:57:ARG:HG2	2.07	0.54
1:C:38:VAL:N	1:C:39:PRO:HD2	2.23	0.54
1:C:77:THR:HG23	1:C:78:GLY:N	2.22	0.54
1:A:214:VAL:CG1	1:A:254:LEU:HD21	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD11	1:B:98:GLU:OE2	2.07	0.54
1:A:32:LEU:O	1:A:36:LEU:HG	2.08	0.54
1:C:72:LEU:HD13	1:C:84:LEU:HB3	1.90	0.54
1:C:66:MET:HG3	1:C:153:TYR:HH	1.73	0.54
1:A:135:LEU:HB2	1:A:209:VAL:CG2	2.35	0.54
1:B:55:VAL:HG23	1:B:102:LEU:HD13	1.90	0.53
1:A:96:LEU:O	1:A:100:GLU:HB2	2.08	0.53
1:B:14:ARG:O	1:B:18:GLN:HG2	2.08	0.53
1:B:25:LEU:CB	1:B:79:LEU:HD11	2.29	0.53
1:B:193:ASN:O	1:B:194:GLY:C	2.46	0.53
1:C:208:ALA:O	1:C:209:VAL:HG23	2.08	0.53
1:B:127:THR:HG23	1:B:128:LYS:HG3	1.91	0.53
1:C:222:ARG:HG2	1:C:223:GLY:N	2.21	0.53
1:A:179:MET:HG2	1:A:221:LEU:HD11	1.88	0.53
1:A:193:ASN:O	1:A:194:GLY:C	2.45	0.53
1:A:187:LEU:HD21	1:A:200:LEU:HD23	1.90	0.53
1:B:19:THR:HG21	1:B:90:ARG:HG3	1.90	0.53
1:B:229:VAL:CG1	1:B:235:ALA:O	2.57	0.53
1:B:81:ARG:HB2	1:B:81:ARG:HH11	1.73	0.53
1:C:54:ALA:HA	1:C:57:ARG:NH1	2.24	0.53
1:B:253:LEU:N	1:B:255:PRO:HD2	2.23	0.52
1:A:11:HIS:CD2	1:A:57:ARG:HD3	2.44	0.52
1:A:165:GLN:O	1:A:167:ALA:N	2.35	0.52
1:C:80:ASP:OD1	1:C:82:VAL:N	2.41	0.52
1:C:193:ASN:O	1:C:194:GLY:C	2.48	0.52
1:A:77:THR:OG1	1:A:79:LEU:HD12	2.08	0.52
1:A:-1:GLN:O	1:A:1:MET:N	2.43	0.52
1:B:11:HIS:C	1:B:11:HIS:CD2	2.83	0.52
1:B:252:ARG:HG3	1:B:253:LEU:HD23	1.91	0.52
1:A:192:ARG:HH11	1:A:192:ARG:HB2	1.75	0.52
1:A:233:PRO:HG2	1:A:234:GLY:H	1.74	0.52
1:B:70:ASP:OD2	1:B:74:ASP:OD2	2.27	0.52
1:A:142:ALA:HA	1:A:145:TYR:CE2	2.45	0.52
1:B:15:CYS:O	1:B:19:THR:OG1	2.22	0.52
1:C:81:ARG:HB3	1:C:81:ARG:CZ	2.39	0.52
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.10	0.52
1:B:25:LEU:HD13	1:B:79:LEU:HD13	1.91	0.52
1:B:49:PRO:HG2	1:B:50:ASP:H	1.74	0.52
1:B:187:LEU:HD21	1:B:204:MET:CE	2.41	0.51
1:C:9:ARG:CB	1:C:36:LEU:HD13	2.39	0.51
1:C:139:ARG:NH1	1:C:179:MET:HE3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:HIS:ND1	1:C:107:LYS:NZ	2.59	0.51
1:C:73:MET:HG3	1:C:74:ASP:OD1	2.11	0.51
1:C:116:ASP:OD1	1:C:148:THR:HG21	2.11	0.51
1:C:135:LEU:HD13	1:C:213:ASP:HB3	1.92	0.51
1:A:51:ARG:NH1	1:A:102:LEU:O	2.44	0.51
1:C:60:ALA:HA	1:C:63:ILE:HD12	1.92	0.51
1:C:162:GLY:O	1:C:163:GLU:O	2.28	0.51
1:B:222:ARG:HB2	1:B:246:THR:HG21	1.91	0.51
1:B:48:ASP:OD2	1:B:51:ARG:CB	2.59	0.51
1:C:180:THR:HG23	1:C:221:LEU:HB3	1.92	0.51
1:A:19:THR:OG1	1:A:90:ARG:HG3	2.10	0.51
1:B:16:VAL:CG1	1:B:26:VAL:HG13	2.41	0.51
1:C:52:ARG:HG3	1:C:52:ARG:HH11	1.75	0.51
1:C:87:VAL:O	1:C:91:LEU:HG	2.10	0.51
1:C:147:SER:O	1:C:175:GLU:HG2	2.11	0.51
1:B:-2:PHE:O	1:B:2:LEU:CD1	2.59	0.51
1:B:89:LEU:O	1:B:93:LEU:HG	2.10	0.51
1:B:252:ARG:C	1:B:253:LEU:HD23	2.31	0.51
1:B:8:ASN:OD1	1:B:57:ARG:HA	2.11	0.50
1:B:104:ARG:HH11	1:B:159:ALA:CA	2.22	0.50
1:C:46:THR:HB	1:C:52:ARG:HG2	1.92	0.50
1:C:124:GLN:HG2	2:C:500:GPP:H93	1.92	0.50
1:C:192:ARG:HB3	1:C:192:ARG:NH1	2.26	0.50
1:B:80:ASP:OD2	1:C:129:ARG:NH2	2.44	0.50
1:C:9:ARG:NE	1:C:30:ALA:O	2.40	0.50
1:B:129:ARG:HH22	1:C:82:VAL:HB	1.76	0.50
1:A:147:SER:O	1:A:175:GLU:HG2	2.12	0.50
1:B:25:LEU:HD13	1:B:79:LEU:CD1	2.41	0.50
1:C:62:ASP:O	1:C:65:SER:HB3	2.12	0.50
1:C:138:TRP:CE2	1:C:200:LEU:HB2	2.46	0.50
1:A:83:GLU:O	1:A:84:LEU:C	2.50	0.50
1:C:40:HIS:CE1	1:C:52:ARG:HH22	2.29	0.50
1:C:183:MET:CE	1:C:200:LEU:HD21	2.42	0.50
1:A:239:VAL:O	1:A:243:HIS:HD2	1.95	0.49
1:A:249:VAL:HA	1:A:253:LEU:CG	2.40	0.49
1:C:45:TRP:HB2	1:C:165:GLN:NE2	2.27	0.49
1:C:45:TRP:CZ3	1:C:238:LEU:HD11	2.48	0.49
1:C:144:THR:HG23	1:C:145:TYR:H	1.77	0.49
1:B:16:VAL:HG12	1:B:26:VAL:HG13	1.95	0.49
1:C:52:ARG:HG3	1:C:52:ARG:NH1	2.27	0.49
1:A:19:THR:HG21	1:A:87:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:HIS:NE2	1:A:144:THR:HG22	2.27	0.49
1:B:67:LYS:HE3	1:B:71:ASP:OD2	2.13	0.49
1:A:201:ALA:CB	1:A:257:HIS:HE1	2.24	0.49
1:B:11:HIS:CD2	1:B:61:LEU:HD21	2.47	0.49
1:B:166:PRO:HB2	1:B:169:SER:HB2	1.93	0.49
1:C:125:ILE:O	1:C:129:ARG:HG2	2.13	0.49
1:A:63:ILE:HG22	1:A:64:VAL:N	2.27	0.49
1:B:89:LEU:HD12	1:B:93:LEU:HG	1.94	0.49
1:C:80:ASP:OD1	1:C:82:VAL:HG23	2.13	0.49
1:C:92:HIS:CD2	1:C:92:HIS:C	2.86	0.49
1:A:70:ASP:C	1:A:72:LEU:N	2.65	0.48
1:B:1:MET:HE1	1:B:37:ARG:CZ	2.43	0.48
1:B:107:LYS:HE3	1:B:111:ASP:OD1	2.13	0.48
1:A:70:ASP:C	1:A:72:LEU:H	2.16	0.48
1:B:82:VAL:O	1:B:86:CYS:SG	2.59	0.48
1:A:-3:TYR:C	1:A:-1:GLN:H	2.12	0.48
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.77	0.48
1:A:127:THR:CG2	1:A:128:LYS:N	2.76	0.48
1:A:133:THR:O	1:A:134:ASN:HB3	2.13	0.48
1:B:9:ARG:CB	1:B:9:ARG:CZ	2.90	0.48
1:B:203:LEU:HB3	1:B:209:VAL:HG23	1.95	0.48
1:B:187:LEU:HD21	1:B:204:MET:HE2	1.95	0.48
1:C:138:TRP:HH2	1:C:183:MET:HG2	1.77	0.48
1:A:190:TYR:CE1	1:A:205:ARG:NH2	2.80	0.48
1:B:62:ASP:O	1:B:65:SER:HB3	2.14	0.48
1:B:127:THR:HG23	1:B:128:LYS:N	2.28	0.48
1:C:70:ASP:C	1:C:72:LEU:H	2.17	0.48
1:C:187:LEU:HD12	1:C:253:LEU:HD13	1.94	0.48
1:B:-1:GLN:C	1:B:-1:GLN:OE1	2.52	0.48
1:B:254:LEU:N	1:B:255:PRO:HD2	2.27	0.48
1:C:9:ARG:NH1	1:C:30:ALA:O	2.44	0.48
1:B:90:ARG:NH1	1:C:117:ALA:HB3	2.28	0.48
1:B:129:ARG:NH2	1:C:82:VAL:HB	2.28	0.48
1:B:232:PRO:HA	1:B:233:PRO:O	2.14	0.48
1:C:28:HIS:ND1	1:C:79:LEU:HD11	2.28	0.48
1:C:153:TYR:CA	1:C:156:LEU:HD12	2.30	0.48
1:A:11:HIS:CE1	1:A:57:ARG:HD3	2.49	0.48
1:B:168:ASP:OD2	1:B:168:ASP:N	2.39	0.48
1:C:252:ARG:HG2	1:C:252:ARG:HH11	1.78	0.48
1:A:127:THR:OG1	1:A:141:HIS:HB3	2.13	0.47
1:A:135:LEU:C	1:A:137:GLU:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:THR:HG21	1:C:30:ALA:HB2	1.95	0.47
1:C:75:ASP:OD1	1:C:81:ARG:NH2	2.41	0.47
1:C:199:ASN:O	1:C:203:LEU:HG	2.14	0.47
1:C:184:ALA:HA	1:C:253:LEU:HD11	1.97	0.47
1:A:112:ILE:HD13	1:A:155:ALA:CB	2.45	0.47
1:B:-1:GLN:O	1:B:1:MET:N	2.47	0.47
1:C:83:GLU:O	1:C:84:LEU:C	2.50	0.47
1:C:108:ALA:O	1:C:111:ASP:HB2	2.14	0.47
1:A:57:ARG:HG3	1:A:58:ALA:N	2.30	0.47
1:A:75:ASP:CG	1:A:75:ASP:O	2.54	0.47
1:B:67:LYS:HD3	1:B:67:LYS:C	2.35	0.47
1:B:73:MET:HE3	2:B:500:GPP:H93	1.97	0.47
1:C:126:ARG:O	1:C:126:ARG:HG2	2.14	0.47
1:A:107:LYS:O	1:A:111:ASP:OD2	2.33	0.47
1:B:127:THR:CG2	1:B:128:LYS:N	2.78	0.47
1:B:135:LEU:C	1:B:137:GLU:N	2.68	0.47
1:C:28:HIS:CD2	1:C:32:LEU:HD11	2.49	0.47
1:A:38:VAL:HG11	1:A:150:LEU:HD11	1.96	0.46
1:A:129:ARG:HA	1:A:129:ARG:HD3	1.53	0.46
1:A:135:LEU:H	1:A:209:VAL:CG2	2.27	0.46
1:B:135:LEU:CD1	1:B:213:ASP:HB3	2.46	0.46
1:C:9:ARG:HA	1:C:36:LEU:CD2	2.45	0.46
1:C:192:ARG:CB	1:C:192:ARG:HH11	2.28	0.46
1:C:222:ARG:HG3	1:C:222:ARG:HH11	1.80	0.46
1:C:-1:GLN:O	1:C:0:SER:C	2.53	0.46
1:C:33:ARG:O	1:C:37:ARG:HG2	2.15	0.46
1:C:249:VAL:HG13	1:C:253:LEU:CD1	2.45	0.46
1:C:-1:GLN:O	1:C:1:MET:N	2.49	0.46
1:C:169:SER:OG	1:C:231:ALA:HB3	2.15	0.46
1:A:38:VAL:N	1:A:39:PRO:CD	2.78	0.46
1:B:108:ALA:O	1:B:111:ASP:HB2	2.15	0.46
1:C:112:ILE:HG21	1:C:155:ALA:HB3	1.96	0.46
1:A:113:LEU:O	1:A:152:ARG:NH1	2.47	0.46
1:B:19:THR:HA	1:C:118:VAL:HG13	1.98	0.46
1:B:83:GLU:O	1:B:84:LEU:C	2.53	0.46
1:C:9:ARG:HG2	1:C:9:ARG:HH21	1.80	0.46
1:C:10:ASP:C	1:C:10:ASP:OD2	2.54	0.46
1:C:135:LEU:HD22	3:C:617:HOH:O	2.15	0.46
1:A:51:ARG:NH2	1:A:162:GLY:CA	2.79	0.46
1:C:26:VAL:CG1	1:C:27:ALA:N	2.77	0.46
1:C:59:LEU:O	1:C:63:ILE:CG1	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ASP:O	1:C:189:ASP:CB	2.61	0.46
1:A:139:ARG:HG3	1:A:217:LEU:HD11	1.98	0.46
1:A:166:PRO:O	1:A:170:VAL:HG23	2.16	0.46
1:A:244:LEU:HD23	1:A:245:TYR:CD2	2.51	0.46
1:B:92:HIS:CD2	1:B:96:LEU:HD11	2.51	0.46
1:C:70:ASP:C	1:C:72:LEU:N	2.69	0.46
1:C:73:MET:HE3	2:C:500:GPP:H92	1.98	0.46
1:C:133:THR:O	1:C:134:ASN:HB3	2.16	0.46
1:A:12:VAL:CG2	1:A:61:LEU:HD23	2.46	0.46
1:A:230:ALA:O	1:A:231:ALA:C	2.54	0.46
1:A:5:GLU:HG3	1:A:37:ARG:HB2	1.97	0.46
1:A:82:VAL:HG12	1:A:83:GLU:N	2.31	0.46
1:B:33:ARG:NH1	3:B:602:HOH:O	2.49	0.45
1:B:16:VAL:HG12	1:B:17:ALA:N	2.31	0.45
1:C:108:ALA:O	1:C:112:ILE:HG13	2.16	0.45
1:B:-2:PHE:O	1:B:2:LEU:HD12	2.16	0.45
1:C:45:TRP:CD1	1:C:166:PRO:CG	2.99	0.45
1:C:49:PRO:HG2	1:C:50:ASP:H	1.81	0.45
1:A:92:HIS:O	1:A:94:ARG:N	2.49	0.45
1:A:120:LEU:O	1:A:120:LEU:HD12	2.16	0.45
1:A:231:ALA:HA	1:A:232:PRO:HD2	1.74	0.45
1:C:104:ARG:HH11	1:C:162:GLY:N	2.12	0.45
1:A:9:ARG:HB2	1:A:36:LEU:CD1	2.45	0.45
1:A:12:VAL:HG12	1:A:13:THR:N	2.31	0.45
1:A:58:ALA:HB1	1:A:99:LEU:HG	1.98	0.45
1:A:249:VAL:CB	1:A:253:LEU:HD12	2.44	0.45
1:B:149:PHE:CE1	2:B:500:GPP:H51	2.52	0.45
1:C:236:PRO:HG2	1:C:237:GLY:N	2.31	0.45
1:B:-1:GLN:O	1:B:0:SER:C	2.53	0.45
1:C:152:ARG:HG3	1:C:153:TYR:N	2.32	0.45
1:A:11:HIS:CE1	1:A:57:ARG:CD	2.99	0.45
1:A:232:PRO:HA	1:A:233:PRO:O	2.17	0.45
1:C:92:HIS:O	1:C:93:LEU:C	2.55	0.45
1:A:189:ASP:CG	1:A:192:ARG:HH22	2.20	0.45
1:A:225:ALA:O	1:A:229:VAL:HG13	2.16	0.45
1:B:90:ARG:HH11	1:B:90:ARG:HG2	1.81	0.45
1:A:80:ASP:OD1	1:A:81:ARG:N	2.50	0.45
1:B:173:PHE:HE1	1:B:242:VAL:HG22	1.82	0.45
1:C:77:THR:OG1	1:C:79:LEU:HD12	2.17	0.44
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.32	0.44
1:B:80:ASP:OD2	1:B:83:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASP:CG	1:C:49:PRO:HD2	2.38	0.44
1:A:35:TYR:OH	1:A:67:LYS:HE3	2.16	0.44
1:A:51:ARG:NH2	1:A:162:GLY:HA2	2.33	0.44
1:A:105:ASP:O	1:A:108:ALA:HB3	2.17	0.44
1:A:108:ALA:O	1:A:111:ASP:HB2	2.17	0.44
1:A:139:ARG:O	1:A:139:ARG:HD3	2.17	0.44
1:A:153:TYR:HA	1:A:156:LEU:CD1	2.45	0.44
1:C:239:VAL:N	1:C:240:PRO:CD	2.81	0.44
1:A:51:ARG:HH22	1:A:162:GLY:HA2	1.82	0.44
1:A:89:LEU:O	1:A:93:LEU:HG	2.18	0.44
1:B:93:LEU:CD2	1:C:113:LEU:HD13	2.48	0.44
1:B:135:LEU:HD12	1:B:213:ASP:HB3	1.98	0.44
1:C:9:ARG:N	1:C:36:LEU:HD22	2.33	0.44
1:C:114:GLU:O	1:C:116:ASP:N	2.51	0.44
1:A:135:LEU:O	1:A:137:GLU:N	2.51	0.44
1:C:135:LEU:C	1:C:137:GLU:N	2.70	0.44
1:A:187:LEU:N	1:A:187:LEU:CD2	2.81	0.44
1:A:257:HIS:N	1:A:257:HIS:CD2	2.85	0.44
1:B:133:THR:O	1:B:134:ASN:HB3	2.18	0.44
1:C:-2:PHE:CZ	1:C:244:LEU:HD22	2.52	0.44
1:C:66:MET:HE2	1:C:66:MET:HA	1.98	0.44
1:C:187:LEU:HD12	1:C:249:VAL:HG13	2.00	0.44
1:B:162:GLY:O	1:B:163:GLU:O	2.36	0.44
1:B:-3:TYR:C	1:B:-1:GLN:N	2.67	0.44
1:B:38:VAL:HB	1:B:39:PRO:HD3	1.99	0.44
1:C:34:LEU:HA	1:C:37:ARG:HG2	1.99	0.44
1:C:44:GLU:HA	1:C:52:ARG:NH2	2.33	0.43
1:C:107:LYS:O	1:C:111:ASP:OD2	2.36	0.43
1:C:139:ARG:NH1	1:C:179:MET:HE1	2.22	0.43
1:A:139:ARG:HG3	1:A:139:ARG:NH2	2.31	0.43
1:A:211:GLY:O	1:A:215:VAL:HG23	2.17	0.43
1:B:49:PRO:HG2	1:B:50:ASP:N	2.33	0.43
1:C:188:THR:OG1	1:C:253:LEU:HD21	2.18	0.43
1:A:-1:GLN:O	1:A:0:SER:C	2.56	0.43
1:A:135:LEU:N	1:A:209:VAL:CG2	2.82	0.43
1:A:244:LEU:HD23	1:A:245:TYR:CE2	2.53	0.43
1:B:11:HIS:ND1	1:B:57:ARG:HD3	2.33	0.43
1:B:254:LEU:N	1:B:255:PRO:CD	2.81	0.43
1:C:41:PHE:CZ	1:C:241:VAL:HG11	2.53	0.43
1:C:183:MET:HE2	1:C:200:LEU:HD21	2.00	0.43
1:C:252:ARG:O	1:C:252:ARG:CG	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ARG:NH1	1:C:253:LEU:CD2	2.78	0.43
1:A:81:ARG:HB3	1:A:81:ARG:CZ	2.48	0.43
1:B:94:ARG:O	1:B:97:HIS:HB3	2.19	0.43
1:B:180:THR:HG23	1:B:218:LEU:HD21	2.00	0.43
1:B:190:TYR:CD2	1:B:201:ALA:HB3	2.53	0.43
1:A:129:ARG:HH11	1:A:129:ARG:CA	2.32	0.43
1:A:202:HIS:O	1:A:205:ARG:N	2.51	0.43
1:B:124:GLN:C	1:B:127:THR:HG22	2.38	0.43
1:C:34:LEU:O	1:C:38:VAL:HG23	2.18	0.43
1:C:135:LEU:C	1:C:137:GLU:H	2.22	0.43
1:C:135:LEU:O	1:C:137:GLU:N	2.52	0.43
1:C:180:THR:HG23	1:C:221:LEU:CB	2.48	0.43
1:A:105:ASP:O	1:A:106:PRO:C	2.57	0.43
1:B:-3:TYR:CG	1:B:-2:PHE:N	2.86	0.43
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.84	0.43
1:C:66:MET:O	1:C:70:ASP:OD1	2.37	0.43
1:A:128:LYS:CB	1:A:129:ARG:HH12	2.32	0.43
1:A:222:ARG:CZ	1:A:246:THR:HG21	2.48	0.43
1:B:19:THR:CG2	1:B:90:ARG:HG3	2.48	0.43
1:A:208:ALA:O	1:A:209:VAL:HG23	2.19	0.43
1:B:248:ASP:OD1	1:B:252:ARG:HG2	2.18	0.43
1:C:-1:GLN:OE1	1:C:0:SER:N	2.51	0.43
1:C:173:PHE:CE1	1:C:177:PHE:HB2	2.54	0.43
1:A:192:ARG:NH1	1:A:192:ARG:CB	2.81	0.43
1:B:13:THR:HG21	1:B:30:ALA:CB	2.48	0.43
1:B:205:ARG:HG3	1:B:205:ARG:HH11	1.83	0.43
1:C:52:ARG:O	1:C:52:ARG:HD3	2.19	0.43
1:C:59:LEU:HD11	1:C:157:ALA:HB2	2.00	0.43
1:C:190:TYR:CG	1:C:201:ALA:HB3	2.54	0.43
1:B:92:HIS:O	1:B:93:LEU:C	2.57	0.43
1:C:252:ARG:HG2	1:C:252:ARG:NH1	2.34	0.43
1:A:127:THR:CG2	1:A:128:LYS:HG3	2.49	0.42
1:B:100:GLU:HB3	1:C:107:LYS:HE2	2.00	0.42
1:C:75:ASP:O	1:C:75:ASP:OD2	2.36	0.42
1:C:131:ARG:NH1	1:C:133:THR:CG2	2.82	0.42
1:A:70:ASP:HA	1:A:73:MET:HG2	2.01	0.42
1:A:256:ARG:HB2	1:A:257:HIS:CD2	2.52	0.42
1:B:100:GLU:OE1	1:B:100:GLU:CA	2.67	0.42
1:A:234:GLY:O	1:A:236:PRO:HD2	2.18	0.42
1:B:218:LEU:HD13	1:B:250:LEU:HD23	2.01	0.42
1:C:135:LEU:H	1:C:209:VAL:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:O	1:A:34:LEU:HD12	2.19	0.42
1:B:11:HIS:CD2	1:B:11:HIS:O	2.72	0.42
1:B:127:THR:CG2	1:B:128:LYS:HG3	2.50	0.42
1:B:202:HIS:O	1:B:205:ARG:N	2.52	0.42
1:C:135:LEU:HB2	1:C:209:VAL:CG2	2.47	0.42
1:C:149:PHE:HE1	1:C:153:TYR:HH	1.67	0.42
1:A:9:ARG:HA	1:A:36:LEU:HD13	2.01	0.42
1:A:181:ILE:O	1:A:184:ALA:HB3	2.19	0.42
1:A:192:ARG:HH11	1:A:192:ARG:CB	2.33	0.42
1:B:-1:GLN:C	1:B:1:MET:N	2.73	0.42
1:C:141:HIS:O	1:C:144:THR:CG2	2.67	0.42
1:C:236:PRO:HG2	1:C:237:GLY:H	1.84	0.42
1:C:124:GLN:HE22	2:C:500:GPP:H41	1.83	0.42
1:C:149:PHE:CE1	1:C:153:TYR:HE2	2.37	0.42
1:A:120:LEU:HD11	2:A:500:GPP:H103	2.00	0.42
1:A:135:LEU:C	1:A:137:GLU:H	2.22	0.42
1:B:70:ASP:C	1:B:72:LEU:H	2.22	0.42
1:B:96:LEU:HB3	1:C:110:THR:HG22	2.02	0.42
1:B:253:LEU:N	1:B:253:LEU:HD23	2.34	0.42
1:C:19:THR:O	1:C:19:THR:HG22	2.19	0.42
1:C:54:ALA:CB	1:C:102:LEU:HD11	2.42	0.42
1:C:73:MET:CE	2:C:500:GPP:H92	2.49	0.42
1:B:70:ASP:C	1:B:72:LEU:N	2.71	0.42
1:A:177:PHE:CZ	1:A:181:ILE:HD11	2.54	0.42
1:B:61:LEU:CD1	1:B:94:ARG:CG	2.91	0.42
1:B:105:ASP:O	1:B:106:PRO:C	2.58	0.42
1:B:135:LEU:C	1:B:137:GLU:H	2.23	0.42
1:B:148:THR:O	1:B:152:ARG:HD3	2.20	0.42
1:C:202:HIS:O	1:C:205:ARG:N	2.52	0.42
1:A:144:THR:OG1	1:A:145:TYR:N	2.52	0.42
1:C:105:ASP:O	1:C:108:ALA:HB3	2.20	0.42
1:A:35:TYR:HB3	1:A:63:ILE:CG2	2.50	0.41
1:A:80:ASP:HB3	1:A:83:GLU:HG3	2.01	0.41
1:B:35:TYR:HB3	1:B:63:ILE:CG2	2.50	0.41
1:B:62:ASP:HB2	1:B:95:ALA:CB	2.50	0.41
1:A:57:ARG:NH1	1:A:57:ARG:HG2	2.34	0.41
1:C:218:LEU:CD1	1:C:249:VAL:HG11	2.50	0.41
1:C:42:LEU:HD11	1:C:150:LEU:HD21	2.00	0.41
1:C:105:ASP:O	1:C:106:PRO:C	2.57	0.41
1:B:120:LEU:HD12	1:B:120:LEU:O	2.20	0.41
1:C:84:LEU:O	1:C:88:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:108:ALA:CB	2.69	0.41
1:A:226:LEU:CD2	1:A:242:VAL:HB	2.49	0.41
1:B:51:ARG:O	1:B:54:ALA:HB3	2.21	0.41
1:A:135:LEU:C	1:A:135:LEU:HD23	2.41	0.41
1:B:135:LEU:O	1:B:139:ARG:HG2	2.20	0.41
1:A:11:HIS:ND1	1:A:57:ARG:HD3	2.35	0.41
1:A:14:ARG:O	1:A:14:ARG:HG3	2.20	0.41
1:B:13:THR:CG2	1:B:30:ALA:HB2	2.48	0.41
1:B:113:LEU:HB3	1:C:93:LEU:CD2	2.48	0.41
1:B:124:GLN:O	1:B:124:GLN:HG3	2.21	0.41
1:C:210:ALA:HB3	1:C:213:ASP:OD2	2.20	0.41
1:A:45:TRP:CD1	1:A:166:PRO:HG3	2.56	0.41
1:A:114:GLU:O	1:A:116:ASP:N	2.54	0.41
1:B:135:LEU:O	1:B:137:GLU:N	2.54	0.41
1:A:183:MET:SD	1:A:217:LEU:HD22	2.60	0.41
1:B:-3:TYR:CD2	1:B:-1:GLN:N	2.89	0.41
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.67	0.41
1:C:44:GLU:OE1	1:C:237:GLY:HA3	2.21	0.41
1:A:112:ILE:HD13	1:A:155:ALA:HB1	2.03	0.41
1:C:104:ARG:HD3	1:C:163:GLU:OE2	2.20	0.41
2:C:500:GPP:H41	2:C:500:GPP:H62	1.79	0.41
1:A:195:GLU:O	1:A:196:ARG:HB2	2.21	0.40
1:A:203:LEU:HD23	1:A:203:LEU:H	1.82	0.40
1:C:-3:TYR:C	1:C:-1:GLN:H	2.24	0.40
1:C:85:ALA:O	1:C:88:CYS:HB3	2.21	0.40
1:C:183:MET:HE2	1:C:183:MET:HB3	1.93	0.40
1:A:183:MET:SD	1:A:217:LEU:CD2	3.09	0.40
1:B:105:ASP:HB3	1:B:108:ALA:HB2	2.03	0.40
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.71	0.40
1:C:124:GLN:NE2	2:C:500:GPP:H41	2.36	0.40
1:C:141:HIS:O	1:C:144:THR:HG23	2.21	0.40
1:B:65:SER:OG	1:B:92:HIS:HB2	2.21	0.40
1:C:72:LEU:HD21	1:C:85:ALA:HB2	2.03	0.40
1:C:168:ASP:OD2	1:C:168:ASP:N	2.55	0.40
1:B:124:GLN:HA	1:B:127:THR:CG2	2.52	0.40
1:C:67:LYS:O	1:C:71:ASP:OD1	2.39	0.40
1:C:135:LEU:N	1:C:209:VAL:CG2	2.84	0.40
1:A:9:ARG:O	1:A:9:ARG:CG	2.65	0.40
1:B:32:LEU:O	1:B:36:LEU:HG	2.21	0.40
1:B:222:ARG:HG2	1:B:226:LEU:HD11	1.98	0.40
1:C:9:ARG:HA	1:C:36:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:HIS:O	1:C:95:ALA:N	2.54	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	259/294 (88%)	214 (83%)	32 (12%)	13 (5%)	2	10
1	B	259/294 (88%)	213 (82%)	34 (13%)	12 (5%)	2	11
1	C	259/294 (88%)	216 (83%)	32 (12%)	11 (4%)	3	13
All	All	777/882 (88%)	643 (83%)	98 (13%)	36 (5%)	2	11

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ASP
1	A	77	THR
1	A	115	GLN
1	A	163	GLU
1	B	71	ASP
1	B	77	THR
1	B	115	GLN
1	B	163	GLU
1	C	71	ASP
1	C	77	THR
1	C	115	GLN
1	C	163	GLU
1	A	0	SER
1	A	167	ALA
1	A	192	ARG
1	A	194	GLY

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Mol	Chain	Res	Type
1	A	196	ARG
1	B	167	ALA
1	B	192	ARG
1	B	194	GLY
1	B	196	ARG
1	C	70	ASP
1	C	167	ALA
1	C	192	ARG
1	C	194	GLY
1	C	196	ARG
1	A	70	ASP
1	A	107	LYS
1	A	233	PRO
1	B	0	SER
1	B	70	ASP
1	B	233	PRO
1	C	0	SER
1	C	233	PRO
1	B	166	PRO
1	A	166	PRO

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	205/232 (88%)	172 (84%)	33 (16%)	2	10
1	B	205/232 (88%)	174 (85%)	31 (15%)	3	12
1	C	205/232 (88%)	157 (77%)	48 (23%)	1	3
All	All	615/696 (88%)	503 (82%)	112 (18%)	1	7

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	10	ASP

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Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	CYS
1	A	18	GLN
1	A	19	THR
1	A	47	THR
1	A	52	ARG
1	A	55	VAL
1	A	57	ARG
1	A	63	ILE
1	A	76	ASP
1	A	77	THR
1	A	81	ARG
1	A	82	VAL
1	A	90	ARG
1	A	96	LEU
1	A	115	GLN
1	A	118	VAL
1	A	124	GLN
1	A	127	THR
1	A	129	ARG
1	A	130	SER
1	A	131	ARG
1	A	139	ARG
1	A	180	THR
1	A	185	ASP
1	A	187	LEU
1	A	189	ASP
1	A	191	ASP
1	A	216	ASP
1	A	246	THR
1	A	254	LEU
1	B	5	GLU
1	B	10	ASP
1	B	14	ARG
1	B	18	GLN
1	B	39	PRO
1	B	48	ASP
1	B	52	ARG
1	B	56	SER
1	B	63	ILE
1	B	77	THR
1	B	81	ARG

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Mol	Chain	Res	Type
1	B	90	ARG
1	B	94	ARG
1	B	100	GLU
1	B	106	PRO
1	B	118	VAL
1	B	129	ARG
1	B	134	ASN
1	B	135	LEU
1	B	148	THR
1	B	150	LEU
1	B	168	ASP
1	B	169	SER
1	B	186	ASP
1	B	196	ARG
1	B	205	ARG
1	B	217	LEU
1	B	218	LEU
1	B	251	VAL
1	B	253	LEU
1	B	254	LEU
1	C	-2	PHE
1	C	-1	GLN
1	C	0	SER
1	C	9	ARG
1	C	10	ASP
1	C	15	CYS
1	C	18	GLN
1	C	24	ASP
1	C	29	THR
1	C	34	LEU
1	C	43	THR
1	C	47	THR
1	C	51	ARG
1	C	52	ARG
1	C	56	SER
1	C	62	ASP
1	C	67	LYS
1	C	70	ASP
1	C	71	ASP
1	C	74	ASP
1	C	76	ASP
1	C	81	ARG

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Mol	Chain	Res	Type
1	C	84	LEU
1	C	90	ARG
1	C	92	HIS
1	C	110	THR
1	C	124	GLN
1	C	127	THR
1	C	131	ARG
1	C	134	ASN
1	C	139	ARG
1	C	144	THR
1	C	150	LEU
1	C	152	ARG
1	C	160	CYS
1	C	168	ASP
1	C	171	ARG
1	C	172	GLU
1	C	179	MET
1	C	180	THR
1	C	196	ARG
1	C	197	ASP
1	C	205	ARG
1	C	214	VAL
1	C	216	ASP
1	C	222	ARG
1	C	236	PRO
1	C	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	HIS
1	B	11	HIS
1	B	18	GLN
1	C	18	GLN
1	C	40	HIS
1	C	97	HIS
1	C	124	GLN
1	C	141	HIS
1	C	165	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	GPP	B	500	-	16,18,18	1.02	0	21,25,25	1.29	1 (4%)
2	GPP	C	500	-	16,18,18	0.76	0	21,25,25	1.19	2 (9%)
2	GPP	A	500	-	16,18,18	0.71	0	21,25,25	1.24	4 (19%)

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	GPP	B	500	-	-	8/19/19/19	-
2	GPP	C	500	-	-	5/19/19/19	-
2	GPP	A	500	-	-	3/19/19/19	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	GPP	C4-C3-C5	3.68	121.46	115.27
2	C	500	GPP	C4-C3-C5	3.41	121.00	115.27
2	A	500	GPP	C10-C8-C9	2.62	120.40	114.60
2	A	500	GPP	C4-C3-C5	2.58	119.61	115.27
2	A	500	GPP	C10-C8-C7	-2.32	115.93	122.65
2	C	500	GPP	C5-C3-C2	-2.18	116.70	121.12
2	A	500	GPP	O3B-PB-O3A	2.16	111.89	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	GPP	C2-C3-C5-C6
2	B	500	GPP	C4-C3-C5-C6
2	C	500	GPP	C4-C3-C5-C6
2	C	500	GPP	C3-C5-C6-C7
2	C	500	GPP	C2-C3-C5-C6
2	B	500	GPP	O1-C1-C2-C3
2	B	500	GPP	C3-C5-C6-C7
2	A	500	GPP	PB-O3A-PA-O1A
2	A	500	GPP	PB-O3A-PA-O1
2	B	500	GPP	PA-O3A-PB-O2B
2	B	500	GPP	PA-O3A-PB-O3B
2	B	500	GPP	C1-O1-PA-O3A
2	B	500	GPP	C1-O1-PA-O2A
2	A	500	GPP	C3-C5-C6-C7
2	C	500	GPP	O1-C1-C2-C3
2	C	500	GPP	C1-O1-PA-O1A

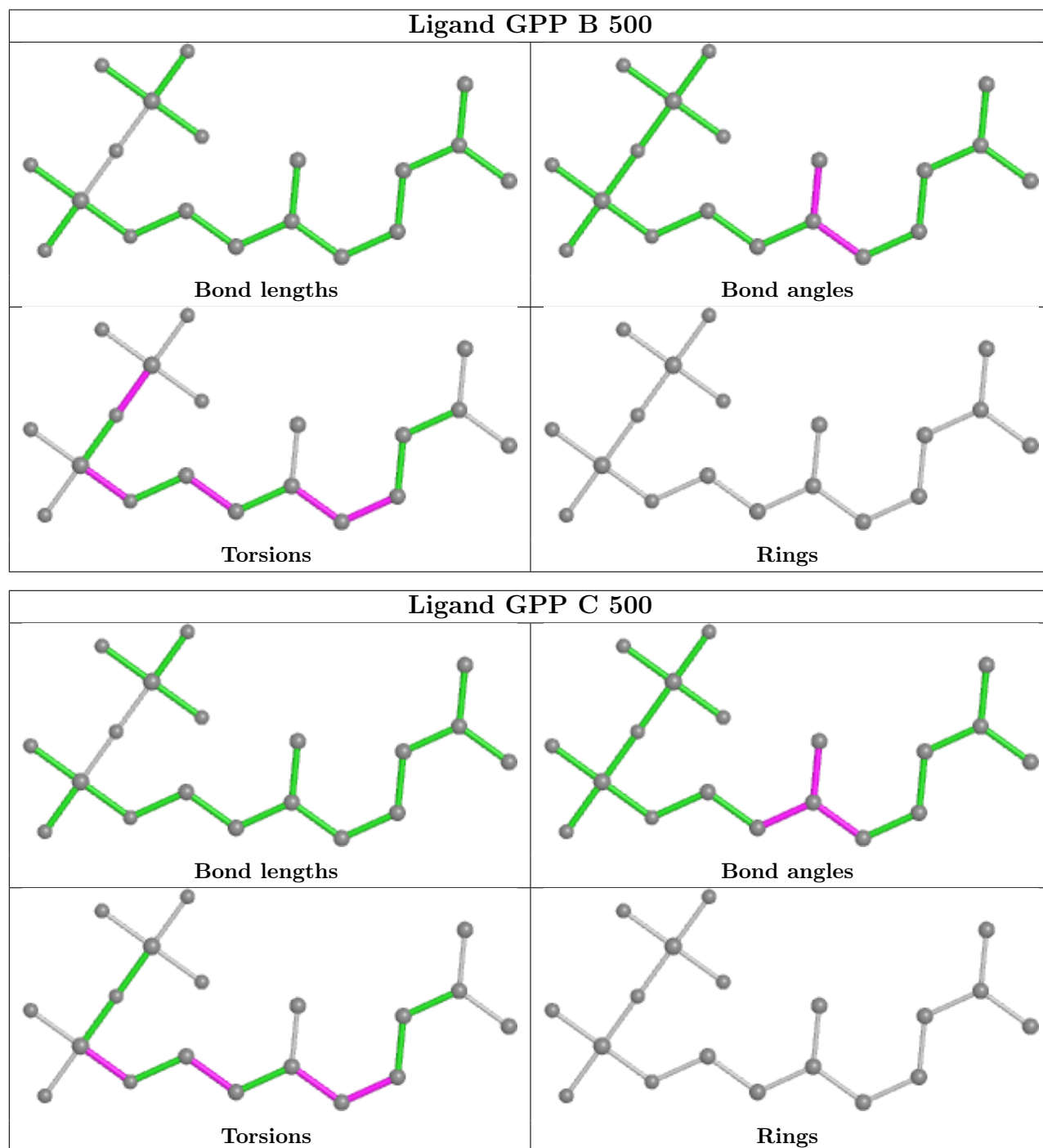
There are no ring outliers.

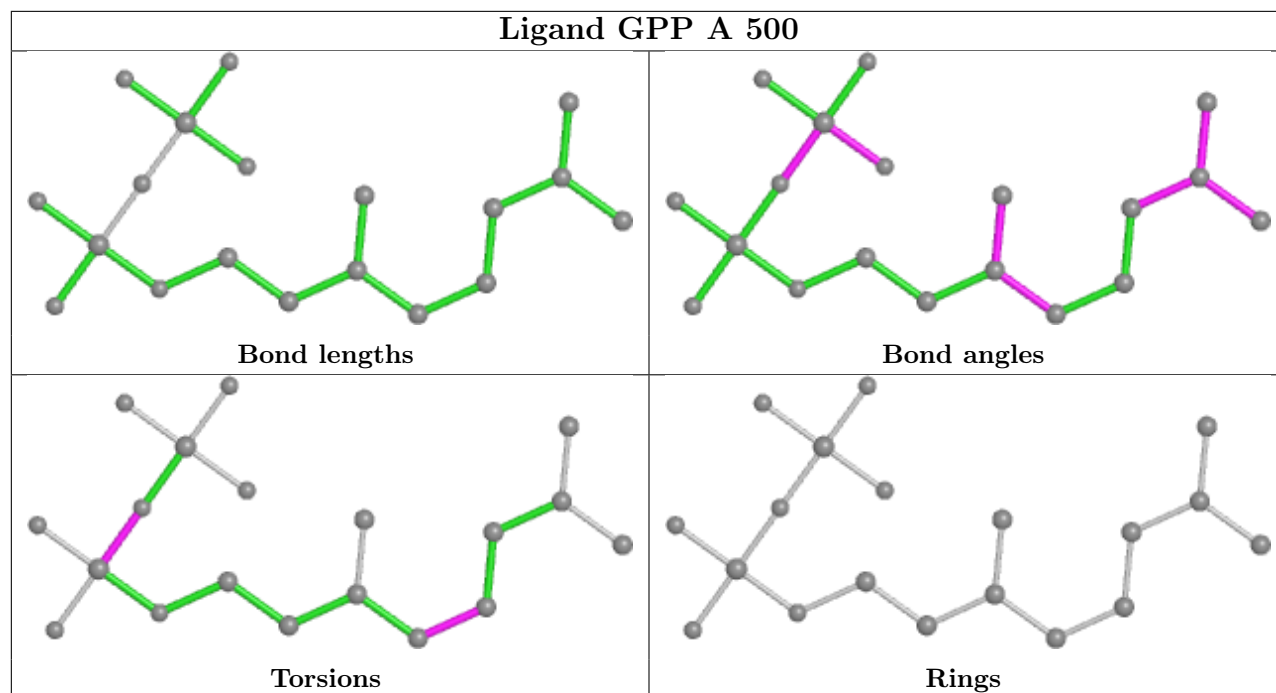
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	GPP	2	0
2	C	500	GPP	7	0
2	A	500	GPP	1	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.





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	261/294 (88%)	0.35	15 (5%) 23 14	60, 88, 136, 168	0
1	B	261/294 (88%)	0.46	17 (6%) 18 11	68, 96, 133, 167	0
1	C	261/294 (88%)	0.89	41 (15%) 2 1	70, 117, 155, 172	0
All	All	783/882 (88%)	0.57	73 (9%) 8 5	60, 100, 153, 172	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	SER	6.5
1	B	195	GLU	6.0
1	C	191	ASP	5.8
1	A	192	ARG	5.5
1	B	193	ASN	5.2
1	C	208	ALA	5.0
1	C	256	ARG	4.9
1	A	195	GLU	4.8
1	C	253	LEU	4.5
1	A	194	GLY	4.5
1	C	252	ARG	4.5
1	B	196	ARG	4.4
1	C	193	ASN	4.4
1	B	194	GLY	4.4
1	C	192	ARG	4.1
1	A	191	ASP	4.1
1	C	207	GLY	4.0
1	C	232	PRO	4.0
1	C	-2	PHE	4.0
1	B	192	ARG	3.9
1	A	129	ARG	3.8
1	B	127	THR	3.8
1	C	257	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	202	HIS	3.6
1	B	257	HIS	3.6
1	B	76	ASP	3.6
1	C	197	ASP	3.6
1	B	197	ASP	3.5
1	B	129	ARG	3.5
1	B	141	HIS	3.5
1	B	77	THR	3.4
1	C	163	GLU	3.3
1	C	131	ARG	3.2
1	C	168	ASP	3.2
1	C	129	ARG	3.2
1	C	255	PRO	3.2
1	C	103	ALA	3.1
1	C	209	VAL	3.0
1	C	244	LEU	3.0
1	C	119	HIS	2.9
1	C	190	TYR	2.9
1	C	195	GLU	2.9
1	C	164	GLY	2.9
1	A	196	ARG	2.8
1	A	163	GLU	2.8
1	C	194	GLY	2.8
1	C	49	PRO	2.8
1	A	193	ASN	2.8
1	C	196	ARG	2.7
1	B	106	PRO	2.6
1	C	254	LEU	2.5
1	B	33	ARG	2.4
1	B	256	ARG	2.4
1	C	248	ASP	2.4
1	C	136	ARG	2.3
1	C	189	ASP	2.2
1	C	231	ALA	2.2
1	C	251	VAL	2.2
1	A	76	ASP	2.2
1	C	43	THR	2.2
1	C	104	ARG	2.2
1	C	203	LEU	2.1
1	A	190	TYR	2.1
1	A	207	GLY	2.1
1	C	124	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	ALA	2.1
1	A	141	HIS	2.1
1	B	50	ASP	2.1
1	C	76	ASP	2.1
1	C	200	LEU	2.0
1	A	210	ALA	2.0
1	C	245	TYR	2.0
1	A	209	VAL	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](#)

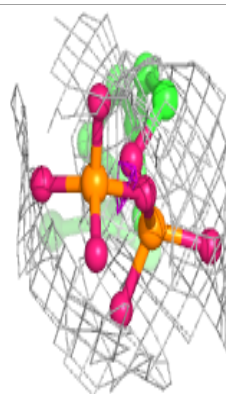
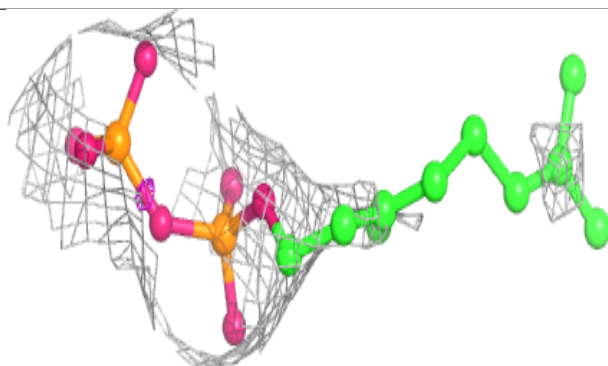
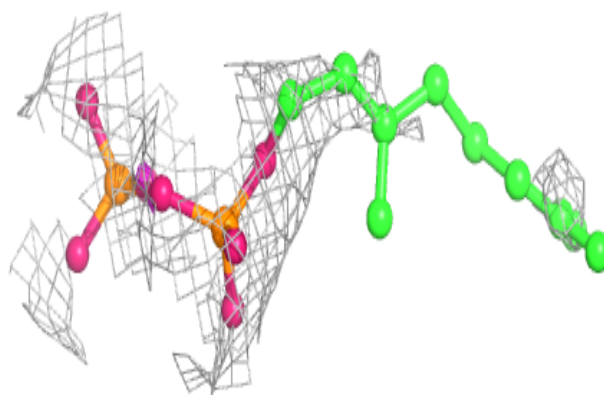
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GPP	B	500	19/19	0.84	0.29	143,153,166,167	0
2	GPP	C	500	19/19	0.84	0.29	146,150,160,160	0
2	GPP	A	500	19/19	0.85	0.31	133,147,162,162	0

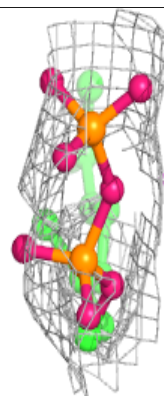
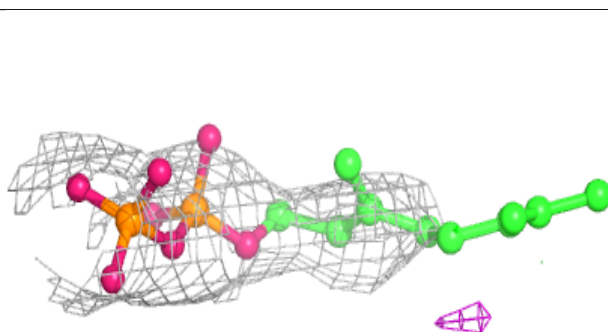
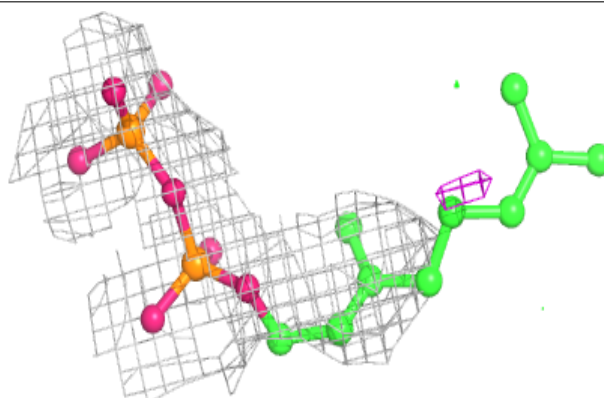
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

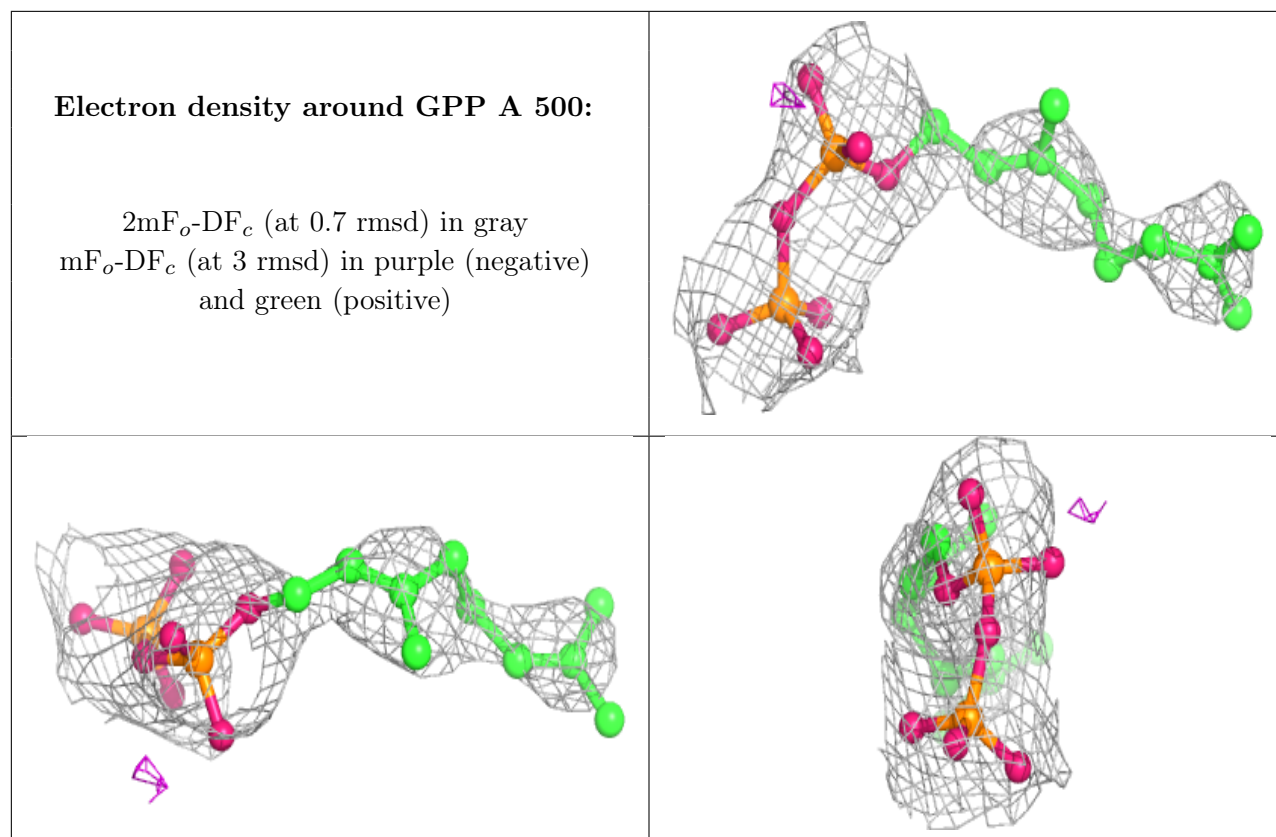
Electron density around GPP B 500:

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

**Electron density around GPP C 500:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.