



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 04:43 PM JST

PDB ID : 8Z8Y
Title : Crystal structure of CrtAgo/CrtTIR-APAZ complex
Authors : Hu, R.; Chen, J.; Liu, L.
Deposited on : 2024-04-22
Resolution : 3.18 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

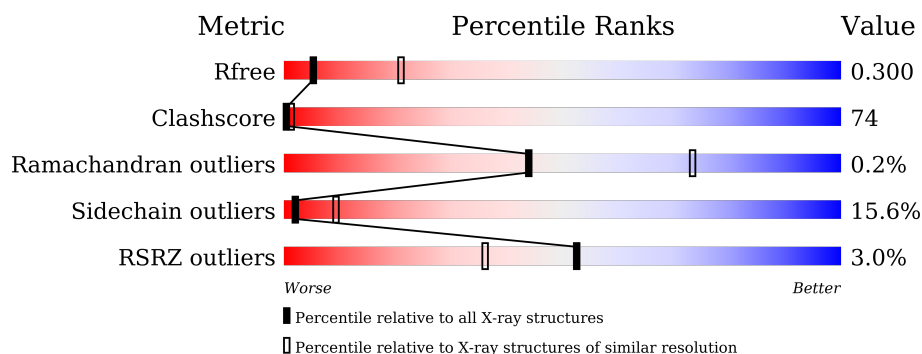
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	507	<div> <div> <div>5%</div> <div>38%</div> <div>50%</div> <div>10%</div> <div>.</div> </div> </div>
2	B	450	<div> <div>5%</div> <div>32%</div> <div>51%</div> <div>16%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7770 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 Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4109	2663	681	753	12			

- Molecule 2 is a protein called TIR domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	446	Total	C	N	O	S	0	0	0
			3652	2350	612	679	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		

V422	T423	E425	E426	E427	S428	V429	D432	I433	N434	N435	F436	E437	E438	D439	T440	E441	D442	L443	D444	E445	L446	GLU	ASP	ILE	GLU																																		
G347	I348	N349	L350	I351	I356	Q357	S360	S361	Q364	G365	K366	N367	W368	W369	N370	D371	K372	W373	R374	F380	I381	L384	S385	D386	D387	Q388	N389	A390	I391	Y392	G396	S397	E398	E399	K400	I401	L402	L403	S404	N405	L408	G412	K413	M414	S415	Y416	V417	T418	P419	S420	E421								
L275	R276	N277	K280		I283	E284	Y285	Q286	W287	S288	K289	T290	F291	A292	Y293	W294	I295	E296		L300	E301	K302	D303	K304	F305		L310	V311	G312	K313	Q314		W319	H320	F321	G322	I323	S324	A325	A326	G327	K328	L329	Y330	F331	V334	L335	W336	S339	H340	I341	I342	F343	T344	W345	D346			
R200	T201	T202	L203	A204	F205	T206	A207	L208	R209	K211	E212	Y213	L214		F217	A218	W219	E220	Y221	D222			L227	P228	K229	Q156	T230	E231	T232		R240	L241		G249	R250	L251	P252	T253	D254	T255	L256	R257	N258	Y259	E260	C261	Q262	R263	L264	T265	V266	Q267	L268	I269	P269	F270	K271	E274	
N69	K70	R71	E72	G73	V74	L75	K76	E77	L78	A79	V80	A81	T82	K83	W84	K85	K86	H87	L88	Q89	D90	D91	N92	F93	I94	P95	P96	L97	A98	I99	D100	E101	N102		Y105	D106	D107	I108	N109	I110	E111	I112	V113	R114	L115	N116	A117	I118	D119	F120	K121		W124	A125	K126	G127	L128	Q129	D130

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	198.36Å 198.36Å 184.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.61 – 3.18 40.61 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.61-3.18) 99.8 (40.61-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.274 , 0.299 0.275 , 0.300	Depositor DCC
R_{free} test set	1881 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	117.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	9/4213 (0.2%)	0.83	14/5702 (0.2%)
2	B	0.56	3/3738 (0.1%)	0.73	10/5049 (0.2%)
All	All	0.67	12/7951 (0.2%)	0.79	24/10751 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	CYS	CB-SG	-7.27	1.69	1.82
2	B	12	PRO	N-CD	5.60	1.55	1.47
1	A	99	GLU	CB-CG	5.53	1.62	1.52
2	B	419	PRO	N-CD	5.42	1.55	1.47
1	A	499	PRO	N-CD	5.35	1.55	1.47
2	B	177	PRO	N-CD	5.33	1.55	1.47
1	A	276	PRO	N-CD	5.27	1.55	1.47
1	A	220	PRO	N-CD	5.17	1.55	1.47
1	A	354	PRO	N-CD	5.15	1.55	1.47
1	A	332	PRO	N-CD	5.13	1.55	1.47
1	A	99	GLU	CG-CD	5.11	1.59	1.51
1	A	500	PRO	N-CD	5.09	1.54	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LEU	CA-CB-CG	-6.54	100.27	115.30
2	B	408	LEU	CA-CB-CG	6.43	130.08	115.30
1	A	392	LYS	C-N-CD	6.25	141.52	128.40
1	A	240	ALA	C-N-CD	6.10	141.20	128.40
1	A	267	LYS	C-N-CD	6.06	141.12	128.40
2	B	153	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	22	ASP	C-N-CD	5.99	140.97	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	PHE	C-N-CD	5.94	140.87	128.40
1	A	62	LYS	C-N-CD	5.92	140.83	128.40
1	A	152	ARG	C-N-CD	5.81	140.60	128.40
1	A	331	LYS	C-N-CD	5.78	140.54	128.40
1	A	499	PRO	C-N-CD	5.77	140.52	128.40
2	B	194	LEU	C-N-CD	5.76	140.49	128.40
1	A	353	TYR	C-N-CD	5.74	140.46	128.40
2	B	176	PHE	C-N-CD	5.70	140.37	128.40
1	A	498	THR	C-N-CD	5.63	140.22	128.40
1	A	275	ARG	C-N-CD	5.57	140.09	128.40
1	A	433	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	A	219	ILE	C-N-CD	5.47	139.88	128.40
2	B	418	THR	C-N-CD	5.40	139.74	128.40
2	B	442	ASP	CB-CG-OD2	5.24	123.01	118.30
2	B	444	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	439	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	432	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4109	0	4126	506	1
2	B	3652	0	3565	701	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
All	All	7770	0	7691	1147	1

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 74.

All (1147) 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:178:ILE:HG21	2:B:181:PHE:CE2	1.26	1.61
2:B:178:ILE:CG2	2:B:181:PHE:HE2	1.15	1.56
2:B:203:LEU:CD1	2:B:207:ALA:HB3	1.39	1.50
2:B:58:CYS:SG	2:B:140:VAL:HG13	1.55	1.44
2:B:208:ILE:CD1	2:B:268:LEU:CD2	1.98	1.42
2:B:80:VAL:C	2:B:84:VAL:HG23	1.04	1.41
2:B:80:VAL:O	2:B:84:VAL:CG2	1.70	1.40
1:A:14:PHE:CE1	1:A:26:GLY:HA3	1.56	1.39
2:B:81:ALA:HA	2:B:84:VAL:CB	1.54	1.36
2:B:82:THR:CG2	2:B:111:GLU:OE2	1.72	1.36
2:B:385:SER:HB3	2:B:405:ASN:ND2	1.43	1.33
1:A:308:GLY:HA3	1:A:465:LEU:CD2	1.55	1.32
2:B:80:VAL:C	2:B:84:VAL:CG2	1.93	1.32
2:B:28:LEU:O	2:B:145:PRO:CA	1.77	1.32
1:A:271:LEU:HD11	1:A:306:ASP:O	1.16	1.31
2:B:166:GLU:HA	2:B:414:MET:SD	1.68	1.31
2:B:82:THR:HG21	2:B:111:GLU:CD	1.49	1.31
1:A:302:GLN:NE2	1:A:479:THR:O	1.65	1.30
2:B:58:CYS:SG	2:B:140:VAL:CG1	2.19	1.30
2:B:81:ALA:CA	2:B:84:VAL:HB	1.62	1.29
1:A:145:GLU:OE1	1:A:225:ARG:NH2	1.63	1.28
1:A:207:HIS:NE2	2:B:442:ASP:OD1	1.66	1.27
2:B:367:ASN:HA	2:B:427:GLU:OE2	1.19	1.26
2:B:14:ASP:O	2:B:18:THR:OG1	1.53	1.26
2:B:101:GLU:OE1	2:B:121:LYS:HG2	1.35	1.25
2:B:367:ASN:CA	2:B:427:GLU:OE2	1.86	1.24
1:A:18:GLN:HG3	1:A:30:PHE:CD1	1.72	1.23
1:A:50:LEU:HD23	1:A:93:PHE:CE1	1.72	1.23
2:B:82:THR:HG21	2:B:111:GLU:OE2	1.04	1.22
1:A:346:TYR:CE2	1:A:354:PRO:HB3	1.75	1.21
1:A:159:ASN:O	1:A:162:VAL:HG23	1.38	1.21
2:B:27:GLY:O	2:B:146:ASP:N	1.74	1.20
2:B:208:ILE:CD1	2:B:268:LEU:HD23	1.63	1.19
2:B:28:LEU:O	2:B:145:PRO:HA	1.02	1.18
1:A:215:LEU:HD21	1:A:506:TYR:HE2	1.05	1.17
2:B:28:LEU:C	2:B:145:PRO:HA	1.63	1.17
1:A:14:PHE:CE1	1:A:26:GLY:CA	2.28	1.17
2:B:199:ASP:O	2:B:202:THR:OG1	1.59	1.16
2:B:85:LYS:HD2	2:B:94:ILE:HD12	1.27	1.16
2:B:85:LYS:HA	2:B:88:LEU:HD21	1.28	1.16
2:B:276:ARG:HH21	2:B:280:LYS:NZ	1.42	1.15
2:B:208:ILE:CD1	2:B:268:LEU:HD21	1.65	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	1:A:306:ASP:C	1.68	1.14
2:B:283:ARG:CD	2:B:296:GLU:OE1	1.94	1.14
1:A:148:TYR:CE2	2:B:440:THR:OG1	2.01	1.14
1:A:271:LEU:CD1	1:A:306:ASP:O	1.94	1.14
1:A:394:LEU:HD12	1:A:395:LYS:N	1.65	1.12
2:B:8:SER:HB2	2:B:74:VAL:HG12	1.23	1.12
1:A:50:LEU:CD2	1:A:93:PHE:CD1	2.32	1.11
2:B:385:SER:CB	2:B:405:ASN:HD21	1.62	1.11
2:B:210:TYR:OH	2:B:256:ILE:CD1	1.99	1.11
2:B:80:VAL:O	2:B:84:VAL:N	1.84	1.10
1:A:4:LEU:HD21	1:A:411:TYR:HB2	1.26	1.10
2:B:81:ALA:HA	2:B:84:VAL:CG2	1.82	1.10
1:A:305:LEU:HD11	1:A:349:GLN:NE2	1.67	1.09
2:B:80:VAL:O	2:B:84:VAL:HG23	0.91	1.09
1:A:215:LEU:HD21	1:A:506:TYR:CE2	1.85	1.08
1:A:308:GLY:HA3	1:A:465:LEU:HD22	1.26	1.08
1:A:308:GLY:HA3	1:A:465:LEU:HD21	1.28	1.08
2:B:283:ARG:HD2	2:B:296:GLU:OE1	1.51	1.08
2:B:101:GLU:OE2	2:B:121:LYS:HB3	1.54	1.08
1:A:18:GLN:OE1	2:B:151:ASN:ND2	1.88	1.07
2:B:179:ILE:HD11	2:B:404:SER:HB2	1.36	1.07
1:A:183:PHE:O	1:A:187:ASN:ND2	1.88	1.07
1:A:50:LEU:HD23	1:A:93:PHE:CD1	1.90	1.07
2:B:258:ASN:ND2	2:B:262:GLN:OE1	1.88	1.07
2:B:203:LEU:HD13	2:B:207:ALA:CB	1.84	1.06
2:B:178:ILE:CG2	2:B:181:PHE:CE2	2.03	1.06
2:B:265:ILE:HG22	2:B:269:ILE:HD11	1.10	1.06
1:A:275:ARG:HH12	1:A:454:GLN:HG3	1.17	1.06
1:A:390:LYS:H	1:A:390:LYS:HD3	1.21	1.06
2:B:81:ALA:C	2:B:84:VAL:HB	1.77	1.06
1:A:262:TYR:OH	1:A:309:ASP:OD1	1.74	1.05
1:A:304:PHE:HE1	1:A:478:VAL:CG2	1.67	1.05
2:B:193:ARG:NE	2:B:232:THR:OG1	1.89	1.05
2:B:208:ILE:HD12	2:B:268:LEU:HD21	1.11	1.05
2:B:203:LEU:CD1	2:B:207:ALA:CB	2.35	1.04
2:B:62:ILE:CG1	2:B:78:LEU:HD21	1.87	1.04
2:B:81:ALA:CA	2:B:84:VAL:CG2	2.34	1.04
2:B:163:GLN:OE1	2:B:164:ALA:N	1.89	1.04
2:B:208:ILE:HD12	2:B:268:LEU:CD2	1.73	1.04
1:A:304:PHE:CD1	1:A:478:VAL:HG13	1.91	1.04
1:A:307:ASN:OD1	1:A:309:ASP:N	1.89	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ILE:HD11	2:B:268:LEU:CD2	1.73	1.03
1:A:228:THR:OG1	2:B:441:GLU:OE1	1.75	1.03
1:A:18:GLN:OE1	2:B:151:ASN:CG	1.97	1.02
2:B:1:MET:HG2	2:B:2:ARG:NH1	1.73	1.02
2:B:81:ALA:HA	2:B:84:VAL:HB	1.13	1.02
2:B:436:PHE:HA	2:B:438:GLU:OE1	1.57	1.02
2:B:62:ILE:HD12	2:B:78:LEU:CD2	1.89	1.02
1:A:18:GLN:HG3	1:A:30:PHE:CE1	1.93	1.01
1:A:304:PHE:HE1	1:A:478:VAL:HG22	1.25	1.01
2:B:62:ILE:HG13	2:B:78:LEU:HD21	1.41	1.01
2:B:80:VAL:HG12	2:B:84:VAL:CG2	1.91	1.00
1:A:305:LEU:CD1	1:A:349:GLN:NE2	2.25	1.00
2:B:8:SER:HB2	2:B:74:VAL:CG1	1.92	1.00
2:B:81:ALA:N	2:B:84:VAL:CG2	2.24	1.00
1:A:184:GLU:OE2	1:A:185:GLU:N	1.94	0.99
2:B:62:ILE:CD1	2:B:78:LEU:CD2	2.39	0.99
1:A:50:LEU:CD2	1:A:93:PHE:CE1	2.45	0.99
2:B:81:ALA:O	2:B:85:LYS:N	1.95	0.99
2:B:210:TYR:OH	2:B:256:ILE:HD12	1.58	0.99
1:A:133:GLU:OE2	1:A:134:GLU:N	1.93	0.99
2:B:203:LEU:HD13	2:B:207:ALA:HB3	1.01	0.98
1:A:271:LEU:H	1:A:271:LEU:HD12	1.28	0.98
2:B:210:TYR:OH	2:B:211:LYS:NZ	1.96	0.98
2:B:387:ASP:OD1	2:B:390:ALA:N	1.96	0.98
2:B:6:PHE:HE2	2:B:33:TRP:HZ3	1.11	0.98
1:A:36:ILE:O	1:A:84:CYS:SG	2.22	0.97
2:B:4:LYS:O	2:B:58:CYS:N	1.97	0.97
2:B:388:GLN:OE1	2:B:388:GLN:N	1.96	0.97
2:B:253:THR:OG1	2:B:256:ILE:N	1.98	0.97
2:B:81:ALA:O	2:B:84:VAL:HB	1.65	0.97
1:A:304:PHE:CE1	1:A:478:VAL:HG13	1.99	0.96
1:A:145:GLU:CD	1:A:225:ARG:HH21	1.67	0.96
1:A:263:LYS:NZ	1:A:507:ILE:O	1.98	0.96
2:B:346:ASP:OD1	2:B:348:ILE:N	1.98	0.96
2:B:88:LEU:HD12	2:B:90:ASP:H	1.30	0.95
2:B:203:LEU:HD12	2:B:207:ALA:HB3	1.44	0.95
1:A:4:LEU:HD21	1:A:411:TYR:CB	1.95	0.95
1:A:304:PHE:CD1	1:A:478:VAL:CG1	2.49	0.95
2:B:137:LYS:HB3	2:B:138:GLN:NE2	1.81	0.95
1:A:215:LEU:CD2	1:A:506:TYR:HE2	1.79	0.95
1:A:347:LYS:NZ	1:A:353:TYR:OH	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:LYS:HZ1	2:B:275:LEU:HD21	1.31	0.95
1:A:152:ARG:O	1:A:155:SER:OG	1.85	0.94
1:A:494:THR:OG1	1:A:495:GLU:OE1	1.85	0.94
2:B:208:ILE:HD11	2:B:268:LEU:HD23	0.96	0.94
1:A:82:PHE:CD1	1:A:261:TYR:CD2	2.54	0.94
1:A:474:ASP:OD2	1:A:481:ARG:HD3	1.66	0.94
1:A:14:PHE:CE1	1:A:26:GLY:C	2.42	0.94
1:A:123:ASP:O	1:A:127:THR:OG1	1.85	0.94
2:B:61:LEU:HD23	2:B:95:ILE:HG13	1.50	0.94
2:B:210:TYR:CE2	2:B:211:LYS:HD2	2.03	0.94
1:A:307:ASN:O	1:A:465:LEU:HD21	1.67	0.93
2:B:81:ALA:N	2:B:84:VAL:HG23	1.81	0.93
1:A:4:LEU:CD2	1:A:411:TYR:HA	1.97	0.93
1:A:304:PHE:CE1	1:A:478:VAL:HG22	2.04	0.93
2:B:100:ASP:OD1	2:B:102:ASN:N	2.01	0.93
1:A:72:ARG:NH1	2:B:426:GLU:OE2	2.01	0.93
2:B:105:TYR:HE1	2:B:113:VAL:CG1	1.82	0.93
2:B:265:ILE:CG2	2:B:269:ILE:HD11	1.97	0.92
1:A:4:LEU:CD2	1:A:411:TYR:CA	2.46	0.92
2:B:300:LEU:HD11	2:B:305:PHE:HB2	1.51	0.92
1:A:304:PHE:CE1	1:A:478:VAL:CG1	2.52	0.92
1:A:24:ARG:HG2	1:A:470:CYS:SG	2.10	0.92
1:A:275:ARG:HH12	1:A:454:GLN:CG	1.83	0.92
2:B:385:SER:CB	2:B:405:ASN:ND2	2.26	0.91
1:A:312:VAL:HG11	1:A:506:TYR:CE1	2.05	0.91
2:B:385:SER:HB2	2:B:387:ASP:O	1.69	0.91
2:B:62:ILE:CD1	2:B:78:LEU:HD21	2.00	0.91
2:B:50:GLU:HA	2:B:53:ILE:HD11	1.52	0.91
2:B:81:ALA:CA	2:B:84:VAL:CB	2.28	0.91
2:B:271:LYS:NZ	2:B:275:LEU:HD21	1.85	0.91
1:A:211:LYS:NZ	1:A:507:ILE:O	2.03	0.90
2:B:193:ARG:HE	2:B:232:THR:HG1	1.18	0.90
1:A:4:LEU:HD22	1:A:410:ALA:C	1.90	0.90
2:B:11:THR:CG2	2:B:12:PRO:HA	2.01	0.90
2:B:300:LEU:HD13	2:B:304:LYS:O	1.70	0.90
2:B:188:HIS:HB3	2:B:190:TYR:CD1	2.07	0.90
2:B:30:TYR:HE1	2:B:135:PHE:HD2	1.20	0.89
1:A:275:ARG:NH1	1:A:454:GLN:HG3	1.87	0.89
2:B:62:ILE:CD1	2:B:78:LEU:HD23	2.03	0.88
1:A:14:PHE:HE1	1:A:26:GLY:HA3	1.35	0.88
2:B:385:SER:HA	2:B:391:ILE:HG12	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:TRP:HB3	2:B:373:TRP:NE1	1.89	0.88
1:A:436:GLU:OE1	2:B:361:ARG:NH2	2.05	0.88
2:B:178:ILE:HG22	2:B:181:PHE:HE2	1.36	0.88
1:A:500:PRO:O	1:A:501:LEU:HD23	1.74	0.88
2:B:108:ILE:HG23	2:B:112:ILE:HG21	1.56	0.87
2:B:58:CYS:O	2:B:59:LYS:HG2	1.73	0.87
2:B:80:VAL:HG12	2:B:84:VAL:HG22	1.54	0.87
1:A:397:TYR:HB3	2:B:374:ARG:HG3	1.56	0.87
1:A:304:PHE:CE1	1:A:478:VAL:CG2	2.56	0.87
1:A:481:ARG:HG3	1:A:481:ARG:HH11	1.39	0.87
1:A:275:ARG:NH1	1:A:454:GLN:CG	2.36	0.87
1:A:347:LYS:HE3	1:A:353:TYR:CE2	2.10	0.87
2:B:249:GLY:HA2	2:B:258:ASN:OD1	1.73	0.87
2:B:445:GLU:OE2	2:B:446:LEU:N	2.08	0.87
1:A:9:GLU:OE1	1:A:464:LYS:NZ	2.07	0.86
2:B:346:ASP:OD1	2:B:349:ASN:N	2.08	0.86
2:B:119:ASP:OD2	2:B:121:LYS:NZ	2.07	0.86
1:A:18:GLN:HE22	2:B:148:SER:HA	1.40	0.86
2:B:82:THR:HG21	2:B:111:GLU:OE1	1.76	0.86
1:A:482:PHE:O	1:A:486:ILE:HG13	1.76	0.86
2:B:6:PHE:CE2	2:B:33:TRP:HZ3	1.94	0.86
2:B:423:THR:O	2:B:427:GLU:N	2.08	0.86
1:A:148:TYR:HE2	2:B:440:THR:OG1	1.49	0.86
2:B:300:LEU:CD1	2:B:304:LYS:O	2.24	0.86
2:B:425:GLU:O	2:B:429:VAL:HG23	1.76	0.86
2:B:30:TYR:CE1	2:B:135:PHE:HD2	1.94	0.86
2:B:25:LEU:HA	2:B:28:LEU:CD1	2.05	0.85
2:B:105:TYR:CE1	2:B:113:VAL:CG1	2.58	0.85
2:B:371:ASP:OD1	2:B:372:LYS:N	2.09	0.85
2:B:28:LEU:HA	2:B:145:PRO:HB3	1.59	0.85
2:B:346:ASP:OD2	2:B:349:ASN:ND2	2.09	0.85
1:A:211:LYS:HZ3	1:A:507:ILE:C	1.79	0.85
2:B:22:SER:O	2:B:25:LEU:HD12	1.76	0.85
2:B:50:GLU:HA	2:B:53:ILE:CD1	2.07	0.85
1:A:212:ALA:O	1:A:215:LEU:HD12	1.76	0.85
1:A:391:SER:CB	1:A:393:PRO:HD3	2.07	0.85
2:B:200:VAL:O	2:B:203:LEU:HG	1.77	0.85
2:B:58:CYS:O	2:B:59:LYS:CG	2.25	0.84
1:A:14:PHE:HE1	1:A:26:GLY:CA	1.82	0.84
1:A:50:LEU:HD12	1:A:50:LEU:O	1.77	0.84
1:A:63:PRO:HG2	2:B:124:TRP:NE1	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:VAL:HG11	1:A:506:TYR:HE1	1.40	0.84
1:A:227:SER:HB2	1:A:243:ARG:NH1	1.93	0.84
1:A:353:TYR:HD1	1:A:378:PRO:HG2	1.40	0.84
2:B:88:LEU:HG	2:B:89:GLN:N	1.91	0.84
2:B:85:LYS:CD	2:B:94:ILE:HD12	2.08	0.84
1:A:499:PRO:HG2	1:A:501:LEU:HD21	1.58	0.84
2:B:22:SER:HA	2:B:25:LEU:CD1	2.08	0.84
2:B:276:ARG:NH2	2:B:280:LYS:NZ	2.24	0.84
1:A:18:GLN:HE22	2:B:148:SER:CA	1.91	0.83
2:B:208:ILE:CG1	2:B:268:LEU:CD2	2.56	0.83
1:A:320:TRP:CE3	1:A:330:LEU:HD13	2.13	0.83
1:A:227:SER:HB2	1:A:243:ARG:HH11	1.43	0.83
2:B:50:GLU:O	2:B:53:ILE:HD12	1.79	0.83
2:B:80:VAL:O	2:B:84:VAL:CB	2.27	0.83
1:A:148:TYR:CD2	2:B:440:THR:OG1	2.31	0.83
1:A:308:GLY:CA	1:A:465:LEU:HD21	2.09	0.83
2:B:101:GLU:OE1	2:B:121:LYS:CG	2.24	0.83
2:B:108:ILE:CG2	2:B:112:ILE:CG2	2.58	0.82
2:B:22:SER:O	2:B:26:ILE:HG13	1.79	0.82
2:B:27:GLY:O	2:B:146:ASP:C	2.18	0.82
2:B:120:PHE:CD1	2:B:127:GLY:HA3	2.14	0.82
1:A:346:TYR:HE2	1:A:354:PRO:HB3	1.45	0.82
2:B:276:ARG:HH21	2:B:280:LYS:HZ2	1.26	0.82
2:B:381:ILE:CG2	2:B:405:ASN:OD1	2.28	0.81
1:A:4:LEU:HD23	1:A:411:TYR:HA	1.62	0.81
2:B:105:TYR:HE1	2:B:113:VAL:HG11	1.45	0.81
1:A:4:LEU:CD2	1:A:411:TYR:HB2	2.10	0.81
1:A:4:LEU:HD22	1:A:411:TYR:N	1.96	0.81
2:B:219:TRP:HZ3	2:B:240:ARG:NH2	1.79	0.81
2:B:120:PHE:CE1	2:B:127:GLY:HA3	2.15	0.81
2:B:436:PHE:CA	2:B:438:GLU:OE1	2.28	0.81
1:A:63:PRO:HG2	2:B:124:TRP:CE2	2.15	0.81
2:B:367:ASN:C	2:B:427:GLU:OE2	2.18	0.81
2:B:252:ASP:OD2	2:B:257:ARG:HD3	1.81	0.81
1:A:271:LEU:HD13	1:A:306:ASP:HB2	1.63	0.80
1:A:9:GLU:OE2	1:A:472:TYR:OH	1.98	0.80
1:A:479:THR:C	1:A:480:LEU:HD23	2.01	0.80
2:B:252:ASP:OD2	2:B:257:ARG:HG3	1.80	0.80
1:A:16:HIS:ND1	2:B:147:HIS:ND1	2.28	0.80
1:A:275:ARG:HH11	1:A:454:GLN:HE21	1.28	0.80
2:B:6:PHE:HE2	2:B:33:TRP:CZ3	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:ILE:HG22	2:B:405:ASN:OD1	1.81	0.80
1:A:14:PHE:CD1	1:A:26:GLY:C	2.54	0.80
1:A:82:PHE:HD1	1:A:261:TYR:CD2	2.00	0.80
2:B:27:GLY:HA2	2:B:146:ASP:O	1.79	0.80
2:B:81:ALA:HA	2:B:84:VAL:HG21	1.62	0.80
2:B:210:TYR:HH	2:B:256:ILE:HD12	1.44	0.80
1:A:253:ALA:O	1:A:257:SER:OG	2.00	0.80
2:B:85:LYS:CA	2:B:88:LEU:HD21	2.10	0.80
1:A:207:HIS:NE2	2:B:442:ASP:CG	2.36	0.79
2:B:33:TRP:HH2	2:B:49:ILE:HG22	1.47	0.79
2:B:300:LEU:CD1	2:B:305:PHE:HB2	2.12	0.79
1:A:159:ASN:O	1:A:162:VAL:CG2	2.28	0.79
1:A:482:PHE:HD2	1:A:503:PHE:HZ	1.30	0.79
2:B:53:ILE:O	2:B:57:THR:OG1	1.99	0.79
2:B:211:LYS:HG2	2:B:212:GLU:N	1.97	0.79
1:A:212:ALA:HA	1:A:215:LEU:CD1	2.12	0.79
1:A:110:THR:OG1	1:A:113:ARG:NH2	2.15	0.79
2:B:88:LEU:HG	2:B:89:GLN:H	1.48	0.79
2:B:105:TYR:OH	2:B:113:VAL:HB	1.81	0.79
1:A:207:HIS:CD2	2:B:442:ASP:OD1	2.35	0.79
2:B:25:LEU:O	2:B:28:LEU:HD12	1.83	0.79
2:B:165:ILE:O	2:B:414:MET:SD	2.40	0.79
2:B:438:GLU:HB2	2:B:441:GLU:HB3	1.65	0.79
1:A:18:GLN:HG3	1:A:30:PHE:CG	2.17	0.78
2:B:271:LYS:NZ	2:B:275:LEU:CD2	2.46	0.78
2:B:1:MET:HG2	2:B:2:ARG:HH11	1.48	0.78
2:B:208:ILE:CG1	2:B:268:LEU:HD21	2.12	0.78
2:B:3:ASN:O	2:B:142:LYS:NZ	2.15	0.78
1:A:35:GLN:NE2	1:A:82:PHE:O	2.15	0.78
1:A:370:TRP:CE2	1:A:447:LYS:HB3	2.18	0.78
2:B:108:ILE:CG2	2:B:112:ILE:HG21	2.14	0.78
1:A:437:VAL:CG2	2:B:370:ASN:HB2	2.14	0.78
1:A:305:LEU:HD11	1:A:349:GLN:HE22	1.45	0.78
1:A:394:LEU:HD12	1:A:395:LYS:H	1.45	0.78
1:A:474:ASP:OD2	1:A:481:ARG:CD	2.32	0.78
2:B:58:CYS:O	2:B:59:LYS:CD	2.32	0.78
1:A:436:GLU:CD	2:B:361:ARG:HH22	1.85	0.77
2:B:21:LEU:HD12	2:B:25:LEU:HD11	1.65	0.77
2:B:88:LEU:HD12	2:B:90:ASP:N	1.98	0.77
1:A:312:VAL:CG1	1:A:506:TYR:HE1	1.98	0.77
2:B:368:TRP:HB3	2:B:373:TRP:HE1	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:N	1:A:446:ASN:OD1	2.17	0.77
1:A:426:VAL:HG11	1:A:472:TYR:HE2	1.48	0.77
1:A:390:LYS:H	1:A:390:LYS:CD	1.96	0.77
1:A:304:PHE:HD1	1:A:478:VAL:CG1	1.93	0.77
2:B:188:HIS:HB3	2:B:190:TYR:CE1	2.20	0.77
1:A:18:GLN:HE22	2:B:148:SER:N	1.82	0.76
1:A:344:GLU:OE2	1:A:353:TYR:OH	2.03	0.76
2:B:6:PHE:CE2	2:B:33:TRP:CZ3	2.72	0.76
2:B:82:THR:HG23	2:B:111:GLU:OE2	1.79	0.76
2:B:253:THR:CG2	2:B:256:ILE:HG22	2.16	0.76
1:A:133:GLU:OE2	1:A:134:GLU:HG2	1.86	0.76
1:A:437:VAL:HG22	2:B:370:ASN:HB2	1.67	0.76
2:B:178:ILE:HG22	2:B:181:PHE:CE2	2.14	0.76
2:B:385:SER:HA	2:B:391:ILE:CG1	2.16	0.76
1:A:40:LYS:O	1:A:136:VAL:HG13	1.87	0.75
1:A:187:ASN:HD22	1:A:187:ASN:H	1.35	0.75
1:A:346:TYR:CD2	1:A:354:PRO:HD3	2.21	0.75
2:B:71:ARG:CA	2:B:71:ARG:HH11	2.00	0.75
1:A:212:ALA:HA	1:A:215:LEU:HD12	1.67	0.75
2:B:194:LEU:HD11	2:B:209:ARG:NH1	2.02	0.75
1:A:18:GLN:OE1	2:B:151:ASN:OD1	2.04	0.75
1:A:271:LEU:HD12	1:A:271:LEU:N	2.02	0.75
1:A:14:PHE:CZ	1:A:26:GLY:HA3	2.19	0.75
1:A:103:ARG:HG2	1:A:104:TYR:CD1	2.21	0.75
2:B:210:TYR:OH	2:B:256:ILE:HD13	1.87	0.75
2:B:415:SER:OG	2:B:416:TYR:N	2.20	0.74
2:B:17:PHE:HZ	2:B:120:PHE:HE2	1.35	0.74
2:B:384:LEU:O	2:B:391:ILE:HG12	1.87	0.74
1:A:271:LEU:HD11	1:A:306:ASP:CA	2.16	0.74
2:B:81:ALA:N	2:B:84:VAL:HG21	2.02	0.74
2:B:193:ARG:NH2	2:B:232:THR:O	2.20	0.74
2:B:81:ALA:CA	2:B:84:VAL:HG21	2.13	0.74
2:B:105:TYR:CE1	2:B:113:VAL:HG12	2.22	0.74
2:B:196:LYS:HA	2:B:209:ARG:NH1	2.03	0.74
1:A:4:LEU:HD22	1:A:410:ALA:O	1.87	0.74
2:B:11:THR:HG22	2:B:12:PRO:HA	1.70	0.74
2:B:101:GLU:OE1	2:B:101:GLU:N	2.21	0.74
2:B:175:TRP:NE1	2:B:336:MET:HG2	2.02	0.74
2:B:200:VAL:HG21	2:B:209:ARG:H	1.53	0.74
1:A:38:GLY:N	1:A:84:CYS:SG	2.61	0.74
2:B:88:LEU:CD1	2:B:90:ASP:H	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:LYS:HZ1	2:B:275:LEU:CD2	2.00	0.74
2:B:205:PHE:HE1	2:B:397:SER:N	1.85	0.73
1:A:312:VAL:CB	1:A:506:TYR:HE1	2.01	0.73
1:A:270:LYS:HG2	1:A:271:LEU:HD12	1.70	0.73
2:B:285:TYR:HD2	2:B:286:GLN:N	1.85	0.73
2:B:140:VAL:HG12	2:B:141:PRO:HD2	1.71	0.73
1:A:367:ASP:O	1:A:371:ASN:ND2	2.21	0.73
2:B:109:ASN:H	2:B:112:ILE:HD12	1.54	0.73
1:A:347:LYS:CE	1:A:353:TYR:CE2	2.70	0.73
1:A:103:ARG:HG2	1:A:104:TYR:CE1	2.22	0.73
1:A:476:GLU:OE1	1:A:481:ARG:HA	1.88	0.73
2:B:4:LYS:O	2:B:57:THR:HA	1.89	0.73
2:B:28:LEU:O	2:B:145:PRO:N	2.20	0.73
2:B:25:LEU:HA	2:B:28:LEU:HD12	1.70	0.73
1:A:397:TYR:CB	2:B:374:ARG:HG3	2.18	0.72
2:B:8:SER:CB	2:B:74:VAL:HG12	2.14	0.72
1:A:215:LEU:CD2	1:A:506:TYR:CE2	2.63	0.72
2:B:25:LEU:HA	2:B:28:LEU:HD11	1.70	0.72
1:A:4:LEU:CD2	1:A:411:TYR:CB	2.65	0.72
1:A:18:GLN:HB3	1:A:30:PHE:CE2	2.24	0.72
2:B:346:ASP:CG	2:B:348:ILE:H	1.93	0.72
1:A:391:SER:C	1:A:393:PRO:HD3	2.09	0.72
2:B:120:PHE:HE1	2:B:127:GLY:C	1.93	0.72
2:B:265:ILE:HG22	2:B:269:ILE:CD1	2.06	0.72
1:A:271:LEU:CD1	1:A:306:ASP:HB2	2.20	0.72
1:A:340:THR:HG23	1:A:376:VAL:HG11	1.72	0.72
1:A:261:TYR:O	1:A:264:ALA:HB3	1.89	0.72
2:B:193:ARG:CZ	2:B:232:THR:OG1	2.37	0.72
2:B:366:LYS:O	2:B:427:GLU:OE2	2.07	0.72
1:A:79:GLU:HG2	2:B:125:ALA:CB	2.20	0.72
2:B:80:VAL:O	2:B:84:VAL:CA	2.37	0.72
2:B:12:PRO:O	2:B:15:ASP:CG	2.28	0.72
2:B:193:ARG:NH2	2:B:232:THR:OG1	2.22	0.72
2:B:118:ILE:HD12	2:B:131:LEU:HD12	1.70	0.71
1:A:347:LYS:NZ	1:A:353:TYR:CZ	2.57	0.71
2:B:2:ARG:HB2	2:B:56:ASN:O	1.90	0.71
2:B:283:ARG:HD3	2:B:296:GLU:OE1	1.86	0.71
2:B:28:LEU:HA	2:B:145:PRO:CB	2.20	0.71
1:A:18:GLN:NE2	2:B:147:HIS:C	2.43	0.71
1:A:312:VAL:HG21	1:A:506:TYR:CE1	2.25	0.71
2:B:73:GLY:O	2:B:77:GLU:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:HB3	2:B:138:GLN:HE21	1.53	0.71
2:B:82:THR:O	2:B:85:LYS:HB2	1.91	0.71
2:B:344:THR:OG1	2:B:347:GLY:HA2	1.91	0.71
2:B:71:ARG:HH11	2:B:71:ARG:CB	2.03	0.71
1:A:50:LEU:HD22	1:A:93:PHE:CD1	2.25	0.71
2:B:211:LYS:HG2	2:B:212:GLU:H	1.55	0.71
2:B:283:ARG:NH1	2:B:348:ILE:O	2.24	0.71
2:B:381:ILE:HG22	2:B:405:ASN:CG	2.12	0.70
1:A:15:ALA:HB2	1:A:32:PRO:O	1.90	0.70
2:B:75:LEU:HD23	2:B:75:LEU:N	2.05	0.70
2:B:180:SER:C	2:B:181:PHE:HD2	1.94	0.70
2:B:79:ALA:HA	2:B:82:THR:OG1	1.91	0.70
2:B:9:HIS:CB	2:B:18:THR:HG21	2.21	0.70
2:B:11:THR:HG23	2:B:12:PRO:HA	1.73	0.70
1:A:305:LEU:CD1	1:A:349:GLN:HE21	2.01	0.70
2:B:178:ILE:HG21	2:B:181:PHE:CZ	2.14	0.70
2:B:388:GLN:HG2	2:B:389:ASN:ND2	2.06	0.70
1:A:312:VAL:HG21	1:A:506:TYR:CD1	2.27	0.70
2:B:192:TRP:HZ2	2:B:193:ARG:NH2	1.89	0.70
1:A:14:PHE:HE1	1:A:26:GLY:C	1.89	0.70
1:A:18:GLN:HE22	2:B:147:HIS:C	1.95	0.70
1:A:487:GLY:O	1:A:491:THR:HG23	1.92	0.70
1:A:126:ILE:HD13	1:A:217:HIS:CE1	2.27	0.69
1:A:16:HIS:CE1	2:B:147:HIS:CE1	2.80	0.69
2:B:193:ARG:CG	2:B:229:LYS:O	2.40	0.69
2:B:62:ILE:HG13	2:B:78:LEU:CD2	2.20	0.69
1:A:481:ARG:HH22	2:B:444:ASP:CG	1.95	0.69
2:B:208:ILE:HG13	2:B:268:LEU:CD2	2.21	0.69
2:B:260:GLU:CD	2:B:263:ARG:HH21	1.94	0.69
1:A:145:GLU:OE2	1:A:227:SER:OG	2.10	0.69
2:B:74:VAL:HA	2:B:77:GLU:OE1	1.93	0.69
2:B:252:ASP:OD2	2:B:257:ARG:CD	2.41	0.69
2:B:426:GLU:HA	2:B:426:GLU:OE1	1.91	0.69
1:A:82:PHE:HD1	1:A:261:TYR:CE2	2.09	0.69
2:B:109:ASN:O	2:B:112:ILE:HB	1.93	0.69
2:B:260:GLU:OE2	2:B:263:ARG:NH2	2.24	0.69
1:A:304:PHE:CD1	1:A:478:VAL:HG11	2.27	0.69
1:A:480:LEU:HD23	1:A:480:LEU:N	2.04	0.69
1:A:482:PHE:HD2	1:A:503:PHE:CZ	2.10	0.69
2:B:17:PHE:CZ	2:B:120:PHE:CE2	2.81	0.69
2:B:22:SER:HA	2:B:25:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:HG11	1:A:472:TYR:CE2	2.29	0.68
2:B:71:ARG:HH11	2:B:71:ARG:HA	1.58	0.68
1:A:133:GLU:OE2	1:A:133:GLU:N	2.25	0.68
2:B:178:ILE:HD13	2:B:181:PHE:CZ	2.29	0.68
1:A:306:ASP:OD1	1:A:307:ASN:N	2.26	0.68
2:B:193:ARG:HG2	2:B:229:LYS:O	1.94	0.68
1:A:270:LYS:HG2	1:A:271:LEU:N	2.08	0.68
2:B:33:TRP:CH2	2:B:49:ILE:HG22	2.28	0.68
2:B:166:GLU:CA	2:B:414:MET:SD	2.64	0.68
2:B:27:GLY:CA	2:B:147:HIS:HA	2.24	0.68
1:A:18:GLN:HB2	1:A:30:PHE:CD2	2.29	0.67
1:A:109:SER:OG	1:A:200:TYR:OH	2.09	0.67
1:A:481:ARG:HG2	1:A:482:PHE:CE1	2.29	0.67
1:A:463:THR:HB	1:A:474:ASP:O	1.95	0.67
1:A:13:LEU:C	1:A:14:PHE:HD2	1.97	0.67
1:A:390:LYS:HD3	1:A:390:LYS:N	2.02	0.67
2:B:27:GLY:O	2:B:146:ASP:CA	2.42	0.67
1:A:184:GLU:OE2	1:A:184:GLU:N	2.28	0.67
1:A:304:PHE:HE1	1:A:478:VAL:CG1	2.01	0.67
2:B:88:LEU:HD11	2:B:90:ASP:O	1.94	0.67
2:B:140:VAL:HG12	2:B:141:PRO:CD	2.25	0.67
2:B:12:PRO:O	2:B:15:ASP:OD1	2.12	0.67
2:B:151:ASN:HA	2:B:154:TYR:HB3	1.75	0.67
2:B:22:SER:C	2:B:25:LEU:HD12	2.15	0.66
1:A:358:PHE:HE1	1:A:455:VAL:HG22	1.58	0.66
2:B:253:THR:N	2:B:256:ILE:O	2.27	0.66
1:A:346:TYR:CE2	1:A:354:PRO:CB	2.68	0.66
1:A:303:MET:O	1:A:304:PHE:HD2	1.78	0.66
2:B:55:GLU:HB3	2:B:56:ASN:OD1	1.96	0.66
2:B:194:LEU:C	2:B:194:LEU:HD12	2.15	0.66
2:B:62:ILE:HD11	2:B:78:LEU:HD23	1.76	0.66
2:B:214:LEU:C	2:B:214:LEU:HD23	2.15	0.66
1:A:115:TYR:CE2	1:A:213:ARG:NH2	2.63	0.66
2:B:196:LYS:HA	2:B:209:ARG:HH12	1.59	0.66
1:A:15:ALA:O	1:A:16:HIS:HB2	1.96	0.65
1:A:308:GLY:CA	1:A:465:LEU:HD22	2.14	0.65
2:B:177:PRO:HA	2:B:334:VAL:HG12	1.79	0.65
2:B:252:ASP:OD2	2:B:257:ARG:CG	2.43	0.65
1:A:262:TYR:CZ	1:A:504:LYS:HB3	2.32	0.65
1:A:305:LEU:CD1	1:A:349:GLN:HE22	1.99	0.65
2:B:5:ILE:HG13	2:B:31:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:HG23	2:B:112:ILE:CG2	2.22	0.65
2:B:341:ILE:O	2:B:342:ILE:HD13	1.97	0.65
1:A:234:PHE:O	1:A:242:ILE:HG13	1.97	0.65
2:B:21:LEU:HD12	2:B:21:LEU:O	1.95	0.65
1:A:115:TYR:O	1:A:119:THR:OG1	2.14	0.65
2:B:369:TRP:CZ2	2:B:423:THR:HB	2.31	0.65
2:B:22:SER:CA	2:B:25:LEU:HD12	2.27	0.65
2:B:212:GLU:HB3	2:B:213:TYR:CE2	2.31	0.65
1:A:245:PHE:HD2	1:A:252:LEU:HD13	1.62	0.65
1:A:349:GLN:HB3	1:A:350:ASN:OD1	1.97	0.65
2:B:314:GLN:NE2	2:B:360:SER:OG	2.29	0.65
1:A:18:GLN:CB	1:A:30:PHE:CD2	2.80	0.65
1:A:245:PHE:CD2	1:A:252:LEU:CD1	2.80	0.65
1:A:346:TYR:O	1:A:346:TYR:HD1	1.80	0.65
2:B:1:MET:HG2	2:B:2:ARG:HH12	1.59	0.65
2:B:17:PHE:HZ	2:B:120:PHE:CE2	2.13	0.65
2:B:71:ARG:HA	2:B:71:ARG:NH1	2.11	0.65
2:B:369:TRP:HZ2	2:B:427:GLU:HB2	1.62	0.65
1:A:471:ILE:CG2	2:B:446:LEU:HD21	2.27	0.64
1:A:225:ARG:NH1	2:B:438:GLU:HG2	2.13	0.64
1:A:316:GLU:HB2	1:A:334:GLU:OE2	1.97	0.64
1:A:500:PRO:C	1:A:501:LEU:HD23	2.18	0.64
2:B:108:ILE:CG2	2:B:112:ILE:HB	2.27	0.64
1:A:14:PHE:CD1	1:A:26:GLY:O	2.49	0.64
1:A:14:PHE:HD1	1:A:26:GLY:O	1.79	0.64
1:A:394:LEU:HD12	1:A:394:LEU:C	2.17	0.64
2:B:112:ILE:O	2:B:115:LEU:HB2	1.97	0.64
1:A:347:LYS:HB2	1:A:353:TYR:HE2	1.63	0.64
2:B:108:ILE:HG22	2:B:112:ILE:HB	1.80	0.64
2:B:137:LYS:HB3	2:B:138:GLN:HE22	1.63	0.64
2:B:262:GLN:HG3	2:B:329:LEU:CD1	2.27	0.64
2:B:346:ASP:OD1	2:B:347:GLY:N	2.31	0.64
2:B:253:THR:OG1	2:B:256:ILE:HG22	1.97	0.64
1:A:347:LYS:HB2	1:A:353:TYR:CE2	2.33	0.64
2:B:81:ALA:O	2:B:84:VAL:CB	2.43	0.64
1:A:459:ILE:HA	1:A:462:LEU:HD12	1.80	0.64
2:B:204:ALA:O	2:B:205:PHE:HD2	1.80	0.64
1:A:274:ILE:HG12	1:A:275:ARG:N	2.13	0.64
1:A:308:GLY:CA	1:A:465:LEU:CD2	2.52	0.64
2:B:2:ARG:HB3	2:B:56:ASN:HA	1.80	0.64
1:A:426:VAL:HG12	1:A:429:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:HG22	2:B:446:LEU:HD21	1.79	0.63
2:B:17:PHE:CZ	2:B:120:PHE:HE2	2.17	0.63
2:B:2:ARG:HB2	2:B:56:ASN:C	2.19	0.63
1:A:481:ARG:HG3	1:A:481:ARG:NH1	2.13	0.63
2:B:29:GLY:HA3	2:B:143:LYS:O	1.99	0.63
2:B:105:TYR:HD1	2:B:105:TYR:O	1.80	0.63
2:B:132:LEU:HA	2:B:135:PHE:HB2	1.80	0.63
1:A:405:ILE:HD11	1:A:421:TRP:NE1	2.13	0.63
2:B:108:ILE:HG21	2:B:112:ILE:CG2	2.28	0.63
1:A:336:LYS:O	1:A:340:THR:OG1	2.15	0.63
2:B:65:SER:OG	2:B:68:GLY:N	2.32	0.63
1:A:79:GLU:HG2	2:B:125:ALA:HB3	1.81	0.62
2:B:210:TYR:HB3	2:B:213:TYR:O	1.99	0.62
2:B:252:ASP:CG	2:B:257:ARG:HG3	2.18	0.62
1:A:275:ARG:HH11	1:A:454:GLN:NE2	1.97	0.62
2:B:350:LEU:C	2:B:351:ILE:HD12	2.19	0.62
1:A:126:ILE:HG22	1:A:130:LYS:HD2	1.81	0.62
2:B:72:GLU:HG3	2:B:76:LYS:HE3	1.81	0.62
2:B:436:PHE:C	2:B:438:GLU:OE1	2.36	0.62
1:A:309:ASP:O	1:A:503:PHE:HB3	1.98	0.62
2:B:128:LEU:O	2:B:132:LEU:HD23	1.99	0.62
1:A:245:PHE:CD2	1:A:252:LEU:HD13	2.35	0.62
2:B:30:TYR:CD2	2:B:142:LYS:HB3	2.35	0.62
2:B:58:CYS:O	2:B:59:LYS:HD3	1.99	0.62
2:B:283:ARG:CG	2:B:296:GLU:OE1	2.47	0.62
2:B:321:PHE:HE2	2:B:339:SER:HB3	1.65	0.62
2:B:265:ILE:O	2:B:269:ILE:HG12	2.00	0.61
1:A:18:GLN:CB	1:A:30:PHE:CE2	2.83	0.61
2:B:252:ASP:OD1	2:B:253:THR:N	2.33	0.61
1:A:481:ARG:NH2	2:B:444:ASP:OD2	2.33	0.61
2:B:2:ARG:CB	2:B:56:ASN:HA	2.31	0.61
1:A:11:SER:O	1:A:272:GLY:N	2.30	0.61
1:A:218:THR:C	1:A:505:TYR:HE1	2.03	0.61
1:A:273:ASP:N	1:A:273:ASP:OD2	2.33	0.61
1:A:281:LEU:HD13	1:A:303:MET:HG3	1.82	0.61
1:A:451:GLU:HG2	1:A:454:GLN:H	1.65	0.61
2:B:82:THR:O	2:B:86:LYS:HD3	2.01	0.61
2:B:2:ARG:HH11	2:B:2:ARG:H	1.48	0.61
2:B:81:ALA:C	2:B:84:VAL:CB	2.62	0.61
2:B:200:VAL:O	2:B:203:LEU:CG	2.47	0.61
2:B:200:VAL:HB	2:B:203:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ILE:O	2:B:348:ILE:HG22	2.00	0.61
2:B:386:ASP:HB2	2:B:392:TYR:CE2	2.35	0.61
1:A:69:ASN:HA	1:A:72:ARG:O	2.01	0.61
2:B:71:ARG:HH11	2:B:71:ARG:CG	2.13	0.61
2:B:361:ARG:HH11	2:B:361:ARG:CG	2.14	0.61
1:A:9:GLU:OE1	1:A:10:PRO:HD2	2.00	0.61
2:B:119:ASP:OD1	2:B:121:LYS:HD3	2.01	0.61
1:A:320:TRP:CE3	1:A:330:LEU:CD1	2.85	0.60
2:B:102:ASN:N	2:B:102:ASN:OD1	2.34	0.60
1:A:212:ALA:HB2	1:A:489:ILE:HG23	1.83	0.60
1:A:360:HIS:HD2	1:A:386:VAL:HB	1.65	0.60
1:A:426:VAL:CG1	1:A:472:TYR:HE2	2.14	0.60
1:A:484:ASN:OD1	1:A:484:ASN:N	2.34	0.60
2:B:85:LYS:O	2:B:88:LEU:HG	2.01	0.60
2:B:11:THR:HG22	2:B:12:PRO:CA	2.31	0.60
1:A:16:HIS:CE1	2:B:147:HIS:ND1	2.68	0.60
2:B:5:ILE:HD11	2:B:142:LYS:HE3	1.82	0.60
2:B:27:GLY:HA2	2:B:147:HIS:HA	1.84	0.60
1:A:306:ASP:O	1:A:465:LEU:HD11	2.01	0.60
1:A:396:LEU:HD12	1:A:421:TRP:CH2	2.37	0.60
2:B:149:LYS:O	2:B:153:LEU:HD22	2.02	0.60
1:A:50:LEU:HD12	1:A:50:LEU:C	2.20	0.60
2:B:30:TYR:CE1	2:B:135:PHE:CD2	2.83	0.60
2:B:190:TYR:O	2:B:193:ARG:HB2	2.01	0.60
2:B:386:ASP:OD2	2:B:392:TYR:N	2.19	0.60
1:A:496:ILE:O	1:A:496:ILE:HG22	2.01	0.60
2:B:62:ILE:HG12	2:B:63:VAL:H	1.67	0.60
2:B:81:ALA:HA	2:B:84:VAL:CG1	2.29	0.60
2:B:85:LYS:CG	2:B:94:ILE:CD1	2.80	0.60
2:B:120:PHE:HE1	2:B:127:GLY:CA	2.15	0.60
2:B:146:ASP:OD2	2:B:149:LYS:HB2	2.02	0.60
2:B:210:TYR:HH	2:B:256:ILE:CD1	2.00	0.60
2:B:384:LEU:HB2	2:B:391:ILE:HD13	1.83	0.60
1:A:57:LEU:HD21	1:A:86:TRP:CD2	2.37	0.60
1:A:212:ALA:HA	1:A:215:LEU:HD11	1.83	0.60
1:A:212:ALA:CA	1:A:215:LEU:HD12	2.31	0.60
2:B:1:MET:CG	2:B:2:ARG:NH1	2.60	0.60
2:B:37:LEU:HD13	2:B:37:LEU:O	2.02	0.60
1:A:390:LYS:O	1:A:390:LYS:HG2	2.01	0.59
2:B:81:ALA:O	2:B:85:LYS:HG3	2.02	0.59
2:B:169:GLU:O	2:B:412:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LYS:N	1:A:393:PRO:HD3	2.16	0.59
2:B:323:ILE:HD13	2:B:380:PHE:CD1	2.36	0.59
2:B:370:ASN:HD22	2:B:371:ASP:N	2.00	0.59
1:A:4:LEU:CD2	1:A:410:ALA:O	2.50	0.59
1:A:13:LEU:C	1:A:14:PHE:CD2	2.76	0.59
2:B:344:THR:HG22	2:B:349:ASN:O	2.02	0.59
1:A:147:ILE:O	1:A:151:CYS:HB2	2.02	0.59
1:A:262:TYR:CZ	1:A:309:ASP:OD1	2.55	0.59
2:B:192:TRP:CZ2	2:B:193:ARG:CZ	2.86	0.59
2:B:346:ASP:CG	2:B:349:ASN:HB2	2.23	0.59
1:A:391:SER:HB3	1:A:393:PRO:HD3	1.83	0.59
1:A:105:LEU:O	1:A:113:ARG:HG3	2.03	0.59
2:B:25:LEU:CA	2:B:28:LEU:HD12	2.33	0.59
2:B:88:LEU:CD1	2:B:90:ASP:O	2.51	0.59
2:B:120:PHE:CE1	2:B:127:GLY:CA	2.86	0.59
2:B:194:LEU:HD12	2:B:194:LEU:O	2.03	0.59
2:B:323:ILE:HD13	2:B:380:PHE:HD1	1.67	0.59
1:A:4:LEU:HD22	1:A:411:TYR:CA	2.23	0.59
2:B:351:ILE:HD12	2:B:351:ILE:N	2.18	0.58
2:B:253:THR:HG21	2:B:256:ILE:HG22	1.85	0.58
2:B:345:MET:HG2	2:B:346:ASP:H	1.67	0.58
1:A:396:LEU:HD12	1:A:421:TRP:CZ2	2.39	0.58
2:B:85:LYS:HG3	2:B:94:ILE:HD11	1.86	0.58
2:B:105:TYR:CZ	2:B:113:VAL:HB	2.38	0.58
2:B:271:LYS:HZ2	2:B:275:LEU:CD2	2.16	0.58
1:A:37:TYR:HA	1:A:84:CYS:SG	2.44	0.58
1:A:288:ILE:H	1:A:297:ALA:HA	1.69	0.58
1:A:353:TYR:CD1	1:A:378:PRO:HG2	2.30	0.58
2:B:178:ILE:CD1	2:B:181:PHE:HZ	2.16	0.58
1:A:18:GLN:NE2	2:B:148:SER:N	2.50	0.58
2:B:58:CYS:SG	2:B:140:VAL:HG12	2.33	0.58
2:B:205:PHE:CE1	2:B:396:GLY:HA2	2.39	0.58
2:B:210:TYR:CZ	2:B:211:LYS:CD	2.86	0.58
1:A:399:THR:O	2:B:374:ARG:NH1	2.35	0.58
2:B:436:PHE:HA	2:B:438:GLU:CD	2.24	0.58
1:A:472:TYR:HD1	1:A:472:TYR:O	1.86	0.58
2:B:6:PHE:CD2	2:B:33:TRP:CE3	2.92	0.58
2:B:6:PHE:HD2	2:B:33:TRP:CE3	2.21	0.58
1:A:153:PRO:O	1:A:154:ASN:HB2	2.03	0.58
1:A:181:THR:HG21	1:A:186:PHE:HD1	1.68	0.58
1:A:405:ILE:HD11	1:A:421:TRP:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:CG	1:A:482:PHE:CE1	2.86	0.58
2:B:30:TYR:HE1	2:B:135:PHE:CD2	2.11	0.58
2:B:188:HIS:CB	2:B:190:TYR:CE1	2.86	0.58
2:B:384:LEU:HB2	2:B:391:ILE:CD1	2.33	0.58
1:A:56:TYR:OH	1:A:252:LEU:HD23	2.03	0.58
1:A:436:GLU:CD	2:B:361:ARG:NH2	2.53	0.58
1:A:479:THR:HB	1:A:480:LEU:HD23	1.85	0.58
2:B:205:PHE:CE1	2:B:397:SER:N	2.69	0.58
1:A:18:GLN:NE2	2:B:148:SER:HA	2.16	0.58
1:A:347:LYS:NZ	1:A:353:TYR:CE2	2.72	0.58
2:B:58:CYS:C	2:B:59:LYS:HG2	2.24	0.58
2:B:344:THR:HA	2:B:351:ILE:CD1	2.34	0.58
1:A:347:LYS:O	1:A:351:LYS:N	2.34	0.57
2:B:28:LEU:CA	2:B:145:PRO:HA	2.33	0.57
2:B:74:VAL:O	2:B:77:GLU:N	2.37	0.57
2:B:194:LEU:HD12	2:B:195:PRO:O	2.03	0.57
2:B:241:ILE:HG21	2:B:246:ILE:HD11	1.86	0.57
1:A:187:ASN:ND2	1:A:187:ASN:H	2.01	0.57
1:A:82:PHE:CE1	1:A:261:TYR:CG	2.93	0.57
2:B:120:PHE:HD1	2:B:127:GLY:HA3	1.66	0.57
1:A:275:ARG:NH1	1:A:454:GLN:HG2	2.19	0.57
2:B:4:LYS:O	2:B:57:THR:CA	2.52	0.57
2:B:386:ASP:HB2	2:B:392:TYR:CD2	2.40	0.57
1:A:30:PHE:HZ	2:B:151:ASN:HB3	1.68	0.57
2:B:20:TRP:CE3	2:B:124:TRP:CE3	2.93	0.57
1:A:109:SER:HG	1:A:200:TYR:HH	1.49	0.57
1:A:503:PHE:CE1	1:A:507:ILE:HD11	2.40	0.57
2:B:385:SER:CA	2:B:391:ILE:HG12	2.31	0.57
1:A:218:THR:HG22	1:A:501:LEU:HD13	1.86	0.57
2:B:21:LEU:HD12	2:B:21:LEU:C	2.25	0.57
1:A:217:HIS:CD2	1:A:217:HIS:N	2.73	0.56
2:B:188:HIS:CB	2:B:190:TYR:CD1	2.85	0.56
2:B:17:PHE:CZ	2:B:21:LEU:HD23	2.40	0.56
2:B:192:TRP:CZ2	2:B:193:ARG:NH1	2.73	0.56
2:B:27:GLY:HA3	2:B:147:HIS:HA	1.85	0.56
2:B:108:ILE:CG2	2:B:112:ILE:CB	2.83	0.56
2:B:151:ASN:HB2	2:B:155:GLN:OE1	2.05	0.56
2:B:192:TRP:CZ2	2:B:193:ARG:NH2	2.73	0.56
1:A:245:PHE:CE2	1:A:252:LEU:HD12	2.41	0.56
1:A:329:HIS:HB3	1:A:366:ASN:ND2	2.20	0.56
2:B:62:ILE:HD12	2:B:78:LEU:HD21	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:PHE:HE1	2:B:127:GLY:HA3	1.70	0.56
1:A:370:TRP:CE2	1:A:447:LYS:CB	2.87	0.56
1:A:207:HIS:CE1	2:B:442:ASP:OD1	2.53	0.56
2:B:101:GLU:CD	2:B:121:LYS:HB3	2.26	0.56
2:B:300:LEU:HD12	2:B:304:LYS:O	2.03	0.56
1:A:337:ALA:HA	1:A:340:THR:OG1	2.06	0.56
2:B:259:TYR:CD2	2:B:260:GLU:N	2.73	0.56
2:B:262:GLN:HA	2:B:329:LEU:HD12	1.87	0.56
1:A:245:PHE:HD2	1:A:252:LEU:CD1	2.18	0.56
2:B:212:GLU:HB3	2:B:213:TYR:CD2	2.41	0.56
2:B:435:ASN:O	2:B:438:GLU:OE2	2.24	0.56
1:A:18:GLN:CG	1:A:30:PHE:CE1	2.79	0.55
1:A:304:PHE:CD2	1:A:310:GLY:HA2	2.41	0.55
2:B:210:TYR:CD2	2:B:211:LYS:N	2.73	0.55
2:B:368:TRP:CB	2:B:373:TRP:HE1	2.18	0.55
2:B:385:SER:HB3	2:B:405:ASN:HD21	0.66	0.55
1:A:304:PHE:HE1	1:A:478:VAL:CB	2.20	0.55
1:A:48:LYS:O	1:A:52:ILE:HG13	2.06	0.55
2:B:262:GLN:HG3	2:B:329:LEU:HD12	1.88	0.55
2:B:30:TYR:HA	2:B:142:LYS:HD2	1.87	0.55
2:B:39:LEU:HD12	2:B:39:LEU:O	2.07	0.55
2:B:369:TRP:O	2:B:373:TRP:HD1	1.89	0.55
2:B:72:GLU:HA	2:B:75:LEU:HG	1.89	0.55
2:B:343:PHE:H	2:B:357:GLN:HE22	1.55	0.55
2:B:178:ILE:HD13	2:B:181:PHE:HZ	1.71	0.55
2:B:388:GLN:HG2	2:B:389:ASN:HD22	1.69	0.55
2:B:85:LYS:HD2	2:B:94:ILE:CD1	2.19	0.55
2:B:12:PRO:C	2:B:15:ASP:OD1	2.45	0.55
2:B:203:LEU:O	2:B:204:ALA:HB3	2.07	0.55
1:A:5:ILE:CD1	1:A:412:ILE:HD11	2.36	0.55
1:A:236:ASN:OD1	1:A:240:ALA:N	2.40	0.55
2:B:180:SER:O	2:B:181:PHE:HD2	1.89	0.55
2:B:271:LYS:O	2:B:275:LEU:HG	2.06	0.54
2:B:85:LYS:CG	2:B:94:ILE:HD11	2.38	0.54
2:B:285:TYR:CD2	2:B:286:GLN:N	2.73	0.54
2:B:300:LEU:HD12	2:B:304:LYS:C	2.28	0.54
2:B:433:ILE:O	2:B:437:GLU:HG3	2.07	0.54
2:B:168:GLU:CB	2:B:412:GLY:O	2.56	0.54
2:B:183:ASN:OD1	2:B:183:ASN:N	2.38	0.54
1:A:334:GLU:OE1	1:A:334:GLU:HA	2.07	0.54
2:B:369:TRP:CZ2	2:B:427:GLU:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:C	1:A:215:LEU:HD12	2.27	0.54
1:A:391:SER:OG	1:A:393:PRO:HD3	2.08	0.54
2:B:110:ILE:O	2:B:113:VAL:HG22	2.06	0.54
1:A:372:ALA:HA	1:A:375:GLU:OE1	2.08	0.54
1:A:99:GLU:OE1	1:A:102:ARG:NH1	2.41	0.54
1:A:403:PHE:CZ	2:B:419:PRO:HG2	2.43	0.54
1:A:419:PHE:CE1	1:A:442:PHE:HB2	2.43	0.54
1:A:471:ILE:HG21	2:B:446:LEU:CD2	2.38	0.54
2:B:213:TYR:CD2	2:B:213:TYR:N	2.76	0.54
2:B:276:ARG:HH21	2:B:280:LYS:HZ1	1.45	0.54
1:A:121:PHE:O	1:A:125:ILE:HG13	2.08	0.53
1:A:207:HIS:NE2	2:B:442:ASP:OD2	2.40	0.53
1:A:184:GLU:HA	1:A:187:ASN:ND2	2.23	0.53
1:A:307:ASN:OD1	1:A:308:GLY:N	2.41	0.53
1:A:284:VAL:HB	1:A:300:ALA:HB3	1.90	0.53
2:B:227:LEU:HD22	2:B:230:THR:HG23	1.90	0.53
2:B:364:GLN:HA	2:B:364:GLN:OE1	2.08	0.53
2:B:274:GLU:O	2:B:277:MET:HB2	2.09	0.53
2:B:280:LYS:NZ	2:B:386:ASP:OD1	2.38	0.53
1:A:398:LYS:HE3	2:B:169:GLU:OE2	2.09	0.53
2:B:262:GLN:HG3	2:B:329:LEU:HD13	1.89	0.53
1:A:108:ALA:HB3	1:A:166:SER:HB2	1.91	0.53
1:A:222:GLN:HG2	1:A:263:LYS:NZ	2.24	0.53
2:B:191:ASP:O	2:B:193:ARG:N	2.42	0.53
2:B:262:GLN:CG	2:B:329:LEU:HD12	2.39	0.53
1:A:446:ASN:O	1:A:447:LYS:HD3	2.09	0.53
2:B:129:GLN:OE1	2:B:129:GLN:HA	2.09	0.53
2:B:82:THR:HA	2:B:85:LYS:HD3	1.90	0.53
2:B:345:MET:HG2	2:B:346:ASP:N	2.23	0.53
1:A:27:LEU:O	1:A:31:GLY:N	2.40	0.52
1:A:364:ARG:CA	1:A:446:ASN:OD1	2.57	0.52
2:B:17:PHE:CE2	2:B:21:LEU:HB2	2.44	0.52
2:B:84:VAL:O	2:B:88:LEU:HD23	2.09	0.52
1:A:14:PHE:HE1	1:A:27:LEU:N	2.08	0.52
1:A:194:GLU:O	1:A:198:LYS:HG3	2.10	0.52
1:A:391:SER:CA	1:A:393:PRO:HD3	2.39	0.52
1:A:275:ARG:NH1	1:A:454:GLN:HE21	2.04	0.52
2:B:274:GLU:HG2	2:B:293:TYR:OH	2.08	0.52
1:A:51:GLN:HG3	1:A:52:ILE:N	2.23	0.52
1:A:340:THR:HG23	1:A:376:VAL:CG1	2.39	0.52
2:B:438:GLU:HB2	2:B:441:GLU:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:HIS:HE1	2:B:147:HIS:CE1	2.27	0.52
1:A:203:ASP:O	1:A:209:GLN:NE2	2.42	0.52
1:A:455:VAL:HA	1:A:458:ASP:HB2	1.91	0.52
2:B:193:ARG:HG3	2:B:229:LYS:O	2.10	0.52
2:B:285:TYR:CE1	2:B:342:ILE:HD12	2.45	0.52
2:B:429:VAL:HG12	2:B:429:VAL:O	2.09	0.52
1:A:302:GLN:OE1	1:A:486:ILE:CD1	2.57	0.52
2:B:141:PRO:O	2:B:142:LYS:HD3	2.10	0.52
2:B:369:TRP:NE1	2:B:427:GLU:OE1	2.42	0.52
1:A:282:GLY:HA3	1:A:302:GLN:HG3	1.92	0.52
2:B:88:LEU:HD12	2:B:90:ASP:HB3	1.92	0.52
1:A:92:VAL:HG21	1:A:136:VAL:CG2	2.40	0.52
2:B:62:ILE:HD12	2:B:78:LEU:CG	2.39	0.52
2:B:88:LEU:HD12	2:B:90:ASP:CA	2.38	0.52
2:B:157:ILE:HB	2:B:158:PHE:CE2	2.45	0.52
1:A:122:ASN:O	1:A:126:ILE:HG13	2.10	0.52
1:A:126:ILE:HG22	1:A:130:LYS:CD	2.39	0.52
1:A:246:SER:OG	1:A:247:LYS:HE3	2.10	0.52
2:B:132:LEU:HD23	2:B:132:LEU:H	1.74	0.51
2:B:194:LEU:CD1	2:B:209:ARG:NH1	2.73	0.51
2:B:222:ASP:OD1	2:B:397:SER:OG	2.24	0.51
2:B:30:TYR:CD1	2:B:142:LYS:HG3	2.44	0.51
2:B:191:ASP:O	2:B:192:TRP:C	2.48	0.51
2:B:351:ILE:N	2:B:351:ILE:CD1	2.73	0.51
2:B:62:ILE:HD12	2:B:78:LEU:HD23	1.70	0.51
2:B:154:TYR:HA	2:B:158:PHE:CD2	2.45	0.51
2:B:344:THR:HA	2:B:351:ILE:HD11	1.92	0.51
1:A:13:LEU:HD11	1:A:17:GLY:HA2	1.93	0.51
1:A:178:TYR:HB2	1:A:194:GLU:HB2	1.91	0.51
2:B:192:TRP:HZ2	2:B:193:ARG:HH22	1.58	0.51
1:A:274:ILE:HG12	1:A:275:ARG:O	2.10	0.51
2:B:50:GLU:C	2:B:53:ILE:HD12	2.31	0.51
1:A:384:VAL:HG21	1:A:450:ALA:HB2	1.91	0.51
2:B:276:ARG:HH21	2:B:280:LYS:HZ3	1.50	0.51
1:A:6:TYR:CD2	1:A:7:ILE:N	2.79	0.51
2:B:78:LEU:O	2:B:82:THR:OG1	2.29	0.51
2:B:251:TYR:O	2:B:258:ASN:HB2	2.10	0.51
1:A:391:SER:HB3	1:A:393:PRO:CD	2.39	0.51
2:B:200:VAL:C	2:B:203:LEU:HG	2.30	0.51
1:A:92:VAL:HG21	1:A:136:VAL:HG21	1.92	0.51
1:A:312:VAL:CG2	1:A:506:TYR:HE1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:PRO:O	1:A:381:THR:HG23	2.11	0.51
1:A:465:LEU:HD23	1:A:465:LEU:O	2.11	0.51
2:B:17:PHE:HA	2:B:124:TRP:CH2	2.46	0.51
2:B:17:PHE:CD1	2:B:99:ILE:HG21	2.46	0.51
1:A:302:GLN:OE1	1:A:486:ILE:HD11	2.10	0.51
1:A:419:PHE:HE1	1:A:442:PHE:HB2	1.76	0.51
1:A:428:LYS:HD2	1:A:428:LYS:O	2.10	0.51
1:A:479:THR:CB	1:A:480:LEU:HD23	2.41	0.50
2:B:25:LEU:C	2:B:28:LEU:HD12	2.31	0.50
2:B:287:MET:N	2:B:290:THR:O	2.45	0.50
2:B:50:GLU:CA	2:B:53:ILE:CD1	2.85	0.50
2:B:178:ILE:CD1	2:B:181:PHE:CZ	2.93	0.50
1:A:57:LEU:O	1:A:60:ILE:HG12	2.12	0.50
1:A:482:PHE:CD2	1:A:503:PHE:HZ	2.20	0.50
2:B:366:LYS:O	2:B:427:GLU:CD	2.50	0.50
2:B:388:GLN:CG	2:B:389:ASN:ND2	2.73	0.50
1:A:358:PHE:CE1	1:A:455:VAL:HG22	2.44	0.50
2:B:105:TYR:CE1	2:B:113:VAL:HB	2.46	0.50
2:B:210:TYR:CZ	2:B:256:ILE:CD1	2.92	0.50
2:B:345:MET:H	2:B:351:ILE:HD11	1.76	0.50
2:B:416:TYR:C	2:B:416:TYR:CD1	2.85	0.50
1:A:50:LEU:HD22	1:A:93:PHE:CE1	2.41	0.50
1:A:285:TYR:CD2	1:A:328:TYR:HB2	2.47	0.50
2:B:79:ALA:CA	2:B:82:THR:OG1	2.60	0.50
2:B:86:LYS:N	2:B:86:LYS:CD	2.73	0.50
2:B:262:GLN:O	2:B:266:VAL:HG23	2.12	0.50
1:A:5:ILE:HD13	1:A:412:ILE:HD11	1.93	0.50
1:A:66:ASN:OD1	1:A:250:GLY:N	2.45	0.50
2:B:2:ARG:CB	2:B:56:ASN:O	2.59	0.50
1:A:9:GLU:OE2	1:A:472:TYR:CZ	2.65	0.50
1:A:97:THR:HG23	1:A:100:GLU:OE2	2.11	0.50
1:A:329:HIS:HB3	1:A:366:ASN:HD22	1.77	0.50
1:A:37:TYR:CA	1:A:84:CYS:SG	3.00	0.49
1:A:40:LYS:O	1:A:136:VAL:CG1	2.58	0.49
2:B:8:SER:OG	2:B:62:ILE:HA	2.12	0.49
2:B:71:ARG:O	2:B:75:LEU:HD21	2.11	0.49
2:B:179:ILE:CD1	2:B:404:SER:HB2	2.24	0.49
2:B:341:ILE:HB	2:B:361:ARG:HG3	1.94	0.49
1:A:56:TYR:OH	1:A:252:LEU:CD2	2.60	0.49
1:A:202:TYR:CE1	1:A:494:THR:HG23	2.46	0.49
1:A:245:PHE:CE2	1:A:252:LEU:CD1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TYR:CD1	1:A:472:TYR:C	2.85	0.49
2:B:176:PHE:N	2:B:176:PHE:CD2	2.80	0.49
2:B:210:TYR:CZ	2:B:211:LYS:HD2	2.41	0.49
1:A:481:ARG:NH1	1:A:481:ARG:CG	2.73	0.49
2:B:200:VAL:HG21	2:B:209:ARG:N	2.24	0.49
2:B:212:GLU:C	2:B:213:TYR:CD2	2.85	0.49
2:B:381:ILE:HG23	2:B:405:ASN:OD1	2.10	0.49
2:B:370:ASN:ND2	2:B:371:ASP:N	2.60	0.49
1:A:95:GLU:HG2	1:A:96:ILE:N	2.27	0.49
1:A:187:ASN:ND2	1:A:187:ASN:N	2.60	0.49
1:A:269:TRP:CD1	1:A:269:TRP:C	2.86	0.49
2:B:74:VAL:HG23	2:B:75:LEU:HD23	1.95	0.49
2:B:108:ILE:HG21	2:B:112:ILE:HG22	1.93	0.49
2:B:253:THR:HG1	2:B:256:ILE:N	2.06	0.49
1:A:284:VAL:HG22	1:A:483:ALA:HB1	1.94	0.49
2:B:208:ILE:HD11	2:B:267:GLN:HB2	1.93	0.49
1:A:79:GLU:OE1	1:A:85:LYS:HE3	2.13	0.49
1:A:225:ARG:HH11	2:B:438:GLU:HG2	1.76	0.49
1:A:391:SER:O	1:A:439:ASN:OD1	2.30	0.49
2:B:259:TYR:CD2	2:B:259:TYR:C	2.86	0.49
1:A:113:ARG:HD3	1:A:157:LEU:HD12	1.95	0.49
2:B:1:MET:CG	2:B:2:ARG:HH12	2.21	0.49
2:B:326:ALA:O	2:B:335:LEU:HD12	2.12	0.49
1:A:391:SER:CB	1:A:393:PRO:CD	2.85	0.49
2:B:24:LYS:O	2:B:28:LEU:HG	2.12	0.49
2:B:105:TYR:HD1	2:B:105:TYR:C	2.15	0.49
2:B:285:TYR:CD2	2:B:285:TYR:C	2.85	0.49
1:A:126:ILE:CG2	1:A:130:LYS:HD2	2.43	0.48
1:A:405:ILE:HD11	1:A:421:TRP:CD1	2.47	0.48
2:B:116:ASN:C	2:B:116:ASN:HD22	2.16	0.48
2:B:133:ASP:O	2:B:137:LYS:N	2.42	0.48
2:B:138:GLN:NE2	2:B:138:GLN:N	2.60	0.48
2:B:193:ARG:HG2	2:B:230:THR:HA	1.96	0.48
1:A:304:PHE:CE1	1:A:478:VAL:HG21	2.46	0.48
1:A:392:LYS:N	1:A:393:PRO:CD	2.76	0.48
2:B:17:PHE:CZ	2:B:21:LEU:CD2	2.95	0.48
2:B:75:LEU:HD23	2:B:75:LEU:H	1.77	0.48
1:A:20:CYS:SG	2:B:154:TYR:HE1	2.36	0.48
1:A:35:GLN:HG3	1:A:36:ILE:N	2.29	0.48
2:B:30:TYR:CE2	2:B:142:LYS:HB3	2.49	0.48
2:B:105:TYR:C	2:B:105:TYR:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:VAL:CG1	2:B:141:PRO:CD	2.91	0.48
2:B:260:GLU:OE1	2:B:260:GLU:HA	2.14	0.48
1:A:14:PHE:HD2	1:A:14:PHE:N	2.12	0.48
1:A:14:PHE:CD2	1:A:14:PHE:N	2.80	0.48
2:B:17:PHE:C	2:B:17:PHE:CD2	2.85	0.48
2:B:361:ARG:CG	2:B:361:ARG:NH1	2.73	0.48
1:A:149:LYS:HD2	1:A:149:LYS:O	2.14	0.48
1:A:184:GLU:O	1:A:187:ASN:N	2.47	0.48
1:A:350:ASN:OD1	1:A:350:ASN:N	2.46	0.48
2:B:6:PHE:HB2	2:B:57:THR:HG21	1.95	0.48
2:B:30:TYR:O	2:B:32:VAL:HG23	2.13	0.48
2:B:82:THR:HA	2:B:85:LYS:CD	2.44	0.48
2:B:271:LYS:HZ2	2:B:275:LEU:HD23	1.79	0.48
2:B:147:HIS:O	2:B:150:SER:N	2.38	0.48
1:A:94:LYS:HA	1:A:94:LYS:HD3	1.67	0.48
1:A:429:LEU:CD1	1:A:472:TYR:HD2	2.27	0.48
2:B:200:VAL:O	2:B:203:LEU:CD1	2.61	0.48
2:B:346:ASP:OD2	2:B:349:ASN:HB2	2.13	0.48
1:A:63:PRO:HG3	1:A:76:PRO:O	2.14	0.48
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.61	0.48
1:A:432:THR:OG1	1:A:433:LEU:N	2.47	0.48
2:B:71:ARG:NH1	2:B:71:ARG:CG	2.73	0.48
2:B:386:ASP:CB	2:B:392:TYR:CD2	2.97	0.48
1:A:16:HIS:CE1	2:B:147:HIS:HD1	2.31	0.47
1:A:275:ARG:H	1:A:275:ARG:HD3	1.79	0.47
2:B:345:MET:N	2:B:351:ILE:HD11	2.28	0.47
1:A:194:GLU:HG2	1:A:198:LYS:HE3	1.95	0.47
1:A:346:TYR:HD1	1:A:346:TYR:C	2.18	0.47
1:A:82:PHE:CE1	1:A:261:TYR:CD2	3.02	0.47
1:A:480:LEU:N	1:A:480:LEU:CD2	2.73	0.47
2:B:191:ASP:C	2:B:193:ARG:N	2.66	0.47
2:B:328:LYS:HD2	2:B:336:MET:HE1	1.96	0.47
1:A:72:ARG:HH12	2:B:426:GLU:CD	2.15	0.47
1:A:120:LEU:O	1:A:120:LEU:HD12	2.13	0.47
1:A:2:LYS:NZ	1:A:413:VAL:O	2.47	0.47
1:A:312:VAL:CG1	1:A:506:TYR:CE1	2.81	0.47
2:B:386:ASP:OD2	2:B:392:TYR:CD2	2.67	0.47
1:A:18:GLN:HG3	1:A:30:PHE:CZ	2.46	0.47
1:A:245:PHE:CD2	1:A:252:LEU:HD12	2.49	0.47
1:A:346:TYR:C	1:A:346:TYR:CD1	2.88	0.47
1:A:479:THR:HB	1:A:480:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:OG1	2:B:256:ILE:CA	2.62	0.47
2:B:301:GLU:CG	2:B:302:LYS:HE3	2.45	0.47
1:A:14:PHE:CD1	1:A:26:GLY:CA	2.89	0.47
1:A:78:PHE:CE1	1:A:82:PHE:HB2	2.50	0.47
2:B:69:ASN:OD1	2:B:107:ASP:O	2.32	0.47
2:B:246:ILE:O	2:B:258:ASN:OD1	2.33	0.47
2:B:361:ARG:HH11	2:B:361:ARG:HG3	1.80	0.47
2:B:30:TYR:CE1	2:B:142:LYS:HG3	2.50	0.47
2:B:319:TRP:HB3	2:B:343:PHE:CD1	2.50	0.47
2:B:356:ILE:O	2:B:360:SER:HB2	2.15	0.47
1:A:20:CYS:HG	2:B:154:TYR:HE1	1.62	0.47
1:A:181:THR:OG1	1:A:183:PHE:O	2.32	0.47
1:A:187:ASN:HA	1:A:190:LEU:HB2	1.96	0.47
2:B:182:PRO:HD3	2:B:401:ILE:HG12	1.97	0.47
1:A:425:PHE:CD1	2:B:416:TYR:CD2	3.03	0.46
2:B:182:PRO:HB3	2:B:399:GLU:OE1	2.15	0.46
2:B:445:GLU:CD	2:B:446:LEU:H	2.18	0.46
1:A:37:TYR:C	1:A:84:CYS:SG	2.94	0.46
2:B:208:ILE:HG13	2:B:268:LEU:HD22	1.95	0.46
2:B:366:LYS:O	2:B:427:GLU:HG3	2.15	0.46
1:A:148:TYR:CD1	1:A:148:TYR:C	2.89	0.46
1:A:271:LEU:CD1	1:A:306:ASP:C	2.58	0.46
1:A:138:VAL:HG12	1:A:140:PHE:CE2	2.51	0.46
2:B:396:GLY:HA3	2:B:399:GLU:HB2	1.98	0.46
2:B:188:HIS:HB3	2:B:190:TYR:HD1	1.68	0.46
2:B:276:ARG:NH2	2:B:280:LYS:HZ3	2.10	0.46
1:A:115:TYR:CD2	1:A:213:ARG:NH2	2.84	0.46
1:A:436:GLU:OE2	2:B:361:ARG:NH2	2.49	0.46
1:A:330:LEU:HD13	1:A:330:LEU:HA	1.79	0.46
2:B:81:ALA:O	2:B:84:VAL:N	2.49	0.46
2:B:121:LYS:HE2	2:B:121:LYS:HB2	1.82	0.46
2:B:2:ARG:CA	2:B:56:ASN:O	2.64	0.46
2:B:62:ILE:HG22	2:B:96:PRO:HA	1.97	0.46
2:B:205:PHE:HE1	2:B:396:GLY:C	2.20	0.46
1:A:346:TYR:CZ	1:A:354:PRO:HB3	2.43	0.45
2:B:113:VAL:HG23	2:B:114:ARG:N	2.30	0.45
1:A:347:LYS:CB	1:A:353:TYR:HE2	2.29	0.45
1:A:478:VAL:HG22	1:A:478:VAL:O	2.16	0.45
2:B:153:LEU:O	2:B:157:ILE:HG12	2.16	0.45
2:B:423:THR:O	2:B:426:GLU:N	2.49	0.45
2:B:105:TYR:CE1	2:B:113:VAL:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ILE:O	2:B:320:HIS:ND1	2.37	0.45
2:B:388:GLN:OE1	2:B:389:ASN:N	2.45	0.45
1:A:18:GLN:CG	1:A:30:PHE:CG	2.93	0.45
1:A:157:LEU:HD21	1:A:161:LEU:HB2	1.98	0.45
1:A:403:PHE:CE2	2:B:419:PRO:O	2.70	0.45
1:A:481:ARG:NH2	2:B:444:ASP:CG	2.68	0.45
2:B:81:ALA:O	2:B:84:VAL:CA	2.64	0.45
2:B:189:ARG:HD3	2:B:213:TYR:CZ	2.52	0.45
2:B:266:VAL:O	2:B:269:ILE:HG12	2.17	0.45
1:A:285:TYR:OH	1:A:330:LEU:HD23	2.17	0.45
1:A:307:ASN:C	1:A:465:LEU:HD21	2.35	0.45
1:A:57:LEU:HD23	1:A:60:ILE:HD11	1.99	0.45
1:A:285:TYR:HE1	1:A:330:LEU:HD21	1.82	0.45
1:A:377:THR:OG1	1:A:383:LEU:HD22	2.16	0.45
2:B:28:LEU:HG	2:B:28:LEU:H	1.58	0.45
2:B:219:TRP:CZ3	2:B:240:ARG:NH2	2.70	0.45
1:A:443:ILE:HD12	1:A:456:LEU:HD22	1.99	0.45
1:A:18:GLN:HB3	2:B:151:ASN:ND2	2.31	0.45
1:A:70:ILE:H	1:A:70:ILE:HG13	1.64	0.45
1:A:194:GLU:CG	1:A:198:LYS:HE3	2.46	0.45
1:A:447:LYS:HD3	1:A:447:LYS:HA	1.70	0.45
2:B:151:ASN:O	2:B:154:TYR:N	2.50	0.45
1:A:64:ILE:HG13	1:A:75:PHE:HD1	1.82	0.45
2:B:341:ILE:C	2:B:342:ILE:HD13	2.37	0.45
1:A:72:ARG:CZ	2:B:426:GLU:OE2	2.63	0.44
1:A:271:LEU:CD1	1:A:271:LEU:H	2.02	0.44
1:A:373:PHE:HB3	1:A:383:LEU:HD21	2.00	0.44
1:A:471:ILE:HG21	2:B:446:LEU:HD23	1.99	0.44
2:B:69:ASN:OD1	2:B:108:ILE:HA	2.16	0.44
2:B:71:ARG:CA	2:B:71:ARG:NH1	2.73	0.44
2:B:140:VAL:O	2:B:142:LYS:HG2	2.17	0.44
2:B:286:GLN:OE1	2:B:291:PHE:CZ	2.70	0.44
2:B:88:LEU:C	2:B:89:GLN:CG	2.85	0.44
2:B:263:ARG:O	2:B:266:VAL:HG23	2.17	0.44
2:B:392:TYR:HE1	2:B:402:LEU:HD21	1.82	0.44
1:A:13:LEU:O	1:A:269:TRP:HB2	2.17	0.44
1:A:304:PHE:CE2	1:A:310:GLY:HA2	2.52	0.44
1:A:335:ALA:HB1	1:A:373:PHE:CE1	2.52	0.44
1:A:481:ARG:HG3	1:A:482:PHE:CD1	2.51	0.44
1:A:14:PHE:CE1	1:A:27:LEU:N	2.84	0.44
1:A:271:LEU:CD1	1:A:306:ASP:CB	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PHE:CD2	2:B:17:PHE:O	2.70	0.44
2:B:188:HIS:CD2	2:B:190:TYR:CE1	3.05	0.44
2:B:280:LYS:HG3	2:B:384:LEU:HD22	1.99	0.44
1:A:82:PHE:CD1	1:A:261:TYR:CG	3.05	0.44
1:A:333:LYS:CD	1:A:333:LYS:C	2.86	0.44
2:B:25:LEU:CA	2:B:28:LEU:CD1	2.85	0.44
1:A:42:GLY:N	1:A:136:VAL:HG11	2.32	0.44
1:A:52:ILE:HG23	1:A:230:ALA:HB2	2.00	0.44
2:B:214:LEU:HD23	2:B:214:LEU:O	2.17	0.44
1:A:6:TYR:CE2	1:A:7:ILE:O	2.70	0.44
1:A:159:ASN:HA	1:A:162:VAL:CG2	2.47	0.44
1:A:245:PHE:N	1:A:245:PHE:CD1	2.86	0.44
2:B:88:LEU:C	2:B:89:GLN:HG2	2.37	0.44
2:B:151:ASN:O	2:B:155:GLN:N	2.41	0.44
2:B:262:GLN:O	2:B:266:VAL:CG2	2.66	0.44
1:A:50:LEU:HD22	1:A:93:PHE:CG	2.52	0.44
2:B:210:TYR:CZ	2:B:211:LYS:NZ	2.73	0.44
1:A:203:ASP:HB2	1:A:492:ALA:HA	1.99	0.44
1:A:259:ALA:O	1:A:263:LYS:HG3	2.18	0.44
2:B:6:PHE:CD2	2:B:33:TRP:CZ3	3.05	0.44
2:B:246:ILE:HD12	2:B:261:CYS:CB	2.48	0.44
1:A:267:LYS:H	1:A:267:LYS:HG2	1.57	0.43
2:B:21:LEU:C	2:B:21:LEU:CD1	2.85	0.43
1:A:312:VAL:HG21	1:A:506:TYR:HD1	1.80	0.43
1:A:364:ARG:HA	1:A:446:ASN:OD1	2.17	0.43
1:A:364:ARG:HB3	1:A:446:ASN:OD1	2.19	0.43
2:B:72:GLU:OE1	2:B:76:LYS:NZ	2.51	0.43
2:B:213:TYR:N	2:B:213:TYR:HD2	2.16	0.43
2:B:285:TYR:HB2	2:B:294:TRP:HE1	1.82	0.43
2:B:290:THR:OG1	2:B:291:PHE:N	2.52	0.43
2:B:262:GLN:CG	2:B:329:LEU:CD1	2.95	0.43
1:A:185:GLU:OE2	1:A:185:GLU:HA	2.18	0.43
2:B:75:LEU:N	2:B:75:LEU:CD2	2.77	0.43
2:B:23:LEU:HD23	2:B:23:LEU:HA	1.89	0.43
2:B:184:GLU:OE1	2:B:240:ARG:HD3	2.18	0.43
1:A:218:THR:O	1:A:505:TYR:HE1	2.01	0.43
2:B:218:ALA:HB1	2:B:222:ASP:OD2	2.18	0.43
2:B:301:GLU:HG3	2:B:302:LYS:HE2	2.01	0.43
1:A:112:LYS:HE2	1:A:116:ASP:OD2	2.19	0.43
1:A:281:LEU:HA	1:A:281:LEU:HD12	1.67	0.43
1:A:366:ASN:OD1	1:A:369:GLU:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:HD13	2:B:251:TYR:HE1	1.84	0.43
1:A:184:GLU:N	1:A:184:GLU:CD	2.72	0.43
1:A:304:PHE:CE2	1:A:310:GLY:CA	3.01	0.43
1:A:320:TRP:HZ3	1:A:331:LYS:HB2	1.84	0.43
2:B:49:ILE:O	2:B:52:GLU:N	2.52	0.43
2:B:80:VAL:CG1	2:B:84:VAL:CG2	2.80	0.43
1:A:245:PHE:N	1:A:245:PHE:HD1	2.17	0.43
1:A:421:TRP:CE3	1:A:440:PRO:HB3	2.54	0.43
2:B:259:TYR:CG	2:B:260:GLU:N	2.87	0.43
1:A:366:ASN:OD1	1:A:368:GLU:HG3	2.19	0.42
1:A:421:TRP:CD2	1:A:440:PRO:HB3	2.54	0.42
2:B:180:SER:O	2:B:181:PHE:CD2	2.71	0.42
2:B:366:LYS:C	2:B:427:GLU:OE2	2.57	0.42
2:B:28:LEU:O	2:B:144:PRO:C	2.57	0.42
2:B:219:TRP:HZ3	2:B:240:ARG:CZ	2.32	0.42
1:A:142:ILE:O	1:A:144:PRO:HD3	2.19	0.42
1:A:395:LYS:HB3	1:A:397:TYR:CE2	2.54	0.42
2:B:21:LEU:HD11	2:B:25:LEU:HD21	2.00	0.42
2:B:87:HIS:ND1	2:B:87:HIS:C	2.73	0.42
2:B:345:MET:CG	2:B:346:ASP:N	2.83	0.42
2:B:389:ASN:ND2	2:B:389:ASN:N	2.66	0.42
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.86	0.42
2:B:384:LEU:C	2:B:391:ILE:HG12	2.37	0.42
2:B:420:SER:O	2:B:421:GLU:HB2	2.20	0.42
1:A:233:ASP:O	1:A:235:LYS:HG2	2.20	0.42
1:A:370:TRP:CZ2	1:A:447:LYS:CB	3.01	0.42
2:B:6:PHE:CD2	2:B:33:TRP:HE3	2.36	0.42
2:B:32:VAL:HG12	2:B:33:TRP:N	2.33	0.42
2:B:199:ASP:OD1	2:B:202:THR:OG1	2.38	0.42
2:B:392:TYR:CE1	2:B:402:LEU:HD21	2.54	0.42
2:B:72:GLU:CG	2:B:76:LYS:HE3	2.48	0.42
2:B:116:ASN:C	2:B:116:ASN:ND2	2.73	0.42
2:B:134:ALA:HA	2:B:137:LYS:HB2	2.01	0.42
2:B:187:PHE:CE2	2:B:241:ILE:HD12	2.54	0.42
2:B:310:LEU:HD23	2:B:310:LEU:HA	1.87	0.42
2:B:330:TYR:HD2	2:B:331:PRO:HA	1.84	0.42
1:A:5:ILE:HD11	1:A:412:ILE:HD11	2.00	0.42
1:A:16:HIS:HD1	2:B:147:HIS:CG	2.31	0.42
1:A:110:THR:HA	1:A:113:ARG:NH2	2.35	0.42
1:A:357:VAL:C	1:A:358:PHE:HD2	2.23	0.42
2:B:22:SER:CA	2:B:25:LEU:CD1	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLY:CA	2:B:146:ASP:O	2.61	0.42
2:B:88:LEU:HD23	2:B:88:LEU:H	1.85	0.42
1:A:16:HIS:ND1	2:B:147:HIS:CE1	2.86	0.42
1:A:474:ASP:OD2	1:A:481:ARG:NE	2.53	0.42
2:B:58:CYS:C	2:B:59:LYS:CG	2.87	0.42
2:B:119:ASP:CG	2:B:121:LYS:NZ	2.73	0.42
2:B:258:ASN:ND2	2:B:258:ASN:C	2.73	0.42
2:B:300:LEU:CD1	2:B:304:LYS:C	2.84	0.42
2:B:368:TRP:C	2:B:373:TRP:HE1	2.23	0.42
1:A:18:GLN:NE2	2:B:147:HIS:HB3	2.35	0.42
1:A:6:TYR:CD2	1:A:6:TYR:C	2.93	0.42
1:A:202:TYR:CZ	1:A:494:THR:HG23	2.55	0.42
1:A:324:GLU:H	1:A:324:GLU:HG3	1.51	0.42
2:B:193:ARG:HH21	2:B:232:THR:CB	2.33	0.42
2:B:210:TYR:CZ	2:B:256:ILE:HD13	2.54	0.42
2:B:285:TYR:CD1	2:B:342:ILE:HD12	2.54	0.42
2:B:388:GLN:CD	2:B:389:ASN:ND2	2.73	0.42
2:B:30:TYR:CD2	2:B:30:TYR:N	2.88	0.41
2:B:58:CYS:SG	2:B:140:VAL:HG11	2.41	0.41
1:A:14:PHE:HZ	1:A:23:PRO:HA	1.85	0.41
1:A:262:TYR:CD2	1:A:262:TYR:C	2.93	0.41
1:A:262:TYR:CD1	1:A:467:TYR:HD2	2.38	0.41
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.73	0.41
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.90	0.41
2:B:389:ASN:O	2:B:404:SER:HA	2.19	0.41
2:B:56:ASN:OD1	2:B:56:ASN:N	2.53	0.41
2:B:71:ARG:NH1	2:B:71:ARG:HG3	2.35	0.41
2:B:108:ILE:HG23	2:B:112:ILE:CB	2.49	0.41
2:B:205:PHE:HE1	2:B:396:GLY:HA2	1.83	0.41
2:B:346:ASP:CG	2:B:349:ASN:N	2.72	0.41
1:A:24:ARG:CZ	1:A:73:PRO:HD2	2.50	0.41
2:B:8:SER:OG	2:B:62:ILE:HG13	2.21	0.41
2:B:137:LYS:CB	2:B:138:GLN:HE21	2.27	0.41
2:B:319:TRP:C	2:B:320:HIS:CD2	2.94	0.41
1:A:174:LYS:HB2	1:A:174:LYS:HE2	1.70	0.41
1:A:216:GLU:HB2	1:A:217:HIS:CD2	2.56	0.41
2:B:28:LEU:CA	2:B:145:PRO:HB3	2.41	0.41
2:B:370:ASN:ND2	2:B:370:ASN:C	2.73	0.41
2:B:387:ASP:HB2	2:B:388:GLN:OE1	2.20	0.41
1:A:124:LYS:HA	1:A:127:THR:OG1	2.21	0.41
1:A:139:TRP:HB2	1:A:221:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CD2	1:A:503:PHE:CZ	3.00	0.41
2:B:61:LEU:HD22	2:B:97:LEU:HD11	2.02	0.41
2:B:189:ARG:HD3	2:B:213:TYR:CE1	2.55	0.41
1:A:446:ASN:O	1:A:447:LYS:HE2	2.20	0.41
2:B:168:GLU:HA	2:B:412:GLY:O	2.20	0.41
2:B:264:LEU:HD23	2:B:264:LEU:HA	1.85	0.41
1:A:23:PRO:HB2	1:A:269:TRP:CZ3	2.56	0.41
1:A:110:THR:CA	1:A:113:ARG:NH2	2.84	0.41
1:A:247:LYS:N	1:A:247:LYS:HD3	2.34	0.41
1:A:332:PRO:HB3	1:A:372:ALA:HB2	2.03	0.41
1:A:346:TYR:CG	1:A:354:PRO:HD3	2.56	0.41
1:A:370:TRP:O	1:A:373:PHE:HB2	2.20	0.41
1:A:464:LYS:HE3	1:A:472:TYR:HE1	1.86	0.41
2:B:311:VAL:HG22	2:B:320:HIS:CG	2.55	0.41
2:B:429:VAL:O	2:B:429:VAL:CG1	2.69	0.41
1:A:312:VAL:CG2	1:A:506:TYR:CE1	2.95	0.41
1:A:370:TRP:CZ2	1:A:447:LYS:HB3	2.53	0.41
1:A:391:SER:C	1:A:393:PRO:CD	2.85	0.41
2:B:70:LYS:HE3	2:B:70:LYS:HB2	1.93	0.41
1:A:142:ILE:HD12	1:A:142:ILE:HG23	1.83	0.40
1:A:472:TYR:HD1	1:A:472:TYR:C	2.22	0.40
2:B:85:LYS:CG	2:B:94:ILE:HD12	2.46	0.40
2:B:109:ASN:O	2:B:113:VAL:HG13	2.21	0.40
2:B:191:ASP:O	2:B:194:LEU:N	2.48	0.40
1:A:112:LYS:CD	1:A:196:GLU:HG3	2.52	0.40
2:B:179:ILE:N	2:B:402:LEU:O	2.55	0.40
2:B:23:LEU:HB3	2:B:150:SER:OG	2.21	0.40
2:B:112:ILE:O	2:B:115:LEU:N	2.53	0.40
2:B:313:LYS:HB3	2:B:313:LYS:HE2	1.67	0.40
2:B:388:GLN:N	2:B:388:GLN:CD	2.72	0.40
1:A:107:ASN:ND2	1:A:164:THR:HB	2.36	0.40
1:A:117:LEU:O	1:A:120:LEU:HB3	2.22	0.40
1:A:304:PHE:CE1	1:A:478:VAL:HG11	2.42	0.40
1:A:460:LEU:HA	1:A:460:LEU:HD12	1.81	0.40
2:B:101:GLU:OE1	2:B:101:GLU:CA	2.70	0.40
2:B:384:LEU:CB	2:B:391:ILE:HD13	2.48	0.40
1:A:113:ARG:NH1	1:A:157:LEU:HB2	2.36	0.40
1:A:245:PHE:HE2	1:A:252:LEU:HD12	1.84	0.40
2:B:246:ILE:HD12	2:B:261:CYS:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:O	2:B:114:ARG:NH1[12_544]	2.02	0.18

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	505/507 (100%)	486 (96%)	18 (4%)	1 (0%)	44	73
2	B	444/450 (99%)	415 (94%)	28 (6%)	1 (0%)	44	73
All	All	949/957 (99%)	901 (95%)	46 (5%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	228	PRO
1	A	392	LYS

5.3.2 Protein sidechains [i](#)

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	444/446 (100%)	391 (88%)	53 (12%)	4	18
2	B	392/415 (94%)	315 (80%)	77 (20%)	1	5
All	All	836/861 (97%)	706 (84%)	130 (16%)	2	9

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	50	LEU
1	A	54	LYS
1	A	55	SER
1	A	57	LEU
1	A	62	LYS
1	A	64	ILE
1	A	78	PHE
1	A	84	CYS
1	A	89	GLN
1	A	93	PHE
1	A	127	THR
1	A	133	GLU
1	A	155	SER
1	A	162	VAL
1	A	164	THR
1	A	169	SER
1	A	184	GLU
1	A	187	ASN
1	A	211	LYS
1	A	213	ARG
1	A	217	HIS
1	A	222	GLN
1	A	227	SER
1	A	235	LYS
1	A	237	THR
1	A	267	LYS
1	A	270	LYS
1	A	271	LEU
1	A	273	ASP
1	A	274	ILE
1	A	275	ARG
1	A	330	LEU
1	A	333	LYS
1	A	334	GLU
1	A	338	LEU
1	A	339	LEU
1	A	340	THR
1	A	346	TYR
1	A	347	LYS
1	A	350	ASN
1	A	368	GLU
1	A	390	LYS

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Mol	Chain	Res	Type
1	A	391	SER
1	A	394	LEU
1	A	446	ASN
1	A	451	GLU
1	A	470	CYS
1	A	471	ILE
1	A	472	TYR
1	A	480	LEU
1	A	484	ASN
1	A	497	LYS
2	B	1	MET
2	B	2	ARG
2	B	12	PRO
2	B	17	PHE
2	B	18	THR
2	B	21	LEU
2	B	22	SER
2	B	25	LEU
2	B	28	LEU
2	B	46	TRP
2	B	53	ILE
2	B	56	ASN
2	B	57	THR
2	B	71	ARG
2	B	74	VAL
2	B	75	LEU
2	B	78	LEU
2	B	82	THR
2	B	83	LYS
2	B	86	LYS
2	B	87	HIS
2	B	88	LEU
2	B	89	GLN
2	B	91	ASP
2	B	95	ILE
2	B	101	GLU
2	B	102	ASN
2	B	105	TYR
2	B	106	ASP
2	B	107	ASP
2	B	110	ILE
2	B	114	ARG

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Mol	Chain	Res	Type
2	B	116	ASN
2	B	121	LYS
2	B	128	LEU
2	B	131	LEU
2	B	132	LEU
2	B	136	GLU
2	B	150	SER
2	B	163	GLN
2	B	183	ASN
2	B	189	ARG
2	B	191	ASP
2	B	193	ARG
2	B	194	LEU
2	B	202	THR
2	B	211	LYS
2	B	212	GLU
2	B	213	TYR
2	B	221	TYR
2	B	254	ASP
2	B	256	ILE
2	B	257	ARG
2	B	258	ASN
2	B	262	GLN
2	B	263	ARG
2	B	269	ILE
2	B	283	ARG
2	B	285	TYR
2	B	287	MET
2	B	288	SER
2	B	289	LYS
2	B	290	THR
2	B	300	LEU
2	B	301	GLU
2	B	324	SER
2	B	345	MET
2	B	360	SER
2	B	361	ARG
2	B	370	ASN
2	B	374	ARG
2	B	388	GLN
2	B	408	LEU
2	B	420	SER

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Mol	Chain	Res	Type
2	B	425	GLU
2	B	426	GLU
2	B	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	187	ASN
1	A	217	HIS
1	A	349	GLN
1	A	360	HIS
1	A	371	ASN
1	A	454	GLN
2	B	116	ASN
2	B	138	GLN
2	B	258	ASN
2	B	262	GLN
2	B	314	GLN
2	B	340	HIS
2	B	389	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	507/507 (100%)	0.07	5 (0%) 79 65	53, 96, 135, 156	0
2	B	446/450 (99%)	0.39	24 (5%) 32 21	88, 129, 167, 195	0
All	All	953/957 (99%)	0.22	29 (3%) 52 36	53, 114, 158, 195	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	ALA	4.7
2	B	78	LEU	4.7
2	B	9	HIS	3.8
2	B	427	GLU	3.8
1	A	496	ILE	3.4
2	B	10	ALA	3.4
2	B	217	PHE	3.3
2	B	110	ILE	3.2
2	B	115	LEU	3.0
2	B	5	ILE	3.0
2	B	405	ASN	2.9
2	B	80	VAL	2.9
2	B	436	PHE	2.8
2	B	425	GLU	2.8
1	A	289	GLU	2.7
2	B	446	LEU	2.5
2	B	36	ILE	2.4
2	B	95	ILE	2.4
2	B	118	ILE	2.4
1	A	186	PHE	2.3
2	B	442	ASP	2.3
2	B	77	GLU	2.3
2	B	96	PRO	2.3
2	B	99	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	221	TYR	2.2
1	A	65	TYR	2.2
2	B	93	PHE	2.1
1	A	109	SER	2.1
2	B	60	PHE	2.1

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
3	MG	A	601	1/1	0.89	0.34	33,33,33,33	0
3	MG	B	501	1/1	0.90	0.09	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.