



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:57 PM UTC

PDB ID : 2VGL / pdb_00002vgl
Title : AP2 CLATHRIN ADAPTOR CORE
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Deposited on : 2007-11-14
Resolution : 2.60 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

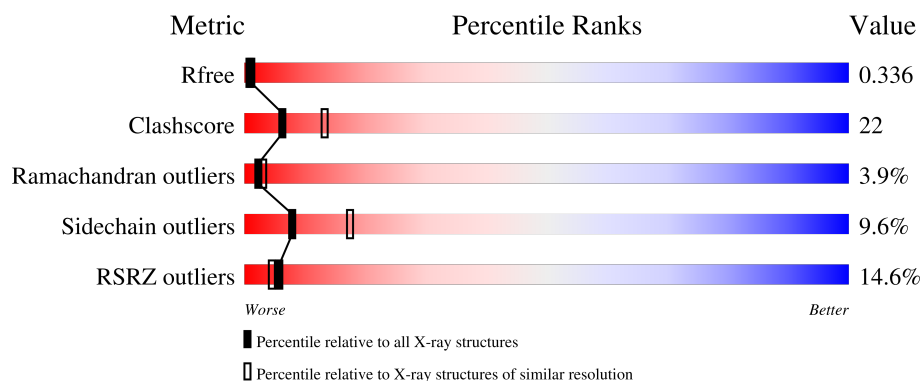
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	621	
2	B	591	
3	M	435	
4	S	142	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13755 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 ADAPTOR PROTEIN COMPLEX AP-2, ALPHA 2 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4737	3017	815	884	21			

- Molecule 2 is a protein called AP-2 COMPLEX SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	579	Total	C	N	O	S	0	0	0
			4578	2919	762	872	25			

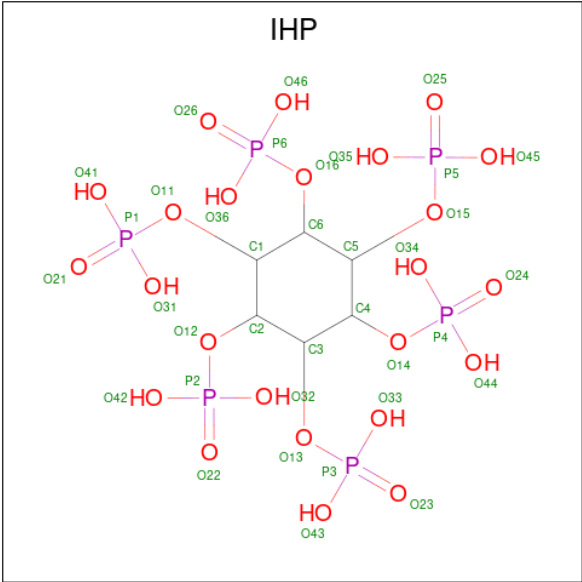
- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	396	Total	C	N	O	S	0	0	0
			3192	2053	559	561	19			

- Molecule 4 is a protein called AP-2 COMPLEX SUBUNIT SIGMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			36	6	24	6		

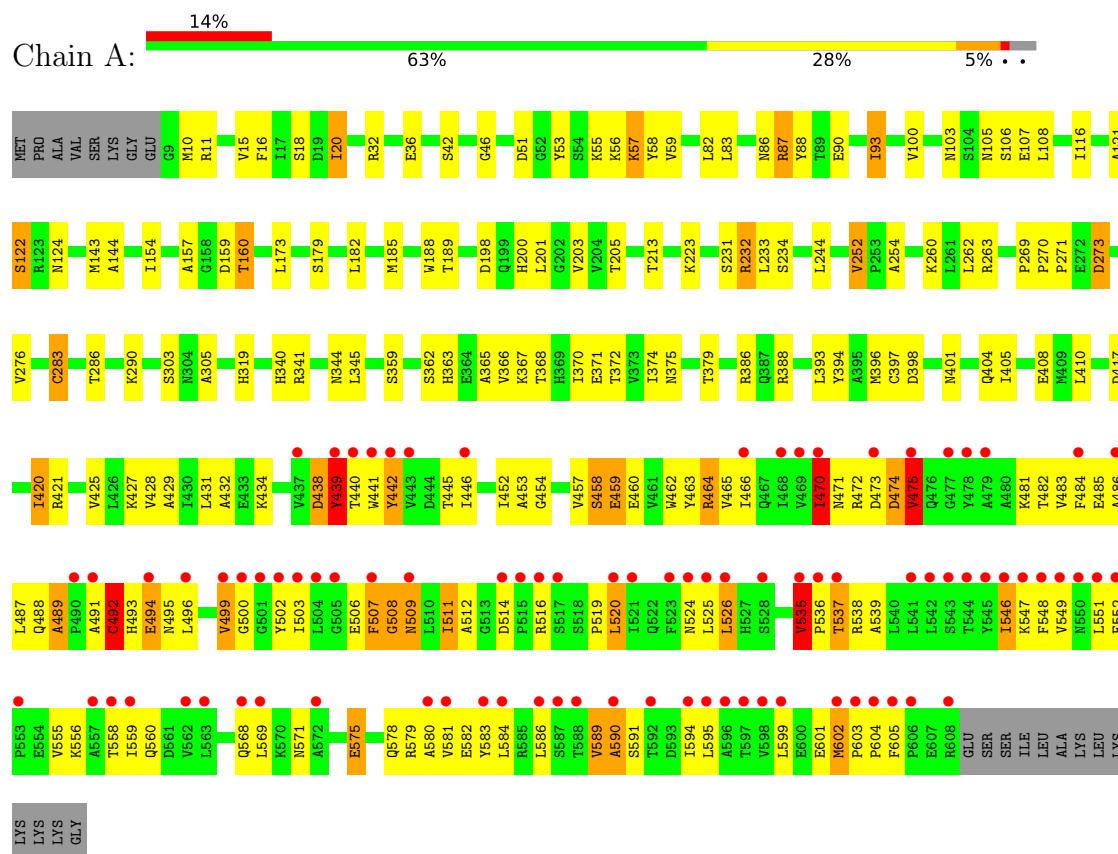
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	1	Total	O	0	0
			1	1		
6	M	2	Total	O	0	0
			2	2		
6	S	5	Total	O	0	0
			5	5		

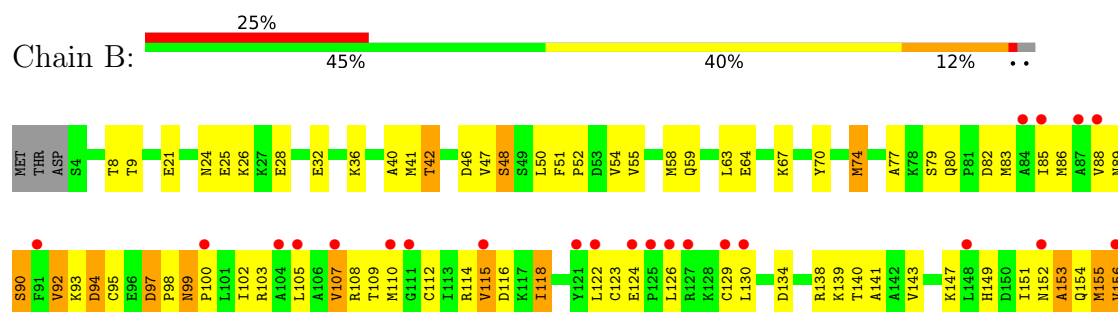
3 Residue-property plots [i](#)

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: ADAPTOR PROTEIN COMPLEX AP-2, ALPHA 2 SUBUNIT

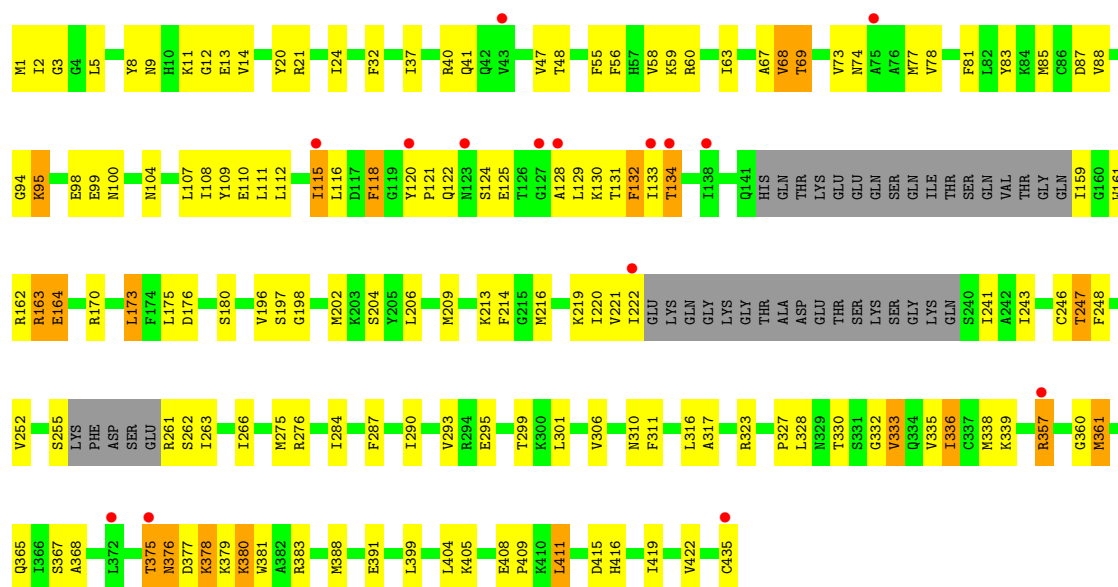


• Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1

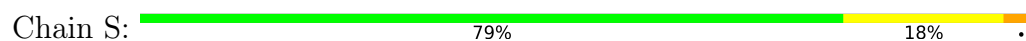




• Molecule 3: AP-2 COMPLEX SUBUNIT MU-1



• Molecule 4: AP-2 COMPLEX SUBUNIT SIGMA-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.75Å 121.75Å 258.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.67 – 2.60 66.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (66.67-2.60) 99.2 (66.67-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.339 0.258 , 0.336	Depositor DCC
R_{free} test set	3498 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13755	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: IHP

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	1.08	2/4822 (0.0%)	1.14	10/6541 (0.2%)
2	B	0.87	0/4650	1.07	16/6309 (0.3%)
3	M	1.07	1/3255 (0.0%)	1.08	7/4382 (0.2%)
4	S	1.34	2/1224 (0.2%)	1.20	4/1650 (0.2%)
All	All	1.04	5/13951 (0.0%)	1.11	37/18882 (0.2%)

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
2	B	0	5
3	M	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	19	TRP	CA-C	-5.98	1.45	1.52
3	M	40	ARG	CA-C	5.64	1.55	1.52
1	A	93	ILE	CA-CB	-5.37	1.47	1.54
4	S	90	VAL	CA-CB	-5.20	1.48	1.54
1	A	100	VAL	C-O	-5.04	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	39	VAL	N-CA-C	8.13	118.93	110.72
2	B	286	PRO	N-CA-C	7.39	119.71	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	MET	N-CA-C	-7.00	103.58	111.07
2	B	200	ASN	N-CA-C	6.84	121.79	112.55
1	A	535	VAL	CA-C-N	-6.76	112.84	119.87
1	A	535	VAL	C-N-CA	-6.76	112.84	119.87
3	M	262	SER	N-CA-C	6.47	117.66	108.74
2	B	248	LEU	N-CA-C	-6.29	102.30	111.30
3	M	266	ILE	CA-C-N	-6.02	115.33	119.66
3	M	266	ILE	C-N-CA	-6.02	115.33	119.66
2	B	330	ASP	CA-C-N	5.99	125.93	119.76
2	B	330	ASP	C-N-CA	5.99	125.93	119.76
2	B	454	GLU	N-CA-C	-5.83	102.97	110.19
2	B	273	ASP	N-CA-C	-5.80	104.33	111.40
1	A	494	GLU	N-CA-C	5.74	120.85	111.37
2	B	577	PRO	O-C-N	5.71	123.83	121.15
2	B	220	ILE	N-CA-C	5.67	121.13	109.34
2	B	193	ASN	N-CA-C	5.66	119.80	113.01
1	A	492	CYS	N-CA-C	5.63	122.79	110.80
3	M	333	VAL	N-CA-C	5.60	115.95	108.27
2	B	253	SER	N-CA-C	5.57	120.34	112.93
2	B	297	GLU	N-CA-C	-5.52	105.34	111.36
4	S	38	VAL	N-CA-C	5.51	115.96	110.23
2	B	214	CYS	N-CA-C	5.45	118.18	110.50
4	S	60	ARG	CA-C-N	-5.44	114.27	122.81
4	S	60	ARG	C-N-CA	-5.44	114.27	122.81
1	A	493	HIS	N-CA-C	5.42	118.10	109.81
3	M	68	VAL	N-CA-C	5.38	116.02	108.17
3	M	198	GLY	N-CA-C	5.34	119.08	111.12
2	B	209	THR	N-CA-C	-5.25	106.20	113.18
3	M	219	LYS	N-CA-C	5.24	118.78	112.38
1	A	232	ARG	N-CA-C	5.24	117.07	111.36
1	A	438	ASP	N-CA-C	5.18	116.75	107.80
1	A	489	ALA	N-CA-C	-5.13	103.31	109.72
2	B	548	ILE	N-CA-C	-5.05	104.50	110.21
1	A	203	VAL	CB-CA-C	-5.04	105.26	112.22
1	A	252	VAL	N-CA-C	-5.03	102.14	107.77

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	190	SER	Peptide
2	B	191	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	B	197	LEU	Peptide
2	B	199	LEU	Peptide
2	B	273	ASP	Peptide
3	M	379	LYS	Peptide

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	4737	0	4830	206	0
2	B	4578	0	4686	297	3
3	M	3192	0	3295	113	0
4	S	1200	0	1195	23	0
5	A	36	0	6	4	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	M	2	0	0	1	0
6	S	5	0	0	0	0
All	All	13755	0	14012	619	3

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 22.

All (619) 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)
3:M:1:MET:O	3:M:69:THR:HG21	1.28	1.22
1:A:103:ASN:HD21	1:A:108:LEU:HD12	1.06	1.17
2:B:251:ALA:HB3	2:B:255:VAL:HG23	1.27	1.16
3:M:361:MET:HE2	3:M:361:MET:HA	1.26	1.08
2:B:85:ILE:HD11	2:B:115:VAL:HG21	1.39	1.04
3:M:163:ARG:O	3:M:209:MET:HE1	1.54	1.04
2:B:186:GLU:OE2	3:M:1:MET:HE2	1.59	1.03
1:A:483:VAL:HG21	1:A:503:ILE:HD12	1.40	1.01
2:B:411:ILE:HD12	2:B:448:MET:HE3	1.40	1.01
1:A:509:ASN:HD22	1:A:509:ASN:N	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ALA:HB1	1:A:579:ARG:NH2	1.77	1.00
2:B:411:ILE:CD1	2:B:448:MET:HE3	1.93	0.98
2:B:351:ILE:HD11	2:B:384:VAL:HG11	1.46	0.97
4:S:93:GLU:CG	4:S:132:LEU:HD11	1.93	0.97
3:M:1:MET:SD	3:M:77:MET:HE1	2.05	0.97
2:B:541:VAL:HG12	2:B:542:LEU:HD23	1.49	0.94
3:M:1:MET:O	3:M:69:THR:CG2	2.15	0.94
2:B:186:GLU:OE2	3:M:1:MET:CE	2.15	0.94
1:A:509:ASN:H	1:A:509:ASN:ND2	1.58	0.94
1:A:198:ASP:O	1:A:232:ARG:NH2	2.00	0.94
3:M:361:MET:HA	3:M:361:MET:CE	1.97	0.94
1:A:103:ASN:ND2	1:A:108:LEU:HD12	1.82	0.93
1:A:344:ASN:HD21	4:S:48:ASN:HD22	0.99	0.93
1:A:10:MET:HE3	1:A:56:LYS:HE3	1.50	0.93
2:B:292:LEU:HD21	2:B:303:LEU:HD21	1.50	0.93
1:A:507:PHE:HA	1:A:509:ASN:HD21	1.33	0.92
1:A:539:ALA:HB1	1:A:579:ARG:CZ	2.01	0.91
2:B:289:VAL:HG22	2:B:323:VAL:HG21	1.54	0.89
1:A:507:PHE:C	1:A:509:ASN:ND2	2.31	0.89
2:B:271:PRO:HB2	2:B:272:LYS:HG2	1.54	0.89
2:B:153:ALA:HB1	2:B:155:MET:HG2	1.56	0.88
1:A:546:ILE:HG23	1:A:599:LEU:CD1	2.05	0.87
2:B:488:ILE:HD12	2:B:506:VAL:HG21	1.57	0.87
2:B:251:ALA:O	2:B:253:SER:N	2.07	0.86
3:M:163:ARG:O	3:M:209:MET:CE	2.25	0.85
4:S:93:GLU:HG2	4:S:132:LEU:HD11	1.57	0.85
1:A:507:PHE:C	1:A:509:ASN:HD22	1.85	0.85
2:B:143:VAL:CG2	2:B:179:ASN:OD1	2.25	0.85
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.58	0.85
2:B:143:VAL:HG22	2:B:179:ASN:OD1	1.76	0.85
3:M:220:ILE:HD12	3:M:399:LEU:HD13	1.60	0.84
1:A:507:PHE:HA	1:A:509:ASN:ND2	1.93	0.84
2:B:143:VAL:HG21	3:M:122:GLN:NE2	1.92	0.83
3:M:310:ASN:CG	3:M:310:ASN:O	2.21	0.83
2:B:251:ALA:HB3	2:B:255:VAL:CG2	2.07	0.83
2:B:58:MET:HE3	2:B:70:TYR:CE1	2.14	0.83
2:B:85:ILE:HD11	2:B:115:VAL:CG2	2.08	0.83
2:B:143:VAL:HG21	3:M:122:GLN:HE22	1.44	0.83
1:A:374:ILE:HD13	1:A:408:GLU:HG3	1.61	0.82
3:M:88:VAL:HG11	3:M:111:LEU:HD22	1.61	0.82
1:A:507:PHE:CA	1:A:509:ASN:HD21	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ALA:CB	2:B:155:MET:HG2	2.09	0.81
2:B:411:ILE:CD1	2:B:448:MET:CE	2.59	0.81
2:B:374:VAL:HG21	2:B:409:GLU:HB3	1.62	0.81
2:B:476:GLU:HB3	2:B:480:VAL:CG1	2.11	0.81
2:B:411:ILE:HD11	2:B:448:MET:CE	2.10	0.81
1:A:56:LYS:HG2	1:A:93:ILE:HD13	1.63	0.81
2:B:364:GLU:HA	2:B:364:GLU:OE1	1.81	0.80
4:S:93:GLU:HG3	4:S:132:LEU:HD11	1.62	0.80
2:B:103:ARG:O	2:B:107:VAL:HG23	1.82	0.79
2:B:292:LEU:HD21	2:B:303:LEU:CD2	2.11	0.79
2:B:351:ILE:CD1	2:B:384:VAL:HG11	2.12	0.79
1:A:546:ILE:HG23	1:A:599:LEU:HD11	1.64	0.79
2:B:381:ALA:HB2	2:B:391:CYS:SG	2.22	0.79
2:B:90:SER:O	2:B:94:ASP:HB2	1.83	0.79
2:B:511:THR:CG2	2:B:524:TYR:CE2	2.65	0.79
4:S:3:ARG:HB3	4:S:21:MET:CE	2.13	0.79
1:A:370:ILE:HA	1:A:396:MET:HE1	1.66	0.78
2:B:511:THR:HG22	2:B:512:GLN:NE2	1.99	0.78
2:B:215:THR:HG22	2:B:217:TRP:H	1.49	0.78
2:B:83:MET:HA	2:B:86:MET:HE2	1.63	0.78
2:B:476:GLU:HB3	2:B:480:VAL:HG11	1.66	0.77
1:A:483:VAL:CG2	1:A:503:ILE:HD12	2.15	0.77
4:S:3:ARG:HB3	4:S:21:MET:HE2	1.65	0.77
1:A:344:ASN:HD21	4:S:48:ASN:ND2	1.79	0.77
2:B:251:ALA:CB	2:B:255:VAL:HG23	2.13	0.77
2:B:374:VAL:CG2	2:B:409:GLU:HB3	2.15	0.77
3:M:5:LEU:CD2	3:M:85:MET:HE1	2.15	0.77
1:A:386:ARG:CD	1:A:420:ILE:HD11	2.15	0.77
1:A:507:PHE:CA	1:A:509:ASN:ND2	2.48	0.77
2:B:374:VAL:HG21	2:B:409:GLU:CB	2.15	0.76
1:A:520:LEU:HD22	1:A:524:ASN:ND2	2.01	0.75
2:B:152:ASN:O	2:B:153:ALA:HB2	1.86	0.75
2:B:63:LEU:CD1	2:B:102:ILE:HD11	2.16	0.74
2:B:155:MET:O	2:B:158:ASP:HB2	1.87	0.74
2:B:269:LEU:O	2:B:271:PRO:HD3	1.85	0.74
2:B:251:ALA:O	2:B:252:ASN:C	2.30	0.74
2:B:429:ILE:HG21	2:B:459:ILE:HD11	1.70	0.74
2:B:250:HIS:O	2:B:252:ASN:N	2.21	0.74
1:A:470:ILE:HD13	1:A:605:PHE:HD1	1.52	0.73
2:B:260:VAL:HG21	2:B:288:LEU:HD21	1.70	0.73
1:A:386:ARG:HD2	1:A:420:ILE:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASN:O	2:B:153:ALA:CB	2.37	0.73
2:B:511:THR:HG21	2:B:524:TYR:CE2	2.23	0.73
1:A:370:ILE:CA	1:A:396:MET:HE1	2.18	0.73
3:M:81:PHE:CE1	3:M:116:LEU:HD13	2.24	0.73
3:M:63:ILE:HD11	3:M:98:GLU:N	2.03	0.73
1:A:16:PHE:CZ	1:A:20:ILE:HD11	2.24	0.73
1:A:438:ASP:O	1:A:440:THR:N	2.22	0.72
2:B:408:GLN:O	2:B:411:ILE:HG22	1.89	0.72
1:A:16:PHE:CE1	1:A:20:ILE:HD11	2.24	0.72
1:A:410:LEU:HD11	1:A:445:THR:HG23	1.72	0.71
1:A:473:ASP:O	1:A:475:VAL:N	2.23	0.71
3:M:162:ARG:O	3:M:209:MET:HE1	1.91	0.70
1:A:375:ASN:O	1:A:379:THR:HG22	1.91	0.70
3:M:375:THR:HG22	3:M:376:ASN:N	2.06	0.70
1:A:370:ILE:CB	1:A:396:MET:HE1	2.20	0.70
2:B:74:MET:HE2	2:B:74:MET:HA	1.72	0.70
2:B:297:GLU:HB2	3:M:83:TYR:OH	1.92	0.70
3:M:164:GLU:HA	3:M:209:MET:HE3	1.74	0.70
2:B:411:ILE:HD11	2:B:448:MET:HE2	1.71	0.70
3:M:361:MET:CE	3:M:361:MET:CA	2.67	0.70
2:B:153:ALA:HB1	2:B:155:MET:HE3	1.74	0.69
3:M:81:PHE:CZ	3:M:116:LEU:HD13	2.27	0.69
2:B:292:LEU:CD2	2:B:303:LEU:HD21	2.22	0.69
2:B:63:LEU:HD12	2:B:102:ILE:HD11	1.74	0.69
1:A:470:ILE:HD13	1:A:605:PHE:CD1	2.28	0.68
1:A:470:ILE:CD1	1:A:605:PHE:HD1	2.05	0.68
1:A:483:VAL:HG21	1:A:503:ILE:CD1	2.19	0.68
1:A:472:ARG:HG3	1:A:472:ARG:HH11	1.57	0.68
2:B:295:GLU:O	2:B:298:VAL:HG12	1.94	0.68
2:B:92:VAL:HG23	2:B:93:LYS:H	1.58	0.68
1:A:569:LEU:HD22	1:A:581:VAL:HG22	1.76	0.68
3:M:336:ILE:HG23	3:M:367:SER:OG	1.94	0.67
1:A:10:MET:HE1	1:A:56:LYS:HG2	1.75	0.67
1:A:586:LEU:HG	2:B:540:VAL:HG11	1.74	0.67
3:M:108:ILE:O	3:M:112:LEU:HD13	1.93	0.67
2:B:257:LEU:HD13	2:B:305:ASN:HD22	1.58	0.67
1:A:10:MET:CE	1:A:56:LYS:HG2	2.25	0.67
2:B:249:SER:OG	2:B:250:HIS:N	2.22	0.66
1:A:56:LYS:CG	1:A:93:ILE:HD13	2.25	0.66
2:B:129:CYS:HB3	2:B:141:ALA:HB2	1.76	0.66
3:M:20:TYR:CE1	3:M:116:LEU:HD23	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:PHE:C	1:A:509:ASN:H	2.03	0.66
2:B:173:ASN:HB3	2:B:176:VAL:HG23	1.78	0.66
2:B:205:ASN:HA	2:B:243:ARG:HH12	1.61	0.66
2:B:502:LEU:O	2:B:504:GLN:N	2.29	0.65
1:A:233:LEU:HD21	1:A:262:LEU:HD21	1.77	0.65
1:A:32:ARG:NH1	1:A:36:GLU:HG2	2.11	0.65
3:M:241:ILE:O	3:M:243:ILE:HD12	1.96	0.65
1:A:56:LYS:HG2	1:A:93:ILE:CD1	2.26	0.65
1:A:507:PHE:O	1:A:509:ASN:N	2.30	0.65
1:A:507:PHE:O	1:A:509:ASN:ND2	2.30	0.65
3:M:248:PHE:CE2	3:M:275:MET:HE3	2.31	0.65
1:A:56:LYS:CG	1:A:93:ILE:CD1	2.74	0.65
1:A:205:THR:HG23	1:A:260:LYS:HD2	1.79	0.65
1:A:10:MET:HE3	1:A:56:LYS:CE	2.24	0.65
2:B:470:LEU:HD11	2:B:506:VAL:CG2	2.27	0.65
2:B:511:THR:HG23	2:B:524:TYR:CE2	2.30	0.65
3:M:246:CYS:SG	3:M:275:MET:HE2	2.36	0.64
2:B:186:GLU:OE2	3:M:1:MET:HE3	1.97	0.64
1:A:568:GLN:HB3	1:A:580:ALA:HB1	1.77	0.64
2:B:130:LEU:O	2:B:138:ARG:HD3	1.97	0.64
2:B:74:MET:HE2	2:B:77:ALA:HB2	1.79	0.64
2:B:155:MET:O	2:B:158:ASP:CB	2.46	0.64
3:M:293:VAL:HG11	3:M:383:ARG:HE	1.62	0.64
4:S:3:ARG:HD2	4:S:21:MET:HE2	1.79	0.64
1:A:344:ASN:ND2	4:S:48:ASN:HD22	1.84	0.64
3:M:3:GLY:N	3:M:69:THR:HG23	2.13	0.64
2:B:46:ASP:OD1	2:B:48:SER:OG	2.16	0.64
1:A:370:ILE:HB	1:A:396:MET:CE	2.28	0.63
2:B:92:VAL:O	2:B:95:CYS:SG	2.57	0.63
1:A:470:ILE:CD1	1:A:605:PHE:CD1	2.81	0.63
1:A:179:SER:HB3	1:A:182:LEU:HD12	1.80	0.63
2:B:492:PHE:HB3	2:B:530:LEU:HD11	1.80	0.63
1:A:549:VAL:HG13	1:A:556:LYS:HB2	1.81	0.62
1:A:370:ILE:HB	1:A:396:MET:HE1	1.82	0.62
1:A:454:GLY:HA2	1:A:457:VAL:HG23	1.81	0.62
1:A:507:PHE:C	1:A:509:ASN:N	2.56	0.62
1:A:590:ALA:HB1	1:A:594:ILE:HG21	1.82	0.62
1:A:520:LEU:HD22	1:A:524:ASN:HD21	1.63	0.61
1:A:546:ILE:HG23	1:A:599:LEU:HD13	1.81	0.61
1:A:58:TYR:OH	5:A:1609:IHP:O25	2.17	0.61
1:A:495:ASN:O	1:A:499:VAL:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASN:HB3	1:A:405:ILE:CD1	2.31	0.61
3:M:58:VAL:HG11	3:M:60:ARG:HE	1.65	0.61
2:B:511:THR:HG23	2:B:524:TYR:CZ	2.36	0.61
1:A:103:ASN:HD21	1:A:108:LEU:CD1	1.99	0.61
2:B:511:THR:HG22	2:B:512:GLN:HE21	1.63	0.61
1:A:397:CYS:SG	1:A:431:LEU:HD22	2.41	0.61
2:B:529:LEU:HD23	2:B:537:ALA:HA	1.83	0.61
2:B:90:SER:O	2:B:94:ASP:CB	2.48	0.60
2:B:470:LEU:HD11	2:B:506:VAL:HG23	1.83	0.60
3:M:94:GLY:O	3:M:95:LYS:O	2.19	0.60
2:B:153:ALA:CB	2:B:155:MET:HE3	2.32	0.60
1:A:460:GLU:O	1:A:464:ARG:N	2.34	0.60
2:B:8:THR:HG22	2:B:8:THR:O	2.02	0.60
2:B:253:SER:CB	2:B:298:VAL:HG21	2.32	0.60
1:A:386:ARG:HD3	1:A:420:ILE:HD11	1.82	0.59
3:M:173:LEU:HD12	3:M:173:LEU:C	2.27	0.59
2:B:474:HIS:O	2:B:476:GLU:HG2	2.02	0.59
1:A:512:ALA:HB2	1:A:552:PHE:CZ	2.38	0.59
1:A:159:ASP:OD1	1:A:159:ASP:N	2.36	0.59
1:A:201:LEU:HD11	1:A:244:LEU:HD22	1.82	0.59
1:A:547:LYS:HG3	1:A:599:LEU:HD22	1.83	0.59
2:B:526:TYR:O	2:B:529:LEU:N	2.32	0.59
1:A:16:PHE:O	1:A:20:ILE:HD12	2.02	0.59
1:A:365:ALA:O	1:A:368:THR:HB	2.03	0.59
3:M:162:ARG:O	3:M:163:ARG:O	2.19	0.59
2:B:220:ILE:HD11	2:B:254:ALA:HB3	1.84	0.59
3:M:175:LEU:HD23	3:M:202:MET:HG3	1.84	0.59
3:M:221:VAL:HG12	3:M:222:ILE:H	1.67	0.59
2:B:220:ILE:CD1	2:B:254:ALA:HB3	2.33	0.58
3:M:335:VAL:HG22	3:M:368:ALA:HB2	1.85	0.58
4:S:36:HIS:CE1	4:S:40:THR:HG21	2.38	0.58
2:B:174:PRO:HA	2:B:177:VAL:CG1	2.33	0.58
2:B:508:SER:OG	2:B:509:LEU:HD23	2.03	0.58
2:B:271:PRO:CB	2:B:272:LYS:HG2	2.31	0.58
2:B:493:LEU:HD21	2:B:537:ALA:HB3	1.86	0.58
1:A:442:TYR:CE2	1:A:446:ILE:HD11	2.39	0.58
1:A:473:ASP:CG	1:A:474:ASP:H	2.11	0.58
2:B:299:GLN:O	2:B:303:LEU:HG	2.04	0.58
2:B:74:MET:HE1	2:B:112:CYS:CB	2.34	0.58
2:B:173:ASN:OD1	2:B:175:MET:HG2	2.04	0.58
2:B:305:ASN:OD1	2:B:572:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HH12	1:A:36:GLU:HG2	1.69	0.57
2:B:74:MET:HE1	2:B:112:CYS:HB2	1.87	0.57
2:B:227:SER:OG	2:B:262:VAL:HG22	2.05	0.57
2:B:267:LEU:HD11	2:B:277:TYR:CE1	2.39	0.57
3:M:3:GLY:H	3:M:69:THR:HG23	1.68	0.57
2:B:435:ASN:HA	2:B:437:ASP:OD1	2.04	0.57
1:A:506:GLU:HB3	1:A:507:PHE:CE1	2.40	0.57
3:M:5:LEU:HD21	3:M:85:MET:SD	2.44	0.57
3:M:377:ASP:O	3:M:378:LYS:CB	2.52	0.57
1:A:370:ILE:HG23	1:A:371:GLU:N	2.20	0.57
2:B:21:GLU:OE1	2:B:36:LYS:NZ	2.38	0.56
2:B:67:LYS:HZ3	2:B:105:LEU:HD13	1.71	0.56
1:A:519:PRO:HB3	1:A:552:PHE:CD2	2.40	0.56
2:B:63:LEU:HD11	2:B:102:ILE:HD11	1.85	0.56
2:B:155:MET:HE2	2:B:155:MET:HA	1.86	0.56
3:M:107:LEU:O	3:M:110:GLU:N	2.38	0.56
1:A:546:ILE:HD12	1:A:583:TYR:CD1	2.41	0.56
3:M:120:TYR:O	3:M:122:GLN:N	2.38	0.56
1:A:509:ASN:HD22	1:A:509:ASN:H	0.77	0.56
1:A:442:TYR:CE2	1:A:446:ILE:CD1	2.88	0.56
1:A:509:ASN:N	1:A:509:ASN:ND2	2.30	0.56
1:A:555:VAL:HG22	1:A:555:VAL:O	2.06	0.56
2:B:110:MET:O	2:B:118:ILE:HD11	2.05	0.56
2:B:325:PHE:O	2:B:338:LYS:NZ	2.35	0.56
3:M:159:ILE:HG22	3:M:161:TRP:H	1.70	0.55
1:A:359:SER:O	1:A:363:HIS:N	2.39	0.55
1:A:520:LEU:CD2	1:A:524:ASN:HD21	2.20	0.55
2:B:123:CYS:SG	2:B:124:GLU:N	2.79	0.55
1:A:200:HIS:CE1	4:S:130:LYS:HZ2	2.25	0.55
1:A:442:TYR:HE2	1:A:446:ILE:CD1	2.19	0.55
3:M:88:VAL:HG11	3:M:111:LEU:CD2	2.35	0.55
3:M:2:ILE:HD12	3:M:116:LEU:HD11	1.88	0.55
3:M:216:MET:SD	3:M:399:LEU:HD11	2.47	0.55
1:A:340:HIS:CE1	1:A:345:LEU:HD12	2.42	0.55
1:A:486:ALA:HB1	1:A:496:LEU:HD21	1.89	0.55
2:B:217:TRP:O	2:B:221:PHE:CE1	2.60	0.55
1:A:549:VAL:HG23	1:A:559:ILE:HD13	1.89	0.55
2:B:408:GLN:OE1	2:B:441:GLU:HB2	2.06	0.55
2:B:350:ASN:O	2:B:352:ALA:N	2.40	0.54
2:B:306:ILE:HD13	2:B:324:PHE:HZ	1.73	0.54
2:B:50:LEU:O	2:B:54:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:375:THR:O	3:M:376:ASN:C	2.51	0.54
2:B:85:ILE:CD1	2:B:115:VAL:HG21	2.26	0.54
3:M:100:ASN:O	3:M:104:ASN:ND2	2.33	0.54
3:M:202:MET:HE2	3:M:204:SER:HB3	1.89	0.54
3:M:377:ASP:O	3:M:378:LYS:HB2	2.08	0.54
2:B:155:MET:HB2	2:B:158:ASP:HB2	1.90	0.54
1:A:549:VAL:HG23	1:A:559:ILE:HG21	1.89	0.54
2:B:156:VAL:O	2:B:159:GLN:N	2.38	0.54
3:M:41:GLN:HG2	3:M:284:ILE:HD13	1.90	0.54
2:B:67:LYS:NZ	2:B:105:LEU:HD13	2.23	0.54
2:B:477:SER:O	2:B:480:VAL:HG12	2.08	0.54
3:M:316:LEU:HD22	3:M:357:ARG:HB3	1.89	0.54
2:B:310:VAL:HG21	2:B:345:LEU:HD21	1.90	0.54
1:A:42:SER:O	1:A:46:GLY:N	2.40	0.53
1:A:454:GLY:HA2	1:A:457:VAL:CG2	2.38	0.53
1:A:485:GLU:HA	1:A:488:GLN:HG2	1.91	0.53
2:B:267:LEU:HD11	2:B:277:TYR:CD1	2.43	0.53
3:M:20:TYR:CZ	3:M:116:LEU:HD23	2.43	0.53
1:A:487:LEU:HB3	1:A:525:LEU:HD21	1.89	0.53
1:A:568:GLN:HB3	1:A:580:ALA:CB	2.37	0.53
2:B:156:VAL:HG12	2:B:159:GLN:NE2	2.23	0.53
2:B:476:GLU:HB3	2:B:480:VAL:HG12	1.90	0.53
3:M:73:VAL:CG1	3:M:74:ASN:N	2.71	0.53
4:S:3:ARG:CB	4:S:21:MET:HE2	2.37	0.53
1:A:569:LEU:HD22	1:A:581:VAL:CG2	2.38	0.53
2:B:149:HIS:CD2	2:B:187:ILE:HG23	2.44	0.53
1:A:11:ARG:NE	5:A:1609:IHP:O34	2.33	0.53
2:B:262:VAL:C	2:B:264:MET:H	2.17	0.53
2:B:42:THR:HG23	3:M:109:TYR:OH	2.09	0.53
2:B:88:VAL:HG12	2:B:110:MET:HE1	1.90	0.53
2:B:174:PRO:HA	2:B:177:VAL:HG12	1.90	0.53
2:B:377:ILE:CG2	2:B:395:LEU:HD21	2.39	0.53
3:M:252:VAL:HG13	3:M:263:ILE:HG23	1.91	0.53
1:A:185:MET:HE3	1:A:185:MET:HA	1.91	0.52
2:B:249:SER:OG	2:B:255:VAL:HG11	2.08	0.52
2:B:310:VAL:CG2	2:B:345:LEU:HD21	2.38	0.52
3:M:9:ASN:OD1	3:M:13:GLU:HB2	2.09	0.52
2:B:153:ALA:HB1	2:B:155:MET:CE	2.37	0.52
3:M:338:MET:HE2	3:M:338:MET:HA	1.91	0.52
1:A:428:VAL:O	1:A:429:ALA:C	2.53	0.52
2:B:306:ILE:HD13	2:B:324:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:SER:CB	2:B:298:VAL:CG2	2.88	0.52
1:A:200:HIS:CE1	4:S:130:LYS:NZ	2.78	0.52
1:A:489:ALA:C	1:A:491:ALA:H	2.18	0.52
1:A:483:VAL:CG1	1:A:500:GLY:HA2	2.39	0.52
2:B:328:TYR:CE1	2:B:329:ASN:HB3	2.46	0.51
1:A:470:ILE:HG22	1:A:471:ASN:N	2.25	0.51
3:M:381:TRP:CZ3	3:M:383:ARG:HG2	2.46	0.51
2:B:110:MET:CG	2:B:122:LEU:HD13	2.40	0.51
2:B:307:ASN:ND2	2:B:575:HIS:CE1	2.78	0.51
1:A:116:ILE:HD11	1:A:143:MET:HE2	1.91	0.51
2:B:115:VAL:O	2:B:151:ILE:HD11	2.11	0.51
1:A:556:LYS:NZ	1:A:560:GLN:NE2	2.58	0.51
2:B:322:LYS:HA	2:B:325:PHE:CE1	2.46	0.51
1:A:370:ILE:HD12	1:A:396:MET:HE3	1.93	0.51
2:B:154:GLN:O	2:B:155:MET:O	2.28	0.51
2:B:267:LEU:CD1	2:B:277:TYR:CE1	2.94	0.51
1:A:116:ILE:CD1	1:A:143:MET:HE2	2.39	0.51
1:A:466:ILE:HD11	1:A:499:VAL:HG13	1.93	0.51
2:B:211:LEU:HD12	2:B:211:LEU:O	2.11	0.51
1:A:124:ASN:C	1:A:124:ASN:OD1	2.53	0.51
1:A:438:ASP:O	1:A:439:TYR:C	2.53	0.51
2:B:153:ALA:HB3	2:B:155:MET:HG2	1.91	0.51
1:A:512:ALA:CB	1:A:552:PHE:CZ	2.94	0.51
2:B:88:VAL:CG1	2:B:110:MET:HE1	2.41	0.51
2:B:155:MET:CB	2:B:158:ASP:HB2	2.41	0.51
2:B:449:ILE:CG2	2:B:483:THR:HG22	2.41	0.51
2:B:126:LEU:O	2:B:130:LEU:HD12	2.10	0.51
2:B:343:ILE:O	2:B:346:ALA:HB3	2.10	0.51
3:M:295:GLU:HA	3:M:301:LEU:HD12	1.93	0.51
2:B:24:ASN:OD1	2:B:25:GLU:N	2.45	0.50
2:B:216:GLU:HG3	2:B:251:ALA:HB2	1.92	0.50
2:B:404:ASN:O	2:B:408:GLN:HG3	2.11	0.50
2:B:510:ALA:O	2:B:520:ARG:HA	2.12	0.50
2:B:103:ARG:O	2:B:107:VAL:CG2	2.58	0.50
3:M:328:LEU:H	3:M:328:LEU:HD12	1.76	0.50
1:A:535:VAL:HG12	1:A:538:ARG:HH21	1.76	0.50
2:B:182:ALA:HB2	2:B:221:PHE:CG	2.46	0.50
3:M:408:GLU:HG2	3:M:411:LEU:HB2	1.93	0.50
1:A:370:ILE:CB	1:A:396:MET:CE	2.86	0.50
3:M:287:PHE:CG	3:M:388:MET:HE1	2.47	0.50
1:A:121:ALA:C	1:A:122:SER:O	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:HA	1:A:283:CYS:SG	2.51	0.50
1:A:10:MET:HE2	1:A:57:LYS:N	2.27	0.50
2:B:292:LEU:HD12	2:B:292:LEU:N	2.26	0.50
2:B:347:SER:H	2:B:350:ASN:HD21	1.59	0.50
4:S:39:VAL:CG1	4:S:66:TYR:CD2	2.94	0.50
2:B:305:ASN:OD1	2:B:572:SER:CB	2.60	0.50
2:B:397:ASP:O	2:B:401:THR:HG23	2.12	0.49
1:A:340:HIS:O	1:A:341:ARG:C	2.55	0.49
3:M:1:MET:HE3	3:M:120:TYR:CE2	2.48	0.49
1:A:601:GLU:O	1:A:602:MET:HB2	2.10	0.49
2:B:511:THR:CG2	2:B:524:TYR:CZ	2.95	0.49
2:B:548:ILE:HG22	2:B:549:SER:O	2.11	0.49
1:A:536:PRO:O	1:A:539:ALA:HB3	2.12	0.49
3:M:56:PHE:CG	3:M:78:VAL:HG11	2.48	0.49
2:B:88:VAL:C	2:B:90:SER:H	2.20	0.49
2:B:383:LYS:NZ	2:B:550:GLU:CB	2.75	0.49
3:M:111:LEU:HG	3:M:133:ILE:HD13	1.93	0.49
2:B:289:VAL:HG22	2:B:323:VAL:CG2	2.37	0.49
1:A:57:LYS:NZ	5:A:1609:IHP:O14	2.37	0.49
2:B:51:PHE:HB3	2:B:52:PRO:HD3	1.94	0.49
2:B:256:VAL:O	2:B:259:ALA:HB3	2.13	0.49
2:B:488:ILE:HG22	2:B:488:ILE:O	2.12	0.49
1:A:458:SER:OG	1:A:459:GLU:N	2.46	0.48
2:B:173:ASN:HB3	2:B:176:VAL:CG2	2.43	0.48
2:B:184:LEU:HA	2:B:187:ILE:HD12	1.94	0.48
2:B:275:ASP:HB3	2:B:278:ASN:HB2	1.94	0.48
2:B:466:LEU:HD13	2:B:488:ILE:HG12	1.93	0.48
2:B:114:ARG:HG3	2:B:151:ILE:HD12	1.96	0.48
2:B:285:ALA:HB3	2:B:286:PRO:CD	2.37	0.48
4:S:69:ILE:HG22	4:S:71:VAL:HG13	1.96	0.48
1:A:273:ASP:OD1	1:A:273:ASP:C	2.56	0.48
1:A:486:ALA:CB	1:A:496:LEU:HD21	2.43	0.48
1:A:370:ILE:HG23	1:A:371:GLU:H	1.77	0.48
1:A:483:VAL:HG11	1:A:500:GLY:HA2	1.95	0.48
1:A:575:GLU:OE1	2:B:482:LEU:HD22	2.14	0.48
1:A:466:ILE:HD11	1:A:499:VAL:CG1	2.44	0.48
2:B:99:ASN:HD22	2:B:100:PRO:HD2	1.79	0.48
2:B:377:ILE:HG21	2:B:395:LEU:HD21	1.94	0.48
1:A:393:LEU:HD23	1:A:396:MET:HE2	1.94	0.48
2:B:24:ASN:OD1	2:B:26:LYS:N	2.43	0.48
2:B:209:THR:HA	2:B:212:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:GLU:OE1	2:B:458:ARG:NH1	2.47	0.48
2:B:581:PHE:CD2	2:B:581:PHE:N	2.80	0.48
1:A:512:ALA:HB1	1:A:519:PRO:HG3	1.95	0.48
1:A:87:ARG:O	1:A:88:TYR:C	2.56	0.48
2:B:216:GLU:CD	2:B:250:HIS:NE2	2.72	0.48
2:B:305:ASN:ND2	2:B:567:ILE:O	2.47	0.48
1:A:441:TRP:O	1:A:442:TYR:C	2.56	0.48
1:A:549:VAL:CG2	1:A:559:ILE:HG21	2.44	0.48
2:B:64:GLU:HB2	3:M:134:THR:HG21	1.95	0.48
2:B:182:ALA:HB2	2:B:221:PHE:CB	2.44	0.48
2:B:267:LEU:HD21	2:B:281:LEU:HD21	1.96	0.48
2:B:328:TYR:OH	3:M:213:LYS:NZ	2.43	0.48
2:B:492:PHE:C	2:B:494:LYS:H	2.22	0.48
3:M:311:PHE:CZ	3:M:317:ALA:HB2	2.48	0.48
2:B:226:LEU:O	2:B:228:ASN:N	2.47	0.47
1:A:252:VAL:HG21	1:A:305:ALA:HB3	1.96	0.47
2:B:143:VAL:HG13	3:M:120:TYR:CE1	2.49	0.47
1:A:16:PHE:CE1	1:A:20:ILE:CD1	2.97	0.47
1:A:556:LYS:NZ	1:A:560:GLN:HE22	2.12	0.47
1:A:188:TRP:O	1:A:189:THR:C	2.58	0.47
1:A:481:LYS:HB2	1:A:511:ILE:CD1	2.44	0.47
2:B:198:ASP:N	2:B:198:ASP:OD1	2.47	0.47
3:M:306:VAL:HG22	3:M:365:GLN:HB2	1.96	0.47
2:B:382:ILE:HG22	2:B:382:ILE:O	2.14	0.47
1:A:546:ILE:CG2	1:A:599:LEU:HD11	2.39	0.47
2:B:222:ILE:O	2:B:223:LEU:C	2.57	0.47
1:A:56:LYS:CG	1:A:93:ILE:HD12	2.44	0.47
1:A:370:ILE:HB	1:A:396:MET:HE3	1.97	0.47
1:A:526:LEU:N	1:A:526:LEU:HD23	2.28	0.47
2:B:115:VAL:HG12	2:B:116:ASP:H	1.78	0.47
2:B:459:ILE:HG22	2:B:462:ALA:N	2.30	0.47
3:M:1:MET:CG	3:M:77:MET:HE1	2.44	0.47
1:A:440:THR:HG23	1:A:475:VAL:HG11	1.97	0.47
2:B:8:THR:O	2:B:9:THR:C	2.58	0.47
2:B:40:ALA:O	2:B:41:MET:C	2.58	0.47
2:B:502:LEU:O	2:B:505:GLN:N	2.48	0.47
2:B:524:TYR:O	2:B:525:ILE:C	2.58	0.47
2:B:153:ALA:HB1	2:B:155:MET:CG	2.38	0.47
2:B:154:GLN:O	2:B:154:GLN:HG3	2.15	0.47
2:B:272:LYS:HD3	2:B:278:ASN:HD21	1.79	0.47
2:B:308:LEU:O	2:B:309:ILE:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:THR:CG2	2:B:512:GLN:HE21	2.26	0.47
1:A:56:LYS:HG3	1:A:93:ILE:CD1	2.45	0.46
1:A:271:PRO:HB3	1:A:276:VAL:CG1	2.45	0.46
2:B:208:LEU:HD23	2:B:211:LEU:HD23	1.96	0.46
1:A:53:TYR:CD2	1:A:53:TYR:C	2.94	0.46
2:B:205:ASN:HA	2:B:243:ARG:NH1	2.29	0.46
2:B:375:ARG:HA	2:B:413:VAL:CG2	2.45	0.46
3:M:336:ILE:HG23	3:M:367:SER:HG	1.81	0.46
4:S:93:GLU:HG2	4:S:132:LEU:CD1	2.38	0.46
2:B:154:GLN:O	2:B:155:MET:C	2.58	0.46
1:A:55:LYS:O	1:A:59:VAL:HG23	2.15	0.46
2:B:184:LEU:HD23	2:B:196:LEU:HD23	1.97	0.46
2:B:165:LEU:HD23	2:B:184:LEU:HD13	1.97	0.46
1:A:494:GLU:OE2	1:A:537:THR:OG1	2.33	0.46
2:B:341:ILE:HG22	2:B:341:ILE:O	2.16	0.46
2:B:404:ASN:OD1	2:B:404:ASN:C	2.58	0.46
2:B:429:ILE:CG2	2:B:459:ILE:HD11	2.42	0.46
4:S:19:TRP:CG	4:S:28:LYS:HE2	2.51	0.46
1:A:286:THR:O	1:A:290:LYS:HG2	2.16	0.46
2:B:506:VAL:O	2:B:508:SER:N	2.49	0.46
3:M:3:GLY:HA2	3:M:21:ARG:HG3	1.97	0.46
2:B:92:VAL:HG23	2:B:93:LYS:N	2.28	0.46
2:B:350:ASN:C	2:B:352:ALA:N	2.70	0.46
3:M:111:LEU:HA	3:M:133:ILE:HD11	1.98	0.46
3:M:375:THR:O	3:M:377:ASP:OD1	2.35	0.45
1:A:51:ASP:OD1	1:A:51:ASP:N	2.47	0.45
2:B:470:LEU:HD21	2:B:506:VAL:HG22	1.98	0.45
1:A:442:TYR:HE2	1:A:446:ILE:HD12	1.81	0.45
3:M:196:VAL:CG1	3:M:197:SER:N	2.80	0.45
1:A:589:VAL:CG1	1:A:590:ALA:N	2.80	0.45
2:B:492:PHE:C	2:B:494:LYS:N	2.74	0.45
1:A:401:ASN:HB3	1:A:405:ILE:HD12	1.98	0.45
1:A:470:ILE:HG22	1:A:471:ASN:OD1	2.17	0.45
4:S:132:LEU:HD23	4:S:132:LEU:HA	1.85	0.45
1:A:154:ILE:HG23	1:A:160:THR:HG21	1.98	0.45
3:M:170:ARG:NH1	3:M:419:ILE:HD13	2.32	0.45
1:A:386:ARG:HD3	1:A:420:ILE:CD1	2.45	0.44
1:A:472:ARG:HG3	1:A:472:ARG:NH1	2.29	0.44
1:A:548:PHE:HB3	1:A:559:ILE:HD11	1.99	0.44
2:B:143:VAL:HG23	2:B:179:ASN:OD1	2.13	0.44
2:B:350:ASN:O	2:B:351:ILE:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LYS:O	2:B:422:PRO:HD3	2.18	0.44
1:A:482:THR:O	1:A:486:ALA:HB2	2.17	0.44
2:B:200:ASN:HA	2:B:203:ASN:HB2	1.99	0.44
2:B:491:LEU:HD23	2:B:491:LEU:C	2.42	0.44
1:A:397:CYS:HB2	1:A:405:ILE:HD13	1.98	0.44
2:B:139:LYS:O	2:B:143:VAL:HG23	2.16	0.44
2:B:408:GLN:HB3	2:B:444:ALA:HB2	1.98	0.44
3:M:311:PHE:O	3:M:360:GLY:HA3	2.17	0.44
1:A:514:ASP:OD1	1:A:514:ASP:C	2.60	0.44
2:B:374:VAL:HG21	2:B:409:GLU:HB2	1.98	0.44
2:B:423:ASN:HA	2:B:426:GLU:OE2	2.17	0.44
1:A:105:ASN:O	1:A:107:GLU:N	2.51	0.44
1:A:269:PRO:O	1:A:270:PRO:C	2.60	0.44
1:A:502:TYR:C	1:A:502:TYR:CD2	2.96	0.44
2:B:288:LEU:O	2:B:289:VAL:C	2.60	0.44
2:B:322:LYS:HA	2:B:325:PHE:CZ	2.52	0.44
3:M:9:ASN:ND2	3:M:11:LYS:H	2.15	0.44
1:A:452:ILE:HD13	1:A:452:ILE:HA	1.82	0.44
1:A:489:ALA:C	1:A:491:ALA:N	2.76	0.44
2:B:378:GLY:O	2:B:379:ARG:C	2.59	0.44
3:M:94:GLY:O	3:M:95:LYS:C	2.60	0.44
1:A:481:LYS:HB2	1:A:511:ILE:HD11	1.99	0.44
2:B:348:GLN:HA	2:B:351:ILE:HD11	1.99	0.44
3:M:98:GLU:O	3:M:99:GLU:C	2.60	0.44
1:A:549:VAL:HG13	1:A:556:LYS:CB	2.47	0.44
1:A:507:PHE:O	1:A:508:GLY:C	2.57	0.43
2:B:441:GLU:O	2:B:445:ARG:HG3	2.18	0.43
3:M:8:TYR:CE2	3:M:14:VAL:HG22	2.52	0.43
2:B:272:LYS:CD	2:B:278:ASN:HD21	2.31	0.43
2:B:474:HIS:C	2:B:476:GLU:N	2.76	0.43
2:B:509:LEU:HD22	2:B:513:ASP:OD2	2.18	0.43
2:B:559:LEU:HD11	2:B:577:PRO:HG3	2.01	0.43
4:S:38:VAL:O	4:S:41:VAL:HG12	2.17	0.43
2:B:351:ILE:HD13	2:B:387:SER:HB3	2.01	0.43
2:B:41:MET:HG2	2:B:47:VAL:CG2	2.49	0.43
2:B:536:THR:HA	2:B:539:GLU:OE2	2.18	0.43
1:A:319:HIS:O	3:M:378:LYS:NZ	2.52	0.43
2:B:126:LEU:HD11	2:B:141:ALA:O	2.19	0.43
2:B:251:ALA:C	2:B:253:SER:N	2.72	0.43
2:B:448:MET:O	2:B:451:ILE:HB	2.19	0.43
3:M:361:MET:HE3	3:M:361:MET:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASN:HD22	2:B:100:PRO:CD	2.31	0.43
2:B:108:ARG:HG3	2:B:109:THR:N	2.34	0.43
2:B:140:THR:O	2:B:141:ALA:C	2.61	0.43
2:B:399:ILE:HA	2:B:407:VAL:HG22	2.01	0.43
2:B:502:LEU:C	2:B:504:GLN:N	2.75	0.43
3:M:375:THR:HG22	3:M:376:ASN:H	1.82	0.43
2:B:28:GLU:O	2:B:32:GLU:HG2	2.19	0.43
2:B:82:ASP:HA	2:B:85:ILE:HD12	2.00	0.43
2:B:262:VAL:C	2:B:264:MET:N	2.77	0.43
3:M:1:MET:HE3	3:M:1:MET:HB2	1.87	0.43
4:S:69:ILE:HG22	4:S:71:VAL:CG1	2.48	0.43
2:B:190:SER:O	2:B:192:PRO:CD	2.67	0.43
2:B:408:GLN:O	2:B:411:ILE:CG2	2.65	0.43
3:M:1:MET:N	6:M:2001:HOH:O	2.21	0.43
3:M:162:ARG:NH2	3:M:206:LEU:O	2.51	0.43
3:M:327:PRO:O	3:M:330:THR:OG1	2.34	0.43
2:B:9:THR:O	2:B:9:THR:HG23	2.19	0.42
3:M:1:MET:SD	3:M:77:MET:CE	2.92	0.42
3:M:56:PHE:HB2	3:M:67:ALA:HB3	2.00	0.42
3:M:214:PHE:CD1	3:M:404:LEU:HD13	2.54	0.42
4:S:106:ASN:O	4:S:109:LYS:N	2.51	0.42
1:A:394:TYR:CD1	1:A:427:LYS:HG2	2.53	0.42
1:A:506:GLU:C	1:A:507:PHE:CG	2.96	0.42
1:A:549:VAL:HG22	1:A:559:ILE:HD12	2.01	0.42
2:B:147:LYS:HG2	3:M:118:PHE:CD1	2.54	0.42
2:B:485:LEU:HD22	2:B:506:VAL:CG1	2.48	0.42
2:B:488:ILE:O	2:B:488:ILE:CG2	2.66	0.42
3:M:247:THR:CG2	3:M:248:PHE:N	2.79	0.42
1:A:546:ILE:HD13	1:A:599:LEU:HD11	2.00	0.42
1:A:549:VAL:HG23	1:A:559:ILE:CD1	2.49	0.42
2:B:207:LEU:C	2:B:209:THR:H	2.27	0.42
2:B:466:LEU:CD1	2:B:488:ILE:HG12	2.49	0.42
2:B:508:SER:OG	2:B:509:LEU:CD2	2.67	0.42
1:A:546:ILE:HD12	1:A:583:TYR:CG	2.54	0.42
2:B:63:LEU:HD11	2:B:102:ILE:CD1	2.49	0.42
3:M:12:GLY:HA2	3:M:37:ILE:HD13	2.01	0.42
1:A:569:LEU:C	1:A:571:ASN:H	2.26	0.42
2:B:309:ILE:N	2:B:564:ILE:HD11	2.34	0.42
3:M:175:LEU:HD12	3:M:422:VAL:HG22	2.01	0.42
1:A:10:MET:HE2	1:A:57:LYS:CA	2.50	0.42
1:A:462:TRP:O	1:A:465:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:O	1:A:486:ALA:CB	2.68	0.42
2:B:515:ASP:O	2:B:517:PRO:HD3	2.19	0.42
1:A:82:LEU:HB3	1:A:90:GLU:O	2.19	0.42
2:B:200:ASN:O	2:B:203:ASN:N	2.52	0.42
2:B:265:LYS:C	2:B:267:LEU:H	2.27	0.42
2:B:273:ASP:N	2:B:273:ASP:OD1	2.53	0.42
2:B:357:GLU:O	2:B:360:GLU:N	2.52	0.42
2:B:411:ILE:HG23	2:B:412:VAL:N	2.34	0.42
2:B:467:GLU:HB2	2:B:502:LEU:HD11	2.02	0.42
3:M:209:MET:N	3:M:408:GLU:OE1	2.42	0.42
1:A:586:LEU:HG	2:B:540:VAL:HG21	2.02	0.42
2:B:272:LYS:CD	2:B:278:ASN:ND2	2.83	0.42
2:B:485:LEU:HD22	2:B:485:LEU:HA	1.84	0.42
1:A:496:LEU:O	1:A:500:GLY:N	2.41	0.42
1:A:512:ALA:CB	1:A:552:PHE:CE1	3.03	0.42
2:B:499:THR:O	2:B:503:VAL:HG22	2.20	0.42
3:M:112:LEU:HA	3:M:115:ILE:HG22	2.02	0.42
2:B:259:ALA:O	2:B:260:VAL:C	2.63	0.41
3:M:405:LYS:NZ	3:M:415:ASP:OD2	2.45	0.41
2:B:169:ILE:HG23	2:B:177:VAL:HG23	2.01	0.41
3:M:115:ILE:HG23	3:M:116:LEU:HB2	2.02	0.41
3:M:383:ARG:HD3	3:M:435:CYS:SG	2.60	0.41
4:S:83:ALA:O	4:S:84:ILE:C	2.60	0.41
1:A:263:ARG:NH2	4:S:74:ASN:O	2.53	0.41
2:B:297:GLU:O	2:B:300:TYR:HB3	2.19	0.41
2:B:307:ASN:ND2	2:B:575:HIS:HE1	2.17	0.41
3:M:58:VAL:HG12	3:M:60:ARG:HG2	2.02	0.41
1:A:144:ALA:HB1	1:A:182:LEU:HD13	2.03	0.41
1:A:425:VAL:HG21	1:A:453:ALA:HB1	2.02	0.41
1:A:603:PRO:HA	1:A:604:PRO:HD3	1.93	0.41
2:B:244:VAL:CG1	2:B:263:LEU:HD21	2.50	0.41
2:B:505:GLN:O	2:B:508:SER:HB3	2.19	0.41
2:B:83:MET:CA	2:B:86:MET:HE2	2.43	0.41
2:B:200:ASN:O	2:B:201:PRO:C	2.63	0.41
2:B:253:SER:HB2	2:B:298:VAL:HG21	2.01	0.41
2:B:272:LYS:HD3	2:B:278:ASN:ND2	2.35	0.41
2:B:548:ILE:HG22	2:B:549:SER:N	2.34	0.41
3:M:129:LEU:O	3:M:130:LYS:C	2.63	0.41
1:A:56:LYS:HG3	1:A:93:ILE:HD12	2.01	0.41
1:A:367:LYS:NZ	1:A:398:ASP:OD2	2.54	0.41
1:A:421:ARG:HH12	1:A:452:ILE:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:HG13	1:A:500:GLY:CA	2.50	0.41
2:B:97:ASP:OD1	2:B:97:ASP:N	2.46	0.41
3:M:128:ALA:O	3:M:132:PHE:HE1	2.04	0.41
1:A:431:LEU:O	1:A:432:ALA:C	2.64	0.41
1:A:509:ASN:C	1:A:511:ILE:H	2.28	0.41
1:A:578:GLN:HG3	1:A:582:GLU:OE1	2.21	0.41
2:B:88:VAL:C	2:B:90:SER:N	2.77	0.41
2:B:198:ASP:HB3	2:B:200:ASN:HD22	1.86	0.41
2:B:244:VAL:HB	2:B:263:LEU:HD21	2.03	0.41
2:B:248:LEU:HD12	2:B:248:LEU:C	2.46	0.41
3:M:5:LEU:HD21	3:M:85:MET:HE1	1.97	0.41
3:M:24:ILE:O	3:M:24:ILE:HG22	2.21	0.41
3:M:328:LEU:HD12	3:M:328:LEU:N	2.36	0.41
1:A:362:SER:O	1:A:366:VAL:HG23	2.20	0.41
2:B:217:TRP:O	2:B:221:PHE:CZ	2.74	0.41
2:B:385:GLU:C	2:B:387:SER:H	2.29	0.41
2:B:387:SER:O	2:B:388:ALA:C	2.64	0.41
2:B:485:LEU:HD11	2:B:510:ALA:HB2	2.03	0.41
3:M:32:PHE:HB2	3:M:55:PHE:CE2	2.56	0.41
5:A:1609:IHP:O42	5:A:1609:IHP:O21	2.38	0.40
3:M:332:GLY:C	3:M:333:VAL:HG23	2.46	0.40
1:A:484:PHE:CD2	1:A:484:PHE:C	3.00	0.40
2:B:506:VAL:HG12	2:B:507:LEU:N	2.35	0.40
3:M:287:PHE:CD2	3:M:388:MET:HE1	2.57	0.40
1:A:271:PRO:CB	1:A:276:VAL:HG12	2.51	0.40
2:B:470:LEU:HD11	2:B:506:VAL:HG22	2.01	0.40
1:A:157:ALA:HB1	1:A:159:ASP:OD1	2.21	0.40
2:B:157:GLU:O	2:B:160:GLY:N	2.55	0.40
2:B:473:PHE:C	2:B:474:HIS:O	2.63	0.40
1:A:173:LEU:HD11	1:A:213:THR:OG1	2.21	0.40
2:B:83:MET:SD	2:B:86:MET:HE1	2.61	0.40
2:B:208:LEU:HB3	2:B:243:ARG:HD2	2.03	0.40
2:B:285:ALA:CB	2:B:286:PRO:HD3	2.39	0.40
2:B:361:TYR:C	2:B:363:THR:H	2.30	0.40
2:B:566:HIS:O	2:B:567:ILE:C	2.65	0.40

All (3) 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)
2:B:290:THR:CG2	2:B:290:THR:CG2[4_555]	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLU:O	2:B:213:GLU:O[4_555]	1.84	0.36
2:B:290:THR:CB	2:B:290:THR:CG2[4_555]	2.12	0.08

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	598/621 (96%)	525 (88%)	57 (10%)	16 (3%)	4	7
2	B	577/591 (98%)	435 (75%)	103 (18%)	39 (7%)	1	1
3	M	388/435 (89%)	348 (90%)	29 (8%)	11 (3%)	4	6
4	S	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	18	38
All	All	1703/1789 (95%)	1441 (85%)	195 (12%)	67 (4%)	2	3

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	ASP
1	A	439	TYR
1	A	474	ASP
1	A	492	CYS
2	B	153	ALA
2	B	155	MET
2	B	179	ASN
2	B	219	GLN
2	B	227	SER
2	B	252	ASN
2	B	289	VAL
2	B	309	ILE
2	B	503	VAL
2	B	506	VAL
2	B	553	ASP

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Mol	Chain	Res	Type
3	M	95	LYS
3	M	121	PRO
3	M	163	ARG
3	M	375	THR
3	M	378	LYS
3	M	380	LYS
1	A	223	LYS
1	A	442	TYR
1	A	458	SER
1	A	463	TYR
1	A	508	GLY
1	A	590	ALA
2	B	59	GLN
2	B	89	ASN
2	B	220	ILE
2	B	251	ALA
2	B	316	ILE
2	B	387	SER
2	B	507	LEU
2	B	525	ILE
3	M	118	PHE
3	M	376	ASN
2	B	79	SER
2	B	99	ASN
2	B	178	ALA
2	B	271	PRO
2	B	308	LEU
2	B	474	HIS
2	B	552	THR
3	M	131	THR
1	A	122	SER
1	A	464	ARG
1	A	470	ILE
1	A	602	MET
2	B	216	GLU
2	B	226	LEU
2	B	350	ASN
2	B	351	ILE
2	B	437	ASP
2	B	528	ARG
3	M	124	SER
4	S	96	HIS

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Mol	Chain	Res	Type
1	A	254	ALA
2	B	92	VAL
2	B	245	THR
3	M	409	PRO
1	A	475	VAL
2	B	94	ASP
2	B	98	PRO
2	B	263	LEU
2	B	418	PHE
2	B	256	VAL

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	526/543 (97%)	486 (92%)	40 (8%)	12	27
2	B	516/532 (97%)	446 (86%)	70 (14%)	3	7
3	M	353/387 (91%)	324 (92%)	29 (8%)	10	24
4	S	131/131 (100%)	123 (94%)	8 (6%)	17	37
All	All	1526/1593 (96%)	1379 (90%)	147 (10%)	8	17

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	18	SER
1	A	20	ILE
1	A	57	LYS
1	A	83	LEU
1	A	86	ASN
1	A	87	ARG
1	A	106	SER
1	A	160	THR
1	A	231	SER
1	A	273	ASP

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Mol	Chain	Res	Type
1	A	283	CYS
1	A	303	SER
1	A	372	THR
1	A	388	ARG
1	A	404	GLN
1	A	420	ILE
1	A	434	LYS
1	A	439	TYR
1	A	459	GLU
1	A	470	ILE
1	A	475	VAL
1	A	492	CYS
1	A	499	VAL
1	A	507	PHE
1	A	509	ASN
1	A	511	ILE
1	A	516	ARG
1	A	520	LEU
1	A	526	LEU
1	A	535	VAL
1	A	537	THR
1	A	546	ILE
1	A	551	LEU
1	A	558	THR
1	A	575	GLU
1	A	584	LEU
1	A	589	VAL
1	A	591	SER
1	A	595	LEU
2	B	42	THR
2	B	48	SER
2	B	55	VAL
2	B	74	MET
2	B	80	GLN
2	B	90	SER
2	B	97	ASP
2	B	107	VAL
2	B	115	VAL
2	B	118	ILE
2	B	134	ASP
2	B	156	VAL
2	B	158	ASP

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Mol	Chain	Res	Type
2	B	172	SER
2	B	177	VAL
2	B	188	SER
2	B	198	ASP
2	B	206	LYS
2	B	212	ASN
2	B	214	CYS
2	B	215	THR
2	B	221	PHE
2	B	224	ASP
2	B	233	ASP
2	B	245	THR
2	B	264	MET
2	B	267	LEU
2	B	269	LEU
2	B	270	LEU
2	B	272	LYS
2	B	273	ASP
2	B	274	SER
2	B	281	LEU
2	B	282	LYS
2	B	284	LEU
2	B	289	VAL
2	B	290	THR
2	B	310	VAL
2	B	313	ARG
2	B	316	ILE
2	B	323	VAL
2	B	351	ILE
2	B	354	VAL
2	B	364	GLU
2	B	396	LEU
2	B	399	ILE
2	B	406	VAL
2	B	432	LEU
2	B	436	LEU
2	B	437	ASP
2	B	457	GLU
2	B	464	GLU
2	B	471	GLU
2	B	475	ASP
2	B	480	VAL

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Mol	Chain	Res	Type
2	B	483	THR
2	B	485	LEU
2	B	488	ILE
2	B	501	GLU
2	B	507	LEU
2	B	508	SER
2	B	524	TYR
2	B	536	THR
2	B	548	ILE
2	B	554	LEU
2	B	556	GLU
2	B	567	ILE
2	B	570	LEU
2	B	572	SER
2	B	581	PHE
3	M	47	VAL
3	M	48	THR
3	M	59	LYS
3	M	68	VAL
3	M	69	THR
3	M	87	ASP
3	M	115	ILE
3	M	125	GLU
3	M	132	PHE
3	M	134	THR
3	M	164	GLU
3	M	173	LEU
3	M	176	ASP
3	M	180	SER
3	M	247	THR
3	M	255	SER
3	M	261	ARG
3	M	276	ARG
3	M	290	ILE
3	M	299	THR
3	M	323	ARG
3	M	336	ILE
3	M	339	LYS
3	M	357	ARG
3	M	361	MET
3	M	380	LYS
3	M	391	GLU

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Mol	Chain	Res	Type
3	M	411	LEU
3	M	416	HIS
4	S	8	GLN
4	S	13	LYS
4	S	15	ARG
4	S	41	VAL
4	S	54	ASN
4	S	69	ILE
4	S	127	SER
4	S	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	166	GLN
1	A	200	HIS
1	A	245	GLN
1	A	320	HIS
1	A	401	ASN
1	A	476	GLN
1	A	509	ASN
1	A	524	ASN
1	A	560	GLN
2	B	10	ASN
2	B	56	ASN
2	B	80	GLN
2	B	99	ASN
2	B	149	HIS
2	B	152	ASN
2	B	154	GLN
2	B	159	GLN
2	B	200	ASN
2	B	278	ASN
2	B	307	ASN
2	B	311	GLN
2	B	353	GLN
2	B	435	ASN
2	B	505	GLN
2	B	512	GLN
2	B	579	ASN
3	M	72	ASN

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Mol	Chain	Res	Type
4	S	48	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](#)

1 ligand is 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$
5	IHP	A	1609	-	36,36,36	3.08	13 (36%)	60,60,60	1.44	12 (20%)

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
5	IHP	A	1609	-	-	2/30/54/54	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1609	IHP	P6-O26	7.15	1.72	1.50
5	A	1609	IHP	P2-O22	6.24	1.69	1.50
5	A	1609	IHP	P4-O24	6.12	1.69	1.50
5	A	1609	IHP	P5-O25	5.93	1.68	1.50
5	A	1609	IHP	P1-O21	5.86	1.68	1.50
5	A	1609	IHP	P2-O32	4.61	1.71	1.54
5	A	1609	IHP	P6-O36	4.42	1.71	1.54
5	A	1609	IHP	P3-O43	4.39	1.71	1.54
5	A	1609	IHP	P1-O41	4.24	1.70	1.54
5	A	1609	IHP	P5-O35	4.10	1.70	1.54
5	A	1609	IHP	P3-O33	3.96	1.69	1.54
5	A	1609	IHP	P4-O34	3.22	1.66	1.54
5	A	1609	IHP	P4-O44	-2.33	1.46	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1609	IHP	P5-O15-C5	-4.39	111.71	123.43
5	A	1609	IHP	O16-C6-C1	-2.96	102.46	108.76
5	A	1609	IHP	O41-P1-O11	2.78	116.68	105.85
5	A	1609	IHP	O16-C6-C5	2.69	114.48	108.76
5	A	1609	IHP	P6-O16-C6	-2.65	116.36	123.43
5	A	1609	IHP	P1-O11-C1	-2.56	116.58	123.43
5	A	1609	IHP	P3-O13-C3	-2.54	116.64	123.43
5	A	1609	IHP	O41-P1-O21	-2.32	101.78	110.83
5	A	1609	IHP	O12-C2-C3	2.19	113.42	108.76
5	A	1609	IHP	C5-C4-C3	-2.18	105.63	110.43
5	A	1609	IHP	P2-O12-C2	-2.14	117.73	123.43
5	A	1609	IHP	O15-C5-C4	2.06	113.15	108.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

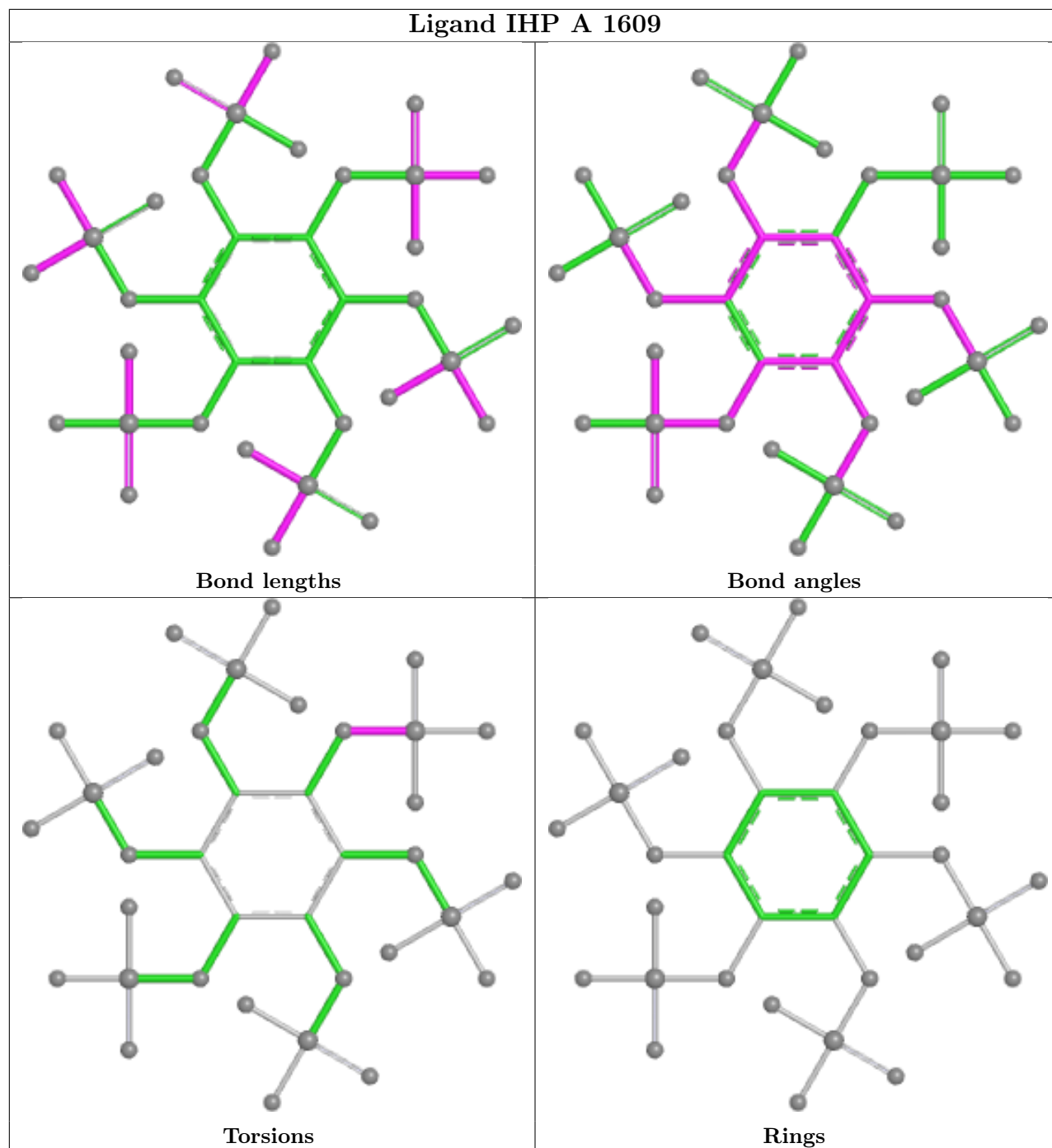
Mol	Chain	Res	Type	Atoms
5	A	1609	IHP	C4-O14-P4-O34
5	A	1609	IHP	C4-O14-P4-O24

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1609	IHP	4	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	600/621 (96%)	0.66	87 (14%) 6 4	23, 50, 93, 114	0
2	B	579/591 (97%)	1.40	148 (25%) 1 1	47, 79, 103, 116	0
3	M	396/435 (91%)	0.53	15 (3%) 44 38	24, 55, 75, 86	0
4	S	142/142 (100%)	-0.20	0 100 100	21, 33, 46, 57	0
All	All	1717/1789 (95%)	0.81	250 (14%) 6 4	21, 59, 101, 116	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	GLY	9.4
2	B	525	ILE	7.1
1	A	504	LEU	6.7
1	A	515	PRO	6.5
2	B	510	ALA	6.5
1	A	546	ILE	6.4
1	A	501	GLY	6.2
1	A	548	PHE	5.8
2	B	489	VAL	5.8
2	B	507	LEU	5.7
2	B	521	ASP	5.5
2	B	530	LEU	5.2
1	A	549	VAL	5.1
1	A	541	LEU	4.9
1	A	598	VAL	4.7
1	A	581	VAL	4.6
2	B	529	LEU	4.5
2	B	253	SER	4.4
2	B	250	HIS	4.2
2	B	519	LEU	4.1
2	B	582	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	595	LEU	4.1
2	B	270	LEU	4.1
1	A	505	GLY	4.1
1	A	586	LEU	4.1
2	B	248	LEU	4.0
2	B	199	LEU	3.9
1	A	594	ILE	3.9
2	B	540	VAL	3.9
1	A	583	TYR	3.8
2	B	196	LEU	3.8
2	B	493	LEU	3.8
1	A	542	LEU	3.8
1	A	551	LEU	3.8
2	B	104	ALA	3.8
2	B	169	ILE	3.8
2	B	182	ALA	3.8
2	B	537	ALA	3.8
1	A	544	THR	3.7
1	A	599	LEU	3.7
1	A	521	ILE	3.7
2	B	223	LEU	3.6
1	A	597	THR	3.6
2	B	527	TRP	3.6
1	A	590	ALA	3.5
2	B	204	ILE	3.5
1	A	547	LYS	3.4
1	A	580	ALA	3.4
2	B	88	VAL	3.3
2	B	229	TYR	3.3
2	B	536	THR	3.3
1	A	596	ALA	3.3
2	B	553	ASP	3.3
2	B	122	LEU	3.3
2	B	526	TYR	3.3
2	B	488	ILE	3.3
2	B	269	LEU	3.2
2	B	495	LYS	3.2
2	B	168	LEU	3.2
2	B	487	ALA	3.2
2	B	524	TYR	3.2
2	B	263	LEU	3.1
2	B	178	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	477	GLY	3.1
1	A	491	ALA	3.1
1	A	557	ALA	3.1
1	A	516	ARG	3.1
1	A	503	ILE	3.1
2	B	380	CYS	3.1
1	A	545	TYR	3.1
2	B	280	LEU	3.1
2	B	517	PRO	3.1
2	B	473	PHE	3.1
1	A	524	ASN	3.0
2	B	548	ILE	3.0
2	B	528	ARG	3.0
1	A	442	TYR	3.0
1	A	558	THR	3.0
2	B	444	ALA	3.0
1	A	528	SER	2.9
1	A	553	PRO	2.9
2	B	274	SER	2.9
1	A	509	ASN	2.9
1	A	550	ASN	2.9
2	B	552	THR	2.9
1	A	475	VAL	2.9
1	A	526	LEU	2.9
2	B	220	ILE	2.9
1	A	440	THR	2.9
1	A	563	LEU	2.9
2	B	485	LEU	2.9
1	A	552	PHE	2.9
2	B	110	MET	2.8
1	A	605	PHE	2.8
3	M	43	VAL	2.8
2	B	227	SER	2.8
2	B	105	LEU	2.8
2	B	277	TYR	2.8
2	B	580	ALA	2.8
1	A	562	VAL	2.8
2	B	466	LEU	2.8
2	B	551	GLU	2.8
1	A	606	PRO	2.8
2	B	249	SER	2.7
2	B	317	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	469	VAL	2.7
3	M	120	TYR	2.7
1	A	584	LEU	2.7
2	B	547	LEU	2.7
1	A	520	LEU	2.7
2	B	514	SER	2.7
2	B	187	ILE	2.7
1	A	525	LEU	2.7
2	B	522	ARG	2.7
2	B	289	VAL	2.7
2	B	374	VAL	2.7
1	A	608	ARG	2.6
1	A	486	ALA	2.6
1	A	484	PHE	2.6
2	B	244	VAL	2.6
2	B	496	PRO	2.6
1	A	602	MET	2.6
2	B	130	LEU	2.6
2	B	520	ARG	2.6
2	B	192	PRO	2.6
2	B	252	ASN	2.6
2	B	271	PRO	2.6
2	B	239	SER	2.6
2	B	243	ARG	2.6
2	B	218	GLY	2.6
2	B	523	GLY	2.6
2	B	221	PHE	2.6
2	B	469	PHE	2.6
3	M	375	THR	2.5
2	B	158	ASP	2.5
2	B	309	ILE	2.5
3	M	357	ARG	2.5
1	A	502	TYR	2.5
2	B	276	TYR	2.5
1	A	499	VAL	2.5
2	B	87	ALA	2.5
2	B	91	PHE	2.5
2	B	341	ILE	2.5
2	B	490	LYS	2.5
1	A	437	VAL	2.5
2	B	156	VAL	2.5
2	B	85	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	491	LEU	2.5
1	A	588	THR	2.5
1	A	441	TRP	2.5
2	B	162	LEU	2.5
2	B	502	LEU	2.5
1	A	470	ILE	2.4
2	B	197	LEU	2.4
2	B	511	THR	2.4
2	B	217	TRP	2.4
3	M	435	CYS	2.4
2	B	505	GLN	2.4
1	A	572	ALA	2.4
2	B	126	LEU	2.4
2	B	542	LEU	2.4
2	B	152	ASN	2.4
2	B	115	VAL	2.4
3	M	75	ALA	2.4
1	A	559	ILE	2.4
2	B	215	THR	2.4
2	B	245	THR	2.4
2	B	283	LYS	2.4
2	B	567	ILE	2.3
1	A	514	ASP	2.3
2	B	497	SER	2.3
2	B	174	PRO	2.3
2	B	161	PHE	2.3
2	B	306	ILE	2.3
2	B	509	LEU	2.3
1	A	439	TYR	2.3
2	B	127	ARG	2.3
3	M	372	LEU	2.3
1	A	466	ILE	2.3
3	M	133	ILE	2.3
1	A	443	VAL	2.3
2	B	539	GLU	2.2
2	B	516	ASN	2.2
1	A	604	PRO	2.2
1	A	496	LEU	2.2
2	B	251	ALA	2.2
3	M	138	ILE	2.2
2	B	425	TYR	2.2
2	B	111	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	568	GLY	2.2
2	B	257	LEU	2.2
2	B	541	VAL	2.2
1	A	446	ILE	2.2
1	A	468	ILE	2.2
2	B	84	ALA	2.2
3	M	134	THR	2.2
2	B	100	PRO	2.2
2	B	281	LEU	2.2
2	B	538	LYS	2.2
2	B	503	VAL	2.2
2	B	535	VAL	2.2
1	A	523	PHE	2.2
3	M	222	ILE	2.2
2	B	121	TYR	2.2
3	M	127	GLY	2.2
1	A	473	ASP	2.2
2	B	107	VAL	2.2
2	B	260	VAL	2.2
2	B	492	PHE	2.2
2	B	183	ALA	2.1
1	A	592	THR	2.1
2	B	479	GLN	2.1
1	A	569	LEU	2.1
2	B	165	LEU	2.1
2	B	226	LEU	2.1
2	B	345	LEU	2.1
2	B	316	ILE	2.1
2	B	259	ALA	2.1
1	A	490	PRO	2.1
2	B	256	VAL	2.1
1	A	517	SER	2.1
1	A	537	THR	2.1
2	B	482	LEU	2.1
2	B	212	ASN	2.1
2	B	241	CYS	2.1
1	A	478	TYR	2.1
1	A	507	PHE	2.1
1	A	479	ALA	2.1
2	B	290	THR	2.1
2	B	148	LEU	2.1
2	B	555	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	115	ILE	2.1
2	B	354	VAL	2.1
2	B	266	PHE	2.1
2	B	581	PHE	2.1
2	B	124	GLU	2.0
1	A	536	PRO	2.0
2	B	125	PRO	2.0
1	A	568	GLN	2.0
3	M	123	ASN	2.0
1	A	535	VAL	2.0
2	B	129	CYS	2.0
1	A	494	GLU	2.0
2	B	170	ALA	2.0
2	B	533	ASP	2.0
3	M	128	ALA	2.0
1	A	543	SER	2.0
1	A	587	SER	2.0
1	A	603	PRO	2.0
2	B	323	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 oligosaccharides in this entry.

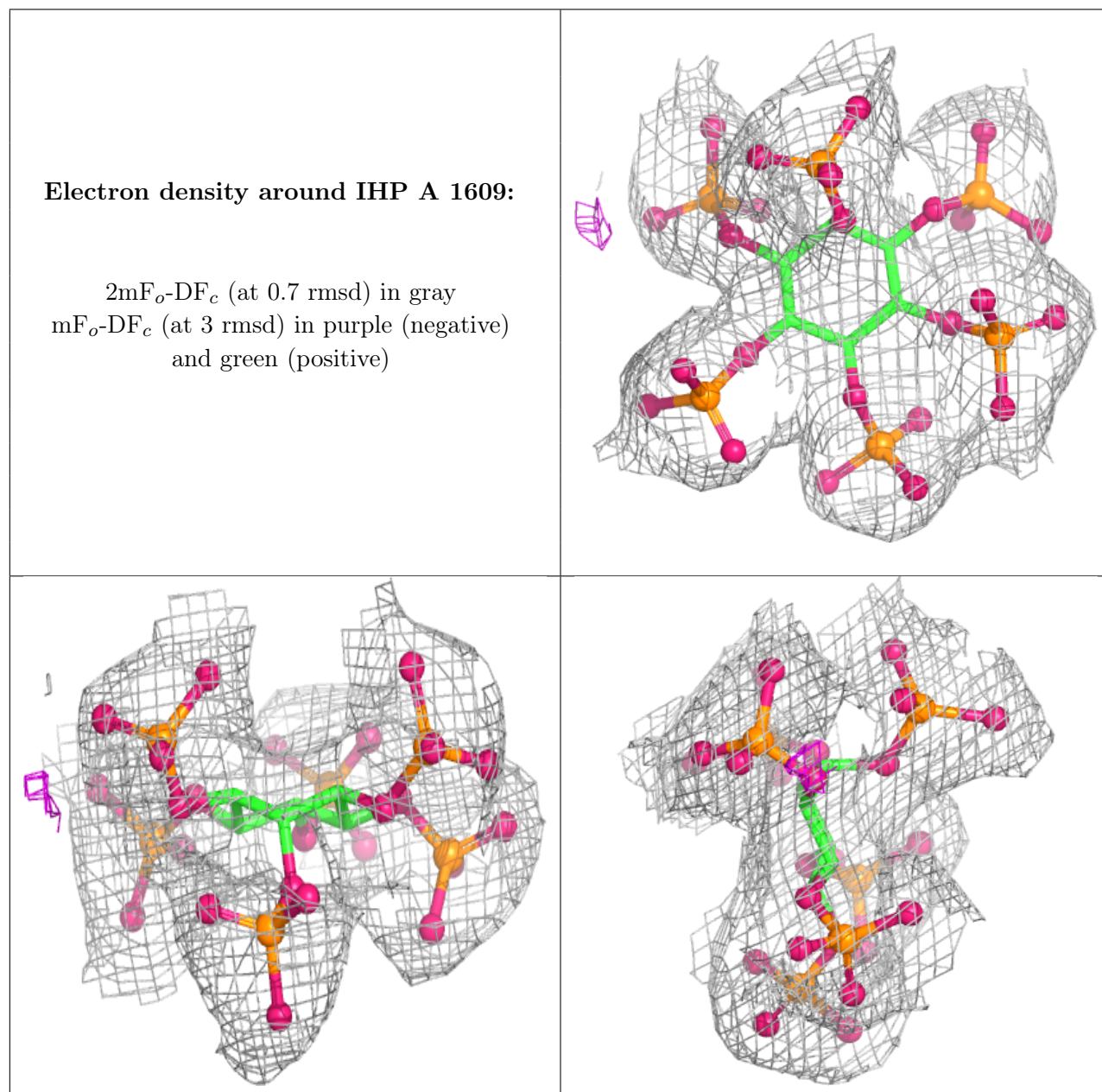
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
5	IHP	A	1609	36/36	0.92	0.07	43,60,68,69	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.