



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:06 PM EDT

PDB ID : 9P05 / pdb\_00009p05  
Title : Structure of human Sec23a/Sec24a/Sec22b bound to CPD11  
Authors : Goldberg, J.  
Deposited on : 2025-06-06  
Resolution : 2.31 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](mailto: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>.

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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

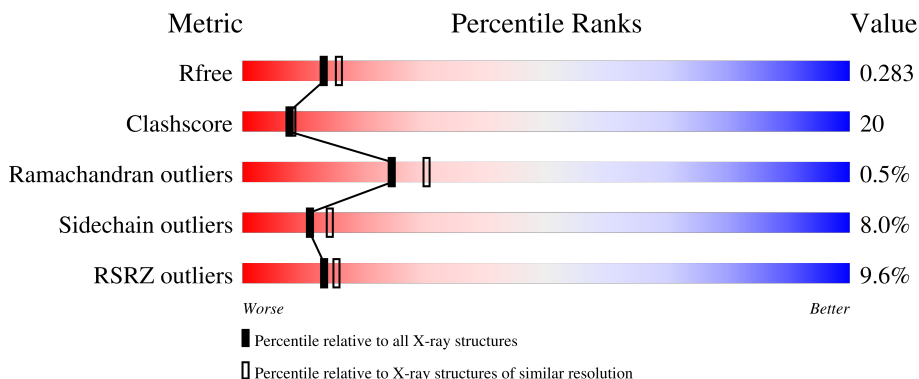
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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  $\geq 3$ , 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	765	<div> <div>11%</div> <div>58%</div> <div>28%</div> <div>•</div> <div>10%</div> </div>
2	B	748	<div> <div>6%</div> <div>61%</div> <div>33%</div> <div>• •</div> </div>
3	C	157	<div> <div>13%</div> <div>49%</div> <div>30%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12226 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5372	3437	901	995	39			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5651	3620	945	1053	33			

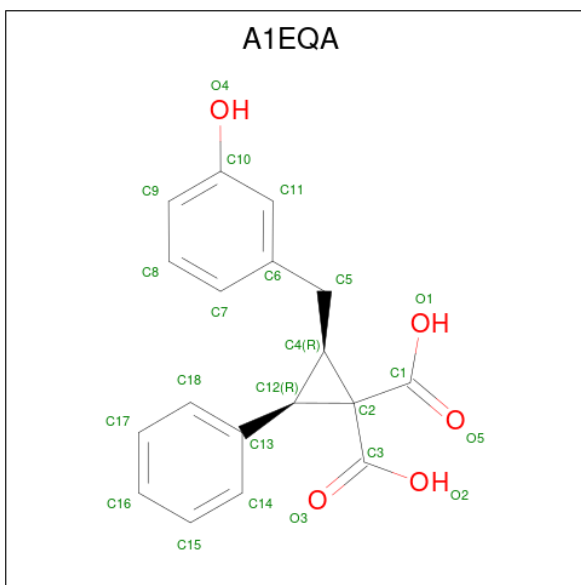
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1016	658	159	193	6			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2 {R},3 {R})-2-[(3-hydroxyphenyl)methyl]-3-phenyl-cyclopropane-1,1-dicarboxylic acid (CCD ID: A1EQA) (formula: C<sub>18</sub>H<sub>16</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			23	18	5		

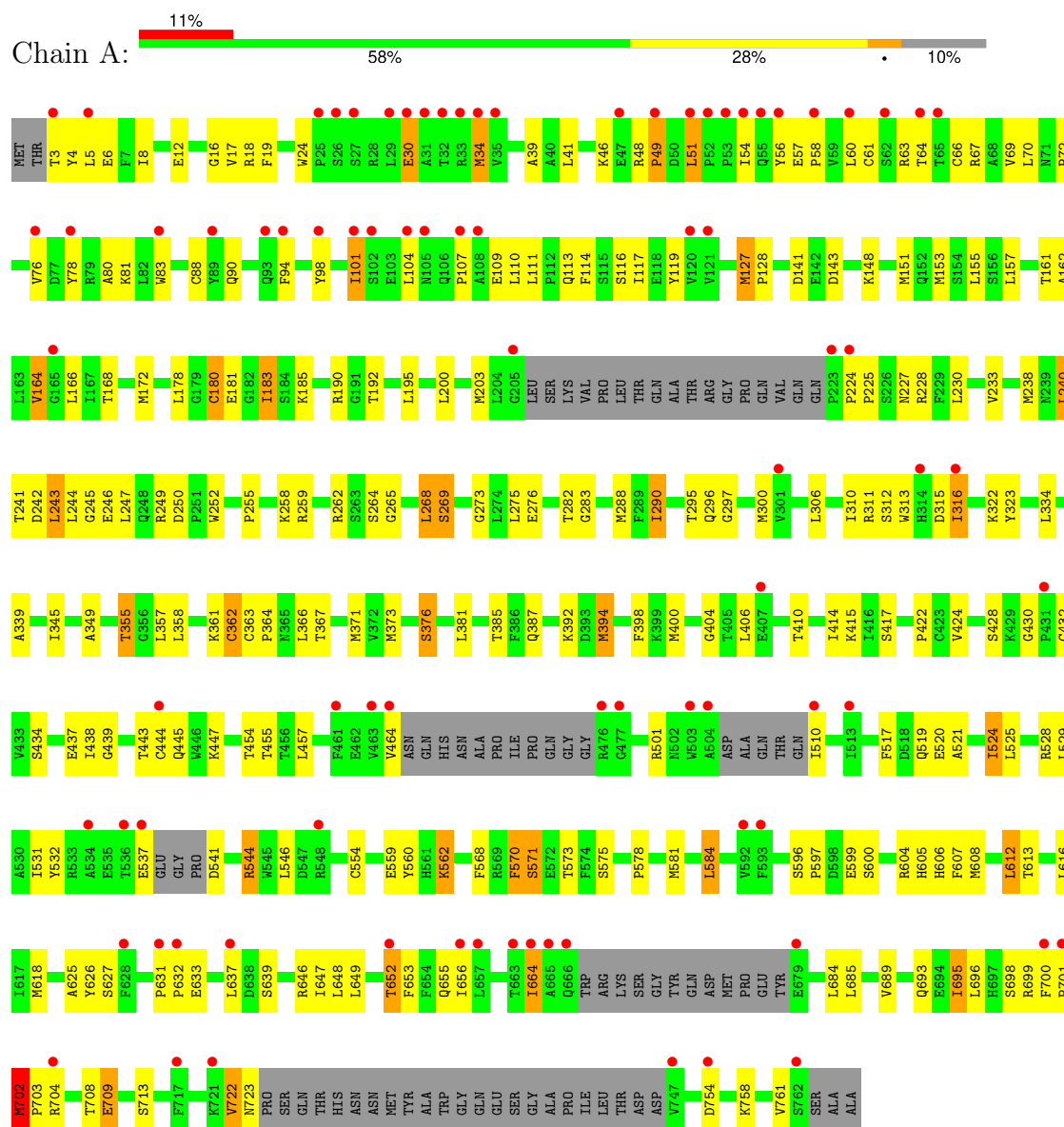
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	59	Total O 59 59	0	0
6	B	93	Total O 93 93	0	0
6	C	10	Total O 10 10	0	0

### 3 Residue-property plots

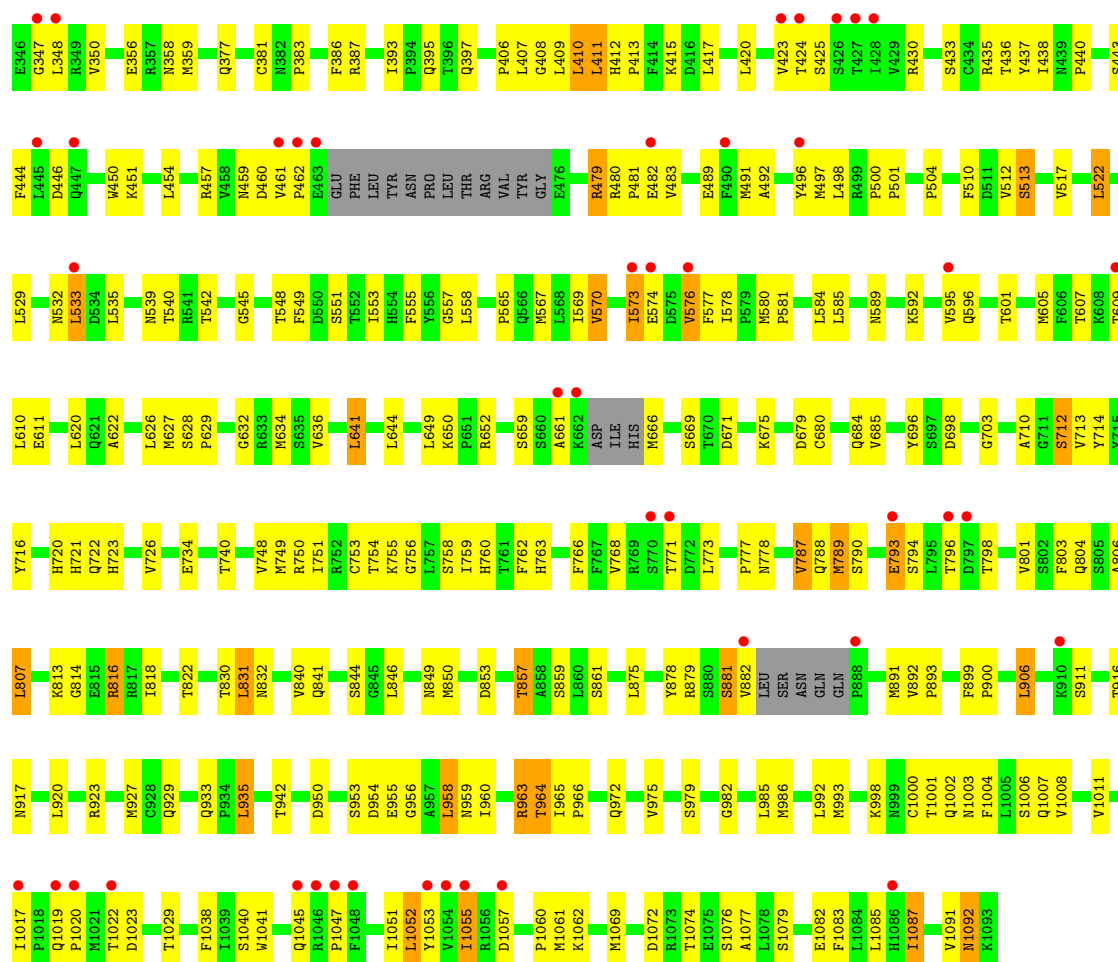
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Protein transport protein Sec23A

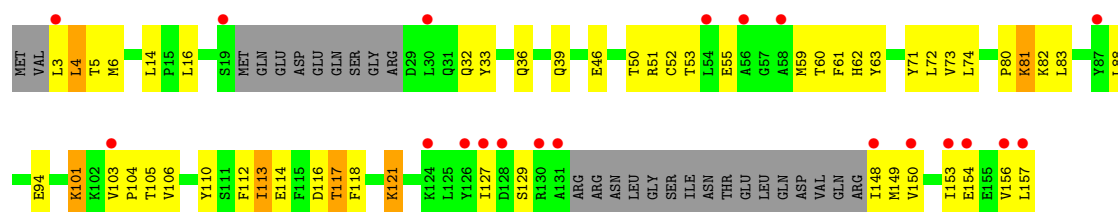


#### • Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.15Å 97.66Å 128.77Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.39 – 2.31 64.39 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.0 (64.39-2.31) 94.9 (64.39-2.31)	Depositor EDS
$R_{merge}$	0.96	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.232 , 0.286 0.232 , 0.283	Depositor DCC
$R_{free}$ test set	2016 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1EQA, ZN

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	0.43	0/5496	0.65	2/7454 (0.0%)
2	B	0.47	0/5773	0.66	2/7862 (0.0%)
3	C	0.37	0/1035	0.58	0/1399
All	All	0.45	0/12304	0.65	4/16715 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1060	PRO	N-CA-CB	6.42	110.63	103.44
1	A	652	THR	CA-C-N	-6.14	110.75	122.53
1	A	652	THR	C-N-CA	-6.14	110.75	122.53
2	B	956	GLY	N-CA-C	-5.53	106.38	114.90

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	5372	0	5267	223	0
2	B	5651	0	5635	207	0
3	C	1016	0	995	56	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	B	23	0	0	4	0
6	A	59	0	0	14	0
6	B	93	0	0	7	0
6	C	10	0	0	1	0
All	All	12226	0	11897	479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (479) 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:750:ARG:HH12	2:B:771:THR:HG22	1.23	1.01
2:B:609:THR:HG22	2:B:611:GLU:H	1.32	0.94
1:A:269:SER:HB3	1:A:334:LEU:HD21	1.46	0.94
1:A:288:MET:HE2	1:A:290:ILE:HD11	1.51	0.93
1:A:528:ARG:HA	1:A:608:MET:HE1	1.48	0.92
1:A:652:THR:HG22	1:A:653:PHE:H	1.33	0.91
1:A:394:MET:HE3	1:A:394:MET:H	1.34	0.90
1:A:656:ILE:HD11	1:A:695:ILE:HG12	1.54	0.90
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.53	0.89
1:A:723:ASN:HB3	6:A:902:HOH:O	1.75	0.86
1:A:153:MET:HE2	1:A:157:LEU:HD11	1.58	0.85
2:B:496:TYR:HD2	2:B:818:ILE:HD11	1.40	0.84
1:A:562:LYS:NZ	1:A:562:LYS:HB3	1.94	0.83
1:A:410:THR:HB	1:A:414:ILE:HB	1.59	0.82
2:B:750:ARG:NH1	2:B:771:THR:O	2.12	0.81
1:A:107:PRO:HG2	1:A:110:LEU:HD12	1.63	0.81
2:B:395:GLN:HE21	2:B:796:THR:HA	1.43	0.81
3:C:50:THR:O	3:C:51:ARG:HG2	1.79	0.81
1:A:127:MET:HE2	1:A:128:PRO:HD2	1.61	0.81
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.22	0.79
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.61	0.79
3:C:114:GLU:HB2	6:C:203:HOH:O	1.84	0.78
1:A:652:THR:HG22	1:A:653:PHE:N	1.97	0.78
2:B:959:ASN:OD1	2:B:964:THR:HB	1.83	0.77
1:A:297:GLY:H	1:A:300:MET:CE	1.98	0.77
2:B:1074:THR:HG23	2:B:1076:SER:H	1.49	0.77
3:C:81:LYS:HD3	3:C:81:LYS:H	1.49	0.76
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:MET:HE1	1:A:225:PRO:HG3	1.67	0.75
1:A:148:LYS:HE3	6:A:901:HOH:O	1.85	0.75
2:B:750:ARG:NH1	2:B:771:THR:HG22	2.00	0.75
2:B:513:SER:O	2:B:517:VAL:HG23	1.86	0.75
1:A:297:GLY:H	1:A:300:MET:HE2	1.52	0.75
1:A:631:PRO:O	1:A:633:GLU:HG3	1.86	0.75
1:A:323:TYR:HB2	6:A:926:HOH:O	1.88	0.73
1:A:153:MET:CE	1:A:157:LEU:HD11	2.19	0.73
2:B:750:ARG:HH22	2:B:771:THR:HG21	1.54	0.73
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.69	0.72
2:B:1041:TRP:O	2:B:1045:GLN:HG2	1.88	0.72
2:B:395:GLN:NE2	2:B:796:THR:HA	2.03	0.72
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.24	0.72
2:B:750:ARG:HH22	2:B:771:THR:CG2	2.03	0.72
2:B:671:ASP:OD2	2:B:675:LYS:HE3	1.91	0.71
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.20	0.71
1:A:155:LEU:HD22	1:A:240:LEU:HD13	1.73	0.70
2:B:409:LEU:C	2:B:410:LEU:HD12	2.17	0.70
1:A:72:PRO:HB3	1:A:110:LEU:O	1.91	0.70
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.74	0.70
2:B:993:MET:HB3	2:B:1055:ILE:HD11	1.74	0.69
1:A:224:PRO:HB2	6:A:919:HOH:O	1.91	0.69
2:B:580:MET:HG2	2:B:581:PRO:HD2	1.75	0.69
2:B:1057:ASP:HA	2:B:1062:LYS:HD3	1.73	0.69
2:B:420:LEU:HD21	2:B:489:GLU:HB2	1.74	0.69
6:A:910:HOH:O	2:B:605:MET:HG2	1.92	0.68
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.76	0.68
2:B:750:ARG:NE	5:B:1101:A1EQA:O2	2.23	0.68
1:A:48:ARG:HE	1:A:49:PRO:HD2	1.59	0.68
1:A:560:TYR:CD2	1:A:761:VAL:HG12	2.29	0.68
2:B:953:SER:OG	2:B:955:GLU:HG2	1.94	0.67
1:A:88:CYS:SG	1:A:90:GLN:HB3	2.35	0.67
3:C:80:PRO:HB2	3:C:83:LEU:HG	1.76	0.66
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.25	0.66
3:C:101:LYS:H	3:C:101:LYS:HE3	1.61	0.66
1:A:422:PRO:HD2	1:A:457:LEU:HD13	1.78	0.66
2:B:830:THR:HG22	2:B:832:ASN:H	1.61	0.66
1:A:596:SER:OG	1:A:599:GLU:HG3	1.96	0.65
2:B:814:GLY:O	3:C:113:ILE:HD12	1.97	0.65
6:B:1203:HOH:O	3:C:117:THR:HG23	1.95	0.65
2:B:634:MET:HE2	2:B:636:VAL:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LYS:HB3	1:A:562:LYS:HZ2	1.62	0.65
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.79	0.64
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.33	0.64
1:A:168:THR:HG21	1:A:247:LEU:CD2	2.27	0.64
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.78	0.64
3:C:149:MET:O	3:C:150:VAL:HG23	1.97	0.64
2:B:859:SER:HB2	6:B:1206:HOH:O	1.97	0.64
2:B:540:THR:HG22	2:B:589:ASN:ND2	2.12	0.64
2:B:748:VAL:HB	2:B:773:LEU:HD11	1.80	0.64
2:B:753:CYS:HB3	2:B:803:PHE:HD1	1.64	0.63
2:B:975:VAL:HG23	2:B:1072:ASP:OD2	1.99	0.63
1:A:24:TRP:CZ2	1:A:501:ARG:HG3	2.34	0.63
1:A:183:ILE:CD1	2:B:565:PRO:HG2	2.28	0.63
3:C:121:LYS:NZ	3:C:121:LYS:HB3	2.13	0.63
1:A:524:ILE:HD11	1:A:616:LEU:HD23	1.80	0.63
3:C:80:PRO:HG2	3:C:83:LEU:CD1	2.29	0.63
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.80	0.62
1:A:70:LEU:HD23	1:A:109:GLU:HG3	1.79	0.62
2:B:750:ARG:HH21	5:B:1101:A1EQA:C3	2.11	0.62
1:A:153:MET:HE1	1:A:387:GLN:HB2	1.80	0.62
2:B:703:GLY:HA3	6:B:1264:HOH:O	1.99	0.62
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.82	0.62
2:B:1003:ASN:O	2:B:1007:GLN:HB2	2.00	0.62
1:A:148:LYS:CE	6:A:901:HOH:O	2.44	0.61
3:C:4:LEU:HD12	3:C:5:THR:N	2.14	0.61
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.81	0.61
1:A:168:THR:HG21	1:A:247:LEU:HD21	1.82	0.61
2:B:555:PHE:HE1	2:B:570:VAL:CG1	2.13	0.61
2:B:788:GLN:NE2	2:B:850:MET:HE3	2.16	0.61
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.82	0.60
2:B:965:ILE:N	2:B:965:ILE:HD12	2.16	0.60
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.32	0.60
1:A:153:MET:CE	1:A:387:GLN:HB2	2.33	0.59
1:A:345:ILE:HG21	1:A:363:CYS:HB3	1.84	0.59
1:A:17:VAL:O	1:A:18:ARG:HG3	2.02	0.59
1:A:430:GLY:HA3	6:A:916:HOH:O	2.01	0.59
1:A:127:MET:HE1	1:A:225:PRO:CG	2.31	0.59
2:B:410:LEU:HD12	2:B:410:LEU:N	2.17	0.59
1:A:245:GLY:C	6:A:901:HOH:O	2.45	0.58
2:B:377:GLN:OE1	2:B:377:GLN:HA	2.03	0.58
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:HG2	3:C:83:LEU:HD11	1.85	0.58
1:A:127:MET:HE2	1:A:127:MET:HA	1.84	0.58
1:A:546:LEU:HD21	1:A:584:LEU:HD23	1.86	0.58
2:B:1083:PHE:O	2:B:1087:ILE:HD12	2.03	0.58
3:C:50:THR:C	3:C:51:ARG:HG2	2.29	0.58
3:C:113:ILE:O	3:C:116:ASP:HB2	2.04	0.58
2:B:553:ILE:HD13	2:B:576:VAL:CG1	2.34	0.57
2:B:846:LEU:O	2:B:850:MET:HG3	2.05	0.57
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.39	0.57
1:A:151:MET:HE3	1:A:244:LEU:HD22	1.87	0.57
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.87	0.57
1:A:700:PHE:C	1:A:702:MET:H	2.13	0.57
2:B:963:ARG:HG3	2:B:965:ILE:HD11	1.86	0.57
1:A:16:GLY:HA2	1:A:46:LYS:HD3	1.87	0.57
1:A:438:ILE:HG21	1:A:529:LEU:HD21	1.85	0.57
2:B:620:LEU:HD22	2:B:634:MET:CE	2.35	0.57
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.87	0.56
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.40	0.56
1:A:143:ASP:OD1	1:A:376:SER:HB2	2.06	0.56
1:A:313:TRP:CA	1:A:316:ILE:HG22	2.31	0.56
2:B:1053:TYR:HE2	2:B:1061:MET:CB	2.19	0.56
2:B:906:LEU:CD1	2:B:942:THR:HG21	2.35	0.56
1:A:238:MET:O	1:A:241:THR:HG22	2.04	0.56
2:B:916:THR:HG22	2:B:917:ASN:N	2.20	0.56
2:B:959:ASN:C	2:B:960:ILE:HD13	2.30	0.56
2:B:411:LEU:N	2:B:411:LEU:HD23	2.21	0.56
2:B:753:CYS:HB3	2:B:803:PHE:CD1	2.41	0.56
2:B:906:LEU:HD12	2:B:942:THR:HG21	1.87	0.56
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.36	0.55
3:C:149:MET:HG2	3:C:150:VAL:H	1.70	0.55
3:C:80:PRO:HB3	3:C:82:LYS:HE2	1.88	0.55
2:B:601:THR:HB	2:B:605:MET:HE3	1.88	0.55
2:B:846:LEU:HG	2:B:850:MET:SD	2.47	0.55
2:B:986:MET:CE	2:B:1069:MET:HE3	2.37	0.55
1:A:541:ASP:HB3	1:A:544:ARG:HB2	1.89	0.55
1:A:422:PRO:HD2	1:A:457:LEU:CD1	2.37	0.55
1:A:148:LYS:NZ	6:A:901:HOH:O	2.39	0.54
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.89	0.54
3:C:101:LYS:HE3	3:C:101:LYS:N	2.21	0.54
2:B:853:ASP:O	2:B:857:THR:HB	2.07	0.54
3:C:32:GLN:O	3:C:36:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:GLU:O	3:C:153:ILE:HG22	2.08	0.54
1:A:625:ALA:HA	1:A:648:LEU:HD23	1.90	0.54
2:B:1004:PHE:CE1	2:B:1008:VAL:HG11	2.42	0.54
2:B:578:ILE:HD11	2:B:626:LEU:CA	2.33	0.54
3:C:121:LYS:NZ	3:C:121:LYS:CB	2.71	0.54
2:B:408:GLY:HA3	2:B:787:VAL:O	2.07	0.54
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.90	0.54
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.90	0.53
1:A:70:LEU:HD23	1:A:109:GLU:CG	2.38	0.53
1:A:517:PHE:CE2	1:A:519:GLN:HA	2.44	0.53
1:A:166:LEU:CD2	1:A:243:LEU:HD13	2.39	0.53
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.91	0.53
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.24	0.53
1:A:381:LEU:HD12	1:A:702:MET:HG2	1.90	0.53
2:B:480:ARG:HG3	2:B:481:PRO:HD2	1.91	0.53
2:B:763:HIS:HB3	2:B:849:ASN:OD1	2.09	0.53
1:A:3:THR:HG22	1:A:5:LEU:H	1.73	0.53
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.91	0.53
2:B:407:LEU:HG	2:B:789:MET:HG3	1.91	0.52
2:B:1022:THR:O	2:B:1023:ASP:HB2	2.08	0.52
2:B:712:SER:OG	6:B:1201:HOH:O	2.19	0.52
1:A:428:SER:O	1:A:443:THR:HA	2.09	0.52
1:A:60:LEU:HD21	1:A:69:VAL:HG22	1.92	0.52
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.33	0.52
1:A:185:LYS:HE3	2:B:569:ILE:CD1	2.39	0.52
1:A:282:THR:CG2	1:A:283:GLY:N	2.72	0.52
3:C:81:LYS:HD3	3:C:81:LYS:N	2.23	0.52
1:A:56:TYR:O	1:A:57:GLU:C	2.54	0.51
2:B:609:THR:HG22	2:B:611:GLU:N	2.14	0.51
2:B:807:LEU:O	2:B:818:ILE:HA	2.09	0.51
1:A:313:TRP:CE3	1:A:316:ILE:HG21	2.45	0.51
1:A:364:PRO:O	1:A:367:THR:O	2.28	0.51
1:A:190:ARG:HG3	2:B:577:PHE:CE1	2.44	0.51
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.40	0.51
1:A:48:ARG:HB3	1:A:49:PRO:HD2	1.93	0.51
1:A:4:TYR:O	1:A:8:ILE:HG13	2.10	0.51
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.92	0.51
1:A:30:GLU:CG	1:A:510:ILE:HD11	2.41	0.51
1:A:700:PHE:O	1:A:702:MET:N	2.44	0.51
1:A:394:MET:HE3	1:A:394:MET:N	2.15	0.51
1:A:521:ALA:HA	1:A:612:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.93	0.51
1:A:700:PHE:C	1:A:702:MET:N	2.69	0.51
2:B:348:LEU:HA	6:B:1229:HOH:O	2.11	0.51
2:B:410:LEU:HD23	2:B:935:LEU:HG	1.92	0.51
2:B:950:ASP:OD2	2:B:982:GLY:HA2	2.10	0.51
2:B:1092:ASN:HB3	6:B:1282:HOH:O	2.10	0.51
1:A:3:THR:HB	1:A:6:GLU:CD	2.36	0.50
2:B:350:VAL:CG1	2:B:891:MET:HE3	2.41	0.50
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.93	0.50
2:B:510:PHE:HB2	2:B:548:THR:HG22	1.94	0.50
2:B:540:THR:HG22	2:B:589:ASN:HD22	1.76	0.50
2:B:788:GLN:HE22	2:B:850:MET:HE3	1.73	0.50
1:A:12:GLU:HG2	1:A:46:LYS:NZ	2.26	0.50
2:B:551:SER:HA	2:B:644:LEU:HD23	1.93	0.50
1:A:56:TYR:HD1	1:A:57:GLU:O	1.94	0.50
1:A:541:ASP:CB	1:A:544:ARG:HD2	2.41	0.50
3:C:127:ILE:HG22	3:C:127:ILE:O	2.12	0.50
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.42	0.50
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.92	0.50
3:C:101:LYS:H	3:C:101:LYS:CE	2.24	0.50
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.93	0.50
2:B:381:CYS:HB2	2:B:822:THR:O	2.12	0.50
1:A:559:GLU:O	1:A:568:PHE:HA	2.12	0.50
2:B:840:VAL:HG13	2:B:841:GLN:N	2.27	0.50
1:A:111:LEU:HD12	1:A:114:PHE:HE2	1.77	0.49
1:A:439:GLY:HA2	1:A:532:TYR:CE1	2.46	0.49
2:B:430:ARG:NH2	2:B:435:ARG:HB3	2.27	0.49
2:B:497:MET:HE2	2:B:816:ARG:HG3	1.94	0.49
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.93	0.49
1:A:148:LYS:HG2	1:A:244:LEU:O	2.12	0.49
1:A:708:THR:OG1	1:A:709:GLU:N	2.45	0.49
1:A:722:VAL:HG13	1:A:723:ASN:N	2.27	0.49
1:A:723:ASN:CB	6:A:902:HOH:O	2.46	0.49
2:B:424:THR:HG22	2:B:491:MET:HG3	1.93	0.49
2:B:592:LYS:O	2:B:596:GLN:HG3	2.11	0.49
2:B:749:MET:HA	2:B:806:ALA:O	2.13	0.49
2:B:960:ILE:HD13	2:B:960:ILE:N	2.27	0.49
1:A:30:GLU:HG3	1:A:510:ILE:HD11	1.94	0.49
1:A:385:THR:OG1	1:A:702:MET:HB3	2.13	0.49
3:C:80:PRO:HD2	3:C:83:LEU:HD12	1.93	0.49
1:A:113:GLN:CD	1:A:113:GLN:H	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:HA	1:A:300:MET:HE2	1.95	0.49
3:C:121:LYS:CB	3:C:121:LYS:HZ2	2.26	0.49
1:A:559:GLU:O	1:A:560:TYR:HB3	2.11	0.49
2:B:433:SER:OG	2:B:457:ARG:HD3	2.13	0.49
1:A:517:PHE:HB3	1:A:573:THR:HG22	1.95	0.49
1:A:417:SER:O	1:A:437:GLU:HA	2.12	0.48
1:A:696:LEU:HD23	1:A:703:PRO:HG2	1.95	0.48
2:B:555:PHE:HE1	2:B:570:VAL:HG11	1.77	0.48
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.78	0.48
1:A:3:THR:HB	1:A:6:GLU:CG	2.43	0.48
1:A:111:LEU:HD12	1:A:114:PHE:CE2	2.48	0.48
1:A:310:ILE:HG22	1:A:311:ARG:HD3	1.94	0.48
1:A:689:VAL:O	1:A:693:GLN:HG2	2.14	0.48
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.95	0.48
3:C:121:LYS:HB3	3:C:121:LYS:HZ3	1.77	0.48
1:A:546:LEU:HD21	1:A:584:LEU:CD2	2.43	0.48
2:B:412:HIS:CE1	2:B:415:LYS:HG3	2.48	0.48
1:A:12:GLU:HG2	1:A:46:LYS:HZ3	1.78	0.48
1:A:297:GLY:H	1:A:300:MET:HE3	1.75	0.48
1:A:652:THR:CG2	1:A:653:PHE:H	2.14	0.47
1:A:54:ILE:O	1:A:119:TYR:HA	2.14	0.47
1:A:172:MET:HE3	1:A:252:TRP:CZ2	2.49	0.47
1:A:107:PRO:HG2	1:A:110:LEU:CD1	2.41	0.47
1:A:162:ALA:O	1:A:233:VAL:HG23	2.15	0.47
3:C:80:PRO:HG2	3:C:83:LEU:HD12	1.97	0.47
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.49	0.47
3:C:3:LEU:HA	3:C:74:LEU:O	2.15	0.47
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.96	0.47
1:A:652:THR:CG2	1:A:653:PHE:N	2.68	0.47
2:B:387:ARG:HD2	2:B:935:LEU:HD12	1.96	0.47
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.15	0.47
1:A:227:ASN:HB2	1:A:230:LEU:H	1.80	0.47
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.50	0.47
1:A:339:ALA:O	1:A:447:LYS:HE3	2.14	0.47
1:A:357:LEU:HA	1:A:357:LEU:HD23	1.65	0.47
2:B:397:GLN:OE1	2:B:790:SER:HB2	2.14	0.47
2:B:620:LEU:HD21	2:B:636:VAL:HG21	1.95	0.47
2:B:721:HIS:CD2	2:B:722:GLN:HG3	2.50	0.47
3:C:154:GLU:OE1	3:C:154:GLU:HA	2.15	0.47
1:A:297:GLY:CA	1:A:300:MET:HB2	2.44	0.47
1:A:312:SER:H	1:A:315:ASP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.97	0.47
2:B:406:PRO:HB2	2:B:846:LEU:HD23	1.97	0.47
2:B:661:ALA:HB3	2:B:861:SER:OG	2.15	0.47
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.96	0.47
2:B:1079:SER:OG	2:B:1082:GLU:HG3	2.15	0.47
3:C:14:LEU:CD2	3:C:106:VAL:HG23	2.45	0.47
1:A:363:CYS:HB2	1:A:364:PRO:HD3	1.95	0.47
1:A:562:LYS:HB3	1:A:562:LYS:HZ3	1.75	0.46
2:B:553:ILE:HD13	2:B:576:VAL:HG11	1.98	0.46
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.50	0.46
1:A:605:HIS:HD2	1:A:606:HIS:CD2	2.34	0.46
2:B:350:VAL:HG12	2:B:891:MET:HE3	1.96	0.46
3:C:60:THR:HG22	3:C:62:HIS:NE2	2.29	0.46
1:A:107:PRO:CG	1:A:110:LEU:HD12	2.38	0.46
1:A:700:PHE:C	1:A:700:PHE:CD1	2.92	0.46
2:B:1011:VAL:HG21	2:B:1017:ILE:HG12	1.97	0.46
1:A:76:VAL:HG11	1:A:78:TYR:CE1	2.50	0.46
1:A:268:LEU:HG	1:A:288:MET:SD	2.55	0.46
3:C:39:GLN:HB3	3:C:157:LEU:HD22	1.97	0.46
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.98	0.46
2:B:992:LEU:O	2:B:1052:LEU:HA	2.15	0.46
1:A:754:ASP:O	1:A:758:LYS:HG3	2.16	0.46
2:B:350:VAL:HG22	2:B:878:TYR:OH	2.16	0.46
2:B:578:ILE:HG23	2:B:584:LEU:HD12	1.97	0.46
2:B:754:THR:HG22	2:B:755:LYS:O	2.16	0.46
2:B:1074:THR:HG23	2:B:1076:SER:N	2.26	0.46
2:B:393:ILE:HG13	2:B:801:VAL:HG21	1.97	0.46
2:B:410:LEU:N	2:B:410:LEU:CD1	2.79	0.46
2:B:965:ILE:N	2:B:965:ILE:CD1	2.77	0.46
3:C:61:PHE:HB3	3:C:72:LEU:HD11	1.97	0.46
1:A:180:CYS:HB3	1:A:183:ILE:HG22	1.97	0.46
1:A:282:THR:HG22	1:A:283:GLY:N	2.30	0.46
2:B:620:LEU:CD2	2:B:636:VAL:HG21	2.45	0.46
3:C:94:GLU:HG2	3:C:118:PHE:CD2	2.51	0.46
2:B:512:VAL:HG22	2:B:549:PHE:O	2.16	0.46
2:B:777:PRO:C	2:B:778:ASN:HD22	2.23	0.46
1:A:246:GLU:C	6:A:901:HOH:O	2.59	0.45
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.98	0.45
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.46	0.45
2:B:750:ARG:NH2	5:B:1101:A1EQA:O2	2.50	0.45
2:B:923:ARG:O	2:B:927:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:VAL:N	3:C:104:PRO:HD2	2.30	0.45
1:A:51:LEU:HD22	1:A:51:LEU:HA	1.80	0.45
1:A:80:ALA:O	1:A:81:LYS:C	2.60	0.45
2:B:879:ARG:CB	6:B:1290:HOH:O	2.64	0.45
1:A:656:ILE:HD11	1:A:695:ILE:CG1	2.36	0.45
2:B:720:HIS:HB3	2:B:723:HIS:HB2	1.98	0.45
1:A:168:THR:HG21	1:A:247:LEU:HD22	1.95	0.45
1:A:183:ILE:HD12	1:A:183:ILE:HA	1.67	0.45
3:C:149:MET:O	3:C:150:VAL:CG2	2.65	0.45
1:A:164:VAL:O	1:A:230:LEU:HA	2.17	0.45
1:A:454:THR:O	1:A:455:THR:C	2.60	0.45
2:B:758:SER:O	2:B:789:MET:HA	2.16	0.45
1:A:647:ILE:HG13	1:A:664:ILE:HD12	1.98	0.45
2:B:522:LEU:HD23	2:B:522:LEU:HA	1.79	0.45
2:B:986:MET:HE1	2:B:1069:MET:HE3	1.97	0.45
1:A:101:ILE:HA	1:A:101:ILE:HD12	1.67	0.45
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.51	0.45
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.99	0.45
1:A:531:ILE:HD12	1:A:607:PHE:CD2	2.52	0.45
2:B:444:PHE:HE1	2:B:461:VAL:HG21	1.80	0.45
2:B:794:SER:C	2:B:796:THR:H	2.25	0.45
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.99	0.45
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.72	0.45
2:B:620:LEU:CD2	2:B:634:MET:HE1	2.44	0.45
2:B:964:THR:C	2:B:965:ILE:HD12	2.42	0.45
2:B:985:LEU:C	2:B:985:LEU:HD23	2.42	0.45
1:A:373:MET:HE1	1:A:599:GLU:HG2	1.99	0.44
1:A:575:SER:O	1:A:578:PRO:HD2	2.17	0.44
2:B:759:ILE:CG2	2:B:787:VAL:HG22	2.47	0.44
3:C:80:PRO:CG	3:C:83:LEU:HD12	2.47	0.44
1:A:181:GLU:OE1	1:A:181:GLU:N	2.48	0.44
1:A:560:TYR:HD2	1:A:761:VAL:HG12	1.81	0.44
2:B:620:LEU:CD2	2:B:634:MET:CE	2.96	0.44
2:B:675:LYS:O	2:B:679:ASP:OD1	2.34	0.44
1:A:19:PHE:HA	1:A:39:ALA:O	2.17	0.44
1:A:297:GLY:N	1:A:300:MET:HB2	2.32	0.44
2:B:504:PRO:HG2	2:B:542:THR:OG1	2.18	0.44
1:A:276:GLU:HB2	6:A:921:HOH:O	2.18	0.44
1:A:524:ILE:CD1	1:A:616:LEU:HD23	2.47	0.44
1:A:647:ILE:HD11	1:A:685:LEU:HD23	1.99	0.44
2:B:417:LEU:HD12	2:B:420:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:ARG:HG3	2:B:482:GLU:OE1	2.18	0.44
3:C:81:LYS:H	3:C:81:LYS:CD	2.15	0.44
1:A:265:GLY:O	1:A:269:SER:OG	2.36	0.44
3:C:16:LEU:HD22	3:C:112:PHE:HE2	1.83	0.44
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.52	0.44
2:B:433:SER:OG	2:B:457:ARG:CD	2.66	0.44
3:C:63:TYR:CD1	3:C:63:TYR:C	2.96	0.44
1:A:600:SER:O	1:A:604:ARG:HG3	2.17	0.44
2:B:411:LEU:HB2	2:B:413:PRO:HD3	1.99	0.44
2:B:450:TRP:CE2	2:B:459:ASN:HB2	2.53	0.43
2:B:480:ARG:HG3	2:B:481:PRO:CD	2.48	0.43
2:B:714:TYR:N	2:B:714:TYR:CD1	2.86	0.43
2:B:760:HIS:CE1	2:B:788:GLN:HB3	2.53	0.43
2:B:814:GLY:O	3:C:113:ILE:CD1	2.65	0.43
1:A:57:GLU:HA	1:A:58:PRO:HD2	1.84	0.43
2:B:437:TYR:HD1	2:B:804:GLN:OE1	2.00	0.43
2:B:840:VAL:CG1	2:B:841:GLN:N	2.81	0.43
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.48	0.43
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.52	0.43
3:C:6:MET:HE2	3:C:6:MET:HB3	1.97	0.43
1:A:3:THR:HG22	1:A:5:LEU:N	2.33	0.43
1:A:404:GLY:O	1:A:447:LYS:HA	2.18	0.43
2:B:545:GLY:HA3	2:B:585:LEU:HD23	2.01	0.43
2:B:766:PHE:HE1	2:B:768:VAL:CG2	2.31	0.43
1:A:54:ILE:CG2	1:A:56:TYR:CZ	3.02	0.43
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.99	0.43
2:B:881:SER:O	2:B:882:VAL:CG1	2.66	0.43
1:A:249:ARG:O	1:A:250:ASP:C	2.61	0.43
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.85	0.43
1:A:392:LYS:HE2	1:A:398:PHE:CE1	2.54	0.43
1:A:63:ARG:O	1:A:66:CYS:N	2.52	0.43
2:B:535:LEU:HB3	2:B:740:THR:HG22	2.01	0.43
2:B:567:MET:HE2	2:B:569:ILE:HD11	2.01	0.43
3:C:33:TYR:CE1	3:C:59:MET:HG3	2.54	0.43
1:A:394:MET:H	1:A:394:MET:CE	2.18	0.42
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.54	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.74	0.42
2:B:955:GLU:O	2:B:955:GLU:HG3	2.19	0.42
1:A:61:CYS:O	1:A:67:ARG:HA	2.19	0.42
1:A:63:ARG:O	1:A:64:THR:C	2.63	0.42
1:A:664:ILE:HD13	1:A:684:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:LEU:HD21	2:B:595:VAL:HG23	2.01	0.42
2:B:592:LYS:O	2:B:595:VAL:HG22	2.19	0.42
1:A:571:SER:HB2	1:A:573:THR:H	1.85	0.42
1:A:698:SER:O	1:A:699:ARG:C	2.62	0.42
2:B:500:PRO:O	2:B:501:PRO:C	2.59	0.42
2:B:830:THR:O	2:B:831:LEU:C	2.62	0.42
1:A:704:ARG:HE	1:A:704:ARG:HB3	1.53	0.42
3:C:14:LEU:HD23	3:C:106:VAL:HG23	2.00	0.42
3:C:148:ILE:HG22	3:C:149:MET:N	2.33	0.42
2:B:479:ARG:HD2	2:B:479:ARG:HA	1.60	0.42
3:C:53:THR:O	3:C:150:VAL:HA	2.20	0.42
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.84	0.42
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.69	0.42
1:A:242:ASP:O	1:A:243:LEU:C	2.62	0.42
1:A:361:LYS:O	1:A:362:CYS:C	2.62	0.42
2:B:436:THR:HG21	2:B:454:LEU:HD13	2.02	0.42
2:B:557:GLY:C	2:B:558:LEU:HG	2.43	0.42
2:B:532:ASN:O	2:B:533:LEU:C	2.61	0.42
2:B:356:GLU:C	2:B:358:ASN:H	2.27	0.42
3:C:82:LYS:H	3:C:82:LYS:HG2	1.66	0.42
1:A:30:GLU:O	1:A:34:MET:HE2	2.19	0.42
1:A:185:LYS:HE3	2:B:569:ILE:HD11	2.02	0.42
2:B:762:PHE:HB3	2:B:766:PHE:CZ	2.55	0.42
2:B:1083:PHE:CZ	2:B:1087:ILE:HD11	2.54	0.42
3:C:4:LEU:HD12	3:C:5:THR:H	1.83	0.42
1:A:83:TRP:CD1	1:A:94:PHE:CE1	3.08	0.42
2:B:383:PRO:HA	2:B:386:PHE:O	2.20	0.42
2:B:393:ILE:HG13	2:B:801:VAL:CG2	2.49	0.42
1:A:70:LEU:O	1:A:109:GLU:HB2	2.20	0.41
1:A:181:GLU:H	1:A:181:GLU:CD	2.28	0.41
1:A:607:PHE:HD2	1:A:608:MET:HE2	1.85	0.41
2:B:440:PRO:HB3	2:B:483:VAL:O	2.20	0.41
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.55	0.41
1:A:406:LEU:O	1:A:445:GLN:HA	2.19	0.41
1:A:581:MET:HE2	1:A:581:MET:HA	2.01	0.41
2:B:438:ILE:HD13	2:B:450:TRP:CE2	2.56	0.41
2:B:641:LEU:HD22	2:B:649:LEU:HB2	2.01	0.41
2:B:881:SER:O	2:B:882:VAL:HG13	2.20	0.41
1:A:273:GLY:HA3	6:A:906:HOH:O	2.19	0.41
1:A:618:MET:HG2	1:A:653:PHE:HB3	2.02	0.41
2:B:754:THR:O	2:B:755:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:CG1	1:A:723:ASN:N	2.83	0.41
2:B:529:LEU:HD23	2:B:529:LEU:HA	1.67	0.41
1:A:48:ARG:HB3	1:A:49:PRO:CD	2.50	0.41
2:B:423:VAL:CG1	2:B:425:SER:H	2.33	0.41
2:B:878:TYR:CD2	2:B:893:PRO:HD3	2.56	0.41
2:B:1006:SER:HA	2:B:1011:VAL:O	2.21	0.41
2:B:929:GLN:O	2:B:933:GLN:HG3	2.21	0.41
1:A:3:THR:HB	1:A:6:GLU:HG3	2.02	0.41
1:A:297:GLY:N	1:A:300:MET:HE2	2.27	0.41
2:B:377:GLN:OE1	2:B:377:GLN:CA	2.69	0.41
2:B:533:LEU:HD12	2:B:533:LEU:HA	1.76	0.41
2:B:573:ILE:HA	2:B:573:ILE:HD12	1.62	0.41
2:B:627:MET:HE1	2:B:632:GLY:C	2.46	0.41
2:B:666:MET:HE1	2:B:927:MET:SD	2.61	0.41
2:B:1051:ILE:H	2:B:1051:ILE:HG12	1.75	0.41
2:B:1069:MET:HE2	2:B:1069:MET:CA	2.48	0.41
1:A:141:ASP:OD1	1:A:249:ARG:HD3	2.21	0.41
1:A:238:MET:HE3	1:A:238:MET:HB3	1.96	0.41
2:B:610:LEU:HA	2:B:610:LEU:HD23	1.65	0.41
1:A:56:TYR:CD1	1:A:56:TYR:C	2.99	0.40
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.35	0.40
1:A:537:GLU:N	1:A:537:GLU:OE1	2.53	0.40
2:B:831:LEU:HD23	2:B:831:LEU:HA	1.89	0.40
5:B:1101:A1EQA:C14	5:B:1101:A1EQA:C5	2.99	0.40
1:A:12:GLU:CG	1:A:46:LYS:HZ3	2.35	0.40
1:A:190:ARG:HB3	1:A:192:THR:HG22	2.04	0.40
2:B:539:ASN:HB2	3:C:114:GLU:OE2	2.22	0.40
2:B:555:PHE:CZ	2:B:622:ALA:HB1	2.56	0.40
2:B:609:THR:CG2	2:B:611:GLU:HB2	2.50	0.40
2:B:680:CYS:HB3	2:B:685:VAL:HB	2.02	0.40
1:A:200:LEU:HA	1:A:200:LEU:HD12	1.83	0.40
2:B:684:GLN:HA	2:B:684:GLN:OE1	2.22	0.40
2:B:716:TYR:OH	2:B:734:GLU:OE1	2.32	0.40
1:A:295:THR:C	1:A:300:MET:HG3	2.47	0.40
2:B:611:GLU:OE1	2:B:611:GLU:HA	2.21	0.40
1:A:247:LEU:N	6:A:901:HOH:O	2.54	0.40
1:A:568:PHE:CD1	1:A:568:PHE:C	2.99	0.40
2:B:558:LEU:HD23	2:B:565:PRO:HB3	2.04	0.40
2:B:762:PHE:HB3	2:B:766:PHE:HZ	1.86	0.40
2:B:958:LEU:HD12	2:B:958:LEU:HA	1.87	0.40
3:C:63:TYR:HA	3:C:71:TYR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	675/765 (88%)	624 (92%)	48 (7%)	3 (0%)	30	37
2	B	720/748 (96%)	666 (92%)	50 (7%)	4 (1%)	21	25
3	C	124/157 (79%)	113 (91%)	11 (9%)	0	100	100
All	All	1519/1670 (91%)	1403 (92%)	109 (7%)	7 (0%)	24	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
2	B	462	PRO
2	B	513	SER
1	A	702	MET
2	B	1047	PRO
2	B	347	GLY
1	A	49	PRO

### 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	586/666 (88%)	543 (93%)	43 (7%)	13	17
2	B	636/679 (94%)	582 (92%)	54 (8%)	10	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	108/138 (78%)	98 (91%)	10 (9%)	8	10
All	All	1330/1483 (90%)	1223 (92%)	107 (8%)	11	14

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	34	MET
1	A	41	LEU
1	A	51	LEU
1	A	101	ILE
1	A	116	SER
1	A	127	MET
1	A	161	THR
1	A	164	VAL
1	A	178	LEU
1	A	180	CYS
1	A	183	ILE
1	A	228	ARG
1	A	240	LEU
1	A	243	LEU
1	A	262	ARG
1	A	264	SER
1	A	268	LEU
1	A	269	SER
1	A	290	ILE
1	A	316	ILE
1	A	355	THR
1	A	362	CYS
1	A	376	SER
1	A	394	MET
1	A	524	ILE
1	A	544	ARG
1	A	562	LYS
1	A	570	PHE
1	A	571	SER
1	A	584	LEU
1	A	612	LEU
1	A	613	THR
1	A	637	LEU
1	A	639	SER
1	A	649	LEU

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Mol	Chain	Res	Type
1	A	655	GLN
1	A	664	ILE
1	A	695	ILE
1	A	702	MET
1	A	709	GLU
1	A	713	SER
1	A	722	VAL
2	B	359	MET
2	B	410	LEU
2	B	411	LEU
2	B	446	ASP
2	B	460	ASP
2	B	479	ARG
2	B	498	LEU
2	B	522	LEU
2	B	533	LEU
2	B	570	VAL
2	B	573	ILE
2	B	574	GLU
2	B	576	VAL
2	B	607	THR
2	B	641	LEU
2	B	650	LYS
2	B	659	SER
2	B	669	SER
2	B	712	SER
2	B	713	VAL
2	B	726	VAL
2	B	751	ILE
2	B	787	VAL
2	B	789	MET
2	B	793	GLU
2	B	798	THR
2	B	807	LEU
2	B	813	LYS
2	B	816	ARG
2	B	831	LEU
2	B	844	SER
2	B	857	THR
2	B	881	SER
2	B	906	LEU
2	B	911	SER

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Mol	Chain	Res	Type
2	B	920	LEU
2	B	935	LEU
2	B	954	ASP
2	B	958	LEU
2	B	963	ARG
2	B	964	THR
2	B	972	GLN
2	B	979	SER
2	B	998	LYS
2	B	1000	CYS
2	B	1001	THR
2	B	1002	GLN
2	B	1029	THR
2	B	1040	SER
2	B	1052	LEU
2	B	1055	ILE
2	B	1085	LEU
2	B	1087	ILE
2	B	1092	ASN
3	C	4	LEU
3	C	46	GLU
3	C	81	LYS
3	C	101	LYS
3	C	105	THR
3	C	113	ILE
3	C	117	THR
3	C	121	LYS
3	C	129	SER
3	C	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	445	GLN
1	A	583	HIS
1	A	591	GLN
1	A	606	HIS
1	A	620	GLN
1	A	660	HIS
2	B	395	GLN
2	B	566	GLN

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Mol	Chain	Res	Type
2	B	604	GLN
2	B	721	HIS
2	B	832	ASN
2	B	943	HIS
3	C	36	GLN
3	C	92	HIS

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	A1EQA	B	1101	-	23,25,25	2.02	7 (30%)	29,37,37	2.54	9 (31%)

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	A1EQA	B	1101	-	-	9/20/33/33	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	A1EQA	O5-C1	5.34	1.38	1.22
5	B	1101	A1EQA	C13-C12	4.14	1.57	1.51
5	B	1101	A1EQA	C12-C4	3.23	1.56	1.50
5	B	1101	A1EQA	C11-C10	2.79	1.43	1.39
5	B	1101	A1EQA	O2-C3	2.64	1.39	1.30
5	B	1101	A1EQA	O4-C10	2.43	1.42	1.37
5	B	1101	A1EQA	C14-C13	2.19	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	A1EQA	C2-C12-C13	-5.86	110.82	121.65
5	B	1101	A1EQA	C5-C6-C11	5.59	130.02	120.43
5	B	1101	A1EQA	C15-C14-C13	5.11	126.76	120.65
5	B	1101	A1EQA	C18-C13-C14	-4.56	112.65	118.30
5	B	1101	A1EQA	C5-C6-C7	-4.48	112.57	120.90
5	B	1101	A1EQA	C13-C12-C4	4.40	129.64	123.07
5	B	1101	A1EQA	O4-C10-C11	2.24	125.72	119.85
5	B	1101	A1EQA	C14-C13-C12	2.13	125.77	120.99
5	B	1101	A1EQA	C4-C2-C1	-2.07	111.08	118.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

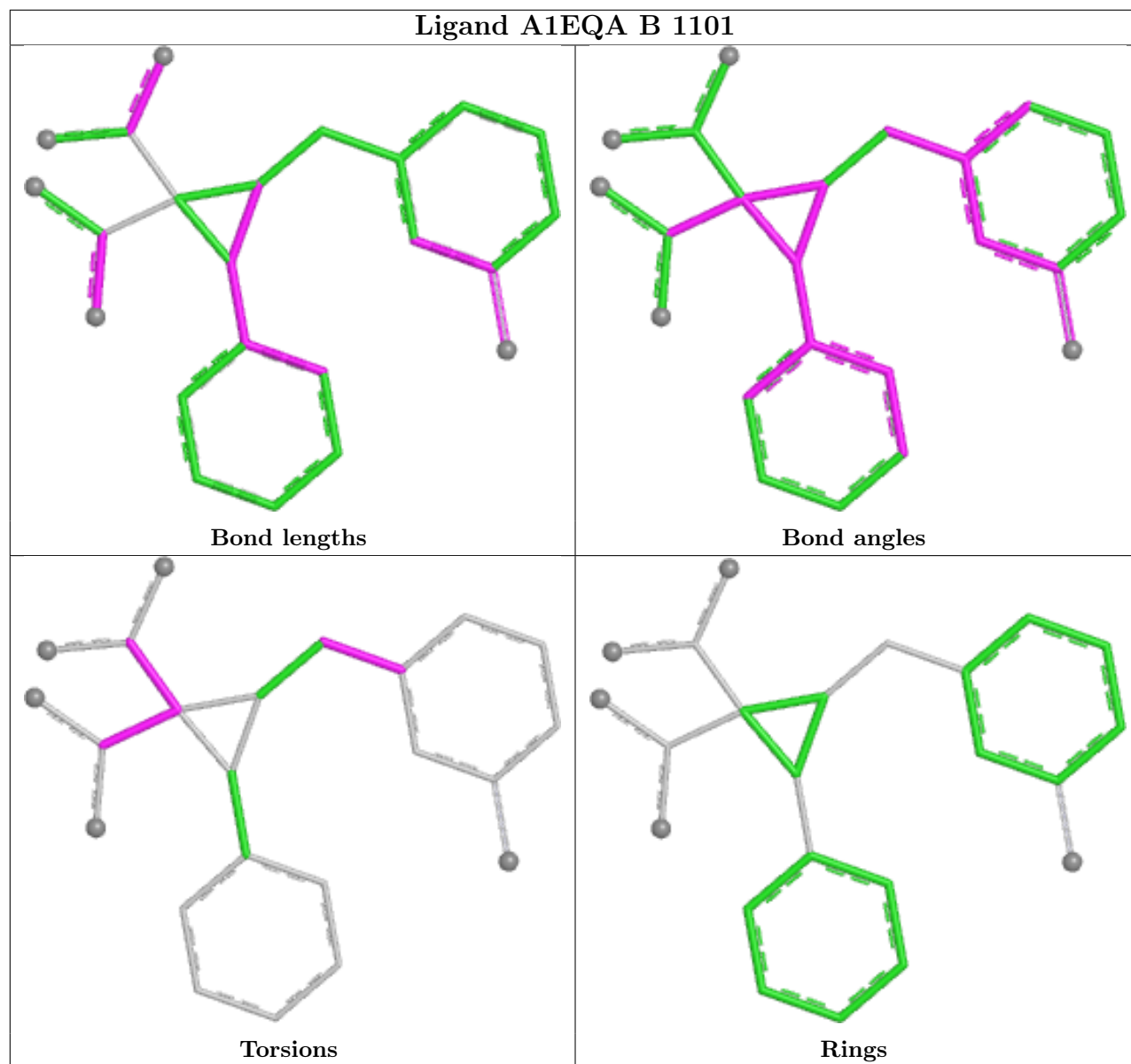
Mol	Chain	Res	Type	Atoms
5	B	1101	A1EQA	O1-C1-C2-C3
5	B	1101	A1EQA	C1-C2-C3-O2
5	B	1101	A1EQA	C12-C2-C3-O3
5	B	1101	A1EQA	C4-C5-C6-C11
5	B	1101	A1EQA	C4-C5-C6-C7
5	B	1101	A1EQA	O1-C1-C2-C12
5	B	1101	A1EQA	O5-C1-C2-C12
5	B	1101	A1EQA	C12-C2-C3-O2
5	B	1101	A1EQA	O5-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	A1EQA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	689/765 (90%)	0.95	85 (12%) <b>8</b> <b>9</b>	40, 59, 87, 118	0
2	B	728/748 (97%)	0.65	44 (6%) <b>27</b> <b>30</b>	37, 54, 79, 120	0
3	C	130/157 (82%)	1.26	20 (15%) <b>5</b> <b>6</b>	51, 75, 106, 119	0
All	All	1547/1670 (92%)	0.84	149 (9%) <b>13</b> <b>15</b>	37, 57, 87, 120	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	127	ILE	5.4
2	B	463	GLU	5.1
1	A	504	ALA	4.8
1	A	94	PHE	4.7
1	A	700	PHE	4.5
3	C	3	LEU	4.3
1	A	51	LEU	4.2
2	B	461	VAL	4.2
2	B	1047	PRO	4.2
1	A	747	VAL	4.1
1	A	49	PRO	4.0
1	A	223	PRO	3.9
1	A	476	ARG	3.8
1	A	29	LEU	3.7
3	C	128	ASP	3.7
1	A	56	TYR	3.7
2	B	888	PRO	3.6
3	C	30	LEU	3.5
1	A	32	THR	3.5
1	A	464	VAL	3.5
1	A	34	MET	3.5
3	C	153	ILE	3.5
2	B	1048	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	701	PRO	3.5
2	B	1020	PRO	3.4
2	B	424	THR	3.4
1	A	35	VAL	3.4
1	A	717	PHE	3.4
1	A	31	ALA	3.4
1	A	101	ILE	3.3
1	A	89	TYR	3.3
1	A	27	SER	3.3
3	C	157	LEU	3.3
2	B	348	LEU	3.2
2	B	1045	GLN	3.2
1	A	762	SER	3.2
1	A	52	PRO	3.2
2	B	1022	THR	3.2
3	C	156	VAL	3.1
2	B	496	TYR	3.1
2	B	793	GLU	3.1
1	A	33	ARG	3.1
1	A	510	ILE	3.1
1	A	62	SER	3.1
2	B	426	SER	3.1
1	A	98	TYR	3.0
1	A	205	GLY	3.0
2	B	1057	ASP	3.0
1	A	78	TYR	3.0
1	A	121	VAL	3.0
2	B	1054	VAL	3.0
1	A	58	PRO	3.0
3	C	131	ALA	2.9
1	A	652	THR	2.9
2	B	427	THR	2.9
1	A	104	LEU	2.9
1	A	105	ASN	2.9
2	B	462	PRO	2.8
1	A	76	VAL	2.8
1	A	463	VAL	2.8
1	A	47	GLU	2.8
1	A	631	PRO	2.8
3	C	58	ALA	2.8
1	A	666	GLN	2.8
2	B	447	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	534	ALA	2.8
2	B	661	ALA	2.8
1	A	503	TRP	2.7
1	A	25	PRO	2.7
2	B	423	VAL	2.7
3	C	148	ILE	2.7
1	A	431	PRO	2.7
1	A	593	PHE	2.7
2	B	533	LEU	2.7
1	A	65	THR	2.6
1	A	224	PRO	2.6
2	B	1019	GLN	2.6
1	A	548	ARG	2.6
1	A	53	PRO	2.6
1	A	107	PRO	2.6
2	B	576	VAL	2.6
1	A	592	VAL	2.6
3	C	126	TYR	2.6
1	A	26	SER	2.5
1	A	665	ALA	2.5
2	B	797	ASP	2.5
2	B	347	GLY	2.5
3	C	56	ALA	2.5
2	B	882	VAL	2.4
1	A	30	GLU	2.4
3	C	130	ARG	2.4
2	B	662	LYS	2.4
3	C	54	LEU	2.4
1	A	704	ARG	2.4
1	A	679	GLU	2.4
1	A	444	CYS	2.4
2	B	573	ILE	2.4
1	A	83	TRP	2.4
1	A	537	GLU	2.4
2	B	910	LYS	2.3
2	B	796	THR	2.3
1	A	656	ILE	2.3
2	B	482	GLU	2.3
1	A	165	GLY	2.3
1	A	3	THR	2.3
1	A	663	THR	2.3
2	B	1046	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	2.3
1	A	60	LEU	2.3
1	A	536	THR	2.3
1	A	102	SER	2.3
1	A	55	GLN	2.3
2	B	1017	ILE	2.3
1	A	637	LEU	2.2
2	B	445	LEU	2.2
2	B	1053	TYR	2.2
2	B	770	SER	2.2
3	C	150	VAL	2.2
3	C	19	SER	2.2
1	A	664	ILE	2.2
2	B	428	ILE	2.2
1	A	632	PRO	2.2
2	B	1086	HIS	2.2
1	A	628	PHE	2.2
1	A	721	LYS	2.2
3	C	124	LYS	2.2
1	A	93	GLN	2.2
1	A	477	GLY	2.2
2	B	609	THR	2.2
1	A	301	VAL	2.1
3	C	103	VAL	2.1
1	A	461	PHE	2.1
3	C	154	GLU	2.1
2	B	771	THR	2.1
1	A	513	ILE	2.1
1	A	120	VAL	2.1
2	B	490	PHE	2.1
1	A	5	LEU	2.1
1	A	64	THR	2.1
1	A	108	ALA	2.1
2	B	574	GLU	2.1
1	A	754	ASP	2.1
3	C	87	TYR	2.1
1	A	314	HIS	2.0
1	A	657	LEU	2.0
1	A	54	ILE	2.0
1	A	316	ILE	2.0
2	B	595	VAL	2.0
1	A	407	GLU	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](#)

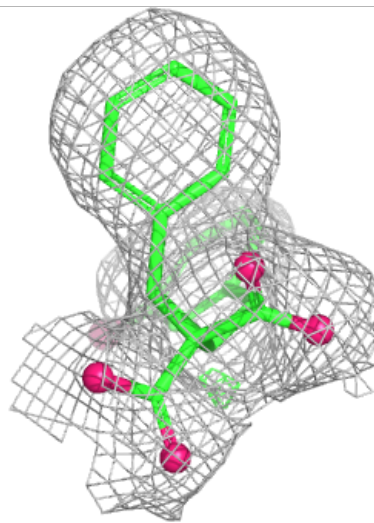
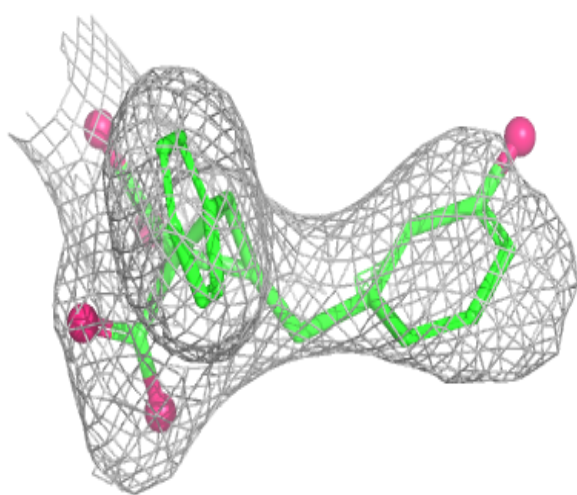
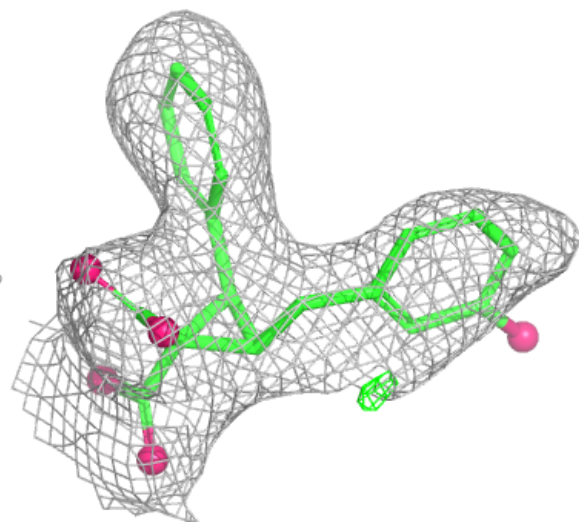
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	A1EQA	B	1101	23/23	0.86	0.14	51,66,73,76	0
4	ZN	A	801	1/1	0.98	0.04	75,75,75,75	0
4	ZN	B	1102	1/1	0.99	0.12	106,106,106,106	0

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

**Electron density around A1EQA B 1101:**

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



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.