



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:10 PM EDT

PDB ID : 9OZM / pdb_00009ozm
Title : Structure of human Sec23a/Sec24a/Sec22b bound to ligand CPD5
Authors : Goldberg, J.
Deposited on : 2025-06-05
Resolution : 3.22 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

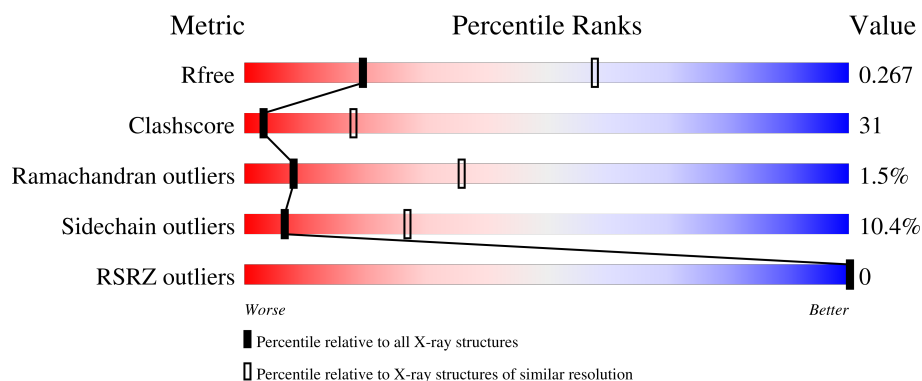
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	B	765	
2	C	748	
3	D	157	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12072 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	B	689	Total	C	N	O	S	0	0	0
			5382	3442	905	996	39			

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

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

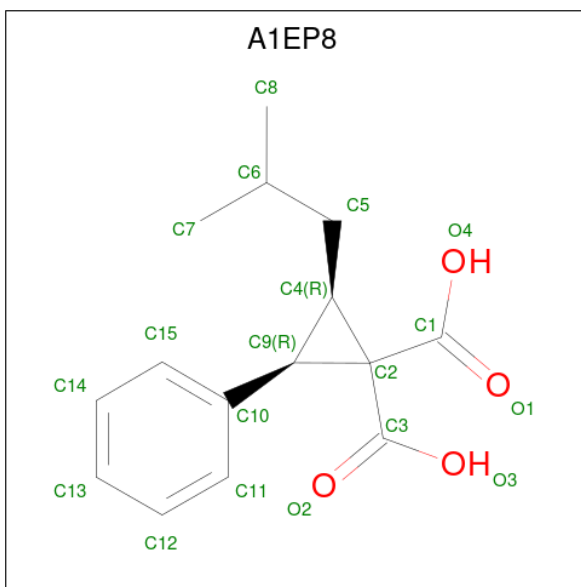
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	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	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2 {R},3 {R})-2-(2-methylpropyl)-3-phenyl-cyclopropane-1,1-dicarboxylic acid (CCD ID: A1EP8) (formula: C₁₅H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			19	15	4		

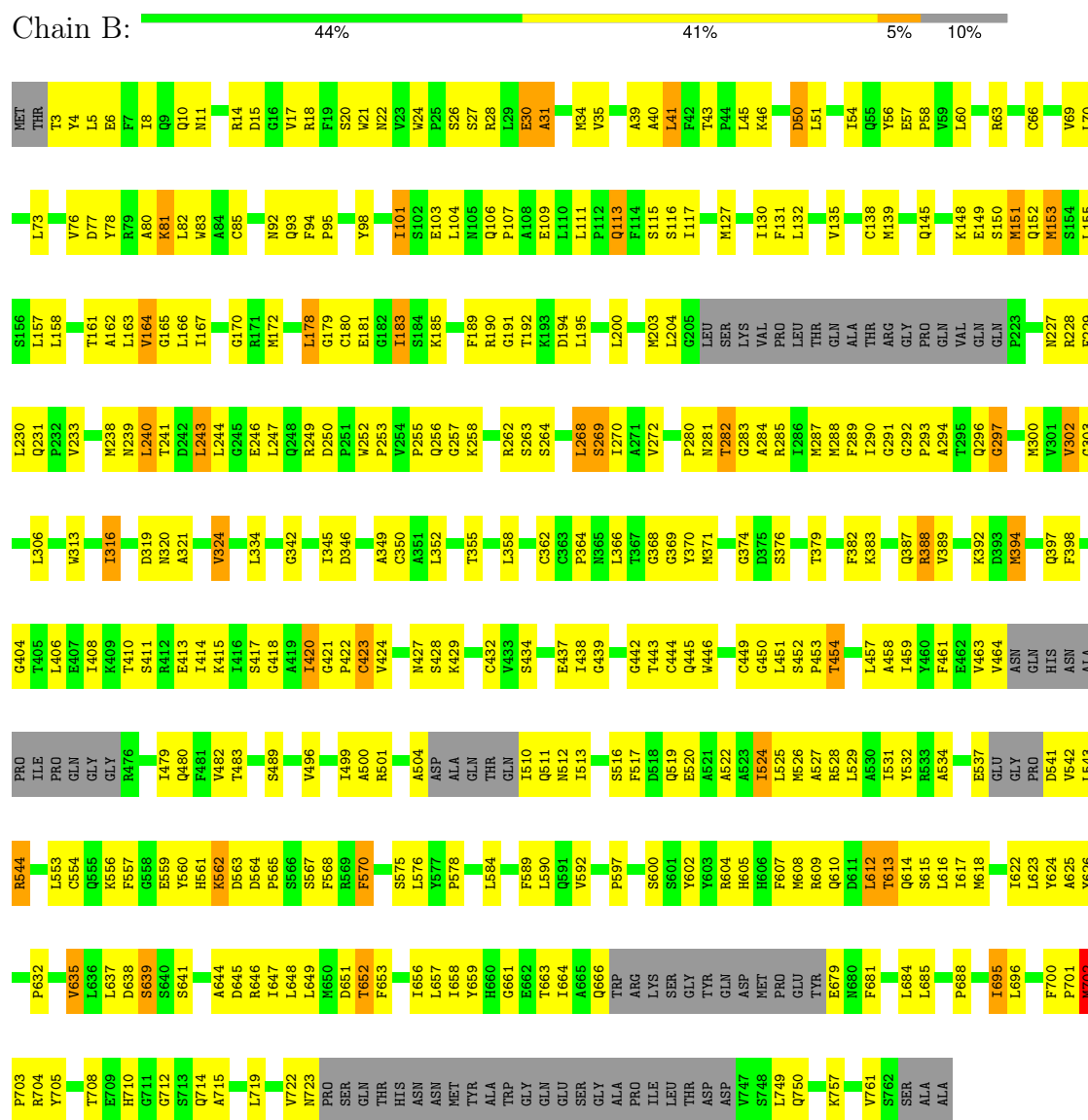
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		

3 Residue-property plots

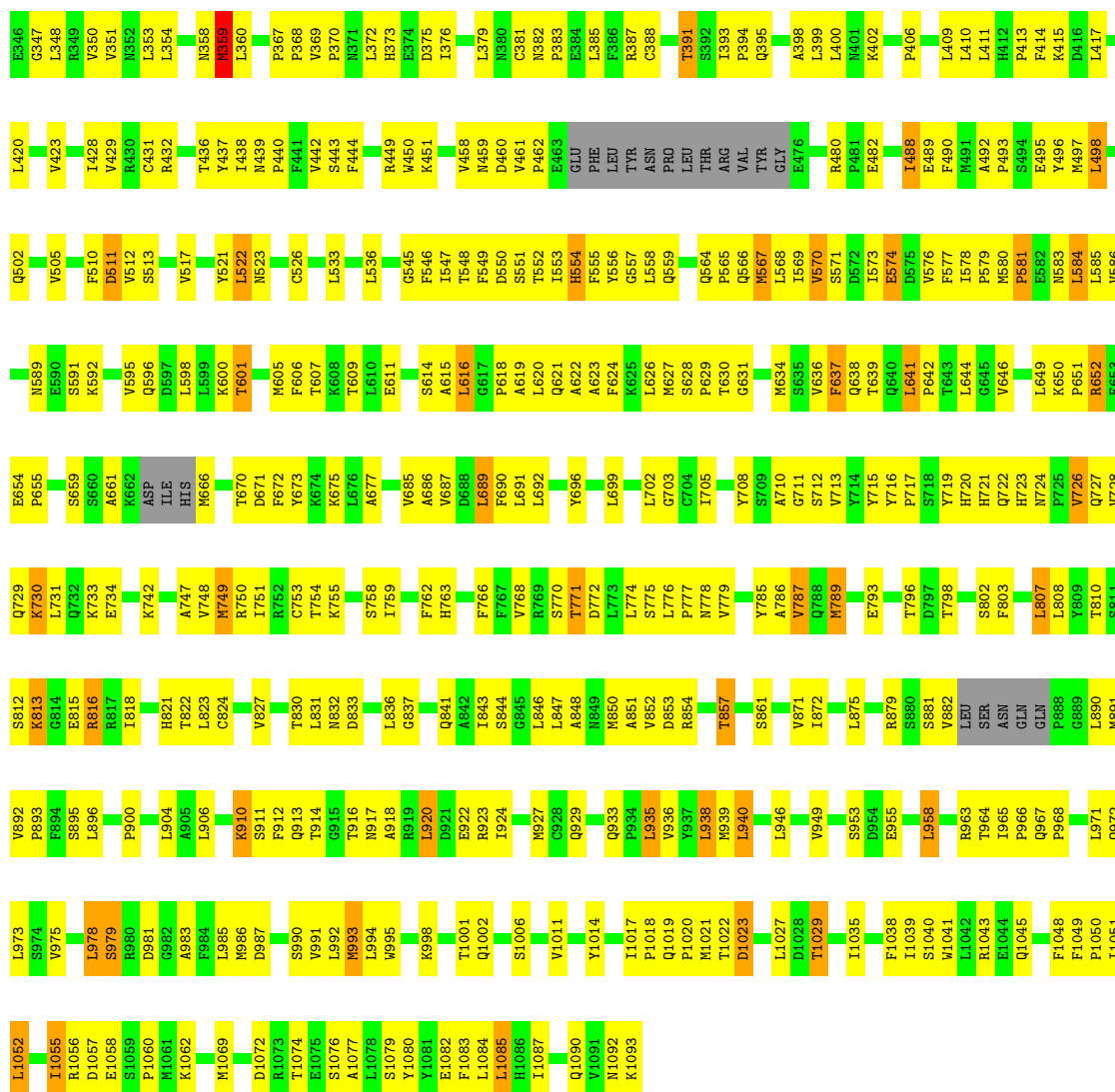
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.44Å 96.68Å 130.54Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	19.84 – 3.22 19.84 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.84-3.22) 99.0 (19.84-3.22)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.22Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.189 , 0.267 0.189 , 0.267	Depositor DCC
R_{free} test set	1457 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	122.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12072	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1EP8

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	B	0.45	0/5506	0.64	2/7466 (0.0%)
2	C	0.48	1/5773 (0.0%)	0.66	1/7862 (0.0%)
3	D	0.41	0/1035	0.60	0/1399
All	All	0.46	1/12314 (0.0%)	0.65	3/16727 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	968	PRO	CA-C	-5.16	1.49	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1060	PRO	N-CA-CB	6.13	110.31	103.44
1	B	652	THR	CA-C-N	-5.68	112.10	120.28
1	B	652	THR	C-N-CA	-5.68	112.10	120.28

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	B	5382	0	5284	338	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5651	0	5635	353	0
3	D	1016	0	995	64	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	19	0	0	1	0
6	B	2	0	0	0	0
All	All	12072	0	11914	748	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 31.

All (748) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLN:HG3	1:B:618:MET:HE1	1.29	1.14
1:B:153:MET:HE2	1:B:157:LEU:HD11	1.27	1.09
2:C:875:LEU:HD22	2:C:892:VAL:HG12	1.36	1.06
2:C:993:MET:HB3	2:C:1055:ILE:HD11	1.35	1.06
1:B:39:ALA:HB3	1:B:525:LEU:HD13	1.42	0.99
2:C:830:THR:HG22	2:C:832:ASN:H	1.32	0.94
2:C:631:GLY:HA2	2:C:685:VAL:HG23	1.46	0.94
1:B:288:MET:HG2	1:B:290:ILE:HD11	1.47	0.93
1:B:70:LEU:HD23	1:B:109:GLU:HG3	1.49	0.93
2:C:949:VAL:HG11	2:C:985:LEU:HB2	1.47	0.93
1:B:560:TYR:CD2	1:B:761:VAL:HG12	2.05	0.91
2:C:975:VAL:HG23	2:C:1072:ASP:OD2	1.71	0.91
1:B:127:MET:HA	1:B:127:MET:HE2	1.50	0.90
2:C:759:ILE:HG23	2:C:787:VAL:HG13	1.54	0.89
2:C:573:ILE:HG23	2:C:618:PRO:HG2	1.53	0.89
1:B:288:MET:HG2	1:B:290:ILE:CD1	2.02	0.89
1:B:3:THR:HB	1:B:6:GLU:HG3	1.55	0.88
1:B:610:GLN:HG3	1:B:618:MET:CE	2.02	0.88
1:B:195:LEU:HD13	1:B:203:MET:HE1	1.54	0.87
1:B:76:VAL:HG12	1:B:77:ASP:H	1.38	0.86
1:B:111:LEU:HB3	1:B:113:GLN:OE1	1.76	0.86
1:B:554:CYS:HA	1:B:570:PHE:CZ	2.09	0.86
2:C:395:GLN:HE21	2:C:796:THR:HA	1.40	0.85
3:D:4:LEU:HD12	3:D:5:THR:N	1.91	0.84
2:C:609:THR:HG22	2:C:611:GLU:H	1.41	0.84
2:C:846:LEU:O	2:C:850:MET:HG3	1.78	0.84
2:C:417:LEU:HD12	2:C:420:LEU:HD13	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:CYS:HA	1:B:570:PHE:HZ	1.43	0.83
2:C:367:PRO:HB3	2:C:387:ARG:NH2	1.93	0.83
2:C:513:SER:O	2:C:517:VAL:HG23	1.77	0.83
3:D:39:GLN:HB3	3:D:157:LEU:HD22	1.61	0.83
2:C:848:ALA:HB2	2:C:906:LEU:HD21	1.59	0.82
1:B:153:MET:HE1	1:B:387:GLN:CB	2.09	0.82
2:C:367:PRO:HB3	2:C:387:ARG:HH22	1.44	0.82
1:B:95:PRO:HG2	1:B:98:TYR:CD1	2.14	0.82
1:B:73:LEU:HD11	1:B:500:ALA:HB2	1.61	0.81
1:B:610:GLN:CG	1:B:618:MET:HE1	2.10	0.81
2:C:413:PRO:HG3	2:C:749:MET:HE1	1.61	0.81
2:C:497:MET:HE2	2:C:816:ARG:HG3	1.61	0.79
1:B:607:PHE:HD2	1:B:608:MET:HE3	1.45	0.79
1:B:3:THR:HB	1:B:6:GLU:CG	2.12	0.79
1:B:238:MET:O	1:B:241:THR:HG22	1.83	0.79
1:B:297:GLY:H	1:B:300:MET:CE	1.95	0.78
1:B:564:ASP:OD2	1:B:567:SER:HB3	1.84	0.78
1:B:439:GLY:HA2	1:B:532:TYR:CZ	2.17	0.78
1:B:148:LYS:O	1:B:152:GLN:HG3	1.84	0.78
1:B:560:TYR:HD2	1:B:761:VAL:HG12	1.43	0.78
1:B:153:MET:HE1	1:B:387:GLN:HB3	1.65	0.78
1:B:531:ILE:HD11	1:B:589:PHE:HB3	1.65	0.78
2:C:724:ASN:ND2	2:C:727:GLN:HG2	1.99	0.77
2:C:580:MET:CE	2:C:583:ASN:HB2	2.15	0.77
2:C:601:THR:HB	2:C:605:MET:HE3	1.66	0.76
1:B:194:ASP:O	1:B:195:LEU:HD23	1.85	0.76
2:C:492:ALA:HB3	2:C:816:ARG:HB3	1.67	0.76
2:C:1079:SER:OG	2:C:1082:GLU:HG3	1.85	0.76
2:C:1019:GLN:CB	2:C:1020:PRO:HD3	2.16	0.75
3:D:50:THR:O	3:D:51:ARG:HG2	1.87	0.75
1:B:45:LEU:HD11	1:B:451:LEU:HD13	1.68	0.75
1:B:183:ILE:HD12	2:C:565:PRO:HG2	1.68	0.75
2:C:631:GLY:HA2	2:C:685:VAL:CG2	2.17	0.74
2:C:993:MET:HB3	2:C:1055:ILE:CD1	2.17	0.74
3:D:80:PRO:HB2	3:D:83:LEU:HG	1.68	0.74
1:B:715:ALA:O	1:B:719:LEU:HG	1.89	0.73
2:C:580:MET:HE3	2:C:583:ASN:HB2	1.70	0.73
1:B:297:GLY:H	1:B:300:MET:HE2	1.51	0.73
1:B:70:LEU:HD23	1:B:109:GLU:CG	2.17	0.73
2:C:406:PRO:HG3	2:C:847:LEU:HD21	1.70	0.73
2:C:654:GLU:OE2	2:C:696:TYR:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:MET:HE2	1:B:157:LEU:CD1	2.12	0.72
2:C:350:VAL:CG1	2:C:891:MET:HE3	2.20	0.72
2:C:388:CYS:HA	2:C:409:LEU:HD23	1.71	0.72
1:B:190:ARG:HG3	2:C:577:PHE:CE2	2.25	0.72
1:B:656:ILE:HD11	1:B:695:ILE:HG12	1.70	0.72
1:B:528:ARG:HA	1:B:608:MET:HE1	1.71	0.71
1:B:200:LEU:HD21	1:B:270:ILE:HG23	1.72	0.71
2:C:875:LEU:CD2	2:C:892:VAL:HG12	2.19	0.71
3:D:61:PHE:HD2	3:D:72:LEU:HD11	1.55	0.71
1:B:394:MET:CE	1:B:394:MET:H	2.03	0.71
1:B:17:VAL:HA	1:B:41:LEU:O	1.90	0.71
2:C:661:ALA:HB3	2:C:861:SER:OG	1.90	0.71
1:B:255:PRO:HG2	1:B:258:LYS:HG3	1.71	0.71
2:C:580:MET:HE2	2:C:584:LEU:HD23	1.73	0.71
2:C:1027:LEU:HB2	2:C:1029:THR:HG23	1.73	0.71
2:C:411:LEU:HD23	2:C:785:TYR:O	1.91	0.70
2:C:391:THR:HG23	2:C:837:GLY:O	1.91	0.70
2:C:438:ILE:HD12	2:C:442:VAL:HG11	1.74	0.70
1:B:183:ILE:CD1	2:C:565:PRO:HG2	2.22	0.70
1:B:45:LEU:HD12	1:B:451:LEU:HB3	1.72	0.69
1:B:69:VAL:HG11	1:B:496:VAL:HG21	1.73	0.69
2:C:692:LEU:HD21	2:C:731:LEU:HD22	1.74	0.69
2:C:991:VAL:O	2:C:992:LEU:HD23	1.91	0.69
3:D:80:PRO:HG2	3:D:83:LEU:CD1	2.22	0.69
1:B:138:CYS:HB2	1:B:262:ARG:NH1	2.06	0.69
2:C:1074:THR:HG22	2:C:1077:ALA:HB3	1.75	0.69
2:C:832:ASN:O	2:C:836:LEU:HG	1.92	0.69
1:B:394:MET:H	1:B:394:MET:HE3	1.56	0.69
2:C:578:ILE:HD11	2:C:626:LEU:HA	1.73	0.69
2:C:841:GLN:HG2	2:C:939:MET:HG3	1.75	0.68
1:B:153:MET:CE	1:B:387:GLN:HB3	2.22	0.68
1:B:528:ARG:HG2	1:B:608:MET:CE	2.23	0.68
1:B:541:ASP:HB3	1:B:544:ARG:HD2	1.74	0.68
1:B:554:CYS:HB3	1:B:568:PHE:CZ	2.29	0.68
1:B:432:CYS:HB2	1:B:444:CYS:SG	2.34	0.68
1:B:3:THR:HG22	1:B:5:LEU:H	1.59	0.68
1:B:397:GLN:HE22	1:B:489:SER:CB	2.06	0.68
1:B:264:SER:HB2	1:B:294:ALA:HB2	1.75	0.68
1:B:313:TRP:HA	1:B:316:ILE:HG22	1.75	0.68
2:C:721:HIS:CD2	2:C:722:GLN:HG3	2.29	0.67
1:B:618:MET:HG2	1:B:653:PHE:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ALA:CB	1:B:525:LEU:HD13	2.23	0.67
2:C:409:LEU:C	2:C:410:LEU:HD12	2.20	0.67
1:B:608:MET:HE2	1:B:608:MET:HA	1.77	0.67
2:C:417:LEU:CD1	2:C:420:LEU:HD13	2.24	0.67
1:B:657:LEU:HD23	1:B:658:ILE:N	2.10	0.67
1:B:18:ARG:NH1	1:B:612:LEU:HD22	2.10	0.66
2:C:1052:LEU:HD23	2:C:1052:LEU:O	1.95	0.66
3:D:113:ILE:O	3:D:116:ASP:HB2	1.96	0.66
1:B:397:GLN:HE22	1:B:489:SER:HB3	1.59	0.66
2:C:385:LEU:HD13	2:C:821:HIS:CE1	2.30	0.66
3:D:81:LYS:H	3:D:81:LYS:HD3	1.60	0.66
2:C:666:MET:HE1	2:C:927:MET:SD	2.37	0.65
1:B:24:TRP:CZ2	1:B:501:ARG:HG3	2.30	0.65
1:B:24:TRP:CZ3	1:B:501:ARG:HB2	2.30	0.65
1:B:268:LEU:HD13	1:B:334:LEU:HD13	1.77	0.65
3:D:10:VAL:HG22	3:D:68:GLY:O	1.97	0.65
2:C:354:LEU:HD12	2:C:890:LEU:H	1.62	0.65
2:C:350:VAL:HG12	2:C:891:MET:HE3	1.79	0.64
1:B:290:ILE:HG22	1:B:292:GLY:H	1.61	0.64
1:B:458:ALA:C	1:B:459:ILE:HD13	2.22	0.64
2:C:573:ILE:HG23	2:C:618:PRO:CG	2.26	0.64
1:B:54:ILE:HG13	1:B:117:ILE:HD11	1.78	0.64
2:C:991:VAL:HG12	2:C:1051:ILE:HG13	1.79	0.64
1:B:418:GLY:HA3	1:B:438:ILE:O	1.97	0.64
1:B:56:TYR:HD1	1:B:57:GLU:O	1.81	0.63
2:C:949:VAL:HG11	2:C:985:LEU:CB	2.25	0.63
1:B:148:LYS:HE3	1:B:244:LEU:O	1.98	0.63
1:B:600:SER:O	1:B:604:ARG:HG3	1.98	0.63
2:C:1011:VAL:HG21	2:C:1017:ILE:HG12	1.79	0.63
2:C:768:VAL:HG22	2:C:774:LEU:HD22	1.80	0.63
1:B:153:MET:CE	1:B:157:LEU:HD11	2.16	0.63
2:C:505:VAL:HG12	2:C:627:MET:HE3	1.81	0.63
1:B:41:LEU:HD13	1:B:525:LEU:HD21	1.81	0.63
3:D:17:ALA:HB2	3:D:112:PHE:O	1.97	0.63
1:B:290:ILE:HG21	1:B:355:THR:HG23	1.79	0.62
2:C:564:GLN:HB2	2:C:565:PRO:HD2	1.80	0.62
2:C:1074:THR:HG23	2:C:1077:ALA:N	2.13	0.62
1:B:700:PHE:HB3	1:B:701:PRO:HD3	1.81	0.62
2:C:558:LEU:HB2	2:C:586:VAL:HG11	1.81	0.62
2:C:592:LYS:O	2:C:596:GLN:HG3	1.99	0.62
2:C:598:LEU:O	2:C:598:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HD13	1:B:316:ILE:O	1.99	0.62
1:B:27:SER:O	1:B:31:ALA:HB2	1.99	0.62
2:C:733:LYS:HD2	2:C:1049:PHE:CD2	2.35	0.62
1:B:95:PRO:HG2	1:B:98:TYR:HD1	1.60	0.61
1:B:658:ILE:HD13	1:B:688:PRO:HB2	1.82	0.61
1:B:93:GLN:HG2	1:B:94:PHE:N	2.15	0.61
1:B:57:GLU:HG3	1:B:58:PRO:HD2	1.81	0.61
1:B:127:MET:HA	1:B:127:MET:CE	2.28	0.61
2:C:724:ASN:HD21	2:C:727:GLN:HG2	1.64	0.61
1:B:166:LEU:HD23	1:B:243:LEU:HD13	1.82	0.61
1:B:45:LEU:CD1	1:B:451:LEU:HD13	2.31	0.61
2:C:372:LEU:HD11	2:C:824:CYS:O	2.00	0.61
3:D:56:ALA:HB2	3:D:153:ILE:HG21	1.83	0.61
1:B:76:VAL:HG12	1:B:77:ASP:N	2.11	0.60
1:B:24:TRP:CH2	1:B:501:ARG:HB2	2.35	0.60
1:B:28:ARG:O	1:B:31:ALA:HB3	2.01	0.60
1:B:417:SER:O	1:B:437:GLU:HA	2.01	0.60
2:C:1041:TRP:O	2:C:1045:GLN:HG2	2.01	0.60
1:B:607:PHE:CD2	1:B:608:MET:HE3	2.32	0.60
1:B:625:ALA:HB2	1:B:635:VAL:HG11	1.82	0.60
2:C:512:VAL:HG21	2:C:548:THR:HB	1.84	0.59
1:B:14:ARG:HD2	1:B:115:SER:OG	2.02	0.59
1:B:30:GLU:HG3	1:B:510:ILE:HD11	1.83	0.59
1:B:528:ARG:HG2	1:B:608:MET:HE1	1.84	0.59
2:C:510:PHE:HB3	2:C:521:TYR:OH	2.01	0.59
2:C:505:VAL:CG1	2:C:627:MET:HE3	2.33	0.59
1:B:195:LEU:HD13	1:B:203:MET:CE	2.31	0.59
1:B:70:LEU:CD2	1:B:109:GLU:HG3	2.27	0.59
2:C:810:THR:HA	2:C:815:GLU:O	2.03	0.59
1:B:369:GLY:O	1:B:609:ARG:NH2	2.35	0.59
2:C:414:PHE:CE2	2:C:742:LYS:HE2	2.37	0.59
3:D:80:PRO:HG2	3:D:83:LEU:HD12	1.84	0.59
2:C:687:VAL:O	2:C:711:GLY:HA3	2.03	0.58
2:C:949:VAL:CG1	2:C:985:LEU:HB2	2.28	0.58
2:C:439:ASN:HB2	2:C:440:PRO:CD	2.33	0.58
1:B:618:MET:HG2	1:B:653:PHE:CB	2.32	0.58
1:B:54:ILE:HG23	1:B:56:TYR:CE2	2.38	0.58
1:B:644:ALA:O	1:B:663:THR:HB	2.04	0.58
3:D:59:MET:HB3	3:D:74:LEU:HD11	1.85	0.58
1:B:183:ILE:HD13	2:C:605:MET:HE1	1.86	0.58
3:D:4:LEU:HD12	3:D:4:LEU:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASP:OD1	1:B:116:SER:HB2	2.04	0.58
1:B:178:LEU:HD11	1:B:229:PHE:O	2.04	0.58
1:B:164:VAL:O	1:B:230:LEU:HA	2.03	0.57
1:B:101:ILE:HD11	1:B:107:PRO:HD3	1.85	0.57
2:C:596:GLN:O	2:C:600:LYS:HG3	2.04	0.57
2:C:641:LEU:HD23	2:C:642:PRO:HD2	1.85	0.57
2:C:750:ARG:NH1	5:C:1101:A1EP8:O2	2.37	0.57
2:C:557:GLY:C	2:C:558:LEU:HG	2.29	0.57
3:D:149:MET:HG2	3:D:150:VAL:H	1.70	0.57
1:B:554:CYS:HB3	1:B:568:PHE:HZ	1.67	0.57
1:B:35:VAL:HG11	1:B:553:LEU:HA	1.86	0.57
1:B:282:THR:CG2	1:B:283:GLY:N	2.67	0.57
1:B:647:ILE:HG23	1:B:659:TYR:O	2.05	0.57
1:B:656:ILE:HD11	1:B:695:ILE:CG1	2.34	0.57
2:C:580:MET:HE2	2:C:584:LEU:CD2	2.33	0.57
2:C:841:GLN:HG2	2:C:939:MET:SD	2.43	0.57
1:B:172:MET:HB3	1:B:189:PHE:O	2.05	0.57
2:C:522:LEU:HD22	2:C:526:CYS:SG	2.44	0.57
2:C:619:ALA:O	2:C:622:ALA:HB3	2.05	0.57
1:B:641:SER:O	1:B:646:ARG:NH2	2.37	0.57
2:C:553:ILE:N	2:C:553:ILE:HD12	2.20	0.57
2:C:554:HIS:HB3	2:C:567:MET:HE3	1.87	0.57
2:C:875:LEU:HD22	2:C:892:VAL:CG1	2.23	0.57
1:B:183:ILE:HD13	2:C:605:MET:CE	2.34	0.57
2:C:348:LEU:O	2:C:348:LEU:HG	2.04	0.57
2:C:609:THR:HG22	2:C:611:GLU:N	2.17	0.57
1:B:130:ILE:HB	1:B:284:ALA:CB	2.35	0.56
2:C:719:TYR:CZ	2:C:728:VAL:HG22	2.40	0.56
3:D:80:PRO:HG2	3:D:83:LEU:HD11	1.85	0.56
1:B:313:TRP:HE3	1:B:316:ILE:HG21	1.70	0.56
2:C:652:ARG:HB2	2:C:696:TYR:CE2	2.40	0.56
2:C:971:LEU:N	2:C:971:LEU:HD23	2.19	0.56
1:B:368:GLY:HA3	1:B:450:GLY:CA	2.36	0.56
2:C:580:MET:HG2	2:C:581:PRO:HD2	1.87	0.56
2:C:618:PRO:HA	2:C:621:GLN:OE1	2.04	0.56
2:C:762:PHE:CZ	2:C:772:ASP:HB3	2.41	0.56
2:C:920:LEU:HD13	2:C:920:LEU:N	2.19	0.56
2:C:1043:ARG:HG2	2:C:1050:PRO:HD2	1.87	0.56
1:B:163:LEU:HA	1:B:231:GLN:O	2.06	0.56
1:B:371:MET:HB3	1:B:605:HIS:CD2	2.41	0.56
2:C:385:LEU:HD21	2:C:415:LYS:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:890:LEU:HD23	2:C:1084:LEU:HD22	1.86	0.56
1:B:397:GLN:HE22	1:B:489:SER:CA	2.18	0.56
1:B:510:ILE:HD13	1:B:513:ILE:HD12	1.88	0.56
1:B:397:GLN:NE2	1:B:489:SER:HB3	2.20	0.56
1:B:411:SER:HB3	1:B:413:GLU:OE1	2.06	0.56
1:B:519:GLN:OE1	1:B:576:LEU:HB2	2.05	0.56
2:C:398:ALA:O	2:C:402:LYS:HG3	2.06	0.56
2:C:438:ILE:HG23	2:C:438:ILE:O	2.06	0.56
3:D:53:THR:O	3:D:150:VAL:HA	2.06	0.56
1:B:285:ARG:NE	1:B:346:ASP:OD2	2.38	0.55
2:C:734:GLU:HA	2:C:1048:PHE:HE1	1.71	0.55
1:B:26:SER:OG	1:B:504:ALA:HB3	2.06	0.55
2:C:350:VAL:HG11	2:C:891:MET:HE3	1.87	0.55
2:C:766:PHE:CD1	2:C:766:PHE:C	2.84	0.55
2:C:910:LYS:HD3	2:C:922:GLU:HB3	1.87	0.55
2:C:830:THR:HG22	2:C:832:ASN:N	2.14	0.55
2:C:808:LEU:HD13	2:C:818:ILE:HG12	1.87	0.55
2:C:1069:MET:HE2	2:C:1069:MET:HA	1.88	0.55
3:D:33:TYR:CZ	3:D:59:MET:HG3	2.41	0.55
1:B:41:LEU:HD13	1:B:525:LEU:CD2	2.37	0.55
2:C:851:ALA:HB3	2:C:912:PHE:CZ	2.42	0.55
1:B:252:TRP:HZ2	2:C:579:PRO:O	1.89	0.54
3:D:7:ILE:HA	3:D:70:CYS:O	2.07	0.54
1:B:289:PHE:C	1:B:290:ILE:HD12	2.32	0.54
2:C:580:MET:HE1	2:C:583:ASN:HB2	1.87	0.54
3:D:52:CYS:SG	3:D:149:MET:HE2	2.48	0.54
2:C:444:PHE:HE1	2:C:461:VAL:HG21	1.72	0.54
1:B:410:THR:HB	1:B:414:ILE:HB	1.90	0.54
2:C:830:THR:HB	2:C:833:ASP:CG	2.31	0.54
3:D:39:GLN:CB	3:D:157:LEU:HD22	2.37	0.54
1:B:302:VAL:HG13	1:B:303:GLY:O	2.07	0.54
1:B:528:ARG:HG2	1:B:608:MET:HE2	1.88	0.54
3:D:61:PHE:CD1	3:D:153:ILE:HD12	2.42	0.54
1:B:166:LEU:HD23	1:B:243:LEU:CD1	2.38	0.54
2:C:512:VAL:HG22	2:C:549:PHE:H	1.72	0.54
2:C:601:THR:CB	2:C:605:MET:HE3	2.37	0.54
3:D:14:LEU:HD12	3:D:15:PRO:HD2	1.89	0.54
1:B:3:THR:CB	1:B:6:GLU:HG3	2.35	0.54
2:C:488:ILE:HG12	2:C:489:GLU:N	2.23	0.54
1:B:408:ILE:HA	1:B:480:GLN:O	2.08	0.53
2:C:702:LEU:O	2:C:705:ILE:HG22	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:986:MET:HE1	2:C:1069:MET:HE3	1.90	0.53
1:B:422:PRO:O	1:B:423:CYS:HB3	2.09	0.53
1:B:705:TYR:C	1:B:705:TYR:CD2	2.86	0.53
2:C:395:GLN:NE2	2:C:796:THR:HA	2.19	0.53
2:C:641:LEU:CD2	2:C:649:LEU:HB2	2.38	0.53
1:B:623:LEU:HD22	1:B:637:LEU:HD23	1.90	0.53
2:C:904:LEU:CD2	2:C:1080:TYR:HA	2.39	0.53
2:C:1056:ARG:C	2:C:1058:GLU:H	2.15	0.53
2:C:779:VAL:HG13	2:C:779:VAL:O	2.07	0.53
3:D:81:LYS:HD3	3:D:81:LYS:N	2.23	0.53
1:B:80:ALA:O	1:B:81:LYS:C	2.51	0.53
1:B:563:ASP:O	1:B:565:PRO:HD3	2.09	0.53
2:C:710:ALA:HB3	2:C:777:PRO:HD2	1.89	0.53
2:C:841:GLN:HG2	2:C:939:MET:CG	2.38	0.53
1:B:392:LYS:HE2	1:B:398:PHE:CE1	2.44	0.53
1:B:626:TYR:CE2	1:B:632:PRO:HG3	2.44	0.53
2:C:428:ILE:HG21	2:C:437:TYR:HE2	1.73	0.53
2:C:505:VAL:HG21	2:C:630:THR:OG1	2.08	0.53
3:D:6:MET:HE1	3:D:38:LYS:HE2	1.89	0.53
3:D:69:VAL:HG22	3:D:103:VAL:HG11	1.89	0.53
1:B:656:ILE:HD11	1:B:695:ILE:CD1	2.38	0.53
1:B:290:ILE:CG2	1:B:292:GLY:H	2.21	0.53
1:B:645:ASP:C	1:B:664:ILE:HD11	2.33	0.53
2:C:580:MET:HE3	2:C:583:ASN:H	1.72	0.53
2:C:372:LEU:HD13	2:C:376:ILE:HG22	1.90	0.53
2:C:1074:THR:C	2:C:1076:SER:H	2.17	0.53
2:C:1039:ILE:HD13	2:C:1052:LEU:HD13	1.91	0.52
2:C:549:PHE:HA	2:C:552:THR:O	2.09	0.52
2:C:638:GLN:HG3	2:C:639:THR:N	2.24	0.52
2:C:686:ALA:HB2	2:C:777:PRO:HB2	1.91	0.52
2:C:1022:THR:O	2:C:1023:ASP:HB2	2.07	0.52
1:B:313:TRP:CE3	1:B:316:ILE:HG21	2.44	0.52
2:C:762:PHE:HB3	2:C:766:PHE:HZ	1.75	0.52
2:C:775:SER:C	2:C:776:LEU:HD23	2.34	0.52
1:B:392:LYS:HA	1:B:397:GLN:O	2.09	0.52
1:B:553:LEU:HD12	1:B:557:PHE:HD2	1.75	0.52
1:B:614:GLN:OE1	1:B:614:GLN:HA	2.10	0.52
1:B:131:PHE:HB3	1:B:287:MET:HE1	1.91	0.52
1:B:368:GLY:HA3	1:B:450:GLY:HA3	1.92	0.52
1:B:297:GLY:H	1:B:300:MET:HE3	1.74	0.52
2:C:497:MET:HE2	2:C:816:ARG:CG	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:CG2	1:B:556:LYS:HD3	2.38	0.52
1:B:524:ILE:HG12	1:B:615:SER:HB3	1.92	0.52
1:B:649:LEU:C	1:B:649:LEU:HD12	2.35	0.52
2:C:439:ASN:HB2	2:C:440:PRO:HD2	1.92	0.52
2:C:555:PHE:C	2:C:556:TYR:CD1	2.87	0.52
2:C:559:GLN:HG2	2:C:583:ASN:CG	2.35	0.52
2:C:637:PHE:CD1	2:C:637:PHE:N	2.78	0.52
2:C:1043:ARG:HG2	2:C:1050:PRO:HG2	1.90	0.52
2:C:353:LEU:CD1	2:C:900:PRO:HG2	2.40	0.52
2:C:406:PRO:HG3	2:C:847:LEU:CD2	2.40	0.52
2:C:552:THR:HA	2:C:573:ILE:HD11	1.91	0.52
3:D:31:GLN:HG2	3:D:32:GLN:N	2.24	0.52
1:B:269:SER:HB3	1:B:334:LEU:HD21	1.91	0.52
2:C:498:LEU:HD12	2:C:498:LEU:N	2.25	0.52
3:D:81:LYS:H	3:D:81:LYS:CD	2.19	0.52
1:B:76:VAL:HG11	1:B:78:TYR:CE1	2.45	0.51
2:C:646:VAL:HG22	2:C:672:PHE:CE2	2.44	0.51
2:C:813:LYS:N	2:C:813:LYS:HE3	2.25	0.51
1:B:559:GLU:O	1:B:568:PHE:HA	2.10	0.51
2:C:754:THR:HG22	2:C:755:LYS:N	2.26	0.51
1:B:527:ALA:HB2	1:B:584:LEU:HD22	1.93	0.51
2:C:350:VAL:CG1	2:C:351:VAL:N	2.73	0.51
2:C:492:ALA:CB	2:C:816:ARG:HB3	2.38	0.51
2:C:719:TYR:CE2	2:C:728:VAL:HA	2.45	0.51
3:D:61:PHE:CD2	3:D:72:LEU:HD11	2.42	0.51
2:C:634:MET:O	2:C:634:MET:HG2	2.10	0.51
2:C:1019:GLN:CB	2:C:1020:PRO:CD	2.88	0.51
3:D:61:PHE:CE1	3:D:153:ILE:HD12	2.45	0.51
2:C:1014:TYR:O	2:C:1017:ILE:HG13	2.10	0.51
1:B:321:ALA:HB1	1:B:324:VAL:HG23	1.92	0.51
2:C:545:GLY:HA3	2:C:585:LEU:HD23	1.93	0.51
2:C:890:LEU:CD2	2:C:1084:LEU:HD22	2.40	0.51
1:B:358:LEU:HD22	1:B:597:PRO:HB3	1.92	0.51
1:B:439:GLY:HA2	1:B:532:TYR:CE2	2.46	0.51
2:C:388:CYS:SG	2:C:393:ILE:HD11	2.51	0.51
2:C:848:ALA:O	2:C:852:VAL:HG23	2.11	0.51
1:B:575:SER:O	1:B:578:PRO:HD2	2.11	0.51
2:C:620:LEU:CD2	2:C:636:VAL:HG21	2.41	0.51
2:C:655:PRO:HD3	2:C:920:LEU:HD21	1.92	0.51
1:B:130:ILE:HB	1:B:284:ALA:HB2	1.92	0.50
2:C:580:MET:HE3	2:C:583:ASN:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:734:GLU:HA	2:C:1048:PHE:CE1	2.46	0.50
3:D:72:LEU:HD12	3:D:73:VAL:H	1.76	0.50
1:B:624:TYR:O	1:B:648:LEU:HD22	2.12	0.50
2:C:381:CYS:HB2	2:C:822:THR:O	2.10	0.50
2:C:566:GLN:O	2:C:566:GLN:HG3	2.10	0.50
2:C:1062:LYS:O	2:C:1062:LYS:HG2	2.11	0.50
1:B:364:PRO:HA	1:B:369:GLY:HA3	1.93	0.50
1:B:623:LEU:HD21	1:B:648:LEU:HD13	1.93	0.50
2:C:388:CYS:CA	2:C:409:LEU:HD23	2.40	0.50
2:C:1006:SER:HA	2:C:1011:VAL:O	2.12	0.50
1:B:3:THR:HB	1:B:6:GLU:CD	2.35	0.50
2:C:616:LEU:HD23	2:C:642:PRO:HG3	1.92	0.50
2:C:443:SER:HB2	2:C:451:LYS:HB3	1.94	0.50
2:C:729:GLN:HG2	2:C:1051:ILE:CG2	2.41	0.50
3:D:87:TYR:CZ	3:D:91:LEU:HD11	2.46	0.50
3:D:149:MET:O	3:D:150:VAL:HG23	2.11	0.50
2:C:753:CYS:HB2	2:C:803:PHE:CD2	2.47	0.50
3:D:33:TYR:CE1	3:D:59:MET:HG3	2.45	0.50
2:C:1074:THR:HG23	2:C:1076:SER:H	1.76	0.50
3:D:60:THR:HG22	3:D:62:HIS:NE2	2.27	0.50
1:B:639:SER:N	1:B:722:VAL:HG13	2.27	0.50
2:C:387:ARG:O	2:C:387:ARG:HG3	2.11	0.50
2:C:762:PHE:HZ	2:C:772:ASP:HB3	1.77	0.50
1:B:3:THR:HG22	1:B:5:LEU:N	2.27	0.50
1:B:618:MET:HE2	1:B:653:PHE:CD2	2.47	0.50
2:C:655:PRO:HD3	2:C:920:LEU:CD2	2.41	0.50
1:B:191:GLY:HA3	1:B:263:SER:OG	2.12	0.49
1:B:293:PRO:HA	1:B:355:THR:O	2.12	0.49
1:B:366:LEU:HD22	1:B:424:VAL:HG22	1.94	0.49
2:C:359:MET:HE2	2:C:1080:TYR:CE2	2.47	0.49
2:C:727:GLN:OE1	2:C:727:GLN:HA	2.12	0.49
2:C:853:ASP:O	2:C:857:THR:HB	2.12	0.49
1:B:17:VAL:HG23	1:B:40:ALA:HB1	1.95	0.49
1:B:45:LEU:CD1	1:B:451:LEU:HB3	2.40	0.49
2:C:710:ALA:CB	2:C:777:PRO:HD2	2.42	0.49
2:C:1074:THR:CG2	2:C:1077:ALA:HB3	2.40	0.49
1:B:700:PHE:CD1	1:B:700:PHE:C	2.88	0.49
2:C:1093:LYS:O	2:C:1093:LYS:HG3	2.11	0.49
2:C:616:LEU:HD22	2:C:638:GLN:NE2	2.27	0.49
3:D:103:VAL:N	3:D:104:PRO:HD2	2.27	0.49
1:B:93:GLN:HG2	1:B:94:PHE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:913:GLN:NE2	2:C:916:THR:HB	2.28	0.49
1:B:113:GLN:H	1:B:113:GLN:CD	2.20	0.49
1:B:153:MET:HE1	1:B:387:GLN:HB2	1.91	0.49
2:C:758:SER:O	2:C:789:MET:HB2	2.12	0.49
1:B:382:PHE:O	1:B:383:LYS:C	2.56	0.49
1:B:522:ALA:O	1:B:526:MET:HG2	2.13	0.49
2:C:354:LEU:HD12	2:C:890:LEU:N	2.27	0.49
1:B:139:MET:HE2	1:B:291:GLY:HA3	1.94	0.48
2:C:511:ASP:HB2	2:C:549:PHE:CZ	2.48	0.48
2:C:766:PHE:C	2:C:766:PHE:HD1	2.20	0.48
1:B:30:GLU:CG	1:B:510:ILE:HD11	2.43	0.48
1:B:313:TRP:O	1:B:316:ILE:HG22	2.13	0.48
1:B:458:ALA:O	1:B:459:ILE:HD13	2.13	0.48
2:C:410:LEU:HD12	2:C:410:LEU:N	2.28	0.48
2:C:953:SER:OG	2:C:955:GLU:HG2	2.13	0.48
1:B:257:GLY:O	1:B:306:LEU:HB2	2.14	0.48
2:C:554:HIS:N	2:C:554:HIS:CD2	2.82	0.48
2:C:616:LEU:HD22	2:C:638:GLN:CD	2.39	0.48
1:B:388:ARG:CG	1:B:388:ARG:HH11	2.27	0.48
1:B:415:LYS:HB3	1:B:434:SER:HB2	1.94	0.48
1:B:638:ASP:OD1	1:B:723:ASN:HB2	2.14	0.48
2:C:671:ASP:OD2	2:C:675:LYS:HE3	2.12	0.48
3:D:44:LEU:HD13	3:D:65:ILE:HD11	1.96	0.48
3:D:110:TYR:HB3	3:D:113:ILE:CG2	2.44	0.48
3:D:55:GLU:O	3:D:153:ILE:HG22	2.13	0.48
1:B:76:VAL:CG1	1:B:77:ASP:H	2.19	0.48
2:C:350:VAL:HG12	2:C:351:VAL:N	2.27	0.48
2:C:929:GLN:O	2:C:933:GLN:HB2	2.12	0.48
1:B:56:TYR:CD1	1:B:57:GLU:O	2.66	0.48
1:B:290:ILE:HD12	1:B:290:ILE:N	2.28	0.48
1:B:626:TYR:HB2	1:B:647:ILE:O	2.14	0.48
2:C:546:PHE:O	2:C:547:ILE:HG13	2.14	0.48
2:C:1083:PHE:CE2	2:C:1087:ILE:HD11	2.49	0.48
3:D:80:PRO:CG	3:D:83:LEU:HD12	2.44	0.48
1:B:35:VAL:HG23	1:B:556:LYS:HD3	1.95	0.48
1:B:24:TRP:CZ2	1:B:501:ARG:CG	2.97	0.47
1:B:82:LEU:HD23	1:B:93:GLN:HA	1.96	0.47
2:C:420:LEU:HD21	2:C:489:GLU:CD	2.39	0.47
2:C:510:PHE:O	2:C:548:THR:HA	2.14	0.47
2:C:720:HIS:HB3	2:C:723:HIS:HB2	1.96	0.47
2:C:726:VAL:O	2:C:727:GLN:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:O	1:B:233:VAL:HG23	2.14	0.47
2:C:991:VAL:HG12	2:C:1051:ILE:CG1	2.43	0.47
2:C:753:CYS:HB3	2:C:803:PHE:HD2	1.79	0.47
2:C:893:PRO:HG2	2:C:896:LEU:HG	1.97	0.47
2:C:990:SER:O	2:C:1050:PRO:HA	2.14	0.47
1:B:34:MET:HE1	1:B:513:ILE:HD13	1.95	0.47
1:B:647:ILE:HD11	1:B:664:ILE:HG21	1.95	0.47
2:C:606:PHE:HB3	2:C:609:THR:OG1	2.14	0.47
1:B:63:ARG:CB	1:B:66:CYS:HB3	2.44	0.47
2:C:553:ILE:C	2:C:554:HIS:HD2	2.23	0.47
1:B:6:GLU:O	1:B:10:GLN:HG3	2.15	0.47
1:B:639:SER:N	1:B:722:VAL:CG1	2.78	0.47
1:B:708:THR:HB	1:B:714:GLN:HB2	1.96	0.47
1:B:82:LEU:HD22	1:B:92:ASN:O	2.15	0.47
1:B:397:GLN:OE1	1:B:489:SER:HB3	2.14	0.47
1:B:461:PHE:CE2	1:B:479:ILE:HD13	2.50	0.47
2:C:994:LEU:O	2:C:1055:ILE:N	2.44	0.47
1:B:185:LYS:HE3	2:C:569:ILE:CD1	2.45	0.47
1:B:296:GLN:O	1:B:297:GLY:O	2.32	0.47
2:C:580:MET:HE3	2:C:583:ASN:N	2.30	0.47
2:C:671:ASP:OD2	2:C:675:LYS:CE	2.63	0.47
2:C:986:MET:CE	2:C:1069:MET:HE3	2.45	0.47
1:B:657:LEU:HD21	1:B:708:THR:HG22	1.96	0.47
2:C:573:ILE:CG2	2:C:618:PRO:HG2	2.35	0.47
2:C:1074:THR:C	2:C:1076:SER:N	2.71	0.47
3:D:7:ILE:O	3:D:16:LEU:HB2	2.14	0.47
1:B:723:ASN:HD21	1:B:749:LEU:HB3	1.79	0.47
1:B:82:LEU:CD2	1:B:93:GLN:HA	2.45	0.46
1:B:394:MET:H	1:B:394:MET:HE2	1.80	0.46
1:B:422:PRO:HG3	1:B:609:ARG:HG2	1.96	0.46
1:B:528:ARG:CG	1:B:608:MET:HE1	2.44	0.46
2:C:615:ALA:HB2	2:C:644:LEU:HD23	1.97	0.46
2:C:719:TYR:HE2	2:C:728:VAL:HA	1.81	0.46
2:C:512:VAL:CG2	2:C:548:THR:HB	2.45	0.46
2:C:729:GLN:HG2	2:C:1051:ILE:HG21	1.97	0.46
2:C:759:ILE:HG23	2:C:787:VAL:CG1	2.35	0.46
2:C:763:HIS:HB2	2:C:786:ALA:HB3	1.97	0.46
3:D:29:ASP:HB3	3:D:31:GLN:OE1	2.15	0.46
2:C:871:VAL:HG12	2:C:875:LEU:HD12	1.96	0.46
1:B:22:ASN:HB2	1:B:516:SER:HB2	1.97	0.46
2:C:432:ARG:HG3	2:C:459:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TYR:O	1:B:8:ILE:HG13	2.16	0.46
2:C:567:MET:HE2	2:C:569:ILE:HD11	1.97	0.46
3:D:29:ASP:CB	3:D:31:GLN:OE1	2.63	0.46
1:B:20:SER:CB	1:B:522:ALA:HB2	2.46	0.46
2:C:488:ILE:HD13	2:C:490:PHE:CZ	2.51	0.46
1:B:98:TYR:O	1:B:101:ILE:HB	2.14	0.46
2:C:802:SER:HA	2:C:823:LEU:O	2.16	0.46
2:C:807:LEU:O	2:C:818:ILE:HA	2.16	0.46
2:C:993:MET:CB	2:C:1055:ILE:HD11	2.26	0.46
1:B:290:ILE:CD1	1:B:290:ILE:N	2.78	0.46
1:B:394:MET:CE	1:B:394:MET:N	2.75	0.46
1:B:411:SER:C	1:B:413:GLU:H	2.24	0.46
1:B:463:VAL:C	1:B:464:VAL:HG23	2.40	0.46
1:B:657:LEU:HD23	1:B:657:LEU:C	2.41	0.46
2:C:770:SER:O	2:C:771:THR:CB	2.63	0.46
2:C:851:ALA:HB1	2:C:912:PHE:CE1	2.49	0.46
3:D:52:CYS:HB3	3:D:63:TYR:CE2	2.50	0.46
3:D:73:VAL:HB	3:D:88:LEU:HD21	1.97	0.46
1:B:722:VAL:CG1	1:B:723:ASN:N	2.79	0.46
2:C:385:LEU:HD13	2:C:821:HIS:HE1	1.78	0.46
2:C:550:ASP:O	2:C:614:SER:HA	2.16	0.46
1:B:60:LEU:CD2	1:B:69:VAL:HG22	2.46	0.45
1:B:664:ILE:HD13	1:B:684:LEU:HD21	1.98	0.45
2:C:411:LEU:HD23	2:C:411:LEU:N	2.31	0.45
2:C:533:LEU:HA	2:C:533:LEU:HD12	1.54	0.45
2:C:1014:TYR:OH	2:C:1057:ASP:N	2.46	0.45
3:D:63:TYR:CD1	3:D:63:TYR:C	2.94	0.45
2:C:567:MET:O	2:C:567:MET:HG2	2.16	0.45
2:C:661:ALA:CB	2:C:861:SER:OG	2.61	0.45
2:C:812:SER:C	2:C:813:LYS:HE3	2.41	0.45
1:B:553:LEU:HD12	1:B:557:PHE:CD2	2.51	0.45
2:C:449:ARG:HA	2:C:459:ASN:O	2.17	0.45
2:C:748:VAL:HG12	2:C:775:SER:HA	1.96	0.45
3:D:33:TYR:HB3	3:D:74:LEU:CD2	2.46	0.45
1:B:345:ILE:O	1:B:369:GLY:HA3	2.16	0.45
1:B:647:ILE:CD1	1:B:685:LEU:HD23	2.46	0.45
1:B:268:LEU:CD1	1:B:334:LEU:HD13	2.44	0.45
1:B:151:MET:HE2	1:B:151:MET:HB2	1.67	0.45
1:B:280:PRO:O	1:B:281:ASN:HB2	2.16	0.45
1:B:564:ASP:CG	1:B:567:SER:HB3	2.40	0.45
1:B:617:ILE:HG22	1:B:651:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:HD23	1:B:703:PRO:HG2	1.98	0.45
2:C:545:GLY:HA3	2:C:585:LEU:CD2	2.47	0.45
2:C:580:MET:CG	2:C:581:PRO:HD2	2.47	0.45
2:C:689:LEU:HD12	2:C:690:PHE:N	2.32	0.45
2:C:966:PRO:HG2	2:C:1038:PHE:HB2	1.99	0.45
2:C:991:VAL:C	2:C:992:LEU:HD23	2.40	0.45
1:B:43:THR:CG2	1:B:46:LYS:HB2	2.47	0.45
1:B:394:MET:HE2	1:B:394:MET:N	2.31	0.45
2:C:716:TYR:CD1	2:C:730:LYS:HE2	2.52	0.45
2:C:721:HIS:NE2	2:C:722:GLN:HG3	2.32	0.45
2:C:940:LEU:HD13	2:C:940:LEU:HA	1.57	0.45
2:C:1043:ARG:HG2	2:C:1050:PRO:CG	2.46	0.45
3:D:14:LEU:HD11	3:D:109:PRO:HA	1.98	0.45
1:B:183:ILE:HD12	1:B:183:ILE:HA	1.79	0.45
1:B:297:GLY:N	1:B:300:MET:HE2	2.24	0.45
1:B:406:LEU:O	1:B:445:GLN:HA	2.17	0.45
1:B:520:GLU:HB3	1:B:616:LEU:HD11	1.98	0.45
2:C:414:PHE:CZ	2:C:742:LYS:HE2	2.52	0.45
2:C:854:ARG:HA	2:C:854:ARG:HD3	1.74	0.45
1:B:195:LEU:HD12	1:B:200:LEU:HD13	1.97	0.45
2:C:388:CYS:HB2	2:C:409:LEU:HD21	1.98	0.45
3:D:14:LEU:HD12	3:D:15:PRO:CD	2.47	0.45
3:D:118:PHE:HA	3:D:121:LYS:HE2	1.99	0.45
3:D:127:ILE:O	3:D:127:ILE:HG22	2.17	0.45
1:B:576:LEU:HA	1:B:576:LEU:HD23	1.50	0.44
2:C:770:SER:O	2:C:771:THR:OG1	2.34	0.44
1:B:625:ALA:HA	1:B:648:LEU:HD23	1.99	0.44
1:B:658:ILE:CD1	1:B:688:PRO:HB2	2.47	0.44
1:B:757:LYS:O	1:B:761:VAL:HG22	2.17	0.44
2:C:584:LEU:HD23	2:C:584:LEU:N	2.32	0.44
2:C:382:ASN:CG	2:C:383:PRO:HD2	2.43	0.44
2:C:546:PHE:C	2:C:547:ILE:HG13	2.43	0.44
2:C:579:PRO:HG2	2:C:584:LEU:HD11	1.99	0.44
2:C:730:LYS:HG3	2:C:1051:ILE:HD11	2.00	0.44
2:C:985:LEU:HD11	2:C:1039:ILE:HG12	1.98	0.44
2:C:1056:ARG:C	2:C:1058:GLU:N	2.76	0.44
1:B:249:ARG:O	1:B:250:ASP:C	2.59	0.44
2:C:747:ALA:HA	2:C:808:LEU:O	2.17	0.44
1:B:179:GLY:HA2	1:B:239:ASN:OD1	2.17	0.44
1:B:180:CYS:HB3	1:B:183:ILE:HG22	1.99	0.44
1:B:645:ASP:O	1:B:664:ILE:HD11	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:496:TYR:CD2	2:C:818:ILE:HD11	2.52	0.44
2:C:555:PHE:HB3	2:C:584:LEU:HD13	1.98	0.44
3:D:94:GLU:HG2	3:D:118:PHE:CD2	2.52	0.44
2:C:627:MET:HE2	2:C:627:MET:HB3	1.84	0.44
2:C:923:ARG:O	2:C:924:ILE:C	2.61	0.44
2:C:975:VAL:HG22	2:C:1069:MET:HG3	2.00	0.44
1:B:181:GLU:CD	1:B:181:GLU:H	2.26	0.44
1:B:428:SER:O	1:B:443:THR:HA	2.18	0.44
1:B:647:ILE:HG13	1:B:664:ILE:CD1	2.48	0.44
1:B:45:LEU:O	1:B:453:PRO:HA	2.17	0.44
1:B:252:TRP:HA	1:B:253:PRO:HD3	1.81	0.44
1:B:607:PHE:C	1:B:609:ARG:H	2.26	0.44
1:B:639:SER:HA	1:B:722:VAL:HG11	1.98	0.44
2:C:649:LEU:HD21	2:C:673:TYR:HE2	1.82	0.44
2:C:753:CYS:CB	2:C:803:PHE:CD2	3.01	0.44
2:C:875:LEU:CD2	2:C:892:VAL:CG1	2.92	0.44
3:D:50:THR:C	3:D:51:ARG:HG2	2.41	0.44
1:B:612:LEU:O	1:B:613:THR:C	2.60	0.44
2:C:496:TYR:HD2	2:C:818:ILE:HD11	1.83	0.44
2:C:620:LEU:HD23	2:C:634:MET:CE	2.48	0.44
1:B:17:VAL:HG22	1:B:18:ARG:N	2.32	0.43
2:C:591:SER:O	2:C:592:LYS:C	2.60	0.43
2:C:851:ALA:CB	2:C:912:PHE:CE1	3.01	0.43
1:B:313:TRP:CE2	1:B:597:PRO:HA	2.53	0.43
1:B:517:PHE:CE2	1:B:519:GLN:HA	2.53	0.43
2:C:808:LEU:CD1	2:C:818:ILE:HG12	2.48	0.43
2:C:1043:ARG:HG2	2:C:1050:PRO:CD	2.48	0.43
1:B:320:ASN:O	1:B:320:ASN:CG	2.59	0.43
2:C:480:ARG:HG3	2:C:482:GLU:OE1	2.18	0.43
2:C:753:CYS:CB	2:C:803:PHE:HD2	2.32	0.43
1:B:282:THR:HG22	1:B:283:GLY:O	2.18	0.43
3:D:109:PRO:O	3:D:110:TYR:C	2.61	0.43
3:D:149:MET:O	3:D:150:VAL:CG2	2.67	0.43
1:B:316:ILE:HD13	1:B:316:ILE:C	2.42	0.43
1:B:541:ASP:CB	1:B:544:ARG:HD2	2.46	0.43
2:C:699:LEU:HD12	2:C:699:LEU:O	2.19	0.43
3:D:32:GLN:O	3:D:36:GLN:HG3	2.19	0.43
1:B:420:ILE:HD12	1:B:529:LEU:HD23	2.01	0.43
1:B:576:LEU:C	1:B:578:PRO:HD2	2.44	0.43
1:B:701:PRO:O	1:B:702:MET:HB3	2.17	0.43
2:C:373:HIS:HE1	2:C:375:ASP:OD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:PRO:HB2	2:C:495:GLU:OE1	2.18	0.43
2:C:720:HIS:CE1	2:C:722:GLN:HB2	2.53	0.43
2:C:906:LEU:HA	2:C:906:LEU:HD12	1.69	0.43
1:B:679:GLU:OE1	1:B:679:GLU:HA	2.18	0.43
2:C:536:LEU:HD23	2:C:536:LEU:HA	1.68	0.43
2:C:843:ILE:O	2:C:847:LEU:HG	2.19	0.43
1:B:617:ILE:HG23	1:B:622:ILE:HG13	2.00	0.43
1:B:666:GLN:OE1	1:B:681:PHE:CZ	2.72	0.43
2:C:958:LEU:HD13	2:C:967:GLN:HG3	1.99	0.43
2:C:985:LEU:C	2:C:985:LEU:HD23	2.44	0.43
1:B:288:MET:CG	1:B:290:ILE:HD11	2.33	0.43
2:C:552:THR:O	2:C:554:HIS:CD2	2.72	0.43
1:B:342:GLY:HA2	1:B:449:CYS:SG	2.59	0.43
1:B:452:SER:C	1:B:454:THR:H	2.27	0.43
2:C:359:MET:CE	2:C:1080:TYR:CE2	3.02	0.43
1:B:101:ILE:HD13	1:B:101:ILE:HA	1.50	0.42
1:B:227:ASN:HB3	1:B:229:PHE:H	1.84	0.42
1:B:423:CYS:C	1:B:424:VAL:HG23	2.44	0.42
2:C:641:LEU:HD11	2:C:651:PRO:HA	2.01	0.42
2:C:759:ILE:CG2	2:C:787:VAL:HG13	2.37	0.42
2:C:904:LEU:HD22	2:C:1080:TYR:HA	2.02	0.42
1:B:41:LEU:CD1	1:B:525:LEU:HD21	2.46	0.42
1:B:442:GLY:O	1:B:443:THR:HB	2.20	0.42
1:B:537:GLU:N	1:B:537:GLU:OE1	2.51	0.42
1:B:647:ILE:HG13	1:B:664:ILE:HD12	2.01	0.42
2:C:497:MET:HB3	2:C:816:ARG:HG3	2.01	0.42
1:B:30:GLU:OE1	1:B:30:GLU:HA	2.18	0.42
1:B:459:ILE:HD13	1:B:459:ILE:N	2.33	0.42
2:C:641:LEU:HD22	2:C:649:LEU:O	2.19	0.42
3:D:72:LEU:HG	3:D:73:VAL:N	2.34	0.42
1:B:240:LEU:HD22	1:B:244:LEU:HD11	2.01	0.42
1:B:659:TYR:CE2	1:B:661:GLY:HA2	2.54	0.42
2:C:592:LYS:O	2:C:595:VAL:HG22	2.19	0.42
2:C:691:LEU:HD12	2:C:691:LEU:HA	1.88	0.42
1:B:132:LEU:HD12	1:B:165:GLY:O	2.19	0.42
1:B:411:SER:O	1:B:413:GLU:N	2.53	0.42
1:B:602:TYR:O	1:B:605:HIS:HB3	2.19	0.42
1:B:700:PHE:CD1	1:B:700:PHE:O	2.72	0.42
2:C:879:ARG:HA	2:C:882:VAL:HG22	2.00	0.42
3:D:110:TYR:HB3	3:D:113:ILE:HG22	2.00	0.42
1:B:138:CYS:HB2	1:B:262:ARG:HH11	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:VAL:C	1:B:464:VAL:CG2	2.93	0.42
1:B:561:HIS:O	1:B:562:LYS:C	2.61	0.42
2:C:353:LEU:HD13	2:C:900:PRO:HG2	2.02	0.42
2:C:395:GLN:O	2:C:395:GLN:HG2	2.19	0.42
2:C:549:PHE:CE2	2:C:616:LEU:HD13	2.55	0.42
1:B:166:LEU:HD12	1:B:167:ILE:N	2.34	0.42
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.81	0.42
2:C:872:ILE:HD13	2:C:1090:GLN:CB	2.49	0.42
2:C:913:GLN:O	2:C:914:THR:HG23	2.20	0.42
1:B:18:ARG:CZ	1:B:612:LEU:HD22	2.49	0.42
2:C:521:TYR:CD1	2:C:521:TYR:C	2.98	0.42
2:C:574:GLU:OE1	2:C:574:GLU:O	2.37	0.42
2:C:774:LEU:N	2:C:774:LEU:HD23	2.34	0.42
2:C:965:ILE:HD12	2:C:965:ILE:N	2.34	0.42
2:C:975:VAL:HG13	2:C:978:LEU:HD12	2.01	0.42
3:D:71:TYR:CE2	3:D:92:HIS:HA	2.55	0.42
1:B:35:VAL:HG11	1:B:553:LEU:CA	2.49	0.42
1:B:534:ALA:HA	1:B:542:VAL:HG21	2.02	0.42
2:C:916:THR:O	2:C:917:ASN:C	2.62	0.42
2:C:1027:LEU:HB2	2:C:1029:THR:CG2	2.46	0.42
1:B:272:VAL:HG21	1:B:334:LEU:HD22	2.01	0.42
1:B:282:THR:HG22	1:B:283:GLY:N	2.35	0.42
2:C:498:LEU:N	2:C:498:LEU:CD1	2.82	0.42
2:C:620:LEU:HD21	2:C:636:VAL:HG21	2.02	0.42
2:C:762:PHE:HB3	2:C:766:PHE:CZ	2.54	0.42
2:C:935:LEU:O	2:C:938:LEU:HB3	2.20	0.42
2:C:394:PRO:HG2	2:C:400:LEU:HB2	2.02	0.41
1:B:264:SER:HB2	1:B:294:ALA:CB	2.46	0.41
1:B:696:LEU:HD23	1:B:703:PRO:HD2	2.02	0.41
1:B:710:HIS:C	1:B:712:GLY:H	2.28	0.41
2:C:702:LEU:O	2:C:703:GLY:C	2.63	0.41
2:C:789:MET:HE3	2:C:789:MET:HB3	1.64	0.41
1:B:625:ALA:CB	1:B:635:VAL:HG11	2.49	0.41
2:C:979:SER:C	2:C:981:ASP:H	2.28	0.41
2:C:983:ALA:HA	2:C:995:TRP:O	2.19	0.41
1:B:145:GLN:O	1:B:149:GLU:HG3	2.19	0.41
1:B:370:TYR:CE2	1:B:389:VAL:HG13	2.55	0.41
1:B:626:TYR:CE2	1:B:632:PRO:CG	3.03	0.41
1:B:653:PHE:HE2	1:B:701:PRO:HG2	1.85	0.41
2:C:394:PRO:HB3	2:C:399:LEU:HG	2.02	0.41
2:C:687:VAL:HG11	2:C:705:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TRP:CZ3	1:B:517:PHE:HB2	2.56	0.41
1:B:443:THR:O	1:B:446:TRP:CZ2	2.74	0.41
2:C:646:VAL:HG13	2:C:672:PHE:CE2	2.56	0.41
2:C:677:ALA:CB	2:C:708:TYR:HB2	2.51	0.41
1:B:50:ASP:OD1	1:B:50:ASP:N	2.50	0.41
1:B:246:GLU:O	1:B:247:LEU:C	2.63	0.41
1:B:349:ALA:HB1	1:B:355:THR:HG21	2.02	0.41
1:B:350:CYS:HA	1:B:374:GLY:O	2.21	0.41
1:B:463:VAL:HG12	1:B:464:VAL:N	2.36	0.41
2:C:431:CYS:HB2	2:C:450:TRP:CH2	2.56	0.41
2:C:1085:LEU:HD12	2:C:1085:LEU:HA	1.76	0.41
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.83	0.41
1:B:155:LEU:HD12	1:B:158:LEU:HD12	2.03	0.41
1:B:255:PRO:O	1:B:256:GLN:C	2.62	0.41
1:B:482:VAL:HG22	1:B:496:VAL:HG22	2.03	0.41
1:B:664:ILE:O	1:B:664:ILE:HG22	2.20	0.41
2:C:522:LEU:HD23	2:C:522:LEU:HA	1.90	0.41
2:C:649:LEU:HD11	2:C:702:LEU:HD21	2.03	0.41
2:C:715:TYR:CE2	2:C:717:PRO:HB3	2.55	0.41
3:D:66:GLU:O	3:D:67:GLN:HB2	2.20	0.41
1:B:153:MET:CE	1:B:387:GLN:CB	2.84	0.41
1:B:534:ALA:CA	1:B:542:VAL:HG21	2.51	0.41
1:B:28:ARG:HA	1:B:31:ALA:CB	2.51	0.41
1:B:313:TRP:HA	1:B:316:ILE:CG2	2.48	0.41
1:B:397:GLN:CD	1:B:489:SER:HB3	2.46	0.41
1:B:421:GLY:HA3	1:B:457:LEU:CD1	2.51	0.41
1:B:423:CYS:SG	1:B:424:VAL:N	2.93	0.41
1:B:428:SER:O	1:B:429:LYS:HD3	2.21	0.41
1:B:446:TRP:N	1:B:446:TRP:CE3	2.89	0.41
1:B:638:ASP:OD1	1:B:723:ASN:CB	2.69	0.41
2:C:368:PRO:HB2	2:C:391:THR:HG21	2.02	0.41
2:C:385:LEU:CD2	2:C:415:LYS:HB3	2.50	0.41
2:C:444:PHE:HE1	2:C:461:VAL:CG2	2.34	0.41
2:C:551:SER:OG	2:C:611:GLU:OE1	2.34	0.41
2:C:555:PHE:HE1	2:C:570:VAL:CG1	2.34	0.41
2:C:750:ARG:HG2	2:C:750:ARG:HH11	1.86	0.41
2:C:1018:PRO:HG2	2:C:1021:MET:HB2	2.02	0.41
3:D:60:THR:HG22	3:D:62:HIS:CD2	2.56	0.41
3:D:80:PRO:HB2	3:D:83:LEU:CG	2.44	0.41
1:B:83:TRP:CZ3	1:B:85:CYS:HB2	2.56	0.41
2:C:410:LEU:N	2:C:410:LEU:CD1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:649:LEU:HD11	2:C:702:LEU:CD2	2.51	0.41
1:B:28:ARG:CZ	1:B:28:ARG:HB3	2.50	0.40
1:B:189:PHE:HZ	1:B:204:LEU:HD21	1.85	0.40
2:C:622:ALA:O	2:C:623:ALA:C	2.64	0.40
2:C:624:PHE:CE2	2:C:628:SER:HB2	2.56	0.40
2:C:813:LYS:HE3	2:C:813:LYS:CA	2.51	0.40
2:C:892:VAL:HB	2:C:893:PRO:HD2	2.03	0.40
2:C:358:ASN:C	2:C:360:LEU:H	2.29	0.40
2:C:717:PRO:HD2	2:C:727:GLN:NE2	2.36	0.40
2:C:987:ASP:HA	2:C:992:LEU:HD22	2.02	0.40
1:B:244:LEU:HA	1:B:244:LEU:HD23	1.83	0.40
2:C:369:VAL:O	2:C:370:PRO:C	2.63	0.40
2:C:578:ILE:HD11	2:C:626:LEU:CA	2.46	0.40
2:C:637:PHE:N	2:C:637:PHE:HD1	2.19	0.40
2:C:691:LEU:HB3	2:C:715:TYR:HD1	1.87	0.40
2:C:973:LEU:HD23	2:C:973:LEU:HA	1.95	0.40
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.82	0.40
1:B:421:GLY:HA3	1:B:457:LEU:HD12	2.04	0.40
1:B:438:ILE:HG21	1:B:529:LEU:CD2	2.51	0.40
2:C:372:LEU:HD13	2:C:376:ILE:CG2	2.51	0.40
2:C:628:SER:N	2:C:629:PRO:CD	2.84	0.40
1:B:749:LEU:O	1:B:750:GLN:C	2.65	0.40
3:D:63:TYR:HA	3:D:71:TYR:O	2.22	0.40
3:D:71:TYR:CD1	3:D:71:TYR:N	2.89	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	B	675/765 (88%)	588 (87%)	76 (11%)	11 (2%)	7 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	720/748 (96%)	629 (87%)	81 (11%)	10 (1%)	9	37
3	D	124/157 (79%)	109 (88%)	13 (10%)	2 (2%)	7	35
All	All	1519/1670 (91%)	1326 (87%)	170 (11%)	23 (2%)	8	36

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	319	ASP
2	C	462	PRO
1	B	31	ALA
1	B	297	GLY
1	B	404	GLY
1	B	104	LEU
2	C	771	THR
2	C	978	LEU
3	D	4	LEU
3	D	11	ALA
1	B	81	LYS
1	B	427	ASN
2	C	359	MET
2	C	523	ASN
2	C	1023	ASP
1	B	423	CYS
1	B	702	MET
2	C	589	ASN
2	C	918	ALA
1	B	324	VAL
1	B	170	GLY
2	C	581	PRO
2	C	347	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	588/666 (88%)	536 (91%)	52 (9%)	9	34
2	C	636/679 (94%)	561 (88%)	75 (12%)	5	22
3	D	108/138 (78%)	97 (90%)	11 (10%)	7	28
All	All	1332/1483 (90%)	1194 (90%)	138 (10%)	7	27

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	30	GLU
1	B	41	LEU
1	B	50	ASP
1	B	51	LEU
1	B	101	ILE
1	B	103	GLU
1	B	106	GLN
1	B	113	GLN
1	B	135	VAL
1	B	150	SER
1	B	151	MET
1	B	153	MET
1	B	161	THR
1	B	164	VAL
1	B	178	LEU
1	B	183	ILE
1	B	192	THR
1	B	228	ARG
1	B	240	LEU
1	B	243	LEU
1	B	268	LEU
1	B	269	SER
1	B	282	THR
1	B	302	VAL
1	B	316	ILE
1	B	362	CYS
1	B	376	SER
1	B	379	THR
1	B	388	ARG
1	B	394	MET
1	B	420	ILE
1	B	454	THR
1	B	483	THR

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Mol	Chain	Res	Type
1	B	499	ILE
1	B	511	GLN
1	B	512	ASN
1	B	524	ILE
1	B	543	LEU
1	B	544	ARG
1	B	562	LYS
1	B	570	PHE
1	B	590	LEU
1	B	592	VAL
1	B	612	LEU
1	B	613	THR
1	B	635	VAL
1	B	639	SER
1	B	652	THR
1	B	695	ILE
1	B	702	MET
1	B	704	ARG
2	C	359	MET
2	C	379	LEU
2	C	391	THR
2	C	423	VAL
2	C	429	VAL
2	C	436	THR
2	C	458	VAL
2	C	460	ASP
2	C	488	ILE
2	C	498	LEU
2	C	502	GLN
2	C	511	ASP
2	C	522	LEU
2	C	554	HIS
2	C	567	MET
2	C	568	LEU
2	C	570	VAL
2	C	571	SER
2	C	574	GLU
2	C	576	VAL
2	C	584	LEU
2	C	601	THR
2	C	607	THR
2	C	616	LEU

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Mol	Chain	Res	Type
2	C	637	PHE
2	C	641	LEU
2	C	650	LYS
2	C	652	ARG
2	C	659	SER
2	C	670	THR
2	C	689	LEU
2	C	712	SER
2	C	713	VAL
2	C	726	VAL
2	C	730	LYS
2	C	749	MET
2	C	751	ILE
2	C	778	ASN
2	C	787	VAL
2	C	789	MET
2	C	793	GLU
2	C	798	THR
2	C	807	LEU
2	C	813	LYS
2	C	816	ARG
2	C	827	VAL
2	C	831	LEU
2	C	844	SER
2	C	857	THR
2	C	881	SER
2	C	895	SER
2	C	910	LYS
2	C	911	SER
2	C	920	LEU
2	C	935	LEU
2	C	936	VAL
2	C	938	LEU
2	C	940	LEU
2	C	946	LEU
2	C	958	LEU
2	C	963	ARG
2	C	964	THR
2	C	972	GLN
2	C	979	SER
2	C	993	MET
2	C	998	LYS

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Mol	Chain	Res	Type
2	C	1001	THR
2	C	1002	GLN
2	C	1029	THR
2	C	1035	ILE
2	C	1040	SER
2	C	1052	LEU
2	C	1055	ILE
2	C	1085	LEU
2	C	1092	ASN
3	D	4	LEU
3	D	12	ASP
3	D	29	ASP
3	D	46	GLU
3	D	67	GLN
3	D	81	LYS
3	D	101	LYS
3	D	113	ILE
3	D	121	LYS
3	D	129	SER
3	D	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	296	GLN
1	B	330	HIS
1	B	397	GLN
1	B	591	GLN
2	C	373	HIS
2	C	724	ASN
2	C	943	HIS
2	C	1002	GLN
2	C	1012	GLN
2	C	1068	ASN
2	C	1086	HIS
2	C	1092	ASN
3	D	92	HIS

5.3.3 RNA ⓘ

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	A1EP8	C	1101	-	18,20,20	2.17	5 (27%)	23,30,30	2.97	6 (26%)

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	A1EP8	C	1101	-	-	5/20/33/33	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1101	A1EP8	C10-C9	4.87	1.58	1.51
5	C	1101	A1EP8	C9-C4	4.34	1.58	1.50
5	C	1101	A1EP8	O1-C1	3.26	1.32	1.22
5	C	1101	A1EP8	C5-C4	3.25	1.59	1.52
5	C	1101	A1EP8	O2-C3	3.09	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	A1EP8	C10-C9-C4	11.12	139.68	123.07
5	C	1101	A1EP8	C6-C5-C4	-5.23	106.41	116.37
5	C	1101	A1EP8	C5-C4-C9	-4.69	112.17	122.20
5	C	1101	A1EP8	C9-C2-C3	-2.72	109.46	117.33
5	C	1101	A1EP8	C2-C9-C10	2.32	125.92	121.65
5	C	1101	A1EP8	C2-C9-C4	-2.09	57.85	60.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

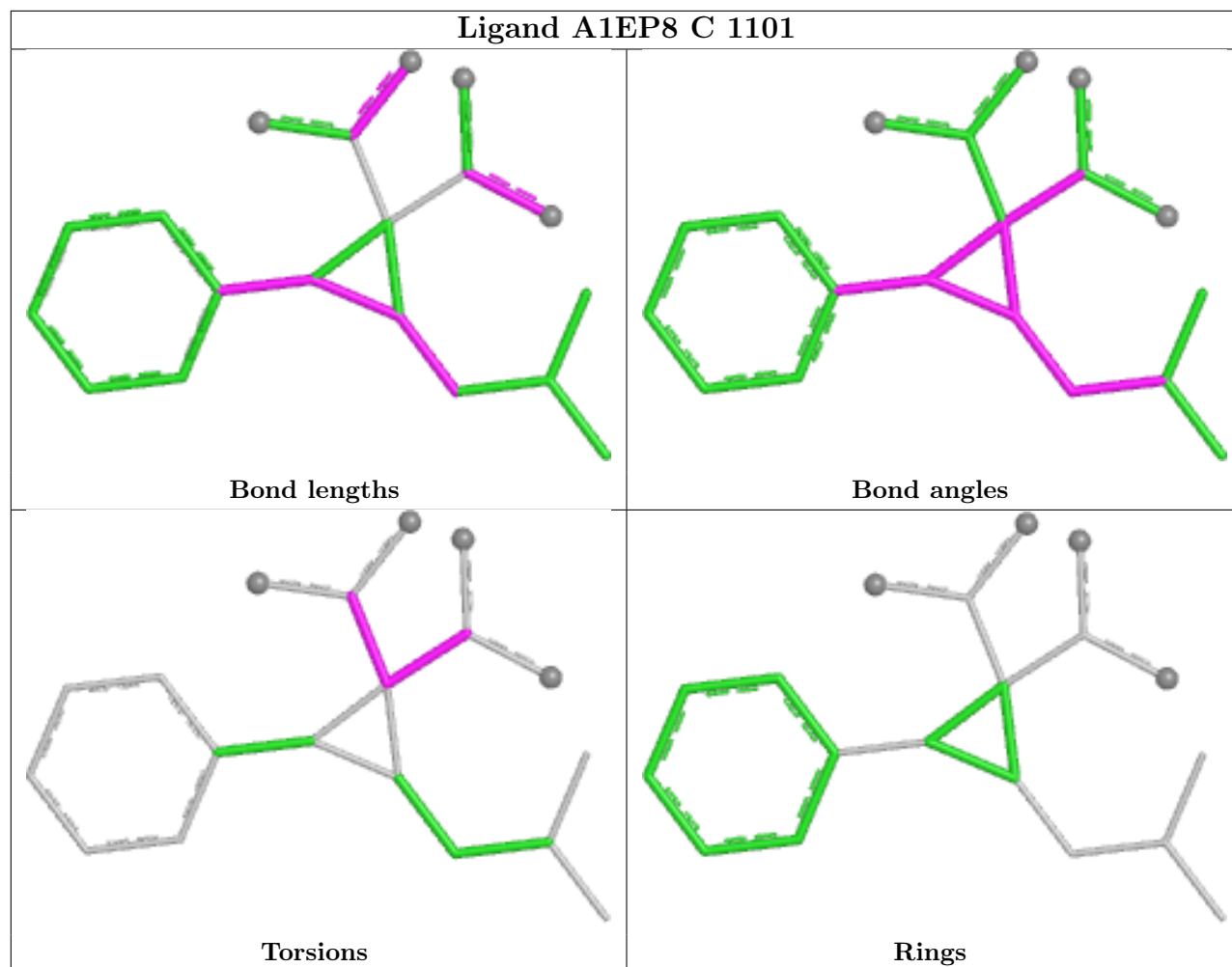
Mol	Chain	Res	Type	Atoms
5	C	1101	A1EP8	O1-C1-C2-C9
5	C	1101	A1EP8	O4-C1-C2-C3
5	C	1101	A1EP8	O4-C1-C2-C9
5	C	1101	A1EP8	C1-C2-C3-O3
5	C	1101	A1EP8	C1-C2-C3-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1101	A1EP8	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	689/765 (90%)	-0.64	0 100 100	81, 123, 160, 194	0
2	C	728/748 (97%)	-0.76	0 100 100	76, 110, 149, 195	0
3	D	130/157 (82%)	-0.67	0 100 100	103, 136, 169, 188	0
All	All	1547/1670 (92%)	-0.70	0 100 100	76, 117, 159, 195	0

There are no RSRZ outliers to report.

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.

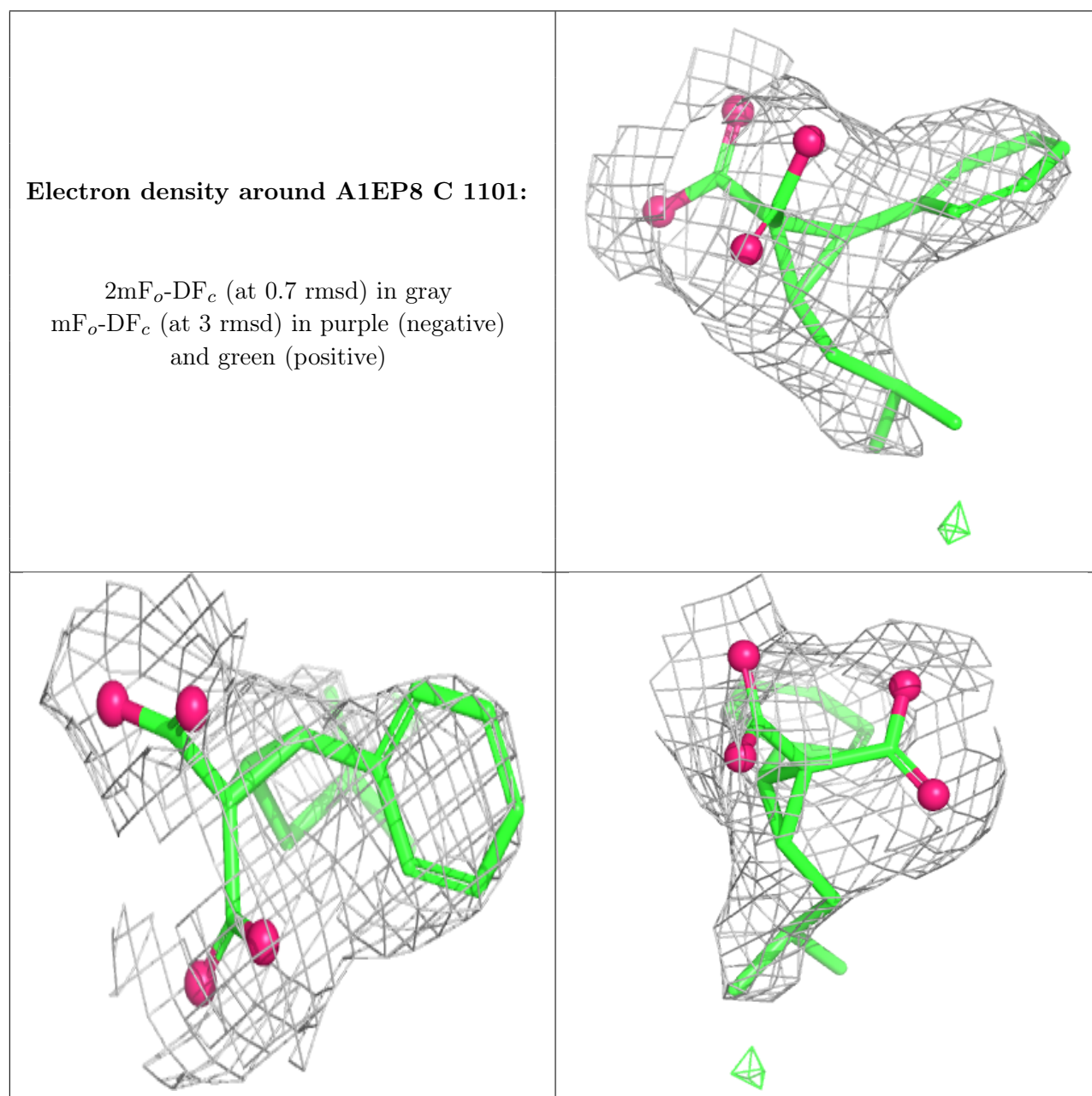
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	A1EP8	C	1101	19/19	0.90	0.09	101,128,135,136	0
4	ZN	C	1102	1/1	0.99	0.05	171,171,171,171	0
4	ZN	B	801	1/1	0.99	0.02	147,147,147,147	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 ⓘ

There are no such residues in this entry.