



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:11 PM EDT

PDB ID : 9P03 / pdb_00009p03
Title : Structure of human Sec23a/Sec24a/Sec22b bound to CPD6
Authors : Goldberg, J.
Deposited on : 2025-06-06
Resolution : 2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

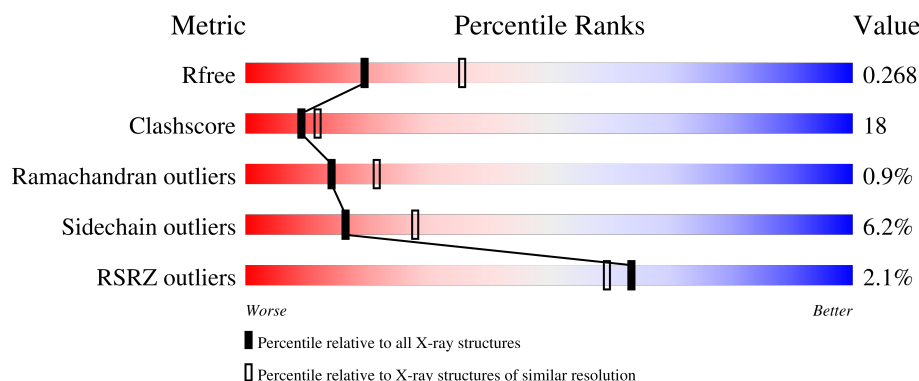
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	765	
2	B	748	
3	C	157	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12344 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	693	Total	C	N	O	S	0	0	0
			5473	3495	934	1005	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5721	3656	961	1070	34			

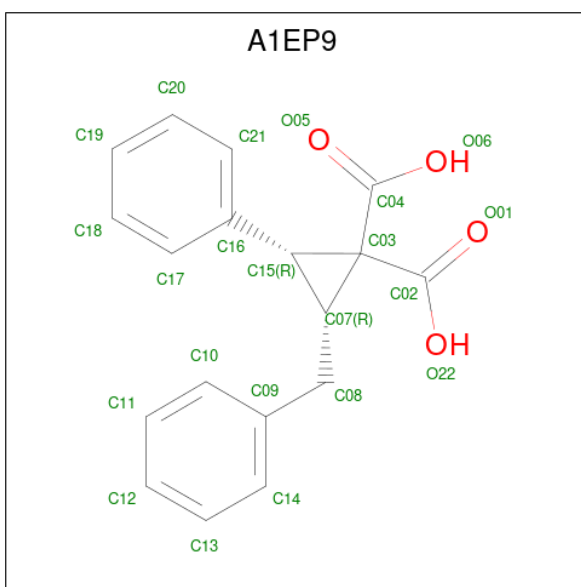
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1063	686	174	196	7			

- 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		

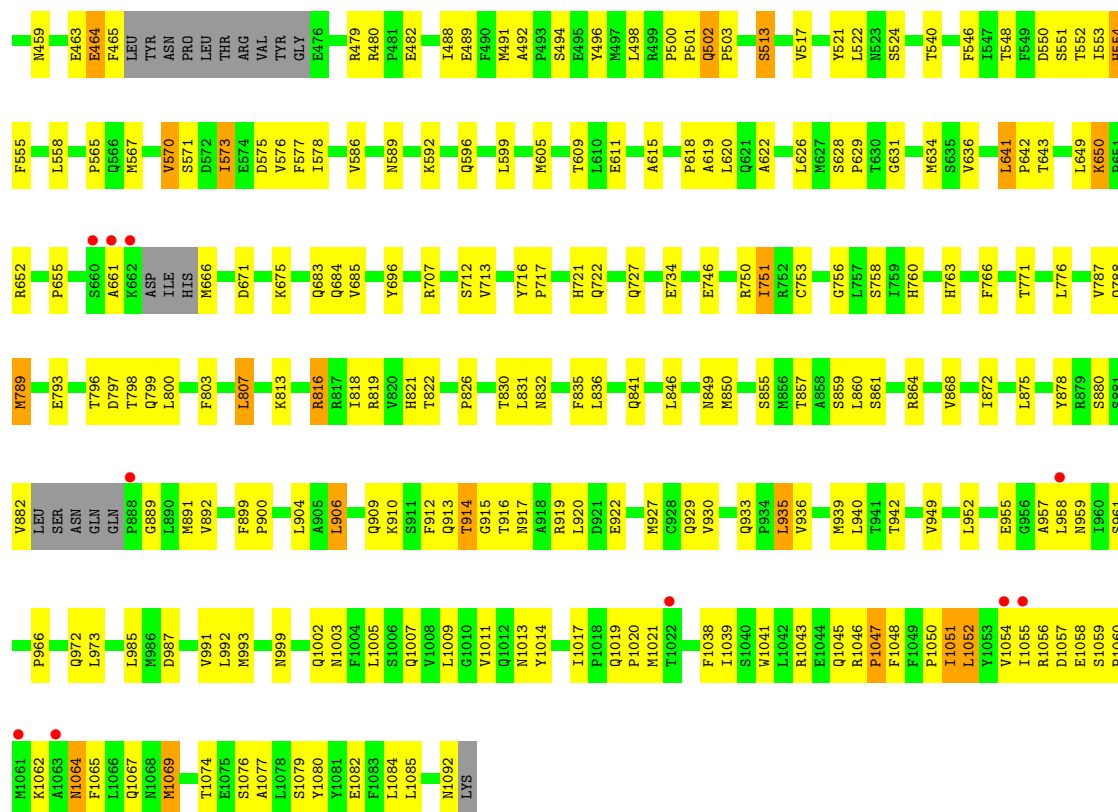
- Molecule 5 is (2 {R},3 {R})-2-phenyl-3-(phenylmethyl)cyclopropane-1,1-dicarboxylic acid (CCD ID: A1EP9) (formula: C₁₈H₁₆O₄) (labeled as "Ligand of Interest" by depositor).



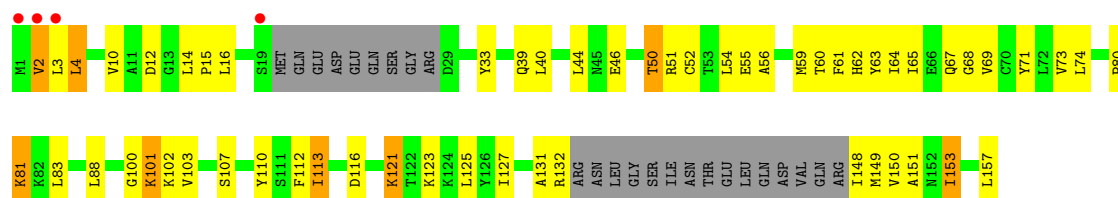
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			22	18	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	32	Total	O	0	0
			32	32		
6	C	4	Total	O	0	0
			4	4		



• 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, α , β , γ	148.19Å 96.49Å 130.80Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.64 50.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.64) 98.0 (50.00-2.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.205 , 0.268 0.205 , 0.268	Depositor DCC
R_{free} test set	2705 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12344	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: A1EP9, 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	0.38	0/5600	0.58	0/7587
2	B	0.41	0/5845	0.61	0/7952
3	C	0.36	0/1082	0.62	2/1458 (0.1%)
All	All	0.39	0/12527	0.60	2/16997 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	LYS	CA-C-N	5.14	123.48	120.24
3	C	102	LYS	C-N-CA	5.14	123.48	120.24

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	5473	0	5416	192	0
2	B	5721	0	5729	211	0
3	C	1063	0	1071	50	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	27	0	0	2	0
6	B	32	0	0	4	0
6	C	4	0	0	0	0
All	All	12344	0	12216	445	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 18.

All (445) 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:A:255:PRO:HG2	1:A:258:LYS:HG3	1.39	1.01
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.39	1.00
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.43	1.00
1:A:153:MET:HE2	1:A:157:LEU:HD11	1.43	0.98
1:A:153:MET:CE	1:A:157:LEU:HD11	2.01	0.89
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.53	0.88
1:A:183:ILE:HD13	2:B:605:MET:HE1	1.55	0.88
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.57	0.87
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.56	0.86
2:B:1074:THR:HG23	2:B:1076:SER:H	1.38	0.86
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.56	0.85
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.57	0.85
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.59	0.84
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.60	0.83
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.59	0.82
3:C:113:ILE:O	3:C:116:ASP:HB2	1.79	0.82
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.62	0.81
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.62	0.81
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.63	0.78
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.66	0.78
1:A:528:ARG:HA	1:A:608:MET:HE1	1.64	0.78
1:A:600:SER:O	1:A:604:ARG:HG3	1.84	0.78
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.65	0.77
2:B:909:GLN:HG2	2:B:910:LYS:N	2.01	0.76
1:A:381:LEU:HA	1:A:702:MET:HE2	1.70	0.74
2:B:991:VAL:HG12	2:B:1051:ILE:CD1	2.17	0.74
1:A:127:MET:HE2	1:A:127:MET:HA	1.69	0.74
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.23	0.73
2:B:513:SER:O	2:B:517:VAL:HG23	1.88	0.73
2:B:830:THR:HG22	2:B:832:ASN:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG12	1:A:77:ASP:H	1.56	0.71
1:A:288:MET:HG2	1:A:290:ILE:CD1	2.20	0.71
1:A:422:PRO:HG3	1:A:609:ARG:HG2	1.73	0.70
3:C:55:GLU:O	3:C:153:ILE:HG22	1.91	0.70
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.74	0.70
1:A:695:ILE:HD11	1:A:699:ARG:HH22	1.57	0.69
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.74	0.69
2:B:609:THR:HG22	2:B:611:GLU:H	1.55	0.69
2:B:620:LEU:HD22	2:B:634:MET:CE	2.22	0.69
1:A:101:ILE:HD11	1:A:106:GLN:HA	1.75	0.69
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.27	0.69
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.75	0.69
2:B:721:HIS:CD2	2:B:722:GLN:HG3	2.28	0.69
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.75	0.69
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.32	0.69
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.08	0.69
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.22	0.68
2:B:395:GLN:HE21	2:B:796:THR:HA	1.57	0.68
2:B:1057:ASP:O	2:B:1060:PRO:HD3	1.92	0.68
2:B:395:GLN:NE2	2:B:796:THR:HA	2.08	0.68
3:C:81:LYS:HD3	3:C:81:LYS:H	1.58	0.68
1:A:259:ARG:NH1	1:A:306:LEU:HD23	2.09	0.68
2:B:991:VAL:HG12	2:B:1051:ILE:HD11	1.75	0.67
1:A:288:MET:HG2	1:A:290:ILE:HD13	1.74	0.67
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.75	0.67
1:A:652:THR:HG22	1:A:653:PHE:N	2.10	0.67
2:B:496:TYR:HD2	2:B:818:ILE:HD11	1.58	0.67
1:A:288:MET:HE2	1:A:290:ILE:HD11	1.77	0.67
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.77	0.67
2:B:411:LEU:N	2:B:411:LEU:HD23	2.10	0.66
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.25	0.66
3:C:149:MET:HG2	3:C:150:VAL:H	1.61	0.66
1:A:482:VAL:HG22	1:A:496:VAL:HG22	1.77	0.66
1:A:26:SER:OG	1:A:504:ALA:HB3	1.95	0.65
1:A:692:ALA:O	1:A:696:LEU:HB2	1.96	0.65
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.21	0.65
1:A:313:TRP:O	1:A:316:ILE:HG22	1.97	0.65
1:A:76:VAL:HG12	1:A:77:ASP:N	2.11	0.64
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.12	0.64
1:A:195:LEU:HD13	1:A:203:MET:CE	2.21	0.64
2:B:480:ARG:HG3	2:B:482:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HG3	1:A:608:MET:HE1	1.78	0.64
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.79	0.64
1:A:528:ARG:HG3	1:A:608:MET:CE	2.28	0.64
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.32	0.64
2:B:1060:PRO:O	2:B:1062:LYS:HG3	1.97	0.64
1:A:524:ILE:HG13	1:A:615:SER:HB3	1.81	0.63
1:A:183:ILE:O	1:A:183:ILE:HG23	1.98	0.63
1:A:153:MET:HE2	1:A:157:LEU:CD1	2.26	0.63
3:C:3:LEU:HD13	3:C:123:LYS:HZ2	1.64	0.63
1:A:296:GLN:O	1:A:296:GLN:HG2	1.99	0.62
2:B:799:GLN:O	2:B:800:LEU:HD23	1.99	0.62
1:A:410:THR:HB	1:A:414:ILE:HB	1.81	0.62
2:B:578:ILE:HD11	2:B:626:LEU:CA	2.30	0.61
3:C:4:LEU:HD23	3:C:74:LEU:HD23	1.82	0.61
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.30	0.61
2:B:831:LEU:HD22	2:B:835:PHE:HE2	1.65	0.61
2:B:832:ASN:O	2:B:836:LEU:HG	2.00	0.61
2:B:348:LEU:HG	2:B:348:LEU:O	2.00	0.61
2:B:502:GLN:HG3	2:B:503:PRO:O	2.01	0.61
1:A:652:THR:HG22	1:A:653:PHE:H	1.65	0.60
3:C:50:THR:O	3:C:51:ARG:HG2	2.01	0.60
2:B:831:LEU:HD22	2:B:835:PHE:CE2	2.36	0.60
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.83	0.60
2:B:830:THR:HG22	2:B:832:ASN:N	2.16	0.60
2:B:576:VAL:CG1	2:B:622:ALA:HB2	2.26	0.60
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.37	0.59
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.29	0.59
3:C:10:VAL:HG23	3:C:68:GLY:O	2.03	0.59
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.83	0.59
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.85	0.58
2:B:991:VAL:HG12	2:B:1051:ILE:HD13	1.85	0.58
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.85	0.58
1:A:405:THR:O	1:A:483:THR:HA	2.03	0.58
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.38	0.58
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.30	0.58
1:A:297:GLY:H	1:A:300:MET:HB2	1.69	0.58
3:C:113:ILE:HD13	3:C:113:ILE:H	1.66	0.58
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.38	0.58
2:B:1064:ASN:HA	2:B:1067:GLN:HG3	1.85	0.58
2:B:1069:MET:HA	2:B:1069:MET:CE	2.31	0.57
1:A:695:ILE:HD11	1:A:699:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.69	0.57
2:B:846:LEU:O	2:B:850:MET:HG3	2.05	0.57
2:B:1020:PRO:HA	2:B:1055:ILE:CG1	2.32	0.57
1:A:649:LEU:HD11	1:A:656:ILE:HG23	1.86	0.57
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.24	0.57
1:A:148:LYS:HG2	1:A:244:LEU:O	2.05	0.57
2:B:909:GLN:HG2	2:B:910:LYS:H	1.69	0.57
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.40	0.56
1:A:610:GLN:HG3	1:A:618:MET:HE1	1.87	0.56
2:B:1005:LEU:CD2	2:B:1017:ILE:HD11	2.35	0.56
2:B:498:LEU:N	2:B:498:LEU:HD12	2.20	0.56
3:C:121:LYS:NZ	3:C:121:LYS:HB3	2.20	0.56
1:A:477:GLY:O	1:A:500:ALA:HA	2.05	0.56
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.34	0.56
2:B:655:PRO:CD	2:B:920:LEU:HD13	2.35	0.56
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.05	0.56
1:A:141:ASP:OD1	1:A:249:ARG:HD3	2.04	0.56
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	1.86	0.56
2:B:540:THR:HG22	2:B:589:ASN:ND2	2.21	0.56
1:A:695:ILE:HD11	1:A:699:ARG:HH12	1.72	0.55
2:B:350:VAL:CG1	2:B:891:MET:HE3	2.36	0.55
2:B:1005:LEU:O	2:B:1009:LEU:HB2	2.06	0.55
1:A:183:ILE:CD1	2:B:565:PRO:HG2	2.33	0.55
2:B:552:THR:HG22	2:B:571:SER:HA	1.88	0.55
2:B:760:HIS:NE2	2:B:788:GLN:HG2	2.21	0.55
2:B:957:ALA:C	2:B:959:ASN:H	2.14	0.55
1:A:183:ILE:HD13	2:B:605:MET:CE	2.33	0.55
2:B:358:ASN:HA	2:B:972:GLN:OE1	2.06	0.55
1:A:686:GLN:HG2	1:A:690:ASP:OD1	2.07	0.54
2:B:385:LEU:HD13	2:B:821:HIS:CE1	2.43	0.54
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.36	0.54
3:C:125:LEU:N	3:C:125:LEU:HD23	2.22	0.54
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.90	0.54
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.08	0.54
1:A:418:GLY:HA3	1:A:438:ILE:O	2.07	0.54
2:B:913:GLN:NE2	2:B:916:THR:HG21	2.23	0.54
3:C:100:GLY:C	3:C:101:LYS:HE3	2.33	0.54
1:A:581:MET:HE2	1:A:581:MET:N	2.23	0.54
1:A:524:ILE:HG13	1:A:615:SER:CB	2.38	0.53
1:A:257:GLY:O	1:A:306:LEU:HB2	2.09	0.53
3:C:127:ILE:HG22	3:C:127:ILE:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLN:O	1:A:388:ARG:HG2	2.07	0.53
1:A:610:GLN:HG3	1:A:618:MET:CE	2.38	0.53
2:B:385:LEU:HD21	2:B:417:LEU:HD21	1.91	0.53
1:A:70:LEU:HD23	1:A:109:GLU:HG3	1.89	0.53
1:A:541:ASP:CB	1:A:544:ARG:HD2	2.34	0.53
2:B:716:TYR:OH	2:B:734:GLU:OE1	2.26	0.53
3:C:81:LYS:HD3	3:C:81:LYS:N	2.23	0.53
1:A:269:SER:HB3	1:A:334:LEU:HD11	1.90	0.53
2:B:609:THR:HG22	2:B:611:GLU:N	2.23	0.53
2:B:936:VAL:O	2:B:940:LEU:HD23	2.08	0.53
2:B:1005:LEU:HD23	2:B:1009:LEU:HD12	1.90	0.53
1:A:259:ARG:NH2	1:A:308:THR:O	2.42	0.53
1:A:185:LYS:HB2	2:B:567:MET:HB3	1.90	0.53
2:B:411:LEU:HD11	2:B:751:ILE:CD1	2.39	0.53
2:B:949:VAL:HA	2:B:952:LEU:HD21	1.91	0.53
3:C:149:MET:HG2	3:C:150:VAL:N	2.24	0.53
1:A:695:ILE:HD11	1:A:699:ARG:CZ	2.39	0.52
2:B:1079:SER:OG	2:B:1082:GLU:HG3	2.10	0.52
1:A:26:SER:CB	1:A:504:ALA:HB3	2.39	0.52
1:A:238:MET:O	1:A:241:THR:HG22	2.10	0.52
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.91	0.52
3:C:131:ALA:C	3:C:132:ARG:HG2	2.35	0.52
1:A:98:TYR:O	1:A:101:ILE:HB	2.09	0.52
2:B:359:MET:HE2	2:B:1080:TYR:CE2	2.44	0.52
1:A:313:TRP:CE3	1:A:316:ILE:HG21	2.45	0.52
2:B:771:THR:O	2:B:771:THR:HG22	2.09	0.52
3:C:12:ASP:OD1	3:C:12:ASP:N	2.42	0.52
2:B:641:LEU:HD21	2:B:649:LEU:HB2	1.91	0.52
2:B:987:ASP:HA	2:B:992:LEU:HD23	1.92	0.52
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.91	0.51
3:C:14:LEU:HD12	3:C:15:PRO:HD2	1.92	0.51
1:A:310:ILE:HG22	1:A:311:ARG:HD3	1.91	0.51
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.91	0.51
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.40	0.51
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.46	0.51
2:B:750:ARG:HH22	2:B:771:THR:CG2	2.24	0.51
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.41	0.51
2:B:935:LEU:O	2:B:935:LEU:HD22	2.11	0.51
1:A:621:PRO:O	1:A:637:LEU:HD11	2.11	0.50
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.75	0.50
2:B:360:LEU:HD12	2:B:361:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.94	0.50
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.92	0.50
2:B:1074:THR:CG2	2:B:1077:ALA:HB3	2.36	0.50
2:B:763:HIS:HB3	2:B:849:ASN:OD1	2.11	0.50
1:A:282:THR:CG2	1:A:283:GLY:N	2.74	0.50
2:B:420:LEU:HD22	2:B:819:ARG:NH2	2.26	0.50
2:B:882:VAL:HG13	6:B:1201:HOH:O	2.12	0.50
1:A:700:PHE:C	1:A:700:PHE:CD1	2.86	0.50
1:A:754:ASP:O	1:A:758:LYS:HG3	2.12	0.50
2:B:372:LEU:HD21	2:B:826:PRO:HD3	1.94	0.50
2:B:428:ILE:HG21	2:B:437:TYR:HE2	1.77	0.50
1:A:311:ARG:HD3	1:A:311:ARG:N	2.26	0.50
1:A:560:TYR:CD2	1:A:761:VAL:HG12	2.47	0.50
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.27	0.50
2:B:592:LYS:O	2:B:596:GLN:HG3	2.11	0.50
1:A:517:PHE:CE2	1:A:519:GLN:HA	2.47	0.49
3:C:60:THR:HG22	3:C:62:HIS:NE2	2.27	0.49
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.93	0.49
1:A:313:TRP:CA	1:A:316:ILE:HG22	2.42	0.49
1:A:6:GLU:O	1:A:10:GLN:HG3	2.12	0.49
1:A:311:ARG:HH21	1:A:359:GLU:CD	2.21	0.49
2:B:425:SER:HB3	2:B:427:THR:O	2.13	0.49
3:C:39:GLN:HB3	3:C:157:LEU:HD22	1.93	0.49
3:C:63:TYR:CD1	3:C:63:TYR:C	2.90	0.49
1:A:368:GLY:HA3	1:A:450:GLY:O	2.13	0.49
2:B:655:PRO:HD3	2:B:920:LEU:HD13	1.93	0.49
3:C:10:VAL:HG23	3:C:68:GLY:C	2.38	0.49
3:C:39:GLN:CB	3:C:157:LEU:HD22	2.43	0.49
1:A:282:THR:HG22	1:A:283:GLY:N	2.27	0.49
2:B:717:PRO:HD2	2:B:727:GLN:NE2	2.28	0.49
1:A:27:SER:O	1:A:31:ALA:HB2	2.12	0.49
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.95	0.49
2:B:1003:ASN:O	2:B:1007:GLN:HB2	2.13	0.49
2:B:1052:LEU:O	2:B:1052:LEU:HD23	2.13	0.49
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.94	0.48
3:C:52:CYS:SG	3:C:149:MET:HE2	2.53	0.48
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.95	0.48
2:B:1074:THR:HG23	2:B:1076:SER:N	2.20	0.48
1:A:354:GLN:OE1	1:A:597:PRO:HD2	2.13	0.48
1:A:195:LEU:CD1	1:A:203:MET:HE1	2.29	0.48
1:A:657:LEU:CD1	1:A:717:PHE:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:O	1:A:164:VAL:HA	2.13	0.48
1:A:293:PRO:HA	1:A:355:THR:O	2.14	0.48
3:C:51:ARG:HD3	3:C:64:ILE:HG22	1.95	0.48
1:A:582:PHE:O	1:A:586:ARG:HG2	2.13	0.48
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.48	0.48
1:A:54:ILE:CG1	1:A:117:ILE:HD11	2.37	0.48
2:B:500:PRO:O	2:B:501:PRO:C	2.56	0.48
3:C:39:GLN:HA	3:C:39:GLN:OE1	2.13	0.48
1:A:3:THR:HB	1:A:6:GLU:CG	2.44	0.48
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.95	0.48
2:B:620:LEU:CD2	2:B:636:VAL:HG21	2.44	0.48
3:C:3:LEU:HD13	3:C:123:LYS:NZ	2.28	0.48
1:A:183:ILE:HB	2:B:605:MET:HE2	1.96	0.47
1:A:607:PHE:CD2	1:A:608:MET:HE3	2.48	0.47
2:B:441:PHE:O	2:B:453:ASN:HB3	2.13	0.47
1:A:417:SER:O	1:A:437:GLU:HA	2.14	0.47
1:A:679:GLU:HA	1:A:679:GLU:OE1	2.14	0.47
2:B:381:CYS:HB2	2:B:822:THR:O	2.14	0.47
2:B:386:PHE:CE1	2:B:409:LEU:HD13	2.49	0.47
2:B:766:PHE:HB3	2:B:776:LEU:CD2	2.44	0.47
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.96	0.47
2:B:494:SER:HB2	6:B:1217:HOH:O	2.14	0.47
2:B:524:SER:HB2	6:B:1208:HOH:O	2.13	0.47
2:B:875:LEU:CD2	2:B:892:VAL:HG12	2.37	0.47
3:C:61:PHE:CE2	3:C:153:ILE:HD12	2.49	0.47
1:A:121:VAL:HG11	6:A:924:HOH:O	2.13	0.47
1:A:398:PHE:HB3	1:A:400:MET:CG	2.45	0.47
1:A:522:ALA:O	1:A:526:MET:HG2	2.15	0.47
3:C:81:LYS:H	3:C:81:LYS:CD	2.20	0.47
2:B:361:PRO:HG3	2:B:365:LEU:CD2	2.45	0.47
1:A:76:VAL:CG1	1:A:77:ASP:H	2.27	0.47
2:B:935:LEU:O	2:B:939:MET:HG2	2.15	0.47
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.79	0.47
1:A:177:GLU:OE1	1:A:185:LYS:HE2	2.14	0.47
2:B:620:LEU:CD2	2:B:634:MET:CE	2.92	0.47
2:B:1054:VAL:HG12	2:B:1054:VAL:O	2.15	0.47
2:B:350:VAL:HG12	2:B:891:MET:HE3	1.96	0.47
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.30	0.46
1:A:297:GLY:N	1:A:300:MET:HB2	2.29	0.46
2:B:860:LEU:O	2:B:864:ARG:HG3	2.15	0.46
1:A:571:SER:HB2	1:A:573:THR:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.74	0.46
1:A:191:GLY:HA3	1:A:263:SER:OG	2.16	0.46
2:B:411:LEU:N	2:B:411:LEU:CD2	2.79	0.46
2:B:1014:TYR:HH	2:B:1058:GLU:H	1.64	0.46
2:B:1080:TYR:CZ	2:B:1084:LEU:HD11	2.51	0.46
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.97	0.46
1:A:404:GLY:HA2	1:A:484:GLN:O	2.16	0.46
2:B:438:ILE:HD13	2:B:450:TRP:CE2	2.51	0.46
2:B:1055:ILE:O	2:B:1057:ASP:N	2.49	0.46
1:A:15:ASP:O	1:A:16:GLY:C	2.57	0.46
2:B:992:LEU:CB	2:B:1052:LEU:HD12	2.46	0.46
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.15	0.46
2:B:555:PHE:HE1	2:B:570:VAL:HG11	1.81	0.46
2:B:919:ARG:O	2:B:922:GLU:HB2	2.16	0.46
2:B:993:MET:HE2	2:B:1065:PHE:HB2	1.97	0.46
2:B:446:ASP:C	2:B:448:ARG:H	2.23	0.46
1:A:631:PRO:O	1:A:633:GLU:HG3	2.16	0.45
2:B:916:THR:HG22	2:B:917:ASN:N	2.30	0.45
2:B:1009:LEU:HD23	2:B:1009:LEU:HA	1.72	0.45
1:A:361:LYS:O	1:A:362:CYS:C	2.59	0.45
2:B:350:VAL:HG22	2:B:878:TYR:OH	2.17	0.45
1:A:524:ILE:HD12	1:A:524:ILE:HA	1.73	0.45
2:B:348:LEU:HD12	2:B:836:LEU:HD21	1.97	0.45
2:B:350:VAL:HG11	2:B:891:MET:HE3	1.97	0.45
2:B:449:ARG:HA	2:B:459:ASN:O	2.16	0.45
1:A:147:LEU:HD11	1:A:289:PHE:CD2	2.52	0.45
2:B:609:THR:CG2	2:B:611:GLU:HB2	2.46	0.45
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.32	0.45
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.79	0.45
1:A:194:ASP:O	1:A:195:LEU:HD23	2.16	0.45
2:B:553:ILE:HG12	2:B:619:ALA:HA	1.98	0.45
1:A:111:LEU:N	1:A:111:LEU:HD23	2.30	0.45
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.45	0.45
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.98	0.45
1:A:117:ILE:HG13	6:A:904:HOH:O	2.17	0.45
2:B:666:MET:HE1	2:B:927:MET:SD	2.57	0.45
3:C:80:PRO:HB2	3:C:83:LEU:HG	1.99	0.45
1:A:95:PRO:HG2	1:A:98:TYR:HD1	1.83	0.44
1:A:297:GLY:HA3	1:A:300:MET:H	1.81	0.44
1:A:551:ILE:O	1:A:555:GLN:HG3	2.16	0.44
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:GLN:OE1	2:B:746:GLU:HA	2.17	0.44
1:A:190:ARG:HG3	2:B:577:PHE:CE2	2.53	0.44
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.18	0.44
1:A:652:THR:CG2	1:A:653:PHE:N	2.80	0.44
2:B:465:PHE:HA	2:B:480:ARG:HE	1.80	0.44
2:B:807:LEU:O	2:B:818:ILE:HA	2.18	0.44
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.47	0.44
1:A:341:THR:HG22	1:A:343:HIS:CE1	2.53	0.44
2:B:463:GLU:O	2:B:465:PHE:N	2.50	0.44
2:B:766:PHE:HB3	2:B:776:LEU:HD23	1.98	0.44
2:B:973:LEU:HA	2:B:1069:MET:HE1	1.98	0.44
1:A:101:ILE:CD1	1:A:106:GLN:HA	2.44	0.44
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.53	0.44
1:A:297:GLY:CA	1:A:300:MET:HB2	2.47	0.44
1:A:368:GLY:C	1:A:609:ARG:HH22	2.26	0.44
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.47	0.44
1:A:240:LEU:O	1:A:240:LEU:HD22	2.18	0.44
2:B:411:LEU:HD23	2:B:411:LEU:H	1.80	0.44
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.99	0.44
2:B:750:ARG:HH22	2:B:771:THR:HG22	1.82	0.44
1:A:101:ILE:HA	1:A:101:ILE:HD13	1.58	0.43
1:A:190:ARG:NH1	2:B:575:ASP:OD1	2.51	0.43
1:A:521:ALA:HA	1:A:612:LEU:CD1	2.48	0.43
3:C:63:TYR:HA	3:C:71:TYR:O	2.18	0.43
1:A:51:LEU:HD22	1:A:51:LEU:HA	1.82	0.43
1:A:153:MET:HE1	1:A:157:LEU:HD11	1.91	0.43
1:A:415:LYS:HD2	1:A:464:VAL:HG21	2.00	0.43
1:A:17:VAL:HA	1:A:41:LEU:O	2.18	0.43
2:B:620:LEU:CD2	2:B:634:MET:HE3	2.48	0.43
2:B:452:CYS:O	2:B:456:TYR:HA	2.19	0.43
2:B:683:GLN:O	2:B:684:GLN:HB2	2.19	0.43
2:B:860:LEU:HD11	2:B:912:PHE:HA	2.01	0.43
2:B:999:ASN:CG	2:B:999:ASN:O	2.61	0.43
2:B:949:VAL:HG11	2:B:985:LEU:HB2	2.00	0.43
3:C:50:THR:C	3:C:51:ARG:HG2	2.44	0.43
1:A:617:ILE:HG12	1:A:622:ILE:CD1	2.49	0.43
2:B:437:TYR:O	2:B:438:ILE:C	2.61	0.43
2:B:758:SER:O	2:B:789:MET:HB3	2.18	0.43
2:B:868:VAL:HG12	2:B:872:ILE:HD12	1.99	0.43
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.53	0.43
2:B:498:LEU:N	2:B:498:LEU:CD1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ILE:HD13	2:B:573:ILE:HA	1.58	0.43
3:C:61:PHE:CD2	3:C:153:ILE:HD12	2.54	0.43
1:A:397:GLN:HE22	1:A:489:SER:HB3	1.83	0.43
2:B:992:LEU:HB3	2:B:1052:LEU:HD12	2.01	0.43
1:A:30:GLU:CD	1:A:510:ILE:HD11	2.44	0.43
1:A:313:TRP:C	1:A:316:ILE:HG22	2.43	0.43
3:C:121:LYS:HB3	3:C:121:LYS:HZ3	1.83	0.43
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.49	0.42
2:B:438:ILE:O	2:B:438:ILE:HG23	2.19	0.42
2:B:446:ASP:OD2	2:B:449:ARG:HD2	2.19	0.42
2:B:628:SER:CB	2:B:629:PRO:HD3	2.48	0.42
3:C:33:TYR:CD1	3:C:74:LEU:HD21	2.54	0.42
1:A:296:GLN:N	1:A:300:MET:HG3	2.34	0.42
2:B:973:LEU:HB3	2:B:1069:MET:HE2	2.01	0.42
1:A:510:ILE:H	1:A:513:ILE:HG13	1.84	0.42
2:B:1055:ILE:HG21	2:B:1062:LYS:CD	2.40	0.42
2:B:359:MET:SD	2:B:359:MET:N	2.92	0.42
1:A:478:ALA:HA	1:A:499:ILE:O	2.20	0.42
2:B:855:SER:HA	2:B:859:SER:O	2.20	0.42
2:B:1020:PRO:HA	2:B:1055:ILE:CD1	2.50	0.42
3:C:33:TYR:HB3	3:C:74:LEU:CD2	2.49	0.42
1:A:36:VAL:HG11	1:A:522:ALA:HB1	2.01	0.42
1:A:316:ILE:HD13	1:A:316:ILE:O	2.19	0.42
1:A:700:PHE:CB	1:A:701:PRO:CD	2.93	0.42
1:A:608:MET:HE2	1:A:608:MET:HA	2.01	0.42
2:B:352:ASN:ND2	2:B:355:GLN:HG2	2.35	0.42
1:A:164:VAL:O	1:A:230:LEU:HA	2.19	0.42
1:A:397:GLN:NE2	1:A:489:SER:HB3	2.34	0.42
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.82	0.42
2:B:424:THR:HG22	2:B:491:MET:HG3	2.02	0.42
2:B:650:LYS:HE3	2:B:650:LYS:HA	2.01	0.42
2:B:864:ARG:HD2	2:B:914:THR:HG23	2.02	0.42
2:B:929:GLN:O	2:B:933:GLN:HB2	2.20	0.42
3:C:4:LEU:HD23	3:C:74:LEU:CD2	2.47	0.42
2:B:558:LEU:HB2	2:B:586:VAL:HG11	2.00	0.42
2:B:915:GLY:HA3	2:B:1076:SER:HB2	2.02	0.42
3:C:40:LEU:O	3:C:44:LEU:HG	2.19	0.42
1:A:233:VAL:O	1:A:237:ASP:HB3	2.20	0.41
2:B:550:ASP:OD1	2:B:551:SER:N	2.53	0.41
2:B:620:LEU:HD22	2:B:634:MET:HE1	2.00	0.41
2:B:661:ALA:HB3	2:B:861:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:753:CYS:HB3	2:B:803:PHE:HD1	1.85	0.41
3:C:148:ILE:HG22	3:C:149:MET:N	2.34	0.41
1:A:683:HIS:O	1:A:687:ALA:HB2	2.19	0.41
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.95	0.41
3:C:16:LEU:HD22	3:C:112:PHE:HE2	1.85	0.41
1:A:349:ALA:HB1	1:A:355:THR:HG21	2.02	0.41
1:A:438:ILE:HG21	1:A:529:LEU:HD21	2.02	0.41
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.78	0.41
2:B:904:LEU:HD22	2:B:1080:TYR:HA	2.02	0.41
2:B:420:LEU:HD21	2:B:489:GLU:HB2	2.02	0.41
1:A:88:CYS:O	1:A:89:TYR:HB2	2.20	0.41
1:A:295:THR:C	1:A:300:MET:HG3	2.45	0.41
1:A:406:LEU:O	1:A:445:GLN:HA	2.20	0.41
3:C:54:LEU:HA	3:C:151:ALA:O	2.20	0.41
1:A:39:ALA:HB1	1:A:525:LEU:HD22	2.03	0.41
2:B:521:TYR:CD1	2:B:521:TYR:C	2.98	0.41
1:A:3:THR:HB	1:A:6:GLU:HG3	2.00	0.41
1:A:26:SER:HB3	1:A:504:ALA:N	2.36	0.41
1:A:316:ILE:HD13	1:A:316:ILE:C	2.46	0.41
1:A:394:MET:HE3	1:A:394:MET:H	1.85	0.41
2:B:479:ARG:HD2	2:B:479:ARG:HA	1.80	0.41
2:B:615:ALA:O	2:B:618:PRO:HD2	2.20	0.41
1:A:297:GLY:H	1:A:300:MET:HE2	1.86	0.41
2:B:955:GLU:OE1	2:B:955:GLU:N	2.54	0.41
1:A:638:ASP:HB3	1:A:640:SER:OG	2.21	0.41
2:B:546:PHE:CE1	2:B:599:LEU:HD21	2.55	0.41
2:B:750:ARG:NH2	2:B:771:THR:HG22	2.36	0.41
2:B:875:LEU:HD23	2:B:875:LEU:HA	1.81	0.41
3:C:56:ALA:HB2	3:C:153:ILE:CG2	2.49	0.41
1:A:695:ILE:CD1	1:A:699:ARG:HH22	2.28	0.41
3:C:69:VAL:CG2	3:C:103:VAL:HG11	2.50	0.41
2:B:671:ASP:OD2	2:B:675:LYS:CE	2.69	0.40
2:B:766:PHE:CD1	2:B:766:PHE:C	3.00	0.40
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.51	0.40
1:A:559:GLU:O	1:A:568:PHE:HA	2.21	0.40
2:B:973:LEU:HA	2:B:1069:MET:CE	2.50	0.40
2:B:1047:PRO:HD2	2:B:1048:PHE:H	1.86	0.40
2:B:576:VAL:HG11	2:B:622:ALA:CB	2.31	0.40
2:B:707:ARG:NE	6:B:1210:HOH:O	2.54	0.40
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.86	0.40
1:A:42:PHE:CZ	1:A:44:PRO:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:GLU:C	2:B:358:ASN:H	2.29	0.40
2:B:841:GLN:HG2	2:B:939:MET:SD	2.62	0.40
2:B:1074:THR:C	2:B:1076:SER:H	2.29	0.40
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.93	0.40
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.90	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	681/765 (89%)	627 (92%)	51 (8%)	3 (0%)	30	42
2	B	721/748 (96%)	661 (92%)	51 (7%)	9 (1%)	10	15
3	C	127/157 (81%)	117 (92%)	8 (6%)	2 (2%)	7	10
All	All	1529/1670 (92%)	1405 (92%)	110 (7%)	14 (1%)	14	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1056	ARG
3	C	4	LEU
2	B	464	GLU
2	B	1047	PRO
1	A	509	GLN
2	B	438	ILE
2	B	513	SER
2	B	958	LEU
1	A	297	GLY
2	B	880	SER
2	B	961	SER
3	C	2	VAL

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Mol	Chain	Res	Type
1	A	183	ILE
2	B	889	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	A	601/666 (90%)	561 (93%)	40 (7%)	15	24
2	B	652/679 (96%)	617 (95%)	35 (5%)	20	33
3	C	115/138 (83%)	105 (91%)	10 (9%)	9	15
All	All	1368/1483 (92%)	1283 (94%)	85 (6%)	16	28

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	41	LEU
1	A	50	ASP
1	A	51	LEU
1	A	65	THR
1	A	101	ILE
1	A	103	GLU
1	A	116	SER
1	A	135	VAL
1	A	145	GLN
1	A	161	THR
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	268	LEU
1	A	290	ILE
1	A	316	ILE
1	A	355	THR
1	A	362	CYS
1	A	376	SER

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Mol	Chain	Res	Type
1	A	400	MET
1	A	451	LEU
1	A	488	SER
1	A	508	THR
1	A	510	ILE
1	A	511	GLN
1	A	513	ILE
1	A	524	ILE
1	A	528	ARG
1	A	544	ARG
1	A	562	LYS
1	A	570	PHE
1	A	571	SER
1	A	581	MET
1	A	608	MET
1	A	613	THR
1	A	695	ILE
1	A	746	ASP
1	A	747	VAL
1	A	748	SER
2	B	356	GLU
2	B	359	MET
2	B	411	LEU
2	B	423	VAL
2	B	464	GLU
2	B	502	GLN
2	B	522	LEU
2	B	554	HIS
2	B	570	VAL
2	B	573	ILE
2	B	641	LEU
2	B	643	THR
2	B	650	LYS
2	B	712	SER
2	B	713	VAL
2	B	751	ILE
2	B	787	VAL
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	807	LEU
2	B	813	LYS

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Mol	Chain	Res	Type
2	B	816	ARG
2	B	857	THR
2	B	906	LEU
2	B	914	THR
2	B	930	VAL
2	B	935	LEU
2	B	1002	GLN
2	B	1051	ILE
2	B	1052	LEU
2	B	1064	ASN
2	B	1069	MET
2	B	1085	LEU
2	B	1092	ASN
3	C	2	VAL
3	C	46	GLU
3	C	50	THR
3	C	67	GLN
3	C	81	LYS
3	C	101	LYS
3	C	107	SER
3	C	113	ILE
3	C	121	LYS
3	C	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	145	GLN
1	A	231	GLN
1	A	512	ASN
1	A	710	HIS
2	B	352	ASN
2	B	395	GLN
2	B	515	ASN
2	B	532	ASN
2	B	564	GLN
2	B	683	GLN
2	B	780	ASN
2	B	788	GLN
2	B	832	ASN
2	B	913	GLN

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Mol	Chain	Res	Type
2	B	932	ASN
2	B	1092	ASN
3	C	34	GLN
3	C	99	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	A1EP9	B	1101	-	22,24,24	1.48	3 (13%)	27,35,35	2.34	5 (18%)

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	A1EP9	B	1101	-	-	8/20/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	A1EP9	C16-C15	4.08	1.57	1.51
5	B	1101	A1EP9	C08-C09	2.65	1.57	1.51
5	B	1101	A1EP9	C15-C07	2.56	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	A1EP9	C16-C15-C07	9.32	136.99	123.07
5	B	1101	A1EP9	C03-C15-C16	4.53	130.01	121.65
5	B	1101	A1EP9	C02-C03-C04	3.14	120.65	115.36
5	B	1101	A1EP9	C07-C03-C02	-2.31	110.24	118.58
5	B	1101	A1EP9	C15-C03-C04	-2.29	110.69	117.33

There are no chirality outliers.

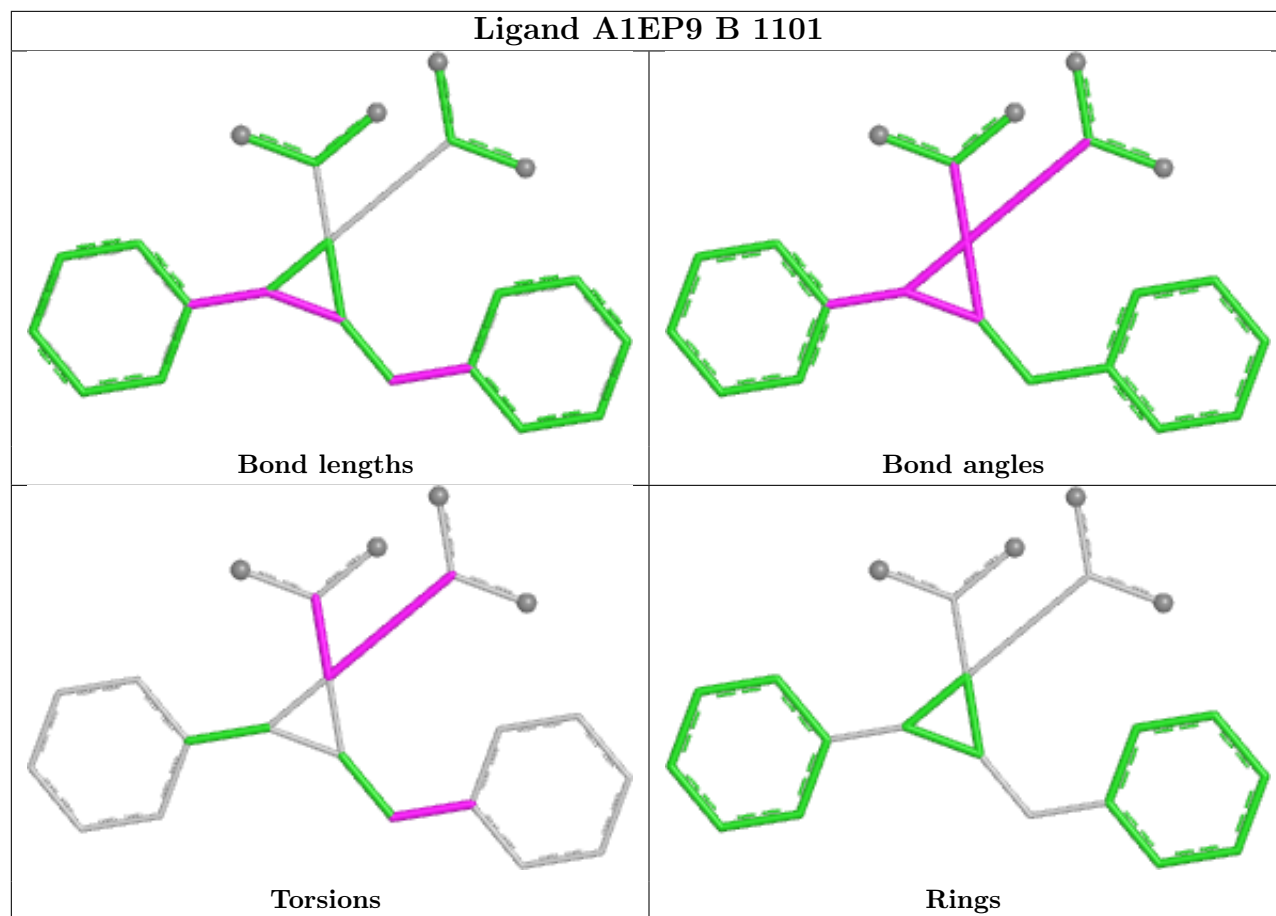
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	A1EP9	O01-C02-C03-C07
5	B	1101	A1EP9	O22-C02-C03-C04
5	B	1101	A1EP9	O22-C02-C03-C07
5	B	1101	A1EP9	C15-C03-C04-O05
5	B	1101	A1EP9	C02-C03-C04-O06
5	B	1101	A1EP9	C07-C08-C09-C10
5	B	1101	A1EP9	C07-C08-C09-C14
5	B	1101	A1EP9	C15-C03-C04-O06

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	693/765 (90%)	0.02	16 (2%) 61 57	45, 69, 106, 152	0
2	B	729/748 (97%)	-0.15	12 (1%) 70 67	41, 61, 99, 152	0
3	C	133/157 (84%)	0.21	4 (3%) 52 47	54, 82, 120, 136	0
All	All	1555/1670 (93%)	-0.04	32 (2%) 63 59	41, 65, 106, 152	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	4.6
1	A	510	ILE	4.0
1	A	31	ALA	3.5
1	A	124	GLY	3.4
3	C	2	VAL	3.3
1	A	504	ALA	3.1
1	A	29	LEU	3.0
1	A	123	ARG	2.8
2	B	1063	ALA	2.8
1	A	223	PRO	2.7
2	B	446	ASP	2.7
2	B	888	PRO	2.5
2	B	445	LEU	2.5
1	A	506	ALA	2.5
2	B	1054	VAL	2.4
2	B	1022	THR	2.4
3	C	3	LEU	2.4
1	A	34	MET	2.4
1	A	224	PRO	2.3
3	C	19	SER	2.3
1	A	32	THR	2.2
1	A	746	ASP	2.2
1	A	30	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	661	ALA	2.2
1	A	105	ASN	2.2
1	A	205	GLY	2.2
2	B	660	SER	2.1
1	A	4	TYR	2.1
2	B	958	LEU	2.1
2	B	662	LYS	2.0
2	B	1061	MET	2.0
3	C	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

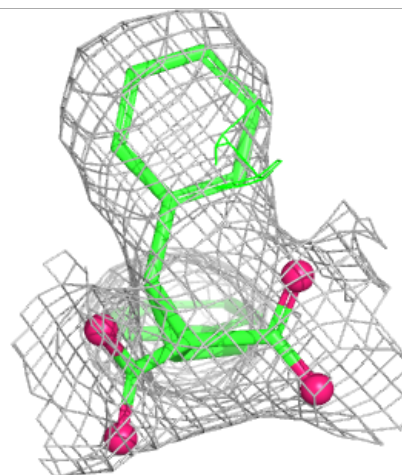
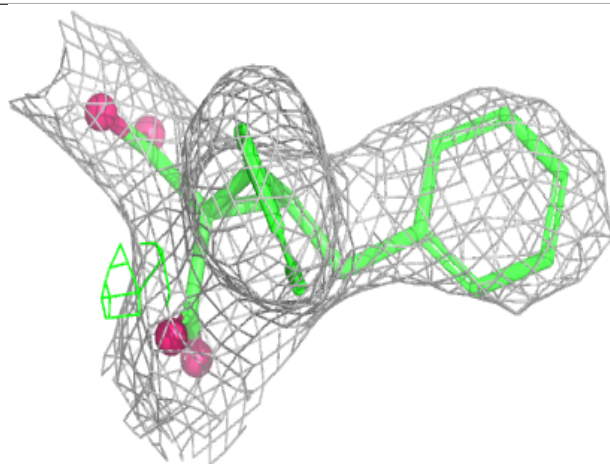
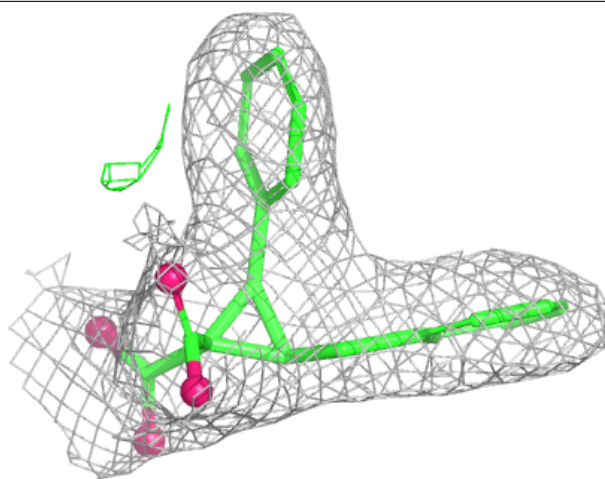
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	A1EP9	B	1101	22/22	0.90	0.13	53,74,81,86	0
4	ZN	A	800	1/1	0.99	0.03	83,83,83,83	0
4	ZN	B	1102	1/1	1.00	0.03	66,66,66,66	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 A1EP9 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.