



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:05 PM EDT

PDB ID : 9P0B / pdb_00009p0b
Title : Structure of human Sec23a/Sec24a/Sec22b bound to CPD15
Authors : Goldberg, J.
Deposited on : 2025-06-06
Resolution : 2.53 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

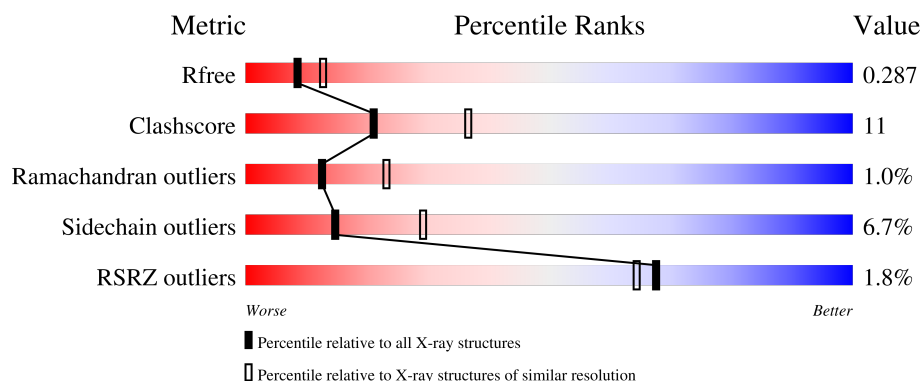
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	<div> <div> <div>0%</div> <div>65%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	748	<div> <div>2%</div> <div>69%</div> <div>25%</div> <div>•</div> <div>•</div> </div>
3	C	157	<div> <div>3%</div> <div>57%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12316 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
			5467	3492	931	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			

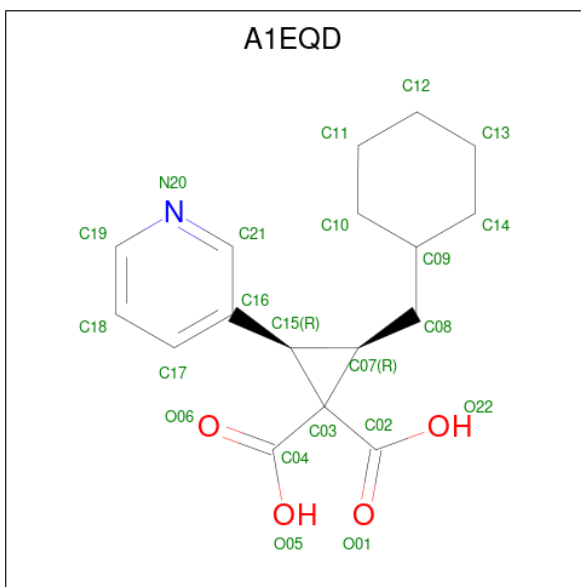
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1042	673	169	194	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-(cyclohexylmethyl)-3-pyridin-3-yl-cyclopropane-1,1-dicarboxylic acid (CCD ID: A1EQD) (formula: C₁₇H₂₁NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			22	17	1	4		

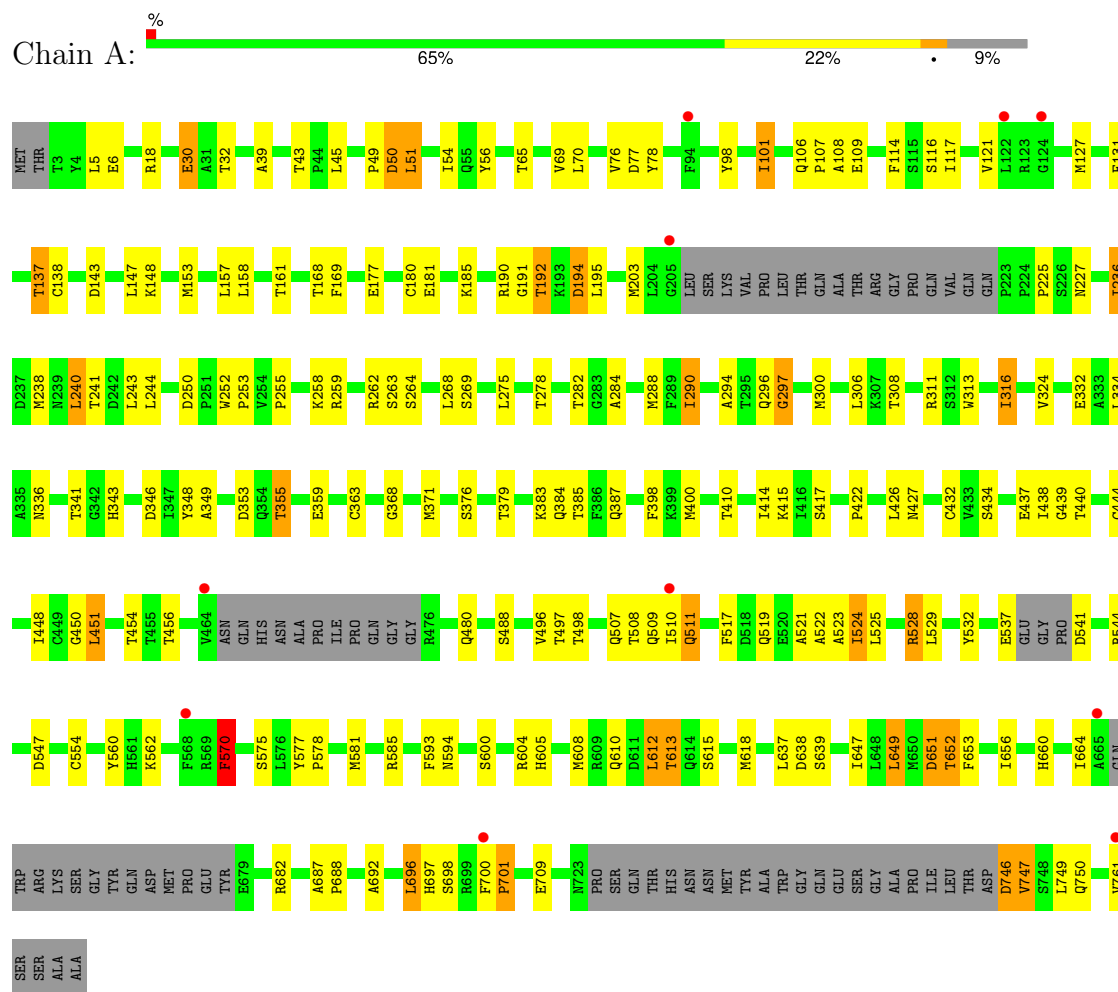
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	32	Total	O	0	0
			32	32		
6	C	4	Total	O	0	0
			4	4		

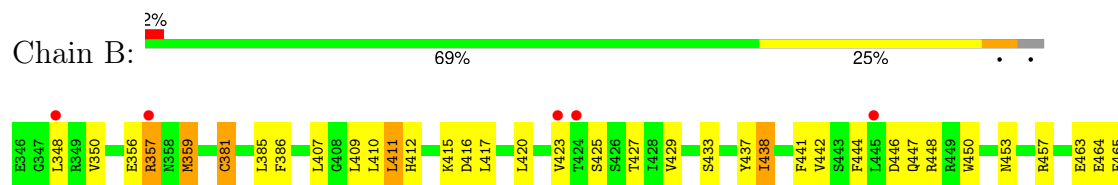
3 Residue-property plots

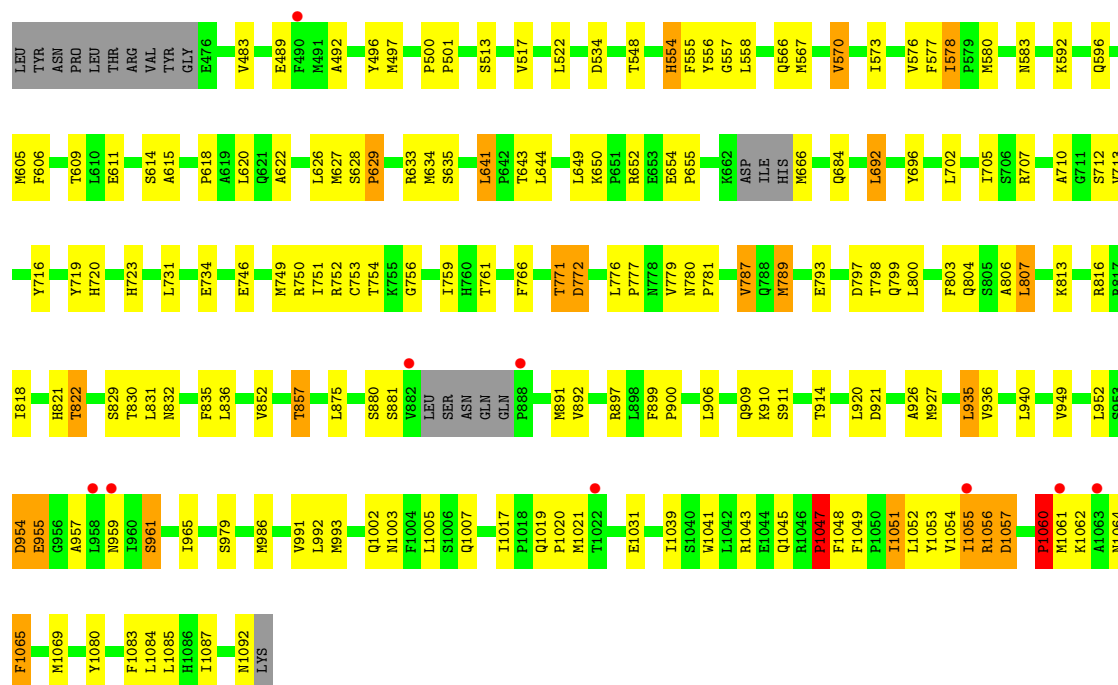
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

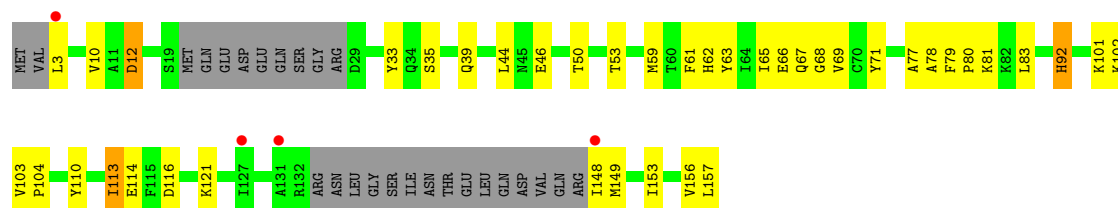


• Molecule 2: Protein transport protein Sec24A





• 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, α , β , γ	147.79Å 96.39Å 129.34Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	129.34 – 2.53 129.34 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.2 (129.34-2.53) 99.2 (129.34-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.218 , 0.288 0.225 , 0.287	Depositor DCC
R_{free} test set	1997 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12316	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EQD, 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	0.54	0/5594	1.12	17/7580 (0.2%)
2	B	0.57	0/5845	1.12	12/7952 (0.2%)
3	C	0.54	0/1061	1.08	3/1431 (0.2%)
All	All	0.56	0/12500	1.12	32/16963 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	CA-CB-OG1	-10.04	94.54	109.60
1	A	282	THR	CA-CB-OG1	-8.09	97.47	109.60
1	A	497	THR	CA-CB-OG1	-7.83	97.85	109.60
2	B	1047	PRO	N-CA-CB	-7.61	95.25	103.25
1	A	43	THR	CA-CB-OG1	-7.55	98.28	109.60
1	A	168	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	570	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	746	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	192	THR	CA-CB-OG1	-6.84	99.33	109.60
2	B	772	ASP	CB-CA-C	6.70	122.17	111.66
2	B	857	THR	CA-CB-OG1	-6.66	99.61	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	PRO	N-CA-C	-6.58	98.92	112.47
1	A	250	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	454	THR	CA-CB-OG1	-6.33	100.10	109.60
2	B	629	PRO	N-CA-C	6.31	121.74	113.86
1	A	747	VAL	N-CA-CB	6.09	117.53	110.65
3	C	12	ASP	CA-CB-CG	5.74	118.34	112.60
2	B	954	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	353	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	416	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	638	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	32	THR	CA-CB-OG1	-5.32	101.63	109.60
2	B	707	ARG	N-CA-CB	5.31	117.71	110.01
3	C	102	LYS	CA-C-N	5.30	123.58	120.24
3	C	102	LYS	C-N-CA	5.30	123.58	120.24
1	A	194	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	1065	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	143	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	921	ASP	CB-CA-C	5.20	119.42	110.79
2	B	1060	PRO	N-CA-CB	-5.10	97.89	103.25
2	B	1057	ASP	CA-CB-CG	5.07	117.67	112.60
2	B	1048	PHE	N-CA-CB	5.04	117.66	110.06

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	ASP	Peptide
2	B	633	ARG	Sidechain
2	B	897	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5467	0	5405	116	0
2	B	5721	0	5729	131	0
3	C	1042	0	1039	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	22	0	0	1	0
6	A	26	0	0	3	0
6	B	32	0	0	1	0
6	C	4	0	0	1	0
All	All	12316	0	12173	269	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 11.

All (269) 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:195:LEU:HD13	1:A:203:MET:HE1	1.59	0.84
1:A:528:ARG:HA	1:A:608:MET:HE1	1.66	0.77
1:A:137:THR:OG1	1:A:169:PHE:O	2.03	0.76
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.67	0.76
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.68	0.76
1:A:153:MET:HE2	1:A:157:LEU:HD11	1.69	0.74
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.69	0.73
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.72	0.71
2:B:1054:VAL:O	2:B:1056:ARG:N	2.23	0.71
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.75	0.68
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.74	0.68
1:A:600:SER:O	1:A:604:ARG:HG3	1.93	0.68
2:B:909:GLN:HG2	2:B:910:LYS:N	2.07	0.67
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.75	0.67
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.76	0.67
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.30	0.66
1:A:131:PHE:CE1	1:A:158:LEU:HD22	2.30	0.66
1:A:410:THR:HB	1:A:414:ILE:HB	1.77	0.66
1:A:127:MET:HE1	1:A:225:PRO:HG3	1.78	0.66
2:B:463:GLU:O	2:B:465:PHE:N	2.30	0.65
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.78	0.65
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.79	0.63
2:B:409:LEU:C	2:B:410:LEU:HD12	2.23	0.63
2:B:949:VAL:HA	2:B:952:LEU:HD21	1.79	0.63
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.80	0.63
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.33	0.63
2:B:592:LYS:O	2:B:596:GLN:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:ASP:C	2:B:448:ARG:H	2.05	0.63
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.81	0.62
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.51	0.62
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.81	0.62
2:B:620:LEU:HD22	2:B:634:MET:CE	2.29	0.62
1:A:456:THR:O	1:A:528:ARG:NH2	2.33	0.62
1:A:651:ASP:OD1	1:A:652:THR:O	2.17	0.62
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.25	0.61
2:B:411:LEU:N	2:B:411:LEU:HD23	2.16	0.61
1:A:101:ILE:HD11	1:A:106:GLN:HA	1.83	0.61
2:B:429:VAL:HG21	2:B:465:PHE:CE1	2.35	0.60
2:B:936:VAL:O	2:B:940:LEU:HD23	2.02	0.60
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.84	0.60
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.32	0.59
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.84	0.59
2:B:412:HIS:CE1	2:B:415:LYS:HB2	2.38	0.59
1:A:537:GLU:N	1:A:537:GLU:OE1	2.36	0.59
3:C:66:GLU:HG3	3:C:92:HIS:CD2	2.38	0.59
3:C:113:ILE:O	3:C:116:ASP:HB2	2.03	0.59
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.33	0.58
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.34	0.58
1:A:76:VAL:HG11	1:A:78:TYR:CE1	2.39	0.58
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.25	0.58
1:A:696:LEU:O	1:A:697:HIS:ND1	2.36	0.58
1:A:153:MET:CE	1:A:157:LEU:HD11	2.33	0.57
1:A:332:GLU:O	1:A:336:ASN:ND2	2.32	0.57
2:B:909:GLN:HG2	2:B:910:LYS:H	1.66	0.57
1:A:560:TYR:CD2	1:A:761:VAL:HG12	2.40	0.57
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.85	0.57
2:B:716:TYR:OH	2:B:734:GLU:OE1	2.18	0.56
2:B:381:CYS:HB2	2:B:822:THR:O	2.06	0.56
2:B:500:PRO:O	2:B:501:PRO:C	2.48	0.56
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.87	0.56
2:B:957:ALA:C	2:B:959:ASN:H	2.11	0.56
1:A:749:LEU:O	1:A:750:GLN:C	2.46	0.56
2:B:425:SER:HB3	2:B:427:THR:O	2.06	0.56
2:B:1055:ILE:O	2:B:1057:ASP:N	2.39	0.55
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.37	0.55
1:A:692:ALA:O	1:A:696:LEU:HB2	2.06	0.55
2:B:655:PRO:HD3	2:B:920:LEU:HD13	1.89	0.55
2:B:1055:ILE:HG21	2:B:1062:LYS:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.37	0.54
2:B:684:GLN:OE1	2:B:746:GLU:HA	2.07	0.54
3:C:113:ILE:HD13	3:C:113:ILE:H	1.72	0.53
3:C:69:VAL:CG2	3:C:103:VAL:HG11	2.38	0.53
1:A:426:LEU:O	1:A:427:ASN:C	2.51	0.53
2:B:750:ARG:HG2	2:B:752:ARG:CZ	2.39	0.53
1:A:422:PRO:O	1:A:448:ILE:HG23	2.08	0.53
2:B:350:VAL:HG12	2:B:891:MET:HE3	1.90	0.53
1:A:108:ALA:HB1	1:A:114:PHE:CD2	2.44	0.53
1:A:76:VAL:HG12	1:A:77:ASP:N	2.24	0.53
1:A:379:THR:O	1:A:383:LYS:HG3	2.09	0.52
2:B:959:ASN:O	2:B:961:SER:N	2.43	0.52
2:B:991:VAL:HG12	2:B:1051:ILE:HD13	1.92	0.52
1:A:194:ASP:O	1:A:195:LEU:HD23	2.09	0.52
2:B:385:LEU:HD21	2:B:417:LEU:HD21	1.92	0.52
2:B:654:GLU:OE2	2:B:696:TYR:HB2	2.08	0.52
3:C:35:SER:O	3:C:39:GLN:HG2	2.10	0.52
2:B:831:LEU:HD22	2:B:835:PHE:CE2	2.43	0.52
2:B:580:MET:HE3	2:B:583:ASN:HB2	1.91	0.52
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.50	0.52
2:B:766:PHE:HB3	2:B:776:LEU:CD2	2.40	0.52
2:B:954:ASP:C	2:B:955:GLU:OE2	2.52	0.52
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.10	0.51
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.75	0.51
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.93	0.51
2:B:359:MET:SD	2:B:359:MET:N	2.83	0.51
1:A:682:ARG:NH1	6:A:902:HOH:O	2.41	0.51
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.91	0.51
1:A:191:GLY:HA3	1:A:263:SER:OG	2.10	0.51
1:A:259:ARG:NH2	1:A:308:THR:O	2.40	0.50
2:B:441:PHE:O	2:B:453:ASN:HB3	2.11	0.50
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.46	0.50
1:A:121:VAL:HG11	6:A:923:HOH:O	2.11	0.50
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.12	0.50
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.47	0.50
2:B:497:MET:HE2	2:B:816:ARG:HG3	1.93	0.50
1:A:76:VAL:HG12	1:A:77:ASP:H	1.76	0.50
1:A:5:LEU:O	1:A:6:GLU:C	2.53	0.49
2:B:578:ILE:HD11	2:B:626:LEU:CA	2.42	0.49
2:B:991:VAL:HG12	2:B:1051:ILE:CD1	2.42	0.49
1:A:180:CYS:O	1:A:181:GLU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:HD12	1:A:649:LEU:C	2.36	0.49
2:B:438:ILE:O	2:B:438:ILE:HG23	2.11	0.49
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.12	0.49
1:A:700:PHE:CD1	1:A:700:PHE:C	2.90	0.49
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.94	0.49
1:A:101:ILE:CD1	1:A:106:GLN:HA	2.42	0.49
2:B:557:GLY:C	2:B:558:LEU:HG	2.36	0.49
2:B:350:VAL:CG1	2:B:891:MET:HE3	2.43	0.48
2:B:993:MET:HE2	2:B:1065:PHE:HB2	1.95	0.48
3:C:69:VAL:HG22	3:C:103:VAL:HG11	1.94	0.48
1:A:341:THR:HG22	1:A:343:HIS:CE1	2.49	0.48
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.95	0.48
2:B:753:CYS:HB3	2:B:803:PHE:HD1	1.79	0.48
2:B:1054:VAL:O	2:B:1055:ILE:C	2.57	0.48
2:B:359:MET:HE2	2:B:1080:TYR:CE2	2.49	0.48
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.43	0.48
2:B:702:LEU:O	2:B:705:ILE:HG22	2.13	0.48
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.96	0.48
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.49	0.47
3:C:77:ALA:O	3:C:78:ALA:C	2.57	0.47
1:A:296:GLN:O	1:A:296:GLN:HG2	2.15	0.47
1:A:69:VAL:HB	1:A:480:GLN:NE2	2.29	0.47
2:B:749:MET:HA	2:B:806:ALA:O	2.15	0.47
2:B:766:PHE:HB3	2:B:776:LEU:HD23	1.97	0.47
1:A:185:LYS:HB2	2:B:567:MET:HB3	1.96	0.47
2:B:433:SER:OG	2:B:457:ARG:HD3	2.15	0.47
2:B:1005:LEU:CD2	2:B:1017:ILE:HD11	2.45	0.47
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.48	0.47
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.97	0.47
2:B:799:GLN:O	2:B:800:LEU:HD23	2.15	0.47
3:C:39:GLN:HB3	3:C:157:LEU:HD22	1.96	0.47
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.44	0.46
1:A:153:MET:HE1	1:A:387:GLN:HB2	1.97	0.46
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.97	0.46
2:B:1049:PHE:CD1	2:B:1049:PHE:C	2.92	0.46
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.98	0.46
2:B:437:TYR:O	2:B:438:ILE:C	2.58	0.46
2:B:609:THR:CG2	2:B:611:GLU:HB2	2.46	0.46
2:B:955:GLU:OE2	2:B:955:GLU:N	2.48	0.46
2:B:807:LEU:O	2:B:818:ILE:HA	2.15	0.46
1:A:288:MET:HG2	1:A:290:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:TRP:CA	1:A:316:ILE:HG22	2.41	0.46
1:A:240:LEU:CD2	1:A:244:LEU:HG	2.46	0.46
1:A:30:GLU:CD	1:A:510:ILE:HD11	2.41	0.46
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.46
2:B:1053:TYR:HD2	2:B:1055:ILE:HB	1.81	0.46
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.51	0.46
2:B:446:ASP:C	2:B:448:ARG:N	2.69	0.46
3:C:63:TYR:CD1	3:C:63:TYR:C	2.94	0.46
1:A:296:GLN:O	1:A:297:GLY:O	2.34	0.45
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.52	0.45
1:A:522:ALA:O	1:A:523:ALA:C	2.59	0.45
2:B:666:MET:HE1	2:B:927:MET:SD	2.56	0.45
2:B:513:SER:O	2:B:517:VAL:HG23	2.15	0.45
1:A:76:VAL:CG1	1:A:78:TYR:CE1	2.99	0.45
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.99	0.45
1:A:346:ASP:HB3	1:A:348:TYR:CE1	2.52	0.45
2:B:573:ILE:HG23	2:B:618:PRO:CG	2.43	0.45
2:B:830:THR:O	2:B:831:LEU:C	2.58	0.45
2:B:986:MET:HE1	2:B:1069:MET:HE3	1.99	0.45
2:B:926:ALA:O	6:B:1301:HOH:O	2.20	0.45
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.99	0.45
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.31	0.45
1:A:190:ARG:HG3	2:B:577:PHE:CE2	2.52	0.45
1:A:368:GLY:HA3	1:A:450:GLY:O	2.18	0.44
2:B:852:VAL:HG22	2:B:927:MET:HG2	1.99	0.44
1:A:227:ASN:HD21	1:A:278:THR:CG2	2.30	0.44
1:A:575:SER:O	1:A:578:PRO:HD2	2.17	0.44
2:B:750:ARG:NH1	2:B:771:THR:O	2.49	0.44
2:B:407:LEU:HG	2:B:789:MET:HG3	1.99	0.44
2:B:1083:PHE:CE2	2:B:1087:ILE:HD11	2.53	0.44
1:A:547:ASP:OD2	1:A:585:ARG:NH2	2.50	0.44
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.98	0.44
2:B:578:ILE:HD11	2:B:626:LEU:N	2.32	0.44
2:B:615:ALA:HB2	2:B:644:LEU:HD23	1.99	0.44
2:B:832:ASN:O	2:B:836:LEU:HG	2.18	0.44
2:B:496:TYR:HD2	2:B:818:ILE:HD11	1.82	0.44
1:A:147:LEU:HD12	1:A:147:LEU:O	2.18	0.43
1:A:451:LEU:HD12	1:A:451:LEU:N	2.33	0.43
2:B:410:LEU:HD22	2:B:935:LEU:HG	2.00	0.43
2:B:444:PHE:CD1	2:B:450:TRP:HB3	2.52	0.43
2:B:556:TYR:HA	2:B:566:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:HD11	1:A:656:ILE:HG23	2.00	0.43
2:B:555:PHE:HE1	2:B:570:VAL:HG11	1.82	0.43
1:A:70:LEU:HB3	1:A:109:GLU:HG3	2.00	0.43
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.83	0.43
1:A:238:MET:HE2	1:A:238:MET:HB3	1.89	0.43
3:C:92:HIS:ND1	3:C:92:HIS:C	2.76	0.43
3:C:103:VAL:N	3:C:104:PRO:CD	2.81	0.43
2:B:438:ILE:HD12	2:B:442:VAL:HG11	2.01	0.43
2:B:965:ILE:N	2:B:965:ILE:HD12	2.34	0.43
2:B:1061:MET:C	2:B:1062:LYS:HG3	2.44	0.43
1:A:384:GLN:O	1:A:385:THR:C	2.62	0.43
2:B:909:GLN:OE1	2:B:911:SER:HB2	2.17	0.43
2:B:1054:VAL:C	2:B:1056:ARG:N	2.76	0.43
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.99	0.43
1:A:238:MET:O	1:A:241:THR:HG22	2.18	0.43
3:C:103:VAL:N	3:C:104:PRO:HD2	2.34	0.43
1:A:49:PRO:O	1:A:50:ASP:CB	2.67	0.43
1:A:127:MET:HE2	1:A:127:MET:HA	2.01	0.43
1:A:297:GLY:H	1:A:300:MET:HG3	1.84	0.43
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.18	0.43
3:C:10:VAL:HG23	3:C:68:GLY:C	2.44	0.43
1:A:148:LYS:HG2	1:A:244:LEU:O	2.18	0.42
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.55	0.42
1:A:290:ILE:HG21	1:A:355:THR:HG23	2.01	0.42
1:A:290:ILE:HG22	1:A:349:ALA:HA	2.00	0.42
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.54	0.42
2:B:831:LEU:HD22	2:B:835:PHE:HE2	1.83	0.42
2:B:1003:ASN:HD21	2:B:1031:GLU:HG2	1.84	0.42
3:C:148:ILE:HG22	3:C:149:MET:N	2.33	0.42
1:A:507:GLN:C	1:A:509:GLN:N	2.78	0.42
1:A:54:ILE:HG13	1:A:117:ILE:HD11	2.01	0.42
2:B:627:MET:O	2:B:628:SER:C	2.62	0.42
2:B:957:ALA:C	2:B:959:ASN:N	2.77	0.42
1:A:593:PHE:O	1:A:594:ASN:HB2	2.19	0.42
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.01	0.42
1:A:269:SER:HB3	1:A:334:LEU:HD21	2.00	0.42
2:B:605:MET:HB2	2:B:606:PHE:CE2	2.54	0.42
3:C:61:PHE:CD2	3:C:153:ILE:HD12	2.54	0.42
1:A:612:LEU:O	1:A:613:THR:C	2.62	0.42
2:B:420:LEU:HD21	2:B:489:GLU:HB2	2.01	0.42
2:B:986:MET:CE	2:B:1069:MET:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:ASN:O	2:B:1007:GLN:HB2	2.20	0.42
3:C:79:PHE:HA	3:C:80:PRO:HD3	1.92	0.42
1:A:101:ILE:HD13	1:A:101:ILE:HA	1.62	0.42
2:B:348:LEU:HG	2:B:348:LEU:O	2.19	0.42
1:A:524:ILE:HG13	1:A:615:SER:HB3	2.01	0.41
1:A:610:GLN:HG3	1:A:618:MET:HE1	2.02	0.41
2:B:357:ARG:C	2:B:359:MET:HE3	2.44	0.41
2:B:666:MET:HE2	2:B:927:MET:HE1	2.02	0.41
2:B:719:TYR:CE2	2:B:731:LEU:HD23	2.54	0.41
2:B:992:LEU:O	2:B:1052:LEU:HA	2.20	0.41
1:A:311:ARG:NE	1:A:359:GLU:OE2	2.35	0.41
2:B:437:TYR:OH	5:B:1201:A1EQD:N20	2.52	0.41
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.55	0.41
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.01	0.41
1:A:51:LEU:HD22	1:A:51:LEU:HA	1.96	0.41
1:A:153:MET:HE1	1:A:387:GLN:CB	2.50	0.41
1:A:438:ILE:HG21	1:A:529:LEU:HD21	2.02	0.41
1:A:69:VAL:HG11	1:A:496:VAL:HG21	2.03	0.41
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.55	0.41
1:A:687:ALA:N	1:A:688:PRO:HD2	2.35	0.41
2:B:1084:LEU:HD23	2:B:1084:LEU:HA	1.88	0.41
1:A:236:ILE:HD12	1:A:236:ILE:HA	1.96	0.41
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.88	0.41
3:C:71:TYR:CE2	3:C:92:HIS:HA	2.56	0.41
1:A:541:ASP:CG	6:A:903:HOH:O	2.63	0.41
2:B:780:ASN:HB2	2:B:781:PRO:HD2	2.03	0.41
2:B:804:GLN:HA	2:B:821:HIS:O	2.21	0.41
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.51	0.41
3:C:114:GLU:HB2	6:C:204:HOH:O	2.21	0.41
1:A:517:PHE:CE2	1:A:519:GLN:HA	2.56	0.40
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.56	0.40
2:B:359:MET:HE2	2:B:1080:TYR:OH	2.21	0.40
2:B:771:THR:O	2:B:772:ASP:C	2.63	0.40
2:B:720:HIS:HB3	2:B:723:HIS:HB2	2.04	0.40
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.56	0.40
1:A:297:GLY:H	1:A:300:MET:CG	2.34	0.40
2:B:692:LEU:HD12	2:B:692:LEU:N	2.36	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%)	617 (91%)	58 (8%)	6 (1%)	14	26
2	B	721/748 (96%)	660 (92%)	52 (7%)	9 (1%)	10	19
3	C	125/157 (80%)	112 (90%)	13 (10%)	0	100	100
All	All	1527/1670 (91%)	1389 (91%)	123 (8%)	15 (1%)	12	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	464	GLU
2	B	1055	ILE
2	B	1056	ARG
1	A	297	GLY
1	A	324	VAL
2	B	447	GLN
1	A	637	LEU
2	B	438	ILE
2	B	381	CYS
2	B	961	SER
1	A	50	ASP
2	B	357	ARG
1	A	511	GLN
2	B	1047	PRO
1	A	363	CYS

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	600/666 (90%)	565 (94%)	35 (6%)	18	36
2	B	652/679 (96%)	606 (93%)	46 (7%)	13	27
3	C	112/138 (81%)	101 (90%)	11 (10%)	7	15
All	All	1364/1483 (92%)	1272 (93%)	92 (7%)	15	29

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	51	LEU
1	A	65	THR
1	A	101	ILE
1	A	116	SER
1	A	161	THR
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	290	ILE
1	A	316	ILE
1	A	355	THR
1	A	376	SER
1	A	440	THR
1	A	451	LEU
1	A	488	SER
1	A	498	THR
1	A	508	THR
1	A	511	GLN
1	A	524	ILE
1	A	528	ARG
1	A	544	ARG
1	A	562	LYS
1	A	570	PHE
1	A	612	LEU
1	A	613	THR
1	A	639	SER
1	A	649	LEU
1	A	652	THR
1	A	696	LEU
1	A	698	SER
1	A	746	ASP

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Mol	Chain	Res	Type
1	A	747	VAL
2	B	356	GLU
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	423	VAL
2	B	483	VAL
2	B	522	LEU
2	B	554	HIS
2	B	570	VAL
2	B	578	ILE
2	B	614	SER
2	B	635	SER
2	B	641	LEU
2	B	643	THR
2	B	650	LYS
2	B	692	LEU
2	B	712	SER
2	B	713	VAL
2	B	751	ILE
2	B	754	THR
2	B	761	THR
2	B	771	THR
2	B	779	VAL
2	B	787	VAL
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	807	LEU
2	B	813	LYS
2	B	822	THR
2	B	829	SER
2	B	857	THR
2	B	880	SER
2	B	881	SER
2	B	906	LEU
2	B	914	THR
2	B	935	LEU
2	B	955	GLU
2	B	979	SER
2	B	1002	GLN
2	B	1047	PRO

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Mol	Chain	Res	Type
2	B	1051	ILE
2	B	1060	PRO
2	B	1064	ASN
2	B	1085	LEU
2	B	1092	ASN
3	C	3	LEU
3	C	12	ASP
3	C	46	GLU
3	C	50	THR
3	C	67	GLN
3	C	81	LYS
3	C	92	HIS
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	145	GLN
1	A	227	ASN
1	A	231	GLN
1	A	239	ASN
1	A	296	GLN
1	A	549	GLN
1	A	591	GLN
1	A	620	GLN
2	B	395	GLN
2	B	527	GLN
2	B	532	ASN
2	B	683	GLN
2	B	788	GLN
2	B	917	ASN
2	B	932	ASN
3	C	36	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	A1EQD	B	1201	-	22,24,24	0.95	1 (4%)	27,35,35	2.44	9 (33%)

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	A1EQD	B	1201	-	-	11/20/41/41	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1201	A1EQD	O01-C02	2.32	1.29	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	A1EQD	C15-C03-C02	7.63	139.43	117.33
5	B	1201	A1EQD	C09-C08-C07	-5.45	108.85	116.41
5	B	1201	A1EQD	C07-C03-C02	-4.20	103.41	118.58
5	B	1201	A1EQD	C15-C03-C04	-3.26	107.89	117.33
5	B	1201	A1EQD	C08-C09-C10	-2.70	105.43	111.71
5	B	1201	A1EQD	C03-C15-C16	2.58	126.41	121.65
5	B	1201	A1EQD	C17-C16-C15	-2.24	115.98	120.99
5	B	1201	A1EQD	C07-C03-C04	-2.20	110.64	118.58
5	B	1201	A1EQD	C08-C07-C15	-2.13	117.65	122.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1201	A1EQD	O01-C02-C03-C15
5	B	1201	A1EQD	O22-C02-C03-C04
5	B	1201	A1EQD	C15-C03-C04-O05
5	B	1201	A1EQD	C15-C03-C04-O06
5	B	1201	A1EQD	C02-C03-C04-O05
5	B	1201	A1EQD	C03-C15-C16-C21
5	B	1201	A1EQD	C03-C15-C16-C17
5	B	1201	A1EQD	C07-C15-C16-C21
5	B	1201	A1EQD	C07-C08-C09-C14
5	B	1201	A1EQD	O22-C02-C03-C15
5	B	1201	A1EQD	C07-C15-C16-C17

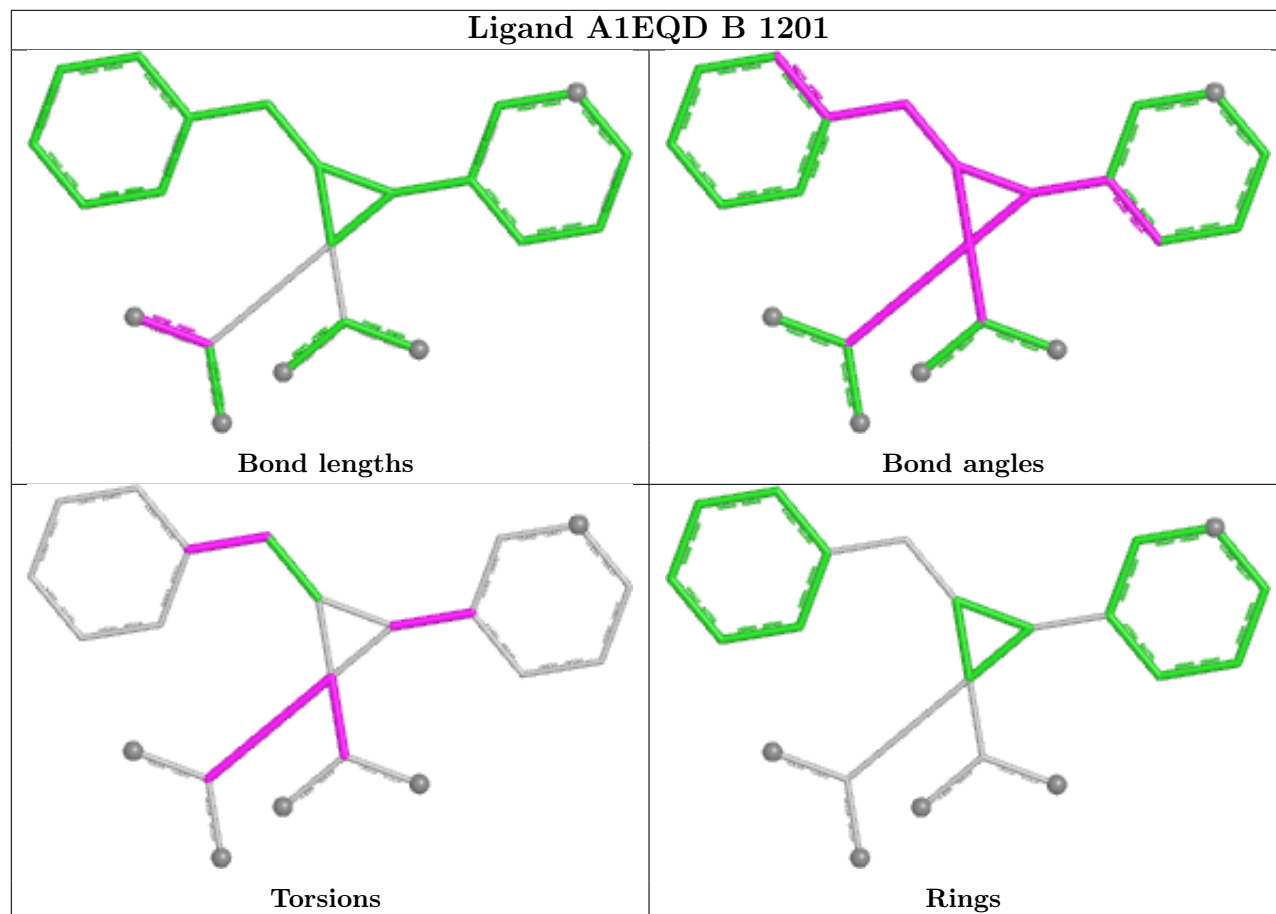
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	A1EQD	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

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%)	0.14	10 (1%) 73 71	51, 81, 125, 168	0
2	B	729/748 (97%)	-0.03	14 (1%) 66 63	46, 69, 115, 169	0
3	C	131/157 (83%)	0.40	4 (3%) 51 48	59, 101, 144, 171	0
All	All	1553/1670 (92%)	0.08	28 (1%) 67 64	46, 77, 126, 171	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	ALA	4.0
3	C	127	ILE	3.9
2	B	1055	ILE	3.1
1	A	700	PHE	2.9
1	A	510	ILE	2.9
1	A	94	PHE	2.9
3	C	148	ILE	2.9
2	B	888	PRO	2.9
3	C	3	LEU	2.8
2	B	490	PHE	2.7
2	B	445	LEU	2.7
2	B	423	VAL	2.5
2	B	882	VAL	2.4
2	B	1061	MET	2.4
2	B	357	ARG	2.3
2	B	424	THR	2.3
1	A	761	VAL	2.3
2	B	1022	THR	2.2
2	B	348	LEU	2.2
1	A	464	VAL	2.2
2	B	958	LEU	2.2
2	B	959	ASN	2.2
1	A	568	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	LEU	2.1
2	B	1063	ALA	2.1
3	C	131	ALA	2.1
1	A	124	GLY	2.0
1	A	205	GLY	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](#)

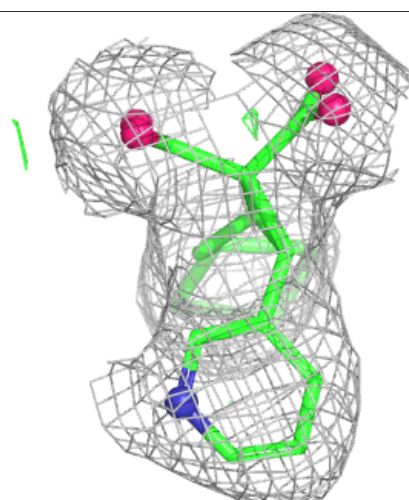
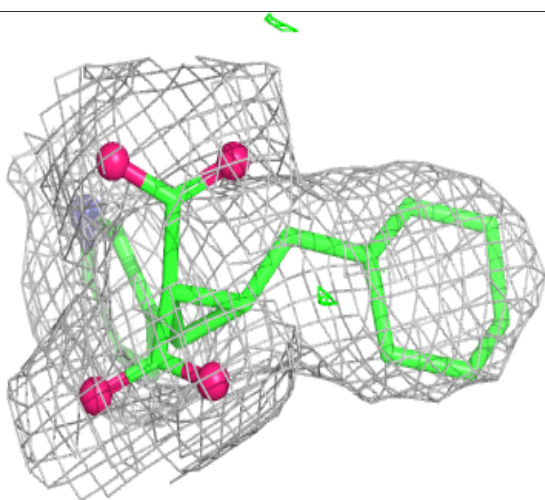
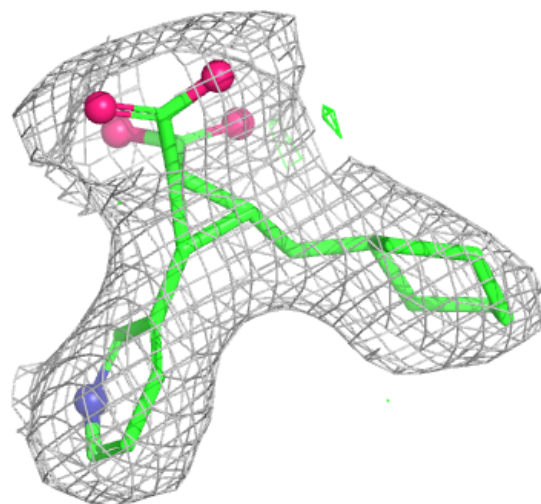
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	A1EQD	B	1201	22/22	0.92	0.09	53,72,89,92	0
4	ZN	B	1202	1/1	0.99	0.02	76,76,76,76	0
4	ZN	A	800	1/1	1.00	0.02	96,96,96,96	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 A1EQD B 1201:

$2mF_o-DF_c$ (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.