



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 AM UTC

PDB ID : 8U15 / pdb_00008u15
Title : The ternary complex structure of DDB1-CRBN-SALL4(ZF1,2)-short bound to CC-220
Authors : Clifton, M.C.; Ma, X.; Ornelas, E.
Deposited on : 2023-08-30
Resolution : 2.95 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

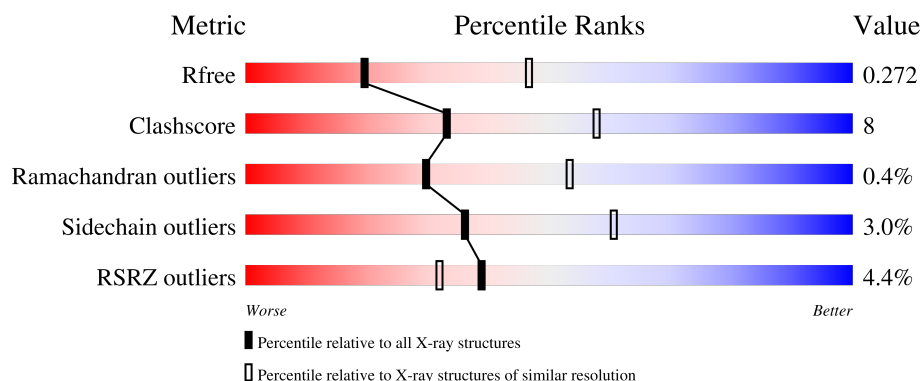
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

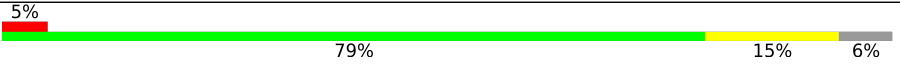
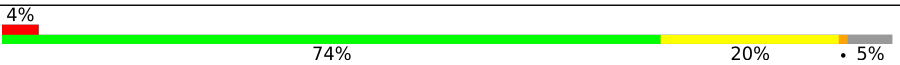
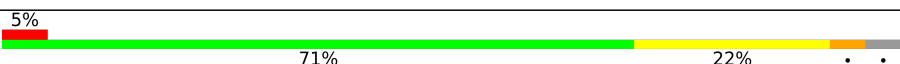
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	373	
1	D	373	
2	B	836	
2	E	836	
3	C	55	

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Mol	Chain	Length	Quality of chain
3	F	55	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	505	-	-	X	-
6	SO4	D	504	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18548 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 cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2752	1768	468	494	22			
1	D	350	Total	C	N	O	S	0	0	0
			2711	1740	453	497	21			

- Molecule 2 is a protein called DDB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	792	Total	C	N	O	S	0	0	0
			6007	3829	1000	1146	32			
2	E	798	Total	C	N	O	S	0	0	0
			6091	3877	1015	1167	32			

- Molecule 3 is a protein called Sal-like protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	53	Total	C	N	O	S	0	0	0
			420	265	83	68	4			
3	F	53	Total	C	N	O	S	0	0	0
			422	264	86	68	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	378	SER	-	expression tag	UNP Q9UJQ4
F	378	SER	-	expression tag	UNP Q9UJQ4

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

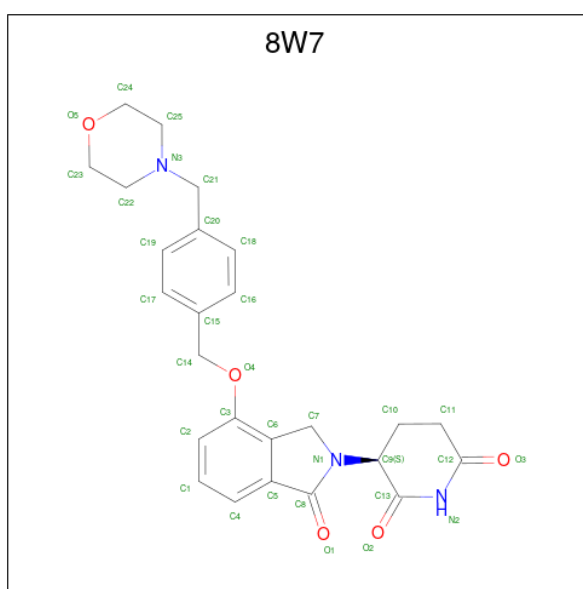
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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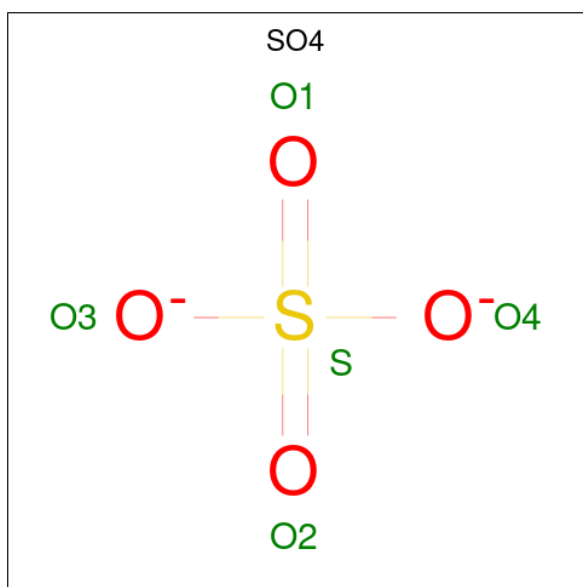
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Zn	0	0
			2	2		
4	D	1	Total	Zn	0	0
			1	1		
4	F	2	Total	Zn	0	0
			2	2		

- Molecule 5 is (3S)-3-[4-({4-[(morpholin-4-yl)methyl]phenyl}methoxy)-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: 8W7) (formula: C₂₅H₂₇N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			33	25	3	5		
5	D	1	Total	C	N	O	0	0
			33	25	3	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

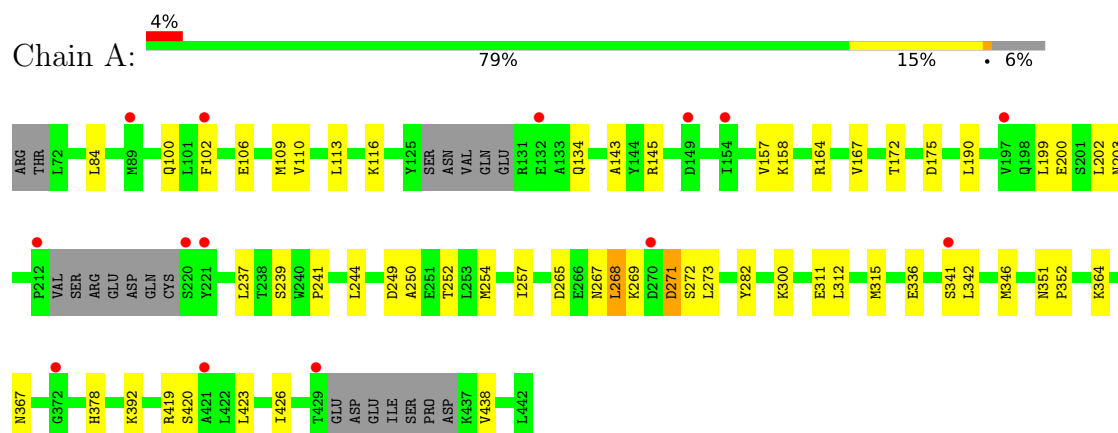
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total 4	O 4	0	0
7	B	4	Total 4	O 4	0	0
7	C	1	Total 1	O 1	0	0
7	D	2	Total 2	O 2	0	0
7	E	1	Total 1	O 1	0	0
7	F	1	Total 1	O 1	0	0

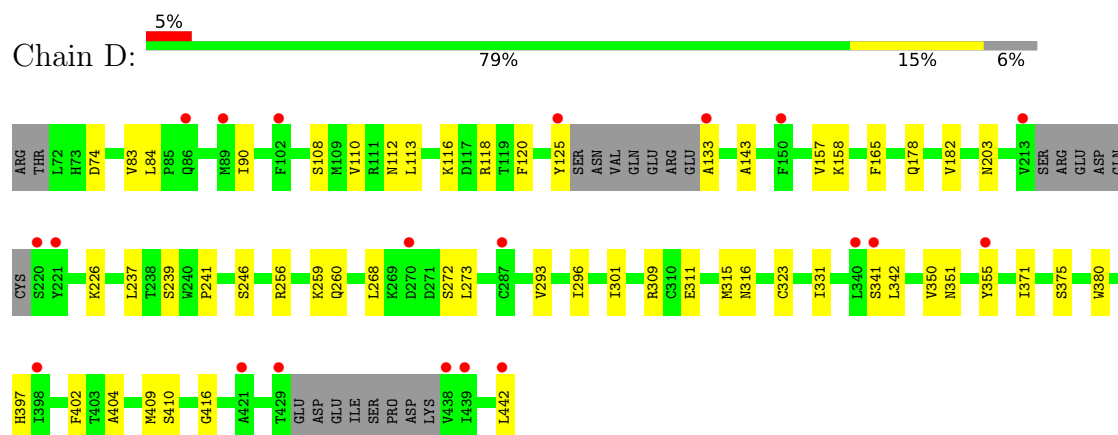
3 Residue-property plots [i](#)

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

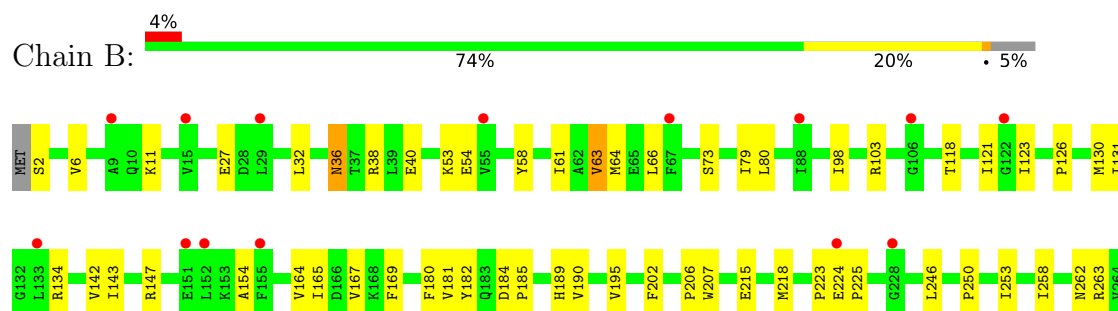
• Molecule 1: Protein cereblon

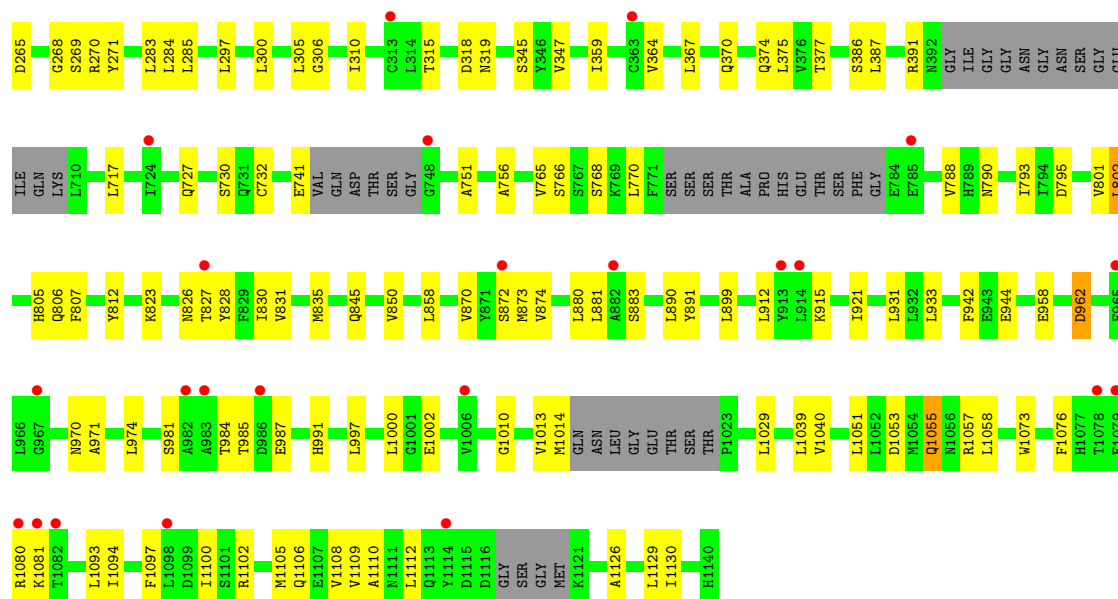


• Molecule 1: Protein cereblon

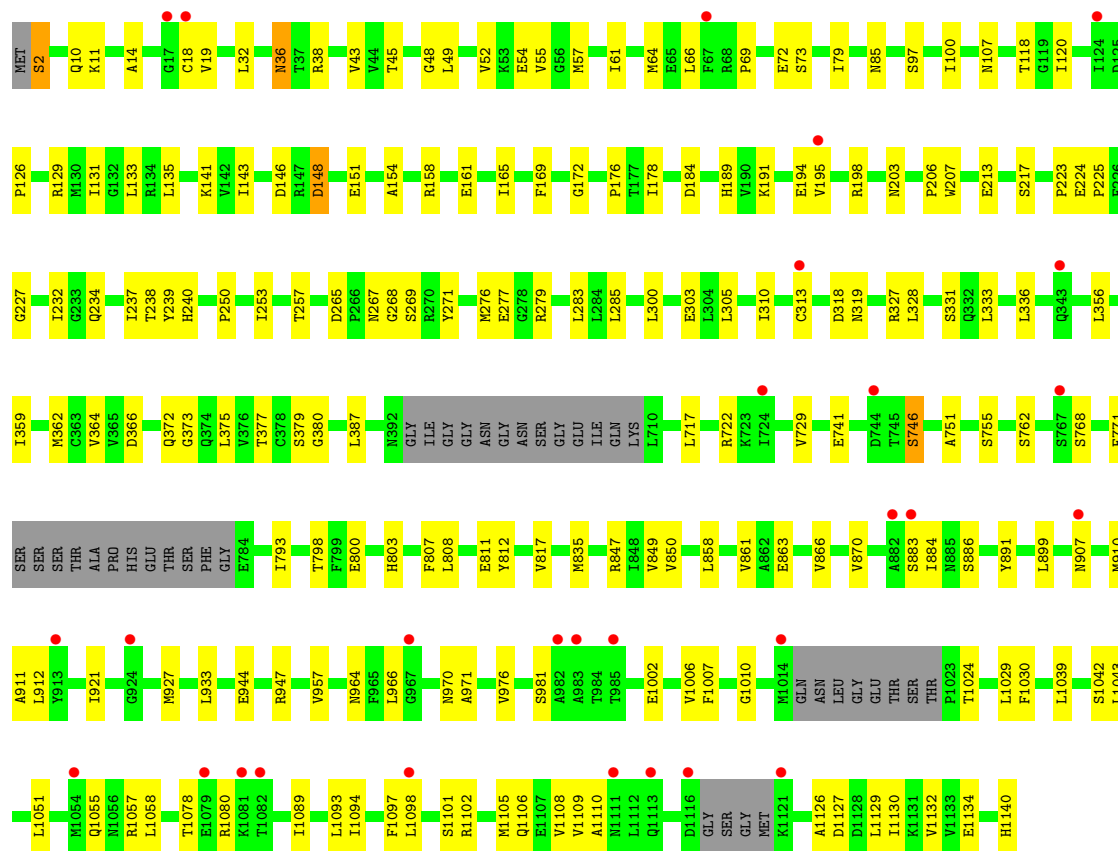
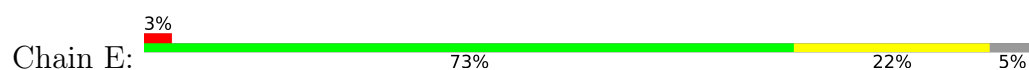


• Molecule 2: DDB1





• Molecule 2: DDB1



• Molecule 3: Sal-like protein 4





● Molecule 3: Sal-like protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.73Å 95.73Å 150.95Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	61.48 – 2.95 61.48 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.48-2.95) 100.0 (61.48-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.94	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.220 , 0.272 0.220 , 0.272	Depositor DCC
R_{free} test set	3235 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18548	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 4.56% 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: 8W7, ZN, SO4

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	0.10	0/2817	0.27	0/3831
1	D	0.09	0/2776	0.26	0/3788
2	B	0.10	0/6117	0.29	0/8311
2	E	0.10	0/6202	0.30	0/8420
3	C	0.10	0/433	0.29	0/579
3	F	0.11	0/434	0.35	0/579
All	All	0.10	0/18779	0.29	0/25508

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2752	0	2679	31	0
1	D	2711	0	2592	32	0
2	B	6007	0	5755	100	0
2	E	6091	0	5875	112	0
3	C	420	0	393	10	0
3	F	422	0	398	10	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
5	A	33	0	0	0	0
5	D	33	0	0	0	0
6	A	15	0	0	3	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	10	0	0	2	0
6	E	15	0	0	0	0
6	F	5	0	0	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	1	0	0	1	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
All	All	18548	0	17692	284	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 8.

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:987:GLU:HG3	2:B:991:HIS:HE1	1.36	0.88
2:B:118:THR:OG1	2:B:134:ARG:NH2	2.11	0.82
2:B:891:TYR:HB3	2:B:899:LEU:HD22	1.69	0.74
2:E:57:MET:HE1	2:E:79:ILE:HG21	1.71	0.73
2:E:250:PRO:HG2	2:E:253:ILE:HG12	1.71	0.72
1:A:267:ASN:O	1:A:269:LYS:N	2.21	0.72
2:E:55:VAL:HG11	2:E:100:ILE:HG13	1.72	0.71
1:D:110:VAL:HG11	1:D:157:VAL:HG21	1.73	0.70
2:B:103:ARG:HH21	2:B:147:ARG:HD2	1.56	0.70
2:B:250:PRO:HG2	2:B:253:ILE:HG12	1.72	0.70
2:B:167:VAL:HG23	2:B:180:PHE:HB3	1.76	0.68
1:A:110:VAL:HG11	1:A:157:VAL:HG21	1.75	0.67
2:B:987:GLU:HG3	2:B:991:HIS:CE1	2.26	0.67
2:E:32:LEU:HD13	2:E:66:LEU:HD11	1.76	0.67
2:B:1057:ARG:NH1	2:B:1110:ALA:O	2.28	0.66
3:C:385:LYS:O	3:C:422:LYS:NZ	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1055:GLN:HG2	2:B:1093:LEU:HD23	1.77	0.66
2:B:270:ARG:HG2	2:B:284:LEU:HD23	1.79	0.64
6:A:504:SO4:O3	3:C:432:HIS:ND1	2.32	0.63
2:B:63:VAL:HG13	2:B:80:LEU:HB3	1.81	0.63
2:E:213:GLU:OE2	2:E:234:GLN:N	2.32	0.62
1:D:143:ALA:HB3	1:D:158:LYS:HB2	1.81	0.62
1:A:199:LEU:HB2	1:A:202:LEU:HD12	1.80	0.62
2:B:1100:ILE:HG13	2:B:1105:MET:HG2	1.82	0.62
1:D:83:VAL:HB	1:D:178:GLN:HG3	1.81	0.62
6:D:504:SO4:O2	3:F:432:HIS:ND1	2.32	0.62
2:E:49:LEU:HD12	2:E:333:LEU:HD11	1.82	0.61
2:E:910:MET:HG2	2:E:912:LEU:HD23	1.81	0.61
2:E:798:THR:OG1	2:E:800:GLU:HG2	2.00	0.61
2:B:195:VAL:HG22	2:B:202:PHE:HE2	1.64	0.61
2:B:915:LYS:HD2	2:B:958:GLU:HA	1.82	0.61
1:A:346:MET:HE1	1:A:419:ARG:HG3	1.82	0.61
2:B:40:GLU:HG3	2:B:54:GLU:HG3	1.82	0.60
1:A:351:ASN:ND2	3:C:413:SER:O	2.32	0.60
2:B:11:LYS:HE2	2:B:38:ARG:HD2	1.84	0.59
2:B:1058:LEU:HD11	2:B:1097:PHE:HB2	1.84	0.59
2:E:771:PHE:HE2	2:E:847:ARG:HG3	1.68	0.59
1:A:367:ASN:HA	1:A:392:LYS:HD2	1.84	0.59
1:A:271:ASP:O	1:A:273:LEU:N	2.35	0.59
2:E:359:ILE:HG21	2:E:362:MET:HE3	1.85	0.59
2:E:148:ASP:OD1	2:E:148:ASP:N	2.36	0.59
2:B:1080:ARG:HD3	2:B:1081:LYS:HB2	1.84	0.58
2:E:1102:ARG:HA	2:E:1105:MET:HB2	1.85	0.58
1:A:145:ARG:NH2	6:A:505:SO4:S	2.71	0.58
1:A:244:LEU:HD11	2:B:912:LEU:HD11	1.85	0.58
2:B:1106:GLN:HA	2:B:1109:VAL:HG22	1.86	0.57
3:C:410:PHE:HB3	3:C:425:LEU:HD22	1.86	0.57
1:D:351:ASN:ND2	3:F:413:SER:O	2.34	0.57
2:E:184:ASP:OD1	2:E:189:HIS:NE2	2.36	0.57
2:E:1078:THR:HG23	2:E:1080:ARG:H	1.70	0.57
3:C:393:THR:OG1	3:C:396:SER:OG	2.21	0.56
1:D:309:ARG:HH22	2:E:910:MET:HE3	1.70	0.56
2:E:176:PRO:HB2	2:E:195:VAL:HG12	1.86	0.56
2:E:372:GLN:NE2	2:E:373:GLY:H	2.03	0.56
2:E:768:SER:HB3	2:E:808:LEU:HD21	1.87	0.56
1:A:164:ARG:NE	1:A:282:TYR:OH	2.38	0.56
2:B:118:THR:HG21	2:B:165:ILE:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:966:LEU:HD12	2:E:976:VAL:HG22	1.88	0.55
2:B:997:LEU:HG	2:B:1076:PHE:CD2	2.42	0.55
2:B:181:VAL:HG22	2:B:190:VAL:HG22	1.87	0.55
2:E:372:GLN:HE21	2:E:373:GLY:H	1.54	0.55
2:E:1098:LEU:HD21	2:E:1134:GLU:HG2	1.89	0.55
2:E:1051:LEU:HB2	2:E:1089:ILE:HD13	1.89	0.55
2:E:118:THR:HG21	2:E:165:ILE:HA	1.88	0.54
2:E:741:GLU:HG2	2:E:751:ALA:HA	1.87	0.54
2:E:1106:GLN:HA	2:E:1109:VAL:HG22	1.87	0.54
1:A:352:PRO:HG3	1:A:378:HIS:CG	2.42	0.54
2:E:238:THR:HG1	2:E:240:HIS:HE2	1.53	0.54
2:E:1129:LEU:HA	2:E:1132:VAL:HG12	1.87	0.54
2:B:765:VAL:HG22	2:B:806:GLN:HB3	1.89	0.54
2:E:366:ASP:HA	2:E:372:GLN:HE22	1.72	0.54
2:B:131:ILE:HB	2:B:143:ILE:HB	1.90	0.54
2:E:318:ASP:OD1	2:E:319:ASN:N	2.41	0.54
3:C:393:THR:HG1	3:C:396:SER:HG	1.53	0.53
2:E:285:LEU:HD22	2:E:300:LEU:HD22	1.89	0.53
2:B:387:LEU:HG	2:B:717:LEU:HD11	1.90	0.53
2:B:223:PRO:HD2	2:B:268:GLY:HA3	1.90	0.53
2:E:129:ARG:HH12	2:E:198:ARG:NH1	2.06	0.53
1:D:113:LEU:HB3	1:D:118:ARG:HA	1.91	0.53
2:B:126:PRO:HD3	2:B:169:PHE:HB3	1.91	0.53
2:B:732:CYS:SG	2:B:793:ILE:HG22	2.49	0.52
2:B:285:LEU:HD22	2:B:300:LEU:HD22	1.91	0.52
2:E:36:ASN:ND2	2:E:1002:GLU:OE2	2.42	0.52
2:B:147:ARG:HA	2:B:147:ARG:NE	2.24	0.52
2:E:1130:ILE:O	2:E:1134:GLU:HG3	2.10	0.52
3:C:388:SER:O	3:C:388:SER:OG	2.19	0.52
1:D:260:GLN:NE2	1:D:316:ASN:OD1	2.34	0.52
1:D:241:PRO:HB3	2:E:812:TYR:CZ	2.45	0.52
2:B:367:LEU:HB2	2:B:374:GLN:NE2	2.25	0.51
2:E:57:MET:HE1	2:E:79:ILE:CG2	2.40	0.51
3:F:388:SER:O	3:F:388:SER:OG	2.20	0.51
2:B:61:ILE:HG23	2:B:79:ILE:HG23	1.91	0.51
2:B:870:VAL:HA	2:B:883:SER:O	2.10	0.51
2:E:223:PRO:HD2	2:E:268:GLY:HA3	1.92	0.51
2:B:984:THR:OG1	2:B:985:THR:N	2.43	0.51
2:E:129:ARG:HH12	2:E:198:ARG:HH12	1.57	0.51
2:B:118:THR:HG1	2:B:134:ARG:HH22	1.50	0.51
2:B:1102:ARG:HA	2:B:1105:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:795:ASP:HB2	2:B:802:LEU:HD21	1.92	0.50
1:D:397:HIS:ND1	6:D:504:SO4:O1	2.32	0.50
2:E:305:LEU:HD22	2:E:336:LEU:HD22	1.93	0.50
2:B:218:MET:HE1	2:B:258:ILE:HG22	1.93	0.50
2:B:36:ASN:ND2	2:B:1002:GLU:OE2	2.41	0.50
2:B:265:ASP:OD1	2:B:269:SER:N	2.41	0.50
2:B:766:SER:HB2	2:B:805:HIS:CE1	2.46	0.50
2:E:61:ILE:HG23	2:E:79:ILE:HG23	1.94	0.50
3:F:421:THR:HG23	3:F:424:ASN:H	1.75	0.50
2:B:206:PRO:HB2	2:B:207:TRP:HD1	1.76	0.50
2:B:793:ILE:HD11	2:B:858:LEU:HD11	1.94	0.50
3:F:394:ASP:O	3:F:398:GLN:HG2	2.12	0.50
1:A:249:ASP:OD2	1:A:252:THR:OG1	2.27	0.49
1:D:108:SER:O	1:D:112:ASN:ND2	2.44	0.49
2:E:271:TYR:HB2	2:E:283:LEU:HB3	1.92	0.49
1:A:250:ALA:O	1:A:254:MET:HG3	2.12	0.49
1:D:350:VAL:O	1:D:380:TRP:NE1	2.42	0.49
2:B:727:GLN:OE1	2:B:730:SER:OG	2.29	0.49
2:E:1057:ARG:NH2	2:E:1110:ALA:O	2.46	0.49
2:B:835:MET:HB2	2:B:845:GLN:HG3	1.94	0.49
2:E:866:VAL:HG21	2:E:884:ILE:HG12	1.95	0.49
2:B:921:ILE:N	2:B:933:LEU:O	2.44	0.49
2:E:131:ILE:HB	2:E:143:ILE:HB	1.95	0.49
2:E:359:ILE:HG23	2:E:377:THR:HB	1.94	0.48
2:E:126:PRO:HD3	2:E:169:PHE:HB3	1.94	0.48
2:E:883:SER:OG	2:E:911:ALA:O	2.27	0.48
2:B:374:GLN:HG2	2:B:391:ARG:HG2	1.94	0.48
2:E:194:GLU:HB2	2:E:203:ASN:HB2	1.94	0.48
2:E:387:LEU:HG	2:E:717:LEU:HD11	1.96	0.48
2:E:1024:THR:HG22	2:E:1043:LEU:HD23	1.95	0.48
2:B:788:VAL:HG12	2:B:790:ASN:HD21	1.79	0.48
1:D:90:ILE:HD13	1:D:296:ILE:HG13	1.95	0.48
1:D:342:LEU:HD12	1:D:342:LEU:H	1.79	0.48
2:E:1039:LEU:HD12	2:E:1140:HIS:HB3	1.95	0.48
2:B:53:LYS:HE3	2:B:98:ILE:HB	1.95	0.48
3:C:418:ARG:NH2	7:C:601:HOH:O	2.46	0.48
1:D:256:ARG:HA	1:D:259:LYS:HE2	1.94	0.48
2:E:944:GLU:CD	2:E:947:ARG:HH21	2.22	0.48
2:E:57:MET:CE	2:E:79:ILE:HG21	2.42	0.48
2:E:172:GLY:HA3	2:E:224:GLU:HG3	1.95	0.48
2:E:746:SER:O	2:E:746:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:NH2	6:A:505:SO4:O4	2.46	0.48
2:E:38:ARG:HE	2:E:54:GLU:CD	2.22	0.48
3:F:395:SER:O	3:F:399:ILE:HD12	2.13	0.48
2:B:130:MET:HE3	2:B:142:VAL:HG13	1.96	0.47
2:E:232:ILE:HG12	2:E:237:ILE:HG23	1.97	0.47
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.95	0.47
2:E:227:GLY:O	2:E:239:TYR:OH	2.26	0.47
1:A:311:GLU:O	1:A:315:MET:HG3	2.14	0.47
2:B:318:ASP:OD1	2:B:319:ASN:N	2.48	0.47
2:B:359:ILE:HG23	2:B:377:THR:HB	1.97	0.47
2:B:375:LEU:HD23	2:B:375:LEU:HA	1.82	0.47
2:B:826:ASN:HB2	2:B:828:TYR:CE2	2.50	0.47
2:E:1105:MET:SD	2:E:1130:ILE:HD11	2.55	0.47
2:B:306:GLY:HA3	2:B:347:VAL:HG22	1.96	0.47
2:E:10:GLN:HG2	2:E:356:LEU:HD12	1.97	0.47
2:B:184:ASP:OD1	2:B:184:ASP:N	2.48	0.46
2:B:1109:VAL:HG11	2:B:1126:ALA:HA	1.97	0.46
2:B:962:ASP:OD1	2:B:962:ASP:N	2.46	0.46
2:E:18:CYS:N	2:E:313:CYS:SG	2.88	0.46
2:E:161:GLU:OE2	2:E:191:LYS:NZ	2.33	0.46
1:A:241:PRO:HB3	2:B:812:TYR:CZ	2.50	0.46
1:D:351:ASN:OD1	1:D:355:TYR:N	2.47	0.46
1:A:199:LEU:HB2	1:A:202:LEU:CD1	2.46	0.46
3:C:394:ASP:O	3:C:398:GLN:HG2	2.16	0.46
1:A:134:GLN:O	1:A:167:VAL:HG12	2.16	0.46
2:B:931:LEU:HD11	2:B:944:GLU:HG3	1.98	0.46
2:E:722:ARG:HD2	2:E:722:ARG:HA	1.65	0.45
2:B:206:PRO:HB2	2:B:207:TRP:CD1	2.52	0.45
1:D:74:ASP:OD1	1:D:74:ASP:N	2.48	0.45
2:E:224:GLU:N	2:E:225:PRO:HD2	2.31	0.45
3:F:410:PHE:HB3	3:F:425:LEU:HD22	1.97	0.45
2:B:766:SER:HB2	2:B:805:HIS:NE2	2.31	0.45
2:E:143:ILE:HG12	2:E:154:ALA:HB2	1.97	0.45
2:B:1105:MET:HE1	2:B:1130:ILE:HD11	1.97	0.45
2:E:43:VAL:HG13	2:E:52:VAL:HG21	1.98	0.45
1:D:125:TYR:HE1	1:D:133:ALA:HB2	1.81	0.45
2:E:375:LEU:HD22	2:E:1029:LEU:HD13	1.98	0.45
2:E:1109:VAL:HG11	2:E:1126:ALA:HA	1.98	0.45
1:D:323:CYS:HB2	1:D:331:ILE:HD11	1.97	0.45
1:D:404:ALA:HB1	1:D:409:MET:HE3	1.98	0.45
2:E:11:LYS:HD2	2:E:38:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ARG:NH2	2:E:910:MET:HE3	2.32	0.45
2:B:807:PHE:CZ	2:B:831:VAL:HG11	2.52	0.45
2:E:257:THR:HB	2:E:276:MET:HE3	1.99	0.45
2:E:1094:ILE:HD13	2:E:1094:ILE:HA	1.86	0.45
2:E:133:LEU:HD12	2:E:141:LYS:HG2	1.98	0.45
2:E:891:TYR:HB3	2:E:899:LEU:HD22	1.99	0.45
2:B:64:MET:HE2	2:B:64:MET:HB3	1.76	0.44
2:B:970:ASN:HA	2:B:971:ALA:HA	1.73	0.44
2:B:1053:ASP:O	2:B:1057:ARG:HG3	2.16	0.44
2:E:19:VAL:HG22	2:E:64:MET:HE3	1.99	0.44
2:B:386:SER:HA	2:B:717:LEU:HD12	1.99	0.44
2:E:198:ARG:HE	2:E:198:ARG:HB2	1.63	0.44
1:A:265:ASP:HB3	1:A:268:LEU:HD22	1.99	0.44
2:B:6:VAL:HG22	2:B:1040:VAL:HG22	1.99	0.44
2:B:246:LEU:HD12	2:B:297:LEU:HD23	2.00	0.44
2:E:14:ALA:HB1	2:E:327:ARG:HD2	1.99	0.44
2:B:370:GLN:O	2:B:1014:MET:HE1	2.17	0.44
3:C:394:ASP:OD1	3:C:398:GLN:NE2	2.49	0.44
1:A:106:GLU:O	1:A:110:VAL:HG23	2.17	0.44
2:B:58:TYR:HB3	2:B:1073:TRP:HB2	1.98	0.44
2:E:120:ILE:HG12	2:E:135:LEU:HD23	2.00	0.44
2:E:970:ASN:HA	2:E:971:ALA:HA	1.76	0.44
2:E:793:ILE:HD11	2:E:858:LEU:HD11	1.99	0.44
2:B:1051:LEU:HD12	2:B:1094:ILE:HD12	2.00	0.44
2:E:870:VAL:HA	2:E:883:SER:O	2.17	0.44
2:E:158:ARG:HE	2:E:158:ARG:HB2	1.71	0.43
1:D:402:PHE:HE2	1:D:416:GLY:HA3	1.83	0.43
2:B:364:VAL:HG11	2:B:1010:GLY:HA3	2.00	0.43
3:F:387:CYS:HB3	3:F:404:HIS:CE1	2.53	0.43
2:B:1000:LEU:HD23	2:B:1002:GLU:HB2	2.00	0.43
2:E:85:ASN:OD1	2:E:107:ASN:ND2	2.51	0.43
1:D:203:ASN:HB3	2:E:118:THR:O	2.18	0.43
1:A:336:GLU:OE1	1:A:364:LYS:NZ	2.42	0.43
2:B:1109:VAL:HG12	2:B:1129:LEU:HD22	2.01	0.43
2:E:206:PRO:HB2	2:E:207:TRP:CD1	2.54	0.43
1:A:200:GLU:HA	1:A:203:ASN:ND2	2.34	0.43
1:A:257:ILE:HG12	1:A:312:LEU:HD13	2.00	0.43
2:B:271:TYR:HB2	2:B:283:LEU:HB3	1.99	0.43
2:E:364:VAL:HG21	2:E:1010:GLY:HA3	2.00	0.43
2:E:277:GLU:OE1	2:E:279:ARG:NH2	2.51	0.43
3:F:404:HIS:O	3:F:409:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ASP:HB2	2:B:185:PRO:HD2	2.01	0.43
2:B:262:ASN:CG	2:B:315:THR:HA	2.43	0.43
1:D:165:PHE:HB2	1:D:182:VAL:HG13	2.01	0.43
2:B:123:ILE:HD13	2:B:167:VAL:HG13	2.01	0.42
2:B:134:ARG:NH1	2:B:164:VAL:HB	2.34	0.42
2:E:921:ILE:N	2:E:933:LEU:O	2.38	0.42
2:B:1112:LEU:HD23	2:B:1112:LEU:HA	1.82	0.42
1:D:226:LYS:HB3	1:D:226:LYS:HE3	1.70	0.42
2:E:886:SER:O	2:E:907:ASN:ND2	2.42	0.42
1:A:143:ALA:HB3	1:A:158:LYS:HB2	2.00	0.42
2:B:874:VAL:HG23	2:B:881:LEU:HB3	2.01	0.42
2:E:64:MET:HE2	2:E:64:MET:HB3	1.85	0.42
2:E:1097:PHE:CE1	2:E:1105:MET:HG2	2.54	0.42
2:E:1140:HIS:CD2	2:E:1140:HIS:H	2.38	0.42
2:B:1057:ARG:HD3	2:B:1108:VAL:O	2.20	0.42
1:A:109:MET:HE3	1:A:113:LEU:HD11	2.01	0.42
1:A:426:ILE:HG21	1:A:438:VAL:HB	2.02	0.42
2:B:768:SER:C	2:B:770:LEU:H	2.27	0.42
2:B:830:ILE:HD13	2:B:850:VAL:HG13	2.01	0.42
1:D:237:LEU:HD11	2:E:328:LEU:HD11	2.01	0.42
1:D:241:PRO:HB3	2:E:812:TYR:OH	2.19	0.42
2:E:1007:PHE:CD1	2:E:1030:PHE:HB3	2.55	0.42
1:D:296:ILE:HD12	1:D:296:ILE:H	1.85	0.42
1:A:199:LEU:HD21	1:A:237:LEU:HD21	2.02	0.42
2:B:121:ILE:HG21	2:B:167:VAL:HG12	2.01	0.42
2:B:182:TYR:CE1	2:B:189:HIS:HB2	2.55	0.42
1:D:371:ILE:HG21	3:F:417:HIS:CE1	2.55	0.42
2:E:2:SER:HB2	2:E:964:ASN:OD1	2.20	0.42
2:B:890:LEU:HB2	2:B:942:PHE:HZ	1.84	0.41
2:E:768:SER:OG	2:E:863:GLU:OE2	2.32	0.41
1:A:300:LYS:HB2	1:A:300:LYS:HE2	1.90	0.41
2:B:823:LYS:HA	2:B:823:LYS:HD3	1.88	0.41
1:D:84:LEU:HD13	1:D:120:PHE:CD2	2.55	0.41
2:E:45:THR:HG1	2:E:48:GLY:H	1.68	0.41
2:E:69:PRO:HG2	2:E:72:GLU:HG3	2.02	0.41
2:E:1102:ARG:NH2	2:E:1127:ASP:OD1	2.53	0.41
2:B:741:GLU:HG2	2:B:751:ALA:HA	2.02	0.41
2:E:807:PHE:HB3	2:E:811:GLU:OE1	2.20	0.41
1:A:100:GLN:HE21	1:A:102:PHE:HE1	1.67	0.41
1:D:311:GLU:O	1:D:315:MET:HG3	2.20	0.41
2:E:803:HIS:CD2	2:E:858:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LEU:HD13	2:B:66:LEU:HD11	2.01	0.41
2:B:263:ARG:HG3	2:B:271:TYR:CE1	2.56	0.41
2:B:1029:LEU:HD23	2:B:1039:LEU:HD13	2.02	0.41
2:E:1078:THR:CG2	2:E:1080:ARG:HG2	2.50	0.41
2:B:756:ALA:HB1	2:B:801:VAL:HG21	2.01	0.41
1:D:301:ILE:HG12	1:D:442:LEU:HD21	2.02	0.41
2:E:1055:GLN:HG2	2:E:1093:LEU:HD23	2.03	0.41
2:E:1101:SER:O	2:E:1105:MET:N	2.47	0.41
2:E:850:VAL:HB	2:E:861:VAL:O	2.21	0.41
2:B:873:MET:HB3	2:B:880:LEU:HD11	2.03	0.41
2:E:771:PHE:CE2	2:E:847:ARG:HG3	2.52	0.41
2:E:811:GLU:HB2	2:E:835:MET:HE1	2.03	0.41
2:E:910:MET:HG2	2:E:912:LEU:CD2	2.48	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.92	0.41
2:E:146:ASP:HB3	2:E:148:ASP:OD1	2.21	0.41
2:E:328:LEU:O	2:E:380:GLY:HA2	2.21	0.41
2:E:1058:LEU:HD12	2:E:1058:LEU:HA	1.90	0.40
2:B:224:GLU:N	2:B:225:PRO:HD2	2.36	0.40
1:D:268:LEU:HD21	1:D:273:LEU:HD21	2.03	0.40
2:E:366:ASP:HA	2:E:372:GLN:NE2	2.36	0.40
1:A:84:LEU:CD2	1:A:109:MET:HE1	2.52	0.40
2:B:974:LEU:HD11	2:B:1000:LEU:HD13	2.03	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	344/373 (92%)	316 (92%)	24 (7%)	4 (1%)	10	28
1	D	342/373 (92%)	327 (96%)	14 (4%)	1 (0%)	36	59
2	B	780/836 (93%)	732 (94%)	46 (6%)	2 (0%)	36	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	788/836 (94%)	740 (94%)	46 (6%)	2 (0%)	36	59
3	C	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
3	F	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
All	All	2356/2528 (93%)	2211 (94%)	136 (6%)	9 (0%)	30	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	A	116	LYS
1	A	271	ASP
2	B	36	ASN
1	D	116	LYS
1	A	272	SER
2	E	36	ASN
2	E	310	ILE
2	B	310	ILE

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	291/340 (86%)	284 (98%)	7 (2%)	43	67
1	D	286/340 (84%)	279 (98%)	7 (2%)	43	67
2	B	626/727 (86%)	612 (98%)	14 (2%)	45	69
2	E	643/727 (88%)	618 (96%)	25 (4%)	28	54
3	C	45/51 (88%)	41 (91%)	4 (9%)	9	24
3	F	45/51 (88%)	44 (98%)	1 (2%)	45	69
All	All	1936/2236 (87%)	1878 (97%)	58 (3%)	36	60

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	A	175	ASP
1	A	239	SER
1	A	341	SER
1	A	342	LEU
1	A	420	SER
1	A	423	LEU
2	B	2	SER
2	B	27	GLU
2	B	63	VAL
2	B	73	SER
2	B	215	GLU
2	B	305	LEU
2	B	345	SER
2	B	802	LEU
2	B	827	THR
2	B	872	SER
2	B	962	ASP
2	B	981	SER
2	B	1013	VAL
2	B	1055	GLN
3	C	388	SER
3	C	395	SER
3	C	396	SER
3	C	401	LEU
1	D	239	SER
1	D	246	SER
1	D	272	SER
1	D	293	VAL
1	D	341	SER
1	D	375	SER
1	D	410	SER
2	E	2	SER
2	E	73	SER
2	E	97	SER
2	E	148	ASP
2	E	151	GLU
2	E	178	ILE
2	E	217	SER
2	E	265	ASP
2	E	267	ASN
2	E	269	SER
2	E	303	GLU

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Mol	Chain	Res	Type
2	E	331	SER
2	E	379	SER
2	E	729	VAL
2	E	746	SER
2	E	755	SER
2	E	762	SER
2	E	817	VAL
2	E	849	VAL
2	E	927	MET
2	E	957	VAL
2	E	981	SER
2	E	1006	VAL
2	E	1042	SER
2	E	1108	VAL
3	F	395	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	112	ASN
1	A	173	GLN
1	A	178	GLN
1	A	233	HIS
1	A	390	GLN
2	B	790	ASN
2	B	826	ASN
2	B	978	GLN
2	B	991	HIS
2	B	1034	ASN
1	D	179	GLN
1	D	198	GLN
1	D	228	GLN
1	D	276	ASN
1	D	369	ASN
1	D	390	GLN
2	E	107	ASN
2	E	156	ASN
2	E	209	GLN
2	E	372	GLN
2	E	790	ASN
2	E	991	HIS

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Mol	Chain	Res	Type
2	E	1059	ASN
3	F	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
6	SO4	E	1201	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	B	1202	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	E	1202	-	4,4,4	0.24	0	6,6,6	0.07	0
5	8W7	A	502	-	37,37,37	0.61	0	50,52,52	0.94	1 (2%)
6	SO4	E	1203	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	F	503	-	4,4,4	0.23	0	6,6,6	0.06	0
6	SO4	B	1201	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.05	0
5	8W7	D	502	-	37,37,37	0.62	0	50,52,52	1.03	4 (8%)

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	8W7	D	502	-	-	2/13/46/46	0/5/5/5
5	8W7	A	502	-	-	2/13/46/46	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	8W7	C11-C10-C9	2.47	114.22	109.77
5	D	502	8W7	C20-C21-N3	-2.39	108.26	113.15
5	D	502	8W7	C13-C9-N1	-2.38	108.12	110.32
5	A	502	8W7	C11-C10-C9	2.36	114.03	109.77
5	D	502	8W7	C2-C3-C6	-2.06	117.36	120.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	8W7	C20-C21-N3-C25
5	D	502	8W7	C20-C21-N3-C25
5	A	502	8W7	C20-C21-N3-C22
5	D	502	8W7	C20-C21-N3-C22

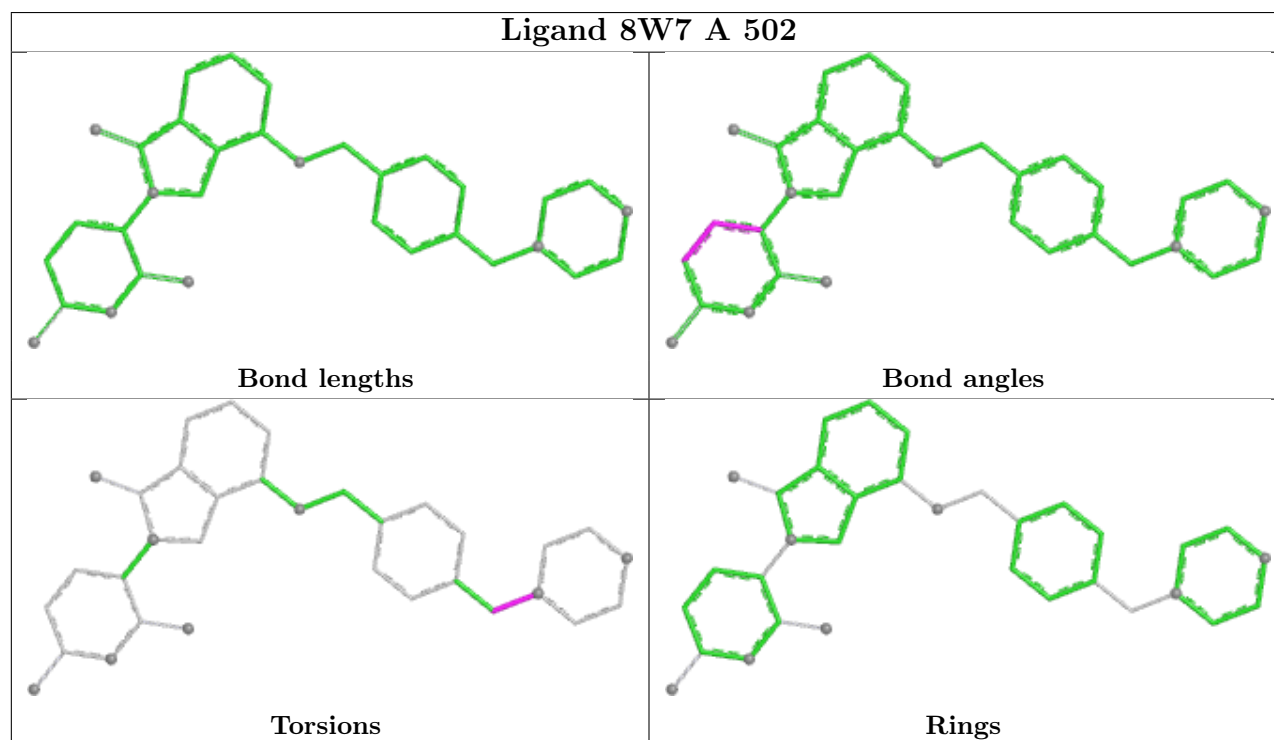
There are no ring outliers.

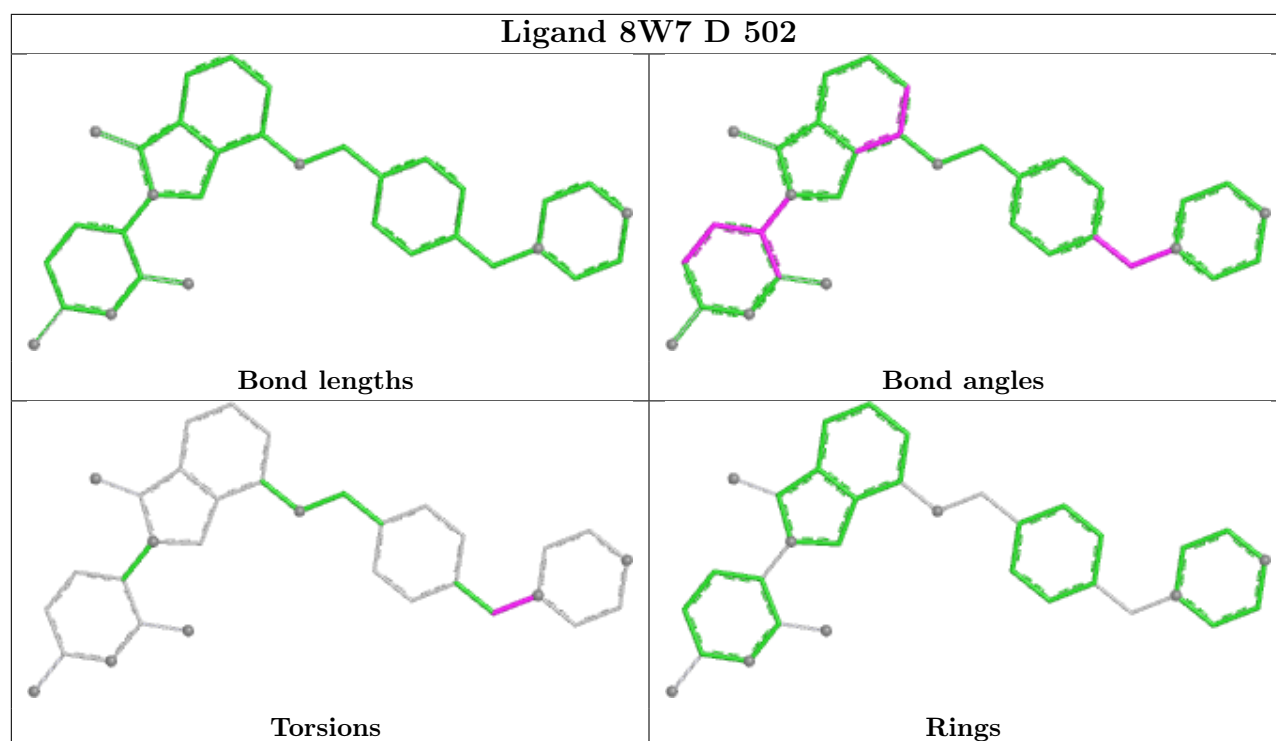
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	SO4	1	0
6	D	504	SO4	2	0
6	A	505	SO4	2	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	352/373 (94%)	0.40	14 (3%)	42	35	38, 62, 111, 140	0
1	D	350/373 (93%)	0.42	20 (5%)	29	24	39, 66, 116, 147	0
2	B	792/836 (94%)	0.42	37 (4%)	36	30	40, 69, 110, 157	0
2	E	798/836 (95%)	0.28	29 (3%)	46	38	39, 62, 104, 166	0
3	C	53/55 (96%)	0.38	3 (5%)	29	24	54, 71, 116, 124	0
3	F	53/55 (96%)	0.68	2 (3%)	44	36	57, 85, 123, 125	0
All	All	2398/2528 (94%)	0.38	105 (4%)	39	32	38, 66, 111, 166	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	SER	7.0
2	B	1098	LEU	5.4
1	A	270	ASP	5.1
3	F	380	TYR	5.1
2	B	914	LEU	4.4
1	D	133	ALA	4.0
2	B	363	CYS	3.7
2	B	1079	GLU	3.6
1	D	421	ALA	3.6
1	D	221	TYR	3.6
3	F	429	PHE	3.5
2	E	924	GLY	3.5
1	D	287	CYS	3.4
2	E	1014	MET	3.4
2	B	913	TYR	3.3
2	B	748	GLY	3.3
2	B	133	LEU	3.2
2	B	224	GLU	3.2
2	B	1114	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	882	ALA	3.2
1	D	89	MET	3.2
2	E	67	PHE	3.1
2	E	967	GLY	3.1
2	E	1098	LEU	3.1
2	E	913	TYR	3.1
2	E	18	CYS	3.1
2	B	1078	THR	3.1
1	A	429	THR	3.0
1	A	197	VAL	3.0
2	E	724	ILE	3.0
1	D	341	SER	3.0
1	D	429	THR	3.0
2	B	872	SER	3.0
1	A	220	SER	2.9
2	E	17	GLY	2.9
2	E	767	SER	2.9
2	B	67	PHE	2.9
2	E	1116	ASP	2.9
2	B	724	ILE	2.9
2	B	106	GLY	2.8
2	E	1081	LYS	2.8
1	D	213	VAL	2.8
1	D	86	GLN	2.8
2	E	1079	GLU	2.8
2	B	1006	VAL	2.7
2	B	986	ASP	2.6
1	D	150	PHE	2.6
2	E	982	ALA	2.6
2	E	1082	THR	2.5
2	B	1081	LYS	2.5
2	B	228	GLY	2.5
1	A	221	TYR	2.5
2	B	1082	THR	2.5
2	B	152	LEU	2.5
2	B	827	THR	2.5
2	B	983	ALA	2.5
1	A	89	MET	2.4
3	C	429	PHE	2.4
1	D	355	TYR	2.4
2	B	29	LEU	2.4
1	A	149	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	PHE	2.4
2	E	985	THR	2.4
2	E	1111	ASN	2.4
1	D	438	VAL	2.3
2	B	88	ILE	2.3
2	E	343	GLN	2.3
2	B	122	GLY	2.3
2	E	907	ASN	2.3
2	B	151	GLU	2.3
2	B	313	CYS	2.3
2	E	313	CYS	2.3
1	D	398	ILE	2.3
2	B	785	GLU	2.3
2	B	1080	ARG	2.3
1	A	212	PRO	2.3
1	A	102	PHE	2.2
1	D	270	ASP	2.2
2	E	883	SER	2.2
1	A	372	GLY	2.2
2	B	982	ALA	2.2
1	D	340	LEU	2.2
1	D	125	TYR	2.2
1	D	442	LEU	2.2
2	B	55	VAL	2.2
2	B	965	PHE	2.2
1	D	439	ILE	2.1
2	E	1054	MET	2.1
2	E	124	ILE	2.1
2	E	1113	GLN	2.1
2	B	9	ALA	2.1
1	A	132	GLU	2.1
1	A	154	ILE	2.1
2	E	744	ASP	2.1
2	E	882	ALA	2.1
3	C	380	TYR	2.1
1	A	341	SER	2.1
2	E	195	VAL	2.1
2	B	967	GLY	2.1
2	E	1121	LYS	2.0
2	B	155	PHE	2.0
3	C	431	ARG	2.0
1	A	421	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	983	ALA	2.0
2	B	15	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

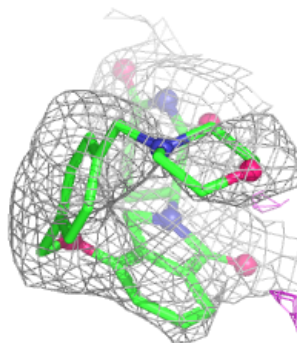
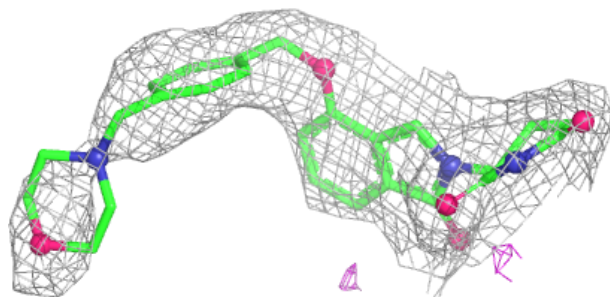
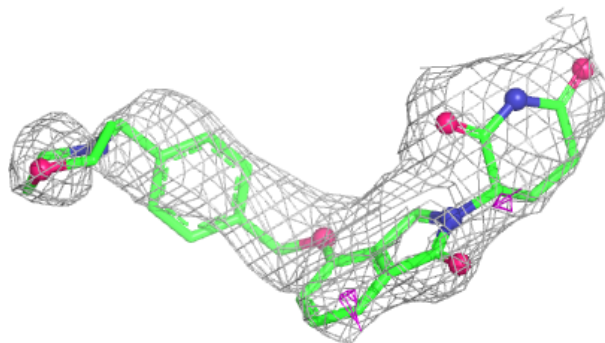
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

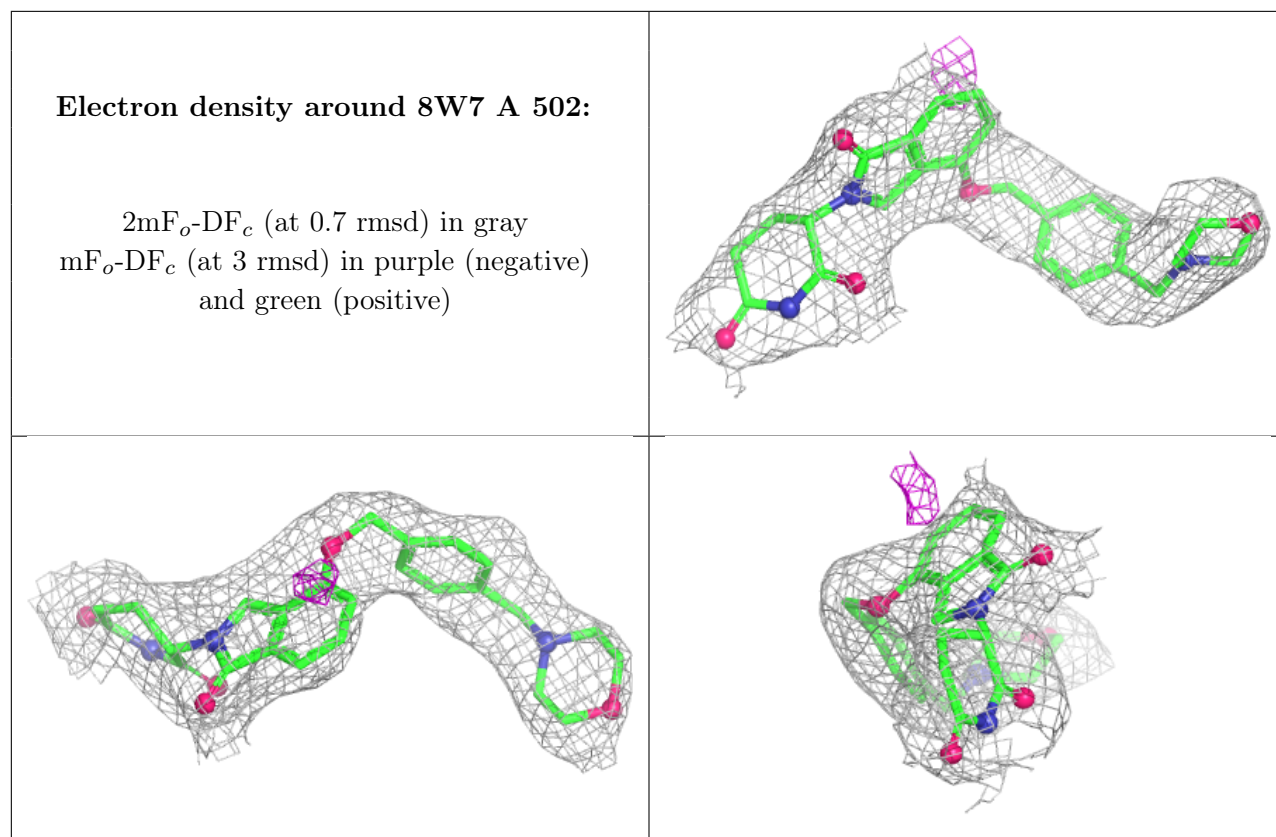
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	E	1202	5/5	0.64	0.13	80,111,139,141	0
6	SO4	F	503	5/5	0.73	0.23	96,100,104,113	0
6	SO4	A	505	5/5	0.75	0.11	65,69,91,97	5
6	SO4	A	503	5/5	0.77	0.15	96,100,118,124	0
6	SO4	B	1202	5/5	0.78	0.17	68,68,77,85	5
6	SO4	D	503	5/5	0.79	0.17	76,95,102,118	0
6	SO4	B	1201	5/5	0.79	0.17	88,107,113,119	0
6	SO4	C	503	5/5	0.79	0.26	75,77,97,106	0
6	SO4	E	1201	5/5	0.82	0.12	82,96,109,124	0
6	SO4	D	504	5/5	0.85	0.23	79,85,95,96	0
6	SO4	A	504	5/5	0.87	0.24	104,105,106,109	0
5	8W7	D	502	33/33	0.89	0.13	50,70,103,108	0
6	SO4	E	1203	5/5	0.91	0.09	70,80,94,155	0
5	8W7	A	502	33/33	0.93	0.11	34,53,86,94	0
4	ZN	F	501	1/1	0.97	0.04	70,70,70,70	0
4	ZN	F	502	1/1	0.98	0.12	87,87,87,87	0
4	ZN	C	502	1/1	0.99	0.02	53,53,53,53	0
4	ZN	A	501	1/1	1.00	0.02	56,56,56,56	0
4	ZN	D	501	1/1	1.00	0.03	66,66,66,66	0
4	ZN	C	501	1/1	1.00	0.02	59,59,59,59	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 8W7 D 502:

$2mF_o-DF_c$ (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.