

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 02:45 PM EST

PDB ID	:	8U15
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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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		
_		250	4%		
	A	373	81%	13%	6%
			5%		
1	D	373	78%	16%	• 6%
			8%		
2	В	836	75%	19%	• 5%
			6%		
2	Ε	836	74%	21%	• 5%
			2%		
3	С	55	71%	22%	• •



Mol	Chain	Length	Quality of chain		
			2%		
3	F	55	67%	25%	• •

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	А	505	-	-	Х	-
6	SO4	D	504	-	-	Х	-



2 Entry composition (i)

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	А	352	Total 2752	C 1768	N 468	0 494	S 22	0	0	0
1	D	350	Total 2711	C 1740	N 453	0 497	S 21	0	0	0

• Molecule 2 is a protein called DDB1.

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	53	Total	С	Ν	Ο	S	0	0	0
5	3 0		420	265	83	68	4	0	0	0
2	Б	52	Total	С	Ν	Ο	S	0	0	0
່ງ	Г		422	264	86	68	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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





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

• 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 (three-letter code: 8W7) (formula: $C_{25}H_{27}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



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

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	Ε	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	F	1	$\begin{array}{c cc} Total & O & S \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 7 is water.



8	U	1	5
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	4	Total O 4 4	0	0
7	В	4	Total O 4 4	0	0
7	С	1	Total O 1 1	0	0
7	D	2	Total O 2 2	0	0
7	Е	1	Total O 1 1	0	0
7	F	1	Total O 1 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 3: Sal-like protein 4





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	110.73Å 95.73Å 150.95Å	Deperitor
a, b, c, α , β , γ	90.00° 91.72° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	61.48 - 2.95	Depositor
Resolution (A)	$90.55 \ - \ 2.95$	EDS
% Data completeness	99.9 (61.48-2.95)	Depositor
(in resolution range)	$100.0 \ (90.55-2.95)$	EDS
R_{merge}	0.10	Depositor
R_{sym}	0.94	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 2.96 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
P. P.	0.220 , 0.272	Depositor
Π, Π_{free}	0.221 , 0.270	DCC
R_{free} test set	3234 reflections $(4.85%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	64.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 41.1	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	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.

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.



¹Intensities estimated from amplitudes.

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: SO4, 8W7, 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).

Mal	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/2817	0.47	1/3831~(0.0%)
1	D	0.24	0/2776	0.46	0/3788
2	В	0.25	0/6117	0.50	0/8311
2	Е	0.25	0/6202	0.49	0/8420
3	С	0.25	0/433	0.47	0/579
3	F	0.24	0/434	0.51	0/579
All	All	0.25	0/18779	0.48	1/25508~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	268	LEU	CA-CB-CG	6.38	129.97	115.30

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	А	2752	0	2679	27	0
1	D	2711	0	2592	32	0
2	В	6007	0	5755	92	0
2	Е	6091	0	5875	105	0



Mol

All

С

D

Е

F

All

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Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
С	420	0	393	10	0		
F	422	0	398	10	0		
А	1	0	0	0	0		
С	2	0	0	0	0		
D	1	0	0	0	0		
F	2	0	0	0	0		
А	33	0	0	0	0		
D	33	0	0	0	0		
А	15	0	0	3	0		
В	10	0	0	0	0		
С	5	0	0	0	0		
D	10	0	0	2	0		
Ε	15	0	0	0	0		
F	5	0	0	0	0		
А	4	0	0	0	0		
В	4	0	0	0	0		

Continued

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 7.

All (266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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: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



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
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	0.60
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: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
3:C:388:SER:O	3:C:388:SER:OG	2.19	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
3:F:388:SER:O	3:F:388:SER:OG	2.20	0.57
1:D:351:ASN:ND2	3:F:413:SER:O	2.34	0.57
2:E:161:GLU:OE2	2:E:191:LYS:NZ	2.33	0.57
2:E:184:ASP:OD1	2:E:189:HIS:NE2	2.36	0.57
2:E:359:ILE:HG21	2:E:362:MET:HE3	1.87	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
2:E:176:PRO:HB2	2:E:195:VAL:HG12	1.86	0.56



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
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	
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:238:THR:HG1	2:E:240:HIS:HE2	1.52	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: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	
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	
3:C:393:THR:HG1	3:C:396:SER:HG	1.54	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	
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: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:1102:ARG:HA	2:B:1105:MET:HG3	1.93	0.51	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:795:ASP:HB2	:795:ASP:HB2 2:B:802:LEU:HD21		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: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: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:E:57:MET:CE	2:E:79:ILE:HG21	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:E:57:MET:HE1	2:E:79:ILE:HG21	1.96	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: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
1:A:145:ARG:NH2	6:A:505:SO4:O4	2.46	0.48
3:F:395:SER:O	3:F:399:ILE:HD12	2.13	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:232:ILE:HG12	2:E:232:ILE:HG12 2:E:237:ILE:HG23		0.47
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.95	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
1:A:241:PRO:HB3	2:B:812:TYR:CZ	2.50	0.46
1:D:404:ALA:HB1	1:D:409:MET:HE3	1.96	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: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
2:E:11:LYS:HD2	2:E:38:ARG:HD2	1.99	0.45
2:B:807:PHE:CZ	2:B:831:VAL:HG11	2.52	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:719:GLU:OE1	2:E:757:SER:OG	2.28	0.45
2:E:891:TYR:HB3	2:E:899:LEU:HD22	1.99	0.45
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



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
1:D:309:ARG:HH22	2:E:910:MET:HE3	1.82	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
2:E:944:GLU:CD	2:E:947:ARG:HH21	2.22	0.43
2:B:1109:VAL:HG12	2:B:1129:LEU:HD22	2.01	0.43
1:D:394:CYS:SG	1:D:396:SER:OG	2.68	0.43
2:E:38:ARG:HE	2:E:54:GLU:CD	2.22	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
2:B:184:ASP:HB2	2:B:185:PRO:HD2	2.01	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



	jue pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:143:ALA:HB3	1:A:143:ALA:HB3 1:A:158:LYS:HB2		0.42	
2:B:874:VAL:HG23	2:B:881:LEU:HB3	2.01	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:426:ILE:HG21	1:A:438:VAL:HB	2.02	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: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	
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: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	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Perce	ntiles
1	А	344/373~(92%)	316 (92%)	24 (7%)	4 (1%)	13	43
1	D	342/373~(92%)	327 (96%)	14 (4%)	1 (0%)	41	73
2	В	780/836~(93%)	732 (94%)	46 (6%)	2(0%)	41	73
2	Е	788/836~(94%)	740 (94%)	46 (6%)	2(0%)	41	73
3	С	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%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	268	LEU
1	А	116	LYS
1	А	271	ASP
2	В	36	ASN
1	D	116	LYS



Continued from previous page...

Mol	Chain	Res	Type
1	А	272	SER
2	Е	36	ASN
2	Е	310	ILE
2	В	310	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	291/340~(86%)	285~(98%)	6(2%)	53 80
1	D	286/340~(84%)	274 (96%)	12 (4%)	30 63
2	В	626/727~(86%)	607~(97%)	19 (3%)	41 72
2	Е	643/727~(88%)	617 (96%)	26 (4%)	31 64
3	С	45/51~(88%)	41 (91%)	4 (9%)	9 32
3	F	45/51~(88%)	42 (93%)	3 (7%)	16 45
All	All	1936/2236~(87%)	1866 (96%)	70 (4%)	35 67

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	72	LEU
1	А	175	ASP
1	А	208	PHE
1	А	239	SER
1	А	283	ARG
1	А	341	SER
2	В	2	SER
2	В	67	PHE
2	В	73	SER
2	В	117	GLU
2	В	265	ASP
2	В	297	LEU
2	В	343	GLN
2	В	345	SER



Mol	Chain	Res	Type
2	В	366	ASP
2	В	392	ASN
2	В	722	ARG
2	В	763	SER
2	В	844	LYS
2	В	962	ASP
2	В	981	SER
2	В	1080	ARG
2	В	1102	ARG
2	В	1115	ASP
2	В	1140	HIS
3	С	380	TYR
3	С	388	SER
3	С	395	SER
3	С	396	SER
1	D	105	GLN
1	D	111	ARG
1	D	188	CYS
1	D	226	LYS
1	D	239	SER
1	D	246	SER
1	D	268	LEU
1	D	272	SER
1	D	341	SER
1	D	375	SER
1	D	410	SER
1	D	441	CYS
2	Е	2	SER
2	E	73	SER
2	Е	74	LYS
2	Е	97	SER
2	Е	146	ASP
2	Е	151	GLU
2	E	188	ARG
2	Е	198	ARG
2	Е	211	ASN
2	E	217	SER
2	E	265	ASP
2	E	267	ASN
2	Е	269	SER
2	E	303	GLU
2	E	331	SER



Mol	Chain	Res	Type
2	Е	379	SER
2	Ε	746	SER
2	Е	755	SER
2	Е	817	VAL
2	Е	947	ARG
2	Ε	957	VAL
2	Е	981	SER
2	Е	1102	ARG
2	Ε	1108	VAL
2	Е	1114	TYR
2	Е	1140	HIS
3	F	385	LYS
3	F	388	SER
3	F	395	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
2	В	790	ASN
2	В	826	ASN
2	В	991	HIS
2	Е	85	ASN
2	Е	107	ASN
2	Е	156	ASN
2	Е	372	GLN
2	E	991	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

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).

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	gles
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	8W7	А	502	-	37,37,37	0.64	0	50,52,52	0.95	3 (6%)
6	SO4	А	504	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	Е	1203	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	В	1201	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	А	503	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	А	505	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	В	1202	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	Е	1201	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	Е	1202	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	С	503	-	4,4,4	0.16	0	6,6,6	0.04	0
6	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.05	0
5	8W7	D	502	-	37,37,37	0.65	0	50,52,52	1.01	3 (6%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
5	D	502	8W7	C20-C21-N3	-2.51	108.26	113.12
5	D	502	8W7	C11-C10-C9	2.37	114.22	109.77



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	D	502	8W7	C2-C3-C6	-2.32	117.36	120.54
5	А	502	8W7	C11-C10-C9	2.26	114.03	109.77
5	А	502	8W7	C2-C3-C6	-2.13	117.62	120.54
5	А	502	8W7	C5-C6-C3	2.13	121.28	120.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	502	8W7	C20-C21-N3-C25
5	D	502	8W7	C20-C21-N3-C25
5	А	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	А	504	SO4	1	0
6	А	505	SO4	2	0
6	D	504	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	А	352/373~(94%)	0.40	16 (4%) 33 21	38, 62, 111, 140	0
1	D	350/373~(93%)	0.44	19 (5%) 25 16	39, 66, 116, 147	0
2	В	792/836~(94%)	0.54	65 (8%) 11 6	40, 69, 110, 157	0
2	Е	798/836~(95%)	0.44	49 (6%) 21 12	39, 62, 104, 166	0
3	С	53/55~(96%)	0.23	1 (1%) 66 49	54, 71, 116, 124	0
3	F	53/55~(96%)	0.45	1 (1%) 66 49	57, 85, 123, 125	0
All	All	2398/2528~(94%)	0.46	151 (6%) 20 11	38, 66, 111, 166	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	88	MET	6.1
2	В	914	LEU	6.1
2	В	1098	LEU	4.9
2	В	133	LEU	4.7
2	В	106	GLY	4.3
1	D	89	MET	4.2
2	В	883	SER	4.1
2	В	1140	HIS	4.1
1	D	177	ILE	4.0
2	В	152	LEU	4.0
2	В	1114	TYR	3.9
2	В	1039	LEU	3.9
2	Ε	19	VAL	3.9
2	В	913	TYR	3.7
2	В	724	ILE	3.7
2	E	724	ILE	3.7
2	Е	67	PHE	3.6
2	В	363	CYS	3.6
2	В	882	ALA	3.6



Mol	Chain	Res	Type	RSRZ
1	А	442	LEU	3.6
2	В	29	LEU	3.5
2	Е	913	TYR	3.5
3	F	429	PHE	3.5
2	В	67	PHE	3.5
2	В	1006	VAL	3.4
1	D	442	LEU	3.4
2	В	5	TYR	3.3
2	В	1128	ASP	3.3
2	В	88	ILE	3.2
2	Е	907	ASN	3.2
2	В	1051	LEU	3.2
2	В	15	VAL	3.2
2	Е	966	LEU	3.2
2	Е	18	CYS	3.1
2	Е	133	LEU	3.1
2	В	966	LEU	3.1
2	Е	1116	ASP	3.1
2	Е	1140	HIS	3.1
2	Е	967	GLY	3.1
2	В	1094	ILE	3.0
2	Е	16	ASN	3.0
2	Е	914	LEU	3.0
2	В	965	PHE	3.0
2	В	17	GLY	3.0
2	Е	1098	LEU	3.0
2	Ε	931	LEU	2.9
1	А	197	VAL	2.9
1	D	220	SER	2.9
2	В	1029	LEU	2.9
1	A	90	ILE	2.9
2	Е	1039	LEU	2.8
2	E	343	GLN	2.8
2	В	725	CYS	2.8
2	В	926	LEU	2.8
2	В	20	THR	2.8
2	В	998	PHE	2.7
2	Е	883	SER	2.7
2	В	19	VAL	2.7
2	В	44	VAL	2.7
2	В	376	VAL	2.7
1	D	199	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	В	1112	LEU	2.7
2	В	151	GLU	2.7
2	В	32	LEU	2.7
2	В	182	TYR	2.7
2	Е	61	ILE	2.7
2	В	907	ASN	2.7
2	Е	806	GLN	2.7
2	Е	1061	VAL	2.7
2	В	872	SER	2.6
1	А	91	LEU	2.6
2	Е	17	GLY	2.6
2	В	16	ASN	2.6
2	В	155	PHE	2.6
1	А	154	ILE	2.6
1	А	124	ALA	2.6
2	В	30	ASN	2.6
1	D	176	GLY	2.6
2	Е	293	GLY	2.6
2	В	1097	PHE	2.6
1	А	441	CYS	2.5
2	Е	923	VAL	2.5
2	В	710	LEU	2.5
1	D	355	TYR	2.5
2	Е	926	LEU	2.5
2	Е	1129	LEU	2.5
2	В	61	ILE	2.5
1	D	421	ALA	2.5
1	D	398	ILE	2.5
1	D	287	CYS	2.5
1	А	92	ILE	2.5
2	Е	15	VAL	2.5
2	Е	925	ASP	2.4
2	Е	108	VAL	2.4
2	Е	930	VAL	2.4
1	А	315	MET	2.4
2	Е	924	GLY	2.4
1	А	155	VAL	2.4
2	Е	965	PHE	2.4
1	D	439	ILE	2.4
1	А	440	LEU	2.3
2	В	829	PHE	2.3
2	В	1050	LEU	2.3



8U15

Mol	Chain	Res	Type	RSRZ
2	В	748	GLY	2.3
2	В	912	LEU	2.3
2	Е	124	ILE	2.3
1	А	240	TRP	2.3
2	В	377	THR	2.3
1	А	143	ALA	2.3
1	D	210	SER	2.2
2	Е	152	LEU	2.2
2	Е	736	LEU	2.2
2	В	63	VAL	2.2
2	В	1065	VAL	2.2
2	В	108	VAL	2.2
2	Е	1133	VAL	2.2
2	В	785	GLU	2.2
3	С	429	PHE	2.2
2	В	1034	ASN	2.2
1	D	240	TRP	2.2
2	В	21	GLY	2.2
2	Е	882	ALA	2.2
2	В	167	VAL	2.2
2	Е	155	PHE	2.2
2	В	45	THR	2.2
1	D	125	TYR	2.2
2	Е	1114	TYR	2.2
2	Е	78	PHE	2.1
2	Е	977	CYS	2.1
2	В	9	ALA	2.1
2	Е	163	HIS	2.1
2	В	974	LEU	2.1
2	Е	785	GLU	2.1
2	В	172	GLY	2.1
2	Е	947	ARG	2.1
2	В	317	LEU	2.1
2	В	2	SER	2.0
2	Е	174	GLN	2.0
2	Е	912	LEU	2.0
1	D	203	ASN	2.0
1	А	237	LEU	2.0
2	В	124	ILE	2.0
2	В	1086	THR	2.0
2	Е	908	ASN	2.0
1	А	198	GLN	2.0



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Mol	Chain	Res Type		RSRZ
1	А	321	LEU	2.0
2	Е	948 ASP		2.0
1	D	102	PHE	2.0
1	D	109	MET	2.0
2	Ε	141	LYS	2.0
1	D	295	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(A^2)$	Q<0.9
6	SO4	Е	1202	5/5	0.69	0.22	80,111,139,141	0
6	SO4	А	505	5/5	0.81	0.34	65,69,91,97	5
6	SO4	А	504	5/5	0.81	0.39	104,105,106,109	0
6	SO4	А	503	5/5	0.82	0.33	96,100,118,124	0
6	SO4	D	503	5/5	0.83	0.32	76,95,102,118	0
6	SO4	В	1202	5/5	0.84	0.20	68,68,77,85	5
6	SO4	Е	1201	5/5	0.84	0.20	82,96,109,124	0
6	SO4	С	503	5/5	0.84	0.33	75,77,97,106	0
6	SO4	D	504	5/5	0.88	0.34	79,85,95,96	0
5	8W7	D	502	33/33	0.89	0.30	50,70,103,108	0
4	ZN	F	502	1/1	0.89	0.27	87,87,87,87	0
6	SO4	В	1201	5/5	0.89	0.21	88,107,113,119	0
6	SO4	Е	1203	5/5	0.91	0.23	70,80,94,155	0
5	8W7	А	502	33/33	0.93	0.23	34,53,86,94	0
6	SO4	F	503	5/5	0.93	0.34	96,100,104,113	0
4	ZN	F	501	1/1	0.96	0.11	70,70,70,70	0
4	ZN	С	501	1/1	0.98	0.12	59,59,59,59	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	ZN	С	502	1/1	0.99	0.14	$53,\!53,\!53,\!53$	0
4	ZN	D	501	1/1	0.99	0.16	66,66,66,66	0
4	ZN	А	501	1/1	1.00	0.16	56, 56, 56, 56	0

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







6.5 Other polymers (i)

There are no such residues in this entry.

