



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 7U8F / pdb_00007u8f
Title : Ternary complex structure of Cereblon-DDB1 bound to IKZF2(ZF2) and the molecular glue DKY709
Authors : Ma, X.; Ornelas, E.; Clifton, M.C.
Deposited on : 2022-03-08
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

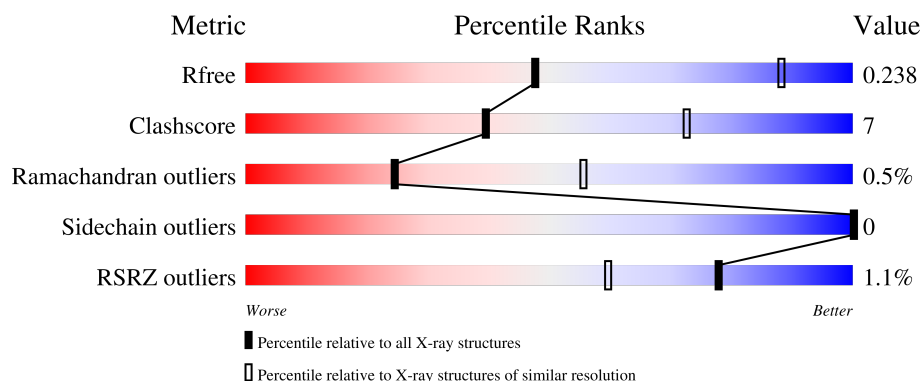
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	405	0% 78% 14% 8%
1	D	405	0% 77% 15% 8%
2	B	836	0% 82% 17% 0%
2	E	836	2% 84% 14% 0%
3	C	28	4% 79% 21% 0%

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Mol	Chain	Length	Quality of chain
3	F	28	 71% 29%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19495 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	374	Total	C	N	O	S	0	0	0
			2986	1904	512	546	24			
1	D	374	Total	C	N	O	S	0	0	0
			2978	1899	509	546	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	expression tag	UNP Q96SW2
A	39	SER	-	expression tag	UNP Q96SW2
D	38	GLY	-	expression tag	UNP Q96SW2
D	39	SER	-	expression tag	UNP Q96SW2

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	826	Total	C	N	O	S	0	0	0
			6472	4099	1093	1244	36			
2	E	826	Total	C	N	O	S	0	0	0
			6471	4099	1093	1243	36			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	700	GLY	-	linker	UNP Q16531
B	701	ASN	-	linker	UNP Q16531
B	702	GLY	-	linker	UNP Q16531
B	703	ASN	-	linker	UNP Q16531
B	704	SER	-	linker	UNP Q16531
B	705	GLY	-	linker	UNP Q16531
E	700	GLY	-	linker	UNP Q16531
E	701	ASN	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
E	702	GLY	-	linker	UNP Q16531
E	703	ASN	-	linker	UNP Q16531
E	704	SER	-	linker	UNP Q16531
E	705	GLY	-	linker	UNP Q16531

- Molecule 3 is a protein called IKZF2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	S	0	0	0
			224	138	46	38	2			
3	F	28	Total	C	N	O	S	0	0	0
			224	138	46	38	2			

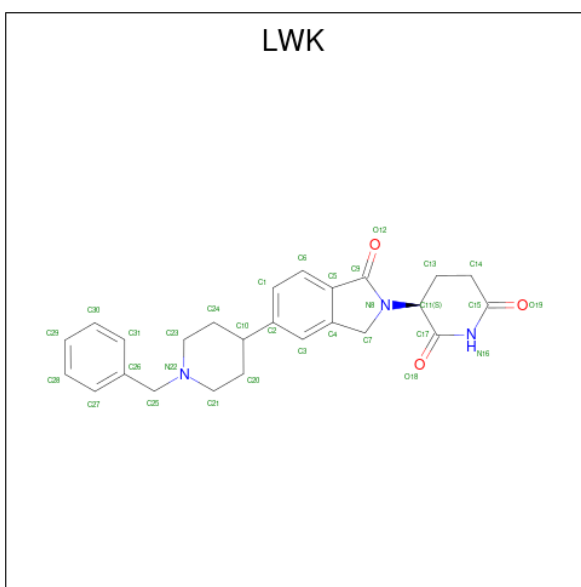
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	SER	-	expression tag	UNP Q53SU9
F	136	SER	-	expression tag	UNP Q53SU9

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

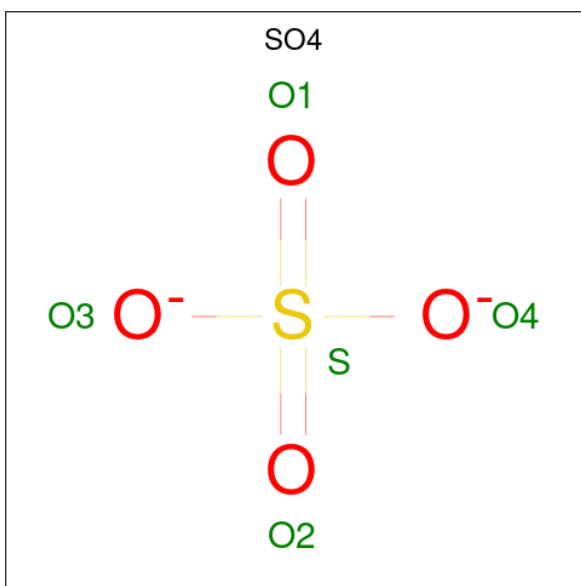
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (3S)-3-[5-(1-benzylpiperidin-4-yl)-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: LWK) (formula: C₂₅H₂₇N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 31	C 25	N 3	O 3	0	0
5	D	1	Total 31	C 25	N 3	O 3	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



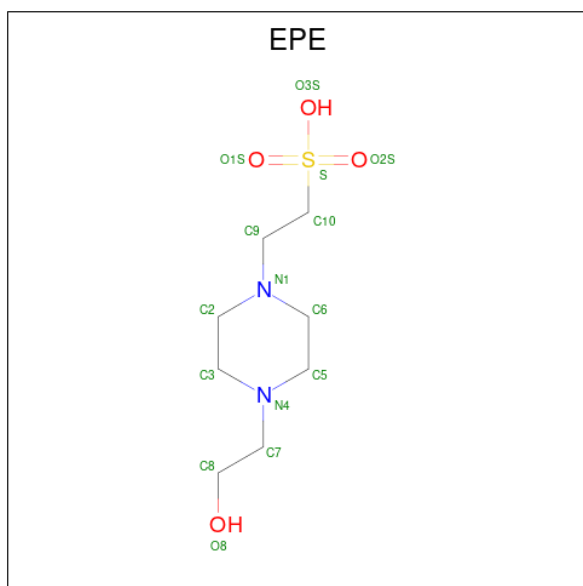
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	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		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	B	8	Total	O	0	0
			8	8		

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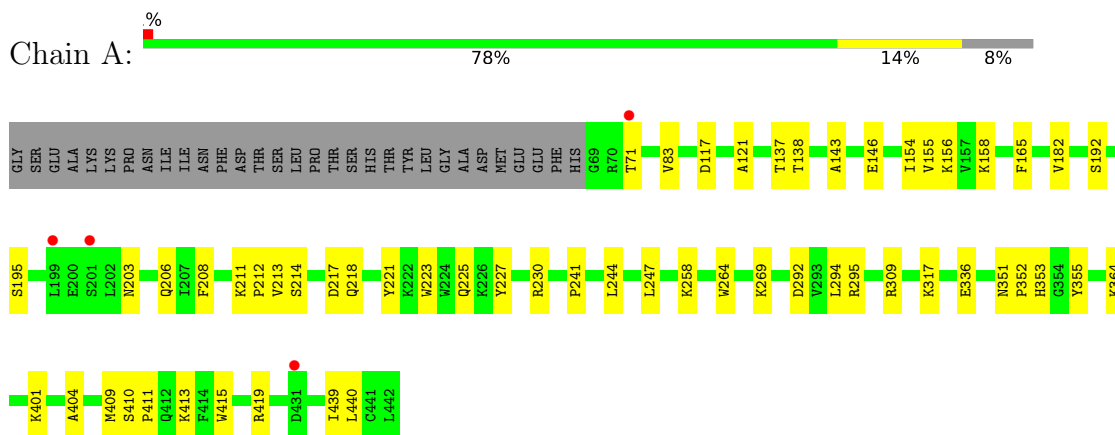
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	O 1	0	0
8	D	1	Total 1	O 1	0	0
8	E	6	Total 6	O 6	0	0
8	F	1	Total 1	O 1	0	0

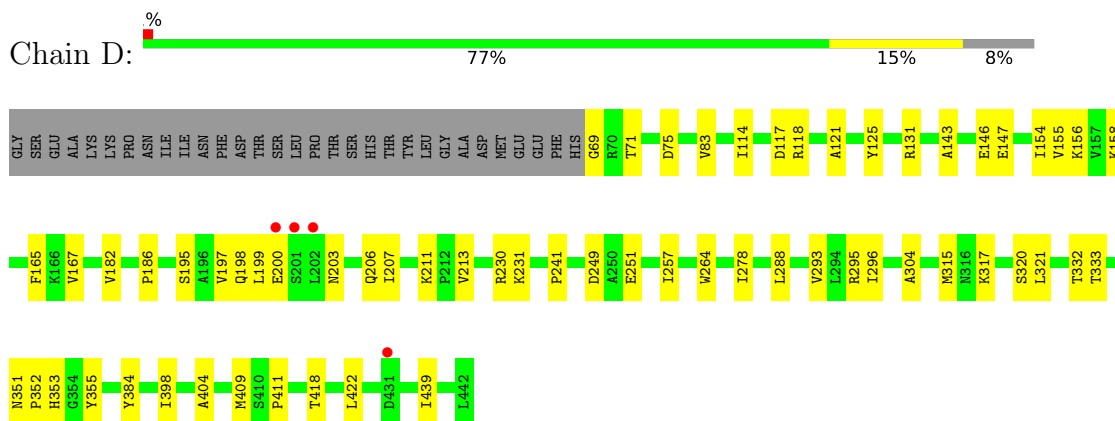
3 Residue-property plots

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.

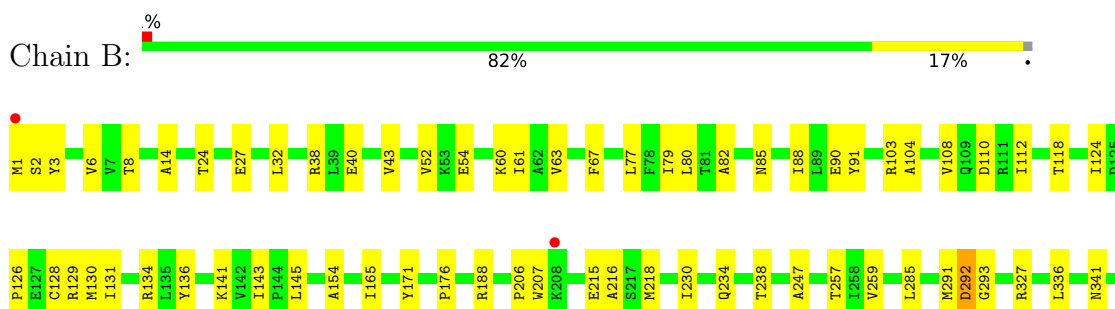
• Molecule 1: Protein cereblon

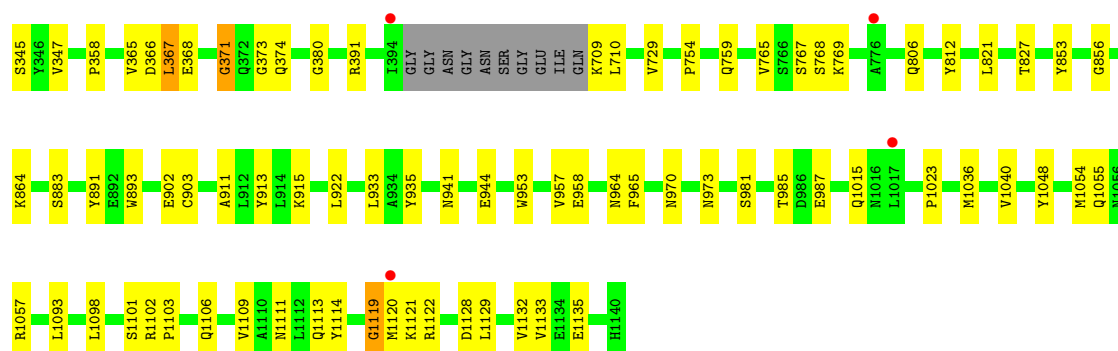


• Molecule 1: Protein cereblon

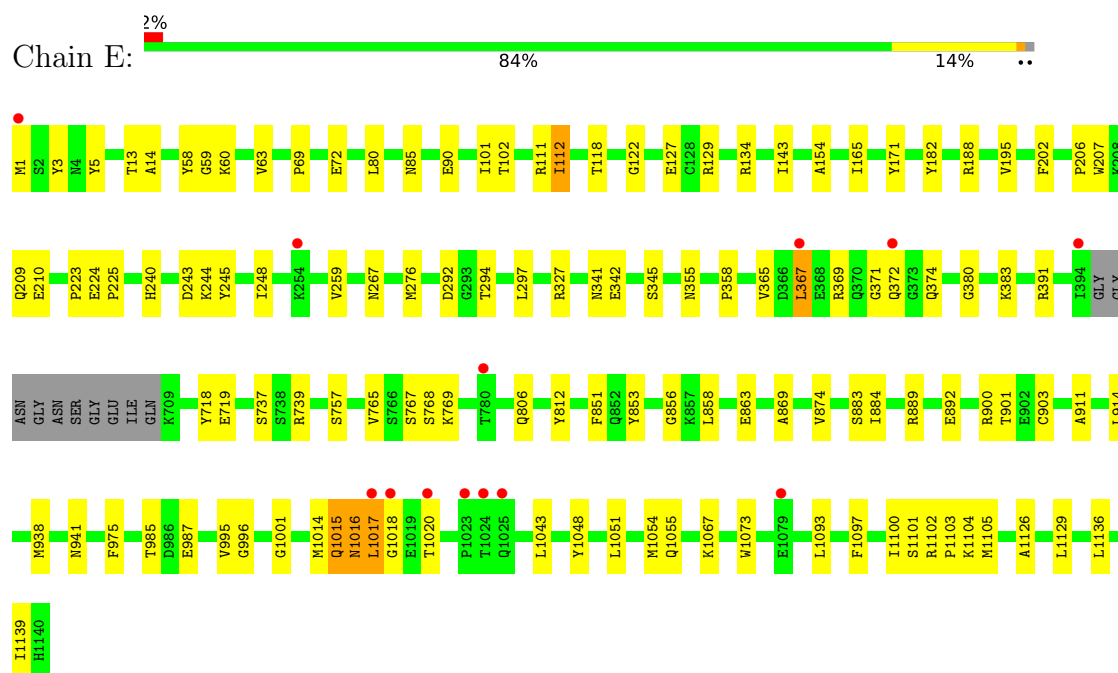


• Molecule 2: DNA damage-binding protein 1

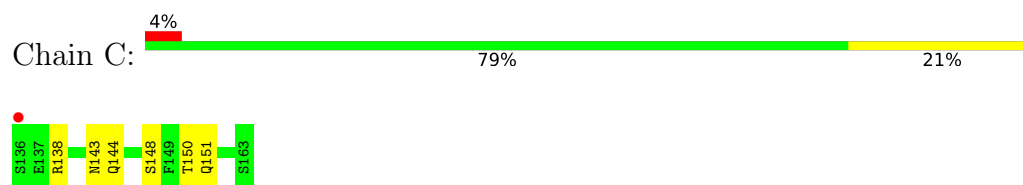




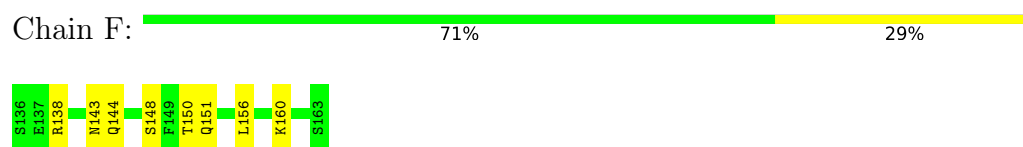
• Molecule 2: DNA damage-binding protein 1



• Molecule 3: IKZF2



• Molecule 3: IKZF2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	180.89Å 180.89Å 555.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.89 – 3.15 49.89 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.89-3.15) 100.0 (49.89-3.15)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.213 , 0.243 0.207 , 0.238	Depositor DCC
R_{free} test set	4704 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19495	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: ZN, SO4, LWK, EPE

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	0.30	0/3055	0.51	0/4147
1	D	0.30	0/3047	0.51	0/4137
2	B	0.30	0/6589	0.53	0/8912
2	E	0.30	0/6588	0.53	1/8910 (0.0%)
3	C	0.32	0/229	0.48	0/305
3	F	0.36	0/229	0.61	0/305
All	All	0.30	0/19737	0.52	1/26716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1017	LEU	CB-CG-CD1	-5.48	94.25	110.70

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	2986	0	2977	44	0
1	D	2978	0	2959	46	0
2	B	6472	0	6424	91	0
2	E	6471	0	6424	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	224	0	216	7	0
3	F	224	0	216	7	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	0	0	0
5	D	31	0	0	0	0
6	B	20	0	0	0	0
6	D	5	0	0	0	0
6	E	15	0	0	0	0
7	E	15	0	17	0	0
8	A	2	0	0	1	0
8	B	8	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	6	0	0	1	0
8	F	1	0	0	0	0
All	All	19495	0	19233	258	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 7.

All (258) 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:D:203:ASN:HD21	2:E:118:THR:HA	1.13	1.14
1:A:203:ASN:HD21	2:B:118:THR:HA	1.21	1.05
2:E:118:THR:HB	2:E:134:ARG:HH22	1.28	0.98
2:B:118:THR:HB	2:B:134:ARG:HH22	1.34	0.90
1:A:203:ASN:ND2	2:B:118:THR:HA	1.93	0.83
1:D:203:ASN:ND2	2:E:118:THR:HA	1.95	0.78
2:E:367:LEU:HD22	2:E:374:GLN:NE2	2.00	0.76
1:A:211:LYS:H	1:A:211:LYS:HD3	1.51	0.76
2:B:767:SER:HB3	2:B:769:LYS:HE2	1.70	0.73
1:D:71:THR:HG21	1:D:117:ASP:HB2	1.69	0.72
2:E:111:ARG:O	2:E:112:ILE:HG12	1.90	0.71
2:B:234:GLN:HG2	2:B:257:THR:HG23	1.73	0.70
2:B:765:VAL:HG12	2:B:806:GLN:HB3	1.74	0.69
1:A:404:ALA:HB1	1:A:409:MET:HG3	1.73	0.69
2:E:1055:GLN:HG2	2:E:1093:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLU:HG3	2:E:1020:THR:C	2.18	0.68
2:E:1017:LEU:HB3	2:E:1020:THR:HB	1.76	0.67
1:A:230:ARG:NH1	2:B:215:GLU:OE1	2.28	0.67
2:E:118:THR:HB	2:E:134:ARG:NH2	2.07	0.66
2:E:118:THR:HG21	2:E:165:ILE:O	1.96	0.66
1:A:264:TRP:O	1:A:419:ARG:NH2	2.29	0.66
2:E:985:THR:HG22	2:E:987:GLU:H	1.61	0.66
1:A:165:PHE:CD1	1:A:182:VAL:HG21	2.31	0.65
3:F:138:ARG:HB3	3:F:148:SER:HB3	1.78	0.65
1:A:317:LYS:NZ	1:A:439:ILE:O	2.30	0.64
1:A:214:SER:HB3	1:A:217:ASP:HB2	1.79	0.64
1:A:212:PRO:HG2	1:A:218:GLN:HB2	1.80	0.64
2:B:1055:GLN:HG2	2:B:1093:LEU:HD23	1.81	0.63
1:D:203:ASN:HA	1:D:206:GLN:HG2	1.80	0.63
1:D:211:LYS:H	1:D:211:LYS:HD3	1.64	0.63
1:A:336:GLU:OE1	1:A:364:LYS:HE3	1.98	0.63
2:B:374:GLN:HG2	2:B:391:ARG:HB3	1.81	0.62
2:E:292:ASP:OD2	2:E:294:THR:OG1	2.13	0.62
1:A:71:THR:HG21	1:A:117:ASP:HB2	1.80	0.62
2:E:1017:LEU:HD23	2:E:1018:GLY:N	2.14	0.62
2:E:1016:ASN:OD1	2:E:1020:THR:HG21	2.00	0.61
1:D:75:ASP:HB3	1:D:186:PRO:HB3	1.81	0.61
1:A:154:ILE:HD11	1:A:156:LYS:HE3	1.83	0.61
2:E:739:ARG:NH1	2:E:757:SER:OG	2.34	0.61
2:B:90:GLU:OE1	2:B:103:ARG:NH1	2.33	0.60
1:D:165:PHE:CD1	1:D:182:VAL:HG21	2.37	0.60
1:A:211:LYS:HG2	1:A:213:VAL:HG13	1.83	0.60
2:E:892:GLU:OE1	2:E:900:ARG:NH1	2.33	0.60
2:E:367:LEU:HD22	2:E:374:GLN:HE22	1.66	0.60
2:B:1098:LEU:HD21	2:B:1133:VAL:HB	1.83	0.59
2:B:883:SER:HB2	2:B:911:ALA:HB3	1.84	0.59
2:B:129:ARG:HH11	2:B:176:PRO:HD3	1.68	0.58
2:E:210:GLU:HG3	2:E:240:HIS:NE2	2.18	0.58
2:E:874:VAL:CG1	2:E:914:LEU:HD22	2.32	0.58
2:E:765:VAL:HG12	2:E:806:GLN:HB3	1.86	0.58
2:E:883:SER:HB2	2:E:911:ALA:HB3	1.85	0.58
2:B:2:SER:HB2	2:B:964:ASN:HD21	1.68	0.57
2:E:767:SER:O	2:E:769:LYS:HE2	2.04	0.57
3:C:138:ARG:HB3	3:C:148:SER:HB3	1.86	0.57
2:E:1101:SER:HB2	2:E:1103:PRO:HD2	1.86	0.57
2:B:2:SER:HB2	2:B:964:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:ASN:ND2	2:B:345:SER:O	2.38	0.56
2:E:14:ALA:HB1	2:E:327:ARG:HD2	1.88	0.56
2:E:1016:ASN:CG	2:E:1020:THR:HG21	2.32	0.55
2:B:118:THR:HG21	2:B:165:ILE:O	2.07	0.55
1:D:199:LEU:HD12	1:D:203:ASN:OD1	2.06	0.55
2:E:243:ASP:N	2:E:243:ASP:OD1	2.39	0.55
2:E:369:ARG:HH11	2:E:1014:MET:HE1	1.72	0.55
1:D:317:LYS:NZ	1:D:439:ILE:O	2.41	0.54
2:E:1016:ASN:OD1	2:E:1017:LEU:N	2.40	0.54
1:A:143:ALA:HB3	1:A:158:LYS:HB2	1.88	0.54
1:D:165:PHE:HB2	1:D:182:VAL:HG22	1.90	0.54
2:E:195:VAL:HG22	2:E:202:PHE:HE1	1.71	0.54
2:B:27:GLU:N	2:B:27:GLU:OE1	2.39	0.54
1:A:258:LYS:CE	1:A:269:LYS:HD3	2.38	0.54
2:E:874:VAL:HG13	2:E:914:LEU:HD22	1.90	0.53
2:B:902:GLU:HG2	2:B:903:CYS:SG	2.48	0.53
2:E:1136:LEU:O	2:E:1139:ILE:HG12	2.08	0.53
1:A:401:LYS:HB2	1:A:415:TRP:CZ3	2.44	0.53
1:A:353:HIS:CG	3:C:143:ASN:HB3	2.44	0.53
2:B:903:CYS:SG	2:B:941:ASN:HA	2.49	0.53
1:A:355:TYR:CD2	3:C:144:GLN:HG3	2.44	0.53
1:D:203:ASN:HD21	2:E:118:THR:CA	2.02	0.53
2:E:769:LYS:HE3	2:E:863:GLU:OE2	2.09	0.53
2:E:1054:MET:SD	2:E:1129:LEU:HD21	2.49	0.53
1:A:292:ASP:OD1	1:A:295:ARG:NH1	2.43	0.52
1:D:154:ILE:HD11	1:D:156:LYS:HE3	1.92	0.52
1:D:251:GLU:OE2	1:D:251:GLU:N	2.42	0.52
1:A:83:VAL:HG22	1:A:121:ALA:HB3	1.92	0.52
2:B:1101:SER:HB2	2:B:1103:PRO:HD2	1.92	0.51
2:B:1113:GLN:HB3	2:B:1121:LYS:HB2	1.91	0.51
1:D:404:ALA:HB1	1:D:409:MET:HG3	1.92	0.51
2:E:365:VAL:HG12	2:E:367:LEU:H	1.74	0.51
2:B:1054:MET:SD	2:B:1129:LEU:HD21	2.51	0.51
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.93	0.51
1:D:69:GLY:N	1:D:118:ARG:HH12	2.08	0.51
1:D:200:GLU:HG3	2:E:327:ARG:HH12	1.75	0.51
2:E:206:PRO:HB2	2:E:207:TRP:CD1	2.46	0.51
1:A:230:ARG:HH12	2:B:215:GLU:CD	2.19	0.50
1:A:353:HIS:CD2	3:C:143:ASN:HB3	2.46	0.50
1:D:353:HIS:CG	3:F:143:ASN:HB3	2.46	0.50
2:E:69:PRO:HD2	2:E:72:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:TYR:CD2	3:F:144:GLN:HG3	2.47	0.50
2:B:110:ASP:OD1	2:B:141:LYS:NZ	2.36	0.50
2:B:1057:ARG:NH2	2:B:1111:ASN:O	2.45	0.49
1:D:195:SER:HB2	1:D:199:LEU:HD21	1.93	0.49
2:E:1100:ILE:HD12	2:E:1104:LYS:HB2	1.94	0.49
1:D:288:LEU:O	1:D:295:ARG:NH2	2.46	0.49
2:B:3:TYR:HB3	2:B:1048:TYR:HB2	1.93	0.49
2:B:129:ARG:NH1	2:B:176:PRO:HD3	2.28	0.49
2:B:188:ARG:NH1	2:B:216:ALA:O	2.43	0.49
1:D:146:GLU:HG2	1:D:155:VAL:HG12	1.93	0.49
2:B:915:LYS:HG3	2:B:958:GLU:HA	1.93	0.49
2:B:24:THR:HA	2:B:91:TYR:CD2	2.47	0.49
2:B:864:LYS:HE2	2:B:891:TYR:HE2	1.78	0.49
1:A:208:PHE:CE2	1:A:227:TYR:HA	2.48	0.48
1:A:221:TYR:O	1:A:225:GLN:N	2.41	0.48
2:B:206:PRO:HB2	2:B:207:TRP:CD1	2.49	0.48
2:B:358:PRO:HD2	2:B:380:GLY:HA2	1.94	0.48
1:A:165:PHE:HB2	1:A:182:VAL:HG22	1.96	0.48
2:B:913:TYR:HB3	2:B:957:VAL:HG12	1.95	0.48
2:B:1120:MET:HG3	2:B:1122:ARG:HE	1.79	0.48
1:D:351:ASN:HB2	1:D:352:PRO:HD2	1.96	0.48
2:E:60:LYS:NZ	2:E:1001:GLY:O	2.46	0.48
1:A:355:TYR:CE2	3:C:144:GLN:HG3	2.48	0.47
2:B:124:ILE:HG12	2:B:131:ILE:HG12	1.95	0.47
2:B:291:MET:O	2:B:292:ASP:C	2.56	0.47
2:B:365:VAL:HG12	2:B:367:LEU:H	1.79	0.47
2:B:985:THR:HG22	2:B:987:GLU:H	1.79	0.47
2:E:244:LYS:NZ	2:E:297:LEU:O	2.44	0.47
2:B:768:SER:O	2:B:769:LYS:HD3	2.15	0.47
2:E:853:TYR:OH	2:E:856:GLY:HA2	2.14	0.47
1:A:211:LYS:H	1:A:211:LYS:CD	2.24	0.47
1:A:413:LYS:NZ	8:A:601:HOH:O	2.34	0.47
2:B:38:ARG:HD2	2:B:54:GLU:OE2	2.13	0.47
2:B:88:ILE:HD13	2:B:104:ALA:HB3	1.95	0.47
2:B:230:ILE:HD11	2:B:285:LEU:HD21	1.96	0.47
2:E:719:GLU:OE2	2:E:737:SER:OG	2.29	0.47
2:E:903:CYS:SG	2:E:941:ASN:HA	2.53	0.47
1:A:208:PHE:HE2	1:A:227:TYR:HA	1.79	0.47
2:B:110:ASP:HB2	2:B:136:TYR:CE2	2.49	0.47
2:B:374:GLN:OE1	2:B:391:ARG:HD3	2.14	0.47
2:E:374:GLN:HG2	2:E:391:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1102:ARG:NH2	2:E:1126:ALA:HB3	2.29	0.47
2:B:1128:ASP:O	2:B:1132:VAL:HG23	2.14	0.47
1:A:244:LEU:O	1:A:244:LEU:HG	2.13	0.47
1:D:143:ALA:HB3	1:D:158:LYS:HB2	1.97	0.47
1:D:257:ILE:HG12	1:D:315:MET:HE1	1.97	0.47
2:E:975:PHE:HA	2:E:996:GLY:O	2.14	0.47
2:B:130:MET:HA	2:B:145:LEU:HD13	1.98	0.46
1:A:241:PRO:HB3	2:B:812:TYR:OH	2.15	0.46
2:B:118:THR:HB	2:B:134:ARG:NH2	2.16	0.46
2:E:889:ARG:HD3	2:E:901:THR:HG23	1.97	0.46
2:B:1120:MET:HG3	2:B:1120:MET:O	2.15	0.46
2:E:80:LEU:HA	2:E:85:ASN:O	2.15	0.46
2:B:126:PRO:HB3	2:B:171:TYR:CE1	2.51	0.46
1:D:167:VAL:HA	1:D:182:VAL:HG23	1.98	0.46
1:D:264:TRP:CH2	1:D:315:MET:HG2	2.50	0.46
3:F:156:LEU:O	3:F:160:LYS:HD3	2.16	0.46
1:A:192:SER:HB3	1:A:195:SER:HB2	1.98	0.46
1:A:258:LYS:HE3	1:A:269:LYS:HD3	1.97	0.46
2:B:131:ILE:HG13	2:B:145:LEU:HD11	1.97	0.46
2:B:215:GLU:CB	2:B:234:GLN:HB2	2.46	0.46
1:D:321:LEU:HD22	1:D:422:LEU:HD13	1.97	0.46
2:B:218:MET:HE1	2:B:259:VAL:HA	1.96	0.46
2:E:342:GLU:N	2:E:342:GLU:OE1	2.49	0.46
2:E:225:PRO:HG2	2:E:267:ASN:HB2	1.97	0.46
2:E:248:ILE:HB	8:E:1306:HOH:O	2.16	0.46
1:A:351:ASN:ND2	3:C:143:ASN:O	2.49	0.45
1:D:211:LYS:HG2	1:D:213:VAL:HG13	1.97	0.45
1:D:114:ILE:HA	1:D:118:ARG:HG2	1.98	0.45
2:B:8:THR:HG23	2:B:1036:MET:HE2	1.99	0.45
2:E:341:ASN:ND2	2:E:345:SER:O	2.39	0.45
2:E:938:MET:SD	2:E:938:MET:N	2.89	0.45
1:A:351:ASN:HB2	1:A:352:PRO:HD2	1.99	0.45
2:B:1:MET:HE1	2:B:981:SER:OG	2.17	0.45
1:D:278:ILE:HG13	1:D:304:ALA:HB2	1.98	0.45
2:E:171:TYR:CD2	2:E:223:PRO:HA	2.52	0.45
2:E:58:TYR:HB3	2:E:1073:TRP:HB2	1.99	0.45
2:E:358:PRO:HD2	2:E:380:GLY:HA2	1.99	0.44
2:B:238:THR:HG22	2:B:247:ALA:CB	2.47	0.44
2:B:729:VAL:HG21	2:B:827:THR:OG1	2.17	0.44
1:D:83:VAL:HG22	1:D:121:ALA:HB3	2.00	0.44
2:E:3:TYR:HB3	2:E:1048:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:TYR:HB2	2:E:1043:LEU:HD11	1.99	0.44
2:B:43:VAL:HG23	2:B:52:VAL:HG21	1.99	0.44
1:D:320:SER:OG	1:D:333:THR:HG22	2.18	0.44
1:D:125:TYR:CE1	1:D:131:ARG:HD3	2.53	0.44
1:D:147:GLU:CD	1:D:156:LYS:HD2	2.43	0.44
1:D:197:VAL:HG12	1:D:197:VAL:O	2.17	0.44
1:D:241:PRO:HB3	2:E:812:TYR:OH	2.18	0.44
2:E:59:GLY:HA2	2:E:1073:TRP:CZ3	2.53	0.44
2:B:108:VAL:O	2:B:141:LYS:HE2	2.18	0.44
2:B:970:ASN:O	2:B:973:ASN:ND2	2.50	0.44
2:E:1014:MET:O	2:E:1015:GLN:C	2.61	0.44
2:B:754:PRO:HB2	2:B:759:GLN:CD	2.44	0.43
2:E:102:THR:HB	2:E:1067:LYS:HE3	1.99	0.43
1:D:293:VAL:HA	1:D:296:ILE:HD12	1.99	0.43
2:E:143:ILE:HG12	2:E:154:ALA:HB2	2.00	0.43
2:B:6:VAL:HG23	2:B:1040:VAL:HG22	2.01	0.43
2:B:371:GLY:O	2:B:1015:GLN:HG2	2.18	0.43
1:D:241:PRO:HB3	2:E:812:TYR:CZ	2.54	0.43
2:B:902:GLU:OE2	2:B:935:TYR:OH	2.28	0.43
2:E:259:VAL:HG11	2:E:276:MET:HG2	1.99	0.43
2:E:372:GLN:HB2	2:E:1014:MET:HE3	2.00	0.43
2:B:14:ALA:HB1	2:B:327:ARG:HD2	1.99	0.43
2:B:336:LEU:CD2	2:B:347:VAL:HG12	2.48	0.43
2:E:1051:LEU:HA	2:E:1054:MET:HB2	2.01	0.43
2:E:1102:ARG:N	2:E:1103:PRO:HD2	2.34	0.43
3:F:150:THR:HG23	3:F:151:GLN:HG3	2.01	0.43
1:A:137:THR:HG22	1:A:138:THR:O	2.19	0.42
1:A:192:SER:O	1:A:195:SER:HB3	2.18	0.42
2:B:933:LEU:HD23	2:B:944:GLU:HA	2.01	0.42
2:E:224:GLU:O	2:E:225:PRO:C	2.61	0.42
1:D:353:HIS:CD2	3:F:143:ASN:HB3	2.54	0.42
2:E:1:MET:HB2	2:E:995:VAL:HG11	2.01	0.42
2:E:13:THR:OG1	2:E:355:ASN:OD1	2.28	0.42
2:E:869:ALA:O	2:E:884:ILE:HA	2.19	0.42
1:A:203:ASN:HA	1:A:206:GLN:HG2	2.01	0.42
1:A:212:PRO:HD3	1:A:223:TRP:NE1	2.34	0.42
2:E:240:HIS:CD2	2:E:245:TYR:CD1	3.07	0.42
1:A:294:LEU:HD11	1:A:440:LEU:HD11	2.01	0.42
1:D:351:ASN:ND2	3:F:143:ASN:O	2.49	0.42
2:B:60:LYS:HB2	2:B:82:ALA:HB2	2.02	0.42
2:B:215:GLU:HB2	2:B:234:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:THR:HG23	3:C:151:GLN:HG3	2.02	0.42
1:D:231:LYS:NZ	1:D:249:ASP:OD1	2.53	0.42
1:A:146:GLU:HG2	1:A:155:VAL:HG12	2.02	0.41
1:A:247:LEU:O	1:A:309:ARG:NH1	2.52	0.41
1:D:321:LEU:HD13	1:D:332:THR:HG23	2.02	0.41
2:B:1121:LYS:H	2:B:1121:LYS:HG2	1.69	0.41
1:D:207:ILE:HD12	1:D:207:ILE:H	1.84	0.41
1:D:207:ILE:O	1:D:230:ARG:NH2	2.53	0.41
2:E:63:VAL:HG11	2:E:122:GLY:HA3	2.02	0.41
2:E:127:GLU:OE2	2:E:129:ARG:NH1	2.53	0.41
2:E:182:TYR:OH	2:E:209:GLN:OE1	2.38	0.41
2:E:851:PHE:HB3	2:E:858:LEU:HD11	2.01	0.41
2:B:953:TRP:HB2	2:B:970:ASN:HB2	2.02	0.41
2:B:1023:PRO:HG3	2:B:1135:GLU:HG3	2.02	0.41
2:E:1097:PHE:CE1	2:E:1105:MET:HG2	2.55	0.41
2:B:61:ILE:HG23	2:B:79:ILE:HG23	2.02	0.41
2:B:366:ASP:HA	2:B:373:GLY:HA2	2.03	0.41
1:A:410:SER:OG	1:A:411:PRO:CD	2.69	0.41
2:B:63:VAL:O	2:B:79:ILE:HA	2.20	0.41
2:B:80:LEU:HA	2:B:85:ASN:O	2.21	0.41
2:B:853:TYR:OH	2:B:856:GLY:HA2	2.21	0.41
2:B:1102:ARG:N	2:B:1103:PRO:HD2	2.36	0.41
2:B:1119:GLY:N	2:B:1121:LYS:HZ2	2.19	0.41
2:E:165:ILE:HD13	2:E:188:ARG:NH1	2.35	0.41
2:E:767:SER:O	2:E:769:LYS:HG3	2.20	0.41
2:B:40:GLU:HG2	2:B:54:GLU:HG2	2.03	0.41
2:B:922:LEU:HD22	2:B:965:PHE:HD1	1.85	0.41
2:B:709:LYS:HG2	2:B:710:LEU:H	1.86	0.40
2:E:1102:ARG:HH21	2:E:1126:ALA:HB3	1.85	0.40
2:B:32:LEU:HD23	2:B:77:LEU:HD22	2.03	0.40
2:B:67:PHE:HB2	2:B:128:CYS:SG	2.61	0.40
2:B:821:LEU:HB3	2:B:893:TRP:HB2	2.03	0.40
2:E:383:LYS:HA	2:E:718:TYR:HA	2.03	0.40
2:B:1114:TYR:O	2:B:1121:LYS:HB3	2.22	0.40
1:D:384:TYR:OH	1:D:411:PRO:HD2	2.21	0.40
2:B:1106:GLN:HA	2:B:1109:VAL:HG22	2.03	0.40
1:D:398:ILE:O	1:D:418:THR:HG22	2.21	0.40
2:E:90:GLU:HB3	2:E:101:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	372/405 (92%)	350 (94%)	22 (6%)	0	100	100
1	D	372/405 (92%)	350 (94%)	21 (6%)	1 (0%)	36	64
2	B	822/836 (98%)	769 (94%)	47 (6%)	6 (1%)	18	49
2	E	822/836 (98%)	770 (94%)	46 (6%)	6 (1%)	18	49
3	C	26/28 (93%)	23 (88%)	3 (12%)	0	100	100
3	F	26/28 (93%)	22 (85%)	4 (15%)	0	100	100
All	All	2440/2538 (96%)	2284 (94%)	143 (6%)	13 (0%)	24	55

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	292	ASP
2	E	112	ILE
2	E	1015	GLN
2	E	1016	ASN
2	B	112	ILE
2	B	367	LEU
2	B	371	GLY
2	B	293	GLY
2	B	1119	GLY
1	D	198	GLN
2	E	367	LEU
2	E	371	GLY
2	E	768	SER

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	332/367 (90%)	332 (100%)	0	100	100
1	D	330/367 (90%)	330 (100%)	0	100	100
2	B	714/727 (98%)	714 (100%)	0	100	100
2	E	714/727 (98%)	714 (100%)	0	100	100
3	C	25/25 (100%)	25 (100%)	0	100	100
3	F	25/25 (100%)	25 (100%)	0	100	100
All	All	2140/2238 (96%)	2140 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	178	GLN
1	A	179	GLN
1	A	198	GLN
1	A	203	ASN
2	B	211	ASN
2	B	337	ASN
2	B	343	GLN
2	B	372	GLN
2	B	790	ASN
2	B	964	ASN
2	B	978	GLN
2	B	1056	ASN
3	C	141	HIS
3	C	143	ASN
1	D	95	GLN
1	D	115	GLN
1	D	203	ASN
1	D	335	ASN
1	D	412	GLN
2	E	337	ASN
2	E	372	GLN
2	E	374	GLN
2	E	727	GLN
2	E	790	ASN

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Mol	Chain	Res	Type
2	E	1056	ASN
3	F	143	ASN

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	B	1204	-	4,4,4	0.29	0	6,6,6	0.22	0
6	SO4	B	1202	-	4,4,4	0.26	0	6,6,6	0.14	0
6	SO4	B	1203	-	4,4,4	0.28	0	6,6,6	0.35	0
6	SO4	E	1202	-	4,4,4	0.24	0	6,6,6	0.23	0
7	EPE	E	1201	-	15,15,15	0.71	1 (6%)	19,20,20	1.82	6 (31%)
5	LWK	A	502	-	35,35,35	1.29	3 (8%)	50,50,50	1.57	8 (16%)
6	SO4	E	1203	-	4,4,4	0.25	0	6,6,6	0.28	0
5	LWK	D	502	-	35,35,35	1.52	5 (14%)	50,50,50	1.47	6 (12%)
6	SO4	D	503	-	4,4,4	0.21	0	6,6,6	0.27	0
6	SO4	B	1201	-	4,4,4	0.25	0	6,6,6	0.28	0
6	SO4	E	1204	-	4,4,4	0.26	0	6,6,6	0.15	0

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	LWK	A	502	-	-	2/12/47/47	0/5/5/5
5	LWK	D	502	-	-	3/12/47/47	0/5/5/5
7	EPE	E	1201	-	-	2/9/19/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	LWK	C9-N8	4.66	1.40	1.36
5	D	502	LWK	C25-N22	3.75	1.54	1.47
5	A	502	LWK	C9-N8	3.58	1.39	1.36
5	D	502	LWK	C15-N16	3.09	1.42	1.37
5	A	502	LWK	C25-N22	2.97	1.53	1.47
5	D	502	LWK	C25-C26	2.75	1.56	1.51
5	D	502	LWK	C17-N16	2.58	1.41	1.37
5	A	502	LWK	C7-N8	2.40	1.49	1.47
7	E	1201	EPE	C10-S	2.13	1.80	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	LWK	C13-C11-N8	-4.87	108.70	114.03
5	D	502	LWK	C17-C11-N8	-4.23	106.41	110.32
7	E	1201	EPE	C5-N4-C3	4.06	117.59	108.84
7	E	1201	EPE	C7-N4-C3	3.77	121.28	111.24
5	A	502	LWK	O12-C9-N8	-3.55	122.52	125.34
5	D	502	LWK	C20-C21-N22	-3.47	105.46	111.08
5	A	502	LWK	C20-C21-N22	-3.40	105.57	111.08
5	D	502	LWK	O12-C9-N8	-3.38	122.65	125.34
5	A	502	LWK	C4-C3-C2	-3.21	117.11	122.17
5	D	502	LWK	C13-C11-N8	-2.84	110.92	114.03
5	D	502	LWK	C24-C23-N22	-2.84	106.48	111.08
5	D	502	LWK	C25-N22-C23	2.79	117.06	111.07
7	E	1201	EPE	O3S-S-C10	2.73	111.36	106.00
5	A	502	LWK	C11-C17-N16	2.58	120.00	116.24
5	A	502	LWK	C17-C11-N8	-2.41	108.09	110.32
7	E	1201	EPE	C7-N4-C5	2.35	117.50	111.24
5	A	502	LWK	C24-C10-C2	-2.32	107.17	112.67
7	E	1201	EPE	C9-N1-C6	-2.16	105.48	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	LWK	C15-N16-C17	-2.09	123.93	126.69
7	E	1201	EPE	C10-C9-N1	-2.00	104.79	112.36

There are no chirality outliers.

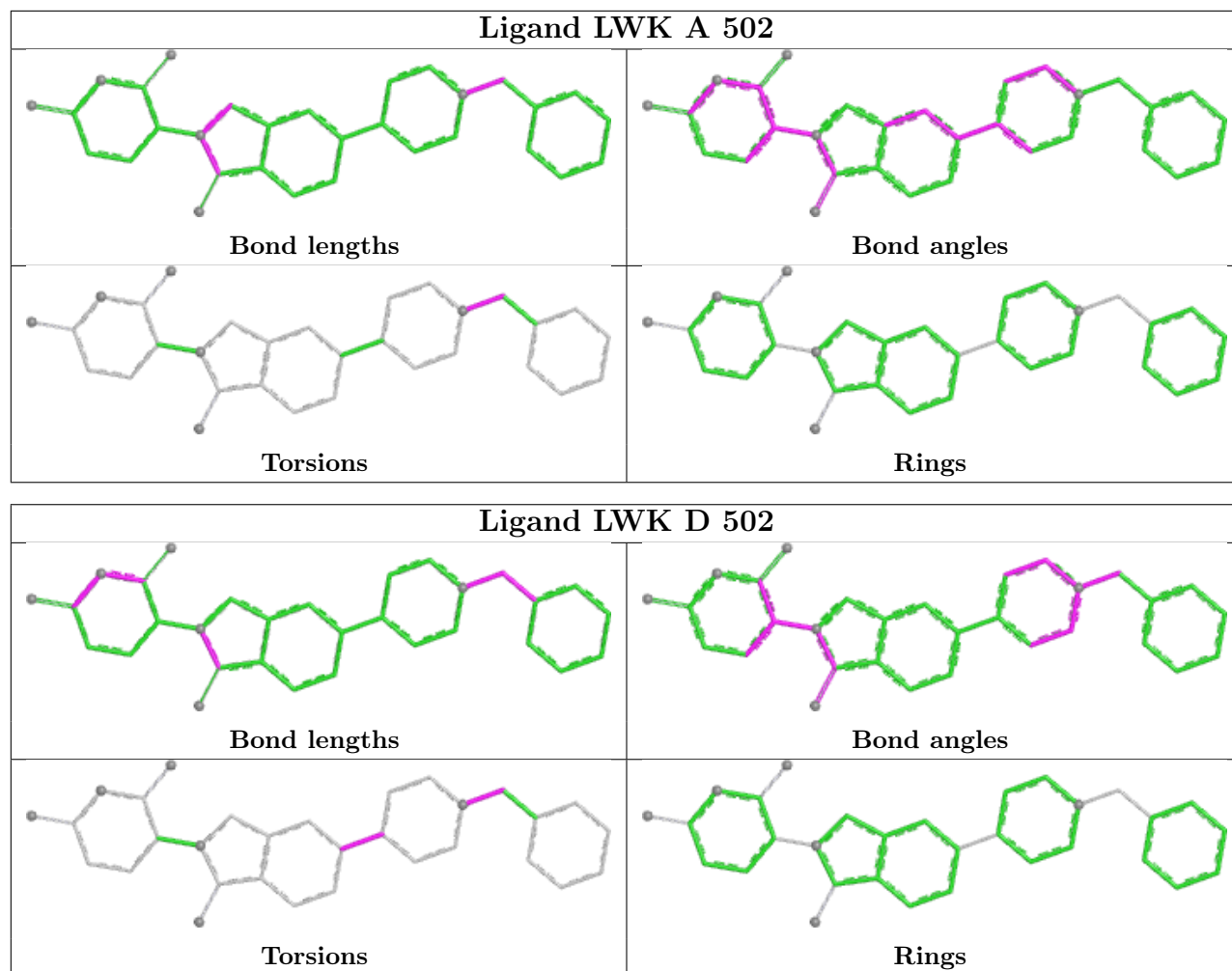
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	1201	EPE	C10-C9-N1-C6
5	A	502	LWK	C26-C25-N22-C23
5	A	502	LWK	C26-C25-N22-C21
5	D	502	LWK	C26-C25-N22-C21
7	E	1201	EPE	C10-C9-N1-C2
5	D	502	LWK	C26-C25-N22-C23
5	D	502	LWK	C20-C10-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/405 (92%)	-0.17	4 (1%) 78 60	85, 115, 183, 268	0
1	D	374/405 (92%)	-0.14	4 (1%) 78 60	80, 110, 176, 234	0
2	B	826/836 (98%)	-0.32	6 (0%) 84 69	73, 108, 178, 251	0
2	E	826/836 (98%)	-0.23	13 (1%) 70 50	73, 109, 181, 279	0
3	C	28/28 (100%)	-0.19	1 (3%) 46 27	92, 104, 139, 155	0
3	F	28/28 (100%)	-0.07	0 100 100	96, 105, 129, 143	0
All	All	2456/2538 (96%)	-0.23	28 (1%) 78 60	73, 110, 181, 279	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1024	THR	3.5
2	B	394	ILE	3.1
1	A	199	LEU	2.9
1	D	431	ASP	2.8
2	E	1018	GLY	2.7
1	A	431	ASP	2.7
2	E	394	ILE	2.7
2	B	1120	MET	2.7
3	C	136	SER	2.7
2	B	776	ALA	2.7
2	E	1023	PRO	2.6
2	E	1079	GLU	2.6
1	D	202	LEU	2.6
2	E	1017	LEU	2.5
2	E	1	MET	2.4
2	E	367	LEU	2.4
2	B	1	MET	2.3
2	B	208	LYS	2.3
2	E	1020	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	780	THR	2.2
1	A	71	THR	2.2
1	D	200	GLU	2.2
2	E	1025	GLN	2.1
2	B	1017	LEU	2.1
1	D	201	SER	2.1
2	E	372	GLN	2.1
2	E	254	LYS	2.0
1	A	201	SER	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.

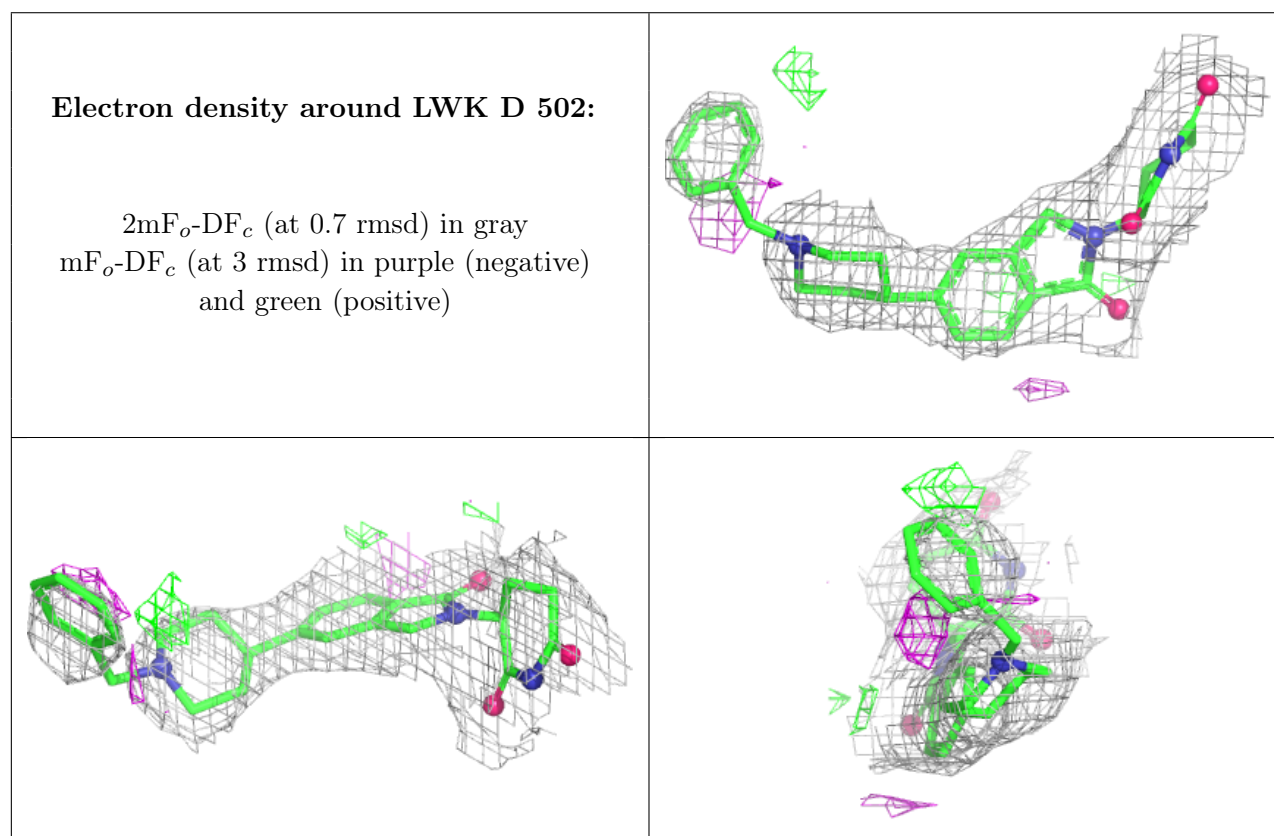
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	503	5/5	0.65	0.08	172,177,197,208	0
6	SO4	B	1203	5/5	0.69	0.09	161,165,201,204	0
6	SO4	E	1204	5/5	0.74	0.07	166,167,178,197	0
6	SO4	B	1204	5/5	0.76	0.06	167,169,173,198	0
7	EPE	E	1201	15/15	0.77	0.20	108,131,170,171	0
6	SO4	B	1202	5/5	0.92	0.07	109,115,131,137	0
6	SO4	E	1202	5/5	0.92	0.08	79,115,127,128	0
6	SO4	E	1203	5/5	0.94	0.15	95,125,139,145	0
5	LWK	D	502	31/31	0.94	0.12	77,96,139,143	0
5	LWK	A	502	31/31	0.94	0.10	83,99,136,148	0
6	SO4	B	1201	5/5	0.95	0.09	90,98,112,122	0
4	ZN	F	201	1/1	1.00	0.02	97,97,97,97	0
4	ZN	A	501	1/1	1.00	0.06	115,115,115,115	0
4	ZN	C	201	1/1	1.00	0.02	92,92,92,92	0

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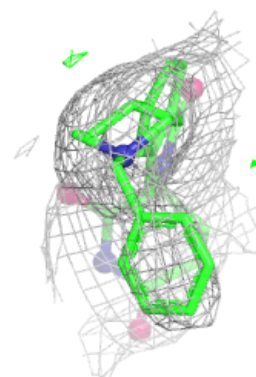
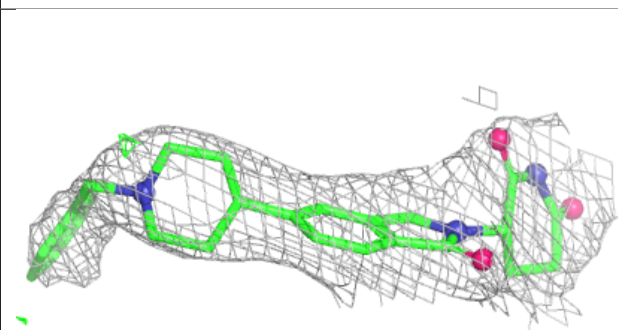
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	D	501	1/1	1.00	0.07	105,105,105,105	0

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 LWK A 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.