



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:42 PM UTC

PDB ID : 4M0V / pdb_00004m0v
Title : Crystal structure of E.coli SbcD with Mn2+
Authors : Liu, S.; Tian, L.F.; Yan, X.X.; Liang, D.C.
Deposited on : 2013-08-02
Resolution : 1.83 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
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

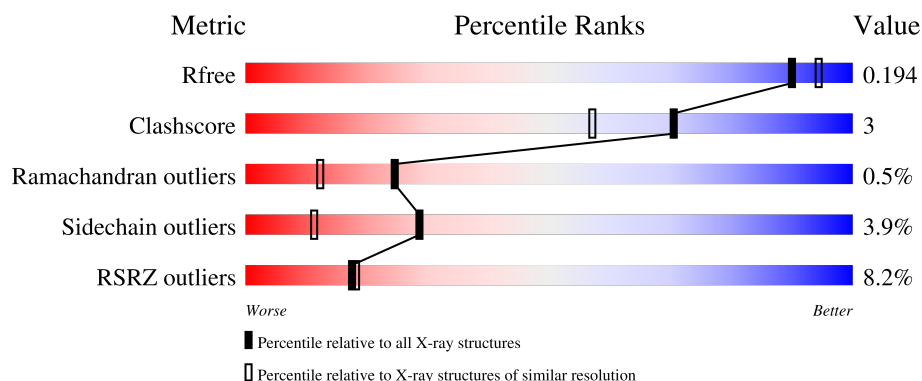
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	354	12% 81% 11% 6%
1	B	354	10% 91% 5%
1	C	354	4% 85% 10%
1	D	354	6% 88% 8%

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
3	MN	C	403	-	-	-	X
3	MN	D	403	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11308 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 Exonuclease subunit SbcD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	5	0
			2509	1593	439	468	9			
1	B	342	Total	C	N	O	S	0	5	0
			2600	1648	455	488	9			
1	C	345	Total	C	N	O	S	0	9	0
			2680	1709	466	494	11			
1	D	345	Total	C	N	O	S	0	7	0
			2651	1689	465	486	11			

There are 56 discrepancies between the modelled and reference sequences:

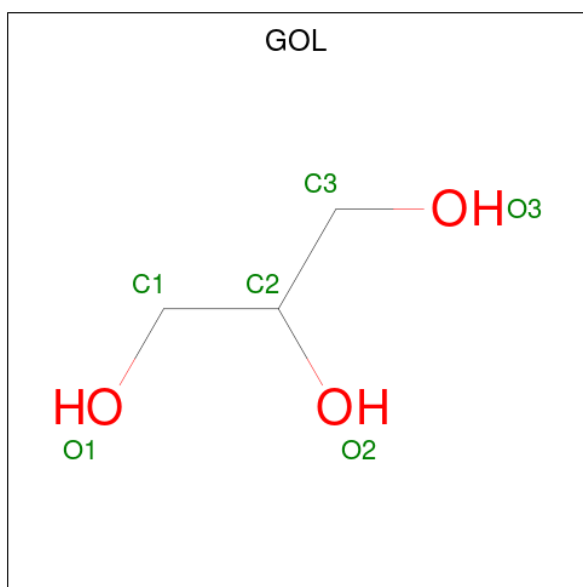
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP E8Y9D8
A	-12	SER	-	expression tag	UNP E8Y9D8
A	-11	HIS	-	expression tag	UNP E8Y9D8
A	-10	HIS	-	expression tag	UNP E8Y9D8
A	-9	HIS	-	expression tag	UNP E8Y9D8
A	-8	HIS	-	expression tag	UNP E8Y9D8
A	-7	HIS	-	expression tag	UNP E8Y9D8
A	-6	HIS	-	expression tag	UNP E8Y9D8
A	-5	SER	-	expression tag	UNP E8Y9D8
A	-4	MET	-	expression tag	UNP E8Y9D8
A	-3	ASP	-	expression tag	UNP E8Y9D8
A	-2	ILE	-	expression tag	UNP E8Y9D8
A	-1	GLU	-	expression tag	UNP E8Y9D8
A	0	PHE	-	expression tag	UNP E8Y9D8
B	-13	MET	-	expression tag	UNP E8Y9D8
B	-12	SER	-	expression tag	UNP E8Y9D8
B	-11	HIS	-	expression tag	UNP E8Y9D8
B	-10	HIS	-	expression tag	UNP E8Y9D8
B	-9	HIS	-	expression tag	UNP E8Y9D8
B	-8	HIS	-	expression tag	UNP E8Y9D8
B	-7	HIS	-	expression tag	UNP E8Y9D8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP E8Y9D8
B	-5	SER	-	expression tag	UNP E8Y9D8
B	-4	MET	-	expression tag	UNP E8Y9D8
B	-3	ASP	-	expression tag	UNP E8Y9D8
B	-2	ILE	-	expression tag	UNP E8Y9D8
B	-1	GLU	-	expression tag	UNP E8Y9D8
B	0	PHE	-	expression tag	UNP E8Y9D8
C	-13	MET	-	expression tag	UNP E8Y9D8
C	-12	SER	-	expression tag	UNP E8Y9D8
C	-11	HIS	-	expression tag	UNP E8Y9D8
C	-10	HIS	-	expression tag	UNP E8Y9D8
C	-9	HIS	-	expression tag	UNP E8Y9D8
C	-8	HIS	-	expression tag	UNP E8Y9D8
C	-7	HIS	-	expression tag	UNP E8Y9D8
C	-6	HIS	-	expression tag	UNP E8Y9D8
C	-5	SER	-	expression tag	UNP E8Y9D8
C	-4	MET	-	expression tag	UNP E8Y9D8
C	-3	ASP	-	expression tag	UNP E8Y9D8
C	-2	ILE	-	expression tag	UNP E8Y9D8
C	-1	GLU	-	expression tag	UNP E8Y9D8
C	0	PHE	-	expression tag	UNP E8Y9D8
D	-13	MET	-	expression tag	UNP E8Y9D8
D	-12	SER	-	expression tag	UNP E8Y9D8
D	-11	HIS	-	expression tag	UNP E8Y9D8
D	-10	HIS	-	expression tag	UNP E8Y9D8
D	-9	HIS	-	expression tag	UNP E8Y9D8
D	-8	HIS	-	expression tag	UNP E8Y9D8
D	-7	HIS	-	expression tag	UNP E8Y9D8
D	-6	HIS	-	expression tag	UNP E8Y9D8
D	-5	SER	-	expression tag	UNP E8Y9D8
D	-4	MET	-	expression tag	UNP E8Y9D8
D	-3	ASP	-	expression tag	UNP E8Y9D8
D	-2	ILE	-	expression tag	UNP E8Y9D8
D	-1	GLU	-	expression tag	UNP E8Y9D8
D	0	PHE	-	expression tag	UNP E8Y9D8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total	O	0	0
			164	164		

Continued on next page...

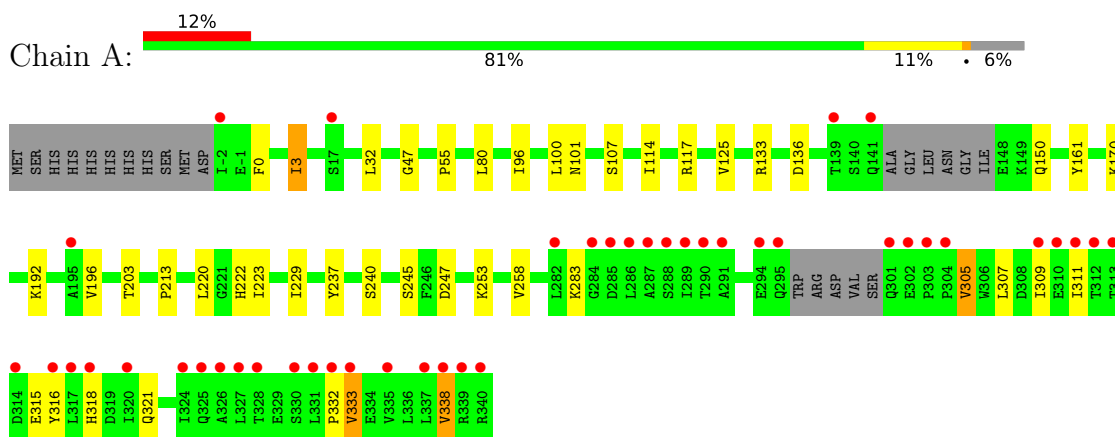
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	194	Total 194	O 194	0	0
4	C	236	Total 236	O 236	0	0
4	D	242	Total 242	O 242	0	0

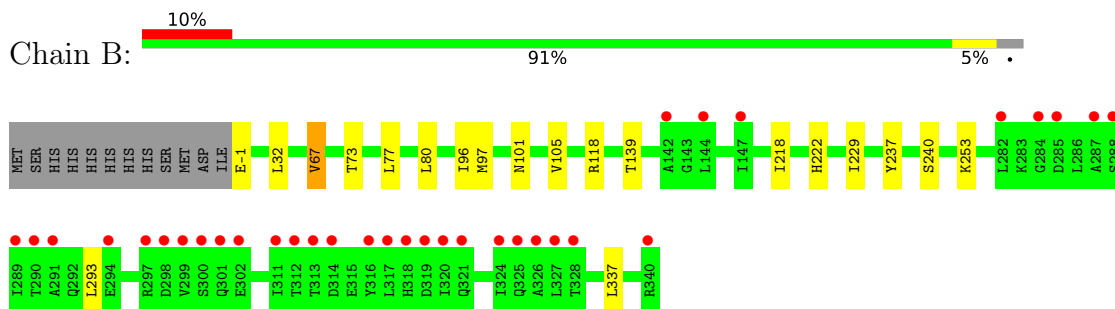
3 Residue-property plots [i](#)

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.

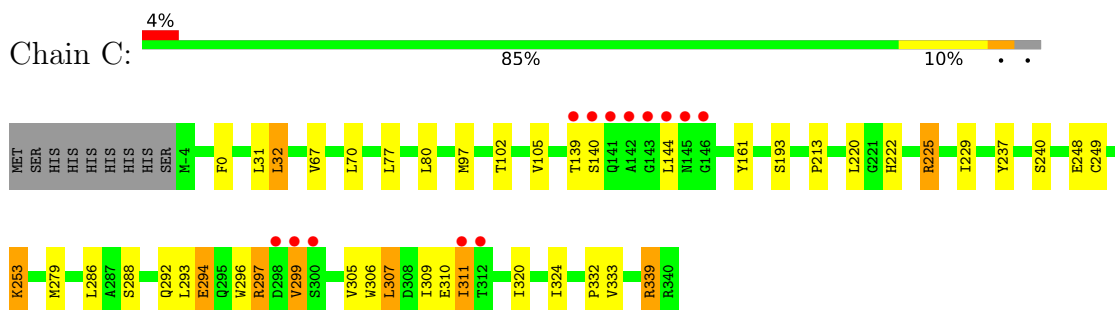
• Molecule 1: Exonuclease subunit SbcD



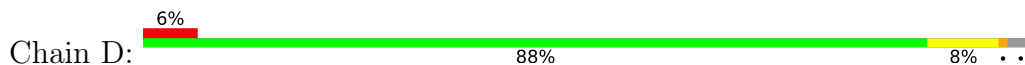
• Molecule 1: Exonuclease subunit SbcD

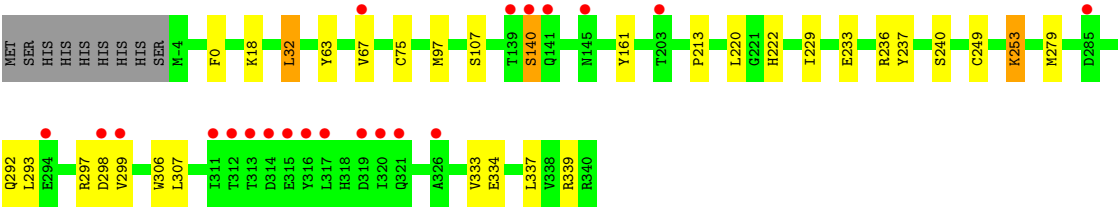


• Molecule 1: Exonuclease subunit SbcD



• Molecule 1: Exonuclease subunit SbcD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.16Å 69.23Å 95.19Å 72.24° 84.00° 83.48°	Depositor
Resolution (Å)	19.97 – 1.83 19.97 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.97-1.83) 97.6 (19.97-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 1.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.162 , 0.199 0.158 , 0.194	Depositor DCC
R_{free} test set	6330 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: MN, GOL

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	0.48	0/2567	0.80	1/3512 (0.0%)
1	B	0.45	0/2662	0.75	0/3646
1	C	0.51	0/2742	0.81	2/3750 (0.1%)
1	D	0.51	0/2714	0.80	1/3713 (0.0%)
All	All	0.49	0/10685	0.79	4/14621 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	LEU	CB-CA-C	-7.85	107.52	116.54
1	C	144	LEU	N-CA-C	7.75	120.09	108.31
1	D	140	SER	N-CA-C	5.20	117.56	110.24
1	A	55	PRO	O-C-N	5.04	123.52	121.15

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	2509	0	2359	22	0
1	B	2600	0	2461	7	0
1	C	2680	0	2595	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2651	0	2555	16	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	164	0	0	1	0
4	B	194	0	0	0	0
4	C	236	0	0	1	0
4	D	242	0	0	0	0
All	All	11308	0	10002	69	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 3.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:O	1:A:333:VAL:HG13	1.55	1.06
1:A:332:PRO:O	1:A:333:VAL:CG1	2.30	0.79
1:C:311:ILE:HD11	1:C:324:ILE:HD11	1.67	0.77
1:A:133[A]:ARG:NH1	1:A:136:ASP:OD2	2.26	0.68
1:D:279[A]:MET:HG2	1:D:306:TRP:HB2	1.78	0.65
1:C:249:CYS:SG	4:C:707:HOH:O	2.55	0.65
1:C:220:LEU:HD12	1:C:229[A]:ILE:HD13	1.83	0.61
1:C:67:VAL:HG11	1:C:97:MET:SD	2.42	0.59
1:A:332:PRO:C	1:A:333:VAL:HG13	2.26	0.59
1:C:279[B]:MET:HG2	1:C:306:TRP:HB2	1.86	0.58
1:C:294:GLU:OE1	1:C:297:ARG:NH2	2.34	0.58
1:D:307:LEU:HD23	1:D:333:VAL:HB	1.85	0.58
1:C:299:VAL:HA	1:C:332:PRO:HG3	1.85	0.58
1:A:220:LEU:HD12	1:A:229:ILE:HD13	1.85	0.58
1:D:67:VAL:HG11	1:D:97:MET:SD	2.44	0.58
1:B:67:VAL:HG11	1:B:97:MET:SD	2.45	0.57
1:D:249:CYS:HB3	1:D:279[B]:MET:HE2	1.86	0.56
1:D:220:LEU:HD12	1:D:229:ILE:HD13	1.90	0.53
1:C:229[B]:ILE:HD11	1:C:237:TYR:CD2	2.44	0.53
1:A:192:LYS:NZ	4:A:591:HOH:O	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HA	1:A:203:THR:O	2.09	0.51
1:B:67:VAL:HG21	1:B:97:MET:SD	2.51	0.51
1:D:337:LEU:HD21	1:D:339:ARG:HD3	1.93	0.51
1:A:161:TYR:HB3	1:A:213:PRO:HD3	1.92	0.50
1:B:80:LEU:HD13	1:B:105:VAL:HB	1.94	0.50
1:A:245:SER:OG	1:A:247:ASP:OD1	2.26	0.50
1:B:67:VAL:HG23	1:B:77:LEU:HD23	1.96	0.48
1:A:196:VAL:HG11	1:A:223:ILE:HD13	1.96	0.48
1:C:161:TYR:HB3	1:C:213:PRO:HD3	1.96	0.47
1:A:309:ILE:HB	1:A:338:VAL:HG12	1.96	0.47
1:B:73:THR:O	1:B:118:ARG:NH1	2.47	0.47
1:C:220:LEU:HD12	1:C:229[A]:ILE:CD1	2.46	0.46
1:A:240:SER:O	1:A:253[A]:LYS:HD3	2.16	0.46
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.69	0.46
1:C:139:THR:HA	1:C:140:SER:HA	1.65	0.46
1:C:240:SER:O	1:C:253[B]:LYS:HD3	2.16	0.46
1:A:3:ILE:HG13	1:A:258:VAL:HB	1.99	0.45
1:C:296:TRP:NE1	1:C:305:VAL:HG21	2.32	0.45
1:C:307:LEU:HD22	1:C:333:VAL:HB	1.99	0.45
1:D:229:ILE:HD11	1:D:237:TYR:CD2	2.52	0.45
1:C:32:LEU:HD12	1:C:32:LEU:HA	1.82	0.45
1:C:70:LEU:CD2	1:C:77:LEU:HB2	2.47	0.45
1:C:310:GLU:CD	1:C:339:ARG:HD2	2.43	0.44
1:D:233:GLU:O	1:D:236:ARG:HD3	2.17	0.44
1:A:318:HIS:O	1:A:321:GLN:HB2	2.18	0.44
1:A:315:GLU:O	1:A:316:TYR:C	2.60	0.44
1:D:67:VAL:HG21	1:D:97:MET:SD	2.58	0.43
1:D:161:TYR:HB3	1:D:213:PRO:HD3	2.00	0.43
1:D:240:SER:O	1:D:253[B]:LYS:HD3	2.18	0.43
1:D:297:ARG:O	1:D:298:ASP:CB	2.67	0.43
1:B:229[B]:ILE:HD11	1:B:237:TYR:CD2	2.53	0.43
1:C:249:CYS:HB3	1:C:279[B]:MET:HE3	2.01	0.43
1:A:0:PHE:O	1:A:117:ARG:NH1	2.51	0.42
1:A:47:GLY:HA2	1:A:80:LEU:O	2.18	0.42
1:A:114:ILE:HD13	1:A:125:VAL:HG22	2.01	0.42
1:C:253[A]:LYS:HE3	1:C:253[A]:LYS:HA	2.01	0.42
1:A:229:ILE:HD11	1:A:237:TYR:CD2	2.54	0.42
1:C:309[B]:ILE:HG22	1:C:311:ILE:HG12	2.01	0.42
1:A:305:VAL:CG1	1:A:333:VAL:HG11	2.50	0.42
1:C:225:ARG:NH1	1:C:248:GLU:OE1	2.53	0.41
1:D:63:TYR:CE1	1:D:97:MET:HE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:MET:HB3	1:C:102:THR:HB	2.02	0.41
1:A:305:VAL:HG22	1:A:307:LEU:HD22	2.02	0.41
1:C:80:LEU:HD13	1:C:105:VAL:HB	2.03	0.41
1:B:240:SER:O	1:B:253[A]:LYS:HD3	2.20	0.41
1:C:288:SER:O	1:C:292:GLN:HG3	2.21	0.41
1:D:18:LYS:NZ	1:D:334:GLU:OE2	2.35	0.41
1:D:32:LEU:HD12	1:D:32:LEU:HA	1.88	0.40
1:D:339:ARG:HE	1:D:339:ARG:HB2	1.63	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	331/354 (94%)	317 (96%)	11 (3%)	3 (1%)	14	4
1	B	345/354 (98%)	334 (97%)	10 (3%)	1 (0%)	36	25
1	C	352/354 (99%)	340 (97%)	10 (3%)	2 (1%)	21	9
1	D	350/354 (99%)	337 (96%)	12 (3%)	1 (0%)	36	25
All	All	1378/1416 (97%)	1328 (96%)	43 (3%)	7 (0%)	24	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ILE
1	C	222	HIS
1	D	222	HIS
1	A	222	HIS
1	B	222	HIS
1	C	299	VAL
1	A	333	VAL

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	251/303 (83%)	241 (96%)	10 (4%)	28	11
1	B	265/303 (88%)	256 (97%)	9 (3%)	32	15
1	C	278/303 (92%)	262 (94%)	16 (6%)	18	4
1	D	273/303 (90%)	262 (96%)	11 (4%)	28	11
All	All	1067/1212 (88%)	1021 (96%)	46 (4%)	28	8

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	32	LEU
1	A	96[A]	ILE
1	A	96[B]	ILE
1	A	100	LEU
1	A	101	ASN
1	A	107	SER
1	A	283	LYS
1	A	305	VAL
1	A	338	VAL
1	B	-1	GLU
1	B	32	LEU
1	B	67	VAL
1	B	96	ILE
1	B	101	ASN
1	B	139	THR
1	B	218	ILE
1	B	293	LEU
1	B	337	LEU
1	C	0	PHE
1	C	31[A]	LEU
1	C	31[B]	LEU
1	C	32	LEU
1	C	193	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	225	ARG
1	C	253[A]	LYS
1	C	253[B]	LYS
1	C	286	LEU
1	C	293	LEU
1	C	294	GLU
1	C	297	ARG
1	C	307	LEU
1	C	311	ILE
1	C	320	ILE
1	C	339	ARG
1	D	0	PHE
1	D	32	LEU
1	D	75[A]	CYS
1	D	75[B]	CYS
1	D	107	SER
1	D	140	SER
1	D	253[A]	LYS
1	D	253[B]	LYS
1	D	292	GLN
1	D	293	LEU
1	D	299	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	175	GLN
1	C	71	GLN
1	C	101	ASN
1	C	152	HIS
1	D	25	GLN
1	D	71	GLN
1	D	101	ASN
1	D	164	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
2	GOL	D	401	-	5,5,5	0.58	0	5,5,5	0.74	0
2	GOL	B	401	-	5,5,5	0.53	0	5,5,5	1.17	1 (20%)
2	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	C	401	-	5,5,5	0.35	0	5,5,5	0.34	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
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GOL	O3-C3-C2	-2.03	101.24	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	332/354 (93%)	0.42	44 (13%) 7 7	10, 31, 52, 79	93 (28%)
1	B	342/354 (96%)	0.15	34 (9%) 13 13	10, 28, 48, 73	84 (24%)
1	C	345/354 (97%)	-0.15	13 (3%) 44 48	7, 25, 54, 65	42 (12%)
1	D	345/354 (97%)	-0.08	21 (6%) 27 28	9, 24, 65, 77	35 (10%)
All	All	1364/1416 (96%)	0.08	112 (8%) 17 18	7, 27, 54, 79	254 (18%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	THR	8.8
1	C	299	VAL	7.1
1	D	299	VAL	6.7
1	A	311	ILE	6.6
1	C	298	ASP	6.5
1	A	287	ALA	6.3
1	D	316	TYR	6.2
1	A	288	SER	6.1
1	C	142	ALA	6.0
1	C	300	SER	6.0
1	A	313	THR	5.9
1	D	313	THR	5.8
1	A	295	GLN	5.4
1	A	303	PRO	5.3
1	A	335	VAL	5.2
1	A	294	GLU	4.9
1	B	326	ALA	4.9
1	A	286	LEU	4.9
1	A	333	VAL	4.9
1	D	314	ASP	4.8
1	C	143	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	331	LEU	4.7
1	A	332	PRO	4.6
1	A	282	LEU	4.6
1	B	312	THR	4.5
1	A	289	ILE	4.5
1	B	311	ILE	4.4
1	B	316	TYR	4.3
1	C	139	THR	4.3
1	C	141	GLN	4.2
1	B	324	ILE	4.2
1	B	147	ILE	4.2
1	B	291	ALA	4.2
1	A	304	PRO	4.1
1	A	327	LEU	4.1
1	D	315	GLU	4.0
1	B	313	THR	4.0
1	A	309	ILE	4.0
1	A	141	GLN	3.9
1	D	141	GLN	3.8
1	A	310	GLU	3.8
1	A	328	THR	3.8
1	B	287	ALA	3.8
1	B	299	VAL	3.8
1	C	145	ASN	3.8
1	B	317	LEU	3.8
1	B	298	ASP	3.8
1	B	318	HIS	3.7
1	A	316	TYR	3.6
1	D	319	ASP	3.6
1	C	144	LEU	3.6
1	D	145	ASN	3.6
1	B	327	LEU	3.5
1	A	291	ALA	3.4
1	D	326	ALA	3.4
1	A	284	GLY	3.3
1	A	139	THR	3.3
1	D	285	ASP	3.3
1	A	314	ASP	3.2
1	C	140	SER	3.2
1	C	146	GLY	3.2
1	A	301	GLN	3.2
1	B	142	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	3.2
1	B	320	ILE	3.2
1	D	312	THR	3.2
1	A	330	SER	3.1
1	A	340	ARG	3.1
1	A	-2	ILE	3.1
1	A	324	ILE	3.0
1	B	319	ASP	3.0
1	B	321	GLN	3.0
1	A	326	ALA	3.0
1	B	314	ASP	2.9
1	B	290	THR	2.9
1	B	328	THR	2.9
1	A	325	GLN	2.8
1	B	297	ARG	2.8
1	B	325	GLN	2.8
1	D	139	THR	2.8
1	B	144	LEU	2.7
1	B	285	ASP	2.7
1	D	294	GLU	2.7
1	D	298	ASP	2.7
1	A	320	ILE	2.7
1	D	140	SER	2.7
1	D	321	GLN	2.7
1	D	317	LEU	2.7
1	B	301	GLN	2.6
1	C	311	ILE	2.6
1	D	311	ILE	2.6
1	A	318	HIS	2.5
1	A	339	ARG	2.5
1	A	285	ASP	2.5
1	B	282	LEU	2.5
1	B	340	ARG	2.4
1	A	195	ALA	2.4
1	B	288	SER	2.3
1	B	284	GLY	2.3
1	B	294	GLU	2.2
1	C	312	THR	2.2
1	D	67	VAL	2.2
1	A	302	GLU	2.2
1	D	320	ILE	2.2
1	B	300	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	203	THR	2.1
1	B	289	ILE	2.1
1	B	302	GLU	2.1
1	A	317	LEU	2.1
1	A	337	LEU	2.1
1	A	17	SER	2.0
1	A	290	THR	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
3	MN	C	403	1/1	0.53	0.53	23,23,23,23	1
3	MN	D	403	1/1	0.53	0.41	19,19,19,19	1
3	MN	A	402	1/1	0.85	0.14	63,63,63,63	1
3	MN	B	403	1/1	0.90	0.20	82,82,82,82	1
2	GOL	B	401	6/6	0.91	0.09	24,27,29,31	0
2	GOL	D	401	6/6	0.91	0.09	30,31,32,33	0
3	MN	B	402	1/1	0.92	0.19	67,67,67,67	1
2	GOL	A	401	6/6	0.94	0.07	23,28,29,32	0
3	MN	D	402	1/1	0.95	0.18	57,57,57,57	1
3	MN	A	403	1/1	0.95	0.21	67,67,67,67	1
3	MN	C	402	1/1	0.96	0.20	69,69,69,69	1
2	GOL	C	401	6/6	0.96	0.07	28,29,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.