



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:31 PM GMT

PDB ID : 4LTY
Title : Crystal Structure of E.coli SbcD at 1.8 Å Resolution
Authors : Liu, S.; Tian, L.F.; Yan, X.X.; Liang, D.C.
Deposited on : 2013-07-24
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

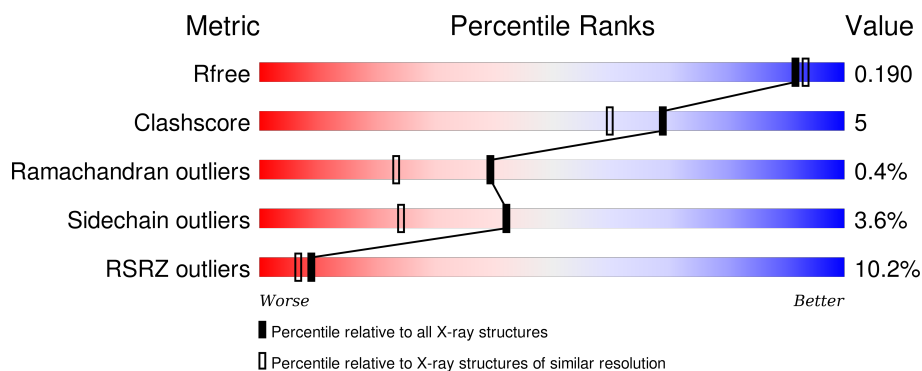
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>7%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	B	354	<div> <div>10%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	C	354	<div> <div>13%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>
1	D	354	<div> <div>9%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11300 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	C	328	Total	C	N	O	S	0	2	0
			2449	1559	429	452	9			
1	B	342	Total	C	N	O	S	0	3	0
			2577	1634	451	483	9			
1	A	345	Total	C	N	O	S	0	11	0
			2697	1718	469	498	12			
1	D	345	Total	C	N	O	S	0	14	0
			2708	1724	476	497	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

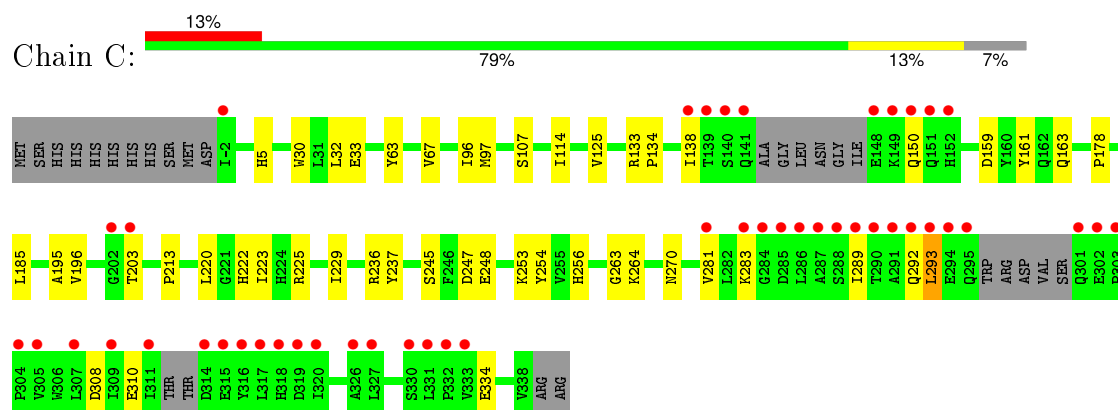
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	171	Total	O	0	0
			171	171		
3	B	206	Total	O	0	0
			206	206		
3	A	231	Total	O	0	0
			231	231		
3	D	237	Total	O	0	0
			237	237		

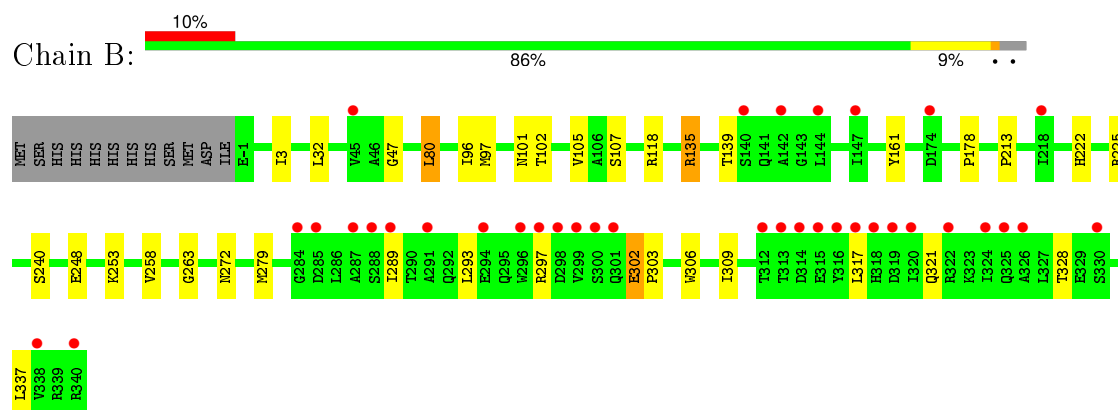
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

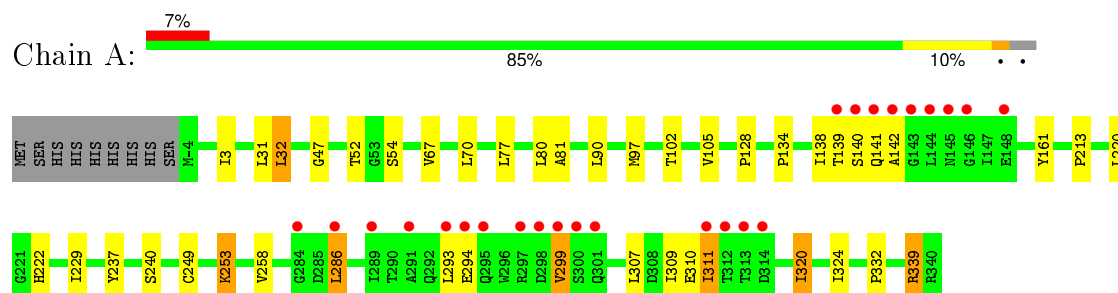
- Molecule 1: Exonuclease subunit SbcD



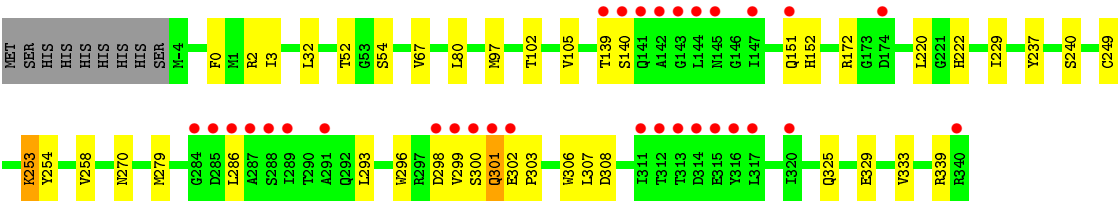
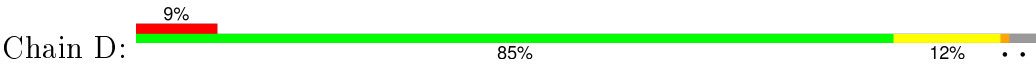
- Molecule 1: Exonuclease subunit SbcD



- 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	62.14Å 69.36Å 95.02Å 72.21° 84.10° 83.77°	Depositor
Resolution (Å)	19.86 – 1.80 32.92 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.86-1.80) 86.7 (32.92-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.156 , 0.193 0.154 , 0.190	Depositor DCC
R_{free} test set	6632 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 144904 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11300	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: 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	0.43	0/2759	0.61	0/3773
1	B	0.36	0/2639	0.56	1/3615 (0.0%)
1	C	0.37	0/2506	0.56	0/3428
1	D	0.43	0/2771	0.61	0/3790
All	All	0.40	0/10675	0.59	1/14606 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	LEU	CA-CB-CG	5.04	126.89	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	A	2697	0	2611	26	0
1	B	2577	0	2431	18	0
1	C	2449	0	2303	25	0
1	D	2708	0	2606	25	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	231	0	0	0	0
3	B	206	0	0	6	0
3	C	171	0	0	2	0
3	D	237	0	0	5	0
All	All	11300	0	9983	94	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 5.

All (94) 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:2:ARG:HD3	3:D:726:HOH:O	1.43	1.17
1:D:52[B]:THR:HG23	1:D:54:SER:H	1.35	0.90
1:A:311:ILE:HD11	1:A:324:ILE:HD11	1.60	0.84
1:D:302:GLU:CB	1:D:303:PRO:HD3	2.10	0.82
1:A:52[A]:THR:HG23	1:A:54:SER:H	1.49	0.76
1:C:236:ARG:NH2	3:C:670:HOH:O	2.21	0.71
1:D:151[A]:GLN:NE2	3:D:682:HOH:O	2.25	0.69
1:A:32:LEU:HD11	1:A:70:LEU:HD13	1.74	0.69
1:D:2:ARG:NH1	3:D:726:HOH:O	2.23	0.68
1:D:302:GLU:CB	1:D:303:PRO:CD	2.73	0.67
1:B:118:ARG:NH2	3:B:693:HOH:O	2.27	0.67
1:A:299:VAL:HA	1:A:332:PRO:HG3	1.77	0.66
1:B:135:ARG:NH2	3:B:695:HOH:O	2.28	0.65
1:D:220:LEU:HD12	1:D:229:ILE:HD13	1.77	0.65
1:D:249:CYS:HB3	1:D:279[B]:MET:HE2	1.79	0.65
1:D:279[A]:MET:HG2	1:D:306:TRP:HB2	1.78	0.64
1:D:52[B]:THR:HG23	1:D:54:SER:N	2.13	0.61
1:A:220:LEU:HD12	1:A:229[A]:ILE:HD13	1.82	0.61
1:A:67:VAL:HG11	1:A:97:MET:SD	2.41	0.61
1:D:307:LEU:HD23	1:D:333:VAL:HB	1.83	0.60
1:D:67:VAL:HG11	1:D:97:MET:SD	2.42	0.60
1:C:289:ILE:O	1:C:293:LEU:HD22	2.01	0.60
1:D:301:GLN:HA	1:D:301:GLN:NE2	2.17	0.60
1:A:134:PRO:O	1:A:138:ILE:HG13	2.02	0.59
1:C:220:LEU:HD12	1:C:229:ILE:HD13	1.85	0.59
1:C:159:ASP:OD2	1:C:163:GLN:NE2	2.37	0.58
1:A:229[B]:ILE:HD11	1:A:237:TYR:CD2	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LEU:O	1:B:321:GLN:N	2.31	0.56
1:C:67:VAL:HG11	1:C:97:MET:SD	2.45	0.56
1:C:107:SER:HB2	3:C:665:HOH:O	2.04	0.56
1:C:63:TYR:O	1:C:67:VAL:HG23	2.07	0.54
1:B:135:ARG:HG2	3:B:694:HOH:O	2.08	0.53
1:C:178:PRO:HD3	1:C:263:GLY:HA2	1.90	0.53
1:B:80:LEU:HD13	1:B:105:VAL:HB	1.91	0.52
1:B:302:GLU:HG3	1:B:303:PRO:HA	1.91	0.52
1:A:220:LEU:HD12	1:A:229[A]:ILE:CD1	2.39	0.52
1:B:240:SER:O	1:B:253[B]:LYS:HD3	2.11	0.51
1:C:195:ALA:HB2	1:C:245:SER:HB3	1.93	0.51
1:B:289:ILE:HD13	1:B:309:ILE:HG23	1.91	0.51
1:C:114:ILE:HD13	1:C:125:VAL:HG22	1.93	0.50
1:C:225:ARG:NH2	1:C:248:GLU:OE2	2.39	0.48
1:B:272:ASN:ND2	3:B:703:HOH:O	2.21	0.48
1:C:281:VAL:HG22	1:C:308:ASP:HB3	1.96	0.48
1:C:229:ILE:HD11	1:C:237:TYR:CD2	2.48	0.47
1:D:229:ILE:HD11	1:D:237:TYR:CD2	2.49	0.47
1:C:245:SER:OG	1:C:247:ASP:OD1	2.30	0.47
1:D:296:TRP:O	1:D:298:ASP:HA	2.15	0.47
1:A:80:LEU:HD13	1:A:105:VAL:HB	1.96	0.47
1:D:80:LEU:HD13	1:D:105:VAL:HB	1.96	0.47
1:A:310:GLU:OE1	1:A:339:ARG:HD2	2.15	0.46
1:A:3:ILE:HG13	1:A:258:VAL:HB	1.97	0.46
1:D:325:GLN:O	1:D:329:GLU:HG2	2.15	0.46
1:A:139:THR:HA	1:A:140:SER:HA	1.56	0.46
1:A:253[A]:LYS:HE3	1:A:253[A]:LYS:HA	1.97	0.46
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.54	0.46
1:D:3:ILE:HG13	1:D:258:VAL:HB	1.98	0.46
1:A:81:ALA:HB2	1:A:90[A]:LEU:HD12	1.98	0.45
1:A:240:SER:O	1:A:253[B]:LYS:HD3	2.16	0.45
1:A:286:LEU:HG	1:A:320:ILE:HD11	1.98	0.45
1:D:240:SER:O	1:D:253[B]:LYS:HD3	2.15	0.45
1:C:161:TYR:HB3	1:C:213:PRO:HD3	1.97	0.45
1:A:52[A]:THR:HG23	1:A:54:SER:N	2.26	0.45
1:C:196:VAL:HG11	1:C:223:ILE:HD13	1.99	0.45
1:D:254:TYR:CD2	1:D:270:ASN:HB3	2.52	0.44
1:B:225:ARG:NH2	1:B:248:GLU:OE1	2.50	0.44
1:A:161:TYR:HB3	1:A:213:PRO:HD3	1.99	0.44
1:B:279:MET:HG2	1:B:306:TRP:HB2	2.00	0.44
1:B:178:PRO:HD3	1:B:263:GLY:HA2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ASP:CG	1:D:339:ARG:HH21	2.21	0.43
1:B:3:ILE:HG13	1:B:258:VAL:HB	2.01	0.43
1:D:97:MET:HB3	1:D:102:THR:HB	2.00	0.43
1:C:150:GLN:HA	1:C:203:THR:O	2.17	0.42
1:C:254:TYR:CD2	1:C:270:ASN:HB3	2.54	0.42
1:D:139:THR:O	1:D:152:HIS:NE2	2.51	0.42
1:D:172[A]:ARG:HD2	3:D:587:HOH:O	2.19	0.42
1:C:223:ILE:HA	1:C:223:ILE:HD13	1.87	0.42
1:B:97:MET:HB3	1:B:102:THR:HB	2.02	0.42
1:B:279:MET:HE3	3:B:700:HOH:O	2.20	0.42
1:D:172[A]:ARG:NH1	3:D:587:HOH:O	2.53	0.42
1:A:141:GLN:HG3	1:A:142:ALA:N	2.35	0.42
1:C:283:LYS:HG2	1:C:310:GLU:HB3	2.00	0.42
1:C:5:HIS:HB3	1:C:256:HIS:HB2	2.02	0.42
1:A:70:LEU:HD23	1:A:77:LEU:HB2	2.02	0.41
1:A:47:GLY:HA2	1:A:80:LEU:O	2.21	0.41
1:C:134:PRO:O	1:C:138:ILE:HG12	2.20	0.41
1:C:253[A]:LYS:HA	1:C:253[A]:LYS:HE2	2.03	0.41
1:A:97:MET:HB3	1:A:102:THR:HB	2.02	0.41
1:A:105:VAL:HG21	1:A:128:PRO:HB2	2.02	0.41
1:C:30:TRP:HA	1:C:33:GLU:HG2	2.02	0.41
1:A:309:ILE:HG22	1:A:311:ILE:HG12	2.03	0.40
1:B:47:GLY:HA2	1:B:80:LEU:O	2.21	0.40
1:B:107:SER:HB2	3:B:690:HOH:O	2.20	0.40
1:B:161:TYR:HB3	1:B:213:PRO:HD3	2.03	0.40
1:C:225:ARG:HE	1:C:225:ARG:HB2	1.69	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	354/354 (100%)	342 (97%)	10 (3%)	2 (1%)	30	14
1	B	343/354 (97%)	334 (97%)	8 (2%)	1 (0%)	46	29
1	C	322/354 (91%)	305 (95%)	16 (5%)	1 (0%)	46	29
1	D	357/354 (101%)	342 (96%)	13 (4%)	2 (1%)	30	14
All	All	1376/1416 (97%)	1323 (96%)	47 (3%)	6 (0%)	39	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	HIS
1	C	222	HIS
1	B	222	HIS
1	A	222	HIS
1	A	299	VAL
1	D	299	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	281/303 (93%)	267 (95%)	14 (5%)	30	13
1	B	260/303 (86%)	250 (96%)	10 (4%)	40	22
1	C	243/303 (80%)	235 (97%)	8 (3%)	45	27
1	D	279/303 (92%)	270 (97%)	9 (3%)	46	29
All	All	1063/1212 (88%)	1022 (96%)	41 (4%)	42	21

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	LEU
1	C	96	ILE
1	C	133	ARG
1	C	185	LEU
1	C	264	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	292	GLN
1	C	293	LEU
1	C	334	GLU
1	B	32	LEU
1	B	96	ILE
1	B	101	ASN
1	B	135	ARG
1	B	139	THR
1	B	293	LEU
1	B	297	ARG
1	B	302	GLU
1	B	328	THR
1	B	337	LEU
1	A	31[A]	LEU
1	A	31[B]	LEU
1	A	32	LEU
1	A	249[A]	CYS
1	A	249[B]	CYS
1	A	253[A]	LYS
1	A	253[B]	LYS
1	A	286	LEU
1	A	293	LEU
1	A	294	GLU
1	A	307	LEU
1	A	311	ILE
1	A	320	ILE
1	A	339	ARG
1	D	0	PHE
1	D	32	LEU
1	D	140	SER
1	D	253[A]	LYS
1	D	253[B]	LYS
1	D	286	LEU
1	D	293	LEU
1	D	300	SER
1	D	301	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	A	401	-	5,5,5	0.29	0	5,5,5	0.35	0
2	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	C	401	-	5,5,5	0.61	0	5,5,5	1.24	1 (20%)
2	GOL	D	401	-	5,5,5	0.56	0	5,5,5	0.83	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	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	GOL	O3-C3-C2	-2.20	99.52	110.18

There are no chirality outliers.

There are no torsion outliers.

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	345/354 (97%)	-0.08	25 (7%) 18 14	13, 26, 70, 98	29 (8%)
1	B	342/354 (96%)	0.17	36 (10%) 8 6	15, 32, 90, 105	57 (16%)
1	C	328/354 (92%)	0.41	47 (14%) 4 2	15, 34, 84, 97	64 (19%)
1	D	345/354 (97%)	0.04	31 (8%) 12 9	13, 26, 78, 99	24 (6%)
All	All	1360/1416 (96%)	0.13	139 (10%) 9 6	13, 29, 81, 105	174 (12%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	12.3
1	A	143	GLY	11.8
1	D	316	TYR	11.7
1	C	139	THR	9.5
1	D	299	VAL	8.8
1	D	142	ALA	8.6
1	B	316	TYR	8.5
1	C	284	GLY	8.1
1	C	287	ALA	7.7
1	C	140	SER	7.4
1	D	143	GLY	7.3
1	D	313	THR	6.9
1	D	144	LEU	6.6
1	B	299	VAL	6.3
1	A	142	ALA	6.2
1	C	317	LEU	6.2
1	D	317	LEU	6.2
1	D	314	ASP	6.1
1	C	320	ILE	6.0
1	A	298	ASP	6.0
1	B	317	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	SER	5.9
1	C	289	ILE	5.8
1	C	148	GLU	5.8
1	C	141	GLN	5.7
1	D	311	ILE	5.7
1	A	299	VAL	5.5
1	B	330	SER	5.4
1	C	316	TYR	5.2
1	C	309	ILE	5.0
1	A	139	THR	4.9
1	D	300	SER	4.9
1	D	312	THR	4.8
1	C	331	LEU	4.7
1	C	295	GLN	4.7
1	C	326	ALA	4.7
1	D	141	GLN	4.6
1	D	286	LEU	4.6
1	C	288	SER	4.6
1	A	141	GLN	4.4
1	C	149	LYS	4.4
1	C	311	ILE	4.2
1	D	315	GLU	4.2
1	C	302	GLU	4.1
1	C	150	GLN	4.1
1	C	138	ILE	4.1
1	C	333	VAL	4.1
1	C	293	LEU	4.1
1	D	285	ASP	4.1
1	D	298	ASP	4.0
1	C	290	THR	3.9
1	D	287	ALA	3.9
1	D	284	GLY	3.9
1	C	332	PRO	3.9
1	D	139	THR	3.8
1	C	286	LEU	3.7
1	B	315	GLU	3.7
1	B	142	ALA	3.7
1	B	144	LEU	3.6
1	B	300	SER	3.6
1	C	330	SER	3.5
1	C	291	ALA	3.5
1	C	315	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	284	GLY	3.4
1	C	285	ASP	3.4
1	B	289	ILE	3.3
1	B	298	ASP	3.3
1	B	312	THR	3.3
1	B	301	GLN	3.3
1	A	145	ASN	3.3
1	A	313	THR	3.2
1	D	302	GLU	3.2
1	B	318	HIS	3.1
1	B	326	ALA	3.1
1	B	297	ARG	3.0
1	B	340	ARG	3.0
1	B	320	ILE	3.0
1	B	285	ASP	3.0
1	C	301	GLN	2.9
1	C	303	PRO	2.9
1	B	319	ASP	2.9
1	C	318	HIS	2.9
1	C	314	ASP	2.9
1	C	283	LYS	2.9
1	C	327	LEU	2.8
1	A	312	THR	2.8
1	D	140	SER	2.8
1	D	174[A]	ASP	2.8
1	A	314	ASP	2.8
1	A	148	GLU	2.8
1	C	307	LEU	2.7
1	A	289	ILE	2.7
1	A	286	LEU	2.7
1	C	151	GLN	2.7
1	B	314	ASP	2.6
1	B	147	ILE	2.6
1	D	301	GLN	2.6
1	B	313	THR	2.6
1	A	146	GLY	2.6
1	C	304	PRO	2.5
1	D	145	ASN	2.5
1	A	300	SER	2.5
1	A	311	ILE	2.5
1	C	152	HIS	2.5
1	A	291	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	291	ALA	2.4
1	C	305	VAL	2.4
1	D	147	ILE	2.4
1	B	45	VAL	2.4
1	B	338	VAL	2.4
1	A	301	GLN	2.4
1	B	287	ALA	2.4
1	B	218	ILE	2.4
1	B	296	TRP	2.4
1	B	294	GLU	2.4
1	D	289	ILE	2.3
1	B	322	ARG	2.3
1	C	203	THR	2.3
1	B	174	ASP	2.3
1	D	340	ARG	2.3
1	C	319	ASP	2.3
1	B	140	SER	2.2
1	C	292	GLN	2.2
1	A	294	GLU	2.2
1	B	291	ALA	2.2
1	A	297	ARG	2.2
1	D	320	ILE	2.2
1	B	325	GLN	2.2
1	C	294	GLU	2.2
1	C	-2	ILE	2.2
1	D	151[A]	GLN	2.2
1	C	202	GLY	2.1
1	A	284	GLY	2.1
1	B	324	ILE	2.0
1	B	288	SER	2.0
1	A	293	LEU	2.0
1	C	281	VAL	2.0
1	A	295	GLN	2.0
1	D	288	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	C	401	6/6	0.95	0.08	1.60	24,31,31,32	0
2	GOL	B	401	6/6	0.96	0.09	1.52	24,27,29,29	0
2	GOL	D	401	6/6	0.91	0.10	0.79	27,32,32,33	0
2	GOL	A	401	6/6	0.93	0.09	0.11	30,31,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.