Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 02:28 PM EDT

PDB ID	:	4LTY
Title	:	Crystal Structure of E.coli SbcD at 1.8 A 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
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:

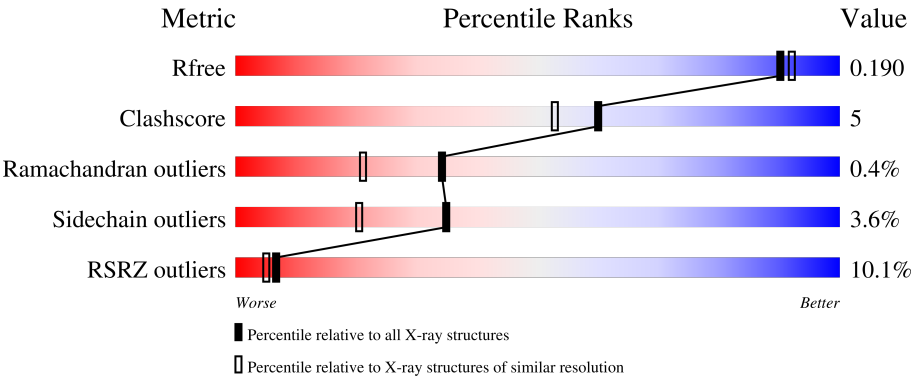
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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
1	A	354	7% 85% 10%
1	B	354	10% 86% 9%
1	C	354	13% 79% 13% 7%
1	D	354	9% 85% 12%

2 Entry composition (i)

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:

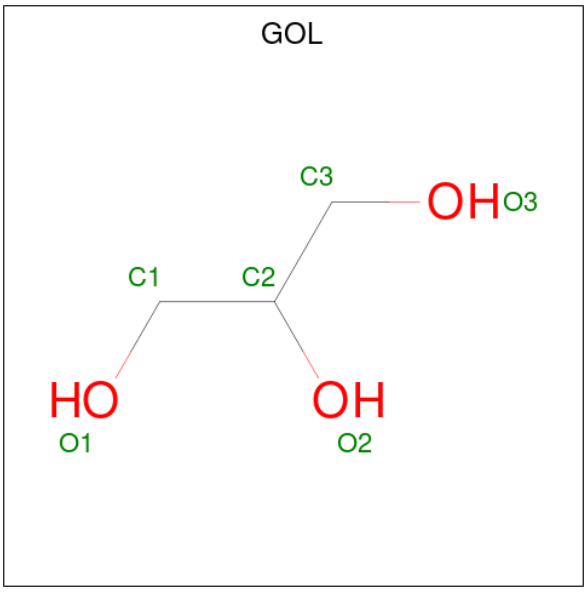
Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	expression tag	UNP E8Y9D8
C	-12	SER	-	expression tag	UNP E8Y9D8
C	-11	HIS	-	expression tag	UNP E8Y9D8
C	-10	HIS	-	expression tag	UNP E8Y9D8
C	-9	HIS	-	expression tag	UNP E8Y9D8
C	-8	HIS	-	expression tag	UNP E8Y9D8
C	-7	HIS	-	expression tag	UNP 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 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

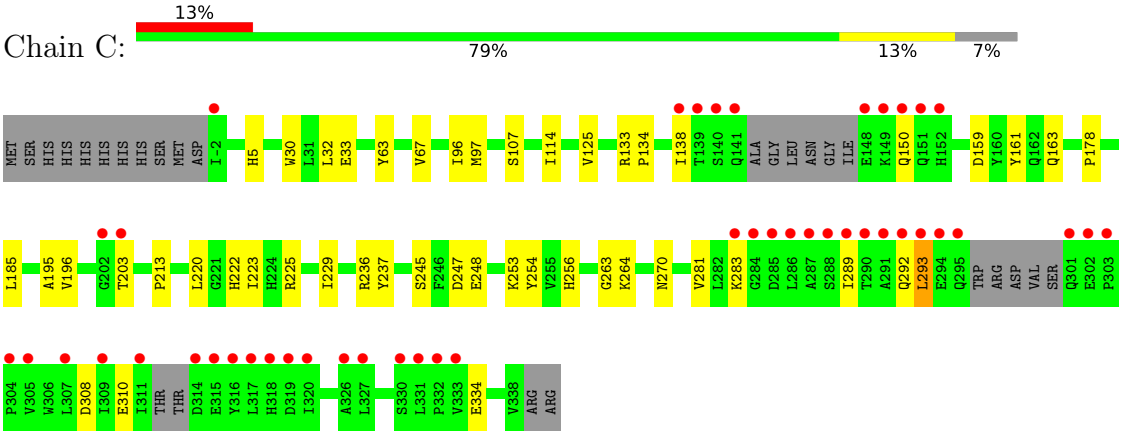
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	171	Total O 171 171	0	0
3	B	206	Total O 206 206	0	0
3	A	231	Total O 231 231	0	0
3	D	237	Total O 237 237	0	0

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.

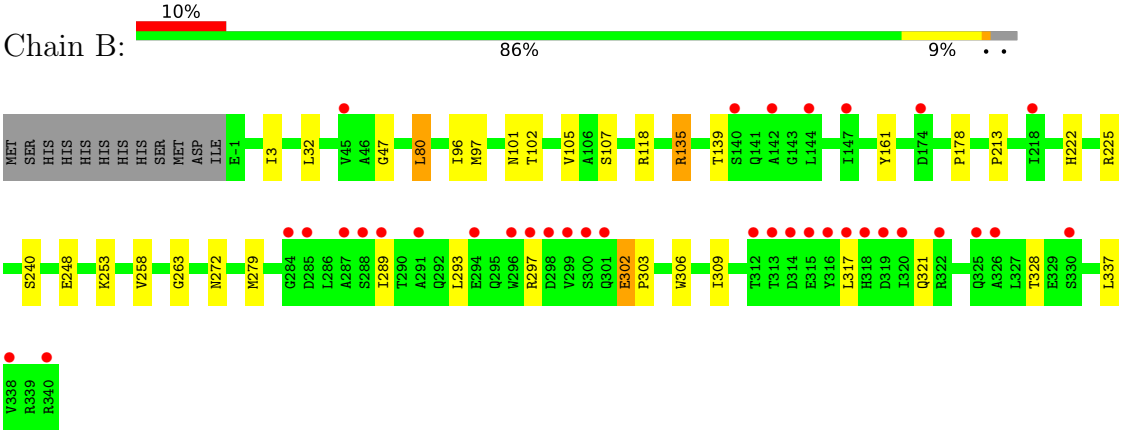
• Molecule 1: Exonuclease subunit SbcD

Chain C:



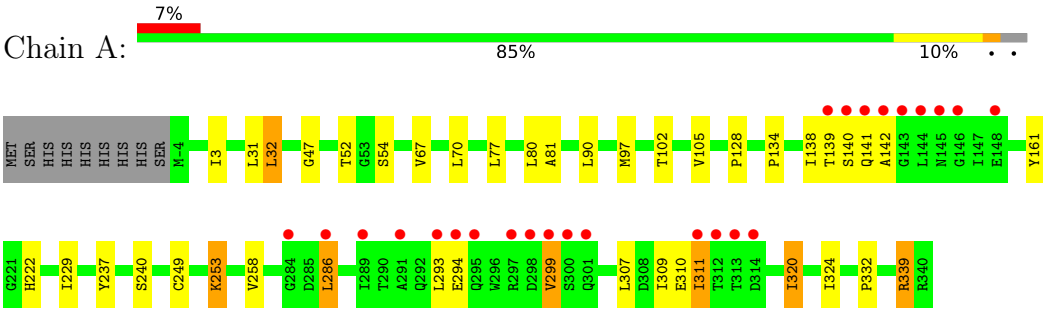
• Molecule 1: Exonuclease subunit SbcD

Chain B:



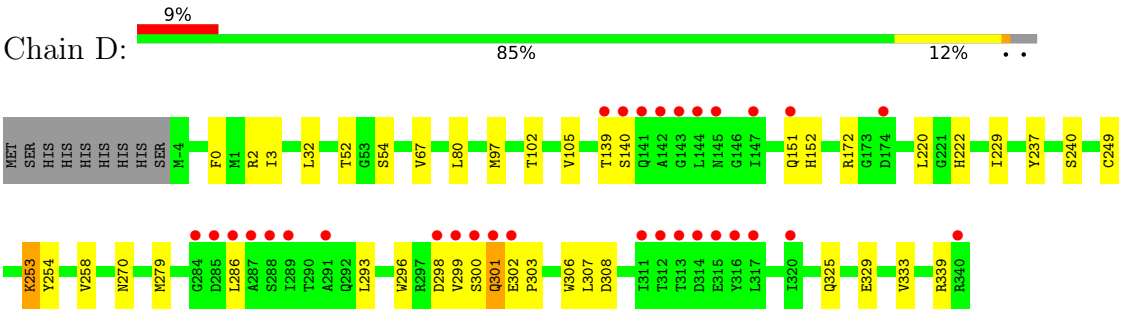
• Molecule 1: Exonuclease subunit SbcD

Chain A:



• Molecule 1: Exonuclease subunit SbcD

Chain D:



4 Data and refinement statistics (i)

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) 95.9 (32.92-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	7221 reflections (4.98%)	wwPDB-VP
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 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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

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:NE2	1:D:301:GLN:HA	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:C:67:VAL:HG11	1:C:97:MET:SD	2.45	0.56
1:B:317:LEU:O	1:B:321:GLN:N	2.31	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:C:195:ALA:HB2	1:C:245:SER:HB3	1.93	0.51
1:B:240:SER:O	1:B:253[B]:LYS:HD3	2.11	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:HA	1:A:253[A]:LYS:HE3	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:C:196:VAL:HG11	1:C:223:ILE:HD13	1.99	0.45
1:A:52[A]:THR:HG23	1:A:54:SER:N	2.26	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:HD13	1:C:223:ILE:HA	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:C:134:PRO:O	1:C:138:ILE:HG12	2.20	0.41
1:A:47:GLY:HA2	1:A:80:LEU:O	2.21	0.41
1:C:253[A]:LYS:HA	1:C:253[A]:LYS:HE2	2.03	0.41
1:C:30:TRP:HA	1:C:33:GLU:HG2	2.02	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: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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	354/354 (100%)	342 (97%)	10 (3%)	2 (1%)	25 12
1	B	343/354 (97%)	334 (97%)	8 (2%)	1 (0%)	41 27
1	C	322/354 (91%)	305 (95%)	16 (5%)	1 (0%)	41 27
1	D	357/354 (101%)	342 (96%)	13 (4%)	2 (1%)	25 12
All	All	1376/1416 (97%)	1323 (96%)	47 (3%)	6 (0%)	34 21

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 (i)

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%)	24 10
1	B	260/303 (86%)	250 (96%)	10 (4%)	33 18
1	C	243/303 (80%)	235 (97%)	8 (3%)	38 23
1	D	279/303 (92%)	270 (97%)	9 (3%)	39 25
All	All	1063/1212 (88%)	1022 (96%)	41 (4%)	35 17

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

Sometimes 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 monosaccharides 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	B	401	-	5,5,5	0.37	0	5,5,5	0.35	0
2	GOL	A	401	-	5,5,5	0.30	0	5,5,5	0.35	0
2	GOL	D	401	-	5,5,5	0.55	0	5,5,5	0.83	0
2	GOL	C	401	-	5,5,5	0.57	0	5,5,5	1.24	1 (20%)

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	B	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	GOL	O3-C3-C2	-2.23	99.52	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	GOL	C1-C2-C3-O3
2	C	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, 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	A	345/354 (97%)	-0.10	25 (7%) 15 12	13, 26, 70, 98	29 (8%)
1	B	342/354 (96%)	0.15	35 (10%) 6 5	15, 32, 90, 105	57 (16%)
1	C	328/354 (92%)	0.38	46 (14%) 2 2	15, 34, 84, 97	64 (19%)
1	D	345/354 (97%)	0.01	31 (8%) 9 7	13, 26, 78, 99	24 (6%)
All	All	1360/1416 (96%)	0.11	137 (10%) 7 5	13, 29, 81, 105	174 (12%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	12.1
1	A	143	GLY	11.8
1	D	316	TYR	11.6
1	C	139	THR	9.3
1	D	142	ALA	8.5
1	D	299	VAL	8.5
1	B	316	TYR	8.4
1	C	284	GLY	7.9
1	C	287	ALA	7.5
1	C	140	SER	7.2
1	D	143	GLY	7.2
1	D	313	THR	6.7
1	D	144	LEU	6.4
1	A	142	ALA	6.2
1	B	299	VAL	6.2
1	C	317	LEU	6.1
1	B	317	LEU	6.0
1	D	317	LEU	6.0
1	D	314	ASP	6.0
1	A	298	ASP	5.9
1	C	320	ILE	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	SER	5.8
1	C	289	ILE	5.8
1	C	148	GLU	5.7
1	C	141	GLN	5.6
1	D	311	ILE	5.6
1	A	299	VAL	5.5
1	B	330	SER	5.4
1	C	316	TYR	5.1
1	A	139	THR	4.9
1	C	309	ILE	4.8
1	D	300	SER	4.8
1	D	312	THR	4.7
1	C	326	ALA	4.7
1	D	141	GLN	4.6
1	C	331	LEU	4.6
1	C	288	SER	4.6
1	C	295	GLN	4.5
1	D	286	LEU	4.5
1	C	149	LYS	4.4
1	A	141	GLN	4.4
1	C	311	ILE	4.2
1	C	302	GLU	4.2
1	C	150	GLN	4.1
1	D	315	GLU	4.1
1	D	285	ASP	4.0
1	C	138	ILE	4.0
1	C	333	VAL	4.0
1	C	293	LEU	4.0
1	C	290	THR	3.9
1	D	298	ASP	3.9
1	D	284	GLY	3.8
1	D	287	ALA	3.8
1	D	139	THR	3.8
1	C	332	PRO	3.8
1	B	315	GLU	3.6
1	B	300	SER	3.6
1	B	142	ALA	3.6
1	C	286	LEU	3.6
1	B	144	LEU	3.5
1	C	330	SER	3.5
1	C	315	GLU	3.5
1	C	291	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	145	ASN	3.4
1	B	284	GLY	3.4
1	B	301	GLN	3.3
1	B	298	ASP	3.3
1	B	312	THR	3.3
1	C	285	ASP	3.3
1	B	289	ILE	3.2
1	A	313	THR	3.2
1	D	302	GLU	3.2
1	B	318	HIS	3.1
1	B	320	ILE	3.0
1	B	340	ARG	3.0
1	B	326	ALA	3.0
1	B	297	ARG	2.9
1	B	285	ASP	2.9
1	C	327	LEU	2.9
1	C	283	LYS	2.9
1	C	318	HIS	2.9
1	C	303	PRO	2.9
1	C	301	GLN	2.8
1	A	312	THR	2.8
1	B	319	ASP	2.8
1	C	314	ASP	2.8
1	A	148	GLU	2.8
1	A	314	ASP	2.8
1	D	140	SER	2.8
1	D	174[A]	ASP	2.7
1	C	307	LEU	2.7
1	A	289	ILE	2.7
1	A	286	LEU	2.7
1	C	151	GLN	2.6
1	D	301	GLN	2.6
1	B	314	ASP	2.6
1	B	147	ILE	2.5
1	A	146	GLY	2.5
1	C	304	PRO	2.5
1	B	313	THR	2.5
1	D	145	ASN	2.5
1	B	296	TRP	2.5
1	C	152	HIS	2.4
1	A	291	ALA	2.4
1	D	291	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	300	SER	2.4
1	A	301	GLN	2.4
1	B	322	ARG	2.4
1	A	311	ILE	2.4
1	C	305	VAL	2.4
1	B	294	GLU	2.4
1	B	287	ALA	2.3
1	D	147	ILE	2.3
1	B	45	VAL	2.3
1	B	338	VAL	2.3
1	D	289	ILE	2.3
1	B	174	ASP	2.3
1	B	218	ILE	2.3
1	D	340	ARG	2.3
1	C	203	THR	2.3
1	B	291	ALA	2.3
1	C	319	ASP	2.3
1	C	292	GLN	2.2
1	D	320	ILE	2.2
1	C	294	GLU	2.2
1	A	297	ARG	2.2
1	A	294	GLU	2.2
1	B	325	GLN	2.2
1	B	140	SER	2.2
1	D	151[A]	GLN	2.2
1	C	202	GLY	2.1
1	C	-2	ILE	2.1
1	B	288	SER	2.1
1	A	284	GLY	2.0
1	A	295	GLN	2.0
1	A	293	LEU	2.0
1	D	288	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 monosaccharides in this entry.

6.4 Ligands

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(Å^2)	Q<0.9
2	GOL	D	401	6/6	0.91	0.10	27,32,32,33	0
2	GOL	A	401	6/6	0.92	0.10	30,31,32,35	0
2	GOL	C	401	6/6	0.94	0.08	24,31,31,32	0
2	GOL	B	401	6/6	0.96	0.09	24,27,29,29	0

6.5 Other polymers

There are no such residues in this entry.