Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:31 PM GMT

PDB ID	:	4LU9
Title	:	Crystal structure of E.coli SbcD at 2.5 angstrom resolution
Authors	:	Liu, S.; Tian, L.F.; Yan, X.X.; Liang, D.C.
Deposited on	:	2013-07-25
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

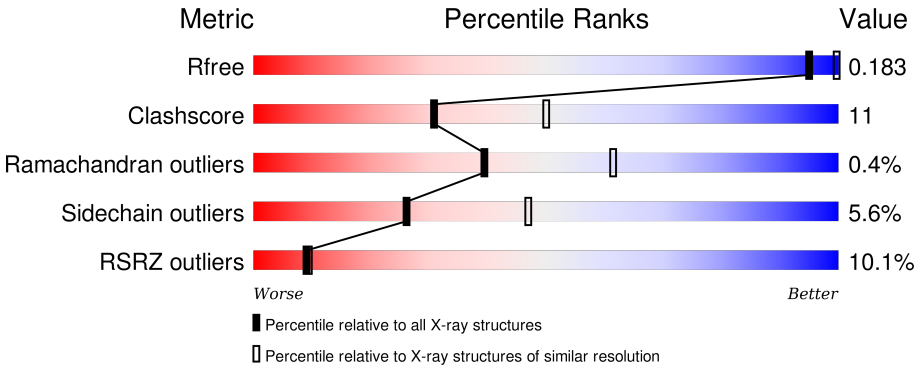
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	5% 77% 16%
1	B	354	10% 78% 18%
1	C	354	13% 71% 20% 5%
1	D	354	11% 78% 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	401	-	-	X	-
2	GOL	B	401	-	-	X	X
2	GOL	D	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10939 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	336	Total	C	N	O	S	0	0	0
			2559	1629	446	475	9			
1	B	342	Total	C	N	O	S	0	0	0
			2579	1637	450	483	9			
1	A	343	Total	C	N	O	S	0	0	0
			2611	1659	457	486	9			
1	D	344	Total	C	N	O	S	0	0	0
			2583	1641	453	480	9			

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

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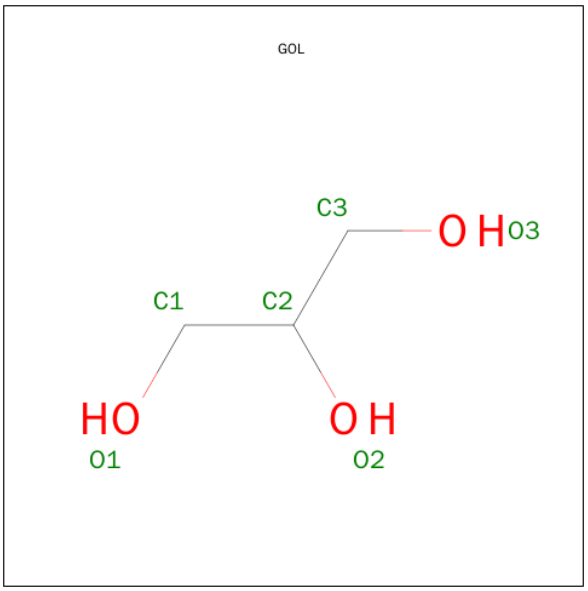
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP E8Y9D8
B	-5	SER	-	EXPRESSION TAG	UNP E8Y9D8
B	-4	MET	-	EXPRESSION TAG	UNP E8Y9D8
B	-3	ASP	-	EXPRESSION TAG	UNP E8Y9D8
B	-2	ILE	-	EXPRESSION TAG	UNP E8Y9D8
B	-1	GLU	-	EXPRESSION TAG	UNP E8Y9D8
B	0	PHE	-	EXPRESSION TAG	UNP E8Y9D8
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.

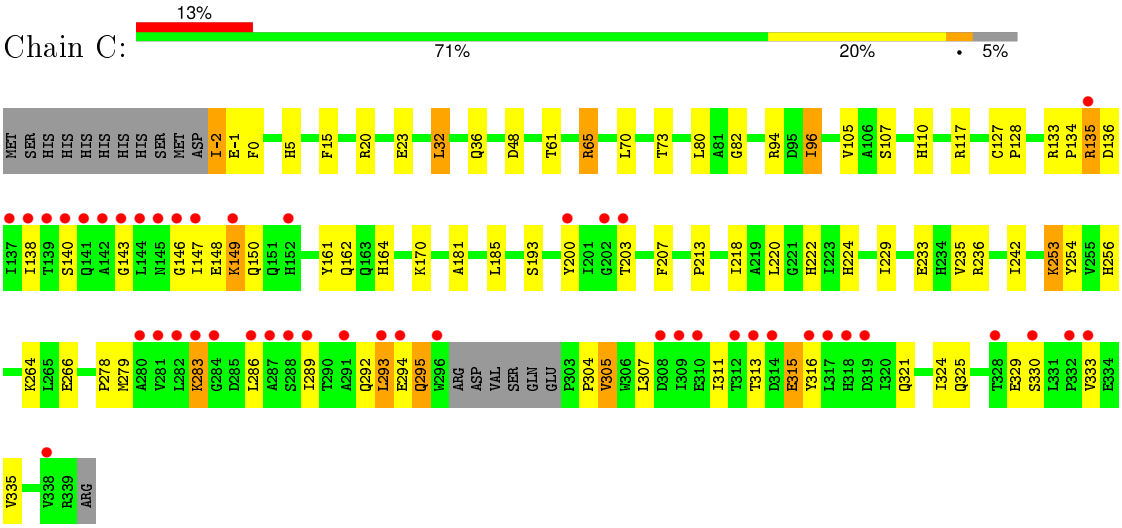
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	132	Total O 132 132	0	0
3	B	135	Total O 135 135	0	0
3	A	164	Total O 164 164	0	0
3	D	152	Total O 152 152	0	0

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.

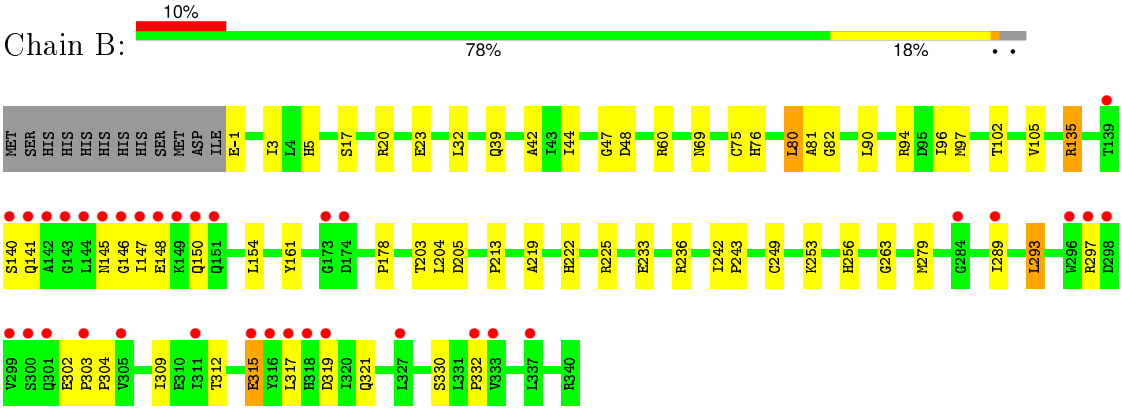
- Molecule 1: Exonuclease subunit SbcD

Chain C:



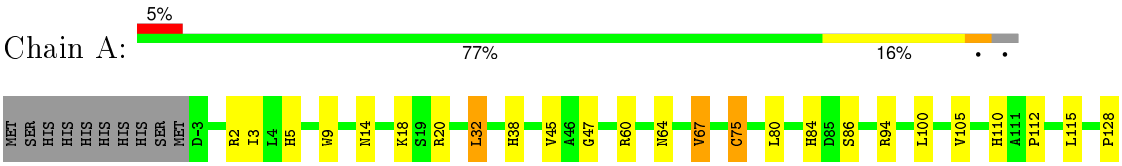
- Molecule 1: Exonuclease subunit SbcD

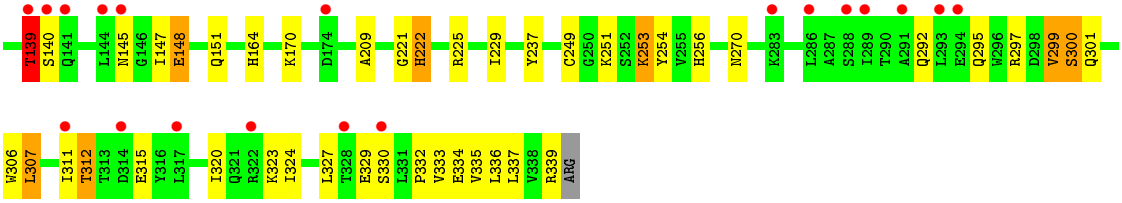
Chain B:



- Molecule 1: Exonuclease subunit SbcD

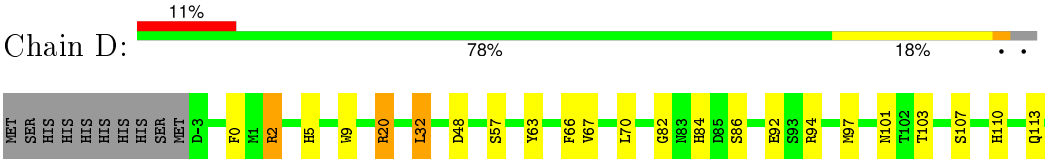
Chain A:





- 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	61.36Å 69.11Å 94.23Å 72.35° 84.24° 83.56°	Depositor
Resolution (Å)	20.00 – 2.50 37.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.50) 88.9 (37.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.176 , 0.235 0.191 , 0.183	Depositor DCC
R_{free} test set	2528 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 49713 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10939	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/2673	0.68	2/3654 (0.1%)
1	B	0.47	0/2641	0.63	2/3613 (0.1%)
1	C	0.51	1/2621 (0.0%)	0.64	3/3580 (0.1%)
1	D	0.51	1/2645 (0.0%)	0.65	1/3620 (0.0%)
All	All	0.51	2/10580 (0.0%)	0.65	8/14467 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	GLU	CD-OE1	-5.07	1.20	1.25
1	D	161	TYR	CE1-CZ	-5.05	1.31	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	80	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	139	THR	CB-CA-C	5.74	127.10	111.60
1	B	80	LEU	CA-CB-CG	5.67	128.35	115.30
1	B	315	GLU	CB-CA-C	5.67	121.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	20	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	295	GLN	CB-CA-C	-5.49	99.43	110.40
1	A	300	SER	N-CA-C	-5.43	96.33	111.00
1	C	295	GLN	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	THR	Peptide
1	C	254	TYR	Peptide
1	D	254	TYR	Peptide

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	2611	0	2531	57	0
1	B	2579	0	2468	52	0
1	C	2559	0	2477	59	0
1	D	2583	0	2471	55	0
2	A	6	0	8	5	0
2	B	6	0	8	6	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
3	A	164	0	0	21	0
3	B	135	0	0	9	0
3	C	132	0	0	22	0
3	D	152	0	0	25	0
All	All	10939	0	9979	221	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 11.

All (221) 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:299:VAL:CB	1:A:300:SER:HA	1.66	1.22
1:C:127:CYS:HB2	3:C:606:HOH:O	1.46	1.15
1:A:45:VAL:HG13	3:A:616:HOH:O	1.46	1.14
1:B:253:LYS:HE3	3:B:623:HOH:O	1.50	1.09
1:B:315:GLU:CB	1:B:319:ASP:CB	2.31	1.08
1:D:70:LEU:HD12	3:D:613:HOH:O	1.56	1.03
1:A:32:LEU:HD23	3:A:624:HOH:O	1.58	1.01
1:A:299:VAL:CB	1:A:300:SER:CA	2.39	1.01
1:A:38:HIS:HE1	3:A:625:HOH:O	1.42	1.01
1:C:207:PHE:HE1	3:C:601:HOH:O	1.46	0.96
1:B:141:GLN:H	1:B:150:GLN:HE21	1.06	0.94
1:D:307:LEU:HD23	1:D:333:VAL:HB	1.58	0.86
1:D:315:GLU:CB	3:D:540:HOH:O	2.24	0.85
1:B:32:LEU:HD21	1:B:69:ASN:HB3	1.60	0.83
3:A:619:HOH:O	1:D:0:PHE:HE2	1.60	0.82
1:A:75:CYS:CB	3:A:632:HOH:O	2.27	0.82
1:A:60:ARG:HH11	2:A:401:GOL:H11	1.43	0.82
1:B:279:MET:SD	3:B:626:HOH:O	2.42	0.77
1:B:141:GLN:N	1:B:150:GLN:HE21	1.84	0.76
1:D:320:ILE:CB	3:D:652:HOH:O	2.34	0.76
1:B:141:GLN:H	1:B:150:GLN:NE2	1.82	0.75
1:B:302:GLU:HB3	1:B:303:PRO:HA	1.69	0.75
3:C:579:HOH:O	1:B:39:GLN:HG2	1.88	0.74
1:A:225:ARG:HH21	1:A:251:LYS:HE3	1.53	0.74
1:C:289:ILE:O	1:C:293:LEU:HD12	1.87	0.74
1:A:60:ARG:HH11	2:A:401:GOL:C1	2.01	0.74
1:A:75:CYS:HB2	3:A:632:HOH:O	1.86	0.73
1:A:251:LYS:HD2	3:A:651:HOH:O	1.89	0.72
1:A:9:TRP:CE2	3:A:616:HOH:O	2.44	0.71
1:C:279:MET:HE3	3:C:616:HOH:O	1.91	0.70
1:A:60:ARG:NH1	2:A:401:GOL:H11	2.05	0.69
1:B:225:ARG:HG3	3:B:618:HOH:O	1.92	0.69
1:B:302:GLU:HG2	1:B:304:PRO:HD3	1.74	0.69
1:B:20:ARG:NH2	1:B:243:PRO:O	2.24	0.69
1:C:65:ARG:HG2	3:A:611:HOH:O	1.94	0.68
1:B:60:ARG:HH11	2:B:401:GOL:C1	2.07	0.68
1:D:236:ARG:HG3	3:D:637:HOH:O	1.94	0.66
1:A:254:TYR:CD2	1:A:270:ASN:HB3	2.31	0.66
1:C:150:GLN:HA	1:C:203:THR:O	1.95	0.66
1:D:307:LEU:CD2	1:D:333:VAL:HB	2.26	0.65
1:B:135:ARG:HG2	3:B:505:HOH:O	1.95	0.65
1:D:63:TYR:O	1:D:67:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:GLU:HA	3:D:649:HOH:O	1.95	0.65
1:C:304:PRO:HD3	3:C:631:HOH:O	1.96	0.65
1:C:220:LEU:HD12	1:C:229:ILE:HD13	1.79	0.65
1:D:134:PRO:O	1:D:138:ILE:HG12	1.98	0.64
1:C:181:ALA:CB	3:C:606:HOH:O	2.45	0.64
1:C:279:MET:CE	3:C:616:HOH:O	2.46	0.63
1:C:94:ARG:HD2	3:C:592:HOH:O	1.99	0.63
1:D:67:VAL:HG11	1:D:97:MET:SD	2.40	0.62
1:A:9:TRP:NE1	3:A:616:HOH:O	2.33	0.61
1:C:181:ALA:HB1	3:C:606:HOH:O	2.00	0.61
1:C:-2:ILE:N	3:C:576:HOH:O	2.34	0.60
1:C:311:ILE:HG12	1:C:313:THR:OG1	2.02	0.60
1:B:302:GLU:CB	1:B:303:PRO:HA	2.32	0.59
1:B:20:ARG:NH1	1:B:242:ILE:HD12	2.17	0.59
1:B:236:ARG:HD2	3:B:619:HOH:O	2.02	0.59
1:C:278:PRO:HB2	1:C:305:VAL:HB	1.84	0.59
1:B:3:ILE:HD13	1:B:44:ILE:HD12	1.84	0.59
1:B:146:GLY:HA3	1:B:148:GLU:N	2.18	0.59
1:B:302:GLU:HA	1:B:303:PRO:C	2.23	0.59
1:D:57:SER:N	3:D:616:HOH:O	2.35	0.59
1:B:94:ARG:HD2	3:B:509:HOH:O	2.03	0.59
1:D:302:GLU:CB	1:D:303:PRO:HD3	2.33	0.58
1:B:289:ILE:HD13	1:B:309:ILE:HG23	1.85	0.58
1:A:337:LEU:HD21	1:A:339:ARG:HE	1.69	0.58
1:A:253:LYS:CE	3:A:654:HOH:O	2.51	0.58
1:A:225:ARG:HG3	3:A:651:HOH:O	2.03	0.58
1:A:253:LYS:NZ	3:A:654:HOH:O	2.24	0.58
1:B:48:ASP:H	1:B:82:GLY:HA3	1.70	0.57
1:D:94:ARG:HD2	3:D:622:HOH:O	2.03	0.57
1:C:48:ASP:H	1:C:82:GLY:HA3	1.69	0.57
1:D:103:THR:HG21	1:D:113:GLN:HE22	1.69	0.57
1:B:20:ARG:HD2	1:B:23:GLU:OE2	2.04	0.57
1:C:305:VAL:HG13	1:C:333:VAL:HG12	1.87	0.57
1:B:5:HIS:CD2	1:B:219:ALA:HB1	2.40	0.56
1:C:61:THR:O	1:C:65:ARG:HG3	2.05	0.56
1:A:64:ASN:O	1:A:67:VAL:HG12	2.05	0.56
1:D:32:LEU:CD1	3:D:613:HOH:O	2.54	0.56
1:A:14:ASN:ND2	1:D:0:PHE:CD2	2.75	0.55
1:C:286:LEU:H	1:C:286:LEU:HD12	1.70	0.55
1:C:96:ILE:HD11	1:A:67:VAL:HG11	1.89	0.55
1:A:306:TRP:HB3	1:A:336:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:GOL:H2	3:D:621:HOH:O	2.06	0.55
1:D:320:ILE:N	3:D:652:HOH:O	2.39	0.54
1:A:147:ILE:HG22	1:A:151:GLN:HE21	1.72	0.54
1:A:5:HIS:HB3	1:A:256:HIS:HB2	1.89	0.54
1:A:2:ARG:HD2	3:A:626:HOH:O	2.07	0.54
1:B:140:SER:HA	1:B:150:GLN:HG3	1.90	0.54
1:A:60:ARG:HG2	2:A:401:GOL:H12	1.90	0.54
1:D:217:TYR:HE1	3:D:637:HOH:O	1.90	0.53
1:B:81:ALA:HB2	1:B:90:LEU:HD12	1.89	0.53
1:A:47:GLY:HA2	1:A:80:LEU:O	2.08	0.53
1:C:36:GLN:HG2	1:C:73:THR:HG22	1.91	0.53
1:D:2:ARG:HH11	1:D:2:ARG:CG	2.21	0.53
1:A:299:VAL:HA	1:A:332:PRO:HG3	1.89	0.53
1:D:66:PHE:HA	3:D:526:HOH:O	2.08	0.53
1:C:283:LYS:O	1:C:292:GLN:NE2	2.41	0.53
1:B:178:PRO:HD3	1:B:263:GLY:HA2	1.89	0.53
1:B:289:ILE:O	1:B:293:LEU:HB2	2.08	0.52
1:B:5:HIS:HB3	1:B:256:HIS:HB2	1.92	0.52
1:D:84:HIS:HE1	3:D:501:HOH:O	1.93	0.52
1:C:146:GLY:O	1:C:149:LYS:NZ	2.38	0.51
1:C:315:GLU:HG2	1:C:316:TYR:N	2.25	0.51
1:B:302:GLU:HB3	1:B:303:PRO:CA	2.40	0.51
1:C:143:GLY:CA	3:C:598:HOH:O	2.58	0.51
1:A:84:HIS:HE1	3:A:501:HOH:O	1.93	0.51
1:B:146:GLY:HA3	1:B:147:ILE:C	2.31	0.51
1:A:14:ASN:ND2	1:D:0:PHE:HD2	2.09	0.51
1:D:251:LYS:HE3	3:D:643:HOH:O	2.10	0.51
1:A:45:VAL:CG1	3:A:616:HOH:O	2.26	0.50
1:B:60:ARG:HH11	2:B:401:GOL:H12	1.77	0.50
1:D:127:CYS:HB2	1:D:181:ALA:HA	1.94	0.50
1:B:317:LEU:O	1:B:321:GLN:HG3	2.12	0.50
1:C:133:ARG:HD3	1:C:136:ASP:OD2	2.12	0.49
1:A:229:ILE:HD11	1:A:237:TYR:CD2	2.47	0.49
1:C:233:GLU:HG2	3:C:614:HOH:O	2.11	0.49
1:C:48:ASP:N	1:C:82:GLY:HA3	2.28	0.49
1:C:133:ARG:HB3	1:C:135:ARG:NH2	2.27	0.49
1:B:-1:GLU:N	3:B:569:HOH:O	2.45	0.49
1:D:110:HIS:HD2	3:D:624:HOH:O	1.96	0.49
1:C:110:HIS:O	1:C:164:HIS:NE2	2.39	0.48
1:A:323:LYS:O	1:A:327:LEU:HD13	2.13	0.48
1:D:311:ILE:HG22	1:D:339:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HA	1:B:42:ALA:O	2.13	0.48
1:D:311:ILE:HG13	1:D:312:THR:N	2.28	0.48
1:D:32:LEU:HD11	3:D:613:HOH:O	2.13	0.48
1:A:145:ASN:O	1:A:148:GLU:HB2	2.14	0.48
1:A:253:LYS:HE2	3:A:654:HOH:O	2.11	0.48
1:D:32:LEU:HD12	3:D:613:HOH:O	2.13	0.48
1:C:307:LEU:HD23	1:C:333:VAL:HB	1.96	0.47
1:D:236:ARG:CG	3:D:637:HOH:O	2.57	0.47
1:C:143:GLY:HA3	3:C:598:HOH:O	2.13	0.47
1:C:110:HIS:HE1	3:C:592:HOH:O	1.98	0.47
1:A:292:GLN:O	1:A:295:GLN:HB3	2.13	0.47
1:C:-1:GLU:HB2	3:C:578:HOH:O	2.14	0.47
1:B:302:GLU:CB	1:B:303:PRO:CA	2.92	0.47
1:D:220:LEU:HD12	1:D:229:ILE:HD13	1.97	0.47
1:C:313:THR:HG23	3:C:618:HOH:O	2.14	0.47
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.97	0.46
1:D:2:ARG:HH11	1:D:2:ARG:HG3	1.80	0.46
1:A:307:LEU:HD22	1:A:333:VAL:HB	1.96	0.46
1:B:154:LEU:HB2	1:B:204:LEU:HD13	1.98	0.46
1:A:311:ILE:CG1	1:A:312:THR:N	2.79	0.46
1:B:332:PRO:HB2	3:B:631:HOH:O	2.15	0.46
1:C:218:ILE:HG13	1:C:235:VAL:HG22	1.97	0.46
1:D:313:THR:CB	3:D:647:HOH:O	2.63	0.46
1:C:48:ASP:H	1:C:82:GLY:CA	2.29	0.46
1:A:324:ILE:CG2	1:A:335:VAL:HG21	2.45	0.46
1:D:250:GLY:HA3	3:D:643:HOH:O	2.15	0.45
1:C:20:ARG:NH2	1:C:242:ILE:HD12	2.31	0.45
1:B:80:LEU:HD13	1:B:105:VAL:HB	1.98	0.45
1:C:236:ARG:HD3	3:C:612:HOH:O	2.17	0.45
1:A:60:ARG:NH1	2:A:401:GOL:C1	2.73	0.45
1:D:217:TYR:CE1	3:D:637:HOH:O	2.56	0.45
1:C:324:ILE:HG13	1:C:325:GLN:N	2.31	0.45
1:D:133:ARG:HD2	3:D:523:HOH:O	2.17	0.45
1:B:297:ARG:HD3	1:B:297:ARG:HA	1.74	0.44
1:A:18:LYS:NZ	1:A:334:GLU:OE2	2.32	0.44
1:B:48:ASP:H	1:B:82:GLY:CA	2.30	0.44
1:D:5:HIS:CD2	1:D:238:CYS:HG	2.36	0.44
1:C:5:HIS:HB3	1:C:256:HIS:HB2	1.99	0.44
1:A:67:VAL:HG13	1:A:100:LEU:HD22	1.99	0.44
1:C:15:PHE:HB2	1:C:20:ARG:HD3	2.00	0.44
1:B:47:GLY:HA2	1:B:80:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ILE:HG13	1:C:148:GLU:H	1.81	0.44
1:B:60:ARG:HH11	2:B:401:GOL:H11	1.80	0.44
1:C:305:VAL:HG22	1:C:307:LEU:HD22	2.00	0.44
1:B:161:TYR:HB3	1:B:213:PRO:HD3	1.99	0.44
1:D:225:ARG:NE	3:D:639:HOH:O	2.50	0.44
1:C:105:VAL:HG21	1:C:128:PRO:HB2	1.99	0.43
1:D:311:ILE:HG13	1:D:312:THR:H	1.83	0.43
1:B:60:ARG:HG2	2:B:401:GOL:H12	2.00	0.43
1:D:2:ARG:HG3	1:D:2:ARG:NH1	2.32	0.43
1:C:294:GLU:CB	3:C:574:HOH:O	2.67	0.43
1:A:105:VAL:HG21	1:A:128:PRO:HB2	2.01	0.43
1:D:296:TRP:NE1	1:D:305:VAL:HG21	2.33	0.43
1:C:138:ILE:C	1:C:140:SER:N	2.72	0.43
1:C:293:LEU:O	1:C:295:GLN:O	2.36	0.43
1:D:223:ILE:HD13	1:D:237:TYR:CZ	2.54	0.43
1:C:148:GLU:HA	3:C:515:HOH:O	2.18	0.43
1:A:139:THR:HA	1:A:140:SER:HA	1.86	0.43
1:A:329:GLU:O	1:A:330:SER:CB	2.67	0.43
1:C:220:LEU:HD12	1:C:229:ILE:CD1	2.48	0.43
1:D:229:ILE:HD11	1:D:237:TYR:CD2	2.54	0.43
1:D:5:HIS:CD2	1:D:238:CYS:SG	3.12	0.43
1:D:139:THR:HA	1:D:140:SER:HA	1.61	0.43
1:A:3:ILE:C	1:A:3:ILE:HD12	2.39	0.43
1:B:23:GLU:HG3	3:B:517:HOH:O	2.19	0.42
1:D:181:ALA:O	1:D:218:ILE:HA	2.19	0.42
1:C:207:PHE:CE1	3:C:601:HOH:O	2.36	0.42
1:B:42:ALA:HA	1:B:76:HIS:O	2.19	0.42
1:A:147:ILE:H	1:A:147:ILE:HD12	1.84	0.42
1:C:161:TYR:HB3	1:C:213:PRO:HD3	2.00	0.42
1:C:32:LEU:HD21	1:C:70:LEU:HA	2.02	0.42
1:A:221:GLY:O	1:A:222:HIS:CB	2.67	0.42
1:D:9:TRP:CD1	1:D:241:PRO:HG3	2.55	0.42
1:A:9:TRP:CD1	3:A:616:HOH:O	2.73	0.41
1:D:20:ARG:NH2	1:D:243:PRO:O	2.42	0.41
1:D:48:ASP:H	1:D:82:GLY:HA3	1.85	0.41
1:A:301:GLN:HB2	1:A:332:PRO:HB2	2.02	0.41
1:C:325:GLN:O	1:C:329:GLU:HG3	2.20	0.41
1:C:224:HIS:HD2	3:C:627:HOH:O	2.02	0.41
1:B:60:ARG:NH1	2:B:401:GOL:C1	2.78	0.41
1:B:97:MET:HB3	1:B:102:THR:HB	2.03	0.41
3:A:619:HOH:O	1:D:0:PHE:CE2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:CD	3:A:626:HOH:O	2.66	0.41
1:A:94:ARG:NH2	1:A:110:HIS:HE1	2.19	0.41
1:A:315:GLU:HG2	1:A:320:ILE:HD11	2.02	0.41
1:C:134:PRO:HD3	1:C:200:TYR:HE1	1.85	0.41
1:A:112:PRO:HD3	1:A:164:HIS:HD2	1.85	0.41
1:C:315:GLU:HB3	3:C:560:HOH:O	2.20	0.41
1:D:246:PHE:O	1:D:249:CYS:HB3	2.21	0.41
1:D:92:GLU:OE2	3:D:619:HOH:O	2.21	0.41
1:B:302:GLU:CA	1:B:303:PRO:C	2.90	0.40
1:B:60:ARG:NH1	2:B:401:GOL:H11	2.36	0.40
1:C:0:PHE:O	1:C:117:ARG:HD3	2.21	0.40
1:D:298:ASP:HA	3:D:650:HOH:O	2.20	0.40
1:A:75:CYS:HB3	3:A:632:HOH:O	2.08	0.40
1:A:209:ALA:HB2	1:A:229:ILE:CG2	2.52	0.40
1:D:314:ASP:O	1:D:315:GLU:CB	2.70	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	341/354 (96%)	322 (94%)	17 (5%)	2 (1%)	30	50
1	B	340/354 (96%)	323 (95%)	16 (5%)	1 (0%)	46	68
1	C	332/354 (94%)	312 (94%)	19 (6%)	1 (0%)	46	68
1	D	342/354 (97%)	325 (95%)	16 (5%)	1 (0%)	46	68
All	All	1355/1416 (96%)	1282 (95%)	68 (5%)	5 (0%)	39	61

All (5) 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

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	273/303 (90%)	260 (95%)	13 (5%)	31	55
1	B	265/303 (88%)	253 (96%)	12 (4%)	34	59
1	C	266/303 (88%)	245 (92%)	21 (8%)	15	28
1	D	264/303 (87%)	250 (95%)	14 (5%)	28	50
All	All	1068/1212 (88%)	1008 (94%)	60 (6%)	26	47

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-2	ILE
1	C	32	LEU
1	C	65	ARG
1	C	96	ILE
1	C	107	SER
1	C	135	ARG
1	C	149	LYS
1	C	162	GLN
1	C	170	LYS
1	C	185	LEU
1	C	193	SER
1	C	253	LYS
1	C	264	LYS
1	C	266	GLU
1	C	283	LYS
1	C	293	LEU
1	C	305	VAL

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Mol	Chain	Res	Type
1	C	315	GLU
1	C	321	GLN
1	C	330	SER
1	C	335	VAL
1	B	17	SER
1	B	75	CYS
1	B	96	ILE
1	B	135	ARG
1	B	145	ASN
1	B	203	THR
1	B	205	ASP
1	B	233	GLU
1	B	249	CYS
1	B	293	LEU
1	B	312	THR
1	B	330	SER
1	A	20	ARG
1	A	32	LEU
1	A	67	VAL
1	A	75	CYS
1	A	86	SER
1	A	115	LEU
1	A	148	GLU
1	A	170	LYS
1	A	249	CYS
1	A	253	LYS
1	A	297	ARG
1	A	307	LEU
1	A	312	THR
1	D	2	ARG
1	D	32	LEU
1	D	86	SER
1	D	101	ASN
1	D	107	SER
1	D	174	ASP
1	D	185	LEU
1	D	193	SER
1	D	249	CYS
1	D	253	LYS
1	D	283	LYS
1	D	286	LEU
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	311	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	C	39	GLN
1	C	84	HIS
1	C	150	GLN
1	C	162	GLN
1	C	224	HIS
1	B	113	GLN
1	B	150	GLN
1	A	38	HIS
1	A	83	ASN
1	A	84	HIS
1	A	110	HIS
1	A	151	GLN
1	A	164	HIS
1	A	222	HIS
1	D	83	ASN
1	D	84	HIS
1	D	113	GLN
1	D	222	HIS
1	D	256	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	0.46	0	5,5,5	0.44	0
2	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.93	0
2	GOL	C	401	-	5,5,5	0.45	0	5,5,5	0.55	0
2	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.45	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.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	5	0
2	B	401	GOL	6	0
2	D	401	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	343/354 (96%)	0.24	19 (5%) 29 32	15, 28, 72, 93	23 (6%)
1	B	342/354 (96%)	0.30	35 (10%) 9 9	16, 31, 80, 118	22 (6%)
1	C	336/354 (94%)	0.50	45 (13%) 4 4	18, 33, 88, 108	31 (9%)
1	D	344/354 (97%)	0.30	39 (11%) 7 7	14, 28, 82, 94	19 (5%)
All	All	1365/1416 (96%)	0.33	138 (10%) 9 9	14, 30, 81, 118	95 (6%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	SER	12.8
1	C	139	THR	11.3
1	C	145	ASN	9.2
1	B	318	HIS	8.6
1	C	142	ALA	7.8
1	C	296	TRP	7.3
1	C	147	ILE	7.2
1	B	316	TYR	7.2
1	C	314	ASP	6.8
1	B	300	SER	6.7
1	D	316	TYR	6.3
1	D	142	ALA	6.3
1	D	144	LEU	5.8
1	D	317	LEU	5.7
1	C	287	ALA	5.7
1	C	141	GLN	5.7
1	C	144	LEU	5.7
1	C	313	THR	5.7
1	C	316	TYR	5.6
1	B	144	LEU	5.5
1	A	317	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	4.8
1	D	143	GLY	4.8
1	C	283	LYS	4.7
1	A	139	THR	4.6
1	C	281	VAL	4.5
1	B	311	ILE	4.4
1	B	145	ASN	4.3
1	D	311	ILE	4.2
1	D	318	HIS	4.2
1	C	143	GLY	4.1
1	B	332	PRO	4.1
1	A	141	GLN	4.1
1	B	140	SER	4.1
1	C	309	ILE	4.0
1	B	317	LEU	4.0
1	A	322	ARG	3.9
1	D	299	VAL	3.9
1	C	317	LEU	3.9
1	B	319	ASP	3.8
1	A	289	ILE	3.8
1	B	298	ASP	3.8
1	C	294	GLU	3.8
1	B	315	GLU	3.7
1	D	290	THR	3.6
1	C	146	GLY	3.5
1	C	149	LYS	3.5
1	A	293	LEU	3.5
1	D	139	THR	3.4
1	B	142	ALA	3.4
1	A	286	LEU	3.3
1	C	289	ILE	3.3
1	C	203	THR	3.3
1	B	174	ASP	3.2
1	C	288	SER	3.2
1	A	328	THR	3.1
1	D	298	ASP	3.1
1	C	312	THR	3.1
1	C	202	GLY	3.1
1	B	143	GLY	3.0
1	D	314	ASP	3.0
1	C	282	LEU	3.0
1	B	284	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	ASN	3.0
1	C	308	ASP	2.9
1	A	291	ALA	2.9
1	A	311	ILE	2.9
1	C	332	PRO	2.9
1	D	285	ASP	2.9
1	D	286	LEU	2.9
1	A	140	SER	2.9
1	D	338	VAL	2.8
1	B	327	LEU	2.8
1	D	331	LEU	2.8
1	D	296	TRP	2.8
1	D	140	SER	2.8
1	C	310	GLU	2.8
1	B	173	GLY	2.8
1	D	174	ASP	2.8
1	B	296	TRP	2.8
1	A	174	ASP	2.8
1	D	328	THR	2.7
1	D	327	LEU	2.7
1	C	293	LEU	2.7
1	B	141	GLN	2.7
1	A	294	GLU	2.7
1	B	139	THR	2.7
1	C	291	ALA	2.7
1	C	286	LEU	2.6
1	C	137	ILE	2.6
1	D	293	LEU	2.6
1	C	284	GLY	2.5
1	B	289	ILE	2.5
1	C	280	ALA	2.5
1	D	326	ALA	2.5
1	D	330	SER	2.4
1	B	303	PRO	2.4
1	C	318	HIS	2.4
1	C	200	TYR	2.3
1	B	151	GLN	2.3
1	A	144	LEU	2.3
1	B	150	GLN	2.3
1	D	283	LYS	2.3
1	B	337	LEU	2.3
1	B	149	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	291	ALA	2.3
1	A	330	SER	2.3
1	D	321	GLN	2.3
1	B	305	VAL	2.3
1	B	333	VAL	2.3
1	D	287	ALA	2.2
1	C	330	SER	2.2
1	D	173	GLY	2.2
1	D	312	THR	2.2
1	B	297	ARG	2.2
1	D	332	PRO	2.2
1	B	147	ILE	2.2
1	C	138	ILE	2.2
1	B	148	GLU	2.2
1	D	281	VAL	2.1
1	D	295	GLN	2.1
1	A	314	ASP	2.1
1	D	175	GLN	2.1
1	C	333	VAL	2.1
1	C	338	VAL	2.1
1	D	339	ARG	2.1
1	C	319	ASP	2.1
1	C	328	THR	2.1
1	B	301	GLN	2.1
1	A	283	LYS	2.1
1	A	288	SER	2.1
1	D	315	GLU	2.1
1	B	146	GLY	2.1
1	C	152	HIS	2.1
1	D	325	GLN	2.0
1	C	135	ARG	2.0
1	D	284	GLY	2.0
1	D	333	VAL	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	D	401	6/6	0.93	0.20	4.31	38,40,40,41	0
2	GOL	B	401	6/6	0.95	0.17	2.95	29,30,31,33	0
2	GOL	A	401	6/6	0.97	0.15	1.27	31,32,33,33	0
2	GOL	C	401	6/6	0.96	0.13	-0.16	28,30,30,33	0

6.5 Other polymers

There are no such residues in this entry.