



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:32 PM BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

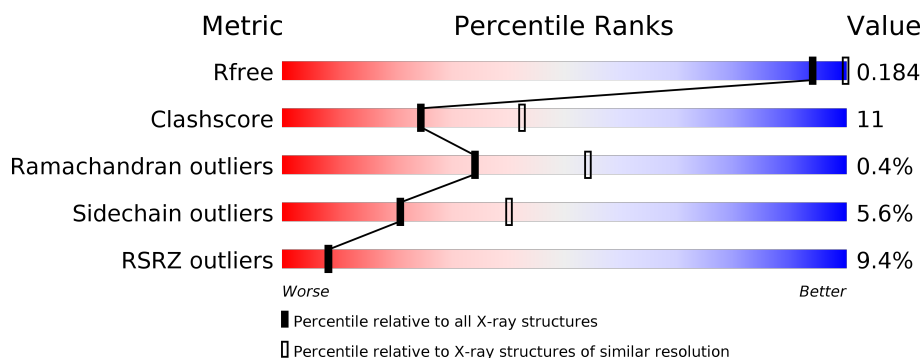
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	354	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	354	<div> <div>12%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	D	354	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>

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	-

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	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		

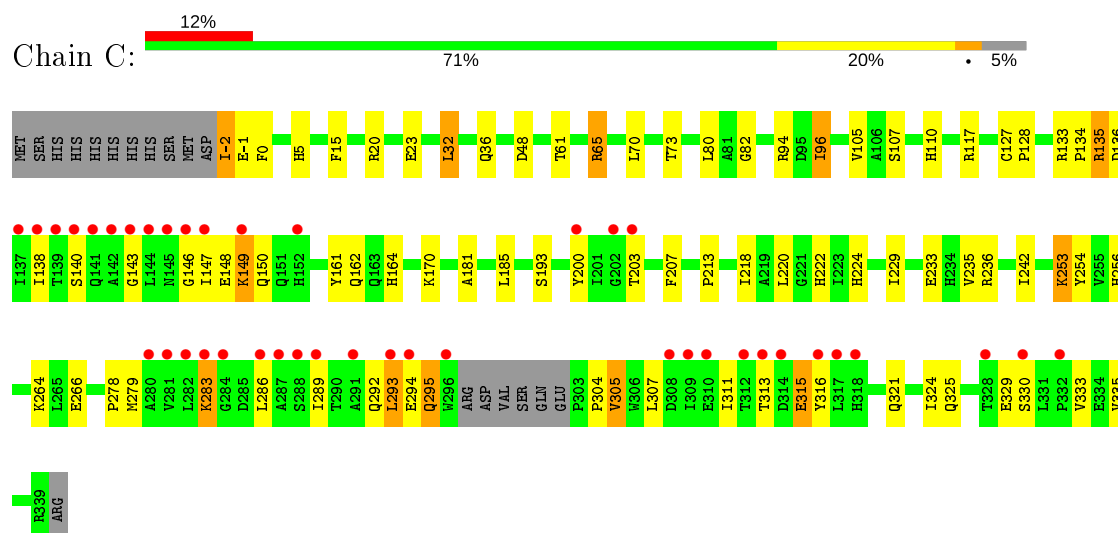
- Molecule 3 is water.

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

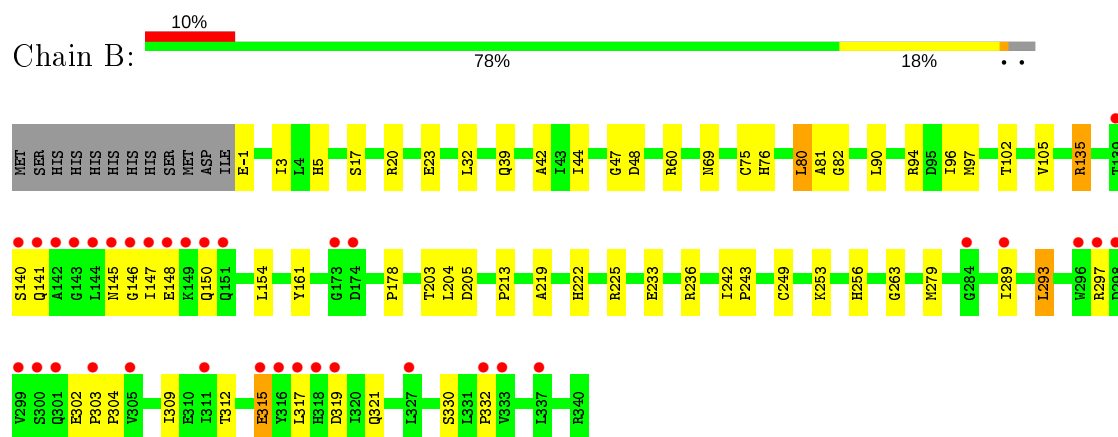
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

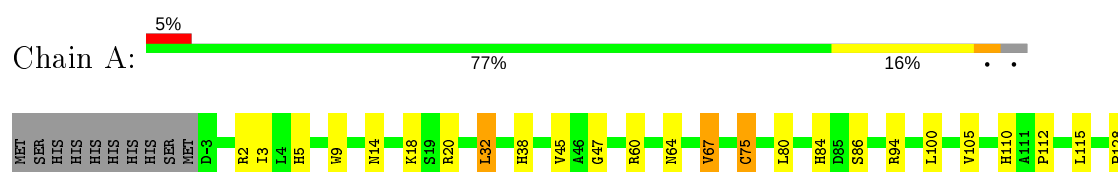
• Molecule 1: Exonuclease subunit SbcD

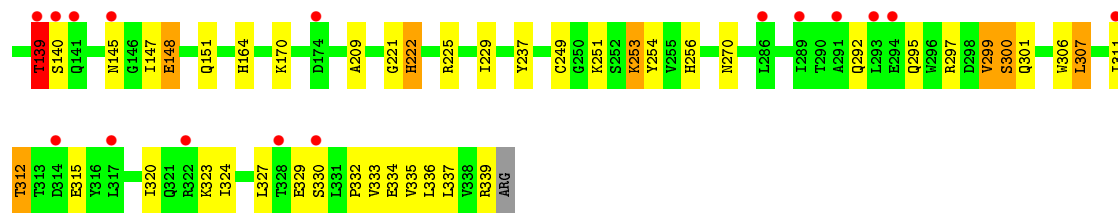


• Molecule 1: Exonuclease subunit SbcD

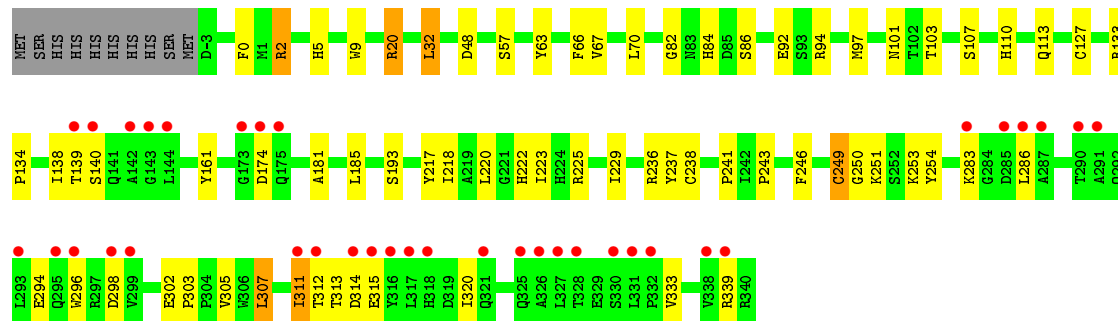
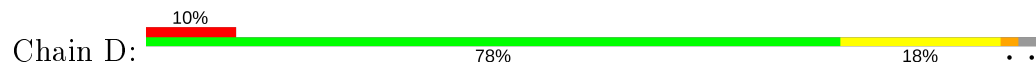


• Molecule 1: Exonuclease subunit SbcD





● 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	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) 98.3 (37.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.176 , 0.235 0.192 , 0.184	Depositor DCC
R_{free} test set	2528 reflections (5.09%)	wwPDB-VP
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 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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 [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	0.54	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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:60:ARG:HH11	2:A:401:GOL:H11	1.43	0.82
1:A:75:CYS:CB	3:A:632:HOH:O	2.27	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:220:LEU:HD12	1:C:229:ILE:HD13	1.79	0.65
1:C:304:PRO:HD3	3:C:631:HOH:O	1.96	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:236:ARG:HD2	3:B:619:HOH:O	2.02	0.59
1:B:20:ARG:NH1	1:B:242:ILE:HD12	2.17	0.59
1:B:302:GLU:CB	1:B:303:PRO:HA	2.32	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:A:253:LYS:CE	3:A:654:HOH:O	2.51	0.58
1:A:337:LEU:HD21	1:A:339:ARG:HE	1.69	0.58
1:B:289:ILE:HD13	1:B:309:ILE:HG23	1.85	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:A:47:GLY:HA2	1:A:80:LEU:O	2.08	0.53
1:B:81:ALA:HB2	1:B:90:LEU:HD12	1.89	0.53
1:D:217:TYR:HE1	3:D:637:HOH:O	1.90	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:A:323:LYS:O	1:A:327:LEU:HD13	2.13	0.48
1:C:110:HIS:O	1:C:164:HIS:NE2	2.39	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:C:143:GLY:HA3	3:C:598:HOH:O	2.13	0.47
1:D:236:ARG:CG	3:D:637:HOH:O	2.57	0.47
1:A:292:GLN:O	1:A:295:GLN:HB3	2.13	0.47
1:C:110:HIS:HE1	3:C:592:HOH:O	1.98	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: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:D:2:ARG:HH11	1:D:2:ARG:HG3	1.80	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:A:324:ILE:CG2	1:A:335:VAL:HG21	2.45	0.46
1:C:48:ASP:H	1:C:82:GLY:CA	2.29	0.46
1:C:20:ARG:NH2	1:C:242:ILE:HD12	2.31	0.45
1:D:250:GLY:HA3	3:D:643:HOH:O	2.15	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:C:324:ILE:HG13	1:C:325:GLN:N	2.31	0.45
1:D:217:TYR:CE1	3:D:637:HOH:O	2.56	0.45
1:D:133:ARG:HD2	3:D:523:HOH:O	2.17	0.45
1:A:18:LYS:NZ	1:A:334:GLU:OE2	2.32	0.44
1:B:297:ARG:HD3	1:B:297:ARG:HA	1.74	0.44
1:B:48:ASP:H	1:B:82:GLY:CA	2.30	0.44
1:C:5:HIS:HB3	1:C:256:HIS:HB2	1.99	0.44
1:D:5:HIS:CD2	1:D:238:CYS:HG	2.36	0.44
1:A:67:VAL:HG13	1:A:100:LEU:HD22	1.99	0.44
1:B:47:GLY:HA2	1:B:80:LEU:O	2.18	0.44
1:C:15:PHE:HB2	1:C:20:ARG:HD3	2.00	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:161:TYR:HB3	1:B:213:PRO:HD3	1.99	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: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:A:105:VAL:HG21	1:A:128:PRO:HB2	2.01	0.43
1:C:138:ILE:C	1:C:140:SER:N	2.72	0.43
1:C:294:GLU:CB	3:C:574:HOH:O	2.67	0.43
1:D:296:TRP:NE1	1:D:305:VAL:HG21	2.33	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:148:GLU:HA	3:C:515:HOH:O	2.18	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:A:3:ILE:C	1:A:3:ILE:HD12	2.39	0.43
1:C:220:LEU:HD12	1:C:229:ILE:CD1	2.48	0.43
1:D:139:THR:HA	1:D:140:SER:HA	1.61	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: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:A:147:ILE:H	1:A:147:ILE:HD12	1.84	0.42
1:B:42:ALA:HA	1:B:76:HIS:O	2.19	0.42
1:C:207:PHE:CE1	3:C:601:HOH:O	2.36	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:224:HIS:HD2	3:C:627:HOH:O	2.02	0.41
1:C:325:GLN:O	1:C:329:GLU:HG3	2.20	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:94:ARG:NH2	1:A:110:HIS:HE1	2.19	0.41
1:A:2:ARG:CD	3:A:626:HOH:O	2.66	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:209:ALA:HB2	1:A:229:ILE:CG2	2.52	0.40
1:A:75:CYS:HB3	3:A:632:HOH:O	2.08	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%)	25	43
1	B	340/354 (96%)	323 (95%)	16 (5%)	1 (0%)	41	61
1	C	332/354 (94%)	312 (94%)	19 (6%)	1 (0%)	41	61
1	D	342/354 (97%)	325 (95%)	16 (5%)	1 (0%)	41	61
All	All	1355/1416 (96%)	1282 (95%)	68 (5%)	5 (0%)	34	54

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 ⓘ

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%)	25	48
1	B	265/303 (88%)	253 (96%)	12 (4%)	27	51
1	C	266/303 (88%)	245 (92%)	21 (8%)	12	24
1	D	264/303 (87%)	250 (95%)	14 (5%)	22	43
All	All	1068/1212 (88%)	1008 (94%)	60 (6%)	21	40

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 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	0.36	0	5,5,5	0.99	1 (20%)
2	GOL	A	401	-	5,5,5	0.46	0	5,5,5	0.50	0
2	GOL	D	401	-	5,5,5	0.36	0	5,5,5	0.47	0
2	GOL	C	401	-	5,5,5	0.46	0	5,5,5	0.59	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	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-

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	C3-C2-C1	-2.16	103.30	111.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

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

There are no ring outliers.

3 monomers are involved in 12 short contacts:

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

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	343/354 (96%)	0.18	16 (4%) 31 33	15, 28, 72, 93	23 (6%)
1	B	342/354 (96%)	0.24	35 (10%) 6 6	16, 31, 80, 118	22 (6%)
1	C	336/354 (94%)	0.44	41 (12%) 4 3	18, 33, 88, 108	31 (9%)
1	D	344/354 (97%)	0.25	36 (10%) 6 6	14, 28, 82, 94	19 (5%)
All	All	1365/1416 (96%)	0.28	128 (9%) 8 8	14, 30, 81, 118	95 (6%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	SER	12.2
1	C	139	THR	10.9
1	C	145	ASN	8.6
1	B	318	HIS	8.4
1	C	142	ALA	7.8
1	C	296	TRP	7.1
1	B	316	TYR	6.9
1	C	147	ILE	6.7
1	B	300	SER	6.6
1	C	314	ASP	6.3
1	D	144	LEU	6.1
1	D	316	TYR	6.1
1	C	144	LEU	5.7
1	D	317	LEU	5.6
1	C	313	THR	5.5
1	C	287	ALA	5.5
1	C	141	GLN	5.5
1	B	144	LEU	5.4
1	D	142	ALA	5.3
1	C	316	TYR	5.2
1	A	317	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	283	LYS	4.6
1	A	139	THR	4.6
1	B	145	ASN	4.4
1	B	299	VAL	4.4
1	B	311	ILE	4.3
1	C	281	VAL	4.2
1	C	143	GLY	4.2
1	B	140	SER	4.2
1	D	143	GLY	4.1
1	A	141	GLN	4.1
1	D	311	ILE	4.0
1	C	317	LEU	4.0
1	D	318	HIS	4.0
1	B	332	PRO	3.9
1	B	317	LEU	3.8
1	B	319	ASP	3.8
1	B	315	GLU	3.8
1	C	309	ILE	3.8
1	A	322	ARG	3.8
1	D	139	THR	3.8
1	A	289	ILE	3.7
1	B	298	ASP	3.7
1	C	294	GLU	3.6
1	D	299	VAL	3.6
1	B	142	ALA	3.5
1	C	149	LYS	3.4
1	D	290	THR	3.4
1	C	146	GLY	3.4
1	A	293	LEU	3.3
1	A	286	LEU	3.2
1	A	145	ASN	3.2
1	C	289	ILE	3.2
1	A	328	THR	3.1
1	A	311	ILE	3.0
1	C	203	THR	3.0
1	C	202	GLY	3.0
1	C	282	LEU	2.9
1	B	143	GLY	2.9
1	D	298	ASP	2.9
1	C	332	PRO	2.9
1	C	312	THR	2.9
1	D	140	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	2.8
1	B	174	ASP	2.8
1	D	286	LEU	2.8
1	D	296	TRP	2.8
1	D	314	ASP	2.8
1	A	291	ALA	2.7
1	D	328	THR	2.7
1	C	288	SER	2.7
1	D	331	LEU	2.7
1	C	310	GLU	2.7
1	C	308	ASP	2.7
1	D	285	ASP	2.7
1	C	293	LEU	2.7
1	B	296	TRP	2.7
1	A	174	ASP	2.7
1	B	141	GLN	2.7
1	B	327	LEU	2.6
1	B	284	GLY	2.6
1	B	139	THR	2.6
1	D	327	LEU	2.6
1	D	338	VAL	2.6
1	A	294	GLU	2.6
1	D	174	ASP	2.6
1	C	286	LEU	2.5
1	D	293	LEU	2.5
1	B	173	GLY	2.5
1	C	137	ILE	2.5
1	C	291	ALA	2.4
1	C	318	HIS	2.4
1	C	284	GLY	2.4
1	A	314	ASP	2.3
1	D	326	ALA	2.3
1	B	289	ILE	2.3
1	B	333	VAL	2.3
1	D	330	SER	2.3
1	B	151	GLN	2.3
1	B	147	ILE	2.3
1	D	283	LYS	2.2
1	D	321	GLN	2.2
1	D	291	ALA	2.2
1	A	330	SER	2.2
1	B	303	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	2.2
1	B	305	VAL	2.2
1	D	287	ALA	2.2
1	D	332	PRO	2.2
1	D	173	GLY	2.2
1	B	150	GLN	2.1
1	B	301	GLN	2.1
1	C	280	ALA	2.1
1	B	337	LEU	2.1
1	C	328	THR	2.1
1	C	330	SER	2.1
1	D	312	THR	2.1
1	B	148	GLU	2.1
1	C	138	ILE	2.1
1	B	146	GLY	2.1
1	D	295	GLN	2.1
1	D	175	GLN	2.0
1	D	315	GLU	2.0
1	D	325	GLN	2.0
1	B	297	ARG	2.0
1	D	339	ARG	2.0
1	B	149	LYS	2.0
1	C	152	HIS	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 [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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	401	6/6	0.94	0.17	29,30,31,33	0
2	GOL	D	401	6/6	0.94	0.20	38,40,40,41	0
2	GOL	C	401	6/6	0.96	0.14	28,30,30,33	0
2	GOL	A	401	6/6	0.97	0.16	31,32,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.