



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 03:10 AM UTC

PDB ID : 2XME / pdb_00002xme
Title : The X-ray structure of CTP:inositol-1-phosphate cytidylyltransferase from *Archaeoglobus fulgidus*
Authors : Brito, J.A.; Borges, N.; Vonrhein, C.; Santos, H.; Archer, M.
Deposited on : 2010-07-27
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

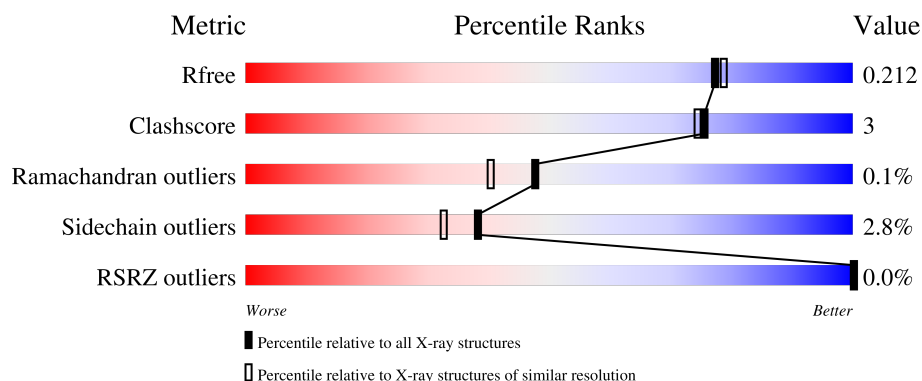
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

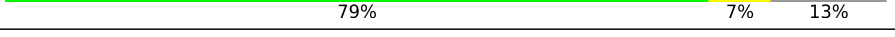
The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	
1	C	232	
1	D	232	
1	E	232	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	232	 80%9%10%
1	G	232	 76%9%14%
1	H	232	 77%7%15%
1	I	232	 78%8%14%
1	J	232	 77%9%14%
1	K	232	 77%8%14%
1	L	232	 75%11%14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	E	501	-	-	X	-

2 Entry composition

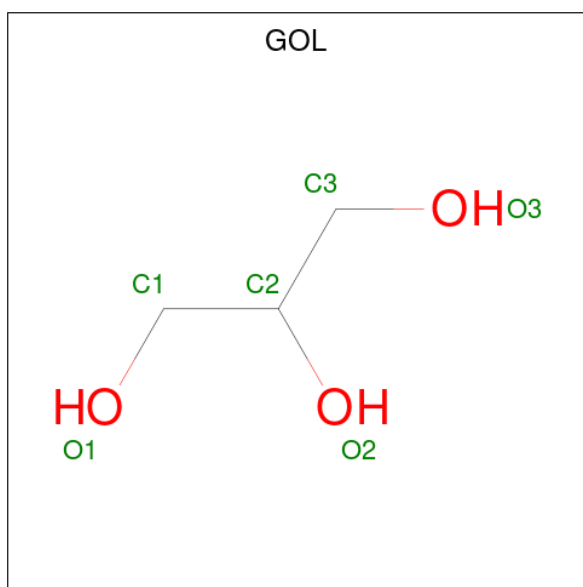
There are 3 unique types of molecules in this entry. The entry contains 20458 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	1	0
			1610	1032	278	294	6			
1	B	198	Total	C	N	O	S	0	0	0
			1582	1012	274	290	6			
1	C	199	Total	C	N	O	S	0	1	0
			1593	1020	275	292	6			
1	D	201	Total	C	N	O	S	0	1	0
			1606	1027	277	296	6			
1	E	204	Total	C	N	O	S	0	1	0
			1627	1040	283	298	6			
1	F	208	Total	C	N	O	S	0	1	0
			1656	1057	288	305	6			
1	G	199	Total	C	N	O	S	0	0	0
			1589	1016	275	292	6			
1	H	198	Total	C	N	O	S	0	1	0
			1594	1022	275	291	6			
1	I	199	Total	C	N	O	S	0	2	0
			1598	1023	275	294	6			
1	J	200	Total	C	N	O	S	0	0	0
			1597	1022	276	293	6			
1	K	200	Total	C	N	O	S	0	0	0
			1598	1022	277	293	6			
1	L	200	Total	C	N	O	S	0	0	0
			1589	1014	276	293	6			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	92	Total	O	0	0
			92	92		
3	C	117	Total	O	0	0
			117	117		
3	D	70	Total	O	0	0
			70	70		

Continued on next page...

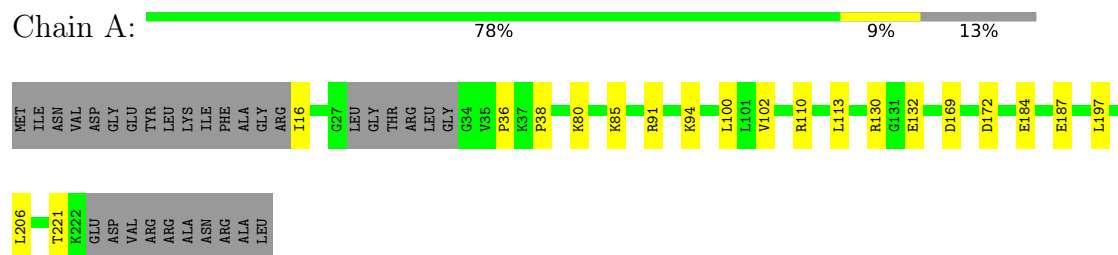
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	132	Total 133	O 133	0	1
3	F	109	Total 109	O 109	0	0
3	G	118	Total 119	O 119	0	1
3	H	98	Total 98	O 98	0	0
3	I	109	Total 110	O 110	0	1
3	J	89	Total 89	O 89	0	0
3	K	77	Total 77	O 77	0	0
3	L	39	Total 39	O 39	0	0

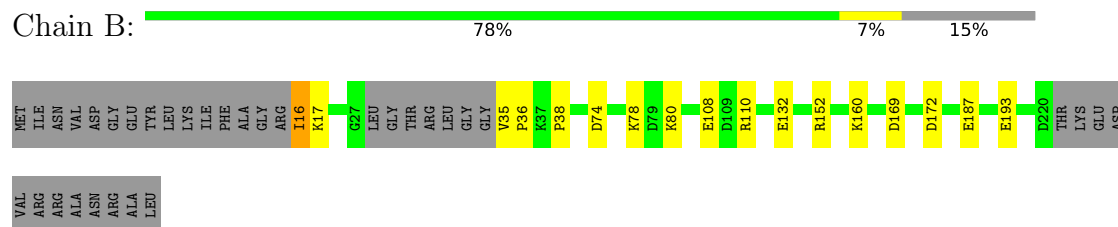
3 Residue-property plots

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.

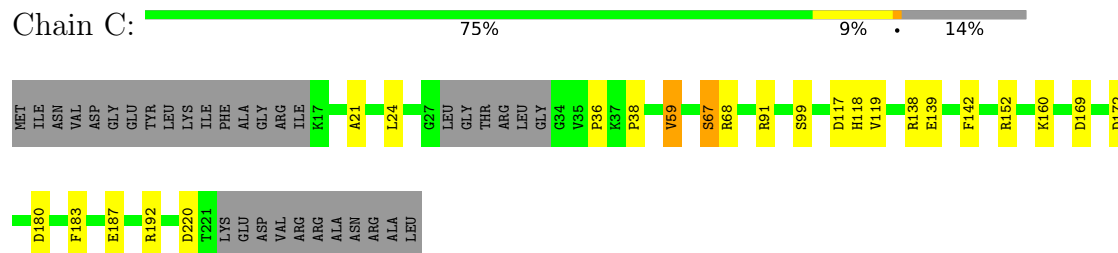
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



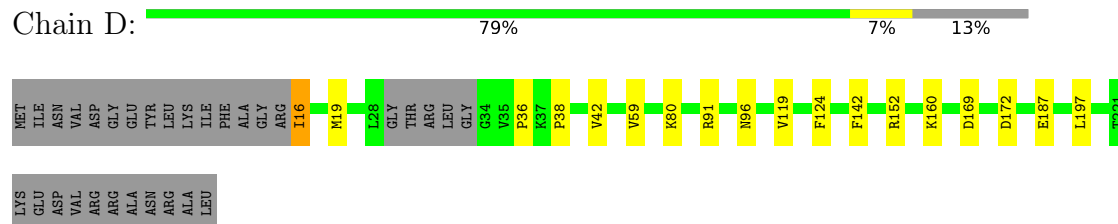
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

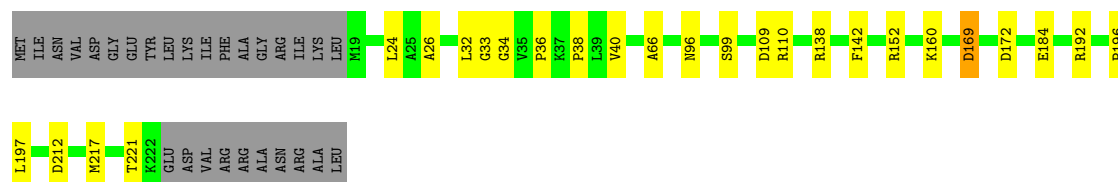


• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



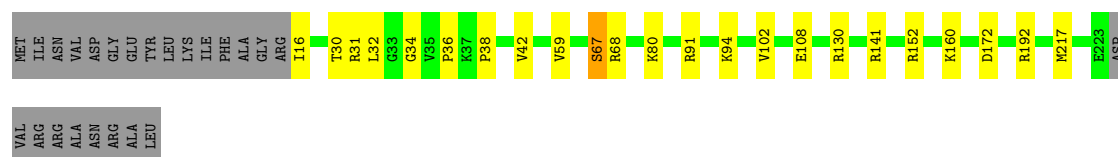
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain E: 



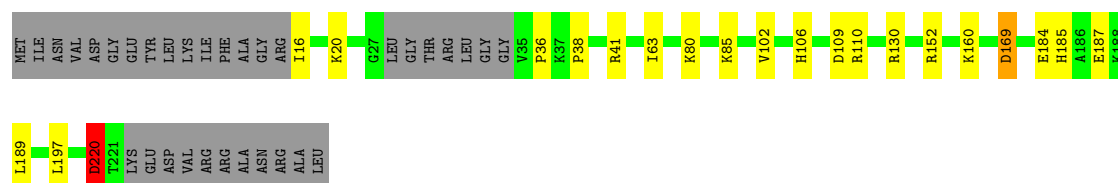
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain F: 



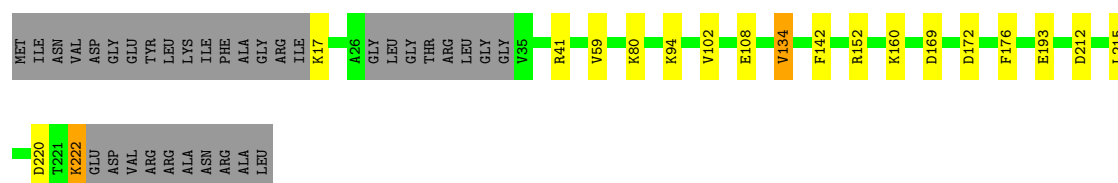
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain G: 



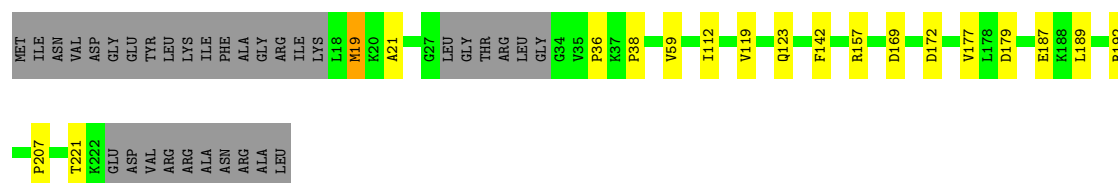
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain H: 



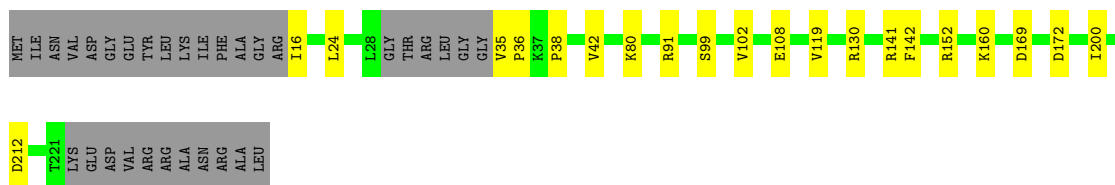
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain I: 



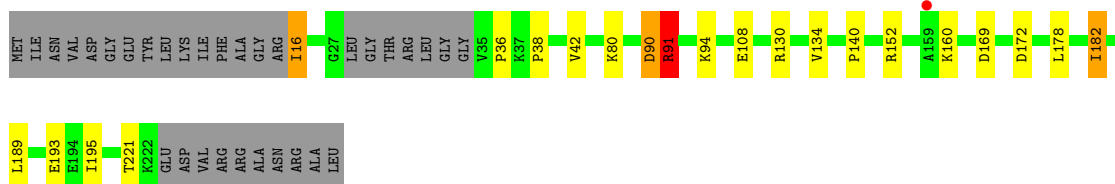
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain J:  77% 9% 14%



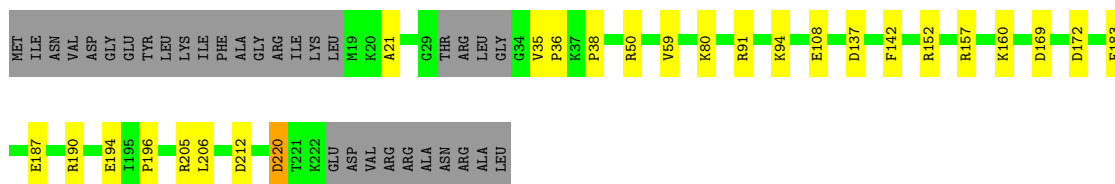
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain K:  77% 8% 14%



- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

Chain L:  75% 11% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.03Å 127.55Å 141.48Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	27.67 – 1.89 27.67 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.67-1.89) 87.9 (27.67-1.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.206 , 0.237 0.196 , 0.212	Depositor DCC
R_{free} test set	10915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.248 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20458	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.86	0/1641	1.23	3/2208 (0.1%)
1	B	0.82	0/1609	1.21	2/2166 (0.1%)
1	C	0.85	0/1624	1.24	6/2186 (0.3%)
1	D	0.85	0/1636	1.22	3/2203 (0.1%)
1	E	0.95	0/1659	1.24	3/2234 (0.1%)
1	F	0.89	0/1687	1.27	9/2271 (0.4%)
1	G	0.89	0/1616	1.25	3/2176 (0.1%)
1	H	0.81	0/1625	1.23	5/2187 (0.2%)
1	I	0.90	1/1632 (0.1%)	1.21	1/2197 (0.0%)
1	J	0.83	0/1624	1.25	5/2187 (0.2%)
1	K	0.77	0/1625	1.26	5/2187 (0.2%)
1	L	0.87	0/1616	1.20	5/2175 (0.2%)
All	All	0.86	1/19594 (0.0%)	1.23	50/26377 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	19	MET	SD-CE	-5.84	1.65	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	220	ASP	CA-CB-CG	10.34	122.94	112.60
1	H	59	VAL	N-CA-C	6.41	117.09	108.11
1	H	172	ASP	CA-CB-CG	6.37	118.97	112.60
1	K	80	LYS	N-CA-C	6.22	120.61	112.89
1	E	172	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	80	LYS	N-CA-C	6.01	120.34	112.89
1	D	80	LYS	N-CA-C	5.98	120.42	113.18
1	D	172	ASP	CA-CB-CG	5.91	118.51	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	80	LYS	N-CA-C	5.89	120.31	113.18
1	J	80	LYS	N-CA-C	5.88	120.29	113.18
1	A	172	ASP	CA-CB-CG	5.83	118.43	112.60
1	L	172	ASP	CA-CB-CG	5.79	118.39	112.60
1	E	169	ASP	CA-CB-CG	5.78	118.38	112.60
1	I	172	ASP	CA-CB-CG	5.78	118.38	112.60
1	H	80	LYS	N-CA-C	5.76	120.03	112.89
1	L	212	ASP	N-CA-C	5.74	118.59	109.24
1	B	172	ASP	CA-CB-CG	5.72	118.33	112.60
1	K	90	ASP	CA-CB-CG	5.67	118.27	112.60
1	L	220	ASP	CA-CB-CG	5.67	118.27	112.60
1	K	140	PRO	CA-C-N	5.61	130.22	120.68
1	K	140	PRO	C-N-CA	5.61	130.22	120.68
1	L	80	LYS	N-CA-C	-5.61	101.73	110.42
1	K	172	ASP	CA-CB-CG	5.58	118.19	112.60
1	D	59	VAL	N-CA-C	5.54	115.86	108.11
1	A	80	LYS	N-CA-C	5.53	119.87	113.18
1	J	172	ASP	CA-CB-CG	5.47	118.08	112.60
1	F	80	LYS	N-CA-C	5.46	119.79	113.18
1	E	212	ASP	N-CA-C	5.46	118.14	109.24
1	H	212	ASP	N-CA-C	5.36	117.98	109.24
1	F	172	ASP	CA-CB-CG	5.35	117.95	112.60
1	J	200	ILE	CA-C-N	5.35	127.30	120.56
1	J	200	ILE	C-N-CA	5.35	127.30	120.56
1	H	220	ASP	CA-CB-CG	5.35	117.95	112.60
1	J	212	ASP	N-CA-C	5.33	118.50	109.76
1	G	169	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	206	LEU	N-CA-C	5.30	115.70	109.60
1	C	172	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	192	ARG	CA-C-N	5.22	127.27	120.28
1	C	192	ARG	C-N-CA	5.22	127.27	120.28
1	F	192	ARG	CA-C-N	5.20	127.50	120.38
1	F	192	ARG	C-N-CA	5.20	127.50	120.38
1	C	183	PHE	CA-C-N	5.19	127.24	120.28
1	C	183	PHE	C-N-CA	5.19	127.24	120.28
1	F	67[A]	SER	CA-C-N	5.18	127.54	120.54
1	F	67[A]	SER	C-N-CA	5.18	127.54	120.54
1	F	67[B]	SER	CA-C-N	5.18	127.54	120.54
1	F	67[B]	SER	C-N-CA	5.18	127.54	120.54
1	C	220	ASP	CA-CB-CG	5.17	117.77	112.60
1	F	59	VAL	N-CA-C	5.11	115.26	108.11
1	L	137	ASP	CA-CB-CG	5.01	117.61	112.60

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	1610	0	1641	8	0
1	B	1582	0	1609	8	0
1	C	1593	0	1617	14	0
1	D	1606	0	1634	11	0
1	E	1627	0	1655	21	0
1	F	1656	0	1692	12	0
1	G	1589	0	1616	12	0
1	H	1594	0	1624	7	0
1	I	1598	0	1621	15	0
1	J	1597	0	1627	10	0
1	K	1598	0	1629	11	0
1	L	1589	0	1611	15	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	3	0
2	E	6	0	8	6	0
2	G	6	0	8	2	0
2	I	6	0	8	0	0
2	L	6	0	8	2	0
3	A	118	0	0	1	0
3	B	92	0	0	0	0
3	C	117	0	0	1	0
3	D	70	0	0	0	0
3	E	133	0	0	1	0
3	F	109	0	0	1	0
3	G	119	0	0	0	0
3	H	98	0	0	0	0
3	I	110	0	0	0	0
3	J	89	0	0	0	0
3	K	77	0	0	1	0
3	L	39	0	0	2	0
All	All	20458	0	19640	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (118) 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:I:19:MET:HE1	1:I:177:VAL:HG13	1.51	0.91
1:E:197:LEU:H	2:E:501:GOL:H12	1.37	0.89
1:D:197:LEU:H	2:D:501:GOL:H11	1.47	0.79
3:K:2009:HOH:O	1:L:220:ASP:HB3	1.81	0.79
1:E:96:ASN:HB2	2:E:501:GOL:H11	1.64	0.78
1:E:32:LEU:HD11	1:E:221:THR:HG23	1.66	0.78
1:G:197:LEU:H	2:G:501:GOL:H2	1.48	0.77
1:D:96:ASN:H	2:D:501:GOL:H32	1.55	0.71
1:A:110:ARG:HH22	1:A:132:GLU:HG3	1.55	0.70
1:L:183:PHE:O	1:L:187:GLU:HG2	1.92	0.70
1:I:221:THR:HG21	1:J:35:VAL:HG11	1.72	0.69
1:I:157:ARG:HD2	1:I:207:PRO:HA	1.74	0.69
1:E:197:LEU:H	2:E:501:GOL:C1	2.07	0.66
1:K:16:ILE:HG12	1:K:130:ARG:HG2	1.78	0.65
1:E:196:PRO:HB3	2:E:501:GOL:H31	1.81	0.63
1:E:196:PRO:HA	2:E:501:GOL:H12	1.81	0.62
1:A:197:LEU:H	2:A:501:GOL:H32	1.64	0.62
1:H:134:VAL:HG13	1:H:176:PHE:CE1	2.35	0.61
1:B:78:LYS:HE3	1:F:68:ARG:HE	1.66	0.61
1:E:197:LEU:N	2:E:501:GOL:H12	2.14	0.60
2:A:501:GOL:H31	3:A:2118:HOH:O	2.02	0.60
1:E:34:GLY:HA3	1:F:32:LEU:O	2.01	0.60
1:B:110:ARG:HH22	1:B:132:GLU:HG3	1.66	0.59
1:F:152:ARG:HB3	1:F:160:LYS:HB2	1.84	0.59
1:G:185:HIS:HD2	1:L:194:GLU:OE2	1.86	0.59
1:C:21:ALA:HB2	1:C:59:VAL:HG21	1.84	0.58
1:I:189:LEU:O	1:I:192:ARG:HG2	2.04	0.58
1:C:118:HIS:HE1	3:C:2095:HOH:O	1.86	0.57
1:H:152:ARG:HB3	1:H:160:LYS:HB2	1.86	0.57
1:I:142[A]:PHE:HZ	1:J:119:VAL:HG11	1.70	0.57
1:E:32:LEU:CD1	1:E:221:THR:HG23	2.34	0.57
1:C:152:ARG:HB3	1:C:160:LYS:HB2	1.88	0.56
1:F:34:GLY:HA2	3:F:2033:HOH:O	2.04	0.56
1:E:217:MET:SD	1:F:217:MET:HE1	2.46	0.56
1:G:16:ILE:HG12	1:G:130:ARG:HA	1.88	0.55
1:G:20:LYS:HD3	1:G:63:ILE:HD11	1.89	0.55
1:K:152:ARG:HB3	1:K:160:LYS:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:HD3	1:F:94:LYS:HD2	1.87	0.54
1:L:91:ARG:HD3	1:L:94:LYS:HD2	1.89	0.54
1:B:152:ARG:HB3	1:B:160:LYS:HB2	1.90	0.54
1:F:16:ILE:HG13	1:F:130:ARG:HG2	1.90	0.54
1:J:152:ARG:HB3	1:J:160:LYS:HB2	1.90	0.53
1:L:196:PRO:HA	2:L:501:GOL:O2	2.08	0.53
1:J:16:ILE:HG13	1:J:130:ARG:HG2	1.91	0.53
1:L:152:ARG:HB3	1:L:160:LYS:HB2	1.90	0.53
1:F:36:PRO:HB2	1:F:38:PRO:HD2	1.91	0.52
1:E:152:ARG:HB3	1:E:160:LYS:HB2	1.91	0.52
1:G:41:ARG:HD2	1:H:222:LYS:HB2	1.91	0.52
1:G:109:ASP:CG	1:G:110:ARG:H	2.18	0.51
1:G:85:LYS:HE3	1:G:106:HIS:ND1	2.25	0.51
1:L:50:ARG:HB2	3:L:2011:HOH:O	2.11	0.51
1:D:152:ARG:HB3	1:D:160:LYS:HB2	1.93	0.50
1:K:42:VAL:HG12	1:L:142:PHE:HE2	1.77	0.50
1:A:91:ARG:HD3	1:A:94:LYS:HD2	1.92	0.50
1:E:142[A]:PHE:HE2	1:F:42:VAL:HG12	1.77	0.49
1:G:152:ARG:HB3	1:G:160:LYS:HB2	1.94	0.49
1:E:36:PRO:HB2	1:E:38:PRO:HD2	1.94	0.49
1:I:19:MET:CE	1:I:177:VAL:HG13	2.32	0.49
1:E:110:ARG:NH2	3:E:2072:HOH:O	2.44	0.49
1:I:123:GLN:HE22	1:J:141:ARG:HH12	1.59	0.49
1:K:221:THR:HG21	1:L:35:VAL:HG11	1.95	0.49
1:C:142[A]:PHE:HE2	1:D:42:VAL:HG12	1.79	0.48
1:K:189:LEU:HB3	1:K:195:ILE:HG23	1.96	0.48
1:E:142[A]:PHE:CE2	1:F:42:VAL:HG12	2.48	0.48
1:A:16:ILE:HG13	1:A:130:ARG:HA	1.96	0.47
1:C:91:ARG:NH2	1:L:190:ARG:HG3	2.29	0.46
1:C:67:SER:HB3	1:C:68:ARG:H	1.61	0.46
1:E:24:LEU:HD22	1:E:99:SER:HB3	1.97	0.46
1:F:16:ILE:HG13	1:F:130:ARG:HA	1.98	0.46
1:G:220:ASP:OD1	1:H:41:ARG:NH1	2.44	0.46
1:H:94:LYS:HG2	1:H:193:GLU:O	2.17	0.45
1:I:142[A]:PHE:HE2	1:J:42:VAL:HG12	1.82	0.45
1:C:142[A]:PHE:CE2	1:D:42:VAL:HG12	2.52	0.45
1:I:21:ALA:HB2	1:I:59:VAL:HG11	1.98	0.44
1:E:32:LEU:HD12	1:E:32:LEU:HA	1.86	0.44
1:I:189:LEU:HD23	1:I:192:ARG:HD2	1.99	0.44
1:L:21:ALA:HB2	1:L:59:VAL:HG11	1.99	0.44
1:B:17:LYS:HB2	1:C:138:ARG:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:ARG:HD2	1:I:207:PRO:CA	2.44	0.44
1:K:178:LEU:HD22	1:K:182:ILE:HD13	2.00	0.44
1:E:32:LEU:HD23	1:E:40:VAL:HG21	1.99	0.44
1:A:16:ILE:HG13	1:A:130:ARG:HG2	2.00	0.43
1:K:36:PRO:HB2	1:K:38:PRO:HD2	2.00	0.43
1:C:24:LEU:HD22	1:C:99:SER:HB3	1.99	0.43
1:J:36:PRO:HB2	1:J:38:PRO:HD2	2.00	0.43
1:K:221:THR:CG2	1:L:35:VAL:HG11	2.48	0.43
1:C:117:ASP:OD1	1:C:118:HIS:HD2	2.01	0.43
2:L:501:GOL:H11	3:L:2004:HOH:O	2.17	0.43
1:I:119:VAL:HG11	1:J:142:PHE:HZ	1.83	0.43
1:I:59:VAL:CG1	1:I:112:ILE:HD12	2.48	0.43
1:K:42:VAL:HG12	1:L:142:PHE:CE2	2.54	0.43
1:B:36:PRO:HB2	1:B:38:PRO:HD2	2.01	0.42
1:B:74:ASP:OD1	1:F:68:ARG:NH1	2.51	0.42
1:D:16:ILE:HD11	1:D:19:MET:HE2	2.01	0.42
1:A:36:PRO:HB2	1:A:38:PRO:HD2	2.01	0.42
1:E:26:ALA:HB2	1:E:66:ALA:HA	2.01	0.42
1:K:91:ARG:CB	1:K:94:LYS:HB2	2.49	0.42
1:G:36:PRO:HB2	1:G:38:PRO:HD2	2.02	0.42
1:I:36:PRO:HB2	1:I:38:PRO:HD2	2.01	0.42
1:J:24:LEU:HD22	1:J:99:SER:HB3	2.00	0.42
1:C:119:VAL:HG11	1:D:142:PHE:HZ	1.83	0.42
1:G:109:ASP:CG	1:G:110:ARG:N	2.78	0.42
1:H:142[B]:PHE:CE2	1:H:215:LEU:HA	2.55	0.42
1:D:96:ASN:H	2:D:501:GOL:C3	2.28	0.42
1:E:138:ARG:HB3	1:H:17:LYS:HB2	2.01	0.42
1:B:16:ILE:O	1:C:139:GLU:HG2	2.19	0.41
1:C:142[A]:PHE:HZ	1:D:119:VAL:HG11	1.84	0.41
1:E:33:GLY:HA3	1:E:34:GLY:HA3	1.93	0.41
1:G:197:LEU:N	2:G:501:GOL:H2	2.27	0.41
1:A:221:THR:HG21	1:B:35:VAL:HG11	2.02	0.41
1:K:91:ARG:HB3	1:K:94:LYS:HB2	2.02	0.41
1:C:36:PRO:HB2	1:C:38:PRO:HD2	2.02	0.41
1:D:36:PRO:HB2	1:D:38:PRO:HD2	2.01	0.41
1:I:142[A]:PHE:CZ	1:J:119:VAL:HG11	2.54	0.41
1:L:157:ARG:NH2	1:L:205:ARG:O	2.54	0.41
1:D:124:PHE:C	1:D:124:PHE:CD1	2.99	0.41
1:A:100:LEU:HD13	1:A:113:LEU:HD13	2.03	0.40
1:L:36:PRO:HB2	1:L:38:PRO:HD2	2.02	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	198/232 (85%)	194 (98%)	4 (2%)	0	100	100
1	B	194/232 (84%)	192 (99%)	2 (1%)	0	100	100
1	C	196/232 (84%)	192 (98%)	4 (2%)	0	100	100
1	D	198/232 (85%)	195 (98%)	3 (2%)	0	100	100
1	E	203/232 (88%)	200 (98%)	2 (1%)	1 (0%)	24	16
1	F	207/232 (89%)	203 (98%)	4 (2%)	0	100	100
1	G	195/232 (84%)	191 (98%)	4 (2%)	0	100	100
1	H	195/232 (84%)	191 (98%)	4 (2%)	0	100	100
1	I	197/232 (85%)	194 (98%)	3 (2%)	0	100	100
1	J	196/232 (84%)	193 (98%)	3 (2%)	0	100	100
1	K	196/232 (84%)	189 (96%)	6 (3%)	1 (0%)	24	16
1	L	196/232 (84%)	195 (100%)	1 (0%)	0	100	100
All	All	2371/2784 (85%)	2329 (98%)	40 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	109	ASP
1	K	91	ARG

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	174/197 (88%)	169 (97%)	5 (3%)	37	31
1	B	171/197 (87%)	166 (97%)	5 (3%)	37	31
1	C	172/197 (87%)	167 (97%)	5 (3%)	37	31
1	D	174/197 (88%)	170 (98%)	4 (2%)	44	40
1	E	175/197 (89%)	172 (98%)	3 (2%)	53	52
1	F	179/197 (91%)	172 (96%)	7 (4%)	28	21
1	G	172/197 (87%)	166 (96%)	6 (4%)	32	24
1	H	173/197 (88%)	168 (97%)	5 (3%)	37	31
1	I	173/197 (88%)	169 (98%)	4 (2%)	44	40
1	J	173/197 (88%)	169 (98%)	4 (2%)	44	40
1	K	173/197 (88%)	165 (95%)	8 (5%)	24	16
1	L	171/197 (87%)	168 (98%)	3 (2%)	51	50
All	All	2080/2364 (88%)	2021 (97%)	59 (3%)	38	32

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	102	VAL
1	A	169	ASP
1	A	184	GLU
1	A	187	GLU
1	B	16	ILE
1	B	108	GLU
1	B	169	ASP
1	B	187	GLU
1	B	193	GLU
1	C	59	VAL
1	C	67	SER
1	C	169	ASP
1	C	180	ASP
1	C	187	GLU
1	D	16	ILE
1	D	91	ARG
1	D	169	ASP
1	D	187	GLU
1	E	169	ASP
1	E	184	GLU
1	E	192	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	30	THR
1	F	31	ARG
1	F	67[A]	SER
1	F	67[B]	SER
1	F	102	VAL
1	F	108	GLU
1	F	141	ARG
1	G	102	VAL
1	G	169	ASP
1	G	184	GLU
1	G	187	GLU
1	G	189	LEU
1	G	220	ASP
1	H	102	VAL
1	H	108	GLU
1	H	134	VAL
1	H	169	ASP
1	H	222	LYS
1	I	169[A]	ASP
1	I	169[B]	ASP
1	I	179	ASP
1	I	187	GLU
1	J	91	ARG
1	J	102	VAL
1	J	108	GLU
1	J	169	ASP
1	K	16	ILE
1	K	90	ASP
1	K	91	ARG
1	K	108	GLU
1	K	134	VAL
1	K	169	ASP
1	K	182	ILE
1	K	193	GLU
1	L	108	GLU
1	L	169	ASP
1	L	206	LEU

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

Mol	Chain	Res	Type
1	A	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185	HIS
1	B	96	ASN
1	B	185	HIS
1	C	118	HIS
1	C	185	HIS
1	D	185	HIS
1	E	96	ASN
1	F	185	HIS
1	G	96	ASN
1	G	185	HIS
1	H	96	ASN
1	H	185	HIS
1	I	185	HIS
1	J	96	ASN
1	J	185	HIS
1	K	89	HIS
1	K	96	ASN
1	K	185	HIS
1	L	185	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	L	501	-	5,5,5	0.84	0	5,5,5	1.40	1 (20%)
2	GOL	B	501	-	5,5,5	0.71	0	5,5,5	0.60	0
2	GOL	E	501	-	5,5,5	1.36	1 (20%)	5,5,5	1.43	1 (20%)
2	GOL	I	501	-	5,5,5	0.35	0	5,5,5	1.52	1 (20%)
2	GOL	D	501	-	5,5,5	0.71	0	5,5,5	1.13	1 (20%)
2	GOL	C	501	-	5,5,5	0.73	0	5,5,5	0.97	0
2	GOL	G	501	-	5,5,5	0.71	0	5,5,5	0.48	0
2	GOL	A	501	-	5,5,5	0.42	0	5,5,5	0.48	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	L	501	-	-	2/4/4/4	-
2	GOL	B	501	-	-	4/4/4/4	-
2	GOL	E	501	-	-	2/4/4/4	-
2	GOL	I	501	-	-	2/4/4/4	-
2	GOL	D	501	-	-	3/4/4/4	-
2	GOL	C	501	-	-	4/4/4/4	-
2	GOL	G	501	-	-	0/4/4/4	-
2	GOL	A	501	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	GOL	C1-C2	2.76	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	GOL	O2-C2-C1	-2.98	96.84	109.18
2	E	501	GOL	O2-C2-C3	-2.31	99.61	109.18
2	D	501	GOL	O2-C2-C1	2.18	118.21	109.18
2	I	501	GOL	O2-C2-C3	2.08	117.77	109.18

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-O2
2	A	501	GOL	O1-C1-C2-C3
2	B	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-C3
2	C	501	GOL	C1-C2-C3-O3
2	D	501	GOL	C1-C2-C3-O3
2	E	501	GOL	C1-C2-C3-O3
2	I	501	GOL	C1-C2-C3-O3
2	L	501	GOL	O1-C1-C2-C3
2	B	501	GOL	O1-C1-C2-O2
2	A	501	GOL	C1-C2-C3-O3
2	B	501	GOL	C1-C2-C3-O3
2	D	501	GOL	O2-C2-C3-O3
2	I	501	GOL	O2-C2-C3-O3
2	L	501	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-O2
2	C	501	GOL	O2-C2-C3-O3
2	E	501	GOL	O2-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	B	501	GOL	O2-C2-C3-O3
2	D	501	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	GOL	2	0
2	E	501	GOL	6	0
2	D	501	GOL	3	0
2	G	501	GOL	2	0
2	A	501	GOL	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	201/232 (86%)	-0.69	0	100	100	23, 42, 77, 108	1 (0%)
1	B	198/232 (85%)	-0.66	0	100	100	30, 44, 77, 107	0
1	C	199/232 (85%)	-0.73	0	100	100	21, 38, 67, 86	1 (0%)
1	D	201/232 (86%)	-0.74	0	100	100	24, 45, 78, 98	1 (0%)
1	E	204/232 (87%)	-1.01	0	100	100	18, 31, 60, 78	1 (0%)
1	F	208/232 (89%)	-0.85	0	100	100	25, 41, 74, 91	1 (0%)
1	G	199/232 (85%)	-0.80	0	100	100	25, 38, 66, 88	0
1	H	198/232 (85%)	-0.81	0	100	100	26, 42, 75, 97	1 (0%)
1	I	199/232 (85%)	-0.96	0	100	100	19, 34, 61, 89	2 (1%)
1	J	200/232 (86%)	-0.83	0	100	100	26, 43, 73, 96	0
1	K	200/232 (86%)	-0.36	1 (0%)	87	89	33, 58, 104, 127	0
1	L	200/232 (86%)	-0.82	0	100	100	27, 38, 63, 92	0
All	All	2407/2784 (86%)	-0.77	1 (0%)	100	100	18, 41, 76, 127	8 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	159	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	501	6/6	0.96	0.08	60,63,64,65	0
2	GOL	D	501	6/6	0.96	0.08	50,51,52,55	0
2	GOL	G	501	6/6	0.97	0.07	61,63,64,65	0
2	GOL	A	501	6/6	0.98	0.05	53,56,58,61	0
2	GOL	E	501	6/6	0.98	0.06	38,39,41,42	0
2	GOL	C	501	6/6	0.98	0.07	51,55,56,56	0
2	GOL	I	501	6/6	0.98	0.06	47,50,52,52	0
2	GOL	L	501	6/6	0.98	0.05	42,45,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.