



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XME
Title : THE X-RAY STRUCTURE OF CTP:INOSITOL-1-PHOSPHATE CYTIDY-
LYLTRANSFERASE 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

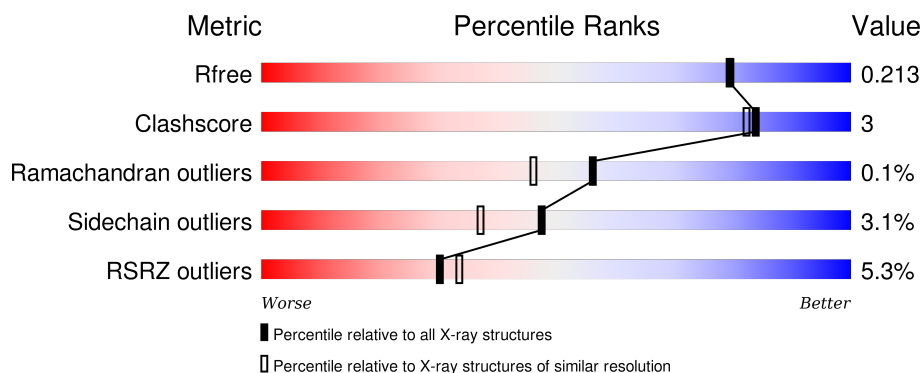
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	<div> <div>4%</div> <div>80%7%13%</div> </div>
1	B	232	<div> <div>3%</div> <div>78%7%15%</div> </div>
1	C	232	<div> <div>3%</div> <div>77%8%14%</div> </div>
1	D	232	<div> <div>7%</div> <div>80%7%13%</div> </div>
1	E	232	<div> <div>77%11%12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	232	
1	G	232	
1	H	232	
1	I	232	
1	J	232	
1	K	232	
1	L	232	

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	D	501	-	-	-	X
2	GOL	E	501	-	-	X	X
2	GOL	I	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 (three-letter code: GOL) (formula: C₃H₈O₃).



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		

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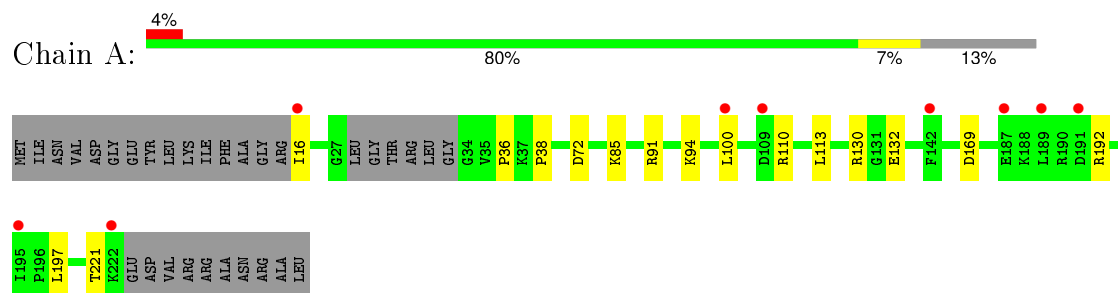
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	132	Total 133	O 133	0	1
3	F	109	Total 109	O 109	0	0
3	G	118	Total 119	O 119	0	1
3	H	98	Total 98	O 98	0	0
3	I	109	Total 110	O 110	0	1
3	J	89	Total 89	O 89	0	0
3	K	77	Total 77	O 77	0	0
3	L	39	Total 39	O 39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

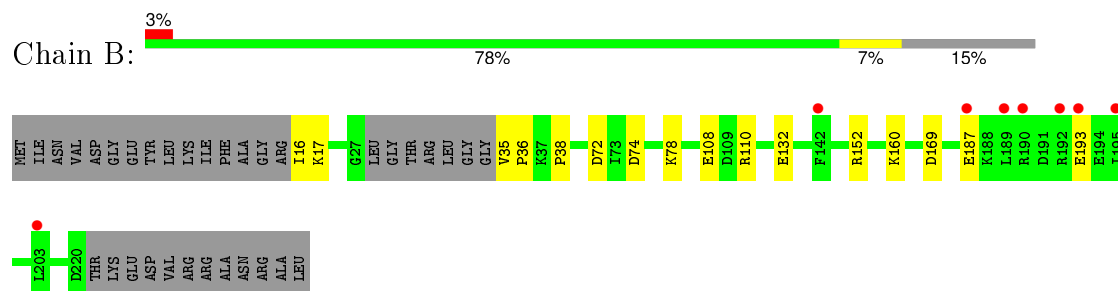
3 Residue-property plots [i](#)

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: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

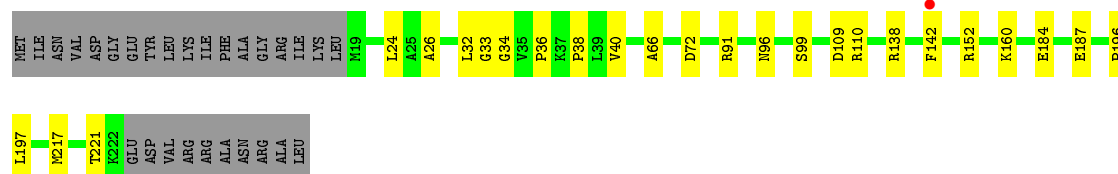
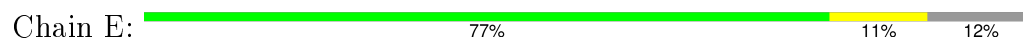


• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

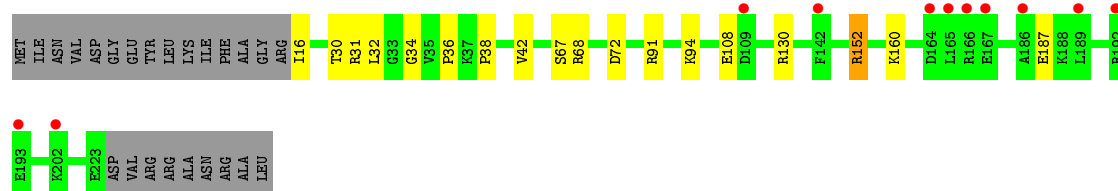
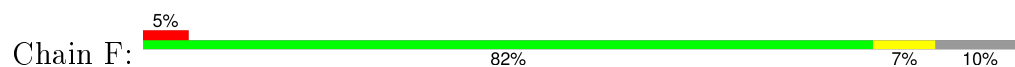




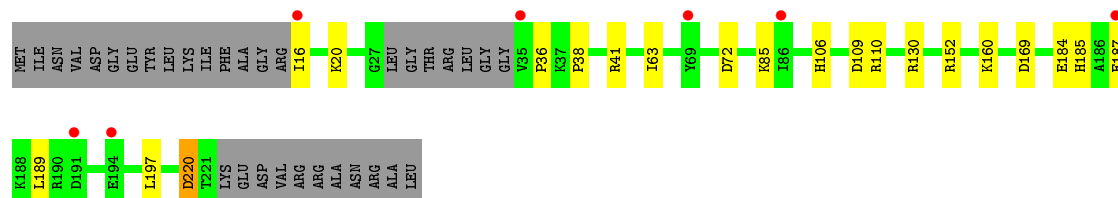
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



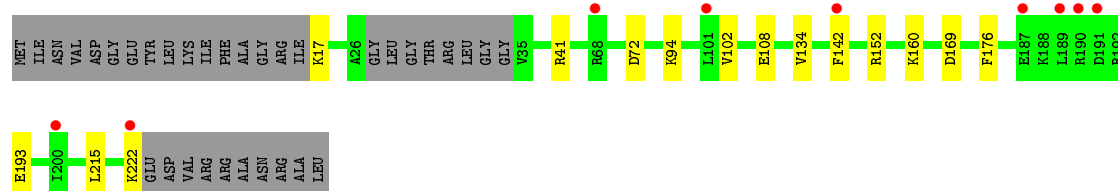
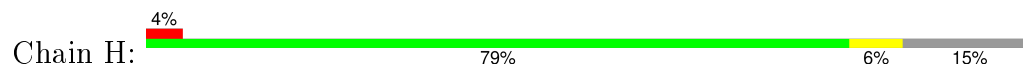
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



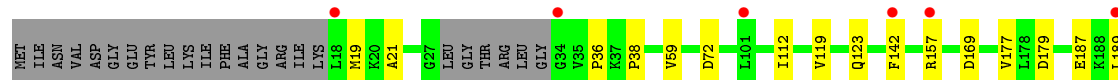
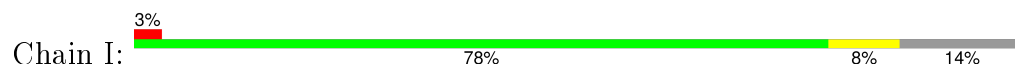
- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

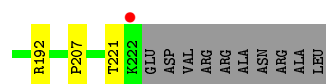


- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

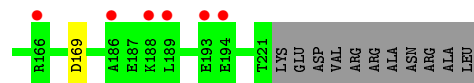
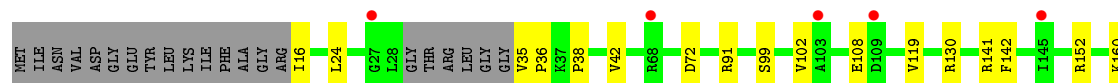
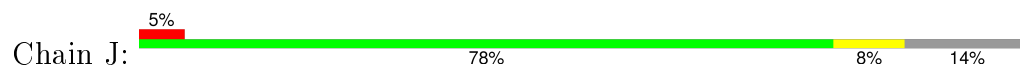


- Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE

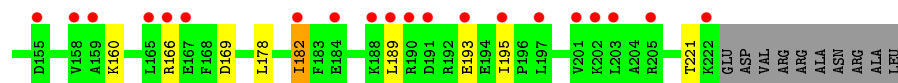
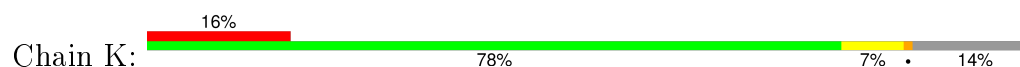




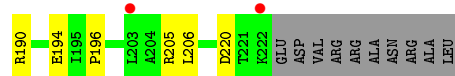
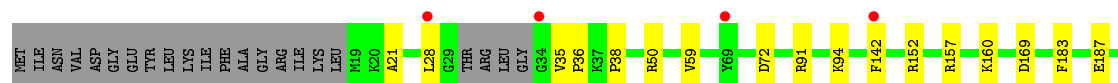
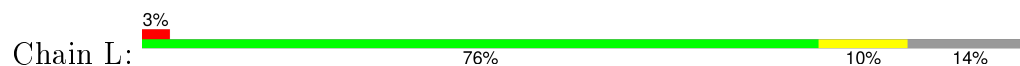
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



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



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



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 27.62 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.67-1.89) 87.9 (27.62-1.89)	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 0.197 , 0.213	Depositor DCC
R_{free} test set	10915 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
Estimated twinning fraction	0.248 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 217329 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/1641	0.67	0/2208
1	B	0.48	0/1609	0.66	0/2166
1	C	0.50	0/1624	0.70	0/2186
1	D	0.49	0/1636	0.67	0/2203
1	E	0.57	0/1659	0.72	0/2234
1	F	0.52	0/1687	0.69	0/2271
1	G	0.52	0/1616	0.69	0/2176
1	H	0.47	0/1625	0.68	0/2187
1	I	0.53	0/1632	0.69	0/2197
1	J	0.48	0/1624	0.68	0/2187
1	K	0.43	0/1625	0.67	0/2187
1	L	0.52	0/1616	0.68	0/2175
All	All	0.50	0/19594	0.68	0/26377

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1610	0	1641	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1582	0	1609	8	0
1	C	1593	0	1617	14	0
1	D	1606	0	1634	9	0
1	E	1627	0	1655	20	0
1	F	1656	0	1692	11	0
1	G	1589	0	1616	11	0
1	H	1594	0	1624	7	0
1	I	1598	0	1621	17	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	116	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 (116) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:19:MET:CE	1:I:177:VAL:HG13	2.32	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:I:142[A]:PHE:HZ	1:J:119:VAL:HG11	1.70	0.57
1:H:152:ARG:HB3	1:H:160:LYS:HB2	1.86	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: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
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:F:16:ILE:HG13	1:F:130:ARG:HG2	1.90	0.54
1:B:152:ARG:HB3	1:B:160:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:19:MET:HE3	1:I:177:VAL:HG13	1.92	0.50
1:K:42:VAL:HG12	1:L:142:PHE:HE2	1.77	0.50
1:D:152:ARG:HB3	1:D:160:LYS:HB2	1.93	0.50
1:I:19:MET:HE1	1:I:177:VAL:HG13	1.94	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:E:110:ARG:NH2	3:E:2072:HOH:O	2.44	0.49
1:K:221:THR:HG21	1:L:35:VAL:HG11	1.95	0.49
1:I:123:GLN:HE22	1:J:141:ARG:HH12	1.59	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:G:109:ASP:CG	1:G:110:ARG:H	2.18	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:I:142[A]:PHE:HE2	1:J:42:VAL:HG12	1.82	0.45
1:H:94:LYS:HG2	1:H:193:GLU:O	2.17	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:HG21	1.99	0.44
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:B:17:LYS:HB2	1:C:138:ARG:HB3	1.99	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:K:221:THR:CG2	1:L:35:VAL:HG11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:74:ASP:OD1	1:F:68:ARG:NH1	2.51	0.42
1:I:19:MET:HE1	1:I:112:ILE:HG13	2.00	0.42
1:B:36:PRO:HB2	1:B:38:PRO:HD2	2.01	0.42
1:E:26:ALA:HB2	1:E:66:ALA:HA	2.01	0.42
1:A:36:PRO:HB2	1:A:38:PRO:HD2	2.01	0.42
1:K:91:ARG:CB	1:K:94:LYS:HB2	2.49	0.42
1:J:24:LEU:HD22	1:J:99:SER:HB3	2.00	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:C:119:VAL:HG11	1:D:142:PHE:HZ	1.83	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:C:142[A]:PHE:HZ	1:D:119:VAL:HG11	1.84	0.41
1:B:16:ILE:O	1:C:139:GLU:HG2	2.19	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:K:91:ARG:HB3	1:K:94:LYS:HB2	2.02	0.41
1:A:221:THR:HG21	1:B:35:VAL:HG11	2.02	0.41
1:I:142[A]:PHE:CZ	1:J:119:VAL:HG11	2.54	0.41
1:D:36:PRO:HB2	1:D:38:PRO:HD2	2.01	0.41
1:C:36:PRO:HB2	1:C:38:PRO:HD2	2.02	0.41
1:L:157:ARG:NH2	1:L:205:ARG:O	2.54	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%)	34	21
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%)	34	21
1	L	196/232 (84%)	195 (100%)	1 (0%)	0	100	100
All	All	2371/2784 (85%)	2329 (98%)	40 (2%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

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

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	174/197 (88%)	170 (98%)	4 (2%)	58	51
1	B	171/197 (87%)	166 (97%)	5 (3%)	50	40
1	C	172/197 (87%)	167 (97%)	5 (3%)	50	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	174/197 (88%)	167 (96%)	7 (4%)	38	26
1	E	175/197 (89%)	170 (97%)	5 (3%)	50	40
1	F	179/197 (91%)	171 (96%)	8 (4%)	34	21
1	G	172/197 (87%)	166 (96%)	6 (4%)	43	31
1	H	173/197 (88%)	169 (98%)	4 (2%)	58	51
1	I	173/197 (88%)	168 (97%)	5 (3%)	50	40
1	J	173/197 (88%)	168 (97%)	5 (3%)	50	40
1	K	173/197 (88%)	164 (95%)	9 (5%)	29	17
1	L	171/197 (87%)	167 (98%)	4 (2%)	58	51
All	All	2080/2364 (88%)	2013 (97%)	67 (3%)	47	35

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	85	LYS
1	A	169	ASP
1	A	192	ARG
1	B	72	ASP
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	72	ASP
1	C	169	ASP
1	C	180	ASP
1	D	16	ILE
1	D	72	ASP
1	D	91	ARG
1	D	110	ARG
1	D	169	ASP
1	D	187	GLU
1	D	191	ASP
1	E	72	ASP
1	E	91	ARG
1	E	184	GLU
1	E	187	GLU

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Mol	Chain	Res	Type
1	E	217	MET
1	F	30	THR
1	F	31	ARG
1	F	67[A]	SER
1	F	67[B]	SER
1	F	72	ASP
1	F	108	GLU
1	F	152	ARG
1	F	187	GLU
1	G	72	ASP
1	G	169	ASP
1	G	184	GLU
1	G	187	GLU
1	G	189	LEU
1	G	220	ASP
1	H	72	ASP
1	H	102	VAL
1	H	108	GLU
1	H	169	ASP
1	I	72	ASP
1	I	169[A]	ASP
1	I	169[B]	ASP
1	I	179	ASP
1	I	187	GLU
1	J	72	ASP
1	J	91	ARG
1	J	102	VAL
1	J	108	GLU
1	J	169	ASP
1	K	16	ILE
1	K	72	ASP
1	K	90	ASP
1	K	91	ARG
1	K	108	GLU
1	K	166	ARG
1	K	169	ASP
1	K	182	ILE
1	K	193	GLU
1	L	28	LEU
1	L	72	ASP
1	L	169	ASP
1	L	206	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	118	HIS
1	D	105	ASN
1	G	185	HIS
1	I	105	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	501	-	5,5,5	0.40	0	5,5,5	0.39	0
2	GOL	B	501	-	5,5,5	0.64	0	5,5,5	0.60	0
2	GOL	C	501	-	5,5,5	0.66	0	5,5,5	0.97	0
2	GOL	D	501	-	5,5,5	0.66	0	5,5,5	1.06	1 (20%)
2	GOL	E	501	-	5,5,5	1.32	1 (20%)	5,5,5	1.30	0
2	GOL	G	501	-	5,5,5	0.65	0	5,5,5	0.53	0
2	GOL	I	501	-	5,5,5	0.30	0	5,5,5	1.39	0
2	GOL	L	501	-	5,5,5	0.80	0	5,5,5	1.22	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	E	501	-	-	0/4/4/4	0/0/0/0
2	GOL	G	501	-	-	0/4/4/4	0/0/0/0
2	GOL	I	501	-	-	0/4/4/4	0/0/0/0
2	GOL	L	501	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	GOL	C1-C2	2.61	1.62	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	GOL	O2-C2-C1	-2.58	96.84	108.65
2	D	501	GOL	O2-C2-C1	2.09	118.21	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	2	0
2	D	501	GOL	3	0
2	E	501	GOL	6	0
2	G	501	GOL	2	0
2	L	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 ⓘ

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	201/232 (86%)	0.50	9 (4%) 37 40	26, 42, 77, 108	0
1	B	198/232 (85%)	0.46	8 (4%) 42 46	30, 44, 77, 107	0
1	C	199/232 (85%)	0.43	6 (3%) 54 57	21, 38, 67, 86	0
1	D	201/232 (86%)	0.62	16 (7%) 15 17	26, 45, 78, 98	1 (0%)
1	E	204/232 (87%)	0.24	1 (0%) 91 92	19, 31, 60, 78	0
1	F	208/232 (89%)	0.48	11 (5%) 30 33	25, 41, 74, 91	0
1	G	199/232 (85%)	0.39	7 (3%) 48 51	25, 38, 66, 88	0
1	H	198/232 (85%)	0.53	9 (4%) 37 40	26, 42, 75, 97	0
1	I	199/232 (85%)	0.38	7 (3%) 48 51	21, 34, 61, 89	0
1	J	200/232 (86%)	0.53	11 (5%) 29 32	26, 43, 73, 96	0
1	K	200/232 (86%)	1.11	36 (18%) 2 2	33, 58, 104, 127	0
1	L	200/232 (86%)	0.37	6 (3%) 54 57	27, 38, 63, 92	0
All	All	2407/2784 (86%)	0.50	127 (5%) 30 33	19, 41, 77, 127	1 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	27	GLY	10.3
1	K	145	ILE	7.9
1	H	222	LYS	7.8
1	K	90	ASP	6.4
1	K	35	VAL	6.3
1	A	191	ASP	5.9
1	K	190	ARG	5.6
1	D	34	GLY	5.4
1	I	222	LYS	5.2
1	C	18	LEU	5.2
1	K	92	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	142[A]	PHE	4.8
1	H	189	LEU	4.8
1	K	222	LYS	4.8
1	C	34	GLY	4.2
1	K	188	LYS	4.0
1	J	188	LYS	3.9
1	A	189	LEU	3.9
1	F	189	LEU	3.7
1	A	16	ILE	3.7
1	L	142	PHE	3.6
1	K	191	ASP	3.6
1	K	165	LEU	3.5
1	H	200	ILE	3.5
1	H	101	LEU	3.5
1	K	166	ARG	3.4
1	K	68	ARG	3.4
1	L	222	LYS	3.4
1	H	191	ASP	3.4
1	J	109	ASP	3.4
1	D	158	VAL	3.4
1	J	68	ARG	3.3
1	A	109	ASP	3.3
1	K	93	GLU	3.3
1	C	69	TYR	3.2
1	I	18	LEU	3.2
1	J	166	ARG	3.1
1	B	192	ARG	3.1
1	D	68	ARG	3.1
1	K	195	ILE	3.1
1	J	145	ILE	3.0
1	F	202	LYS	3.0
1	K	184	GLU	3.0
1	J	194	GLU	2.9
1	F	166	ARG	2.9
1	F	164	ASP	2.9
1	C	142[A]	PHE	2.9
1	H	142[A]	PHE	2.9
1	K	158	VAL	2.9
1	B	142	PHE	2.8
1	K	182	ILE	2.8
1	B	187	GLU	2.7
1	K	69	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	26	ALA	2.7
1	H	68	ARG	2.7
1	A	222	LYS	2.7
1	B	203	LEU	2.7
1	F	165	LEU	2.7
1	A	142[A]	PHE	2.6
1	G	86	ILE	2.6
1	D	171	VAL	2.6
1	J	186	ALA	2.6
1	K	102	VAL	2.6
1	K	79	ASP	2.6
1	I	142[A]	PHE	2.6
1	K	189	LEU	2.6
1	K	101	LEU	2.6
1	H	190	ARG	2.6
1	D	16	ILE	2.6
1	B	195	ILE	2.5
1	I	189	LEU	2.5
1	K	203	LEU	2.5
1	K	205	ARG	2.5
1	G	191	ASP	2.5
1	F	193	GLU	2.5
1	L	28	LEU	2.5
1	K	202	LYS	2.5
1	D	69	TYR	2.5
1	F	142	PHE	2.4
1	D	109[A]	ASP	2.4
1	G	69	TYR	2.4
1	G	194	GLU	2.4
1	K	155	ASP	2.4
1	D	145	ILE	2.4
1	D	188	LYS	2.4
1	F	167	GLU	2.4
1	D	143	VAL	2.4
1	B	193	GLU	2.3
1	G	35	VAL	2.3
1	D	192	ARG	2.3
1	B	190	ARG	2.3
1	C	166	ARG	2.3
1	J	27	GLY	2.3
1	B	189	LEU	2.3
1	A	187	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	186	ALA	2.2
1	J	103	ALA	2.2
1	L	203	LEU	2.2
1	D	164	ASP	2.2
1	H	187	GLU	2.2
1	F	109	ASP	2.2
1	K	152	ARG	2.2
1	L	69	TYR	2.2
1	J	193	GLU	2.1
1	I	157	ARG	2.1
1	L	34	GLY	2.1
1	K	193	GLU	2.1
1	J	189	LEU	2.1
1	A	195	ILE	2.1
1	K	167	GLU	2.1
1	D	189	LEU	2.1
1	G	187	GLU	2.1
1	K	141	ARG	2.1
1	K	151	ILE	2.1
1	A	100	LEU	2.1
1	K	100	LEU	2.1
1	D	193	GLU	2.1
1	K	201	VAL	2.1
1	D	142	PHE	2.0
1	K	197	LEU	2.0
1	I	34	GLY	2.0
1	C	17	LYS	2.0
1	G	16	ILE	2.0
1	D	203	LEU	2.0
1	I	101	LEU	2.0
1	F	192	ARG	2.0
1	K	159	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	D	501	6/6	0.64	0.26	4.77	50,51,52,55	0
2	GOL	I	501	6/6	0.85	0.17	2.79	47,50,52,52	0
2	GOL	E	501	6/6	0.84	0.19	2.73	38,39,41,42	0
2	GOL	G	501	6/6	0.81	0.18	1.84	61,63,64,65	0
2	GOL	B	501	6/6	0.56	0.18	1.13	60,63,64,65	0
2	GOL	C	501	6/6	0.90	0.14	0.74	51,55,56,56	0
2	GOL	A	501	6/6	0.91	0.16	0.73	53,56,58,61	0
2	GOL	L	501	6/6	0.92	0.13	0.73	42,45,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.