



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:28 AM UTC

PDB ID : 1RLM / pdb_00001rlm
Title : Crystal Structure of ybiV from Escherichia coli K12
Authors : Roberts, A.; Lee, S.Y.; McCullagh, E.; Silversmith, R.E.; Wemmer, D.E.
Deposited on : 2003-11-26
Resolution : 1.90 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

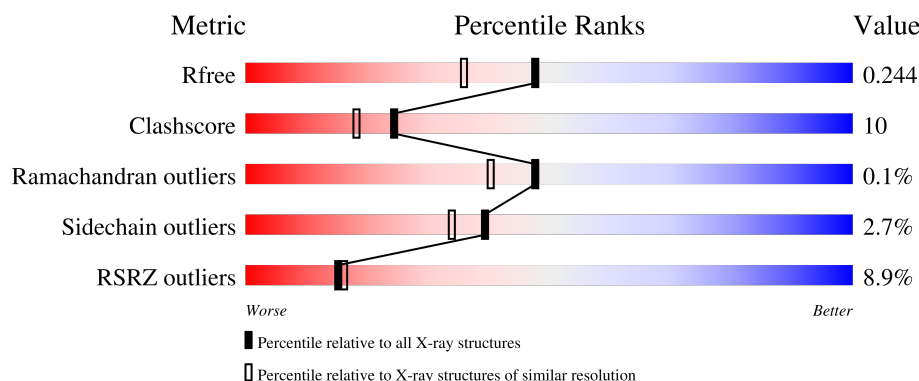
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	271	7% 76% 22% ..
1	B	271	10% 80% 18% ..
1	C	271	15% 73% 25% ..
1	D	271	3% 78% 18% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	804	-	X	-	-
3	GOL	A	806	-	X	-	-
3	GOL	B	807	-	X	-	-
3	GOL	C	808	-	X	-	-
3	GOL	C	809	-	X	-	-
3	GOL	D	810	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9154 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 Phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2134	1369	362	395	8			
1	B	269	Total	C	N	O	S	0	0	0
			2134	1369	362	395	8			
1	C	269	Total	C	N	O	S	0	0	0
			2134	1369	362	395	8			
1	D	269	Total	C	N	O	S	0	0	0
			2134	1369	362	395	8			

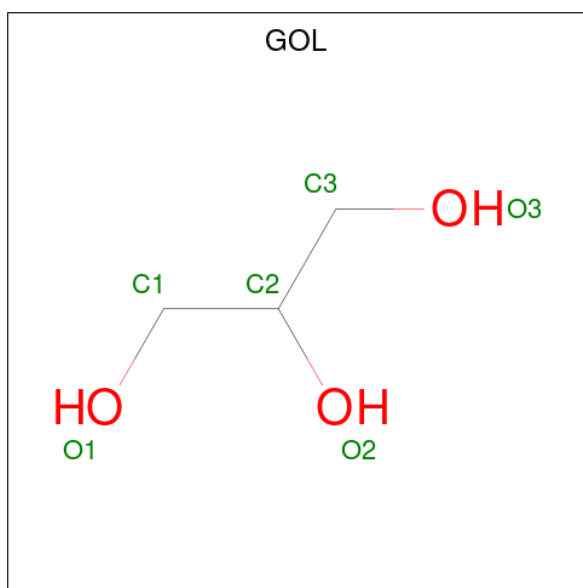
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P75792
A	267	TYR	SER	engineered mutation	UNP P75792
B	2	ALA	SER	engineered mutation	UNP P75792
B	267	TYR	SER	engineered mutation	UNP P75792
C	2	ALA	SER	engineered mutation	UNP P75792
C	267	TYR	SER	engineered mutation	UNP P75792
D	2	ALA	SER	engineered mutation	UNP P75792
D	267	TYR	SER	engineered mutation	UNP P75792

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

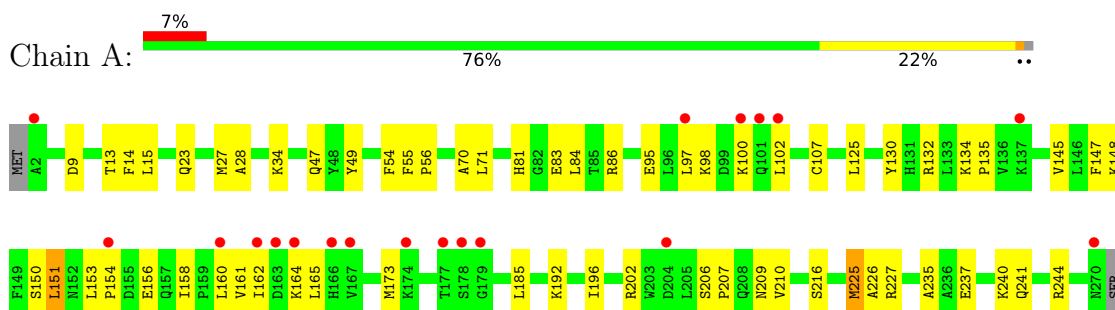
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	150	Total	O	0	0
			150	150		
4	C	107	Total	O	0	0
			107	107		
4	D	170	Total	O	0	0
			170	170		

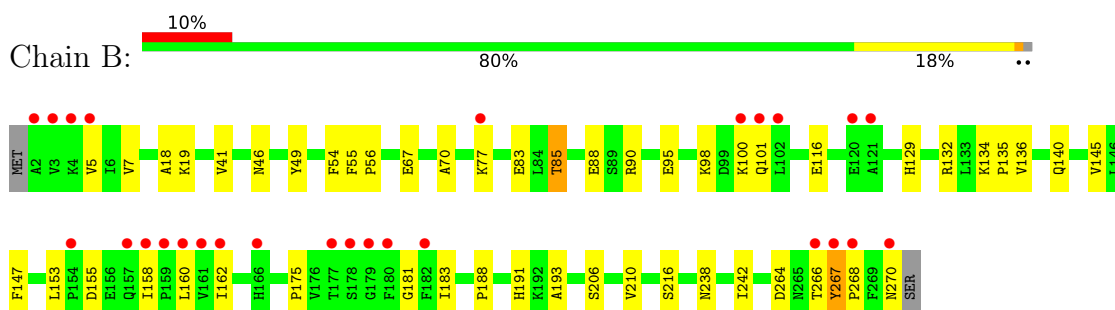
3 Residue-property plots [i](#)

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

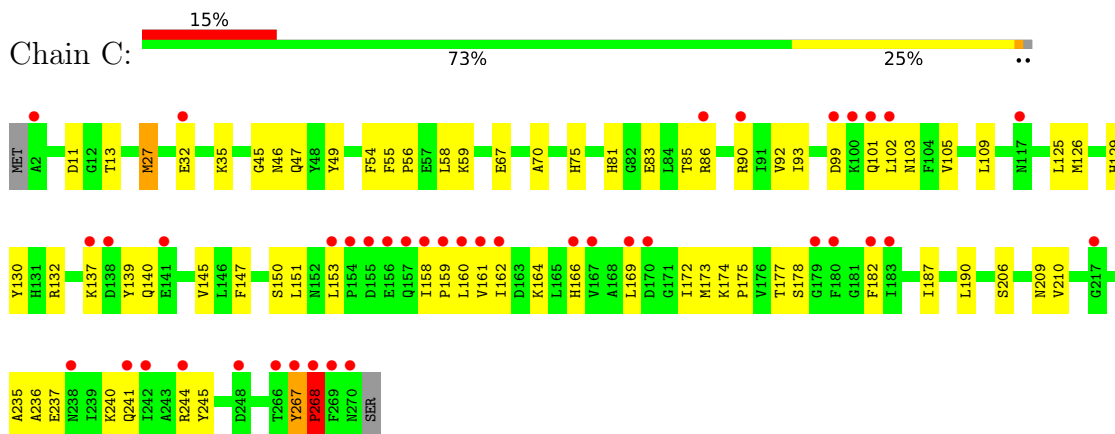
- Molecule 1: Phosphatase



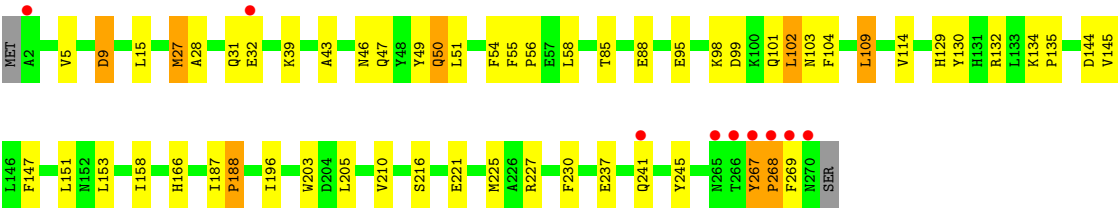
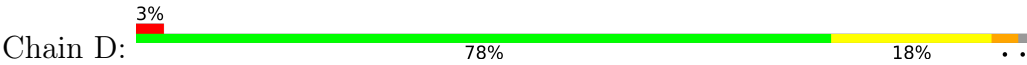
- Molecule 1: Phosphatase



- Molecule 1: Phosphatase



- Molecule 1: Phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.82Å 91.61Å 186.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.96-1.90) 97.1 (19.96-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.248 0.217 , 0.244	Depositor DCC
R_{free} test set	9608 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9154	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: MG, 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	0.40	0/2179	0.89	3/2946 (0.1%)
1	B	0.43	0/2179	1.00	12/2946 (0.4%)
1	C	0.43	1/2179 (0.0%)	1.32	9/2946 (0.3%)
1	D	0.44	0/2179	1.04	13/2946 (0.4%)
All	All	0.43	1/8716 (0.0%)	1.08	37/11784 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	13	THR	CA-C	8.36	1.56	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	TYR	CA-C-N	32.78	160.81	119.84
1	C	267	TYR	C-N-CA	32.78	160.81	119.84
1	C	268	PRO	CA-N-CD	-17.97	86.84	112.00
1	C	268	PRO	N-CA-CB	13.93	117.87	103.25
1	D	267	TYR	CA-C-N	13.81	160.15	127.00
1	D	267	TYR	C-N-CA	13.81	160.15	127.00
1	D	267	TYR	C-N-CD	-13.11	91.75	120.60
1	C	268	PRO	N-CD-CG	11.79	120.89	103.20
1	B	267	TYR	C-N-CD	-11.70	94.86	120.60
1	C	267	TYR	C-N-CD	-11.48	77.92	125.00
1	B	267	TYR	CA-C-N	10.39	151.94	127.00
1	B	267	TYR	C-N-CA	10.39	151.94	127.00
1	B	101	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	D	267	TYR	N-CA-C	8.80	120.81	109.64
1	A	210	VAL	N-CA-C	8.12	119.54	108.17
1	D	210	VAL	N-CA-C	6.99	117.96	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	LYS	N-CA-C	6.77	121.77	112.90
1	B	101	GLN	CG-CD-NE2	6.67	126.41	116.40
1	B	181	GLY	N-CA-C	-6.27	106.59	115.43
1	C	210	VAL	N-CA-C	6.18	117.49	108.53
1	B	188	PRO	CB-CA-C	5.92	119.16	111.64
1	D	103	ASN	N-CA-C	-5.87	98.84	108.76
1	D	187	ILE	N-CA-C	-5.74	103.33	108.95
1	A	9	ASP	N-CA-C	-5.71	103.16	110.53
1	D	158	ILE	N-CA-C	5.66	119.14	112.35
1	C	85	THR	N-CA-C	-5.64	102.94	110.55
1	B	206	SER	CA-C-N	5.62	125.30	119.56
1	B	206	SER	C-N-CA	5.62	125.30	119.56
1	A	216	SER	N-CA-C	5.59	117.11	109.18
1	D	216	SER	N-CA-C	5.57	118.71	110.46
1	B	216	SER	N-CA-C	5.46	118.53	110.46
1	D	188	PRO	CA-N-CD	-5.30	104.57	112.00
1	D	9	ASP	N-CA-C	-5.29	103.42	110.55
1	D	104	PHE	N-CA-C	5.27	117.08	109.07
1	B	85	THR	N-CA-C	-5.20	103.82	110.53
1	C	59	LYS	N-CA-C	5.11	118.29	111.75
1	D	269	PHE	N-CA-C	5.06	117.39	108.24

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	2134	0	2124	42	0
1	B	2134	0	2124	33	0
1	C	2134	0	2124	52	0
1	D	2134	0	2124	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	8	1	0
3	B	6	0	4	0	0
3	C	12	0	8	3	0
3	D	6	0	4	0	0
4	A	151	0	0	4	0
4	B	150	0	0	1	0
4	C	107	0	0	2	0
4	D	170	0	0	3	0
All	All	9154	0	8520	169	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 10.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:MET:HE3	1:D:58:LEU:HD11	1.44	0.98
1:D:99:ASP:OD1	1:D:101:GLN:HG2	1.76	0.85
1:A:102:LEU:HD11	1:A:151:LEU:HD23	1.57	0.83
1:D:27:MET:HE1	1:D:31:GLN:HE21	1.44	0.82
1:C:83:GLU:HG3	1:C:145:VAL:HG13	1.59	0.82
1:B:267:TYR:CD2	1:B:268:PRO:HD3	2.20	0.76
1:A:13:THR:HG22	1:A:14:PHE:N	1.98	0.76
1:A:207:PRO:HB3	1:A:225:MET:HE3	1.68	0.75
1:C:267:TYR:CD2	1:C:268:PRO:HD3	2.23	0.73
1:C:102:LEU:HD23	1:C:103:ASN:N	2.05	0.71
1:C:102:LEU:HD11	1:C:151:LEU:HD23	1.71	0.71
1:A:156:GLU:H	1:A:156:GLU:CD	2.00	0.69
1:C:11:ASP:HB2	3:C:809:GOL:H11	1.73	0.69
1:A:225:MET:HE2	1:A:226:ALA:HA	1.75	0.68
1:C:102:LEU:HD21	1:C:151:LEU:HG	1.74	0.67
1:D:196:ILE:HG21	1:D:225:MET:HE1	1.77	0.67
1:A:164:LYS:HG2	4:A:903:HOH:O	1.93	0.66
1:A:227:ARG:HD2	1:A:244:ARG:NH2	2.12	0.64
1:D:27:MET:HE1	1:D:31:GLN:NE2	2.14	0.63
1:C:161:VAL:HA	1:C:164:LYS:HE2	1.81	0.63
1:A:154:PRO:HB3	1:A:156:GLU:OE2	1.99	0.62
1:C:178:SER:HB3	1:C:182:PHE:HB3	1.82	0.61
1:A:125:LEU:HD12	3:A:806:GOL:O2	2.01	0.60
1:B:85:THR:OG1	1:B:88:GLU:HG3	2.02	0.59
1:D:49:TYR:CG	1:D:132:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG23	1:B:175:PRO:HB2	1.85	0.58
1:C:90:ARG:HD3	1:C:140:GLN:NE2	2.19	0.57
1:C:187:ILE:HB	1:C:190:LEU:HD12	1.86	0.57
1:B:264:ASP:HB2	1:B:266:THR:HG23	1.88	0.55
1:C:45:GLY:H	3:C:809:GOL:C3	2.18	0.55
1:D:27:MET:CE	1:D:31:GLN:HE21	2.18	0.55
1:A:153:LEU:N	1:A:153:LEU:HD23	2.21	0.55
1:A:165:LEU:HD13	1:A:185:LEU:HD21	1.88	0.55
1:D:50:GLN:HG2	1:D:129:HIS:O	2.06	0.55
1:A:237:GLU:O	1:A:241:GLN:HG3	2.07	0.55
1:B:55:PHE:N	1:B:56:PRO:HD3	2.23	0.54
1:A:49:TYR:CG	1:A:132:ARG:HD3	2.42	0.54
1:A:100:LYS:HE2	4:A:938:HOH:O	2.07	0.54
1:B:83:GLU:HG3	1:B:145:VAL:HG13	1.89	0.54
1:D:114:VAL:O	1:D:135:PRO:HA	2.07	0.54
1:D:153:LEU:N	1:D:153:LEU:HD23	2.23	0.54
1:A:225:MET:HE2	1:A:226:ALA:CA	2.37	0.54
1:A:227:ARG:HD2	1:A:244:ARG:HH22	1.71	0.54
1:C:86:ARG:HH11	1:C:86:ARG:HG2	1.72	0.53
1:C:160:LEU:HD23	4:C:871:HOH:O	2.08	0.53
1:A:55:PHE:N	1:A:56:PRO:HD3	2.24	0.53
1:D:27:MET:HA	1:D:27:MET:HE2	1.91	0.53
1:D:166:HIS:HD2	4:D:912:HOH:O	1.92	0.52
1:B:49:TYR:CG	1:B:132:ARG:HD3	2.45	0.52
1:C:162:ILE:HD11	1:C:177:THR:HG22	1.92	0.51
1:A:207:PRO:CB	1:A:225:MET:HE3	2.39	0.51
1:C:150:SER:C	1:C:151:LEU:HD12	2.35	0.51
1:C:153:LEU:HD23	1:C:153:LEU:N	2.26	0.51
1:D:5:VAL:HG23	1:D:205:LEU:HD23	1.93	0.51
1:C:27:MET:HE1	1:C:58:LEU:HD21	1.91	0.51
1:D:99:ASP:HB3	1:D:102:LEU:HD22	1.93	0.51
1:B:160:LEU:C	1:B:160:LEU:HD23	2.36	0.51
1:B:54:PHE:C	1:B:56:PRO:HD3	2.36	0.51
1:D:28:ALA:O	1:D:32:GLU:HG3	2.11	0.51
1:A:151:LEU:HD12	1:A:151:LEU:N	2.26	0.50
1:A:95:GLU:OE2	1:A:98:LYS:HD2	2.12	0.50
1:C:102:LEU:HD21	1:C:151:LEU:CG	2.41	0.50
1:C:237:GLU:O	1:C:241:GLN:HG3	2.11	0.50
1:B:267:TYR:CA	1:B:270:ASN:ND2	2.75	0.50
1:B:267:TYR:HA	1:B:270:ASN:ND2	2.27	0.50
1:C:49:TYR:CG	1:C:132:ARG:HD3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD23	1:B:153:LEU:N	2.26	0.49
1:B:191:HIS:CE1	1:B:193:ALA:HB3	2.47	0.49
1:A:192:LYS:O	1:A:196:ILE:HG13	2.12	0.48
1:A:107:CYS:SG	1:A:148:LYS:HE2	2.53	0.48
1:A:83:GLU:HG3	1:A:145:VAL:HG13	1.94	0.48
1:D:132:ARG:HG2	4:D:812:HOH:O	2.14	0.48
1:C:93:ILE:HD12	1:C:139:TYR:HB3	1.95	0.48
1:C:125:LEU:HD13	1:C:125:LEU:C	2.39	0.48
1:A:153:LEU:CD1	1:A:161:VAL:HG21	2.44	0.47
1:B:18:ALA:O	1:B:19:LYS:HB2	2.13	0.47
1:D:227:ARG:O	1:D:227:ARG:HD2	2.14	0.47
1:D:267:TYR:CD2	1:D:267:TYR:C	2.92	0.47
1:A:206:SER:H	1:A:209:ASN:HD22	1.61	0.47
1:B:191:HIS:HB2	4:B:913:HOH:O	2.13	0.47
1:C:47:GLN:HB2	1:C:130:TYR:CD2	2.49	0.47
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.79	0.47
1:B:158:ILE:O	1:B:162:ILE:HG13	2.15	0.46
1:D:203:TRP:O	1:D:205:LEU:HD13	2.14	0.46
1:C:178:SER:HB3	1:C:182:PHE:CB	2.44	0.46
1:D:196:ILE:CG2	1:D:225:MET:HE1	2.44	0.46
1:B:238:ASN:O	1:B:242:ILE:HG13	2.15	0.46
1:D:46:ASN:HB3	1:D:50:GLN:CG	2.45	0.46
1:A:84:LEU:HD11	1:A:173:MET:CE	2.45	0.46
1:D:46:ASN:HB3	1:D:50:GLN:HG2	1.98	0.46
1:A:54:PHE:C	1:A:56:PRO:HD3	2.41	0.46
1:A:150:SER:C	1:A:151:LEU:HD12	2.40	0.46
1:C:125:LEU:HD11	1:C:182:PHE:CZ	2.51	0.46
1:A:235:ALA:O	1:A:240:LYS:HE3	2.15	0.46
1:C:99:ASP:C	1:C:101:GLN:H	2.22	0.45
1:D:9:ASP:HA	1:D:43:ALA:O	2.16	0.45
1:C:105:VAL:CG2	1:C:126:MET:HE3	2.47	0.45
1:A:160:LEU:C	1:A:160:LEU:HD13	2.42	0.45
1:B:160:LEU:HD23	1:B:160:LEU:O	2.16	0.45
1:C:11:ASP:CB	3:C:809:GOL:H11	2.43	0.45
1:B:267:TYR:CE2	1:B:268:PRO:HD3	2.51	0.45
1:C:162:ILE:HG23	1:C:175:PRO:HB2	1.99	0.45
1:D:245:TYR:CD2	1:D:268:PRO:HG3	2.52	0.45
1:C:132:ARG:HG2	4:C:836:HOH:O	2.16	0.44
1:C:235:ALA:O	1:C:240:LYS:HE3	2.18	0.44
1:D:54:PHE:C	1:D:56:PRO:HD3	2.42	0.44
1:B:95:GLU:OE2	1:B:98:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HB	1:B:210:VAL:HG22	1.99	0.44
1:D:46:ASN:OD1	1:D:129:HIS:HD2	2.00	0.44
1:B:46:ASN:OD1	1:B:129:HIS:ND1	2.42	0.44
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.83	0.44
1:C:54:PHE:C	1:C:56:PRO:HD3	2.43	0.43
1:D:15:LEU:HD21	1:D:54:PHE:CE1	2.53	0.43
1:C:92:VAL:HG22	1:C:169:LEU:HD22	2.01	0.43
1:C:206:SER:H	1:C:209:ASN:HD22	1.66	0.43
1:B:153:LEU:HD23	1:B:153:LEU:H	1.82	0.43
1:D:134:LYS:HA	1:D:135:PRO:HD3	1.86	0.43
1:D:230:PHE:CZ	1:D:268:PRO:HG2	2.53	0.43
1:A:23:GLN:O	1:A:27:MET:HG2	2.18	0.43
1:A:34:LYS:HA	4:A:930:HOH:O	2.18	0.43
1:C:35:LYS:HB3	1:C:35:LYS:HE2	1.81	0.43
1:B:267:TYR:HB2	1:B:270:ASN:ND2	2.33	0.43
1:C:32:GLU:HA	1:C:35:LYS:HE2	2.01	0.43
1:B:267:TYR:HB2	1:B:270:ASN:HD21	1.82	0.42
1:D:55:PHE:N	1:D:56:PRO:HD3	2.34	0.42
1:D:237:GLU:O	1:D:241:GLN:HG3	2.19	0.42
1:B:7:VAL:HG22	1:B:41:VAL:HB	2.01	0.42
1:C:70:ALA:O	1:C:81:HIS:HA	2.20	0.42
1:C:245:TYR:CE2	1:C:268:PRO:HG3	2.54	0.42
1:A:49:TYR:CD1	1:A:132:ARG:HD3	2.54	0.42
1:D:144:ASP:OD2	1:D:145:VAL:N	2.52	0.42
1:C:105:VAL:HG22	1:C:126:MET:HE3	2.00	0.42
1:D:28:ALA:HB3	4:D:897:HOH:O	2.20	0.42
1:D:5:VAL:CG2	1:D:205:LEU:HD23	2.50	0.42
1:C:55:PHE:N	1:C:56:PRO:HD3	2.34	0.41
1:C:125:LEU:HD11	1:C:182:PHE:HZ	1.84	0.41
1:A:28:ALA:HB3	4:A:872:HOH:O	2.20	0.41
1:A:154:PRO:CB	1:A:156:GLU:OE2	2.66	0.41
1:B:155:ASP:HA	1:B:158:ILE:HG13	2.01	0.41
1:D:47:GLN:HB2	1:D:130:TYR:CD2	2.55	0.41
1:D:95:GLU:HA	1:D:98:LYS:HD3	2.03	0.41
1:A:47:GLN:HB2	1:A:130:TYR:CD2	2.55	0.41
1:C:158:ILE:HB	1:C:159:PRO:HD3	2.02	0.41
1:C:46:ASN:OD1	1:C:129:HIS:HD2	2.04	0.41
1:D:39:LYS:HD3	1:D:203:TRP:CE2	2.55	0.41
1:A:70:ALA:O	1:A:81:HIS:HA	2.20	0.41
1:C:245:TYR:CD2	1:C:268:PRO:HG3	2.55	0.41
1:B:134:LYS:HA	1:B:135:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:HG2	1:B:136:VAL:O	2.21	0.41
1:C:99:ASP:C	1:C:101:GLN:N	2.78	0.41
1:C:236:ALA:O	1:C:240:LYS:HG3	2.21	0.41
1:D:227:ARG:HG2	1:D:227:ARG:NH1	2.36	0.41
1:A:102:LEU:HD21	1:A:151:LEU:CD2	2.50	0.41
1:B:158:ILE:HG23	1:B:183:ILE:HD11	2.03	0.41
1:C:166:HIS:ND1	1:C:166:HIS:C	2.79	0.41
1:A:13:THR:HG22	1:A:14:PHE:H	1.79	0.40
1:A:134:LYS:HA	1:A:135:PRO:HD3	1.88	0.40
1:B:153:LEU:N	1:B:153:LEU:CD2	2.84	0.40
1:C:67:GLU:HB2	1:C:70:ALA:HB3	2.01	0.40
1:C:172:ILE:HG22	1:C:173:MET:HG3	2.02	0.40
1:A:158:ILE:O	1:A:162:ILE:HG13	2.21	0.40
1:D:85:THR:OG1	1:D:88:GLU:HG3	2.22	0.40
1:C:86:ARG:HG2	1:C:86:ARG:NH1	2.35	0.40
1:A:225:MET:HE2	1:A:226:ALA:N	2.37	0.40
1:B:67:GLU:HB2	1:B:70:ALA:HB3	2.04	0.40
1:B:90:ARG:HA	1:B:140:GLN:OE1	2.22	0.40
1:C:174:LYS:HA	1:C:175:PRO:HD3	1.86	0.40
1:D:50:GLN:NE2	1:D:51:LEU:HD23	2.36	0.40
1:D:109:LEU:HB2	1:D:145:VAL:HB	2.03	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	267/271 (98%)	255 (96%)	12 (4%)	0	100	100
1	B	267/271 (98%)	254 (95%)	13 (5%)	0	100	100
1	C	267/271 (98%)	254 (95%)	12 (4%)	1 (0%)	30	22
1	D	267/271 (98%)	255 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1068/1084 (98%)	1018 (95%)	49 (5%)	1 (0%)	48 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	PRO

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	228/230 (99%)	220 (96%)	8 (4%)	32 24
1	B	228/230 (99%)	226 (99%)	2 (1%)	70 73
1	C	228/230 (99%)	222 (97%)	6 (3%)	40 35
1	D	228/230 (99%)	219 (96%)	9 (4%)	28 21
All	All	912/920 (99%)	887 (97%)	25 (3%)	39 34

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	71	LEU
1	A	86	ARG
1	A	97	LEU
1	A	147	PHE
1	A	151	LEU
1	A	202	ARG
1	A	225	MET
1	B	77	LYS
1	B	147	PHE
1	C	27	MET
1	C	75	HIS
1	C	109	LEU
1	C	137	LYS

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Mol	Chain	Res	Type
1	C	147	PHE
1	C	268	PRO
1	D	27	MET
1	D	50	GLN
1	D	102	LEU
1	D	109	LEU
1	D	147	PHE
1	D	151	LEU
1	D	188	PRO
1	D	221	GLU
1	D	268	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	78	GLN
1	A	81	HIS
1	A	101	GLN
1	A	110	GLN
1	A	194	ASN
1	A	208	GLN
1	A	209	ASN
1	B	78	GLN
1	B	103	ASN
1	B	152	ASN
1	B	194	ASN
1	B	265	ASN
1	B	270	ASN
1	C	68	ASN
1	C	103	ASN
1	C	117	ASN
1	C	129	HIS
1	C	208	GLN
1	C	209	ASN
1	C	218	ASN
1	D	31	GLN
1	D	50	GLN
1	D	78	GLN
1	D	87	HIS
1	D	101	GLN
1	D	129	HIS

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Mol	Chain	Res	Type
1	D	166	HIS
1	D	209	ASN
1	D	238	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	GOL	C	808	-	5,5,5	4.77	5 (100%)	5,5,5	6.12	3 (60%)
3	GOL	D	810	-	5,5,5	4.90	5 (100%)	5,5,5	6.07	3 (60%)
3	GOL	A	806	-	5,5,5	4.86	5 (100%)	5,5,5	6.01	3 (60%)
3	GOL	C	809	-	5,5,5	4.82	5 (100%)	5,5,5	6.11	3 (60%)
3	GOL	A	804	-	5,5,5	4.73	5 (100%)	5,5,5	6.07	3 (60%)
3	GOL	B	807	-	5,5,5	4.77	5 (100%)	5,5,5	6.13	3 (60%)

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
3	GOL	C	808	-	-	2/4/4/4	-
3	GOL	D	810	-	-	3/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	C	809	-	-	3/4/4/4	-
3	GOL	A	804	-	-	3/4/4/4	-
3	GOL	B	807	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	810	GOL	C3-C2	-8.39	1.19	1.51
3	C	809	GOL	C3-C2	-8.33	1.20	1.51
3	A	806	GOL	C3-C2	-8.27	1.20	1.51
3	B	807	GOL	C3-C2	-8.16	1.20	1.51
3	C	808	GOL	C3-C2	-8.14	1.20	1.51
3	A	804	GOL	C3-C2	-8.09	1.20	1.51
3	A	804	GOL	O1-C1	4.64	1.61	1.42
3	D	810	GOL	O1-C1	4.61	1.61	1.42
3	B	807	GOL	O1-C1	4.52	1.61	1.42
3	C	808	GOL	O1-C1	4.48	1.61	1.42
3	A	806	GOL	O1-C1	4.32	1.60	1.42
3	C	809	GOL	O1-C1	4.17	1.59	1.42
3	D	810	GOL	O2-C2	-3.48	1.33	1.43
3	A	806	GOL	C1-C2	-3.47	1.38	1.51
3	C	809	GOL	C1-C2	-3.35	1.39	1.51
3	C	808	GOL	O3-C3	3.16	1.55	1.42
3	A	806	GOL	O3-C3	3.11	1.55	1.42
3	A	804	GOL	O3-C3	3.10	1.55	1.42
3	B	807	GOL	O3-C3	3.08	1.55	1.42
3	C	809	GOL	O2-C2	-3.06	1.34	1.43
3	D	810	GOL	C1-C2	-3.01	1.40	1.51
3	A	806	GOL	O2-C2	-3.01	1.34	1.43
3	C	808	GOL	C1-C2	-3.01	1.40	1.51
3	B	807	GOL	C1-C2	-2.99	1.40	1.51
3	C	809	GOL	O3-C3	2.98	1.54	1.42
3	C	808	GOL	O2-C2	-2.90	1.34	1.43
3	B	807	GOL	O2-C2	-2.87	1.35	1.43
3	A	804	GOL	C1-C2	-2.84	1.40	1.51
3	D	810	GOL	O3-C3	2.68	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	GOL	O2-C2	-2.65	1.35	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	808	GOL	O3-C3-C2	11.17	160.67	110.38
3	D	810	GOL	O3-C3-C2	11.15	160.57	110.38
3	B	807	GOL	O3-C3-C2	11.15	160.55	110.38
3	A	804	GOL	O3-C3-C2	10.95	159.67	110.38
3	C	809	GOL	O3-C3-C2	10.93	159.60	110.38
3	A	806	GOL	O3-C3-C2	10.71	158.57	110.38
3	A	806	GOL	O2-C2-C3	7.46	140.08	109.18
3	C	809	GOL	O2-C2-C3	7.31	139.44	109.18
3	B	807	GOL	O2-C2-C3	7.16	138.82	109.18
3	A	804	GOL	O2-C2-C3	7.14	138.75	109.18
3	C	808	GOL	O2-C2-C3	7.14	138.72	109.18
3	D	810	GOL	O2-C2-C3	6.93	137.86	109.18
3	A	804	GOL	O1-C1-C2	3.53	126.28	110.38
3	C	809	GOL	O1-C1-C2	3.53	126.26	110.38
3	B	807	GOL	O1-C1-C2	3.39	125.63	110.38
3	C	808	GOL	O1-C1-C2	3.33	125.37	110.38
3	D	810	GOL	O1-C1-C2	3.32	125.31	110.38
3	A	806	GOL	O1-C1-C2	3.10	124.33	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	GOL	O1-C1-C2-C3
3	A	804	GOL	C1-C2-C3-O3
3	A	806	GOL	O1-C1-C2-C3
3	A	806	GOL	C1-C2-C3-O3
3	B	807	GOL	C1-C2-C3-O3
3	C	808	GOL	C1-C2-C3-O3
3	C	809	GOL	C1-C2-C3-O3
3	D	810	GOL	C1-C2-C3-O3
3	C	809	GOL	O1-C1-C2-C3
3	C	809	GOL	O1-C1-C2-O2
3	C	808	GOL	O1-C1-C2-O2
3	B	807	GOL	O1-C1-C2-O2
3	D	810	GOL	O1-C1-C2-O2
3	D	810	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	804	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	806	GOL	1	0
3	C	809	GOL	3	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	269/271 (99%)	0.35	19 (7%) 22 23	13, 24, 52, 83	0
1	B	269/271 (99%)	0.44	27 (10%) 12 13	12, 23, 61, 131	0
1	C	269/271 (99%)	0.74	41 (15%) 5 5	17, 30, 64, 118	0
1	D	269/271 (99%)	0.08	9 (3%) 49 52	12, 22, 43, 76	0
All	All	1076/1084 (99%)	0.40	96 (8%) 15 16	12, 25, 58, 131	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	14.2
1	B	5	VAL	8.7
1	B	4	LYS	7.0
1	B	3	VAL	6.9
1	B	270	ASN	5.8
1	D	268	PRO	5.4
1	C	102	LEU	5.0
1	C	268	PRO	4.7
1	B	266	THR	4.5
1	B	100	LYS	4.5
1	D	32	GLU	4.4
1	A	100	LYS	4.3
1	C	180	PHE	4.2
1	A	2	ALA	4.2
1	B	268	PRO	4.2
1	B	160	LEU	4.1
1	C	100	LYS	4.0
1	A	160	LEU	4.0
1	B	182	PHE	4.0
1	D	267	TYR	4.0
1	A	270	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	101	GLN	3.7
1	A	102	LEU	3.6
1	B	179	GLY	3.5
1	B	178	SER	3.4
1	B	177	THR	3.4
1	C	266	THR	3.4
1	B	267	TYR	3.3
1	D	270	ASN	3.3
1	C	241	GLN	3.1
1	A	101	GLN	3.1
1	A	163	ASP	3.1
1	C	101	GLN	3.1
1	B	102	LEU	3.0
1	C	244	ARG	3.0
1	C	156	GLU	3.0
1	C	2	ALA	3.0
1	C	161	VAL	2.9
1	C	99	ASP	2.9
1	D	2	ALA	2.8
1	C	270	ASN	2.8
1	C	217	GLY	2.8
1	A	167	VAL	2.8
1	A	178	SER	2.7
1	D	266	THR	2.7
1	C	157	GLN	2.7
1	B	77	LYS	2.7
1	C	162	ILE	2.7
1	B	161	VAL	2.6
1	C	117	ASN	2.6
1	C	158	ILE	2.6
1	A	177	THR	2.6
1	C	267	TYR	2.6
1	A	166	HIS	2.5
1	A	164	LYS	2.5
1	C	86	ARG	2.5
1	C	160	LEU	2.5
1	B	120	GLU	2.5
1	C	159	PRO	2.5
1	C	90	ARG	2.5
1	C	238	ASN	2.4
1	B	166	HIS	2.4
1	B	180	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	182	PHE	2.4
1	B	157	GLN	2.4
1	D	241	GLN	2.4
1	A	179	GLY	2.4
1	C	269	PHE	2.3
1	D	269	PHE	2.3
1	B	154	PRO	2.3
1	D	265	ASN	2.3
1	B	162	ILE	2.3
1	C	183	ILE	2.3
1	C	242	ILE	2.3
1	C	167	VAL	2.3
1	C	179	GLY	2.2
1	C	154	PRO	2.2
1	C	32	GLU	2.2
1	A	154	PRO	2.2
1	B	121	ALA	2.2
1	B	158	ILE	2.2
1	A	204	ASP	2.1
1	C	153	LEU	2.1
1	A	137	LYS	2.1
1	C	141	GLU	2.1
1	C	166	HIS	2.1
1	C	138	ASP	2.1
1	C	155	ASP	2.1
1	C	170	ASP	2.1
1	A	97	LEU	2.1
1	B	159	PRO	2.1
1	A	162	ILE	2.0
1	A	174	LYS	2.0
1	C	137	LYS	2.0
1	C	169	LEU	2.0
1	C	248	ASP	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 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($\text{\AA}^2$)	Q<0.9
3	GOL	A	804	6/6	0.73	0.19	22,29,29,29	0
3	GOL	D	810	6/6	0.73	0.17	24,30,32,32	0
3	GOL	B	807	6/6	0.76	0.17	30,33,35,38	0
3	GOL	A	806	6/6	0.77	0.28	28,31,32,36	0
3	GOL	C	808	6/6	0.81	0.12	25,28,29,31	0
3	GOL	C	809	6/6	0.82	0.19	29,30,32,34	0
2	MG	C	803	1/1	0.95	0.07	24,24,24,24	0
2	MG	A	800	1/1	0.96	0.04	18,18,18,18	0
2	MG	B	801	1/1	0.98	0.04	20,20,20,20	0
2	MG	D	802	1/1	0.98	0.05	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.