



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:49 PM UTC

PDB ID : 3M24 / pdb_00003m24
Title : Crystal structure of TagBFP fluorescent protein
Authors : Malashkevich, V.N.; Subach, O.M.; Almo, S.C.; Verkhusha, V.V.
Deposited on : 2010-03-06
Resolution : 2.20 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

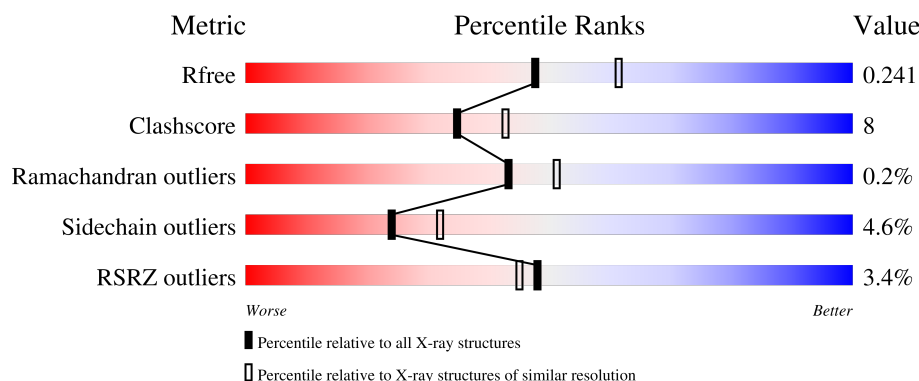
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	% 82% 12% ..
1	B	232	3% 78% 18% ..
1	C	232	% 81% 15% ..
1	D	232	8% 76% 19% ..

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
1	NRP	D	63	-	-	X	-

2 Entry composition [i](#)

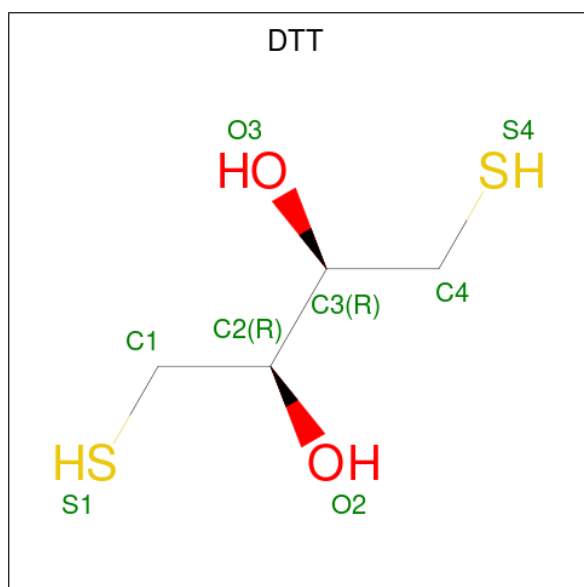
There are 5 unique types of molecules in this entry. The entry contains 7761 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TagBFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1809	1151	302	345	11			
1	B	228	Total	C	N	O	S	0	1	0
			1826	1162	305	348	11			
1	C	227	Total	C	N	O	S	0	0	0
			1817	1157	303	346	11			
1	D	225	Total	C	N	O	S	0	0	0
			1803	1149	301	343	10			

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



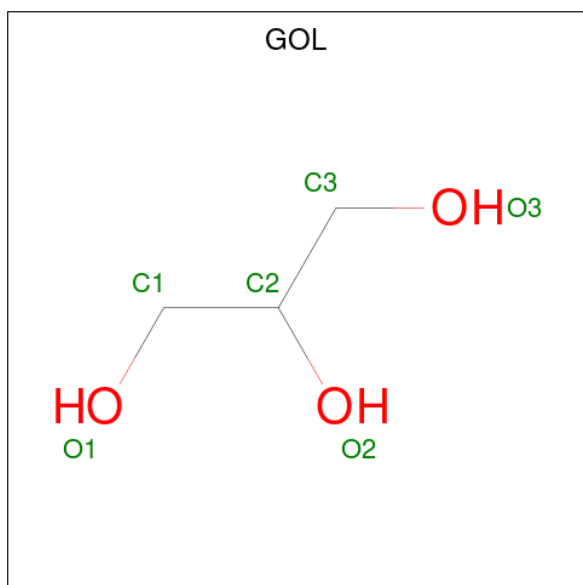
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	S	0	0
			3	2	1		
2	B	1	Total	C	S	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	S	0	0
			3	2	1		
2	D	1	Total	C	S	0	0
			3	2	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	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	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0

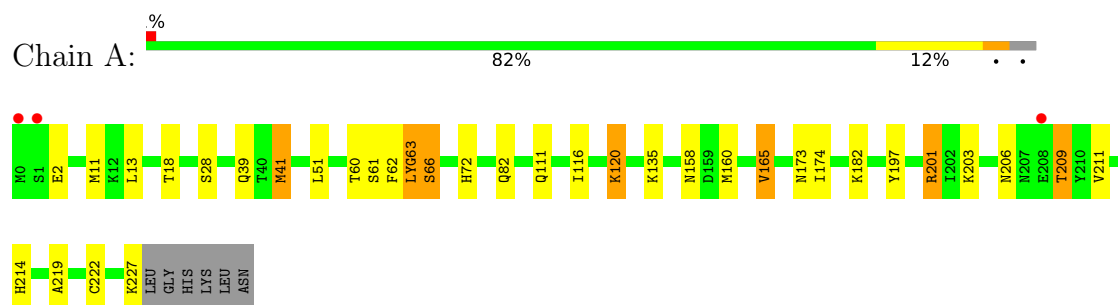
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total 137	O 137	0	0
5	B	126	Total 126	O 126	0	0
5	C	114	Total 114	O 114	0	0
5	D	73	Total 73	O 73	0	0

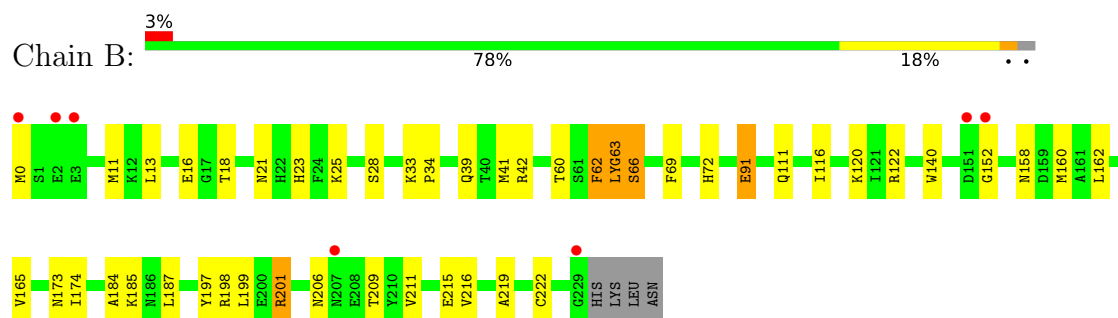
3 Residue-property plots [i](#)

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.

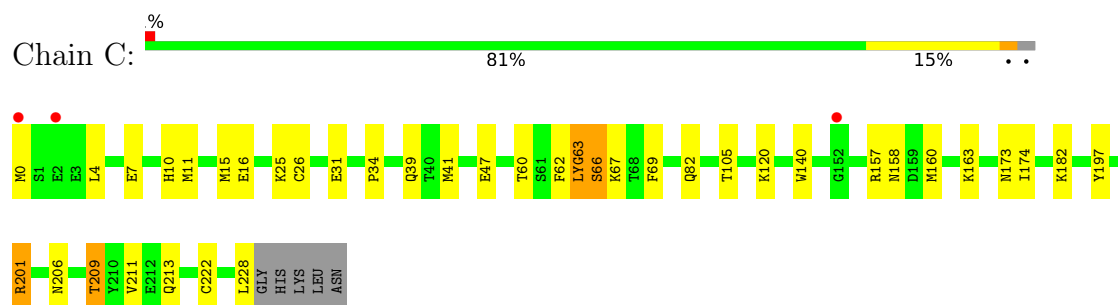
• Molecule 1: TagBFP



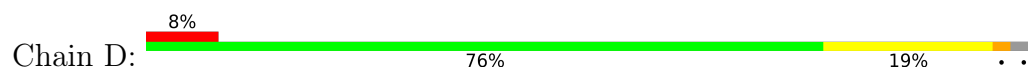
• Molecule 1: TagBFP

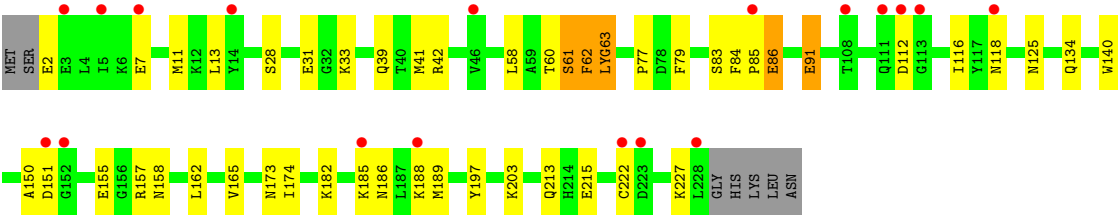


• Molecule 1: TagBFP



• Molecule 1: TagBFP





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.95Å 105.94Å 137.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.20 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.8 (19.94-2.20) 87.6 (19.94-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.238 0.195 , 0.241	Depositor DCC
R_{free} test set	2739 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7761	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: DTT, CL, NRP, 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	0.73	4/1826 (0.2%)	0.81	2/2464 (0.1%)
1	B	0.65	1/1846 (0.1%)	0.80	4/2491 (0.2%)
1	C	0.61	1/1834 (0.1%)	0.81	4/2475 (0.2%)
1	D	0.61	1/1820 (0.1%)	0.79	2/2457 (0.1%)
All	All	0.65	7/7326 (0.1%)	0.80	12/9887 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	PHE	CA-C	-10.83	1.30	1.52
1	D	62	PHE	CA-C	-6.40	1.39	1.52
1	A	66	SER	N-CA	-6.15	1.34	1.46
1	A	61	SER	C-O	-6.02	1.16	1.24
1	B	66	SER	N-CA	-5.77	1.35	1.46
1	A	165	VAL	CA-CB	5.63	1.60	1.54
1	C	67	LYS	C-O	-5.04	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	PHE	CB-CA-C	10.76	130.55	110.10
1	C	62	PHE	CB-CA-C	10.35	129.76	110.10
1	D	62	PHE	CB-CA-C	9.53	128.20	110.10
1	B	66	SER	N-CA-CB	-7.76	97.31	110.50
1	C	66	SER	N-CA-CB	-7.02	98.56	110.50
1	B	62	PHE	CA-C-O	6.85	132.45	120.80
1	C	62	PHE	CA-CB-CG	6.67	120.47	113.80
1	C	62	PHE	N-CA-CB	-5.67	100.86	110.50
1	D	62	PHE	CA-C-O	-5.44	111.56	120.80
1	A	66	SER	N-CA-CB	-5.21	101.65	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LYS	CA-C-N	5.15	124.94	119.28
1	B	33	LYS	C-N-CA	5.15	124.94	119.28

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	1809	0	1762	24	0
1	B	1826	0	1783	29	0
1	C	1817	0	1774	25	0
1	D	1803	0	1757	31	0
2	A	3	0	3	1	0
2	B	3	0	3	1	0
2	C	3	0	3	2	0
2	D	3	0	3	1	0
3	A	24	0	32	0	0
3	B	6	0	8	2	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	137	0	0	1	0
5	B	126	0	0	2	0
5	C	114	0	0	2	0
5	D	73	0	0	2	0
All	All	7761	0	7144	109	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 8.

All (109) 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:C:222:CYS:SG	2:C:501:DTT:S4	2.50	0.98
1:D:150:ALA:HB3	1:D:155:GLU:HG3	1.49	0.93
1:A:82:GLN:O	1:A:182:LYS:HE3	1.75	0.84
1:A:60:THR:HB	1:A:63:NRP:HD1	1.60	0.83
1:B:11:MET:HG3	1:B:41:MET:HE3	1.65	0.78
1:D:63:NRP:HD3A	1:D:213:GLN:HE21	1.47	0.78
1:B:201:ARG:HD2	1:B:211:VAL:HG13	1.72	0.72
1:D:77:PRO:HB3	1:D:188:LYS:HG3	1.73	0.71
1:A:222:CYS:SG	2:A:501:DTT:S4	2.48	0.69
1:A:63:NRP:HD4A	1:A:66:SER:HB3	1.75	0.66
1:D:222:CYS:SG	2:D:501:DTT:S4	2.45	0.66
1:C:82:GLN:O	1:C:182:LYS:HE3	1.94	0.66
1:B:122:ARG:HH22	3:B:506:GOL:H2	1.62	0.64
1:B:222:CYS:SG	2:B:501:DTT:S4	2.49	0.64
1:A:39:GLN:CD	1:A:63:NRP:HD4	2.23	0.63
1:A:111:GLN:HB2	1:A:116:ILE:HD13	1.80	0.63
1:C:11:MET:HE1	1:C:39:GLN:HB2	1.82	0.62
1:D:63:NRP:HD4A	1:D:215:GLU:OE2	2.00	0.62
1:D:150:ALA:HB3	1:D:155:GLU:CG	2.29	0.61
1:D:63:NRP:HD4A	1:D:215:GLU:CD	2.26	0.60
1:D:60:THR:HB	1:D:63:NRP:HD1	1.83	0.60
1:B:16:GLU:HB3	1:B:25:LYS:HG3	1.83	0.60
1:B:11:MET:HE1	1:B:39:GLN:HB2	1.86	0.57
1:B:63:NRP:HD2	1:B:197:TYR:CE2	2.40	0.57
1:B:63:NRP:HD4	1:B:215:GLU:HB2	1.88	0.56
1:D:173:ASN:C	1:D:174:ILE:HD12	2.31	0.56
1:B:111:GLN:HB2	1:B:116:ILE:HD13	1.87	0.55
1:A:214:HIS:HD2	5:A:344:HOH:O	1.88	0.55
1:C:60:THR:HB	1:C:63:NRP:HD1	1.89	0.55
1:A:39:GLN:NE2	1:A:63:NRP:HD4	2.22	0.55
1:D:188:LYS:HA	5:D:368:HOH:O	2.06	0.54
1:A:63:NRP:HD2	1:A:197:TYR:CZ	2.43	0.54
1:A:201:ARG:HD2	1:A:211:VAL:HG13	1.90	0.54
1:C:0:MET:HE3	1:C:4:LEU:HD11	1.90	0.54
1:D:150:ALA:CB	1:D:155:GLU:HG3	2.30	0.54
1:D:63:NRP:HD3A	1:D:213:GLN:NE2	2.21	0.53
1:D:62:PHE:C	1:D:63:NRP:HD3B	2.34	0.53
1:B:34:PRO:HA	1:B:69:PHE:HA	1.90	0.52
1:A:63:NRP:HD4A	1:A:66:SER:CB	2.40	0.52
1:D:58:LEU:O	1:D:61:SER:HB2	2.10	0.52
1:A:158:ASN:ND2	1:A:160:MET:HG3	2.25	0.51
1:C:63:NRP:HD2	1:C:197:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:HD3	1:D:186:ASN:HB3	1.91	0.51
1:C:10:HIS:HD2	1:C:31:GLU:HB3	1.75	0.51
1:D:63:NRP:HD3B	1:D:63:NRP:N1	2.26	0.51
1:B:60:THR:HB	1:B:63:NRP:HD1	1.93	0.50
1:C:82:GLN:O	1:C:182:LYS:CE	2.59	0.50
1:A:51:LEU:O	1:A:135:LYS:HE3	2.12	0.49
1:B:18:THR:HG22	1:B:23:HIS:HA	1.94	0.49
1:C:201:ARG:HD2	1:C:211:VAL:HG13	1.94	0.49
1:A:39:GLN:HE22	1:A:66:SER:HB3	1.78	0.49
1:C:158:ASN:ND2	1:C:160:MET:HG3	2.28	0.48
5:B:379:HOH:O	1:D:125:ASN:HB3	2.12	0.48
1:A:72:HIS:HA	1:A:219:ALA:HB3	1.96	0.47
1:C:7:GLU:HG2	5:C:312:HOH:O	2.14	0.47
1:D:174:ILE:HD12	1:D:174:ILE:N	2.29	0.47
1:D:63:NRP:CD4	1:D:215:GLU:HB2	2.45	0.47
1:A:11:MET:HE1	1:A:39:GLN:HB2	1.96	0.47
1:A:11:MET:HG3	1:A:41:MET:CE	2.45	0.47
1:A:120:LYS:HE3	3:D:503:GOL:H31	1.98	0.46
1:C:63:NRP:OH	1:C:158:ASN:OD1	2.33	0.46
1:B:91:GLU:HG3	5:C:302:HOH:O	2.16	0.46
1:C:34:PRO:HA	1:C:69:PHE:HA	1.97	0.46
1:D:63:NRP:HD2	1:D:197:TYR:CE2	2.50	0.46
1:A:173:ASN:C	1:A:174:ILE:HD12	2.40	0.46
1:B:63:NRP:HD4B	1:B:199:LEU:HD13	1.97	0.46
3:B:506:GOL:H31	1:C:120:LYS:HE3	1.97	0.46
1:D:63:NRP:HB2	1:D:197:TYR:CE1	2.50	0.46
1:B:13:LEU:HB3	1:B:28:SER:OG	2.16	0.46
1:A:11:MET:HG3	1:A:41:MET:HE1	1.98	0.45
1:B:63:NRP:CD4	1:B:199:LEU:HD13	2.46	0.45
1:D:157:ARG:O	1:D:158:ASN:HB3	2.15	0.45
1:D:83:SER:O	1:D:86:GLU:HG2	2.17	0.45
1:A:63:NRP:CD4	1:A:66:SER:HB3	2.46	0.45
1:D:11:MET:HE1	1:D:39:GLN:HE21	1.82	0.45
1:A:51:LEU:O	1:A:135:LYS:CE	2.65	0.44
1:D:11:MET:HE1	1:D:39:GLN:HB2	1.99	0.44
1:D:91:GLU:HG3	5:D:300:HOH:O	2.17	0.44
1:B:140:TRP:CZ3	1:B:162:LEU:HB2	2.53	0.44
1:C:15:MET:HB3	1:C:26:CYS:HB2	1.99	0.43
1:B:173:ASN:C	1:B:174:ILE:HD12	2.44	0.43
1:B:158:ASN:ND2	1:B:160:MET:HG3	2.34	0.43
1:B:72:HIS:HA	1:B:219:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LYS:HB2	1:C:47:GLU:HB2	1.99	0.43
1:D:79:PHE:CD1	1:D:189:MET:HE1	2.54	0.43
1:C:157:ARG:O	1:C:158:ASN:HB3	2.19	0.43
1:D:84:PHE:HB3	1:D:85:PRO:HA	2.01	0.42
1:A:13:LEU:HB3	1:A:28:SER:OG	2.19	0.42
1:B:206:ASN:HB2	1:B:209:THR:HB	2.01	0.42
1:B:42:ARG:NE	5:B:418:HOH:O	2.41	0.42
1:B:158:ASN:HD21	1:B:160:MET:HG3	1.85	0.42
1:B:63:NRP:HD2	1:B:197:TYR:CZ	2.54	0.42
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.84	0.42
1:D:140:TRP:CZ3	1:D:162:LEU:HB2	2.55	0.41
1:C:206:ASN:O	1:C:209:THR:HB	2.20	0.41
1:D:13:LEU:HB3	1:D:28:SER:OG	2.20	0.41
1:C:173:ASN:C	1:C:174:ILE:HD12	2.46	0.41
1:C:174:ILE:HD12	1:C:174:ILE:N	2.35	0.41
1:B:184:ALA:HA	1:B:187:LEU:HD12	2.03	0.41
1:D:31:GLU:OE1	1:D:42:ARG:NH2	2.54	0.41
1:C:63:NRP:HD3A	1:C:213:GLN:HE21	1.84	0.41
1:C:140:TRP:CE3	1:C:160:MET:HE2	2.55	0.41
1:B:120:LYS:HZ1	3:C:502:GOL:H31	1.85	0.41
1:C:39:GLN:HE22	1:C:66:SER:HB3	1.86	0.41
1:C:16:GLU:HB3	1:C:25:LYS:HG3	2.03	0.40
1:A:206:ASN:O	1:A:209:THR:HB	2.20	0.40
1:B:62:PHE:CA	1:B:63:NRP:HB1A	2.51	0.40
1:B:198:ARG:HB3	1:B:216:VAL:CG1	2.51	0.40
1:C:222:CYS:HG	2:C:501:DTT:C4	2.28	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	221/232 (95%)	217 (98%)	4 (2%)	0	100	100
1	B	224/232 (97%)	219 (98%)	4 (2%)	1 (0%)	30	34
1	C	222/232 (96%)	216 (97%)	6 (3%)	0	100	100
1	D	220/232 (95%)	210 (96%)	9 (4%)	1 (0%)	24	27
All	All	887/928 (96%)	862 (97%)	23 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	112	ASP
1	B	152	GLY

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	194/199 (98%)	185 (95%)	9 (5%)	24	32
1	B	196/199 (98%)	190 (97%)	6 (3%)	35	48
1	C	195/199 (98%)	189 (97%)	6 (3%)	35	48
1	D	193/199 (97%)	178 (92%)	15 (8%)	11	13
All	All	778/796 (98%)	742 (95%)	36 (5%)	24	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	THR
1	A	41	MET
1	A	120	LYS
1	A	165	VAL
1	A	201	ARG
1	A	203	LYS
1	A	209	THR
1	A	227	LYS

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Mol	Chain	Res	Type
1	B	0	MET
1	B	21	ASN
1	B	91	GLU
1	B	165	VAL
1	B	185	LYS
1	B	201	ARG
1	C	41	MET
1	C	105	THR
1	C	163	LYS
1	C	201	ARG
1	C	209	THR
1	C	228	LEU
1	D	2	GLU
1	D	7	GLU
1	D	33	LYS
1	D	41	MET
1	D	61	SER
1	D	86	GLU
1	D	91	GLU
1	D	116	ILE
1	D	118	ASN
1	D	134	GLN
1	D	151	ASP
1	D	165	VAL
1	D	185	LYS
1	D	203	LYS
1	D	227	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	206	ASN
1	A	214	HIS
1	B	21	ASN
1	B	23	HIS
1	B	39	GLN
1	B	158	ASN
1	C	10	HIS
1	C	158	ASN
1	C	213	GLN
1	D	8	ASN

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Mol	Chain	Res	Type
1	D	129	ASN
1	D	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	NRP	B	63	1	24,24,25	4.68	11 (45%)	26,33,35	4.99	11 (42%)
1	NRP	C	63	1	24,24,25	4.42	8 (33%)	26,33,35	4.60	10 (38%)
1	NRP	D	63	1	24,24,25	4.69	10 (41%)	26,33,35	5.01	13 (50%)
1	NRP	A	63	1	24,24,25	4.53	10 (41%)	26,33,35	4.92	9 (34%)

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
1	NRP	B	63	1	-	8/9/31/32	0/2/2/2
1	NRP	C	63	1	-	6/9/31/32	0/2/2/2
1	NRP	D	63	1	-	7/9/31/32	0/2/2/2
1	NRP	A	63	1	-	4/9/31/32	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	NRP	CB2-CA2	15.56	1.50	1.35
1	C	63	NRP	CB2-CA2	14.52	1.49	1.35
1	D	63	NRP	CB2-CA2	13.81	1.48	1.35
1	A	63	NRP	CB2-CA2	13.42	1.48	1.35
1	D	63	NRP	CB1-CA1	-10.67	1.33	1.50
1	A	63	NRP	O2-C2	10.22	1.43	1.23
1	B	63	NRP	O2-C2	10.10	1.43	1.23
1	D	63	NRP	O2-C2	9.63	1.42	1.23
1	C	63	NRP	O2-C2	9.16	1.41	1.23
1	B	63	NRP	CA1-N1	8.95	1.47	1.27
1	A	63	NRP	C1-CA1	-7.66	1.36	1.48
1	A	63	NRP	CB1-CA1	-6.93	1.39	1.50
1	D	63	NRP	CA1-N1	6.65	1.42	1.27
1	C	63	NRP	C2-N3	-6.29	1.25	1.40
1	C	63	NRP	CA1-N1	6.04	1.41	1.27
1	C	63	NRP	CA2-C2	-5.42	1.42	1.48
1	A	63	NRP	C2-N3	-5.24	1.27	1.40
1	C	63	NRP	C1-CA1	5.20	1.55	1.48
1	B	63	NRP	C2-N3	-5.17	1.28	1.40
1	D	63	NRP	C2-N3	-5.06	1.28	1.40
1	A	63	NRP	CA2-C2	-4.28	1.43	1.48
1	A	63	NRP	CA3-N3	-4.22	1.39	1.47
1	B	63	NRP	CA2-N2	-4.12	1.29	1.38
1	D	63	NRP	CA2-N2	-3.70	1.30	1.38
1	C	63	NRP	CA2-N2	-3.60	1.30	1.38
1	D	63	NRP	O3-C3	3.51	1.39	1.20
1	C	63	NRP	CA3-N3	-3.10	1.41	1.47
1	A	63	NRP	CA2-N2	-3.10	1.32	1.38
1	D	63	NRP	CA2-C2	-3.09	1.45	1.48
1	B	63	NRP	CA3-N3	-2.91	1.41	1.47
1	B	63	NRP	CB1-CA1	-2.82	1.45	1.50
1	D	63	NRP	C1-N3	-2.60	1.33	1.38
1	B	63	NRP	CA2-C2	-2.43	1.45	1.48
1	B	63	NRP	C1-N2	2.25	1.38	1.33
1	A	63	NRP	CA3-C3	-2.22	1.41	1.49
1	B	63	NRP	C1-N3	-2.22	1.34	1.38
1	D	63	NRP	OH-CZ	-2.10	1.32	1.37
1	B	63	NRP	O3-C3	2.09	1.31	1.20
1	A	63	NRP	C1-N2	2.02	1.37	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	NRP	CG2-CB2-CA2	-14.34	112.82	129.87
1	B	63	NRP	CG2-CB2-CA2	-13.36	113.98	129.87
1	A	63	NRP	O2-C2-CA2	-13.11	122.66	131.02
1	C	63	NRP	O2-C2-CA2	-12.24	123.21	131.02
1	B	63	NRP	C2-CA2-N2	-11.14	100.97	108.95
1	A	63	NRP	CG2-CB2-CA2	-11.11	116.66	129.87
1	B	63	NRP	CA2-C2-N3	10.71	112.49	103.50
1	D	63	NRP	CA2-C2-N3	10.70	112.49	103.50
1	C	63	NRP	CA2-C2-N3	10.55	112.36	103.50
1	A	63	NRP	C2-CA2-N2	-9.95	101.82	108.95
1	D	63	NRP	O2-C2-CA2	-9.61	124.89	131.02
1	C	63	NRP	C2-CA2-N2	-9.60	102.07	108.95
1	A	63	NRP	CA2-C2-N3	9.02	111.07	103.50
1	C	63	NRP	CG2-CB2-CA2	-9.02	119.15	129.87
1	B	63	NRP	O2-C2-CA2	-8.52	125.58	131.02
1	D	63	NRP	C2-CA2-N2	-8.51	102.86	108.95
1	B	63	NRP	CB2-CA2-C2	7.79	131.80	122.36
1	A	63	NRP	CB2-CA2-C2	7.16	131.03	122.36
1	D	63	NRP	CB2-CA2-C2	6.88	130.70	122.36
1	C	63	NRP	CB2-CA2-C2	6.16	129.82	122.36
1	A	63	NRP	N3-C1-N2	-6.05	105.44	112.62
1	D	63	NRP	CA3-N3-C2	5.74	136.28	123.67
1	C	63	NRP	N3-C1-N2	-5.02	106.66	112.62
1	D	63	NRP	CA3-N3-C1	-4.91	118.70	128.39
1	A	63	NRP	CA2-N2-C1	4.57	112.51	104.09
1	B	63	NRP	CA2-N2-C1	4.42	112.22	104.09
1	B	63	NRP	C3-CA3-N3	4.37	122.36	112.43
1	A	63	NRP	CD4-CG1-CB1	-4.25	94.65	111.16
1	B	63	NRP	N3-C1-N2	-4.15	107.69	112.62
1	C	63	NRP	CA2-N2-C1	3.96	111.38	104.09
1	B	63	NRP	CD4-CG1-CB1	-3.54	97.42	111.16
1	D	63	NRP	CD4-CG1-CB1	3.51	124.80	111.16
1	D	63	NRP	C3-CA3-N3	3.41	120.18	112.43
1	D	63	NRP	CD2-CG2-CD1	2.96	122.04	117.65
1	A	63	NRP	CD3-CG1-CB1	2.81	122.09	111.16
1	C	63	NRP	CE1-CD1-CG2	-2.80	117.60	121.22
1	C	63	NRP	C3-CA3-N3	2.76	118.71	112.43
1	C	63	NRP	CD2-CG2-CD1	2.76	121.74	117.65
1	B	63	NRP	CD2-CG2-CD1	2.55	121.43	117.65
1	D	63	NRP	CD3-CG1-CB1	-2.50	101.46	111.16
1	B	63	NRP	CD3-CG1-CB1	2.42	120.57	111.16
1	D	63	NRP	CA2-N2-C1	2.30	108.32	104.09
1	D	63	NRP	CE1-CD1-CG2	-2.07	118.55	121.22

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	NRP	C2-CA2-CB2-CG2
1	A	63	NRP	N2-CA2-CB2-CG2
1	B	63	NRP	C2-CA2-CB2-CG2
1	B	63	NRP	N2-CA2-CB2-CG2
1	B	63	NRP	CA1-CB1-CG1-CD3
1	B	63	NRP	CA1-CB1-CG1-CD4
1	C	63	NRP	C2-CA2-CB2-CG2
1	C	63	NRP	N2-CA2-CB2-CG2
1	C	63	NRP	CA1-CB1-CG1-CD3
1	C	63	NRP	CA1-CB1-CG1-CD4
1	D	63	NRP	C2-CA2-CB2-CG2
1	D	63	NRP	N2-CA2-CB2-CG2
1	D	63	NRP	CA1-CB1-CG1-CD3
1	D	63	NRP	CA1-CB1-CG1-CD4
1	A	63	NRP	CA2-CB2-CG2-CD2
1	B	63	NRP	CA2-CB2-CG2-CD2
1	A	63	NRP	CA2-CB2-CG2-CD1
1	B	63	NRP	CA2-CB2-CG2-CD1
1	D	63	NRP	C3-CA3-N3-C2
1	B	63	NRP	C3-CA3-N3-C1
1	B	63	NRP	C1-CA1-CB1-CG1
1	D	63	NRP	CA2-CB2-CG2-CD2
1	D	63	NRP	CA2-CB2-CG2-CD1
1	C	63	NRP	CA2-CB2-CG2-CD2
1	C	63	NRP	CA2-CB2-CG2-CD1

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRP	7	0
1	C	63	NRP	4	0
1	D	63	NRP	10	0
1	A	63	NRP	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	502	-	5,5,5	0.41	0	5,5,5	0.17	0
3	GOL	D	503	-	5,5,5	0.42	0	5,5,5	0.18	0
2	DTT	A	501	-	2,2,7	0.76	0	0,1,8	-	-
3	GOL	A	505	-	5,5,5	0.46	0	5,5,5	0.40	0
2	DTT	D	501	-	2,2,7	0.70	0	0,1,8	-	-
2	DTT	B	501	-	2,2,7	0.65	0	0,1,8	-	-
2	DTT	C	501	-	2,2,7	0.50	0	0,1,8	-	-
3	GOL	A	504	-	5,5,5	0.42	0	5,5,5	0.26	0
3	GOL	A	507	-	5,5,5	0.40	0	5,5,5	0.58	0
3	GOL	B	506	-	5,5,5	0.51	0	5,5,5	0.30	0
3	GOL	A	503	-	5,5,5	0.41	0	5,5,5	0.17	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
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-
3	GOL	A	507	-	-	4/4/4/4	-
3	GOL	B	506	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	507	GOL	O1-C1-C2-C3
3	A	507	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	C	502	GOL	O2-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	D	503	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	A	507	GOL	O1-C1-C2-O2
3	A	507	GOL	O2-C2-C3-O3
3	D	503	GOL	O2-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GOL	1	0
3	D	503	GOL	1	0
2	A	501	DTT	1	0
2	D	501	DTT	1	0
2	B	501	DTT	1	0
2	C	501	DTT	2	0
3	B	506	GOL	2	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	225/232 (96%)	-0.27	3 (1%) 75 73	3, 10, 24, 45	1 (0%)
1	B	227/232 (97%)	-0.03	7 (3%) 51 48	4, 12, 29, 43	2 (0%)
1	C	226/232 (97%)	-0.11	3 (1%) 75 73	5, 14, 28, 39	1 (0%)
1	D	224/232 (96%)	0.87	18 (8%) 18 16	7, 20, 36, 46	1 (0%)
All	All	902/928 (97%)	0.11	31 (3%) 48 45	3, 14, 32, 46	5 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	4.5
1	D	112	ASP	4.4
1	C	152	GLY	3.7
1	D	14	TYR	3.6
1	B	152	GLY	3.5
1	D	152	GLY	3.4
1	D	223	ASP	3.1
1	C	0	MET	3.1
1	D	151	ASP	2.9
1	D	228	LEU	2.8
1	C	2	GLU	2.8
1	B	207	ASN	2.5
1	D	7	GLU	2.5
1	B	151	ASP	2.5
1	D	46	VAL	2.4
1	B	3	GLU	2.3
1	D	85	PRO	2.3
1	D	111	GLN	2.3
1	D	108	THR	2.3
1	D	5	ILE	2.2
1	A	208	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	0	MET	2.2
1	B	2	GLU	2.2
1	D	185	LYS	2.2
1	D	113	GLY	2.2
1	D	188	LYS	2.1
1	A	0	MET	2.1
1	D	118	ASN	2.1
1	B	229	GLY	2.1
1	D	3	GLU	2.0
1	D	222	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	NRP	D	63	23/24	0.75	0.17	43,44,44,45	0
1	NRP	B	63	23/24	0.79	0.15	34,35,37,37	0
1	NRP	A	63	23/24	0.79	0.14	31,33,34,35	0
1	NRP	C	63	23/24	0.82	0.14	32,33,35,35	0

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
3	GOL	C	502	6/6	0.76	0.14	35,35,39,40	0
3	GOL	A	503	6/6	0.77	0.16	39,39,40,40	0
3	GOL	A	505	6/6	0.80	0.13	31,31,33,33	0
2	DTT	A	501	3/8	0.80	0.15	11,11,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	507	6/6	0.85	0.10	26,27,32,32	0
2	DTT	C	501	3/8	0.85	0.16	16,16,18,19	0
3	GOL	B	506	6/6	0.86	0.12	36,36,38,38	0
3	GOL	A	504	6/6	0.86	0.12	32,32,46,46	0
2	DTT	B	501	3/8	0.87	0.14	16,16,17,18	0
3	GOL	D	503	6/6	0.87	0.11	23,24,26,26	0
2	DTT	D	501	3/8	0.88	0.18	15,15,16,17	0
4	CL	C	509	1/1	0.98	0.07	14,14,14,14	0
4	CL	A	508	1/1	0.99	0.07	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.