



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:06 pm BST

PDB ID : 2YF4
Title : Crystal structure of DR2231, the MazG-like protein from *Deinococcus radiodurans*, Apo structure
Authors : Goncalves, A.M.D.; deSanctis, D.; McSweeney, S.M.
Deposited on : 2011-04-01
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

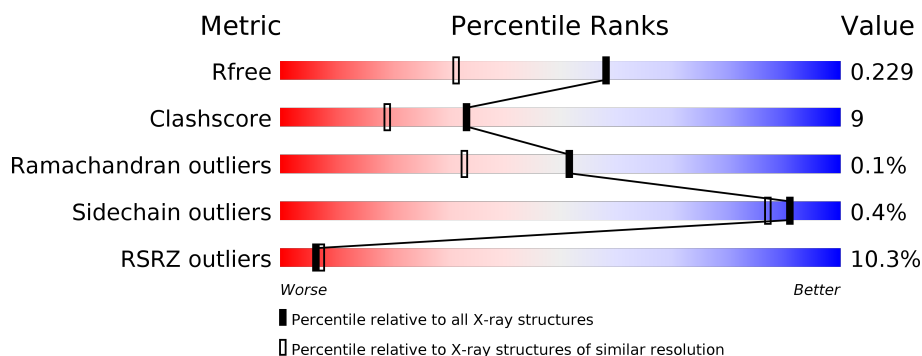
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	154	<div> <div>11%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	154	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	C	154	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	D	154	<div> <div>8%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	154	<div> <div>14%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	F	154	<div> <div>10%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	1146	-	-	X	X
2	GOL	C	1147	-	-	X	-
2	GOL	D	1145	-	-	X	-
2	GOL	D	1149	-	-	X	-
2	GOL	E	1145	-	-	X	-
2	GOL	F	1148	-	-	X	-
3	SO4	B	1152	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14726 atoms, of which 6904 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 MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total	C	H	N	O	S	0	0	0
			2284	716	1136	212	218	2			
1	B	146	Total	C	H	N	O	S	0	0	0
			2224	698	1106	208	211	1			
1	C	149	Total	C	H	N	O	S	0	0	0
			2275	714	1131	211	217	2			
1	D	150	Total	C	H	N	O	S	0	0	0
			2283	716	1135	212	218	2			
1	E	149	Total	C	H	N	O	S	0	0	0
			2276	714	1132	211	217	2			
1	F	143	Total	C	H	N	O	S	0	0	0
			2190	688	1088	205	208	1			

There are 36 discrepancies between the modelled and reference sequences:

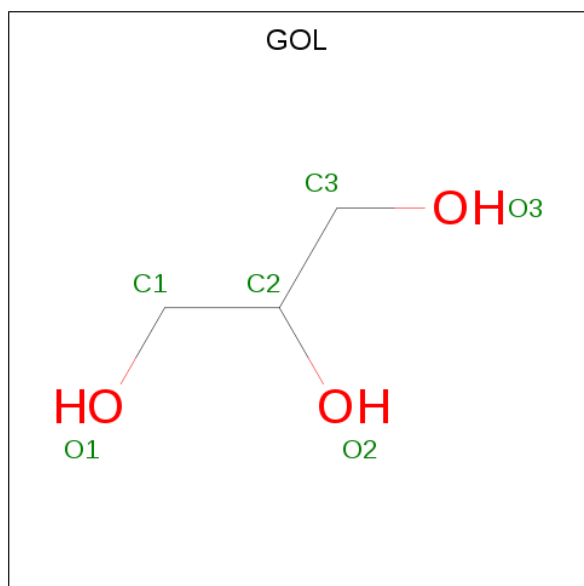
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9RS96
A	-4	ILE	-	expression tag	UNP Q9RS96
A	-3	ASP	-	expression tag	UNP Q9RS96
A	-2	PRO	-	expression tag	UNP Q9RS96
A	-1	PHE	-	expression tag	UNP Q9RS96
A	0	THR	-	expression tag	UNP Q9RS96
B	-5	GLY	-	expression tag	UNP Q9RS96
B	-4	ILE	-	expression tag	UNP Q9RS96
B	-3	ASP	-	expression tag	UNP Q9RS96
B	-2	PRO	-	expression tag	UNP Q9RS96
B	-1	PHE	-	expression tag	UNP Q9RS96
B	0	THR	-	expression tag	UNP Q9RS96
C	-5	GLY	-	expression tag	UNP Q9RS96
C	-4	ILE	-	expression tag	UNP Q9RS96
C	-3	ASP	-	expression tag	UNP Q9RS96
C	-2	PRO	-	expression tag	UNP Q9RS96

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PHE	-	expression tag	UNP Q9RS96
C	0	THR	-	expression tag	UNP Q9RS96
D	-5	GLY	-	expression tag	UNP Q9RS96
D	-4	ILE	-	expression tag	UNP Q9RS96
D	-3	ASP	-	expression tag	UNP Q9RS96
D	-2	PRO	-	expression tag	UNP Q9RS96
D	-1	PHE	-	expression tag	UNP Q9RS96
D	0	THR	-	expression tag	UNP Q9RS96
E	-5	GLY	-	expression tag	UNP Q9RS96
E	-4	ILE	-	expression tag	UNP Q9RS96
E	-3	ASP	-	expression tag	UNP Q9RS96
E	-2	PRO	-	expression tag	UNP Q9RS96
E	-1	PHE	-	expression tag	UNP Q9RS96
E	0	THR	-	expression tag	UNP Q9RS96
F	-5	GLY	-	expression tag	UNP Q9RS96
F	-4	ILE	-	expression tag	UNP Q9RS96
F	-3	ASP	-	expression tag	UNP Q9RS96
F	-2	PRO	-	expression tag	UNP Q9RS96
F	-1	PHE	-	expression tag	UNP Q9RS96
F	0	THR	-	expression tag	UNP Q9RS96

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	C	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	D	1	Total 14	C 3	H 8	O 3	0	0
2	E	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0
2	F	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

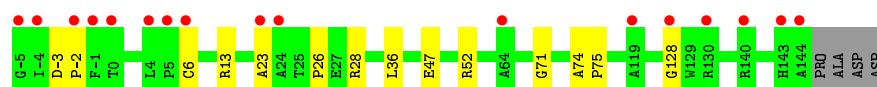
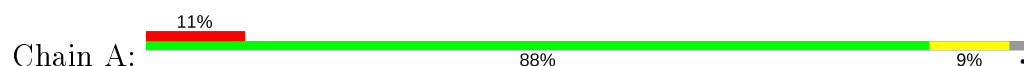
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	125	Total	O	0	0
			125	125		
4	C	165	Total	O	0	0
			165	165		
4	D	150	Total	O	0	0
			150	150		
4	E	108	Total	O	0	0
			108	108		
4	F	111	Total	O	0	0
			111	111		

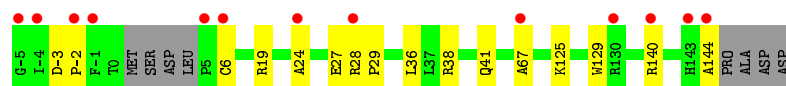
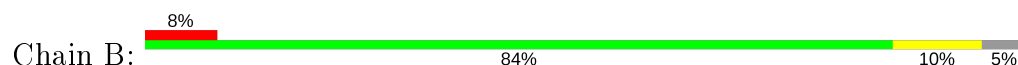
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

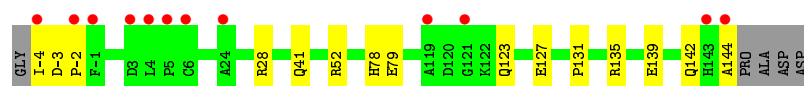
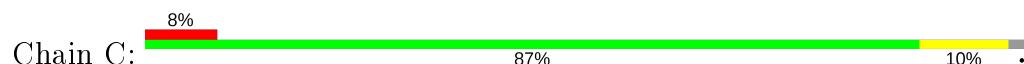
• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



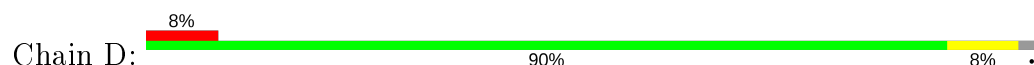
• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



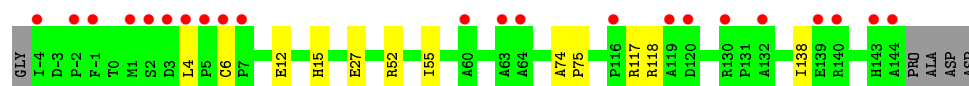
• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



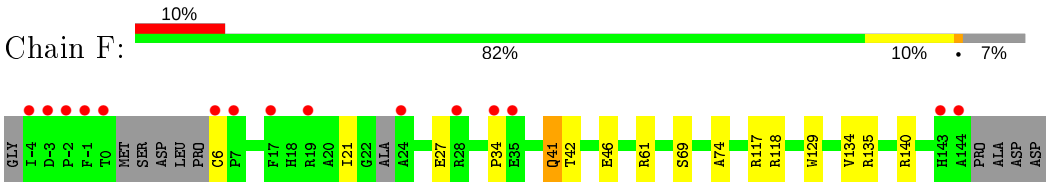
• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



• Molecule 1: MAZG-LIKE NUCLEOSIDE TRIPHOSPHATE PYROPHOSPHOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.78Å 110.83Å 166.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.97 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.70) 99.8 (19.97-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.232 0.208 , 0.229	Depositor DCC
R_{free} test set	6916 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14726	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.65	0/1174	0.72	0/1600
1	B	0.63	0/1143	0.68	0/1556
1	C	0.64	0/1170	0.71	0/1595
1	D	0.64	0/1174	0.70	0/1600
1	E	0.60	0/1170	0.66	0/1595
1	F	0.58	0/1125	0.67	0/1530
All	All	0.62	0/6956	0.69	0/9476

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	1148	1136	1134	20	0
1	B	1118	1106	1105	18	0
1	C	1144	1131	1130	24	0
1	D	1148	1135	1133	24	0
1	E	1144	1132	1131	15	0
1	F	1102	1088	1088	23	1
2	A	24	32	32	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	24	24	6	0
2	C	18	24	24	12	0
2	D	36	48	48	22	0
2	E	6	8	8	5	0
2	F	30	40	40	12	0
3	A	15	0	0	0	0
3	B	25	0	0	2	0
3	C	15	0	0	0	0
3	D	15	0	0	0	1
3	E	20	0	0	1	0
3	F	5	0	0	0	0
4	A	132	0	0	7	0
4	B	125	0	0	5	0
4	C	165	0	0	6	0
4	D	150	0	0	5	0
4	E	108	0	0	2	0
4	F	111	0	0	3	0
All	All	7822	6904	6897	119	1

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 9.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:HB1	4:A:2090:HOH:O	1.26	1.30
1:B:41:GLN:HG3	4:B:2044:HOH:O	1.29	1.27
1:A:6:CYS:HG	1:B:6:CYS:HG	1.07	0.97
1:D:125:LYS:H	2:D:1149:GOL:H11	1.34	0.90
1:F:118:ARG:HH12	2:F:1145:GOL:H32	1.39	0.88
1:D:135:ARG:HG3	2:D:1145:GOL:H31	1.57	0.86
1:D:125:LYS:N	2:D:1149:GOL:H11	1.91	0.85
1:D:135:ARG:H	2:D:1145:GOL:H32	1.42	0.85
1:E:55:ILE:HD13	1:F:41:GLN:HG2	1.65	0.78
1:A:71:GLY:HA3	2:A:1145:GOL:H32	1.66	0.78
1:D:3:ASP:HB3	4:D:2009:HOH:O	1.82	0.78
1:F:134:VAL:HB	2:F:1148:GOL:H31	1.66	0.78
1:A:47:GLU:HG2	4:A:2053:HOH:O	1.83	0.78
1:D:125:LYS:H	2:D:1149:GOL:C1	1.99	0.76
1:E:55:ILE:CD1	1:F:41:GLN:HG2	2.16	0.76
1:A:28:ARG:H	2:A:1147:GOL:H12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:VAL:H	2:F:1148:GOL:C3	2.01	0.73
1:E:52:ARG:HG3	1:F:41:GLN:OE1	1.90	0.72
1:D:125:LYS:HE3	2:D:1149:GOL:H31	1.72	0.71
1:E:15:HIS:CD2	2:E:1145:GOL:H32	2.26	0.70
1:A:26:PRO:O	2:A:1148:GOL:C3	2.39	0.70
1:A:28:ARG:HB2	2:A:1147:GOL:O1	1.91	0.69
1:D:135:ARG:N	2:D:1145:GOL:H32	2.08	0.69
1:F:27:GLU:HA	2:F:1146:GOL:H32	1.74	0.69
1:D:135:ARG:H	2:D:1145:GOL:C3	2.05	0.68
1:F:34:PRO:HB3	4:F:2020:HOH:O	1.93	0.68
1:F:134:VAL:H	2:F:1148:GOL:H32	1.58	0.67
1:D:135:ARG:HG3	2:D:1145:GOL:C3	2.24	0.66
2:C:1145:GOL:H31	4:C:2037:HOH:O	1.95	0.65
1:C:139:GLU:CB	2:C:1146:GOL:H32	2.26	0.64
1:F:118:ARG:HH22	2:F:1145:GOL:H11	1.63	0.63
1:C:139:GLU:HG2	2:C:1146:GOL:H32	1.82	0.61
1:A:23:ALA:CB	4:A:2090:HOH:O	2.06	0.61
2:A:1147:GOL:H11	4:A:2035:HOH:O	1.99	0.61
1:A:71:GLY:H	2:A:1145:GOL:H12	1.66	0.60
1:A:13:ARG:NH1	4:A:2019:HOH:O	2.35	0.59
1:A:71:GLY:H	2:A:1145:GOL:C1	2.16	0.59
1:F:69:SER:HB2	2:F:1149:GOL:H32	1.84	0.58
1:E:12:GLU:HA	2:E:1145:GOL:H31	1.86	0.58
1:F:129:TRP:HE3	2:F:1147:GOL:H2	1.68	0.58
2:C:1147:GOL:C1	4:C:2161:HOH:O	2.53	0.56
1:C:139:GLU:HG2	2:C:1146:GOL:C3	2.35	0.56
1:F:134:VAL:N	2:F:1148:GOL:C3	2.69	0.55
1:D:124:LEU:HA	2:D:1149:GOL:H11	1.89	0.55
1:F:42:THR:O	1:F:46:GLU:HG3	2.07	0.55
1:D:125:LYS:CE	2:D:1149:GOL:H31	2.37	0.54
1:A:128:GLY:HA2	4:A:2120:HOH:O	2.07	0.53
1:F:61:ARG:NH2	4:F:2042:HOH:O	2.41	0.53
1:A:-3:ASP:HB2	1:A:-2:PRO:HD2	1.90	0.53
1:C:52:ARG:HD3	4:D:2054:HOH:O	2.08	0.52
1:D:124:LEU:CA	2:D:1149:GOL:H11	2.38	0.52
1:B:144:ALA:CB	4:B:2117:HOH:O	2.57	0.52
1:B:27:GLU:HG2	2:B:1146:GOL:H31	1.92	0.52
1:F:117:ARG:NH1	4:F:2078:HOH:O	2.42	0.52
1:D:71:GLY:H	2:D:1147:GOL:C3	2.23	0.51
1:C:52:ARG:HA	1:D:41:GLN:OE1	2.11	0.51
1:E:6:CYS:HG	1:F:6:CYS:HG	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:HH12	1:C:144:ALA:H	1.58	0.51
1:C:78:HIS:ND1	2:D:1145:GOL:C1	2.74	0.50
1:C:79:GLU:HG2	4:C:2079:HOH:O	2.11	0.50
1:C:139:GLU:CG	2:C:1146:GOL:H32	2.41	0.50
1:C:135:ARG:HG3	2:C:1147:GOL:C3	2.42	0.50
1:B:19:ARG:CZ	2:B:1145:GOL:H2	2.43	0.49
1:A:-3:ASP:HB2	1:A:-2:PRO:CD	2.42	0.49
1:E:15:HIS:CG	2:E:1145:GOL:H32	2.48	0.49
1:C:52:ARG:CD	4:D:2054:HOH:O	2.59	0.49
1:F:69:SER:OG	2:F:1149:GOL:H11	2.13	0.48
1:B:36:LEU:HD23	1:B:36:LEU:C	2.34	0.48
1:E:118:ARG:NH1	4:E:2088:HOH:O	2.46	0.47
1:E:55:ILE:HD12	1:F:41:GLN:HG2	1.93	0.47
1:B:125:LYS:NZ	2:B:1147:GOL:O1	2.44	0.47
1:B:125:LYS:HD2	2:B:1147:GOL:O2	2.15	0.46
1:C:139:GLU:HB2	2:C:1146:GOL:H12	1.97	0.46
1:E:74:ALA:HB3	1:E:75:PRO:HD3	1.97	0.46
1:F:118:ARG:HH12	2:F:1145:GOL:C3	2.21	0.46
1:B:140:ARG:NH2	4:B:2118:HOH:O	2.48	0.46
1:F:134:VAL:CB	2:F:1148:GOL:H31	2.41	0.46
1:D:125:LYS:HD2	2:D:1149:GOL:H12	1.97	0.46
1:D:41:GLN:HG2	4:D:2049:HOH:O	2.15	0.46
1:D:71:GLY:H	2:D:1147:GOL:H32	1.81	0.46
1:B:-3:ASP:HB2	1:B:-2:PRO:HD2	1.97	0.45
1:A:26:PRO:O	2:A:1148:GOL:H32	2.15	0.45
1:B:38:ARG:HD3	3:B:1152:SO4:O3	2.17	0.45
1:A:52:ARG:HA	4:B:2044:HOH:O	2.16	0.45
1:B:28:ARG:HG2	1:B:29:PRO:HD2	1.99	0.44
1:B:125:LYS:HD3	1:B:129:TRP:CE3	2.53	0.44
1:E:138:ILE:HD12	1:F:74:ALA:HA	1.99	0.44
1:C:139:GLU:HB3	2:C:1146:GOL:H32	2.00	0.44
1:E:27:GLU:HG2	4:E:2028:HOH:O	2.18	0.44
1:B:38:ARG:NH2	3:B:1152:SO4:O2	2.51	0.43
1:C:78:HIS:ND1	2:D:1145:GOL:H12	2.32	0.43
1:C:-3:ASP:HB2	1:C:-2:PRO:HD2	1.99	0.43
1:E:4:LEU:HD12	1:E:4:LEU:O	2.19	0.43
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.99	0.43
1:B:144:ALA:HB3	4:B:2117:HOH:O	2.16	0.43
4:C:2143:HOH:O	1:D:21:ILE:HA	2.18	0.43
2:C:1147:GOL:H11	4:C:2161:HOH:O	2.16	0.43
1:D:124:LEU:HD22	2:D:1149:GOL:H2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ARG:NH2	1:F:21:ILE:HB	2.33	0.43
1:E:15:HIS:HB3	2:E:1145:GOL:H32	2.01	0.43
1:C:123:GLN:OE1	4:C:2143:HOH:O	2.22	0.43
1:D:28:ARG:NH1	1:D:144:ALA:HB2	2.34	0.42
1:A:128:GLY:CA	4:A:2120:HOH:O	2.63	0.42
1:C:135:ARG:H	2:C:1147:GOL:H32	1.84	0.42
1:C:135:ARG:HG3	2:C:1147:GOL:H31	2.00	0.42
1:C:142:GLN:HE22	2:D:1147:GOL:H12	1.85	0.42
1:D:36:LEU:C	1:D:36:LEU:HD23	2.38	0.42
1:C:41:GLN:OE1	1:D:52:ARG:HA	2.19	0.42
1:C:78:HIS:ND1	2:D:1145:GOL:H11	2.34	0.42
1:A:26:PRO:O	2:A:1148:GOL:H31	2.17	0.41
1:B:125:LYS:HZ2	2:B:1147:GOL:H12	1.85	0.41
1:C:28:ARG:NH1	1:C:144:ALA:H	2.18	0.41
1:B:27:GLU:H	2:B:1146:GOL:C2	2.34	0.41
1:A:36:LEU:C	1:A:36:LEU:HD23	2.41	0.41
2:D:1145:GOL:H12	4:D:2138:HOH:O	2.19	0.41
1:D:134:VAL:HB	2:D:1145:GOL:H11	2.02	0.41
2:E:1145:GOL:H11	3:E:1149:SO4:O3	2.20	0.41
2:A:1146:GOL:H11	1:C:131:PRO:HG3	2.03	0.40
1:B:67:ALA:O	1:C:127:GLU:CD	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ARG:HH22	3:D:1152:SO4:O3[1_455]	1.59	0.01

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	148/154 (96%)	144 (97%)	4 (3%)	0	100	100
1	B	142/154 (92%)	139 (98%)	2 (1%)	1 (1%)	22	8
1	C	147/154 (96%)	145 (99%)	2 (1%)	0	100	100
1	D	148/154 (96%)	145 (98%)	3 (2%)	0	100	100
1	E	147/154 (96%)	143 (97%)	4 (3%)	0	100	100
1	F	137/154 (89%)	134 (98%)	3 (2%)	0	100	100
All	All	869/924 (94%)	850 (98%)	18 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ALA

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	117/120 (98%)	117 (100%)	0	100	100
1	B	113/120 (94%)	113 (100%)	0	100	100
1	C	117/120 (98%)	116 (99%)	1 (1%)	78	70
1	D	117/120 (98%)	117 (100%)	0	100	100
1	E	117/120 (98%)	117 (100%)	0	100	100
1	F	112/120 (93%)	110 (98%)	2 (2%)	59	43
All	All	693/720 (96%)	690 (100%)	3 (0%)	91	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-4	ILE
1	F	41	GLN
1	F	140	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	93	GLN

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](#)

41 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
3	SO4	B	1150	-	4,4,4	0.25	0	6,6,6	0.38	0
2	GOL	C	1147	-	5,5,5	0.09	0	5,5,5	0.44	0
3	SO4	C	1149	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	1151	-	4,4,4	0.11	0	6,6,6	0.32	0
2	GOL	A	1148	-	5,5,5	0.53	0	5,5,5	0.34	0
2	GOL	A	1146	-	5,5,5	0.37	0	5,5,5	0.36	0
2	GOL	C	1146	-	5,5,5	0.45	0	5,5,5	0.33	0
2	GOL	B	1146	-	5,5,5	0.09	0	5,5,5	0.47	0
2	GOL	D	1146	-	5,5,5	0.33	0	5,5,5	0.99	0
3	SO4	B	1151	-	4,4,4	0.22	0	6,6,6	0.35	0
2	GOL	F	1148	-	5,5,5	0.63	0	5,5,5	1.43	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	1150	-	5,5,5	0.47	0	5,5,5	0.35	0
3	SO4	D	1151	-	4,4,4	0.12	0	6,6,6	0.37	0
2	GOL	D	1147	-	5,5,5	0.77	0	5,5,5	0.68	0
3	SO4	F	1150	-	4,4,4	0.11	0	6,6,6	0.19	0
2	GOL	B	1145	-	5,5,5	0.38	0	5,5,5	0.36	0
2	GOL	F	1146	-	5,5,5	0.72	0	5,5,5	0.50	0
2	GOL	A	1147	-	5,5,5	0.19	0	5,5,5	0.44	0
2	GOL	D	1148	-	5,5,5	0.24	0	5,5,5	0.45	0
2	GOL	D	1145	-	5,5,5	0.37	0	5,5,5	0.39	0
3	SO4	E	1146	-	4,4,4	0.25	0	6,6,6	0.36	0
3	SO4	D	1152	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	B	1152	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	D	1153	-	4,4,4	0.18	0	6,6,6	0.23	0
3	SO4	B	1148	-	4,4,4	0.14	0	6,6,6	0.42	0
2	GOL	B	1147	-	5,5,5	0.57	0	5,5,5	1.36	1 (20%)
3	SO4	E	1147	-	4,4,4	0.18	0	6,6,6	0.25	0
2	GOL	A	1145	-	5,5,5	0.50	0	5,5,5	0.26	0
3	SO4	C	1150	-	4,4,4	0.16	0	6,6,6	0.25	0
2	GOL	D	1149	-	5,5,5	1.00	0	5,5,5	1.16	0
3	SO4	C	1148	-	4,4,4	0.27	0	6,6,6	0.34	0
2	GOL	F	1145	-	5,5,5	0.52	0	5,5,5	0.62	0
3	SO4	E	1148	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	B	1149	-	4,4,4	0.17	0	6,6,6	0.40	0
3	SO4	E	1149	-	4,4,4	0.16	0	6,6,6	0.34	0
3	SO4	A	1149	-	4,4,4	0.21	0	6,6,6	0.32	0
3	SO4	A	1150	-	4,4,4	0.16	0	6,6,6	0.40	0
2	GOL	C	1145	-	5,5,5	0.54	0	5,5,5	0.35	0
2	GOL	F	1147	-	5,5,5	0.33	0	5,5,5	0.35	0
2	GOL	F	1149	-	5,5,5	0.42	0	5,5,5	0.55	0
2	GOL	E	1145	-	5,5,5	0.56	0	5,5,5	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1147	-	-	0/4/4/4	-
2	GOL	A	1148	-	-	0/4/4/4	-
2	GOL	A	1146	-	-	2/4/4/4	-
2	GOL	C	1146	-	-	1/4/4/4	-
2	GOL	B	1146	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	1146	-	-	2/4/4/4	-
2	GOL	F	1148	-	-	4/4/4/4	-
2	GOL	D	1150	-	-	2/4/4/4	-
2	GOL	D	1147	-	-	0/4/4/4	-
2	GOL	B	1145	-	-	0/4/4/4	-
2	GOL	F	1146	-	-	2/4/4/4	-
2	GOL	A	1147	-	-	2/4/4/4	-
2	GOL	D	1148	-	-	4/4/4/4	-
2	GOL	D	1145	-	-	2/4/4/4	-
2	GOL	B	1147	-	-	4/4/4/4	-
2	GOL	A	1145	-	-	2/4/4/4	-
2	GOL	D	1149	-	-	4/4/4/4	-
2	GOL	F	1145	-	-	4/4/4/4	-
2	GOL	C	1145	-	-	2/4/4/4	-
2	GOL	F	1147	-	-	2/4/4/4	-
2	GOL	F	1149	-	-	2/4/4/4	-
2	GOL	E	1145	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1148	GOL	O2-C2-C1	2.70	121.00	109.12
2	B	1147	GOL	O1-C1-C2	-2.03	100.46	110.20

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1146	GOL	C1-C2-C3-O3
2	F	1148	GOL	O1-C1-C2-C3
2	F	1148	GOL	C1-C2-C3-O3
2	A	1147	GOL	C1-C2-C3-O3
2	D	1148	GOL	O1-C1-C2-O2
2	D	1148	GOL	O1-C1-C2-C3
2	D	1148	GOL	C1-C2-C3-O3
2	B	1147	GOL	C1-C2-C3-O3
2	F	1145	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	F	1147	GOL	C1-C2-C3-O3
2	F	1149	GOL	C1-C2-C3-O3
2	A	1146	GOL	O2-C2-C3-O3
2	F	1148	GOL	O1-C1-C2-O2
2	F	1145	GOL	O1-C1-C2-O2
2	F	1149	GOL	O2-C2-C3-O3
2	A	1146	GOL	C1-C2-C3-O3
2	D	1150	GOL	C1-C2-C3-O3
2	F	1146	GOL	O1-C1-C2-C3
2	D	1145	GOL	O1-C1-C2-C3
2	B	1147	GOL	O1-C1-C2-C3
2	A	1145	GOL	C1-C2-C3-O3
2	D	1149	GOL	C1-C2-C3-O3
2	F	1145	GOL	C1-C2-C3-O3
2	C	1145	GOL	C1-C2-C3-O3
2	E	1145	GOL	O1-C1-C2-C3
2	D	1146	GOL	O2-C2-C3-O3
2	D	1150	GOL	O2-C2-C3-O3
2	A	1147	GOL	O2-C2-C3-O3
2	D	1148	GOL	O2-C2-C3-O3
2	B	1147	GOL	O1-C1-C2-O2
2	B	1147	GOL	O2-C2-C3-O3
2	F	1147	GOL	O2-C2-C3-O3
2	E	1145	GOL	O1-C1-C2-O2
2	A	1145	GOL	O2-C2-C3-O3
2	D	1149	GOL	O2-C2-C3-O3
2	C	1145	GOL	O2-C2-C3-O3
2	D	1145	GOL	O1-C1-C2-O2
2	F	1145	GOL	O2-C2-C3-O3
2	F	1148	GOL	O2-C2-C3-O3
2	D	1149	GOL	O1-C1-C2-O2
2	D	1149	GOL	O1-C1-C2-C3
2	F	1146	GOL	O1-C1-C2-O2
2	C	1146	GOL	O2-C2-C3-O3

There are no ring outliers.

22 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1147	GOL	5	0
2	A	1148	GOL	3	0
2	A	1146	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1146	GOL	6	0
2	B	1146	GOL	2	0
2	F	1148	GOL	5	0
2	D	1147	GOL	3	0
2	B	1145	GOL	1	0
2	F	1146	GOL	1	0
2	A	1147	GOL	3	0
2	D	1145	GOL	10	0
3	D	1152	SO4	0	1
3	B	1152	SO4	2	0
2	B	1147	GOL	3	0
2	A	1145	GOL	3	0
2	D	1149	GOL	9	0
2	F	1145	GOL	3	0
3	E	1149	SO4	1	0
2	C	1145	GOL	1	0
2	F	1147	GOL	1	0
2	F	1149	GOL	2	0
2	E	1145	GOL	5	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	150/154 (97%)	0.41	17 (11%) 5 6	11, 20, 46, 56	0
1	B	146/154 (94%)	0.33	13 (8%) 9 11	11, 20, 52, 77	0
1	C	149/154 (96%)	0.29	12 (8%) 12 14	10, 18, 43, 54	0
1	D	150/154 (97%)	0.23	12 (8%) 12 14	10, 18, 33, 43	0
1	E	149/154 (96%)	0.66	22 (14%) 2 2	13, 29, 49, 58	0
1	F	143/154 (92%)	0.58	15 (10%) 6 7	13, 27, 55, 92	0
All	All	887/924 (95%)	0.41	91 (10%) 6 7	10, 21, 49, 92	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	LEU	11.2
1	F	-1	PHE	10.7
1	A	-1	PHE	9.5
1	C	-1	PHE	9.3
1	F	144	ALA	8.6
1	F	-2	PRO	8.0
1	B	144	ALA	7.9
1	F	6	CYS	7.2
1	F	-4	ILE	7.1
1	E	-1	PHE	7.0
1	E	144	ALA	7.0
1	B	-5	GLY	7.0
1	B	-1	PHE	6.6
1	D	144	ALA	6.3
1	C	144	ALA	5.9
1	A	144	ALA	5.8
1	A	4	LEU	5.7
1	E	5	PRO	5.6
1	D	-5	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	5	PRO	5.4
1	B	24	ALA	5.2
1	A	-5	GLY	5.2
1	C	-2	PRO	5.0
1	A	5	PRO	4.9
1	E	3	ASP	4.8
1	B	-4	ILE	4.6
1	A	-2	PRO	4.6
1	A	23	ALA	4.3
1	A	6	CYS	4.3
1	B	6	CYS	4.2
1	D	143	HIS	4.2
1	F	24	ALA	4.2
1	E	6	CYS	4.1
1	F	7	PRO	4.1
1	C	4	LEU	3.9
1	D	-1	PHE	3.9
1	E	130	ARG	3.8
1	C	-4	ILE	3.8
1	F	0	THR	3.7
1	D	4	LEU	3.6
1	E	63	ALA	3.5
1	A	24	ALA	3.4
1	B	140	ARG	3.4
1	D	119	ALA	3.4
1	D	121	GLY	3.3
1	E	143	HIS	3.2
1	E	119	ALA	3.1
1	B	5	PRO	3.1
1	D	120	ASP	3.0
1	C	6	CYS	3.0
1	F	143	HIS	2.9
1	C	24	ALA	2.9
1	C	143	HIS	2.9
1	A	143	HIS	2.9
1	D	22	GLY	2.8
1	E	7	PRO	2.8
1	B	-2	PRO	2.8
1	F	35	GLU	2.7
1	A	-4	ILE	2.7
1	B	130	ARG	2.6
1	D	23	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	143	HIS	2.6
1	B	67	ALA	2.6
1	B	28	ARG	2.5
1	E	1	MET	2.5
1	D	5	PRO	2.5
1	C	119	ALA	2.5
1	F	17	PHE	2.5
1	E	132	ALA	2.4
1	C	3	ASP	2.4
1	E	2	SER	2.4
1	E	-2	PRO	2.4
1	F	-3	ASP	2.4
1	E	-4	ILE	2.3
1	E	120	ASP	2.3
1	A	119	ALA	2.3
1	A	140	ARG	2.3
1	A	128	GLY	2.3
1	D	24	ALA	2.3
1	F	34	PRO	2.3
1	A	0	THR	2.3
1	E	116	PRO	2.2
1	A	64	ALA	2.2
1	C	121	GLY	2.2
1	E	140	ARG	2.2
1	F	19	ARG	2.2
1	A	130	ARG	2.1
1	E	64	ALA	2.1
1	E	139	GLU	2.1
1	F	28	ARG	2.0
1	E	60	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	C	1146	6/6	0.49	0.55	44,45,46,46	0
2	GOL	F	1148	6/6	0.53	0.25	41,46,49,49	0
2	GOL	F	1146	6/6	0.63	0.32	46,47,48,48	0
2	GOL	C	1145	6/6	0.63	0.27	38,43,45,45	0
2	GOL	A	1145	6/6	0.67	0.20	36,37,39,39	0
2	GOL	A	1146	6/6	0.72	0.25	35,41,46,46	0
2	GOL	F	1145	6/6	0.73	0.18	30,35,39,39	0
2	GOL	D	1150	6/6	0.73	0.29	40,41,44,44	0
2	GOL	B	1147	6/6	0.75	0.35	31,31,36,36	0
2	GOL	D	1148	6/6	0.75	0.20	40,41,44,44	0
3	SO4	C	1149	5/5	0.80	0.28	30,31,32,32	5
2	GOL	D	1146	6/6	0.80	0.26	33,35,38,38	0
2	GOL	E	1145	6/6	0.81	0.36	29,36,41,41	0
2	GOL	F	1147	6/6	0.82	0.43	33,36,39,39	0
2	GOL	F	1149	6/6	0.82	0.16	38,41,42,42	0
2	GOL	D	1145	6/6	0.82	0.28	31,32,34,34	0
2	GOL	D	1147	6/6	0.83	0.25	30,33,38,38	0
2	GOL	A	1148	6/6	0.83	0.26	26,33,36,36	0
2	GOL	A	1147	6/6	0.83	0.39	35,38,41,41	0
2	GOL	B	1146	6/6	0.84	0.35	36,38,41,41	0
3	SO4	E	1147	5/5	0.84	0.19	31,33,34,34	5
3	SO4	D	1152	5/5	0.84	0.22	34,34,36,36	5
3	SO4	D	1153	5/5	0.84	0.16	33,33,35,35	5
2	GOL	D	1149	6/6	0.85	0.29	23,28,30,30	0
3	SO4	E	1149	5/5	0.86	0.33	35,35,38,38	5
2	GOL	B	1145	6/6	0.87	0.38	35,37,39,39	0
2	GOL	C	1147	6/6	0.88	0.18	34,35,37,37	0
3	SO4	B	1151	5/5	0.88	0.30	39,40,41,41	0
3	SO4	A	1151	5/5	0.90	0.29	38,39,40,40	5
3	SO4	C	1150	5/5	0.91	0.24	40,40,41,42	5
3	SO4	F	1150	5/5	0.92	0.14	20,24,25,27	5
3	SO4	A	1149	5/5	0.92	0.15	23,24,24,26	5
3	SO4	B	1149	5/5	0.92	0.21	38,38,38,39	5
3	SO4	E	1148	5/5	0.93	0.21	35,36,37,38	5
3	SO4	B	1148	5/5	0.94	0.10	21,24,26,27	5
3	SO4	A	1150	5/5	0.94	0.12	20,20,24,25	5
3	SO4	B	1150	5/5	0.96	0.22	30,33,35,35	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	1152	5/5	0.97	0.30	38,38,39,39	0
3	SO4	D	1151	5/5	0.98	0.16	29,30,31,31	0
3	SO4	E	1146	5/5	0.98	0.17	18,19,19,20	5
3	SO4	C	1148	5/5	0.99	0.07	23,25,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.