



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:04 AM UTC

PDB ID : 1F0V / pdb_00001f0v
Title : Crystal structure of an Rnase A dimer displaying a new type of 3D domain swapping
Authors : Liu, Y.S.; Gotte, G.; Libonati, M.; Eisenberg, D.S.
Deposited on : 2000-05-17
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 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

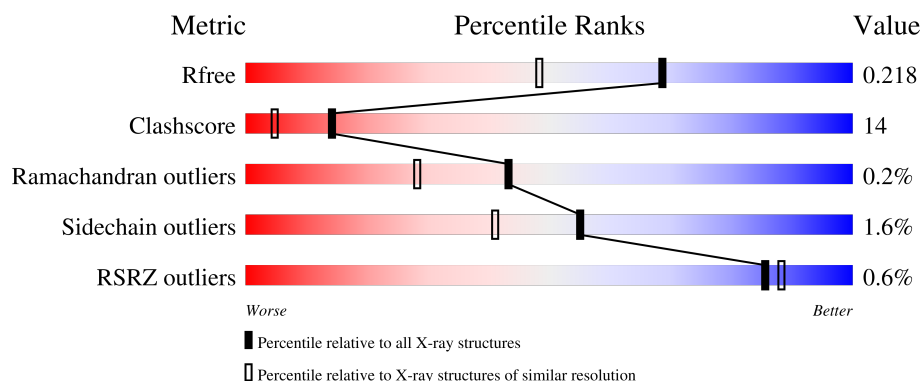
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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.



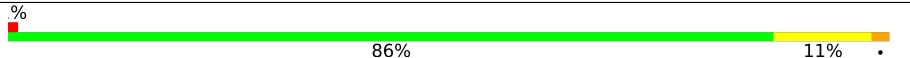
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 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	M	2	50% 50%
1	N	2	100%
1	O	2	100%
1	P	2	100%
2	A	124	87% 12% .

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Mol	Chain	Length	Quality of chain
2	B	124	
2	C	124	
2	D	124	

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	PO4	A	801	-	-	X	-
4	GOL	A	904	-	X	-	-
4	GOL	A	908	-	X	-	-
4	GOL	A	918	-	X	X	-
4	GOL	B	902	-	X	X	-
4	GOL	B	905	-	X	X	-
4	GOL	B	910	-	X	X	-
4	GOL	B	914	-	X	-	-
4	GOL	B	920	-	X	X	-
4	GOL	B	921	-	X	-	-
4	GOL	B	922	-	X	X	-
4	GOL	C	903	-	X	-	-
4	GOL	C	912	-	X	-	-
4	GOL	C	917	-	-	X	-
4	GOL	C	919	-	X	-	-
4	GOL	D	901	-	X	X	-
4	GOL	D	913	-	X	X	-
4	GOL	D	916	-	X	-	-
4	GOL	D	924	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4742 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 DNA chain called 5'-D(*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	N	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	O	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	P	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			

- Molecule 2 is a protein called RIBONUCLEASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	124	Total	C	N	O	S	0	4	0
			960	581	171	196	12			
2	B	124	Total	C	N	O	S	0	9	0
			979	594	174	198	13			
2	C	124	Total	C	N	O	S	0	6	0
			968	586	173	197	12			
2	D	124	Total	C	N	O	S	0	5	0
			965	585	172	196	12			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	3	Total	O		0	0
			3	3			
5	N	7	Total	O		0	0
			7	7			
5	O	3	Total	O		0	0
			3	3			
5	P	7	Total	O		0	0
			7	7			
5	A	154	Total	O		0	0
			154	154			
5	B	129	Total	O		0	0
			129	129			
5	C	132	Total	O		0	0
			132	132			
5	D	119	Total	O		0	0
			119	119			

3 Residue-property plots

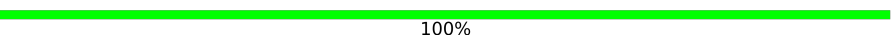
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 5'-D(*CP*G)-3'

Chain M: 

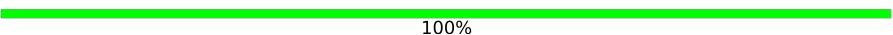


- Molecule 1: 5'-D(*CP*G)-3'

Chain N: 

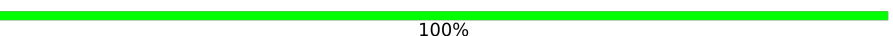
There are no outlier residues recorded for this chain.

- Molecule 1: 5'-D(*CP*G)-3'

Chain O: 

There are no outlier residues recorded for this chain.

- Molecule 1: 5'-D(*CP*G)-3'

Chain P: 

There are no outlier residues recorded for this chain.

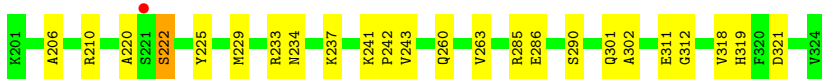
- Molecule 2: RIBONUCLEASE A

Chain A: 

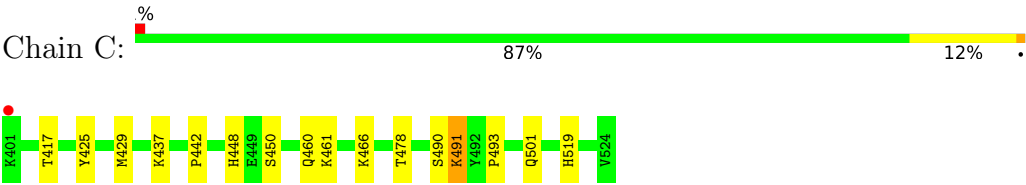


- Molecule 2: RIBONUCLEASE A

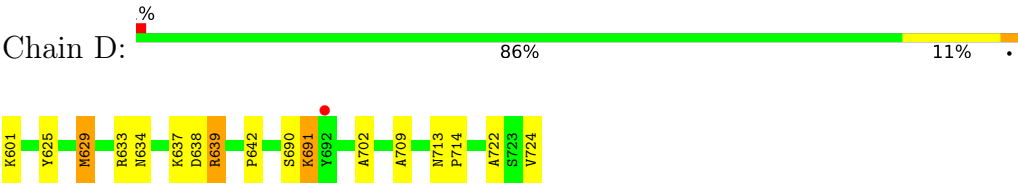
Chain B: 



- Molecule 2: RIBONUCLEASE A



● Molecule 2: RIBONUCLEASE A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.57Å 96.34Å 48.24Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.0 (10.00-1.70) 94.8 (10.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.213 0.189 , 0.218	Depositor DCC
R_{free} test set	7670 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4742	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6604e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, 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	M	0.63	0/42	1.05	0/63
1	N	0.61	0/42	1.00	0/63
1	O	0.64	0/42	1.07	0/63
1	P	0.66	0/42	0.95	0/63
2	A	1.05	1/992 (0.1%)	1.19	2/1335 (0.1%)
2	B	0.99	0/1032	1.17	2/1387 (0.1%)
2	C	0.97	0/1009	1.16	5/1358 (0.4%)
2	D	1.04	1/1001 (0.1%)	1.15	2/1346 (0.1%)
All	All	1.00	2/4202 (0.0%)	1.16	11/5678 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	60	GLN	CA-C	-7.34	1.49	1.53
2	D	629	MET	SD-CE	-7.02	1.62	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	442	PRO	N-CA-C	6.95	122.71	113.40
2	D	642	PRO	N-CA-C	6.75	122.41	113.57
2	A	42	PRO	N-CA-C	6.59	122.23	113.40
2	A	61	LYS	N-CA-C	6.53	118.79	108.67
2	C	461	LYS	N-CA-C	6.45	118.67	108.67
2	C	460	GLN	N-CA-C	6.22	113.88	108.78
2	B	237	LYS	N-CA-C	6.09	117.61	110.97
2	C	478	THR	N-CA-C	-5.73	102.43	110.50
2	B	241	LYS	N-CA-C	-5.31	101.84	109.48
2	C	437	LYS	N-CA-C	5.12	116.55	111.07
2	D	637	LYS	N-CA-C	5.00	116.42	110.97

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	M	38	0	24	1	0
1	N	38	0	24	0	0
1	O	38	0	24	0	0
1	P	38	0	24	0	0
2	A	960	0	913	26	0
2	B	979	0	929	32	0
2	C	968	0	914	10	0
2	D	965	0	919	19	1
3	A	5	0	0	3	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	P	5	0	0	0	0
4	A	36	0	47	8	0
4	B	54	0	72	35	0
4	C	24	0	32	8	1
4	D	30	0	38	19	0
5	A	154	0	0	2	0
5	B	129	0	0	0	0
5	C	132	0	0	0	0
5	D	119	0	0	1	0
5	M	3	0	0	0	0
5	N	7	0	0	0	0
5	O	3	0	0	0	0
5	P	7	0	0	0	0
All	All	4742	0	3960	116	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 14.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:924:GOL:C1	4:D:924:GOL:C2	1.80	1.58
4:C:903:GOL:C1	4:C:903:GOL:C2	1.76	1.54
4:A:923:GOL:C1	4:A:923:GOL:O1	1.65	1.45
4:B:910:GOL:C1	4:B:910:GOL:O1	1.65	1.43
4:B:902:GOL:C3	4:B:902:GOL:O3	1.66	1.43
4:D:901:GOL:C2	4:D:901:GOL:O2	1.67	1.43
4:B:920:GOL:C1	4:B:920:GOL:O1	1.67	1.42
4:A:918:GOL:O2	4:A:918:GOL:C2	1.66	1.42
4:B:905:GOL:O1	4:B:905:GOL:C1	1.70	1.40
4:B:920:GOL:C3	4:B:920:GOL:O3	1.67	1.40
4:D:913:GOL:O2	4:D:913:GOL:C2	1.69	1.39
4:B:914:GOL:O1	4:B:914:GOL:C1	1.66	1.39
4:C:917:GOL:O3	4:C:917:GOL:C3	1.69	1.39
4:A:911:GOL:C3	4:A:911:GOL:O3	1.71	1.38
4:D:913:GOL:C1	4:D:913:GOL:O1	1.70	1.37
4:D:901:GOL:O3	4:D:901:GOL:C3	1.76	1.32
4:B:921:GOL:C3	4:B:921:GOL:O3	1.81	1.26
4:D:924:GOL:C1	4:D:924:GOL:O1	1.83	1.25
2:A:66:LYS:HD3	2:A:67:ASN:H	1.19	1.02
2:B:301:GLN:HG3	4:B:906:GOL:H12	1.37	1.01
2:B:312:GLY:HA2	4:B:910:GOL:H31	1.44	0.97
2:B:210:ARG:HB2	4:B:905:GOL:H32	1.47	0.96
2:A:116:VAL:HG22	4:B:910:GOL:H12	1.51	0.91
2:B:229[B]:MET:HE1	2:B:233:ARG:NH2	1.91	0.86
2:C:450:SER:HB2	4:C:919:GOL:H32	1.68	0.76
2:A:66:LYS:HD3	2:A:67:ASN:N	2.01	0.75
2:D:714:PRO:O	4:D:901:GOL:H11	1.90	0.72
2:D:691[A]:LYS:HB3	2:D:691[A]:LYS:NZ	2.05	0.71
2:C:519[B]:HIS:HD2	2:D:709:ALA:HB2	1.56	0.70
2:C:501:GLN:HG3	4:C:917:GOL:H31	1.74	0.70
2:C:450:SER:CB	4:C:919:GOL:H32	2.23	0.69
2:C:490:SER:O	2:C:491:LYS:HD3	1.94	0.67
2:A:116:VAL:CG2	4:B:910:GOL:H12	2.23	0.67
2:A:34:ASN:HB3	2:A:37:LYS:HZ2	1.59	0.67
2:A:12:HIS:HE1	3:A:801:PO4:O2	1.77	0.66
2:C:519[B]:HIS:HD2	2:D:709:ALA:CB	2.08	0.66
2:B:302:ALA:HA	4:B:902:GOL:H32	1.78	0.65
2:A:12:HIS:HD2	2:A:45:THR:O	1.79	0.65
2:B:234:ASN:HD22	4:B:922:GOL:H32	1.61	0.64
4:D:913:GOL:O2	4:D:913:GOL:H2	1.92	0.63
2:D:702:ALA:HA	4:D:913:GOL:H2	1.79	0.62
2:B:220:ALA:O	2:B:301:GLN:NE2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:923:GOL:C1	4:A:923:GOL:HO1	2.08	0.61
2:B:234:ASN:ND2	4:B:922:GOL:H32	2.16	0.61
2:D:691[A]:LYS:HB3	2:D:691[A]:LYS:HZ3	1.64	0.60
2:B:243:VAL:HG13	2:B:285:ARG:HE	1.66	0.60
2:C:466:LYS:HE2	2:D:722:ALA:HB2	1.84	0.59
2:C:501:GLN:HG3	4:C:917:GOL:C3	2.32	0.59
2:B:206:ALA:HB1	4:B:905:GOL:H12	1.83	0.59
2:D:639:ARG:HH11	2:D:639:ARG:HB3	1.67	0.59
2:B:242:PRO:HD2	4:B:914:GOL:H32	1.84	0.59
4:B:910:GOL:C1	4:B:910:GOL:HO1	2.09	0.59
2:B:229[B]:MET:HE1	2:B:233:ARG:CZ	2.32	0.59
2:A:66:LYS:CD	2:A:67:ASN:H	2.04	0.59
4:A:918:GOL:C2	4:A:918:GOL:HO2	2.10	0.58
2:D:713:ASN:HB3	4:D:901:GOL:H12	1.84	0.58
2:A:34:ASN:HB3	2:A:37:LYS:NZ	2.17	0.58
4:C:917:GOL:C3	4:C:917:GOL:HO3	2.12	0.58
2:D:601:LYS:HD2	2:D:601:LYS:N	2.18	0.58
4:D:901:GOL:H12	5:D:1254:HOH:O	2.03	0.57
2:D:702:ALA:HA	4:D:913:GOL:H31	1.85	0.57
2:A:105:HIS:HE1	5:A:1128:HOH:O	1.89	0.55
2:B:234:ASN:HD22	4:B:922:GOL:C3	2.19	0.55
2:A:66:LYS:HD2	2:B:321:ASP:OD1	2.07	0.55
2:A:65:CYS:HB3	2:A:66:LYS:CD	2.36	0.55
2:A:23:SER:HA	4:A:918:GOL:H11	1.89	0.55
4:B:902:GOL:C3	4:B:902:GOL:HO3	2.10	0.55
2:B:210:ARG:CB	4:B:905:GOL:H32	2.31	0.54
4:D:913:GOL:C2	4:D:913:GOL:HO2	2.12	0.54
2:B:260:GLN:NE2	4:B:921:GOL:H2	2.23	0.53
4:B:905:GOL:C1	4:B:905:GOL:HO1	2.13	0.53
2:A:66:LYS:HE2	5:A:1097:HOH:O	2.08	0.53
2:B:312:GLY:CA	4:B:910:GOL:H31	2.29	0.53
4:B:910:GOL:O3	4:B:920:GOL:H31	2.10	0.52
4:B:920:GOL:C3	4:B:920:GOL:HO3	2.11	0.52
2:D:638:ASP:HB3	2:D:639:ARG:HH12	1.75	0.51
2:A:66:LYS:CD	2:A:66:LYS:N	2.74	0.51
4:B:920:GOL:C1	4:B:920:GOL:HO1	2.11	0.51
1:M:751:DC:C6	2:A:85:ARG:HD2	2.45	0.51
2:A:66:LYS:CD	2:B:321:ASP:OD1	2.59	0.50
4:D:913:GOL:C1	4:D:913:GOL:HO1	2.14	0.50
2:B:285:ARG:HG3	2:B:285:ARG:HH11	1.77	0.50
2:B:225:TYR:CZ	2:B:229[A]:MET:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:914:GOL:C1	4:B:914:GOL:HO1	2.10	0.50
2:B:210:ARG:HB2	4:B:905:GOL:C3	2.30	0.50
2:D:625:TYR:CZ	2:D:629:MET:HG3	2.48	0.49
2:A:65:CYS:HB3	2:A:66:LYS:HD2	1.94	0.48
3:A:801:PO4:O1	2:B:319[A]:HIS:ND1	2.43	0.47
2:A:12:HIS:CE1	3:A:801:PO4:O2	2.64	0.47
4:D:901:GOL:C2	4:D:901:GOL:HO2	2.10	0.46
4:C:903:GOL:C1	4:C:903:GOL:C3	2.84	0.46
2:D:633:ARG:O	2:D:634:ASN:HB2	2.15	0.46
2:B:311:GLU:O	4:B:910:GOL:H2	2.17	0.45
2:B:302:ALA:HA	4:B:902:GOL:C3	2.45	0.45
2:A:66:LYS:HD2	2:A:66:LYS:H	1.82	0.44
2:B:286:GLU:HG3	2:B:290:SER:CB	2.47	0.44
2:D:702:ALA:HA	4:D:913:GOL:C2	2.44	0.44
2:D:702:ALA:CA	4:D:913:GOL:H31	2.47	0.44
2:A:50:SER:OG	4:A:908:GOL:H31	2.18	0.44
2:A:66:LYS:CG	2:A:67:ASN:N	2.81	0.44
2:B:206:ALA:O	4:B:905:GOL:H12	2.19	0.43
2:B:263:VAL:HB	4:B:907:GOL:H32	2.01	0.42
2:A:23:SER:HA	4:A:918:GOL:C1	2.50	0.42
4:D:924:GOL:C1	4:D:924:GOL:C3	2.86	0.42
2:D:702:ALA:HA	4:D:913:GOL:C3	2.48	0.42
2:A:66:LYS:HD2	2:A:66:LYS:N	2.34	0.42
2:B:210:ARG:HD2	4:B:922:GOL:H31	2.01	0.41
2:A:66:LYS:CD	2:A:67:ASN:N	2.75	0.41
2:C:417:THR:O	2:C:448:HIS:HB3	2.21	0.41
2:B:210:ARG:CD	4:B:922:GOL:H31	2.50	0.41
2:A:66:LYS:HE3	2:B:319[A]:HIS:NE2	2.36	0.40
2:B:318:VAL:HG23	2:B:319[B]:HIS:CD2	2.55	0.40
2:B:225:TYR:CZ	2:B:229[B]:MET:HG3	2.57	0.40
2:C:425:TYR:CZ	2:C:429:MET:HG3	2.57	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)
2:D:690:SER:O	4:C:919:GOL:O3[2_555]	1.96	0.24

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	
2	A	125/124 (101%)	121 (97%)	4 (3%)	0	100	100
2	B	130/124 (105%)	123 (95%)	6 (5%)	1 (1%)	16	5
2	C	127/124 (102%)	122 (96%)	5 (4%)	0	100	100
2	D	126/124 (102%)	118 (94%)	8 (6%)	0	100	100
All	All	508/496 (102%)	484 (95%)	23 (4%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	SER

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	
2	A	113/109 (104%)	111 (98%)	2 (2%)	51	36
2	B	118/109 (108%)	117 (99%)	1 (1%)	73	65
2	C	115/109 (106%)	113 (98%)	2 (2%)	53	38
2	D	114/109 (105%)	111 (97%)	3 (3%)	40	23
All	All	460/436 (106%)	452 (98%)	8 (2%)	55	38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1	LYS
2	A	66	LYS
2	B	222	SER
2	C	491	LYS
2	C	493	PRO
2	D	639	ARG
2	D	691[A]	LYS
2	D	691[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	11	GLN
2	A	12	HIS
2	A	105	HIS
2	B	228	GLN
2	B	234	ASN
2	C	434	ASN
2	C	503	ASN
2	C	505	HIS
2	D	634	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](#)

28 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
4	GOL	C	903	-	5,5,5	3.56	2 (40%)	5,5,5	0.77	0
4	GOL	D	916	-	5,5,5	2.65	3 (60%)	5,5,5	1.12	0
4	GOL	C	919	-	5,5,5	2.62	3 (60%)	5,5,5	1.54	2 (40%)
4	GOL	A	904	-	5,5,5	3.63	5 (100%)	5,5,5	0.96	0
4	GOL	D	901	-	5,5,5	5.65	5 (100%)	5,5,5	2.40	3 (60%)
4	GOL	A	923	-	5,5,5	4.14	3 (60%)	5,5,5	1.32	0
3	PO4	P	804	-	4,4,4	1.48	1 (25%)	6,6,6	0.61	0
3	PO4	B	802	-	4,4,4	1.21	0	6,6,6	0.43	0
4	GOL	B	921	-	5,5,5	4.52	3 (60%)	5,5,5	1.20	0
4	GOL	C	917	-	5,5,5	3.21	2 (40%)	5,5,5	1.32	0
4	GOL	D	913	-	5,5,5	5.65	4 (80%)	5,5,5	1.83	2 (40%)
4	GOL	B	902	-	5,5,5	4.39	5 (100%)	5,5,5	1.67	1 (20%)
4	GOL	A	908	-	5,5,5	2.74	4 (80%)	5,5,5	0.63	0
3	PO4	A	801	-	4,4,4	1.32	0	6,6,6	0.67	0
4	GOL	D	924	-	5,5,5	6.17	5 (100%)	5,5,5	0.63	0
4	GOL	B	914	-	5,5,5	4.46	4 (80%)	5,5,5	1.57	1 (20%)
4	GOL	D	909	-	5,5,5	2.30	3 (60%)	5,5,5	0.93	0
4	GOL	A	911	-	5,5,5	3.89	2 (40%)	5,5,5	1.09	0
4	GOL	B	906	-	5,5,5	2.51	2 (40%)	5,5,5	0.77	0
3	PO4	C	803	-	4,4,4	1.06	0	6,6,6	0.58	0
4	GOL	B	910	-	5,5,5	2.87	2 (40%)	5,5,5	2.26	2 (40%)
4	GOL	B	922	-	5,5,5	4.51	5 (100%)	5,5,5	0.72	0
4	GOL	C	912	-	5,5,5	2.96	4 (80%)	5,5,5	0.77	0
4	GOL	A	915	-	5,5,5	2.56	3 (60%)	5,5,5	0.88	0
4	GOL	A	918	-	5,5,5	4.24	3 (60%)	5,5,5	1.60	1 (20%)
4	GOL	B	920	-	5,5,5	4.70	4 (80%)	5,5,5	0.89	0
4	GOL	B	905	-	5,5,5	3.20	1 (20%)	5,5,5	1.99	2 (40%)
4	GOL	B	907	-	5,5,5	2.01	3 (60%)	5,5,5	1.02	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
4	GOL	C	903	-	-	4/4/4/4	-
4	GOL	D	916	-	-	4/4/4/4	-
4	GOL	C	919	-	-	1/4/4/4	-
4	GOL	A	904	-	-	2/4/4/4	-
4	GOL	D	901	-	-	4/4/4/4	-
4	GOL	A	923	-	-	2/4/4/4	-
4	GOL	B	921	-	-	3/4/4/4	-
4	GOL	C	917	-	-	3/4/4/4	-
4	GOL	D	913	-	-	2/4/4/4	-
4	GOL	B	902	-	-	3/4/4/4	-
4	GOL	A	908	-	-	2/4/4/4	-
4	GOL	D	924	-	-	4/4/4/4	-
4	GOL	B	914	-	-	2/4/4/4	-
4	GOL	D	909	-	-	2/4/4/4	-
4	GOL	A	911	-	-	1/4/4/4	-
4	GOL	B	906	-	-	1/4/4/4	-
4	GOL	B	910	-	-	2/4/4/4	-
4	GOL	B	922	-	-	4/4/4/4	-
4	GOL	C	912	-	-	3/4/4/4	-
4	GOL	A	915	-	-	2/4/4/4	-
4	GOL	A	918	-	-	3/4/4/4	-
4	GOL	B	920	-	-	2/4/4/4	-
4	GOL	B	905	-	-	3/4/4/4	-
4	GOL	B	907	-	-	0/4/4/4	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	924	GOL	O1-C1	9.79	1.83	1.42
4	B	921	GOL	O3-C3	9.20	1.81	1.42
4	D	913	GOL	O2-C2	8.93	1.69	1.43
4	D	901	GOL	O2-C2	8.26	1.67	1.43
4	A	918	GOL	O2-C2	8.09	1.66	1.43
4	D	901	GOL	O3-C3	7.99	1.76	1.42
4	D	924	GOL	C1-C2	7.49	1.80	1.51
4	A	911	GOL	O3-C3	7.01	1.71	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	913	GOL	O1-C1	6.78	1.70	1.42
4	B	905	GOL	O1-C1	6.58	1.70	1.42
4	C	903	GOL	C1-C2	6.36	1.76	1.51
4	C	917	GOL	O3-C3	6.35	1.69	1.42
4	B	920	GOL	O1-C1	6.02	1.67	1.42
4	A	923	GOL	O2-C2	5.98	1.60	1.43
4	B	922	GOL	O2-C2	5.97	1.60	1.43
4	B	920	GOL	O3-C3	5.97	1.67	1.42
4	B	902	GOL	O2-C2	5.95	1.60	1.43
4	B	902	GOL	O3-C3	5.83	1.66	1.42
4	B	920	GOL	C1-C2	5.80	1.73	1.51
4	B	914	GOL	O1-C1	5.75	1.66	1.42
4	B	910	GOL	O1-C1	5.57	1.65	1.42
4	B	914	GOL	C1-C2	5.45	1.72	1.51
4	A	923	GOL	O1-C1	5.40	1.65	1.42
4	B	922	GOL	C1-C2	5.25	1.71	1.51
4	D	913	GOL	O3-C3	-4.96	1.21	1.42
4	A	904	GOL	O1-C1	4.83	1.62	1.42
4	B	922	GOL	O1-C1	4.80	1.62	1.42
4	A	904	GOL	C1-C2	4.59	1.69	1.51
4	D	916	GOL	O3-C3	4.46	1.61	1.42
4	D	924	GOL	O3-C3	4.46	1.61	1.42
4	C	912	GOL	C1-C2	4.33	1.68	1.51
4	A	923	GOL	C1-C2	4.29	1.68	1.51
4	A	911	GOL	C3-C2	4.28	1.68	1.51
4	B	914	GOL	C3-C2	4.24	1.68	1.51
4	B	914	GOL	O3-C3	4.21	1.60	1.42
4	C	903	GOL	O3-C3	4.19	1.60	1.42
4	D	901	GOL	O1-C1	4.00	1.59	1.42
4	B	906	GOL	O3-C3	3.92	1.58	1.42
4	A	918	GOL	O3-C3	3.82	1.58	1.42
4	C	919	GOL	O1-C1	3.77	1.58	1.42
4	D	924	GOL	O2-C2	3.73	1.54	1.43
4	A	908	GOL	C1-C2	3.67	1.65	1.51
4	C	912	GOL	O1-C1	3.66	1.57	1.42
4	A	915	GOL	C3-C2	3.63	1.65	1.51
4	B	906	GOL	O2-C2	3.63	1.53	1.43
4	C	919	GOL	C1-C2	3.48	1.65	1.51
4	B	902	GOL	C1-C2	3.31	1.64	1.51
4	D	909	GOL	C3-C2	3.25	1.64	1.51
4	B	902	GOL	C3-C2	3.24	1.64	1.51
4	A	915	GOL	O3-C3	3.24	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	922	GOL	O3-C3	3.05	1.55	1.42
4	A	908	GOL	C3-C2	3.02	1.63	1.51
4	C	917	GOL	O1-C1	2.97	1.54	1.42
4	D	913	GOL	C1-C2	2.97	1.63	1.51
4	A	908	GOL	O1-C1	2.95	1.54	1.42
4	D	909	GOL	O2-C2	2.93	1.51	1.43
4	D	916	GOL	C1-C2	2.80	1.62	1.51
4	D	901	GOL	C1-C2	2.77	1.62	1.51
4	A	904	GOL	O2-C2	2.77	1.51	1.43
4	B	921	GOL	O1-C1	2.77	1.54	1.42
4	B	910	GOL	O3-C3	2.76	1.54	1.42
4	A	918	GOL	C3-C2	2.73	1.62	1.51
4	B	907	GOL	C1-C2	2.69	1.62	1.51
4	A	904	GOL	O3-C3	2.68	1.53	1.42
4	A	904	GOL	C3-C2	2.57	1.61	1.51
4	C	912	GOL	O3-C3	2.54	1.53	1.42
4	B	921	GOL	C1-C2	2.53	1.61	1.51
4	B	907	GOL	O3-C3	2.47	1.52	1.42
3	P	804	PO4	P-O4	-2.45	1.47	1.54
4	B	922	GOL	C3-C2	-2.43	1.42	1.51
4	A	908	GOL	O2-C2	2.42	1.50	1.43
4	A	915	GOL	C1-C2	2.39	1.60	1.51
4	D	916	GOL	O1-C1	2.37	1.52	1.42
4	B	902	GOL	O1-C1	2.34	1.52	1.42
4	B	907	GOL	C3-C2	2.32	1.60	1.51
4	C	912	GOL	C3-C2	2.20	1.60	1.51
4	B	920	GOL	C3-C2	2.11	1.59	1.51
4	D	909	GOL	O3-C3	2.09	1.51	1.42
4	D	924	GOL	C3-C2	2.08	1.59	1.51
4	C	919	GOL	O2-C2	-2.06	1.37	1.43
4	D	901	GOL	C3-C2	2.01	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	910	GOL	O1-C1-C2	4.25	129.51	110.38
4	D	901	GOL	O1-C1-C2	3.59	126.53	110.38
4	A	918	GOL	O2-C2-C3	3.49	123.65	109.18
4	D	913	GOL	O2-C2-C1	3.36	123.11	109.18
4	B	902	GOL	O2-C2-C3	3.06	121.83	109.18
4	D	901	GOL	O2-C2-C3	3.01	121.63	109.18
4	B	905	GOL	O1-C1-C2	2.88	123.34	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	914	GOL	O3-C3-C2	2.68	122.44	110.38
4	B	905	GOL	O2-C2-C1	2.56	119.80	109.18
4	B	910	GOL	O2-C2-C3	-2.48	98.91	109.18
4	C	919	GOL	C3-C2-C1	-2.43	102.89	111.80
4	D	901	GOL	C3-C2-C1	2.40	120.60	111.80
4	D	913	GOL	O2-C2-C3	2.19	118.24	109.18
4	C	919	GOL	O3-C3-C2	2.10	119.82	110.38

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	908	GOL	C1-C2-C3-O3
4	A	923	GOL	O1-C1-C2-C3
4	B	902	GOL	C1-C2-C3-O3
4	B	905	GOL	C1-C2-C3-O3
4	B	910	GOL	O1-C1-C2-O2
4	B	910	GOL	O1-C1-C2-C3
4	B	914	GOL	O1-C1-C2-C3
4	B	920	GOL	O1-C1-C2-C3
4	B	921	GOL	C1-C2-C3-O3
4	C	903	GOL	O1-C1-C2-C3
4	C	903	GOL	C1-C2-C3-O3
4	C	912	GOL	O1-C1-C2-C3
4	C	917	GOL	C1-C2-C3-O3
4	D	901	GOL	C1-C2-C3-O3
4	D	913	GOL	C1-C2-C3-O3
4	D	916	GOL	C1-C2-C3-O3
4	D	924	GOL	O1-C1-C2-O2
4	D	924	GOL	O1-C1-C2-C3
4	D	924	GOL	C1-C2-C3-O3
4	A	908	GOL	O2-C2-C3-O3
4	A	923	GOL	O1-C1-C2-O2
4	B	914	GOL	O1-C1-C2-O2
4	D	913	GOL	O2-C2-C3-O3
4	D	916	GOL	O2-C2-C3-O3
4	D	924	GOL	O2-C2-C3-O3
4	A	904	GOL	O1-C1-C2-C3
4	A	915	GOL	C1-C2-C3-O3
4	A	918	GOL	C1-C2-C3-O3
4	B	902	GOL	O1-C1-C2-C3
4	B	905	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	906	GOL	C1-C2-C3-O3
4	B	922	GOL	O1-C1-C2-C3
4	B	922	GOL	C1-C2-C3-O3
4	C	912	GOL	C1-C2-C3-O3
4	D	901	GOL	O1-C1-C2-C3
4	D	909	GOL	O1-C1-C2-C3
4	D	916	GOL	O1-C1-C2-C3
4	A	904	GOL	O1-C1-C2-O2
4	A	918	GOL	O2-C2-C3-O3
4	B	902	GOL	O1-C1-C2-O2
4	B	905	GOL	O1-C1-C2-O2
4	B	920	GOL	O1-C1-C2-O2
4	B	921	GOL	O2-C2-C3-O3
4	C	903	GOL	O1-C1-C2-O2
4	C	903	GOL	O2-C2-C3-O3
4	C	912	GOL	O1-C1-C2-O2
4	D	901	GOL	O1-C1-C2-O2
4	D	901	GOL	O2-C2-C3-O3
4	D	916	GOL	O1-C1-C2-O2
4	A	918	GOL	O1-C1-C2-O2
4	B	922	GOL	O2-C2-C3-O3
4	C	917	GOL	O1-C1-C2-O2
4	C	917	GOL	O2-C2-C3-O3
4	A	915	GOL	O2-C2-C3-O3
4	D	909	GOL	O1-C1-C2-O2
4	B	921	GOL	O1-C1-C2-O2
4	A	911	GOL	O1-C1-C2-C3
4	B	922	GOL	O1-C1-C2-O2
4	C	919	GOL	O2-C2-C3-O3

There are no ring outliers.

20 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	903	GOL	2	0
4	C	919	GOL	2	1
4	D	901	GOL	6	0
4	A	923	GOL	2	0
4	B	921	GOL	2	0
4	C	917	GOL	4	0
4	D	913	GOL	10	0
4	B	902	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	GOL	1	0
3	A	801	PO4	3	0
4	D	924	GOL	3	0
4	B	914	GOL	3	0
4	A	911	GOL	1	0
4	B	906	GOL	1	0
4	B	910	GOL	8	0
4	B	922	GOL	5	0
4	A	918	GOL	4	0
4	B	920	GOL	5	0
4	B	905	GOL	7	0
4	B	907	GOL	1	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	2/2 (100%)	-0.70	0 100 100	17, 17, 17, 19	0
1	N	2/2 (100%)	-0.68	0 100 100	17, 17, 17, 18	0
1	O	2/2 (100%)	-0.74	0 100 100	18, 18, 18, 20	0
1	P	2/2 (100%)	-0.61	0 100 100	17, 17, 17, 18	0
2	A	124/124 (100%)	-0.28	0 100 100	11, 17, 29, 49	4 (3%)
2	B	124/124 (100%)	-0.28	1 (0%) 82 85	9, 17, 32, 49	9 (7%)
2	C	124/124 (100%)	-0.22	1 (0%) 82 85	10, 18, 30, 47	6 (4%)
2	D	124/124 (100%)	-0.17	1 (0%) 82 85	11, 18, 34, 48	5 (4%)
All	All	504/504 (100%)	-0.24	3 (0%) 85 88	9, 17, 32, 49	24 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	692	TYR	3.5
2	B	221	SER	3.1
2	C	401	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	GOL	A	918	6/6	0.63	0.17	39,51,53,54	0
4	GOL	D	909	6/6	0.78	0.17	49,55,56,59	0
4	GOL	C	903	6/6	0.79	0.13	46,52,53,54	0
4	GOL	A	915	6/6	0.80	0.12	44,51,53,53	0
4	GOL	A	923	6/6	0.82	0.12	40,45,47,53	0
4	GOL	B	902	6/6	0.82	0.11	36,47,52,55	0
4	GOL	D	913	6/6	0.82	0.18	40,45,48,48	0
4	GOL	C	919	6/6	0.83	0.17	37,43,44,46	0
4	GOL	B	920	6/6	0.83	0.13	37,42,44,45	0
4	GOL	B	914	6/6	0.83	0.12	36,43,45,50	0
4	GOL	A	908	6/6	0.84	0.12	38,46,50,57	0
4	GOL	C	917	6/6	0.85	0.10	37,49,51,57	0
4	GOL	A	911	6/6	0.86	0.12	44,52,55,56	0
4	GOL	B	922	6/6	0.87	0.10	49,51,54,57	0
4	GOL	B	921	6/6	0.87	0.12	23,40,42,43	0
4	GOL	D	924	6/6	0.87	0.12	30,42,47,51	0
4	GOL	C	912	6/6	0.88	0.09	51,56,59,64	0
4	GOL	A	904	6/6	0.88	0.12	40,50,52,58	0
4	GOL	D	901	6/6	0.89	0.12	28,37,39,42	0
4	GOL	B	906	6/6	0.90	0.11	28,42,45,51	0
4	GOL	D	916	6/6	0.91	0.10	31,46,48,54	0
4	GOL	B	907	6/6	0.92	0.12	34,42,44,48	0
4	GOL	B	905	6/6	0.92	0.10	27,34,36,38	0
4	GOL	B	910	6/6	0.93	0.12	15,37,44,45	0
3	PO4	P	804	5/5	0.98	0.04	14,14,22,22	0
3	PO4	A	801	5/5	0.98	0.05	13,14,19,24	0
3	PO4	C	803	5/5	0.98	0.05	14,15,19,24	0
3	PO4	B	802	5/5	0.99	0.04	12,14,21,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.