



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:12 PM UTC

PDB ID : 2DG1 / pdb_00002dg1
Title : Crystal structure of Drp35, a 35kDa drug responsive protein from Staphylococcus aureus, complexed with Ca²⁺
Authors : Tanaka, Y.; Ohki, Y.; Morikawa, K.; Yao, M.; Watanabe, N.; Ohta, T.; Tanaka, I.
Deposited on : 2006-03-07
Resolution : 1.72 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:

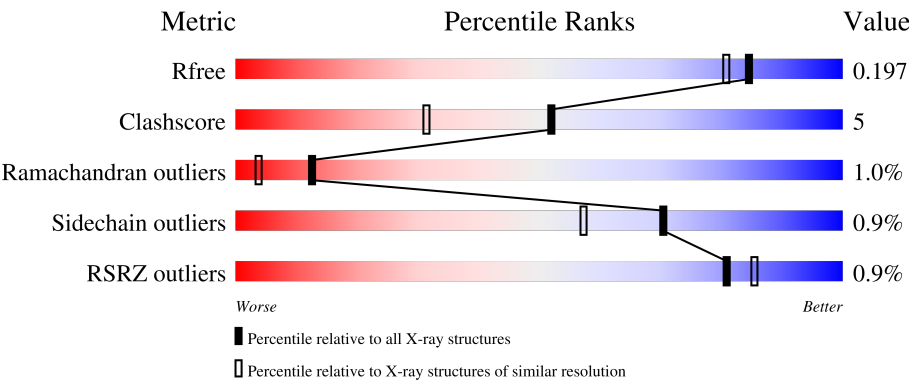
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	333	% 83% 12% . .
1	B	333	% 83% 13% .
1	C	333	% 84% 11% . .
1	D	333	% 80% 15% . .
1	E	333	% 80% 17% .

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Mol	Chain	Length	Quality of chain
1	F	333	% 80% 15% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17301 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 DrP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2511	1604	415	482	10			
1	B	322	Total	C	N	O	S	0	0	0
			2520	1609	416	485	10			
1	C	320	Total	C	N	O	S	0	0	0
			2503	1598	414	481	10			
1	D	322	Total	C	N	O	S	0	0	0
			2520	1609	417	484	10			
1	E	321	Total	C	N	O	S	0	0	0
			2511	1604	415	482	10			
1	F	321	Total	C	N	O	S	0	0	0
			2511	1604	415	482	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q9S0S3
A	2	ALA	-	cloning artifact	UNP Q9S0S3
A	326	LEU	-	expression tag	UNP Q9S0S3
A	327	GLU	-	expression tag	UNP Q9S0S3
A	328	HIS	-	expression tag	UNP Q9S0S3
A	329	HIS	-	expression tag	UNP Q9S0S3
A	330	HIS	-	expression tag	UNP Q9S0S3
A	331	HIS	-	expression tag	UNP Q9S0S3
A	332	HIS	-	expression tag	UNP Q9S0S3
A	333	HIS	-	expression tag	UNP Q9S0S3
B	1	MET	-	cloning artifact	UNP Q9S0S3
B	2	ALA	-	cloning artifact	UNP Q9S0S3
B	326	LEU	-	expression tag	UNP Q9S0S3
B	327	GLU	-	expression tag	UNP Q9S0S3
B	328	HIS	-	expression tag	UNP Q9S0S3
B	329	HIS	-	expression tag	UNP Q9S0S3
B	330	HIS	-	expression tag	UNP Q9S0S3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	331	HIS	-	expression tag	UNP Q9S0S3
B	332	HIS	-	expression tag	UNP Q9S0S3
B	333	HIS	-	expression tag	UNP Q9S0S3
C	1	MET	-	cloning artifact	UNP Q9S0S3
C	2	ALA	-	cloning artifact	UNP Q9S0S3
C	326	LEU	-	expression tag	UNP Q9S0S3
C	327	GLU	-	expression tag	UNP Q9S0S3
C	328	HIS	-	expression tag	UNP Q9S0S3
C	329	HIS	-	expression tag	UNP Q9S0S3
C	330	HIS	-	expression tag	UNP Q9S0S3
C	331	HIS	-	expression tag	UNP Q9S0S3
C	332	HIS	-	expression tag	UNP Q9S0S3
C	333	HIS	-	expression tag	UNP Q9S0S3
D	1	MET	-	cloning artifact	UNP Q9S0S3
D	2	ALA	-	cloning artifact	UNP Q9S0S3
D	326	LEU	-	expression tag	UNP Q9S0S3
D	327	GLU	-	expression tag	UNP Q9S0S3
D	328	HIS	-	expression tag	UNP Q9S0S3
D	329	HIS	-	expression tag	UNP Q9S0S3
D	330	HIS	-	expression tag	UNP Q9S0S3
D	331	HIS	-	expression tag	UNP Q9S0S3
D	332	HIS	-	expression tag	UNP Q9S0S3
D	333	HIS	-	expression tag	UNP Q9S0S3
E	1	MET	-	cloning artifact	UNP Q9S0S3
E	2	ALA	-	cloning artifact	UNP Q9S0S3
E	326	LEU	-	expression tag	UNP Q9S0S3
E	327	GLU	-	expression tag	UNP Q9S0S3
E	328	HIS	-	expression tag	UNP Q9S0S3
E	329	HIS	-	expression tag	UNP Q9S0S3
E	330	HIS	-	expression tag	UNP Q9S0S3
E	331	HIS	-	expression tag	UNP Q9S0S3
E	332	HIS	-	expression tag	UNP Q9S0S3
E	333	HIS	-	expression tag	UNP Q9S0S3
F	1	MET	-	cloning artifact	UNP Q9S0S3
F	2	ALA	-	cloning artifact	UNP Q9S0S3
F	326	LEU	-	expression tag	UNP Q9S0S3
F	327	GLU	-	expression tag	UNP Q9S0S3
F	328	HIS	-	expression tag	UNP Q9S0S3
F	329	HIS	-	expression tag	UNP Q9S0S3
F	330	HIS	-	expression tag	UNP Q9S0S3
F	331	HIS	-	expression tag	UNP Q9S0S3
F	332	HIS	-	expression tag	UNP Q9S0S3

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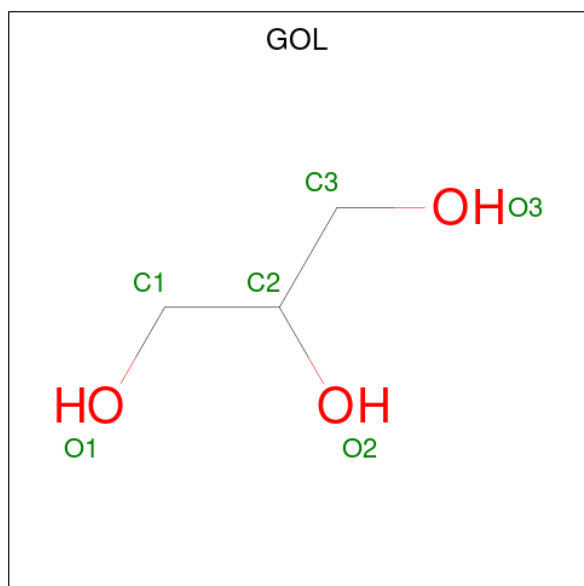
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Chain	Residue	Modelled	Actual	Comment	Reference
F	333	HIS	-	expression tag	UNP Q9S0S3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total 2 Ca 2	0	0
2	B	2	Total 2 Ca 2	0	0
2	C	2	Total 2 Ca 2	0	0
2	D	2	Total 2 Ca 2	0	0
2	E	2	Total 2 Ca 2	0	0
2	F	2	Total 2 Ca 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

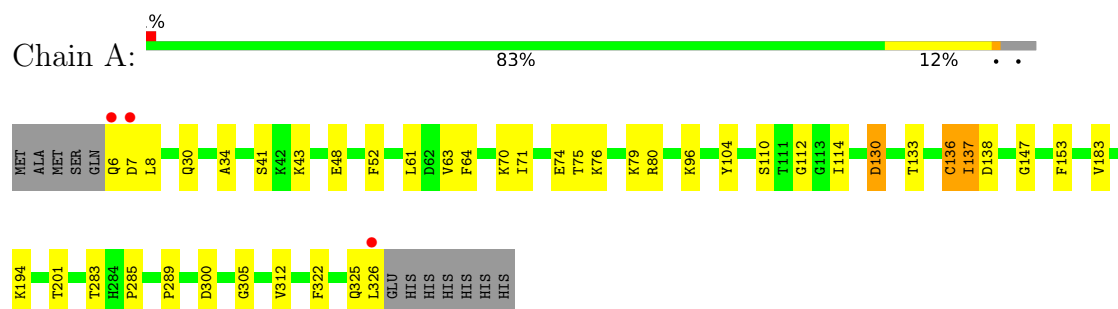
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	361	Total	O	0	0
			361	361		
4	B	365	Total	O	0	0
			365	365		
4	C	355	Total	O	0	0
			355	355		
4	D	350	Total	O	0	0
			350	350		
4	E	377	Total	O	0	0
			377	377		
4	F	333	Total	O	0	0
			333	333		

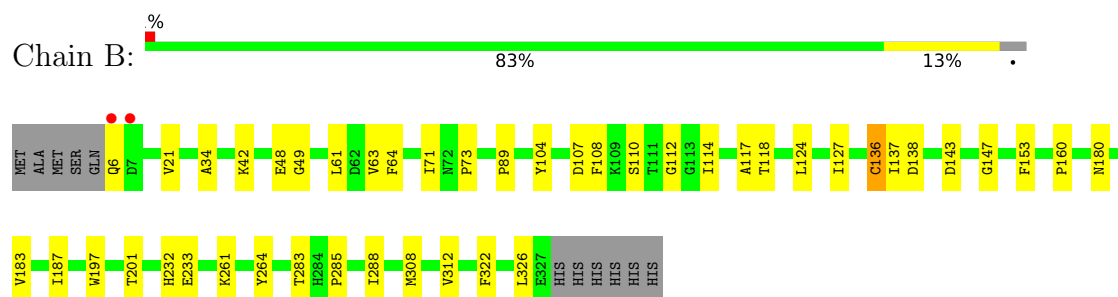
3 Residue-property plots [i](#)

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.

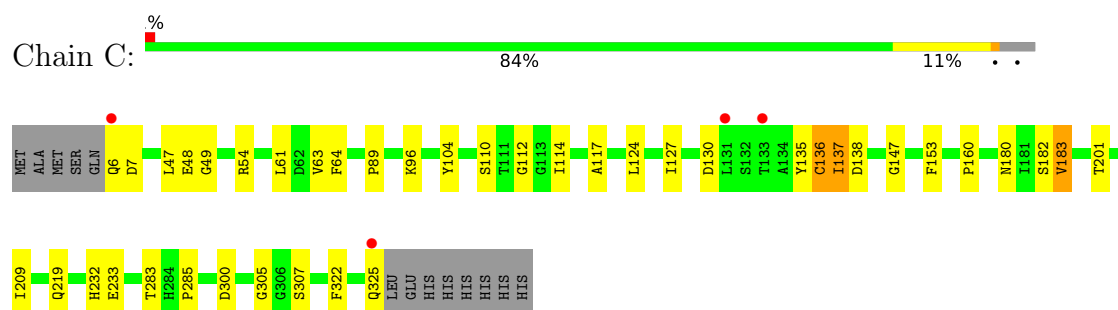
• Molecule 1: DrP35



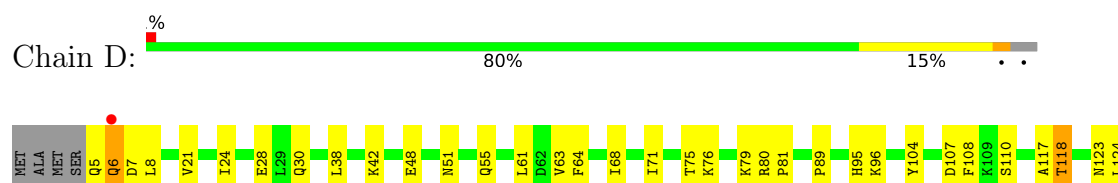
• Molecule 1: DrP35



• Molecule 1: DrP35

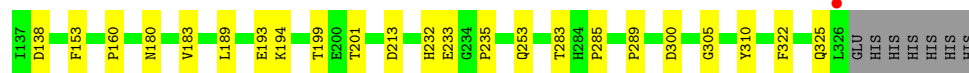
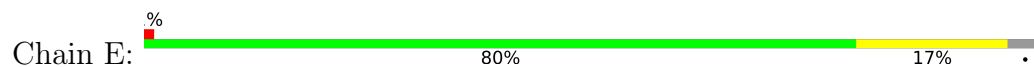


• Molecule 1: DrP35

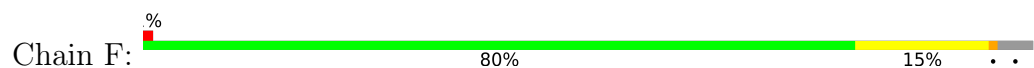




● Molecule 1: DrP35



● Molecule 1: DrP35



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.53Å 181.98Å 81.80Å 90.00° 115.41° 90.00°	Depositor
Resolution (Å)	19.99 – 1.72 19.99 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.99-1.72) 99.1 (19.99-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.169 , 0.197 0.168 , 0.197	Depositor DCC
R_{free} test set	20980 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17301	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: GOL, CA

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	0.31	0/2571	0.94	12/3487 (0.3%)
1	B	0.32	0/2580	0.95	14/3499 (0.4%)
1	C	0.31	0/2563	0.92	11/3476 (0.3%)
1	D	0.31	0/2580	0.94	13/3499 (0.4%)
1	E	0.32	0/2571	0.94	13/3487 (0.4%)
1	F	0.31	0/2571	0.95	11/3487 (0.3%)
All	All	0.31	0/15436	0.94	74/20935 (0.4%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	VAL	N-CA-C	9.26	119.24	110.53
1	F	63	VAL	N-CA-C	8.92	118.98	110.42
1	A	63	VAL	N-CA-C	8.72	118.80	110.42
1	D	63	VAL	N-CA-C	8.53	118.61	110.42
1	D	201	THR	N-CA-C	8.46	120.12	111.07
1	E	63	VAL	N-CA-C	8.44	118.52	110.42
1	E	201	THR	N-CA-C	8.30	120.02	110.97
1	F	288	ILE	N-CA-C	-8.15	100.96	108.95
1	A	130	ASP	N-CA-C	8.15	121.71	111.69
1	C	201	THR	N-CA-C	8.10	119.80	110.97
1	C	63	VAL	N-CA-C	8.02	118.07	110.30
1	A	201	THR	N-CA-C	7.97	119.66	110.97
1	B	201	THR	N-CA-C	7.87	119.49	111.07
1	B	288	ILE	N-CA-C	-7.84	101.26	108.95
1	F	201	THR	N-CA-C	7.80	119.42	111.07
1	B	127	ILE	N-CA-C	-7.43	104.54	111.45
1	F	127	ILE	N-CA-C	-6.97	104.97	111.45
1	E	130	ASP	N-CA-C	6.88	119.79	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	322	PHE	N-CA-C	6.30	118.95	111.33
1	D	322	PHE	N-CA-C	6.29	118.94	111.33
1	A	322	PHE	N-CA-C	6.14	118.75	111.33
1	C	64	PHE	N-CA-C	6.12	118.92	111.82
1	C	135	TYR	N-CA-C	6.12	119.13	110.50
1	F	283	THR	N-CA-C	6.12	121.40	113.88
1	E	64	PHE	N-CA-C	6.10	118.89	111.82
1	A	64	PHE	N-CA-C	5.96	118.73	111.82
1	D	135	TYR	N-CA-C	5.95	118.89	110.50
1	A	283	THR	N-CA-C	5.93	121.17	113.88
1	E	127	ILE	N-CA-C	-5.92	105.08	110.82
1	C	283	THR	N-CA-C	5.92	121.16	113.88
1	D	136	CYS	N-CA-C	-5.82	95.53	107.70
1	D	64	PHE	N-CA-C	5.80	118.55	111.82
1	F	118	THR	N-CA-C	-5.74	103.12	110.53
1	E	283	THR	N-CA-C	5.70	121.26	113.97
1	B	322	PHE	N-CA-C	5.70	118.22	111.33
1	D	80	ARG	CA-C-N	5.69	126.95	119.84
1	D	80	ARG	C-N-CA	5.69	126.95	119.84
1	E	131	LEU	N-CA-C	5.69	118.42	111.82
1	B	283	THR	N-CA-C	5.68	121.24	113.97
1	B	136	CYS	N-CA-C	-5.64	95.90	107.70
1	F	135	TYR	N-CA-C	5.62	118.42	110.50
1	F	136	CYS	N-CA-C	-5.61	95.97	107.70
1	D	283	THR	N-CA-C	5.61	121.15	113.97
1	C	147	GLY	N-CA-C	-5.59	103.84	112.85
1	B	42	LYS	N-CA-C	-5.58	106.42	113.18
1	C	127	ILE	N-CA-C	-5.54	104.97	111.00
1	E	136	CYS	N-CA-C	-5.48	96.25	107.70
1	F	42	LYS	N-CA-C	-5.46	106.12	112.89
1	A	30	GLN	N-CA-C	-5.41	101.90	109.96
1	A	137	ILE	N-CA-C	5.41	116.51	108.23
1	F	147	GLY	N-CA-C	-5.40	103.91	112.66
1	C	136	CYS	N-CA-C	-5.40	96.41	107.70
1	D	118	THR	N-CA-C	-5.39	103.58	110.53
1	A	136	CYS	N-CA-C	-5.35	96.51	107.70
1	A	80	ARG	CA-C-N	5.33	124.78	119.24
1	A	80	ARG	C-N-CA	5.33	124.78	119.24
1	B	308	MET	N-CA-C	5.32	117.90	109.50
1	D	30	GLN	N-CA-C	-5.29	102.07	109.96
1	E	111	THR	N-CA-C	5.29	118.58	112.97
1	B	147	GLY	N-CA-C	-5.25	104.41	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	TYR	N-CA-C	5.22	117.44	110.35
1	C	209	ILE	N-CA-C	5.20	115.06	107.37
1	A	147	GLY	N-CA-C	-5.17	104.69	112.60
1	B	118	THR	N-CA-C	-5.14	103.90	110.53
1	D	137	ILE	N-CA-C	5.14	116.09	108.23
1	F	64	PHE	N-CA-C	5.14	118.70	112.23
1	C	137	ILE	N-CA-C	5.13	116.08	108.23
1	E	42	LYS	N-CA-C	-5.11	106.55	112.89
1	B	64	PHE	N-CA-C	5.08	118.74	112.54
1	B	49	GLY	N-CA-C	5.08	122.90	113.76
1	D	42	LYS	N-CA-C	-5.06	106.95	113.23
1	C	49	GLY	N-CA-C	5.05	122.85	113.76
1	E	118	THR	N-CA-C	-5.04	104.03	110.53
1	B	143	ASP	N-CA-C	-5.02	103.31	110.59

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	2511	0	2436	17	0
1	B	2520	0	2441	17	0
1	C	2503	0	2424	24	0
1	D	2520	0	2443	36	0
1	E	2511	0	2435	26	0
1	F	2511	0	2435	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	16	0	0
3	E	12	0	16	0	0
3	F	12	0	16	0	0
4	A	361	0	0	1	0
4	B	365	0	0	2	0
4	C	355	0	0	3	0
4	D	350	0	0	3	0
4	E	377	0	0	0	0
4	F	333	0	0	3	0
All	All	17301	0	14710	153	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 5.

All (153) 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:F:43:LYS:HD3	1:F:44:GLY:N	1.94	0.82
1:D:96:LYS:HE2	1:D:325:GLN:HB3	1.64	0.77
1:D:232:HIS:CE1	1:D:233:GLU:HG2	2.25	0.71
1:E:232:HIS:CE1	1:E:233:GLU:HG2	2.24	0.71
1:C:232:HIS:CE1	1:C:233:GLU:HG2	2.26	0.71
1:A:41:SER:OG	1:A:43:LYS:HG2	1.91	0.70
1:C:96:LYS:HE2	1:C:325:GLN:HA	1.73	0.69
1:E:194:LYS:NZ	1:E:213:ASP:HA	2.07	0.68
1:D:24:ILE:HG13	1:D:28:GLU:HG3	1.75	0.68
1:D:6:GLN:NE2	1:D:6:GLN:H	1.92	0.67
1:E:194:LYS:HZ1	1:E:213:ASP:HA	1.59	0.67
1:D:24:ILE:CG1	1:D:28:GLU:HG3	2.26	0.66
1:F:96:LYS:HE3	1:F:326:LEU:HB2	1.77	0.65
1:D:5:GLN:HB3	1:D:8:LEU:HG	1.79	0.64
1:C:54:ARG:HH12	1:C:325:GLN:HB2	1.63	0.64
1:C:6:GLN:HG2	1:C:7:ASP:H	1.63	0.63
1:C:54:ARG:HD2	4:C:5238:HOH:O	2.01	0.60
1:F:6:GLN:HG3	1:F:8:LEU:H	1.66	0.60
1:E:232:HIS:NE2	1:E:233:GLU:HG2	2.18	0.59
1:D:232:HIS:NE2	1:D:233:GLU:HG2	2.17	0.58
1:C:232:HIS:NE2	1:C:233:GLU:HG2	2.19	0.57
1:E:6:GLN:HG2	1:E:8:LEU:HG	1.87	0.56
1:C:54:ARG:HG3	4:C:5098:HOH:O	2.06	0.56
1:A:6:GLN:C	1:A:8:LEU:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLN:NE2	4:C:5361:HOH:O	2.40	0.55
1:D:6:GLN:H	1:D:6:GLN:CD	2.15	0.54
1:F:43:LYS:HE3	4:F:5289:HOH:O	2.08	0.54
1:D:172:ARG:HG2	1:D:172:ARG:HH21	1.72	0.54
1:D:5:GLN:HG3	1:D:7:ASP:H	1.73	0.53
1:D:322:PHE:HA	1:D:325:GLN:OE1	2.09	0.53
1:B:326:LEU:N	1:B:326:LEU:HD22	2.25	0.51
1:A:79:LYS:HE2	4:A:5146:HOH:O	2.09	0.51
1:D:232:HIS:CD2	1:D:233:GLU:HG2	2.45	0.51
1:D:96:LYS:HE2	1:D:325:GLN:CB	2.37	0.51
1:F:70:LYS:C	1:F:71:ILE:HD12	2.36	0.51
1:F:42:LYS:HE2	1:F:42:LYS:H	1.76	0.51
1:D:117:ALA:HB2	1:D:124:LEU:HD23	1.92	0.51
1:C:117:ALA:HB2	1:C:124:LEU:HD23	1.92	0.50
1:F:112:GLY:HA3	1:F:136:CYS:HA	1.93	0.50
1:A:112:GLY:HA3	1:A:136:CYS:HA	1.93	0.50
1:B:232:HIS:CE1	1:B:233:GLU:HG2	2.45	0.50
1:A:70:LYS:C	1:A:71:ILE:HD12	2.36	0.50
1:F:194:LYS:NZ	1:F:213:ASP:HA	2.26	0.50
1:A:138:ASP:HB2	1:A:153:PHE:HB2	1.92	0.50
1:A:75:THR:O	1:A:76:LYS:HB2	2.11	0.49
1:F:79:LYS:HE2	4:F:5100:HOH:O	2.12	0.49
1:B:117:ALA:HB2	1:B:124:LEU:HD23	1.94	0.49
1:D:300:ASP:HB3	1:D:305:GLY:HA3	1.95	0.49
1:D:326:LEU:HD22	1:D:326:LEU:N	2.27	0.49
1:A:96:LYS:HD2	1:A:325:GLN:OE1	2.11	0.49
1:A:326:LEU:N	1:A:326:LEU:HD12	2.28	0.49
1:D:24:ILE:HG13	1:D:28:GLU:CG	2.41	0.48
1:F:6:GLN:CG	1:F:313:ASN:HD21	2.25	0.48
1:D:138:ASP:HB2	1:D:153:PHE:HB2	1.95	0.48
1:C:104:TYR:OH	1:C:130:ASP:HB3	2.13	0.48
1:D:68:ILE:O	1:D:81:PRO:HD2	2.14	0.48
1:B:112:GLY:HA3	1:B:136:CYS:HA	1.96	0.47
1:E:38:LEU:HD23	1:E:71:ILE:HD13	1.97	0.47
1:E:77:GLU:OE1	1:E:79:LYS:HE3	2.15	0.47
1:A:104:TYR:OH	1:A:130:ASP:HB3	2.14	0.47
1:C:112:GLY:HA3	1:C:136:CYS:HA	1.96	0.47
1:F:42:LYS:HE2	4:F:5318:HOH:O	2.13	0.47
1:F:123:ASN:O	1:F:125:GLN:HG3	2.14	0.47
1:F:325:GLN:O	1:F:326:LEU:HB3	2.14	0.47
1:F:138:ASP:HB2	1:F:153:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLN:NE2	1:D:6:GLN:N	2.62	0.46
1:F:194:LYS:HZ1	1:F:213:ASP:HA	1.81	0.46
1:D:96:LYS:HE3	1:D:322:PHE:CE1	2.51	0.46
1:E:61:LEU:HD12	1:E:61:LEU:C	2.41	0.46
1:A:194:LYS:HA	1:A:194:LYS:HE3	1.98	0.46
1:F:325:GLN:HG2	1:F:326:LEU:N	2.30	0.46
1:E:75:THR:O	1:E:76:LYS:HB2	2.15	0.46
1:A:300:ASP:HB3	1:A:305:GLY:HA3	1.98	0.45
1:B:160:PRO:HB2	1:B:180:ASN:C	2.41	0.45
1:C:232:HIS:CD2	1:C:233:GLU:HG2	2.52	0.45
1:E:232:HIS:CD2	1:E:233:GLU:HG2	2.52	0.45
1:F:43:LYS:HD3	1:F:44:GLY:H	1.75	0.45
1:B:138:ASP:HB2	1:B:153:PHE:HB2	1.98	0.45
1:C:54:ARG:HH12	1:C:325:GLN:CB	2.27	0.45
1:E:189:LEU:HD13	1:E:193:GLU:HG2	1.97	0.45
1:E:6:GLN:CD	1:E:6:GLN:N	2.74	0.45
1:E:300:ASP:HB3	1:E:305:GLY:HA3	1.98	0.45
1:C:61:LEU:C	1:C:61:LEU:HD12	2.42	0.45
1:C:325:GLN:HG2	1:C:325:GLN:O	2.17	0.45
1:F:300:ASP:HB3	1:F:305:GLY:HA3	1.99	0.45
1:D:81:PRO:HG3	4:D:5237:HOH:O	2.17	0.45
1:F:160:PRO:HB2	1:F:180:ASN:C	2.42	0.45
1:E:116:ALA:HB3	1:E:125:GLN:HG3	1.98	0.45
1:E:138:ASP:HB2	1:E:153:PHE:HB2	1.98	0.45
1:F:43:LYS:HD3	1:F:43:LYS:C	2.42	0.44
1:A:34:ALA:HA	1:A:312:VAL:CG1	2.48	0.44
1:F:232:HIS:CE1	1:F:233:GLU:HG2	2.52	0.44
1:E:253:GLN:HG2	1:F:264:TYR:OH	2.16	0.44
1:A:71:ILE:HD12	1:A:71:ILE:N	2.33	0.44
1:D:79:LYS:HE2	4:D:5080:HOH:O	2.17	0.44
1:B:21:VAL:HG12	1:B:264:TYR:CE2	2.52	0.44
1:D:107:ASP:O	1:D:108:PHE:HB2	2.17	0.44
1:B:6:GLN:HA	4:B:5162:HOH:O	2.17	0.44
1:B:261:LYS:HE2	4:B:5302:HOH:O	2.18	0.44
1:E:160:PRO:HB2	1:E:180:ASN:C	2.43	0.44
1:F:34:ALA:HA	1:F:312:VAL:CG1	2.47	0.44
1:F:96:LYS:CE	1:F:326:LEU:HB2	2.47	0.44
1:B:107:ASP:O	1:B:108:PHE:HB2	2.18	0.44
1:B:232:HIS:NE2	1:B:233:GLU:HG2	2.33	0.44
1:C:300:ASP:HB3	1:C:305:GLY:HA3	2.00	0.44
1:F:52:PHE:CG	1:F:289:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HB2	1:C:180:ASN:C	2.44	0.43
1:E:133:THR:HB	1:E:135:TYR:CD1	2.54	0.43
1:F:232:HIS:NE2	1:F:233:GLU:HG2	2.33	0.43
1:B:187:ILE:HA	1:B:197:TRP:O	2.19	0.43
1:D:61:LEU:C	1:D:61:LEU:HD12	2.43	0.43
1:F:232:HIS:CD2	1:F:233:GLU:HG2	2.53	0.43
1:A:114:ILE:HG13	1:A:137:ILE:HD12	2.01	0.43
1:B:34:ALA:HA	1:B:312:VAL:CG1	2.49	0.43
1:B:61:LEU:C	1:B:61:LEU:HD12	2.44	0.43
1:B:71:ILE:O	1:B:73:PRO:HD3	2.18	0.43
1:D:89:PRO:HA	1:D:104:TYR:HA	2.00	0.43
1:C:89:PRO:HA	1:C:104:TYR:HA	2.00	0.43
1:D:75:THR:O	1:D:76:LYS:HB2	2.19	0.43
1:D:118:THR:CG2	1:D:123:ASN:HD22	2.32	0.43
1:D:104:TYR:OH	1:D:130:ASP:HB3	2.19	0.43
1:F:42:LYS:HE2	1:F:42:LYS:N	2.34	0.43
1:D:160:PRO:HB2	1:D:180:ASN:C	2.43	0.42
1:E:96:LYS:CD	1:E:325:GLN:HB3	2.49	0.42
1:C:47:LEU:HD11	1:C:307:SER:HB3	2.01	0.42
1:C:114:ILE:HG13	1:C:137:ILE:HD12	2.00	0.42
1:E:34:ALA:HB1	1:E:310:TYR:HB3	2.01	0.42
1:A:61:LEU:HD12	1:A:61:LEU:C	2.44	0.42
1:F:62:ASP:OD1	1:F:65:GLU:HB2	2.20	0.42
1:E:107:ASP:O	1:E:108:PHE:HB2	2.20	0.42
1:C:96:LYS:HE3	1:C:322:PHE:CE1	2.55	0.42
1:E:89:PRO:HA	1:E:104:TYR:HA	2.02	0.41
1:C:138:ASP:HB2	1:C:153:PHE:HB2	2.01	0.41
1:F:107:ASP:O	1:F:108:PHE:HB2	2.20	0.41
1:B:89:PRO:HA	1:B:104:TYR:HA	2.01	0.41
1:F:114:ILE:HG13	1:F:137:ILE:HD12	2.01	0.41
1:D:38:LEU:HD23	1:D:71:ILE:HD13	2.02	0.41
1:E:199:THR:HB	1:E:235:PRO:HB2	2.03	0.41
1:F:6:GLN:HG2	1:F:313:ASN:HD21	1.85	0.41
1:A:52:PHE:CG	1:A:289:PRO:HD3	2.55	0.41
1:E:232:HIS:HA	1:E:233:GLU:HA	1.82	0.41
1:D:21:VAL:HG12	1:D:264:TYR:CE2	2.56	0.41
1:D:182:SER:O	1:D:183:VAL:HB	2.21	0.41
1:F:61:LEU:C	1:F:61:LEU:HD12	2.46	0.41
1:E:52:PHE:CG	1:E:289:PRO:HD3	2.55	0.41
1:C:182:SER:O	1:C:183:VAL:HB	2.21	0.40
1:C:232:HIS:HA	1:C:233:GLU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:HIS:ND1	1:D:96:LYS:N	2.70	0.40
1:D:172:ARG:HG2	1:D:172:ARG:NH2	2.34	0.40
1:F:118:THR:CG2	1:F:123:ASN:HD22	2.34	0.40
1:B:114:ILE:HG13	1:B:137:ILE:HD12	2.04	0.40
1:D:5:GLN:HG2	4:D:5213:HOH:O	2.21	0.40
1:E:129:GLU:OE1	1:E:132:SER:OG	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/333 (96%)	306 (96%)	9 (3%)	4 (1%)	9	2
1	B	320/333 (96%)	309 (97%)	8 (2%)	3 (1%)	14	4
1	C	318/333 (96%)	306 (96%)	9 (3%)	3 (1%)	14	4
1	D	320/333 (96%)	309 (97%)	8 (2%)	3 (1%)	14	4
1	E	319/333 (96%)	307 (96%)	9 (3%)	3 (1%)	14	4
1	F	319/333 (96%)	309 (97%)	7 (2%)	3 (1%)	14	4
All	All	1915/1998 (96%)	1846 (96%)	50 (3%)	19 (1%)	12	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	SER
1	A	285	PRO
1	B	110	SER
1	B	285	PRO
1	C	110	SER
1	C	285	PRO

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Mol	Chain	Res	Type
1	D	110	SER
1	D	285	PRO
1	E	110	SER
1	E	285	PRO
1	F	110	SER
1	F	285	PRO
1	A	7	ASP
1	A	183	VAL
1	B	183	VAL
1	C	183	VAL
1	D	183	VAL
1	E	183	VAL
1	F	183	VAL

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	274/285 (96%)	271 (99%)	3 (1%)	65	50
1	B	275/285 (96%)	274 (100%)	1 (0%)	84	76
1	C	273/285 (96%)	272 (100%)	1 (0%)	84	76
1	D	275/285 (96%)	270 (98%)	5 (2%)	51	29
1	E	274/285 (96%)	273 (100%)	1 (0%)	84	76
1	F	274/285 (96%)	270 (98%)	4 (2%)	57	36
All	All	1645/1710 (96%)	1630 (99%)	15 (1%)	70	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	74	GLU
1	A	133	THR
1	B	48	GLU
1	C	48	GLU

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Mol	Chain	Res	Type
1	D	6	GLN
1	D	48	GLU
1	D	51	ASN
1	D	55	GLN
1	D	325	GLN
1	E	48	GLU
1	F	28	GLU
1	F	43	LYS
1	F	48	GLU
1	F	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	286	GLN
1	B	179	GLN
1	B	180	ASN
1	B	286	GLN
1	B	293	GLN
1	C	123	ASN
1	C	179	GLN
1	C	219	GLN
1	C	286	GLN
1	D	6	GLN
1	D	123	ASN
1	D	286	GLN
1	E	55	GLN
1	E	179	GLN
1	E	180	ASN
1	E	232	HIS
1	F	55	GLN
1	F	123	ASN
1	F	159	ASN
1	F	179	GLN
1	F	286	GLN
1	F	313	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	5009	-	5,5,5	0.38	0	5,5,5	0.25	0
3	GOL	F	5012	-	5,5,5	0.39	0	5,5,5	0.29	0
3	GOL	E	5005	-	5,5,5	0.44	0	5,5,5	0.25	0
3	GOL	C	5003	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	D	5004	-	5,5,5	0.38	0	5,5,5	0.27	0
3	GOL	B	5002	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	A	5001	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	B	5008	-	5,5,5	0.42	0	5,5,5	0.27	0
3	GOL	F	5006	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	D	5010	-	5,5,5	0.41	0	5,5,5	0.29	0
3	GOL	E	5011	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	A	5007	-	5,5,5	0.36	0	5,5,5	0.28	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	5009	-	-	0/4/4/4	-
3	GOL	F	5012	-	-	1/4/4/4	-
3	GOL	E	5005	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	5003	-	-	0/4/4/4	-
3	GOL	D	5004	-	-	0/4/4/4	-
3	GOL	B	5002	-	-	0/4/4/4	-
3	GOL	A	5001	-	-	0/4/4/4	-
3	GOL	B	5008	-	-	1/4/4/4	-
3	GOL	F	5006	-	-	0/4/4/4	-
3	GOL	D	5010	-	-	2/4/4/4	-
3	GOL	E	5011	-	-	0/4/4/4	-
3	GOL	A	5007	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5008	GOL	C1-C2-C3-O3
3	D	5010	GOL	C1-C2-C3-O3
3	D	5010	GOL	O2-C2-C3-O3
3	F	5012	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	321/333 (96%)	-0.29	3 (0%) 81 85	10, 16, 28, 51	0
1	B	322/333 (96%)	-0.42	2 (0%) 85 89	10, 14, 24, 51	0
1	C	320/333 (96%)	-0.25	4 (1%) 75 80	9, 16, 32, 46	0
1	D	322/333 (96%)	-0.38	3 (0%) 81 85	9, 15, 26, 49	0
1	E	321/333 (96%)	-0.37	2 (0%) 85 89	10, 15, 26, 48	0
1	F	321/333 (96%)	-0.27	3 (0%) 81 85	10, 16, 27, 47	0
All	All	1927/1998 (96%)	-0.33	17 (0%) 81 85	9, 15, 28, 51	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	326	LEU	5.4
1	B	6	GLN	4.1
1	E	326	LEU	3.3
1	C	325	GLN	3.2
1	D	6	GLN	3.2
1	E	6	GLN	3.2
1	A	326	LEU	3.1
1	B	7	ASP	3.1
1	A	6	GLN	3.0
1	D	326	LEU	3.0
1	D	325	GLN	2.9
1	C	6	GLN	2.7
1	A	7	ASP	2.7
1	C	133	THR	2.3
1	F	6	GLN	2.2
1	C	131	LEU	2.2
1	F	7	ASP	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	5008	6/6	0.77	0.14	33,36,38,41	0
3	GOL	D	5010	6/6	0.81	0.14	33,38,40,43	0
3	GOL	F	5012	6/6	0.86	0.10	27,28,32,36	0
3	GOL	E	5011	6/6	0.89	0.10	23,27,30,34	0
3	GOL	A	5007	6/6	0.89	0.10	26,28,32,35	0
3	GOL	C	5003	6/6	0.90	0.13	20,23,25,29	0
3	GOL	A	5001	6/6	0.90	0.12	15,21,22,25	0
3	GOL	C	5009	6/6	0.92	0.08	25,28,30,32	0
3	GOL	F	5006	6/6	0.92	0.10	19,23,23,27	0
3	GOL	E	5005	6/6	0.92	0.09	14,19,19,24	0
3	GOL	D	5004	6/6	0.93	0.09	16,17,19,20	0
3	GOL	B	5002	6/6	0.93	0.10	14,19,21,24	0
2	CA	A	3007	1/1	0.98	0.09	17,17,17,17	1
2	CA	E	3011	1/1	0.99	0.07	19,19,19,19	1
2	CA	F	3012	1/1	0.99	0.07	18,18,18,18	1
2	CA	A	3001	1/1	0.99	0.02	11,11,11,11	0
2	CA	B	3002	1/1	0.99	0.02	10,10,10,10	0
2	CA	C	3003	1/1	0.99	0.02	12,12,12,12	0
2	CA	C	3009	1/1	0.99	0.10	19,19,19,19	1
2	CA	D	3010	1/1	0.99	0.09	17,17,17,17	1
2	CA	E	3005	1/1	1.00	0.02	11,11,11,11	0
2	CA	D	3004	1/1	1.00	0.04	11,11,11,11	0
2	CA	F	3006	1/1	1.00	0.02	12,12,12,12	0
2	CA	B	3008	1/1	1.00	0.07	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.