



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:56 pm BST

PDB ID : 5OUR
Title : X-ray structure uridine phosphorylase from *Vibrio cholerae* in complex with 2,2'-anhydrouridine at 1.34 Å.
Authors : Prokofev, I.I.; Balaev, V.V.; Gabdoulkhakov, A.G.; Betzel, C.; Lashkov, A.A.
Deposited on : 2017-08-24
Resolution : 1.35 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

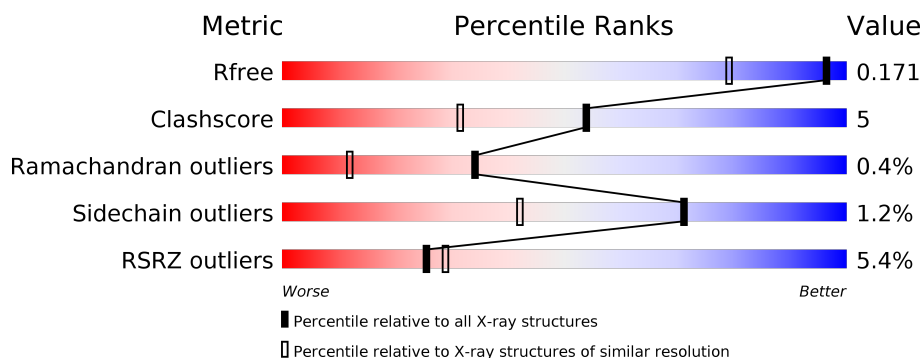
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	253	<div> <div>3%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	253	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	C	253	<div> <div>6%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	D	253	<div> <div>7%</div> <div>87%</div> <div>13%</div> <div></div> </div>
1	E	253	<div> <div>6%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	F	253	<div> <div>6%</div> <div>83%</div> <div>16%</div> <div>.</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
3	BJE	A	302	X	-	-	-
3	BJE	B	302	X	-	-	-
3	BJE	C	302	X	-	-	-
3	BJE	D	301	X	-	-	-
3	BJE	E	302	X	-	-	-
3	BJE	F	301	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14875 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.

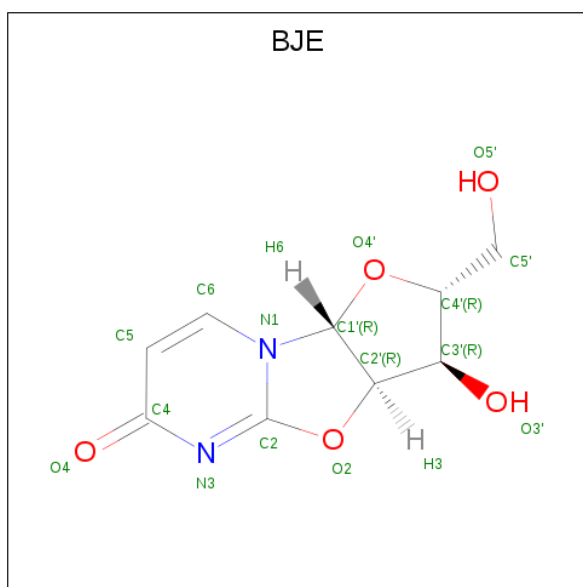
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	22	0
			2062	1287	365	392	18			
1	B	252	Total	C	N	O	S	0	20	0
			2066	1285	370	394	17			
1	C	251	Total	C	N	O	S	0	34	0
			2161	1348	387	408	18			
1	D	252	Total	C	N	O	S	0	27	0
			2101	1310	371	403	17			
1	E	251	Total	C	N	O	S	0	32	0
			2123	1330	372	403	18			
1	F	251	Total	C	N	O	S	0	37	0
			2182	1363	388	413	18			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		

- Molecule 3 is 2,2'-Anhydro-(1-beta-D-ribofuranosyl)uracil (three-letter code: BJE) (formula: C₉H₁₀N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	9	2	5		
3	B	1	Total	C	N	O	0	0
			16	9	2	5		
3	C	1	Total	C	N	O	0	0
			16	9	2	5		
3	D	1	Total	C	N	O	0	0
			16	9	2	5		
3	E	1	Total	C	N	O	0	0
			16	9	2	5		
3	F	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	1
			8	4	4		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	1
			12	6	6		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	1
			12	6	6		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	1
			12	6	6		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Mg	0	0
			1	1		

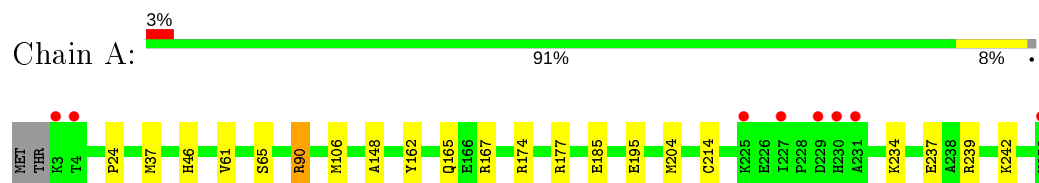
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	345	Total	O	0	8
			353	353		
8	B	344	Total	O	0	3
			347	347		
8	C	325	Total	O	0	5
			331	331		
8	D	308	Total	O	0	2
			310	310		
8	E	318	Total	O	0	3
			321	321		
8	F	330	Total	O	0	8
			338	338		

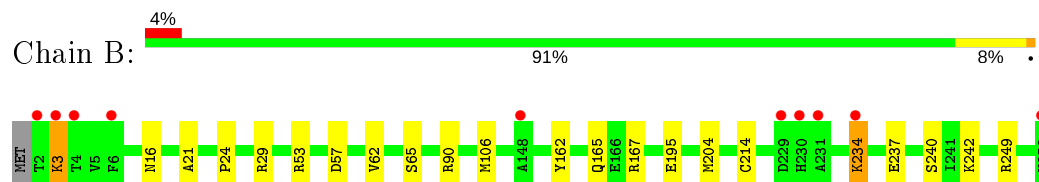
3 Residue-property plots [i](#)

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.

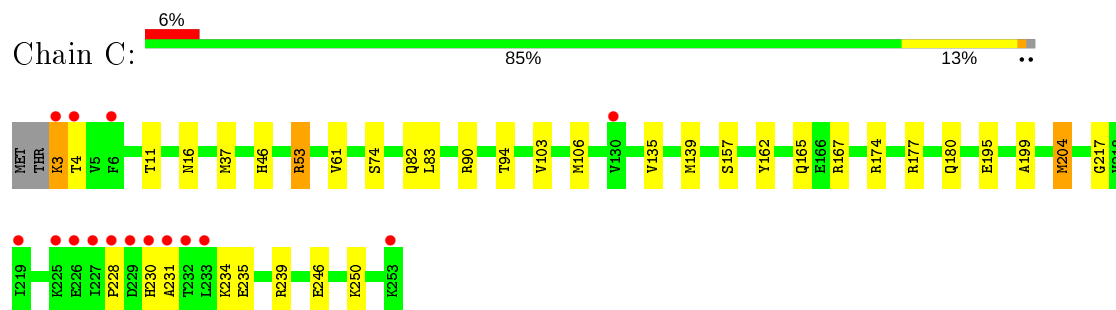
- Molecule 1: Uridine phosphorylase



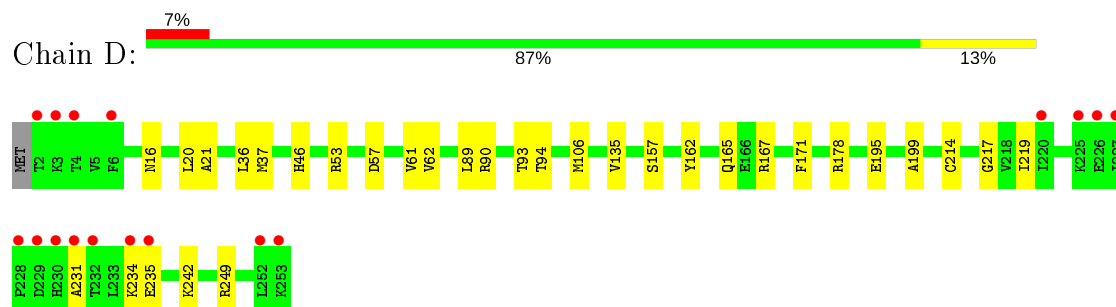
- Molecule 1: Uridine phosphorylase



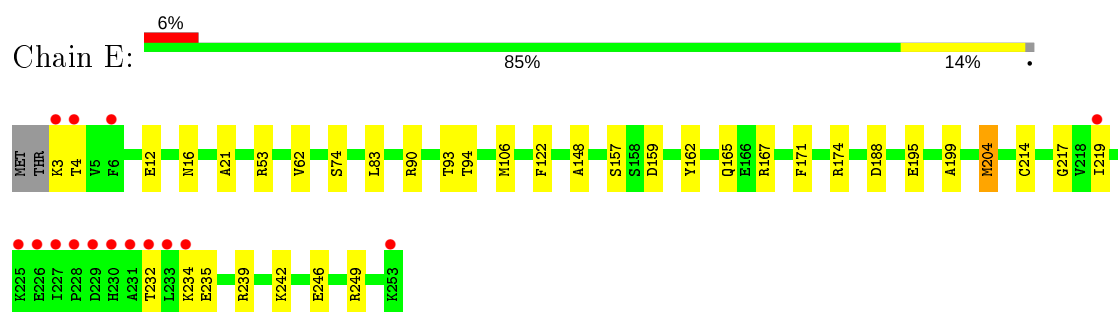
- Molecule 1: Uridine phosphorylase



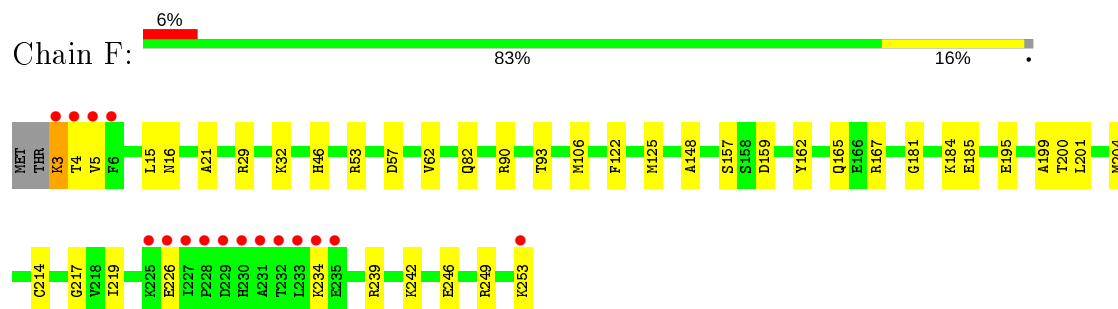
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	93.25Å 93.25Å 152.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.60 – 1.35 46.62 – 1.34	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.60-1.35) 99.8 (46.62-1.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.131 , 0.171 0.132 , 0.171	Depositor DCC
R_{free} test set	3463 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14875	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 33.35 % 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 8.1136e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, MG, CL, NA, BJE, EDO

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	0.66	0/2109	0.81	1/2849 (0.0%)
1	B	0.65	0/2101	0.78	1/2840 (0.0%)
1	C	0.63	0/2201	0.80	3/2971 (0.1%)
1	D	0.65	0/2148	0.76	1/2903 (0.0%)
1	E	0.63	0/2177	0.79	2/2940 (0.1%)
1	F	0.65	0/2233	0.77	2/3012 (0.1%)
All	All	0.65	0/12969	0.79	10/17515 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	F	90	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	90	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	90	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	E	159	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	53[A]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	53[B]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	F	159	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	90	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	E	90	ARG	NE-CZ-NH1	-5.20	117.70	120.30

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	2062	0	2072	16	0
1	B	2066	0	2064	13	0
1	C	2161	0	2166	30	0
1	D	2101	0	2106	23	0
1	E	2123	0	2147	23	0
1	F	2182	0	2200	35	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
3	E	16	0	0	0	0
3	F	16	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	B	4	0	6	0	0
5	D	8	0	12	2	0
5	F	4	0	6	1	0
6	B	12	0	16	0	0
6	D	18	0	24	2	0
6	F	30	0	40	4	0
7	E	1	0	0	0	0
8	A	353	0	0	8	0
8	B	347	0	0	5	0
8	C	331	0	0	10	0
8	D	310	0	0	7	0
8	E	321	0	0	6	0
8	F	338	0	0	11	0
All	All	14875	0	12859	138	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 (138) 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:B:242:LYS:NZ	8:B:401:HOH:O	2.06	0.85
1:C:82:GLN:HG2	5:D:302[A]:EDO:H11	1.62	0.82
1:E:93[B]:THR:HB	1:E:219:ILE:HG23	1.61	0.82
1:A:106[B]:MET:SD	8:A:574:HOH:O	2.39	0.79
1:B:214[A]:CYS:SG	8:B:628:HOH:O	2.39	0.79
1:D:214[B]:CYS:SG	8:D:570:HOH:O	2.41	0.77
1:C:180:GLN:NE2	8:C:403:HOH:O	2.19	0.75
1:C:106[A]:MET:SD	8:C:597:HOH:O	2.43	0.75
1:B:106[B]:MET:SD	8:B:622:HOH:O	2.45	0.74
1:E:106[A]:MET:SD	8:E:552:HOH:O	2.46	0.74
1:F:214[B]:CYS:SG	8:F:585:HOH:O	2.45	0.74
1:F:106[A]:MET:SD	8:F:607:HOH:O	2.46	0.72
1:C:246[B]:GLU:OE2	8:C:401:HOH:O	2.08	0.71
1:F:4[A]:THR:HG22	1:F:5[A]:VAL:H	1.56	0.71
1:F:46[B]:HIS:HD2	8:F:436:HOH:O	1.73	0.70
1:A:177[A]:ARG:NH1	1:C:177:ARG:O	2.24	0.68
1:D:235[A]:GLU:OE1	8:D:401:HOH:O	2.10	0.68
1:D:231:ALA:HB1	8:D:401:HOH:O	1.94	0.68
1:F:226:GLU:OE1	8:F:401:HOH:O	2.11	0.68
1:C:165:GLN:NE2	1:C:167[A]:ARG:HH12	1.94	0.66
1:F:148:ALA:HB2	1:F:239[B]:ARG:HD3	1.77	0.65
1:C:4[B]:THR:O	8:C:402:HOH:O	2.13	0.65
1:D:178:ARG:HG3	6:D:303[B]:GOL:H12	1.79	0.64
1:F:165:GLN:NE2	1:F:167[A]:ARG:HH12	1.95	0.63
1:F:15:LEU:HD22	1:F:62[B]:VAL:HG11	1.82	0.62
1:A:177[A]:ARG:NH1	8:A:402:HOH:O	2.33	0.62
1:E:165:GLN:NE2	1:E:167[A]:ARG:HH12	1.97	0.62
1:E:93[B]:THR:HB	1:E:219:ILE:CG2	2.30	0.62
1:E:246[A]:GLU:OE1	1:E:249[A]:ARG:NH2	2.33	0.61
1:A:165:GLN:NE2	1:A:167[A]:ARG:HH12	1.99	0.61
1:A:185[A]:GLU:OE2	8:A:401:HOH:O	2.16	0.60
1:F:201:LEU:HA	1:F:204[B]:MET:CE	2.31	0.60
1:D:106[A]:MET:SD	8:D:605:HOH:O	2.57	0.59
1:F:29[B]:ARG:NE	8:F:626[B]:HOH:O	2.29	0.59
1:F:253:LYS:HE2	8:F:628:HOH:O	2.01	0.58
1:F:82:GLN:HG2	6:F:305[A]:GOL:H11	1.86	0.58
1:A:242[A]:LYS:HE3	8:A:505:HOH:O	2.05	0.56
8:A:591:HOH:O	1:E:174:ARG:HD2	2.04	0.56
1:E:214[A]:CYS:SG	8:E:616:HOH:O	2.58	0.56
1:B:3:LYS:HG3	8:B:421:HOH:O	2.05	0.55
1:A:174[A]:ARG:HD2	8:C:532:HOH:O	2.07	0.55
1:F:201:LEU:HA	1:F:204[B]:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29[B]:ARG:NH2	1:B:240[B]:SER:OG	2.40	0.54
1:E:16:ASN:HB2	1:E:53[A]:ARG:HD2	1.89	0.54
1:B:16[A]:ASN:HB2	1:B:53[A]:ARG:HD2	1.90	0.54
1:E:3[B]:LYS:HE2	1:E:12:GLU:OE1	2.08	0.54
1:C:16[A]:ASN:HB2	1:C:53[A]:ARG:HD2	1.90	0.53
1:F:16[A]:ASN:HB2	1:F:53[A]:ARG:HD2	1.91	0.53
1:B:57:ASP:OD2	1:B:249[B]:ARG:HG3	2.10	0.52
1:C:230[B]:HIS:CG	1:C:231:ALA:N	2.78	0.52
1:C:174[A]:ARG:HD2	8:E:505:HOH:O	2.09	0.52
1:D:165:GLN:NE2	1:D:167[A]:ARG:HH12	2.08	0.52
1:A:174[C]:ARG:NH1	8:A:404:HOH:O	2.43	0.51
1:D:53[B]:ARG:NH2	8:D:406:HOH:O	2.43	0.51
1:E:148:ALA:HB2	1:E:239[A]:ARG:HD3	1.93	0.51
1:D:20:LEU:HD21	1:D:89[B]:LEU:HD23	1.91	0.51
1:F:46[B]:HIS:CD2	8:F:436:HOH:O	2.55	0.51
1:F:46[A]:HIS:HD2	8:F:428:HOH:O	1.93	0.51
1:B:165:GLN:NE2	1:B:167[A]:ARG:HH12	2.09	0.50
1:D:93[B]:THR:HB	1:D:219:ILE:HG23	1.93	0.49
1:D:36:LEU:HD22	1:D:242:LYS:NZ	2.27	0.49
1:F:93[B]:THR:HB	1:F:219:ILE:HG23	1.94	0.48
1:C:94[B]:THR:N	1:C:217[B]:GLY:O	2.45	0.48
1:C:103:VAL:HG11	1:C:228:PRO:HB3	1.93	0.48
1:C:3[A]:LYS:HA	1:C:3[A]:LYS:HE2	1.95	0.48
1:F:246[B]:GLU:HG2	8:F:414:HOH:O	2.13	0.48
1:C:3[B]:LYS:HE2	1:C:83:LEU:HD23	1.95	0.48
1:E:94[B]:THR:N	1:E:217[B]:GLY:O	2.38	0.48
1:E:242[A]:LYS:HE3	8:E:538:HOH:O	2.14	0.47
1:F:122:PHE:CE1	1:F:204[A]:MET:HG3	2.50	0.47
1:F:200:THR:O	1:F:204[B]:MET:HB3	2.15	0.47
1:E:53[B]:ARG:NH1	8:E:410:HOH:O	2.47	0.47
1:E:122:PHE:CE1	1:E:204[B]:MET:HG3	2.50	0.47
1:D:16[A]:ASN:HB2	1:D:53[A]:ARG:HD2	1.98	0.46
1:B:234:LYS:HE3	1:B:234:LYS:HB3	1.78	0.46
1:C:174[C]:ARG:CZ	1:C:174[C]:ARG:HB2	2.44	0.46
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.98	0.46
1:A:37:MET:SD	1:A:61[B]:VAL:HG21	2.56	0.46
1:C:53[B]:ARG:NH2	8:C:412:HOH:O	2.48	0.46
1:D:93[B]:THR:HB	1:D:219:ILE:CG2	2.46	0.46
1:F:184[B]:LYS:HE3	8:F:686:HOH:O	2.15	0.46
1:C:3[B]:LYS:O	1:C:11:THR:HA	2.16	0.46
1:D:93[B]:THR:HG23	8:D:405:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:THR:HA	1:E:235:GLU:OE1	2.15	0.46
1:E:3[B]:LYS:HE3	1:E:83:LEU:HD23	1.96	0.46
1:C:46[A]:HIS:HD2	8:C:459:HOH:O	1.98	0.45
1:F:93[B]:THR:HB	1:F:219:ILE:CG2	2.46	0.45
1:E:171:PHE:HA	6:F:305[A]:GOL:H12	1.98	0.45
1:F:93[B]:THR:HA	1:F:217[B]:GLY:O	2.16	0.45
1:D:46[A]:HIS:HD2	8:D:469:HOH:O	1.99	0.45
1:F:125:MET:CB	5:F:302:EDO:H22	2.46	0.45
1:F:181:GLY:O	1:F:185[C]:GLU:HG3	2.17	0.44
1:C:239[A]:ARG:NH2	8:C:404:HOH:O	2.21	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.98	0.44
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.98	0.44
1:F:29[B]:ARG:HD2	1:F:32[B]:LYS:HE3	1.99	0.44
1:A:237[A]:GLU:HG2	8:A:468:HOH:O	2.17	0.44
1:A:46[A]:HIS:HD2	8:A:428:HOH:O	2.00	0.44
1:D:21:ALA:HA	1:D:62[B]:VAL:O	2.18	0.44
1:D:171:PHE:HA	5:D:302[A]:EDO:H12	2.00	0.43
1:E:249[B]:ARG:NH2	8:E:401:HOH:O	2.24	0.43
1:B:204[A]:MET:HB3	1:B:204[A]:MET:HE3	1.91	0.43
1:F:234[B]:LYS:HD3	1:F:234[B]:LYS:HA	1.85	0.43
1:F:82:GLN:HG2	6:F:305[B]:GOL:H11	2.00	0.43
1:F:57:ASP:OD2	1:F:249[B]:ARG:HG3	2.18	0.43
1:D:37:MET:SD	1:D:61[B]:VAL:HG21	2.58	0.43
1:D:94[B]:THR:N	1:D:217:GLY:O	2.50	0.43
1:E:94[B]:THR:O	1:E:219:ILE:N	2.37	0.43
1:C:235:GLU:HG3	8:C:558:HOH:O	2.19	0.42
1:C:3[A]:LYS:HB3	1:C:4[A]:THR:H	1.64	0.42
1:F:21:ALA:HA	1:F:62[B]:VAL:O	2.19	0.42
1:B:21:ALA:HA	1:B:62[B]:VAL:O	2.20	0.42
1:E:74:SER:HA	1:E:204[B]:MET:HE1	2.01	0.42
1:C:74:SER:HA	1:C:204[A]:MET:HE1	2.02	0.41
1:C:37:MET:SD	1:C:61[B]:VAL:HG21	2.60	0.41
1:C:157:SER:HB3	1:C:199:ALA:HB2	2.02	0.41
1:C:234:LYS:HD3	1:C:234:LYS:HA	1.88	0.41
1:A:148:ALA:HB2	1:A:239:ARG:HD3	2.03	0.41
1:D:234:LYS:C	1:D:234:LYS:HD3	2.41	0.41
1:A:24:PRO:O	1:A:65:SER:HA	2.20	0.41
1:A:90:ARG:HG2	1:A:214[B]:CYS:SG	2.61	0.41
1:B:24:PRO:O	1:B:65:SER:HA	2.21	0.41
1:D:57:ASP:OD2	1:D:249[B]:ARG:HG3	2.21	0.41
1:E:21:ALA:HA	1:E:62[B]:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ALA:HB2	1:F:62[B]:VAL:HG23	2.03	0.41
1:B:237:GLU:HG3	8:B:441:HOH:O	2.21	0.40
1:F:242[A]:LYS:HD2	8:F:621:HOH:O	2.20	0.40
1:D:178:ARG:CG	6:D:303[B]:GOL:H12	2.49	0.40
1:C:135:VAL:O	1:C:139[B]:MET:HG2	2.22	0.40
1:F:184[A]:LYS:NZ	6:F:304:GOL:O3	2.55	0.40
1:F:3[A]:LYS:HB2	1:F:3[A]:LYS:HE3	1.79	0.40
1:C:250:LYS:NZ	8:C:401:HOH:O	2.53	0.40
1:D:89[B]:LEU:HD12	1:D:135:VAL:HG13	2.04	0.40
1:C:174[C]:ARG:CZ	1:E:188:ASP:HB3	2.51	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	272/253 (108%)	269 (99%)	2 (1%)	1 (0%)	34	12
1	B	271/253 (107%)	265 (98%)	5 (2%)	1 (0%)	34	12
1	C	283/253 (112%)	276 (98%)	6 (2%)	1 (0%)	34	12
1	D	278/253 (110%)	273 (98%)	4 (1%)	1 (0%)	34	12
1	E	281/253 (111%)	276 (98%)	4 (1%)	1 (0%)	34	12
1	F	286/253 (113%)	281 (98%)	4 (1%)	1 (0%)	41	18
All	All	1671/1518 (110%)	1640 (98%)	25 (2%)	6 (0%)	34	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	162	TYR
1	A	162	TYR

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Mol	Chain	Res	Type
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	F	162	TYR

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	224/203 (110%)	221 (99%)	3 (1%)	69	37
1	B	223/203 (110%)	220 (99%)	3 (1%)	69	37
1	C	233/203 (115%)	228 (98%)	5 (2%)	53	19
1	D	228/203 (112%)	227 (100%)	1 (0%)	91	81
1	E	231/203 (114%)	225 (97%)	6 (3%)	46	12
1	F	237/203 (117%)	234 (99%)	3 (1%)	69	37
All	All	1376/1218 (113%)	1355 (98%)	21 (2%)	71	33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	204[A]	MET
1	A	204[B]	MET
1	B	3	LYS
1	B	195	GLU
1	B	234	LYS
1	C	3[A]	LYS
1	C	3[B]	LYS
1	C	195	GLU
1	C	204[A]	MET
1	C	204[B]	MET
1	D	195	GLU
1	E	4[A]	THR
1	E	4[B]	THR

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Mol	Chain	Res	Type
1	E	195	GLU
1	E	204[A]	MET
1	E	204[B]	MET
1	E	234	LYS
1	F	3[A]	LYS
1	F	3[B]	LYS
1	F	195	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	B	165	GLN
1	C	165	GLN
1	D	165	GLN
1	E	165	GLN
1	F	165	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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z > 2$
5	EDO	D	302[A]	-	3,3,3	0.60	0	2,2,2	0.40	0
6	GOL	F	303[A]	-	5,5,5	0.42	0	5,5,5	0.84	0
6	GOL	D	303[B]	-	5,5,5	0.72	0	5,5,5	1.70	2 (40%)
6	GOL	D	304	-	5,5,5	0.23	0	5,5,5	0.49	0
6	GOL	B	304[A]	-	5,5,5	0.54	0	5,5,5	1.21	0
6	GOL	F	304	-	5,5,5	0.40	0	5,5,5	0.34	0
5	EDO	D	302[B]	-	3,3,3	0.50	0	2,2,2	0.25	0
6	GOL	F	305[A]	-	5,5,5	0.31	0	5,5,5	0.61	0
6	GOL	D	303[C]	-	5,5,5	0.44	0	5,5,5	0.42	0
3	BJE	F	301	-	16,18,18	2.36	5 (31%)	13,27,27	1.67	3 (23%)
6	GOL	F	305[B]	-	5,5,5	0.32	0	5,5,5	0.75	0
3	BJE	D	301	-	16,18,18	2.77	4 (25%)	13,27,27	1.35	2 (15%)
5	EDO	F	302	-	3,3,3	0.50	0	2,2,2	0.17	0
3	BJE	E	302	-	16,18,18	2.05	3 (18%)	13,27,27	1.71	3 (23%)
6	GOL	F	303[B]	-	5,5,5	0.53	0	5,5,5	0.55	0
3	BJE	B	302	-	16,18,18	2.40	4 (25%)	13,27,27	2.02	2 (15%)
3	BJE	A	302	-	16,18,18	2.50	6 (37%)	13,27,27	1.77	5 (38%)
3	BJE	C	302	-	16,18,18	3.03	6 (37%)	13,27,27	2.09	4 (30%)
5	EDO	B	303	-	3,3,3	0.37	0	2,2,2	0.62	0
6	GOL	B	304[B]	-	5,5,5	0.43	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
5	EDO	D	302[A]	-	-	1/1/1/1	-
6	GOL	F	303[A]	-	-	2/4/4/4	-
6	GOL	D	303[B]	-	-	2/4/4/4	-
6	GOL	D	304	-	-	4/4/4/4	-
6	GOL	B	304[A]	-	-	3/4/4/4	-
6	GOL	F	304	-	-	3/4/4/4	-
5	EDO	D	302[B]	-	-	1/1/1/1	-
6	GOL	F	305[A]	-	-	1/4/4/4	-
6	GOL	D	303[C]	-	-	2/4/4/4	-
3	BJE	F	301	-	1/1/4/4	0/2/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	F	305[B]	-	-	2/4/4/4	-
3	BJE	D	301	-	1/1/4/4	0/2/26/26	0/3/3/3
5	EDO	F	302	-	-	1/1/1/1	-
3	BJE	E	302	-	1/1/4/4	0/2/26/26	0/3/3/3
6	GOL	F	303[B]	-	-	3/4/4/4	-
3	BJE	B	302	-	1/1/4/4	0/2/26/26	0/3/3/3
3	BJE	A	302	-	1/1/4/4	0/2/26/26	0/3/3/3
3	BJE	C	302	-	1/1/4/4	0/2/26/26	0/3/3/3
5	EDO	B	303	-	-	0/1/1/1	-
6	GOL	B	304[B]	-	-	0/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	BJE	C6-N1	8.05	1.45	1.35
3	D	301	BJE	C6-N1	7.30	1.44	1.35
3	C	302	BJE	C6-C5	6.62	1.52	1.38
3	A	302	BJE	C6-C5	5.90	1.51	1.38
3	B	302	BJE	C6-C5	5.85	1.51	1.38
3	D	301	BJE	C6-C5	5.71	1.50	1.38
3	A	302	BJE	C6-N1	5.64	1.42	1.35
3	F	301	BJE	C6-N1	5.41	1.42	1.35
3	F	301	BJE	C6-C5	5.37	1.49	1.38
3	B	302	BJE	C6-N1	5.34	1.42	1.35
3	E	302	BJE	C6-C5	5.19	1.49	1.38
3	D	301	BJE	C4-N3	4.12	1.40	1.33
3	E	302	BJE	C6-N1	4.02	1.40	1.35
3	E	302	BJE	C4-N3	3.90	1.39	1.33
3	C	302	BJE	C4-N3	3.88	1.39	1.33
3	F	301	BJE	C4-N3	3.49	1.39	1.33
3	A	302	BJE	O2-C2'	-3.20	1.42	1.45
3	B	302	BJE	C4-N3	3.16	1.38	1.33
3	B	302	BJE	O4'-C1'	3.12	1.45	1.41
3	A	302	BJE	C4-N3	2.94	1.38	1.33
3	D	301	BJE	C2-N3	2.84	1.37	1.32
3	C	302	BJE	C2-N3	2.74	1.37	1.32
3	A	302	BJE	C3'-C4'	2.61	1.59	1.53
3	F	301	BJE	O4'-C1'	2.23	1.44	1.41
3	C	302	BJE	O4'-C1'	2.22	1.44	1.41
3	A	302	BJE	C2-N3	2.11	1.36	1.32
3	F	301	BJE	C1'-N1	-2.05	1.46	1.49
3	C	302	BJE	O2-C2'	-2.02	1.43	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	BJE	O2-C2'-C3'	-5.06	103.69	110.59
3	B	302	BJE	O2-C2'-C3'	-4.85	103.98	110.59
3	E	302	BJE	O2-C2'-C3'	-3.84	105.36	110.59
3	B	302	BJE	C5-C6-N1	-3.63	112.57	120.68
3	D	301	BJE	C3'-C2'-C1'	3.49	109.44	102.89
3	C	302	BJE	C5-C6-N1	-3.42	113.06	120.68
3	F	301	BJE	O2-C2'-C3'	-3.06	106.42	110.59
3	F	301	BJE	C3'-C2'-C1'	2.91	108.36	102.89
3	A	302	BJE	O2-C2'-C1'	-2.82	102.08	105.47
3	E	302	BJE	C3'-C2'-C1'	2.82	108.19	102.89
3	F	301	BJE	C5-C6-N1	-2.75	114.55	120.68
3	A	302	BJE	C5-C6-N1	-2.74	114.57	120.68
3	A	302	BJE	O4'-C4'-C5'	2.66	114.95	109.21
6	D	303[B]	GOL	O1-C1-C2	2.65	122.91	110.20
6	D	303[B]	GOL	C3-C2-C1	2.65	122.00	111.70
3	A	302	BJE	O2-C2'-C3'	-2.59	107.07	110.59
3	C	302	BJE	O4'-C4'-C5'	2.55	114.72	109.21
3	A	302	BJE	C3'-C2'-C1'	2.47	107.54	102.89
3	D	301	BJE	C5-C6-N1	-2.16	115.85	120.68
3	E	302	BJE	O4'-C4'-C5'	2.15	113.85	109.21
3	C	302	BJE	C3'-C2'-C1'	2.12	106.87	102.89

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	302	BJE	C2'
3	B	302	BJE	C2'
3	A	302	BJE	C2'
3	C	302	BJE	C2'
3	F	301	BJE	C2'
3	D	301	BJE	C2'

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	304	GOL	O1-C1-C2-C3
6	F	305[B]	GOL	O1-C1-C2-C3
6	F	303[B]	GOL	O1-C1-C2-C3
6	D	303[B]	GOL	O1-C1-C2-C3
6	D	304	GOL	O1-C1-C2-C3
6	D	304	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	F	304	GOL	C1-C2-C3-O3
6	B	304[A]	GOL	O1-C1-C2-C3
6	B	304[A]	GOL	C1-C2-C3-O3
6	F	303[A]	GOL	O1-C1-C2-C3
6	D	303[C]	GOL	C1-C2-C3-O3
6	F	304	GOL	O1-C1-C2-O2
6	B	304[A]	GOL	O1-C1-C2-O2
6	F	303[B]	GOL	O1-C1-C2-O2
6	F	303[A]	GOL	O1-C1-C2-O2
6	D	303[B]	GOL	O1-C1-C2-O2
6	D	304	GOL	O1-C1-C2-O2
5	D	302[A]	EDO	O1-C1-C2-O2
6	F	305[B]	GOL	O1-C1-C2-O2
6	D	304	GOL	O2-C2-C3-O3
5	D	302[B]	EDO	O1-C1-C2-O2
6	F	305[A]	GOL	O2-C2-C3-O3
6	F	303[B]	GOL	C1-C2-C3-O3
5	F	302	EDO	O1-C1-C2-O2
6	D	303[C]	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	302[A]	EDO	2	0
6	D	303[B]	GOL	2	0
6	F	304	GOL	1	0
6	F	305[A]	GOL	2	0
6	F	305[B]	GOL	1	0
5	F	302	EDO	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

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	251/253 (99%)	0.14	8 (3%)	47	53	6, 10, 24, 51	2 (0%)
1	B	252/253 (99%)	0.19	10 (3%)	38	43	6, 10, 23, 62	1 (0%)
1	C	251/253 (99%)	0.34	15 (5%)	21	24	6, 12, 30, 60	3 (1%)
1	D	252/253 (99%)	0.37	17 (6%)	17	20	7, 12, 30, 56	1 (0%)
1	E	251/253 (99%)	0.30	15 (5%)	21	24	6, 11, 32, 58	2 (0%)
1	F	251/253 (99%)	0.23	16 (6%)	19	21	6, 11, 26, 56	1 (0%)
All	All	1508/1518 (99%)	0.26	81 (5%)	25	29	6, 11, 27, 62	10 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	ILE	12.4
1	B	2	THR	11.6
1	E	227	ILE	8.5
1	C	4[A]	THR	7.8
1	D	2	THR	7.6
1	D	227	ILE	7.4
1	C	231	ALA	7.0
1	A	4	THR	6.8
1	E	230	HIS	6.7
1	F	227	ILE	6.5
1	E	4[A]	THR	6.2
1	D	229	ASP	6.0
1	E	225	LYS	5.6
1	D	231	ALA	5.6
1	D	4	THR	5.6
1	C	229	ASP	5.3
1	D	253	LYS	5.2
1	C	230[A]	HIS	5.2
1	B	4	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	231	ALA	5.1
1	F	231	ALA	5.1
1	F	229	ASP	4.9
1	E	3[A]	LYS	4.8
1	C	226[A]	GLU	4.7
1	D	230	HIS	4.5
1	A	227	ILE	4.5
1	D	225	LYS	4.4
1	F	230	HIS	4.2
1	E	226	GLU	4.1
1	D	3	LYS	4.0
1	E	229	ASP	3.9
1	B	253	LYS	3.9
1	B	3	LYS	3.8
1	C	232	THR	3.7
1	B	229	ASP	3.7
1	E	6[A]	PHE	3.7
1	F	226	GLU	3.6
1	A	3	LYS	3.6
1	A	229[A]	ASP	3.5
1	A	253	LYS	3.5
1	C	228	PRO	3.4
1	F	4[A]	THR	3.4
1	A	225	LYS	3.3
1	B	230	HIS	3.3
1	B	6	PHE	3.3
1	F	232	THR	3.2
1	B	231	ALA	3.2
1	F	3[A]	LYS	3.1
1	D	232	THR	3.1
1	A	231	ALA	3.0
1	D	226	GLU	3.0
1	E	233	LEU	3.0
1	A	230	HIS	3.0
1	F	234[A]	LYS	3.0
1	F	225	LYS	2.9
1	C	6[A]	PHE	2.8
1	C	253	LYS	2.7
1	E	232	THR	2.7
1	C	225	LYS	2.7
1	F	228	PRO	2.6
1	C	219[A]	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	234	LYS	2.5
1	E	219	ILE	2.5
1	F	233	LEU	2.5
1	D	235[A]	GLU	2.5
1	D	6	PHE	2.4
1	F	5[A]	VAL	2.4
1	B	234	LYS	2.3
1	E	253	LYS	2.3
1	D	228	PRO	2.3
1	F	6[A]	PHE	2.3
1	D	220	ILE	2.3
1	E	228	PRO	2.3
1	B	148	ALA	2.3
1	C	233	LEU	2.2
1	E	234	LYS	2.2
1	C	3[A]	LYS	2.2
1	C	130[A]	VAL	2.1
1	F	235[A]	GLU	2.0
1	D	252	LEU	2.0
1	F	253	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	F	304	6/6	0.59	0.34	51,52,53,53	6
6	GOL	D	304	6/6	0.75	0.33	55,56,57,57	0
5	EDO	B	303	4/4	0.76	0.17	35,37,38,40	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	F	305[A]	6/6	0.79	0.25	40,40,40,41	6
6	GOL	F	305[B]	6/6	0.79	0.25	31,33,34,35	6
5	EDO	D	302[A]	4/4	0.80	0.16	40,41,41,42	4
5	EDO	D	302[B]	4/4	0.80	0.16	50,50,51,51	4
6	GOL	B	304[A]	6/6	0.81	0.19	21,26,27,29	6
6	GOL	B	304[B]	6/6	0.81	0.19	16,17,18,21	6
5	EDO	F	302	4/4	0.85	0.44	32,32,32,33	4
6	GOL	D	303[B]	6/6	0.86	0.18	14,16,17,17	6
6	GOL	D	303[C]	6/6	0.86	0.18	23,24,25,25	6
6	GOL	F	303[B]	6/6	0.88	0.16	13,15,16,18	6
6	GOL	F	303[A]	6/6	0.88	0.16	18,21,22,22	6
3	BJE	C	302	16/16	0.94	0.09	11,12,16,19	16
3	BJE	F	301	16/16	0.96	0.08	10,12,14,17	0
3	BJE	D	301	16/16	0.96	0.08	11,12,15,17	0
4	CL	B	301	1/1	0.96	0.08	59,59,59,59	0
3	BJE	B	302	16/16	0.97	0.07	9,11,13,15	0
3	BJE	A	302	16/16	0.97	0.07	10,11,13,16	0
3	BJE	E	302	16/16	0.97	0.07	9,10,13,16	16
2	NA	A	301	1/1	0.99	0.05	18,18,18,18	0
4	CL	F	306	1/1	0.99	0.07	25,25,25,25	0
2	NA	C	303	1/1	1.00	0.05	18,18,18,18	0
7	MG	E	303	1/1	1.00	0.23	21,21,21,21	1
4	CL	C	301	1/1	1.00	0.04	26,26,26,26	0
4	CL	B	305	1/1	1.00	0.08	24,24,24,24	0
2	NA	E	301	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.