Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:57 pm BST

PDB ID	:	2OEC
Title	:	Crystal structure of the uridine phosphorylase from Salmonella typhimurium in complex with 2,2'-anhydrouridine and potassium ion at 2.194A resolution
Authors	:	Timofeev, V.I.; Lashkov, A.A.; Pavlyuk, B.P.; Mikhailov, A.M.
Deposited on	:	2006-12-29
Resolution	:	2.19 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 ①) were used in the production of this report:

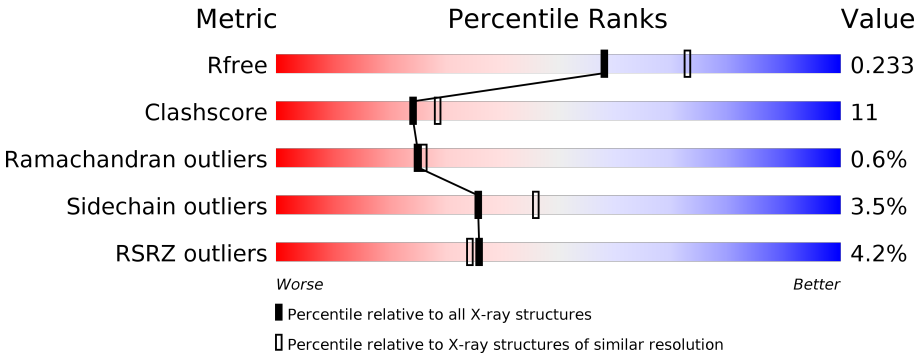
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	252	3% 84% 15%
1	B	252	2% 76% 18% 5%
1	C	252	4% 77% 20%
1	D	252	5% 73% 25%
1	E	252	7% 75% 23%
1	F	252	4% 75% 21%

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
5	GOL	F	16	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11603 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.

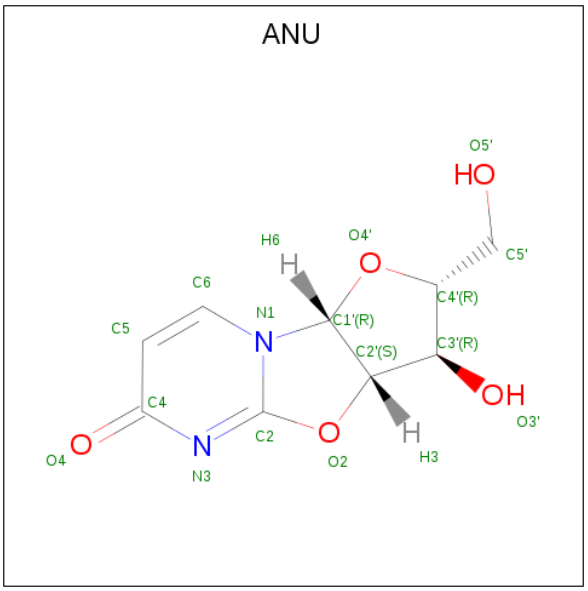
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	3	0
			1912	1195	337	368	12			
1	B	239	Total	C	N	O	S	0	1	0
			1799	1128	319	341	11			
1	C	247	Total	C	N	O	S	0	3	0
			1874	1172	330	360	12			
1	D	251	Total	C	N	O	S	0	0	0
			1882	1177	331	362	12			
1	E	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	F	247	Total	C	N	O	S	0	0	0
			1852	1159	325	356	12			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

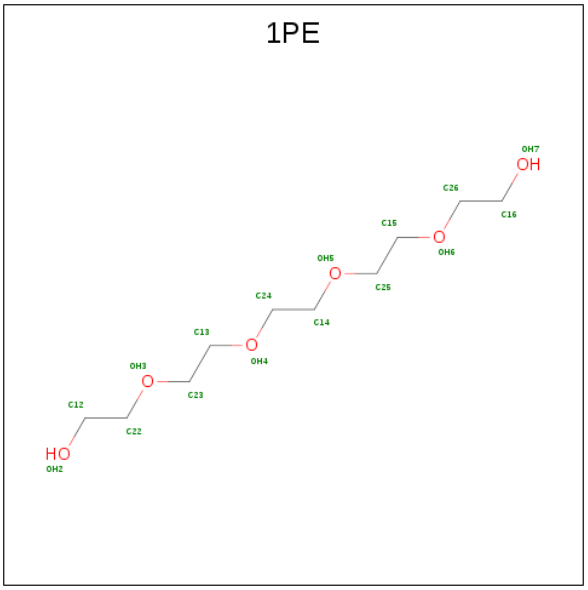
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

- Molecule 3 is 2,2'-Anhydro-(1-beta-D-arabinofuranosyl)uracil (three-letter code: ANU) (formula: $C_9H_{10}N_2O_5$).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0

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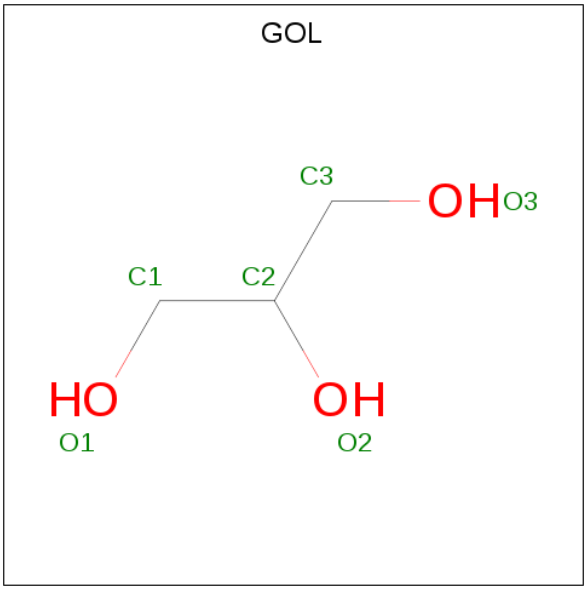
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 16 10 6	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

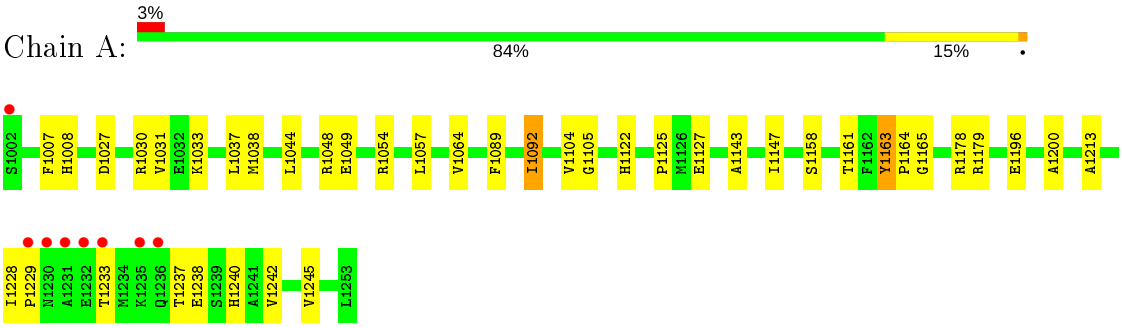
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	B	51	Total O 51 51	0	0
6	C	56	Total O 56 56	0	0
6	D	50	Total O 50 50	0	0
6	E	46	Total O 46 46	0	0
6	F	49	Total O 49 49	0	0

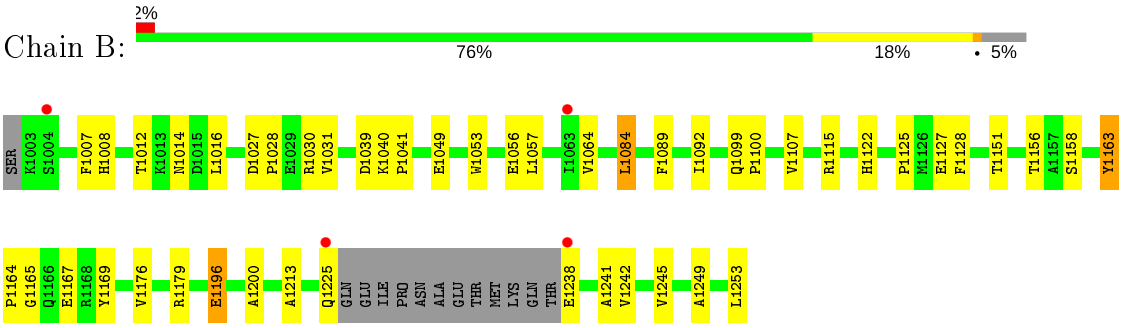
3 Residue-property plots (i)

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.

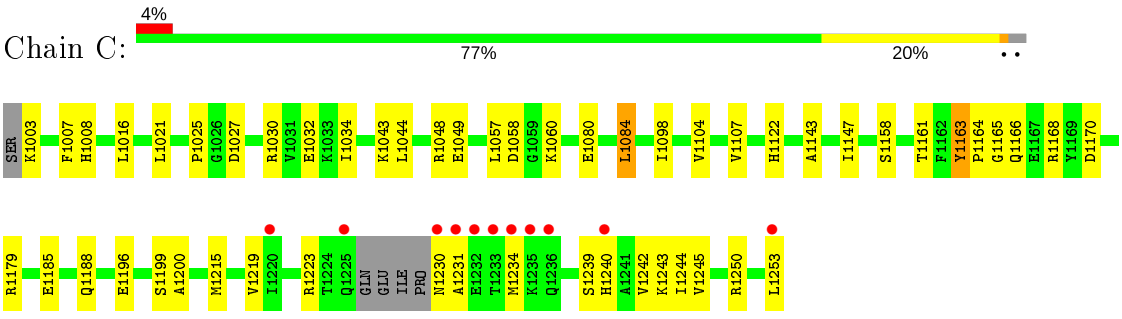
- Molecule 1: Uridine phosphorylase



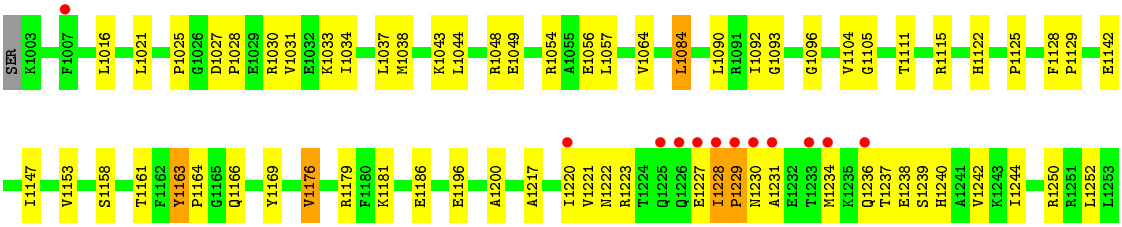
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

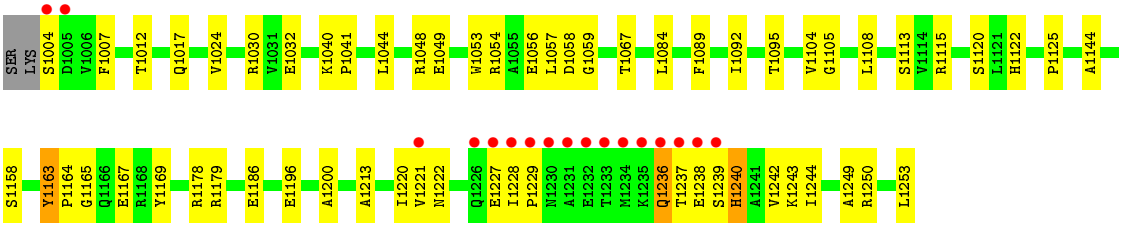


- Molecule 1: Uridine phosphorylase



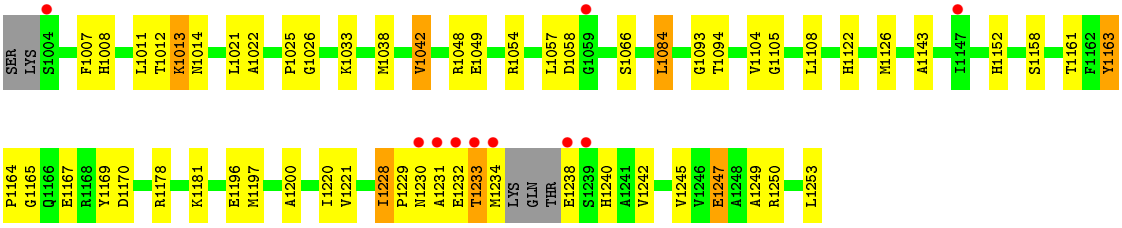
- Molecule 1: Uridine phosphorylase

Chain E:



- Molecule 1: Uridine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.52Å 123.98Å 133.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.19 19.89 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.0 (8.00-2.19) 99.1 (19.89-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.15Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.178 , 0.240 0.189 , 0.233	Depositor DCC
R_{free} test set	3956 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11603	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, K, 1PE, ANU

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	0.27	0/1948	0.48	0/2637
1	B	0.27	0/1830	0.47	0/2476
1	C	0.27	0/1907	0.49	0/2578
1	D	0.26	0/1912	0.47	0/2591
1	E	0.26	0/1907	0.46	0/2584
1	F	0.27	0/1881	0.48	0/2548
All	All	0.27	0/11385	0.48	0/15414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1912	0	1928	31	0
1	B	1799	0	1819	35	0
1	C	1874	0	1889	43	0
1	D	1882	0	1889	47	0
1	E	1877	0	1887	47	0
1	F	1852	0	1858	71	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	B	16	0	10	0	0
3	F	16	0	10	1	0
4	B	32	0	44	2	0
4	D	16	0	22	0	0
5	F	6	0	8	6	0
6	A	66	0	0	0	0
6	B	51	0	0	0	0
6	C	56	0	0	2	0
6	D	50	0	0	0	0
6	E	46	0	0	1	0
6	F	49	0	0	1	0
All	All	11603	0	11364	250	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 11.

All (250) 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:1233:THR:HG23	1:F:1234:MET:HA	1.36	1.07
1:F:1232:GLU:N	1:F:1233:THR:HA	1.71	1.03
1:F:1233:THR:HG23	1:F:1234:MET:CA	2.05	0.85
1:F:1231:ALA:N	1:F:1232:GLU:HG3	1.94	0.82
1:F:1231:ALA:H	1:F:1232:GLU:HG3	1.45	0.79
1:F:1233:THR:CG2	1:F:1234:MET:HA	2.12	0.78
1:A:1104:VAL:HG21	1:A:1229:PRO:HG2	1.64	0.78
1:D:1163:TYR:HB2	1:D:1164:PRO:HD3	1.66	0.77
1:F:1012:THR:HG22	1:F:1014:ASN:H	1.51	0.76
1:B:1030:ARG:HH12	1:B:1242:VAL:HG21	1.52	0.75
1:E:1220:ILE:HG13	1:E:1221:VAL:HG23	1.69	0.73
1:C:1163:TYR:HB2	1:C:1164:PRO:HD3	1.71	0.73
1:B:1012:THR:HG22	1:B:1014:ASN:H	1.55	0.72
1:C:1230:ASN:O	1:C:1234:MET:HG3	1.92	0.70
1:F:1093:GLY:HA2	5:F:16:GOL:H32	1.73	0.69
1:A:1027:ASP:HB3	1:A:1030:ARG:HD3	1.73	0.69
1:F:1231:ALA:C	1:F:1233:THR:HA	2.13	0.69
1:B:1158:SER:HB3	1:B:1200:ALA:HB2	1.76	0.68
1:F:1238:GLU:HA	1:F:1238:GLU:OE1	1.93	0.68
1:C:1032:GLU:HG3	6:C:1272:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:TYR:CE2	1:B:1176:VAL:HG13	2.29	0.67
1:F:1238:GLU:HG3	1:F:1240:HIS:HB2	1.77	0.67
1:C:1158:SER:HB3	1:C:1200:ALA:HB2	1.76	0.66
1:F:1232:GLU:N	1:F:1233:THR:CA	2.55	0.66
1:F:1231:ALA:HB3	1:F:1232:GLU:HA	1.77	0.66
4:B:315:1PE:H152	1:E:1178:ARG:HG3	1.78	0.66
1:D:1104:VAL:HG13	1:D:1220:ILE:HA	1.78	0.66
1:E:1228:ILE:HD12	1:E:1228:ILE:H	1.63	0.64
1:A:1049:GLU:HB3	1:B:1049:GLU:HB3	1.80	0.64
1:D:1025:PRO:HG3	1:D:1034:ILE:HD12	1.80	0.62
1:E:1048:ARG:HB3	1:E:1049:GLU:OE2	2.00	0.61
1:C:1060:LYS:HD3	1:C:1253:LEU:HB3	1.82	0.61
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.83	0.60
1:B:1030:ARG:HH12	1:B:1242:VAL:CG2	2.13	0.60
1:C:1161:THR:OG1	1:D:1122:HIS:HD2	1.85	0.60
1:B:1012:THR:HG22	1:B:1014:ASN:N	2.17	0.60
1:E:1095:THR:HG21	1:E:1108:LEU:HD12	1.83	0.60
1:D:1125:PRO:HG3	6:E:1289:HOH:O	2.01	0.59
1:A:1030:ARG:HG2	1:A:1033:LYS:NZ	2.17	0.59
1:E:1044:LEU:HD11	1:E:1054:ARG:HB2	1.84	0.59
1:C:1027:ASP:HB3	1:C:1030:ARG:CG	2.33	0.58
1:E:1049:GLU:HB3	1:F:1049:GLU:CG	2.33	0.58
1:F:1007:PHE:HD2	1:F:1008:HIS:CE1	2.21	0.58
1:E:1032:GLU:HG3	1:E:1053:TRP:CZ2	2.39	0.58
1:A:1048:ARG:HB3	1:A:1049:GLU:OE1	2.04	0.58
1:D:1129:PRO:HG3	1:E:1113:SER:O	2.03	0.58
1:D:1105:GLY:HA2	1:D:1237:THR:OG1	2.04	0.58
1:F:1231:ALA:H	1:F:1232:GLU:HA	1.69	0.58
1:D:1169:TYR:CE2	1:D:1176:VAL:HG13	2.39	0.57
1:F:1042:VAL:HG11	1:F:1054:ARG:NH1	2.20	0.56
1:B:1007:PHE:HD2	1:B:1008:HIS:CE1	2.24	0.56
1:C:1016:LEU:HD22	1:C:1084:LEU:HB3	1.88	0.56
1:C:1080:GLU:O	1:C:1084:LEU:HD22	2.05	0.56
1:C:1027:ASP:HB3	1:C:1030:ARG:HG3	1.86	0.56
1:E:1057:LEU:HD21	1:E:1250:ARG:HG2	1.88	0.55
1:E:1158:SER:HB3	1:E:1200:ALA:HB2	1.88	0.55
1:C:1057:LEU:HB3	1:C:1253:LEU:HD11	1.89	0.55
1:F:1242:VAL:O	1:F:1245:VAL:HG12	2.07	0.55
1:E:1163:TYR:HB2	1:E:1164:PRO:CD	2.37	0.54
1:C:1057:LEU:HD21	1:C:1250:ARG:HG2	1.90	0.54
1:C:1166:GLN:O	1:C:1223:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1105:GLY:HA2	1:E:1237:THR:OG1	2.08	0.54
1:D:1115:ARG:NH2	1:D:1125:PRO:O	2.41	0.54
1:F:1158:SER:HB3	1:F:1200:ALA:HB2	1.90	0.54
1:F:1247:GLU:OE2	1:F:1250:ARG:HD2	2.07	0.54
1:E:1122:HIS:CD2	1:F:1165:GLY:HA3	2.42	0.53
1:F:1230:ASN:HB2	1:F:1231:ALA:HA	1.90	0.53
1:A:1037:LEU:HD12	1:A:1242:VAL:HG12	1.90	0.53
1:E:1058:ASP:OD2	1:E:1250:ARG:HD2	2.07	0.53
1:A:1143:ALA:O	1:A:1147:ILE:HG12	2.08	0.53
1:D:1030:ARG:O	1:D:1034:ILE:HG13	2.08	0.53
1:F:1108:LEU:HD22	1:F:1152:HIS:HB2	1.91	0.53
1:F:1229:PRO:HB2	1:F:1231:ALA:HB2	1.89	0.53
1:C:1057:LEU:CD2	1:C:1250:ARG:HG2	2.40	0.52
1:C:1048:ARG:HB3	1:C:1049:GLU:OE2	2.09	0.52
1:C:1185:GLU:HA	1:C:1188[A]:GLN:OE1	2.10	0.52
1:F:1094:THR:H	5:F:16:GOL:H12	1.74	0.52
1:D:1163:TYR:CB	1:D:1164:PRO:HD3	2.39	0.52
1:D:1030:ARG:NH2	1:D:1033:LYS:CE	2.73	0.52
1:E:1122:HIS:HD2	1:F:1165:GLY:HA3	1.74	0.52
1:D:1181:LYS:O	1:F:1178:ARG:NH2	2.43	0.52
1:A:1165:GLY:HA3	1:B:1122:HIS:HD2	1.74	0.52
1:B:1115[A]:ARG:NH2	1:B:1125:PRO:O	2.43	0.52
1:E:1049:GLU:HB3	1:F:1049:GLU:HG2	1.92	0.52
1:A:1165:GLY:HA3	1:B:1122:HIS:CD2	2.45	0.52
1:E:1165:GLY:HA3	1:F:1122:HIS:HD2	1.74	0.51
1:F:1011:LEU:HB2	1:F:1084:LEU:HD21	1.91	0.51
1:E:1007:PHE:CE1	1:F:1229:PRO:HG2	2.45	0.51
1:F:1249:ALA:O	1:F:1253:LEU:HG	2.11	0.51
1:D:1030:ARG:HH22	1:D:1033:LYS:HE3	1.76	0.51
1:E:1221:VAL:HG12	1:E:1222:ASN:N	2.25	0.51
1:B:1167:GLU:HG2	1:B:1169:TYR:CE1	2.45	0.51
1:C:1043:LYS:HD3	1:C:1044:LEU:N	2.24	0.51
1:C:1165:GLY:HA3	1:D:1122:HIS:CD2	2.46	0.51
1:F:1167:GLU:HG2	1:F:1169:TYR:CE1	2.45	0.51
1:E:1228:ILE:HG22	1:E:1229:PRO:HD2	1.93	0.51
1:E:1115:ARG:HD2	1:E:1120:SER:OG	2.11	0.51
1:E:1167:GLU:HG2	1:E:1169:TYR:CE1	2.46	0.51
4:B:315:1PE:OH4	4:B:315:1PE:H162	2.11	0.51
1:C:1239:SER:O	1:C:1243:LYS:HG3	2.11	0.51
1:F:1058:ASP:OD2	1:F:1250:ARG:HG3	2.11	0.51
1:F:1093:GLY:HA2	5:F:16:GOL:C3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1163:TYR:HB2	1:B:1164:PRO:CD	2.41	0.50
1:B:1039:ASP:HB2	1:B:1056:GLU:HB3	1.94	0.50
1:D:1030:ARG:NH2	1:D:1033:LYS:HE3	2.27	0.50
1:F:1094:THR:H	5:F:16:GOL:C1	2.24	0.50
1:F:1221:VAL:CG2	1:F:1229:PRO:HD3	2.42	0.50
1:D:1166:GLN:O	1:D:1223:ARG:NH2	2.42	0.50
1:E:1238:GLU:O	1:E:1242:VAL:HG23	2.12	0.50
1:C:1104:VAL:HA	1:C:1219:VAL:HG12	1.93	0.50
1:B:1040:LYS:N	1:B:1041:PRO:HD3	2.27	0.49
1:F:1231:ALA:N	1:F:1232:GLU:HA	2.26	0.49
1:C:1025:PRO:HG3	1:C:1034:ILE:CD1	2.43	0.49
1:E:1115:ARG:NH2	1:E:1125:PRO:O	2.42	0.49
1:F:1220:ILE:HG13	1:F:1221:VAL:HG23	1.93	0.49
1:C:1025:PRO:HG3	1:C:1034:ILE:HD12	1.93	0.49
1:F:1048:ARG:HB3	1:F:1049:GLU:OE2	2.12	0.49
1:D:1237:THR:O	1:D:1240:HIS:HB2	2.13	0.49
1:C:1231:ALA:HA	1:C:1234:MET:CE	2.44	0.48
1:D:1158:SER:HB3	1:D:1200:ALA:HB2	1.94	0.48
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.96	0.48
1:D:1147:ILE:HD12	1:D:1244:ILE:HG12	1.96	0.48
1:D:1031:VAL:HG13	1:D:1064:VAL:HG12	1.95	0.48
1:A:1027:ASP:CB	1:A:1030:ARG:HD3	2.42	0.48
1:E:1057:LEU:CD2	1:E:1250:ARG:HG2	2.44	0.48
1:E:1249:ALA:O	1:E:1253:LEU:HG	2.14	0.48
1:B:1242:VAL:O	1:B:1245:VAL:HG12	2.14	0.48
1:B:1031:VAL:HG12	1:B:1053:TRP:CD1	2.49	0.47
1:E:1165:GLY:HA3	1:F:1122:HIS:CD2	2.49	0.47
1:C:1057:LEU:HG	1:C:1250:ARG:HG2	1.96	0.47
1:E:1163:TYR:CB	1:E:1164:PRO:CD	2.93	0.47
1:D:1044:LEU:HD11	1:D:1054:ARG:HB2	1.96	0.47
1:D:1221:VAL:HG22	1:D:1222:ASN:N	2.30	0.47
1:D:1093:GLY:O	1:D:1217:ALA:HA	2.15	0.47
1:F:1033:LYS:HA	1:F:1033:LYS:HD3	1.59	0.47
1:B:1030:ARG:NH1	1:B:1242:VAL:HG21	2.25	0.47
1:A:1161:THR:OG1	1:B:1122:HIS:HD2	1.98	0.46
1:C:1057:LEU:HB3	1:C:1253:LEU:CD1	2.45	0.46
1:E:1089:PHE:O	1:E:1213:ALA:HA	2.15	0.46
1:F:1163:TYR:HB2	1:F:1164:PRO:CD	2.44	0.46
1:E:1007:PHE:HE1	1:F:1229:PRO:HG2	1.78	0.46
1:A:1092:ILE:C	1:A:1092:ILE:HD13	2.35	0.46
1:A:1178:ARG:NH2	1:F:1181:LYS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1228:ILE:HB	1:D:1229:PRO:HA	1.98	0.46
1:A:1007:PHE:HD2	1:A:1008:HIS:CE1	2.33	0.46
1:B:1107:VAL:O	1:B:1151:THR:HA	2.15	0.46
1:E:1122:HIS:HD2	1:F:1161:THR:OG1	1.98	0.46
1:F:1220:ILE:HG13	1:F:1221:VAL:CG2	2.46	0.46
1:A:1027:ASP:HB3	1:A:1030:ARG:CD	2.44	0.46
1:C:1168:ARG:HG3	1:C:1223:ARG:NH2	2.30	0.46
1:C:1161:THR:OG1	1:D:1122:HIS:CD2	2.67	0.46
1:B:1016:LEU:HD22	1:B:1084:LEU:HB3	1.98	0.45
1:B:1030:ARG:NH1	1:B:1238:GLU:OE2	2.49	0.45
1:C:1122:HIS:HD2	1:D:1161:THR:OG1	2.00	0.45
1:D:1090:LEU:HD11	1:D:1252:LEU:HD12	1.98	0.45
1:B:1092:ILE:HD11	1:B:1241:ALA:HB1	1.97	0.45
1:C:1163:TYR:CB	1:C:1164:PRO:HD3	2.41	0.45
1:D:1231:ALA:HA	1:D:1234:MET:HE2	1.98	0.45
1:A:1122:HIS:CD2	1:B:1165:GLY:HA3	2.51	0.45
1:D:1027:ASP:HA	1:D:1028:PRO:HD2	1.79	0.45
1:F:1025:PRO:O	1:F:1066:SER:HA	2.16	0.45
1:F:1231:ALA:HB1	1:F:1233:THR:HB	1.98	0.45
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.17	0.45
1:D:1236:GLN:HE21	1:D:1240:HIS:CE1	2.35	0.45
1:F:1105:GLY:O	1:F:1238:GLU:HG2	2.17	0.45
1:D:1092:ILE:CD1	1:D:1242:VAL:HA	2.47	0.45
1:C:1234:MET:HB2	1:C:1234:MET:HE3	1.84	0.44
1:E:1163:TYR:HB2	1:E:1164:PRO:HD2	1.98	0.44
1:A:1122:HIS:HD2	1:B:1165:GLY:HA3	1.82	0.44
1:C:1057:LEU:CG	1:C:1250:ARG:HG2	2.47	0.44
1:D:1129:PRO:HG3	1:E:1113:SER:C	2.38	0.44
1:E:1228:ILE:HG22	1:E:1229:PRO:CD	2.48	0.44
1:E:1057:LEU:HB3	1:E:1253:LEU:HD11	1.99	0.44
1:C:1021:LEU:HD23	1:C:1021:LEU:C	2.37	0.44
1:C:1027:ASP:HB3	1:C:1030:ARG:HG2	1.99	0.44
1:E:1040:LYS:N	1:E:1041:PRO:HD3	2.32	0.44
1:D:1021:LEU:HD23	1:D:1021:LEU:C	2.38	0.44
1:F:1231:ALA:H	1:F:1232:GLU:CA	2.30	0.44
1:A:1228:ILE:HA	1:A:1229:PRO:HD3	1.84	0.44
1:B:1031:VAL:HG13	1:B:1064:VAL:HG12	1.99	0.44
1:D:1016:LEU:HD22	1:D:1084:LEU:HB3	2.00	0.44
1:D:1240:HIS:O	1:D:1244:ILE:HG13	2.18	0.44
1:A:1105:GLY:HA2	1:A:1237:THR:HG23	1.99	0.43
1:E:1017:GLN:HG3	1:E:1054:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1143:ALA:HB1	1:F:1247:GLU:HB3	2.00	0.43
1:B:1027:ASP:HA	1:B:1028:PRO:HD2	1.86	0.43
1:D:1037:LEU:HD12	1:D:1242:VAL:HG12	2.00	0.43
1:C:1199:SER:HB3	1:C:1215:MET:CE	2.48	0.43
1:D:1230:ASN:O	1:D:1234:MET:HG3	2.19	0.43
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.49	0.43
1:B:1007:PHE:CD2	1:B:1008:HIS:CE1	3.06	0.43
1:F:1093:GLY:CA	5:F:16:GOL:H11	2.49	0.43
1:A:1030:ARG:HG2	1:A:1033:LYS:HZ2	1.84	0.43
1:C:1143:ALA:O	1:C:1147:ILE:HG12	2.18	0.43
1:D:1048:ARG:HB3	1:D:1049:GLU:OE2	2.19	0.43
1:E:1049:GLU:HB3	1:F:1049:GLU:HG3	2.01	0.43
1:B:1115[A]:ARG:NH2	1:B:1128:PHE:HB3	2.34	0.43
1:B:1249:ALA:O	1:B:1253:LEU:HG	2.19	0.43
1:E:1056:GLU:OE2	1:E:1059:GLY:HA2	2.19	0.43
1:B:1089:PHE:O	1:B:1213:ALA:HA	2.19	0.42
1:F:1038:MET:HG2	1:F:1057:LEU:HD13	2.00	0.42
1:C:1240:HIS:O	1:C:1244:ILE:HG13	2.19	0.42
1:D:1238:GLU:O	1:D:1242:VAL:HG23	2.20	0.42
1:F:1026:GLY:H	5:F:16:GOL:H31	1.85	0.42
1:A:1125:PRO:HB2	1:A:1127:GLU:OE1	2.19	0.42
1:C:1007:PHE:HD2	1:C:1008:HIS:CE1	2.38	0.42
1:D:1220:ILE:HD12	1:D:1221:VAL:HG12	2.00	0.42
1:F:1012:THR:HG22	1:F:1013:LYS:N	2.33	0.42
1:C:1098:ILE:O	1:C:1188[A]:GLN:HG2	2.19	0.42
1:D:1128:PHE:HA	1:D:1129:PRO:HD3	1.85	0.42
1:E:1030:ARG:NE	1:E:1030:ARG:HA	2.35	0.42
1:F:1228:ILE:HG22	6:F:1298:HOH:O	2.20	0.42
1:A:1030:ARG:HD2	1:A:1238:GLU:OE2	2.19	0.42
1:A:1037:LEU:CD1	1:A:1242:VAL:HG12	2.50	0.42
1:B:1099:GLN:HA	1:B:1100:PRO:HD3	1.93	0.42
1:C:1242:VAL:O	1:C:1245:VAL:HG12	2.19	0.42
1:F:1230:ASN:N	1:F:1231:ALA:HA	2.34	0.42
1:E:1004:SER:HB3	1:E:1012:THR:CG2	2.50	0.42
1:C:1058:ASP:OD2	1:C:1250:ARG:HD2	2.20	0.41
1:D:1030:ARG:CZ	1:D:1033:LYS:HD2	2.50	0.41
1:F:1012:THR:HG22	1:F:1014:ASN:N	2.29	0.41
1:F:1197:MET:SD	3:F:6:ANU:H3'	2.60	0.41
1:E:1144:ALA:HA	1:E:1244:ILE:HG12	2.02	0.41
1:F:1221:VAL:HG21	1:F:1229:PRO:HD3	2.02	0.41
1:C:1107:VAL:HG21	1:C:1244:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:TYR:CB	1:A:1164:PRO:CD	2.99	0.41
1:F:1233:THR:HG23	1:F:1234:MET:C	2.40	0.41
1:C:1168:ARG:HB3	6:C:1306:HOH:O	2.21	0.41
1:F:1163:TYR:CB	1:F:1164:PRO:CD	2.99	0.41
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	2.02	0.41
1:C:1057:LEU:HA	1:C:1057:LEU:HD12	1.91	0.41
1:D:1038:MET:HB3	1:D:1056:GLU:O	2.21	0.41
1:F:1247:GLU:O	1:F:1250:ARG:HB3	2.21	0.41
1:A:1242:VAL:O	1:A:1245:VAL:HG12	2.21	0.41
1:D:1038:MET:HG2	1:D:1057:LEU:HG	2.01	0.41
1:D:1111:THR:HG23	1:D:1153:VAL:HG12	2.03	0.41
1:E:1236:GLN:O	1:E:1240:HIS:HB2	2.20	0.41
1:F:1084:LEU:HD12	1:F:1084:LEU:HA	1.92	0.41
1:D:1096:GLY:HA2	1:D:1221:VAL:HG13	2.03	0.41
1:F:1231:ALA:H	1:F:1232:GLU:CG	2.25	0.41
1:B:1127:GLU:HG3	1:F:1126:MET:HE3	2.03	0.41
1:F:1042:VAL:HG11	1:F:1054:ARG:HH12	1.86	0.40
1:B:1057:LEU:HA	1:B:1057:LEU:HD12	1.90	0.40
1:B:1156:THR:HG21	1:B:1196:GLU:HG3	2.02	0.40
1:F:1253:LEU:HA	1:F:1253:LEU:HD23	1.79	0.40
1:A:1044:LEU:HD11	1:A:1054:ARG:HB2	2.03	0.40
1:E:1024:VAL:HB	1:E:1067:THR:HG23	2.02	0.40
1:E:1228:ILE:CG2	1:E:1229:PRO:CD	2.99	0.40
1:E:1239:SER:O	1:E:1243:LYS:HG3	2.22	0.40
1:F:1021:LEU:HD23	1:F:1022:ALA:N	2.37	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	253/252 (100%)	249 (98%)	3 (1%)	1 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	236/252 (94%)	232 (98%)	3 (1%)	1 (0%)	34 37
1	C	245/252 (97%)	239 (98%)	5 (2%)	1 (0%)	34 37
1	D	249/252 (99%)	239 (96%)	6 (2%)	4 (2%)	9 7
1	E	248/252 (98%)	243 (98%)	4 (2%)	1 (0%)	34 37
1	F	243/252 (96%)	237 (98%)	5 (2%)	1 (0%)	34 37
All	All	1474/1512 (98%)	1439 (98%)	26 (2%)	9 (1%)	25 26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1229	PRO
1	A	1163	TYR
1	C	1163	TYR
1	F	1163	TYR
1	B	1163	TYR
1	D	1228	ILE
1	E	1163	TYR
1	D	1163	TYR
1	D	1227	GLU

5.3.2 Protein sidechains (i)

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	204/201 (102%)	199 (98%)	5 (2%)	47 60
1	B	190/201 (94%)	186 (98%)	4 (2%)	53 67
1	C	199/201 (99%)	194 (98%)	5 (2%)	47 60
1	D	199/201 (99%)	190 (96%)	9 (4%)	27 34
1	E	199/201 (99%)	190 (96%)	9 (4%)	27 34
1	F	196/201 (98%)	187 (95%)	9 (5%)	27 34
All	All	1187/1206 (98%)	1146 (96%)	41 (4%)	36 46

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1179	ARG
1	A	1196	GLU
1	A	1233	THR
1	A	1240	HIS
1	B	1084	LEU
1	B	1179	ARG
1	B	1196	GLU
1	B	1225	GLN
1	C	1003	LYS
1	C	1084	LEU
1	C	1170	ASP
1	C	1179	ARG
1	C	1196	GLU
1	D	1043	LYS
1	D	1084	LEU
1	D	1142	GLU
1	D	1176	VAL
1	D	1179	ARG
1	D	1186	GLU
1	D	1196	GLU
1	D	1239	SER
1	D	1250	ARG
1	E	1084	LEU
1	E	1092	ILE
1	E	1104	VAL
1	E	1179	ARG
1	E	1186	GLU
1	E	1196	GLU
1	E	1227	GLU
1	E	1236	GLN
1	E	1240	HIS
1	F	1013	LYS
1	F	1042	VAL
1	F	1084	LEU
1	F	1104	VAL
1	F	1170	ASP
1	F	1196	GLU
1	F	1228	ILE
1	F	1233	THR
1	F	1247	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	HIS
1	A	1122	HIS
1	A	1209	GLN
1	B	1122	HIS
1	B	1209	GLN
1	C	1122	HIS
1	C	1209	GLN
1	C	1236	GLN
1	D	1122	HIS
1	D	1209	GLN
1	D	1236	GLN
1	E	1122	HIS
1	E	1209	GLN
1	F	1017	GLN
1	F	1122	HIS
1	F	1209	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	GOL	F	16	-	5,5,5	0.40	0	5,5,5	0.18	0
3	ANU	B	2	-	16,18,18	1.17	1 (6%)	13,27,27	1.11	0
4	1PE	B	62	-	15,15,15	0.45	0	14,14,14	0.34	0
3	ANU	F	6	-	16,18,18	1.20	1 (6%)	13,27,27	1.23	1 (7%)
4	1PE	D	314	-	15,15,15	0.47	0	14,14,14	0.41	0
4	1PE	B	315	-	15,15,15	0.48	0	14,14,14	0.35	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	GOL	F	16	-	-	2/4/4/4	-
3	ANU	B	2	-	-	2/2/26/26	0/3/3/3
4	1PE	B	62	-	-	7/13/13/13	-
3	ANU	F	6	-	-	2/2/26/26	0/3/3/3
4	1PE	D	314	-	-	8/13/13/13	-
4	1PE	B	315	-	-	9/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	ANU	O2-C2'	-2.09	1.43	1.45
3	B	2	ANU	O2-C2'	-2.02	1.43	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6	ANU	C5'-C4'-C3'	-2.12	109.97	115.09

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	16	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	F	6	ANU	C3'-C4'-C5'-O5'
3	F	6	ANU	O4'-C4'-C5'-O5'
4	D	314	1PE	OH4-C13-C23-OH3
4	D	314	1PE	OH6-C15-C25-OH5
3	B	2	ANU	O4'-C4'-C5'-O5'
4	B	315	1PE	OH2-C12-C22-OH3
3	B	2	ANU	C3'-C4'-C5'-O5'
4	B	62	1PE	OH5-C14-C24-OH4
4	B	62	1PE	OH7-C16-C26-OH6
4	B	315	1PE	OH7-C16-C26-OH6
4	B	315	1PE	OH6-C15-C25-OH5
5	F	16	GOL	O1-C1-C2-O2
4	D	314	1PE	OH5-C14-C24-OH4
4	B	62	1PE	OH6-C15-C25-OH5
4	B	315	1PE	OH5-C14-C24-OH4
4	B	315	1PE	OH4-C13-C23-OH3
4	B	315	1PE	C25-C15-OH6-C26
4	B	62	1PE	C24-C14-OH5-C25
4	B	62	1PE	C16-C26-OH6-C15
4	D	314	1PE	C16-C26-OH6-C15
4	B	315	1PE	C16-C26-OH6-C15
4	D	314	1PE	C14-C24-OH4-C13
4	B	62	1PE	C15-C25-OH5-C14
4	B	315	1PE	C13-C23-OH3-C22
4	B	315	1PE	C24-C14-OH5-C25
4	D	314	1PE	C24-C14-OH5-C25
4	B	62	1PE	C13-C23-OH3-C22
4	D	314	1PE	C25-C15-OH6-C26
4	D	314	1PE	C13-C23-OH3-C22

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	16	GOL	6	0
3	F	6	ANU	1	0
4	B	315	1PE	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	252/252 (100%)	-0.14	8 (3%)	47	45	8, 13, 39, 57	0
1	B	239/252 (94%)	-0.21	4 (1%)	70	68	8, 15, 33, 54	0
1	C	247/252 (98%)	-0.07	11 (4%)	33	32	7, 15, 39, 60	0
1	D	251/252 (99%)	0.18	12 (4%)	30	29	9, 18, 48, 60	0
1	E	250/252 (99%)	0.23	17 (6%)	17	16	9, 20, 53, 60	0
1	F	247/252 (98%)	-0.02	10 (4%)	38	36	9, 16, 38, 60	1 (0%)
All	All	1486/1512 (98%)	-0.00	62 (4%)	36	34	7, 16, 43, 60	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1228	ILE	11.0
1	E	1228	ILE	8.9
1	F	1233	THR	8.3
1	F	1234	MET	7.4
1	E	1226	GLN	6.5
1	D	1231	ALA	6.4
1	E	1231	ALA	6.2
1	D	1226	GLN	6.2
1	E	1230	ASN	6.0
1	C	1231	ALA	5.4
1	D	1229	PRO	5.4
1	E	1236	GLN	5.4
1	E	1229	PRO	5.3
1	A	1231	ALA	5.0
1	F	1231	ALA	4.9
1	E	1233	THR	4.8
1	C	1232	GLU	4.7
1	C	1236	GLN	4.7
1	C	1233	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	1227	GLU	4.4
1	F	1232	GLU	4.1
1	E	1232	GLU	4.0
1	D	1227	GLU	3.9
1	F	1238	GLU	3.8
1	D	1234	MET	3.7
1	D	1233	THR	3.6
1	E	1234	MET	3.5
1	E	1221	VAL	3.4
1	D	1230	ASN	3.4
1	A	1232	GLU	3.4
1	B	1238	GLU	3.3
1	A	1235	LYS	3.3
1	A	1233	THR	3.3
1	A	1230	ASN	3.2
1	D	1236	GLN	3.2
1	C	1230	ASN	3.1
1	E	1238	GLU	3.1
1	D	1220	ILE	3.1
1	E	1235	LYS	3.1
1	E	1239	SER	3.0
1	F	1239	SER	2.9
1	E	1005	ASP	2.8
1	F	1230	ASN	2.8
1	E	1237	THR	2.7
1	C	1225[A]	GLN	2.7
1	E	1004	SER	2.7
1	A	1236	GLN	2.6
1	D	1225	GLN	2.6
1	B	1004	SER	2.5
1	C	1220	ILE	2.5
1	A	1002	SER	2.4
1	C	1235	LYS	2.4
1	B	1225	GLN	2.4
1	C	1253	LEU	2.3
1	F	1147	ILE	2.3
1	F	1004	SER	2.2
1	C	1240	HIS	2.2
1	A	1229	PRO	2.2
1	C	1234	MET	2.0
1	D	1007	PHE	2.0
1	B	1063	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	1059	GLY	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, 95^{th} 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	1PE	B	62	16/16	0.77	0.20	37,46,54,56	0
4	1PE	D	314	16/16	0.78	0.25	35,43,56,57	0
4	1PE	B	315	16/16	0.79	0.25	33,40,50,51	0
3	ANU	F	6	16/16	0.84	0.15	20,27,33,37	0
3	ANU	B	2	16/16	0.84	0.20	25,35,44,45	0
5	GOL	F	16	6/6	0.88	0.20	27,29,33,33	0
2	K	E	502	1/1	0.93	0.12	18,18,18,18	0
2	K	A	503	1/1	0.99	0.04	8,8,8,8	0
2	K	C	501	1/1	0.99	0.05	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.