Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 02:08 AM EDT

PDB ID	:	1BRW
Title	:	THE CRYSTAL STRUCTURE OF PYRIMIDINE NUCLEOSIDE PHOSPHORYLASE IN A CLOSED CONFORMATION
Authors	:	Pugmire, M.J.; Ealick, S.E.
Deposited on	:	1998-08-25
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

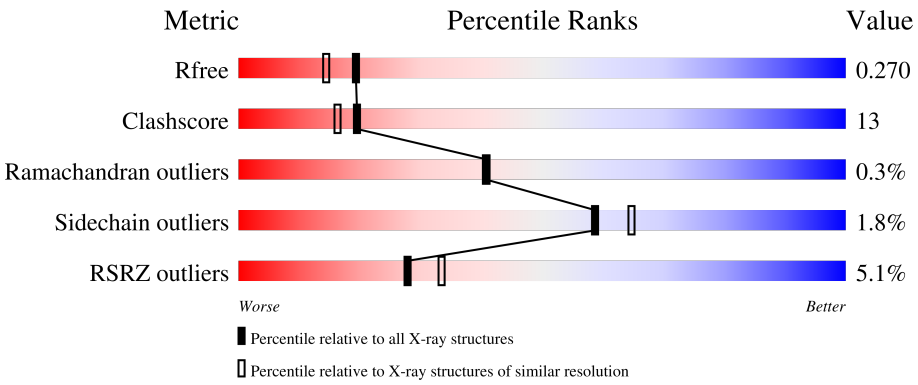
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	433	3% 86% 14%
1	B	433	7% 78% 21% •

2 Entry composition (i)

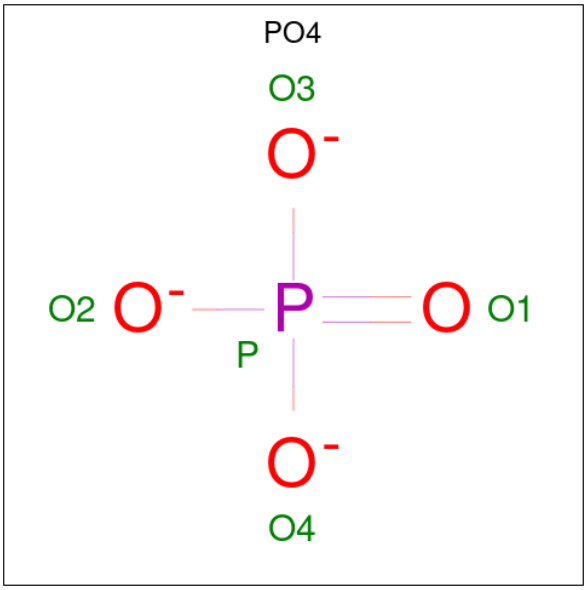
There are 6 unique types of molecules in this entry. The entry contains 6592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (PYRIMIDINE NUCLEOSIDE PHOSPHORYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3217	2021	558	620	18	0	0	0
1	B	433	3221	2024	559	620	18	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

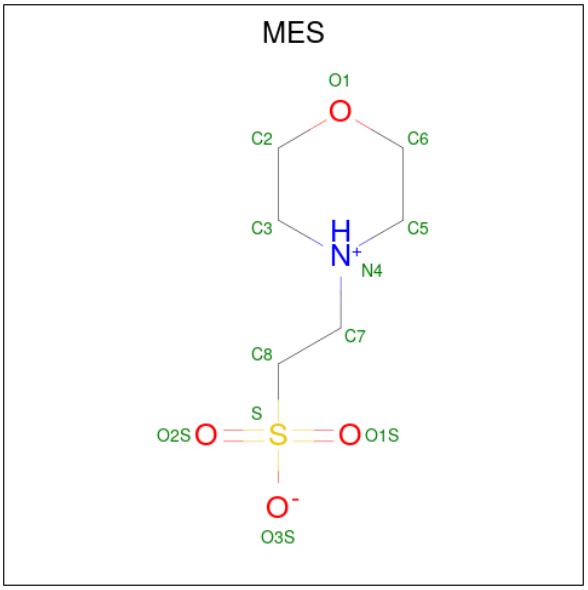


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

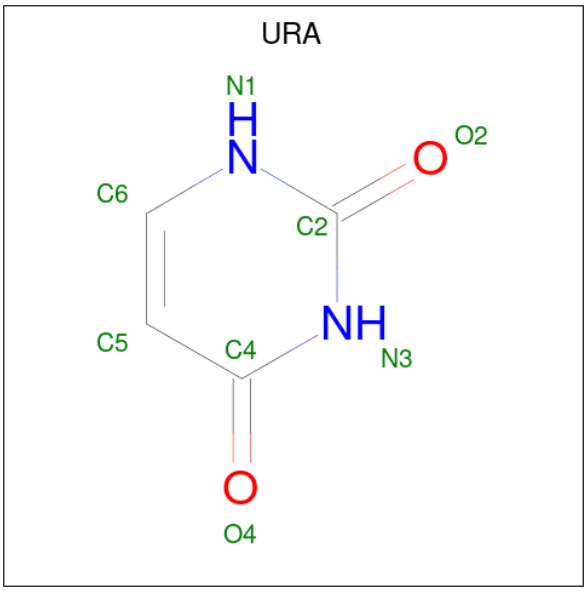
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0

- Molecule 5 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



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

- Molecule 6 is water.

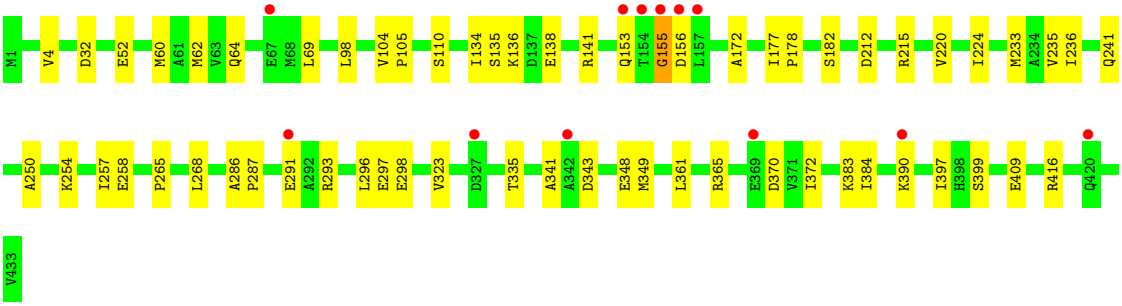
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	68	68	68	0	0
			Total	O		
6	B	42	42	42	0	0

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.

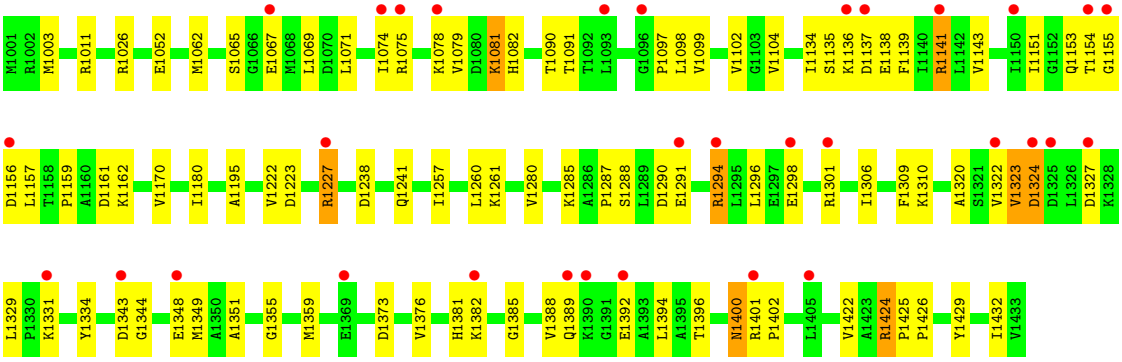
• Molecule 1: PROTEIN (PYRIMIDINE NUCLEOSIDE PHOSPHORYLASE)

Chain A:



• Molecule 1: PROTEIN (PYRIMIDINE NUCLEOSIDE PHOSPHORYLASE)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.57Å 70.45Å 122.78Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 28.12 – 1.99	Depositor EDS
% Data completeness (in resolution range)	82.9 (30.00-2.10) 83.7 (28.12-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.98Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.232 , 0.276 0.234 , 0.270	Depositor DCC
R_{free} test set	2756 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6592	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, URA, PO4, MES

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	0.52	1/3257 (0.0%)	0.67	1/4401 (0.0%)
1	B	0.56	2/3261 (0.1%)	0.71	9/4405 (0.2%)
All	All	0.54	3/6518 (0.0%)	0.69	10/8806 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLY	C-N	-17.63	0.93	1.34
1	B	1324	ASP	C-N	-14.80	1.00	1.34
1	B	1323	VAL	C-N	-11.54	1.07	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	GLY	C-N-CA	15.06	159.34	121.70
1	B	1324	ASP	C-N-CA	10.12	147.00	121.70
1	B	1227	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	B	1294	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	1301	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	B	1141	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	B	1075	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	B	1401	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	B	1323	VAL	C-N-CA	-5.54	107.86	121.70
1	B	1323	VAL	O-C-N	5.26	131.11	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3217	0	3324	41	0
1	B	3221	0	3331	130	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	2	0
5	B	8	0	3	1	0
6	A	68	0	0	0	0
6	B	42	0	0	3	0
All	All	6592	0	6684	169	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 13.

All (169) 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:1074:ILE:HB	1:B:1078:LYS:CE	1.42	1.46
1:B:1074:ILE:HD12	1:B:1078:LYS:NZ	1.37	1.39
1:A:287:PRO:CD	1:A:291:GLU:OE1	1.78	1.31
1:B:1382:LYS:HD3	1:B:1388:VAL:CG1	1.61	1.29
1:A:287:PRO:HD2	1:A:291:GLU:OE1	1.15	1.28
1:B:1074:ILE:CB	1:B:1078:LYS:CE	2.26	1.14
1:B:1071:LEU:HB3	1:B:1078:LYS:NZ	1.63	1.12
1:B:1136:LYS:HE3	1:B:1156:ASP:CB	1.80	1.12
1:A:287:PRO:HD2	1:A:291:GLU:CD	1.70	1.11
1:B:1154:THR:HB	1:B:1162:LYS:NZ	1.61	1.10
1:B:1074:ILE:CD1	1:B:1078:LYS:NZ	2.12	1.10
1:B:1074:ILE:CB	1:B:1078:LYS:HE2	1.81	1.08
1:B:1153:GLN:O	1:B:1154:THR:OG1	1.71	1.08
1:B:1223:ASP:O	1:B:1227:ARG:HG3	1.51	1.08
1:B:1382:LYS:HD3	1:B:1388:VAL:HG11	1.36	1.07
1:B:1074:ILE:CG1	1:B:1078:LYS:HZ1	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1136:LYS:HE3	1:B:1156:ASP:HB2	1.12	1.06
1:B:1382:LYS:HD3	1:B:1388:VAL:HG12	1.38	1.06
1:B:1074:ILE:HB	1:B:1078:LYS:HE3	1.39	1.04
1:A:287:PRO:CG	1:A:291:GLU:OE1	2.08	1.02
1:B:1382:LYS:HD2	1:B:1394:LEU:HD23	1.40	1.02
1:B:1074:ILE:CG2	1:B:1078:LYS:HE2	1.92	0.98
1:B:1074:ILE:HD12	1:B:1078:LYS:HZ3	0.87	0.98
1:B:1074:ILE:HB	1:B:1078:LYS:NZ	1.77	0.98
1:B:1074:ILE:HB	1:B:1078:LYS:HE2	1.34	0.97
1:B:1348:GLU:HG2	1:B:1349:MET:H	1.27	0.97
1:B:1294:ARG:O	1:B:1298:GLU:HG3	1.67	0.95
1:B:1071:LEU:HB3	1:B:1078:LYS:HZ2	1.29	0.93
1:B:1382:LYS:CD	1:B:1388:VAL:CG1	2.45	0.93
1:A:110:SER:O	1:A:153:GLN:HG3	1.73	0.88
1:B:1382:LYS:CD	1:B:1388:VAL:HG12	2.03	0.87
1:B:1074:ILE:CD1	1:B:1078:LYS:HZ1	1.83	0.86
1:B:1348:GLU:HG2	1:B:1349:MET:N	1.91	0.86
1:B:1074:ILE:CB	1:B:1078:LYS:HZ1	1.90	0.84
1:B:1382:LYS:CD	1:B:1388:VAL:HG11	2.09	0.83
1:B:1154:THR:HB	1:B:1162:LYS:HZ2	1.41	0.82
1:A:287:PRO:CD	1:A:291:GLU:CD	2.39	0.82
1:A:52:GLU:HG3	1:A:220:VAL:HG23	1.63	0.80
1:B:1074:ILE:HG21	1:B:1078:LYS:HE2	1.63	0.80
1:B:1074:ILE:CG1	1:B:1078:LYS:NZ	2.42	0.79
1:B:1323:VAL:HG23	1:B:1324:ASP:OD1	1.82	0.79
1:B:1071:LEU:CB	1:B:1078:LYS:HZ2	1.97	0.78
1:A:287:PRO:HG2	1:A:291:GLU:OE1	1.83	0.77
1:B:1382:LYS:CE	1:B:1388:VAL:HG12	2.15	0.76
1:B:1136:LYS:HE2	1:B:1157:LEU:HG	1.69	0.75
1:B:1071:LEU:HB3	1:B:1078:LYS:HZ3	1.52	0.74
1:B:1348:GLU:CG	1:B:1349:MET:H	2.00	0.74
1:B:1137:ASP:O	1:B:1141:ARG:HG3	1.88	0.74
1:B:1074:ILE:CB	1:B:1078:LYS:NZ	2.44	0.73
1:B:1154:THR:OG1	1:B:1162:LYS:HE3	1.76	0.72
1:B:1382:LYS:HD2	1:B:1394:LEU:CD2	2.19	0.72
1:A:341:ALA:O	1:A:390:LYS:HG3	1.91	0.70
1:B:1310:LYS:HE2	1:B:1323:VAL:HG21	1.72	0.69
1:B:1343:ASP:OD1	1:B:1388:VAL:O	2.10	0.68
1:B:1400:ASN:HD22	1:B:1400:ASN:H	1.38	0.68
1:B:1327:ASP:HA	1:B:1331:LYS:HE3	1.75	0.68
1:B:1382:LYS:HZ1	1:B:1392:GLU:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:ASP:HA	1:B:1331:LYS:CE	2.25	0.65
1:A:172:ALA:HB1	1:B:1011:ARG:NH1	2.11	0.65
1:B:1074:ILE:HD12	1:B:1078:LYS:CE	2.27	0.64
1:A:134:ILE:HG23	1:A:138:GLU:HB2	1.80	0.64
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.61	0.64
1:B:1074:ILE:CD1	1:B:1078:LYS:CE	2.76	0.63
1:B:1382:LYS:HZ1	1:B:1392:GLU:CB	2.12	0.63
1:B:1135:SER:OG	1:B:1138:GLU:HG3	1.99	0.61
1:B:1320:ALA:O	1:B:1323:VAL:HG22	2.00	0.61
1:B:1069:LEU:HD21	1:B:1136:LYS:HB3	1.82	0.60
1:B:1153:GLN:HG2	1:B:1154:THR:HG23	1.83	0.59
1:B:1071:LEU:CB	1:B:1078:LYS:NZ	2.52	0.59
1:B:1071:LEU:CA	1:B:1078:LYS:HZ2	2.16	0.59
1:B:1071:LEU:HB3	1:B:1078:LYS:CE	2.33	0.58
1:B:1382:LYS:HZ2	1:B:1388:VAL:HB	1.69	0.58
1:B:1382:LYS:NZ	1:B:1392:GLU:HB2	2.18	0.58
1:A:241:GLN:NE2	1:A:383:LYS:HE2	2.20	0.57
1:B:1257:ILE:HG12	1:B:1309:PHE:HE2	1.69	0.57
1:B:1322:VAL:HG13	1:B:1329:LEU:HG	1.87	0.57
1:B:1081:LYS:HD2	1:B:1082:HIS:N	2.20	0.56
1:B:1026:ARG:HD3	4:B:6001:MES:O1S	2.06	0.56
1:A:172:ALA:HB1	1:B:1011:ARG:HH11	1.69	0.55
1:B:1136:LYS:CE	1:B:1156:ASP:CB	2.71	0.55
1:A:365:ARG:NH2	1:A:372:ILE:HG12	2.21	0.55
1:A:241:GLN:HE22	1:A:384:ILE:H	1.54	0.55
1:B:1343:ASP:OD1	1:B:1344:GLY:N	2.41	0.54
1:B:1071:LEU:O	1:B:1078:LYS:NZ	2.39	0.54
1:B:1071:LEU:HB3	1:B:1078:LYS:CD	2.38	0.54
1:B:1261:LYS:HG3	1:B:1306:ILE:HG21	1.90	0.53
1:A:365:ARG:HB2	1:A:370:ASP:HB2	1.91	0.53
1:B:1071:LEU:C	1:B:1078:LYS:HZ2	2.12	0.53
1:B:1287:PRO:HG2	1:B:1291:GLU:HG3	1.91	0.52
1:A:265:PRO:HG2	1:A:268:LEU:HB3	1.91	0.52
1:B:1153:GLN:C	1:B:1154:THR:HG1	1.89	0.52
1:A:254:LYS:O	1:A:258:GLU:HG3	2.10	0.52
1:B:1382:LYS:NZ	1:B:1388:VAL:HB	2.24	0.52
1:A:241:GLN:HE22	1:A:383:LYS:HB3	1.74	0.51
1:B:1052:GLU:CG	1:B:1227:ARG:HH22	2.24	0.51
1:B:1074:ILE:HG13	1:B:1078:LYS:HZ1	1.65	0.51
1:B:1071:LEU:HD13	1:B:1078:LYS:HD3	1.93	0.51
1:A:69:LEU:HD22	1:A:136:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1382:LYS:NZ	1:B:1388:VAL:CG1	2.74	0.50
1:A:4:VAL:HG13	6:B:4032:HOH:O	2.10	0.50
1:B:1154:THR:CB	1:B:1162:LYS:NZ	2.39	0.50
1:B:1400:ASN:H	1:B:1400:ASN:ND2	2.08	0.50
1:B:1400:ASN:HD22	1:B:1400:ASN:N	2.02	0.50
1:A:361:LEU:HD11	1:A:399:SER:HB3	1.94	0.50
1:B:1382:LYS:NZ	1:B:1388:VAL:HG12	2.27	0.50
1:B:1385:GLY:HA2	1:B:1422:VAL:HG13	1.94	0.49
1:B:1052:GLU:HG2	1:B:1227:ARG:HH22	1.77	0.49
1:B:1280:VAL:HG13	1:B:1285:LYS:HB2	1.94	0.49
1:B:1288:SER:OG	1:B:1291:GLU:HG2	2.12	0.49
1:B:1223:ASP:O	1:B:1227:ARG:CG	2.43	0.49
1:A:134:ILE:CG2	1:A:138:GLU:HB2	2.43	0.49
1:A:250:ALA:O	1:A:254:LYS:HG3	2.13	0.48
1:B:1334:TYR:CZ	1:B:1402:PRO:HG3	2.47	0.48
1:B:1382:LYS:NZ	1:B:1392:GLU:CB	2.74	0.48
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.27	0.48
1:B:1382:LYS:HZ2	1:B:1388:VAL:CG1	2.27	0.48
1:B:1136:LYS:HE3	1:B:1156:ASP:HB3	1.84	0.48
1:A:60:MET:O	1:A:64:GLN:HG3	2.13	0.48
1:A:233:MET:HE2	1:A:235:VAL:HG13	1.96	0.47
1:B:1348:GLU:CG	1:B:1349:MET:N	2.62	0.47
1:B:1134:ILE:HG12	1:B:1151:ILE:HG21	1.96	0.47
1:B:1067:GLU:HB2	1:B:1136:LYS:NZ	2.29	0.47
1:B:1355:GLY:O	1:B:1359:MET:HG2	2.15	0.47
1:B:1260:LEU:O	1:B:1306:ILE:HG23	2.15	0.47
1:B:1238:ASP:HB2	1:B:1429:TYR:HE1	1.80	0.46
1:B:1139:PHE:O	1:B:1143:VAL:HG23	2.15	0.46
1:B:1062:MET:HE3	1:B:1161:ASP:HB2	1.97	0.46
1:A:335:THR:HA	1:A:397:ILE:O	2.17	0.45
1:B:1382:LYS:CE	1:B:1388:VAL:CG1	2.89	0.45
4:B:6001:MES:H31	4:B:6001:MES:H82	1.82	0.45
1:A:4:VAL:HG12	1:B:1170:VAL:O	2.17	0.44
1:A:104:VAL:HA	1:A:105:PRO:HD3	1.85	0.44
1:A:348:GLU:HB2	1:A:416:ARG:HB3	1.99	0.44
1:B:1071:LEU:HB3	1:B:1078:LYS:HD2	2.00	0.44
1:B:1071:LEU:CB	1:B:1078:LYS:HD2	2.48	0.44
1:A:293:ARG:O	1:A:297:GLU:HG3	2.18	0.44
1:B:1074:ILE:CD1	1:B:1078:LYS:HE2	2.47	0.44
1:B:1425:PRO:HA	1:B:1426:PRO:HD3	1.81	0.44
1:B:1067:GLU:HB2	1:B:1136:LYS:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:VAL:HG21	1:B:1280:VAL:HG22	2.00	0.43
1:A:286:ALA:HA	1:A:287:PRO:HD3	1.83	0.43
1:B:1155:GLY:O	1:B:1156:ASP:HB2	2.18	0.43
1:B:1381:HIS:HE1	1:B:1396:THR:OG1	2.02	0.43
1:A:62:MET:CE	1:A:182:SER:HB2	2.49	0.43
1:A:220:VAL:O	1:A:224:ILE:HG13	2.19	0.43
1:B:1074:ILE:CG1	1:B:1078:LYS:CE	2.94	0.43
1:B:1069:LEU:HG	1:B:1157:LEU:HD21	2.02	0.42
1:B:1097:PRO:HG2	1:B:1309:PHE:CD1	2.54	0.42
1:B:1373:ASP:OD2	1:B:1376:VAL:HG13	2.19	0.42
1:A:98:LEU:HG	1:A:296:LEU:HD22	2.02	0.41
1:B:1180:ILE:HG12	5:B:5001:URA:O4	2.19	0.41
1:B:1241:GLN:HA	1:B:1351:ALA:HB2	2.02	0.41
1:B:1291:GLU:HA	1:B:1291:GLU:OE1	2.20	0.41
1:B:1400:ASN:ND2	6:B:4108:HOH:O	2.52	0.41
1:A:135:SER:OG	1:A:138:GLU:HG3	2.20	0.41
1:B:1424:ARG:HD3	6:B:4099:HOH:O	2.21	0.41
1:B:1079:VAL:HG22	1:B:1195:ALA:HB3	2.01	0.41
1:A:177:ILE:HB	1:A:178:PRO:HD3	2.03	0.41
1:A:215:ARG:HA	1:A:236:ILE:HD11	2.02	0.41
1:A:257:ILE:HD13	1:A:323:VAL:HA	2.02	0.41
1:B:1098:LEU:HG	1:B:1296:LEU:HD22	2.02	0.41
1:B:1099:VAL:O	1:B:1102:VAL:HG22	2.21	0.41
1:B:1222:VAL:HG21	1:B:1432:ILE:HG22	2.03	0.41
1:B:1334:TYR:CE2	1:B:1402:PRO:HG3	2.56	0.41
1:B:1389:GLN:O	1:B:1392:GLU:HG2	2.19	0.41
1:B:1392:GLU:HA	1:B:1392:GLU:OE1	2.20	0.41
1:B:1065:SER:OG	1:B:1159:PRO:HD2	2.21	0.40
1:B:1382:LYS:HZ2	1:B:1388:VAL:CB	2.32	0.40
1:B:1154:THR:HB	1:B:1162:LYS:HZ1	1.73	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	431/433 (100%)	416 (96%)	13 (3%)	2 (0%)	29	26
1	B	431/433 (100%)	411 (95%)	19 (4%)	1 (0%)	47	49
All	All	862/866 (100%)	827 (96%)	32 (4%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY
1	A	156	ASP
1	B	1091	THR

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	336/337 (100%)	330 (98%)	6 (2%)	59	65
1	B	337/337 (100%)	331 (98%)	6 (2%)	59	65
All	All	673/674 (100%)	661 (98%)	12 (2%)	59	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	212	ASP
1	A	298	GLU
1	A	343	ASP
1	A	349	MET
1	A	409	GLU
1	B	1003	MET
1	B	1081	LYS
1	B	1090	THR
1	B	1290	ASP

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Mol	Chain	Res	Type
1	B	1400	ASN
1	B	1424	ARG

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

Mol	Chain	Res	Type
1	A	82	HIS
1	A	241	GLN
1	A	316	GLN
1	B	1249	ASN
1	B	1381	HIS
1	B	1400	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	URA	B	5001	-	8,8,8	1.78	2 (25%)	9,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	2001	-	4,4,4	2.03	1 (25%)	6,6,6	0.64	0
2	PO4	B	2002	-	4,4,4	1.95	1 (25%)	6,6,6	0.41	0
4	MES	A	6002	-	12,12,12	9.17	9 (75%)	14,16,16	2.49	5 (35%)
4	MES	B	6001	-	12,12,12	8.91	9 (75%)	14,16,16	2.64	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	B	6001	-	-	0/6/14/14	0/1/1/1
4	MES	A	6002	-	-	0/6/14/14	0/1/1/1
5	URA	B	5001	-	-	-	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6002	MES	C8-S	-24.05	1.43	1.77
4	B	6001	MES	C8-S	-23.25	1.44	1.77
4	A	6002	MES	O2S-S	11.96	1.80	1.45
4	B	6001	MES	O2S-S	11.83	1.79	1.45
4	A	6002	MES	O1S-S	11.74	1.79	1.45
4	B	6001	MES	O1S-S	11.57	1.79	1.45
4	A	6002	MES	O3S-S	9.29	1.80	1.47
4	B	6001	MES	O3S-S	9.07	1.79	1.47
4	A	6002	MES	C7-C8	-5.00	1.39	1.52
4	B	6001	MES	C7-C8	-4.82	1.39	1.52
2	A	2001	PO4	P-O1	3.68	1.59	1.50
5	B	5001	URA	C2-N1	3.56	1.41	1.36
2	B	2002	PO4	P-O1	3.28	1.58	1.50
4	A	6002	MES	C7-N4	-3.14	1.40	1.47
4	A	6002	MES	C3-C2	-3.13	1.38	1.50
4	B	6001	MES	C3-C2	-3.02	1.38	1.50
4	A	6002	MES	C5-C6	-2.93	1.39	1.50
4	B	6001	MES	C5-C6	-2.91	1.39	1.50
4	B	6001	MES	C7-N4	-2.64	1.41	1.47
4	A	6002	MES	C5-N4	-2.50	1.40	1.46
4	B	6001	MES	C5-N4	-2.42	1.40	1.46
5	B	5001	URA	C6-N1	2.19	1.39	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	6001	MES	O3S-S-C8	6.08	115.60	105.77
4	A	6002	MES	O3S-S-C8	5.61	114.84	105.77
4	B	6001	MES	O1S-S-C8	5.23	113.22	106.92
4	A	6002	MES	O1S-S-C8	4.88	112.79	106.92
4	A	6002	MES	O2S-S-C8	3.05	110.59	106.92
4	B	6001	MES	O2S-S-C8	2.89	110.39	106.92
4	B	6001	MES	O3S-S-O2S	-2.52	105.13	111.27
4	B	6001	MES	O2S-S-O1S	-2.44	105.49	113.95
4	A	6002	MES	O2S-S-O1S	-2.43	105.54	113.95
4	A	6002	MES	O3S-S-O2S	-2.15	106.01	111.27
4	B	6001	MES	O3S-S-O1S	-2.07	106.23	111.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5001	URA	1	0
4	B	6001	MES	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1323:VAL	C	1324:ASP	N	1.07
1	B	1324:ASP	C	1325:ASP	N	1.00
1	A	155:GLY	C	156:ASP	N	0.93

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	433/433 (100%)	-0.11	12 (2%)	53	59	7, 21, 39, 52	0
1	B	433/433 (100%)	0.38	32 (7%)	14	18	6, 30, 48, 60	0
All	All	866/866 (100%)	0.13	44 (5%)	28	33	6, 25, 45, 60	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1154	THR	8.2
1	A	154	THR	7.2
1	A	155	GLY	6.3
1	B	1141	ARG	5.9
1	B	1325	ASP	5.6
1	B	1324	ASP	5.5
1	B	1301	ARG	5.4
1	B	1343	ASP	4.9
1	B	1294	ARG	4.8
1	B	1389	GLN	4.7
1	A	156	ASP	4.6
1	B	1382	LYS	4.5
1	B	1075	ARG	4.5
1	B	1327	ASP	4.4
1	B	1156	ASP	4.0
1	B	1298	GLU	4.0
1	B	1136	LYS	3.9
1	A	369	GLU	3.7
1	B	1291	GLU	3.4
1	B	1390	LYS	3.2
1	B	1227	ARG	3.2
1	B	1401	ARG	3.2
1	B	1405	LEU	3.1
1	B	1392	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1369	GLU	3.1
1	B	1331	LYS	2.9
1	B	1067	GLU	2.9
1	B	1078	LYS	2.7
1	A	342	ALA	2.7
1	B	1322	VAL	2.6
1	B	1150	ILE	2.5
1	A	67	GLU	2.5
1	B	1348	GLU	2.5
1	A	420	GLN	2.4
1	B	1074	ILE	2.4
1	A	327	ASP	2.3
1	A	157	LEU	2.3
1	B	1096	GLY	2.3
1	A	153	GLN	2.3
1	A	291	GLU	2.2
1	B	1155	GLY	2.2
1	A	390	LYS	2.2
1	B	1137	ASP	2.1
1	B	1093	LEU	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 monosaccharides 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
5	URA	B	5001	8/8	0.68	0.21	25,33,37,37	0
3	CA	B	3002	1/1	0.79	0.10	22,22,22,22	0
4	MES	B	6001	12/12	0.94	0.14	30,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MES	A	6002	12/12	0.94	0.14	39,47,52,52	0
2	PO4	B	2002	5/5	0.97	0.15	12,17,24,28	0
2	PO4	A	2001	5/5	0.98	0.13	12,17,19,26	0
3	CA	A	3001	1/1	0.98	0.05	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.