



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:39 PM UTC

PDB ID : 1Y1R / pdb_00001y1r
Title : Crystal Structure of the Uridine Phosphorylase from Salmonella Typhimurium
in Complex with Inhibitor and Phosphate Ion at 2.11Å Resolution
Authors : Dontsova, M.V.; Gabdoulkhakov, A.G.; Kachalova, G.S.; Betzel, C.; Ealick,
S.E.; Mikhailov, A.M.
Deposited on : 2004-11-19
Resolution : 2.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

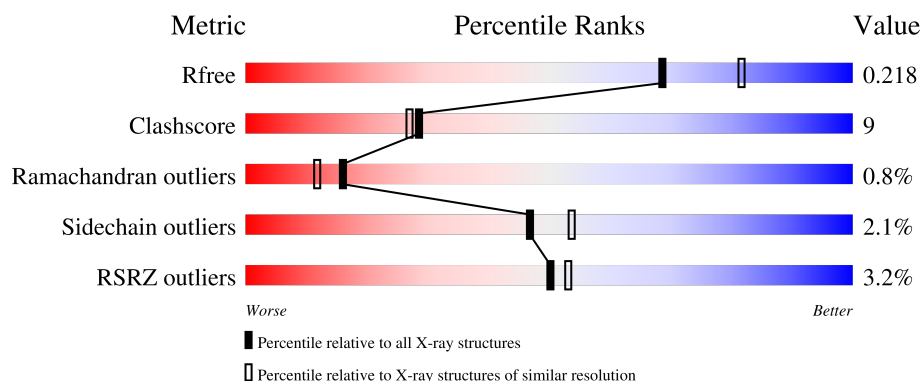
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	 6% 76% 19% ..
1	B	253	 2% 77% 17% . .
1	C	253	 2% 81% 13% . .
1	D	253	 4% 71% 23% . 5%
1	E	253	 2% 81% 13% . 5%

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Mol	Chain	Length	Quality of chain
1	F	253	2% 75% 17% • 5%

2 Entry composition [i](#)

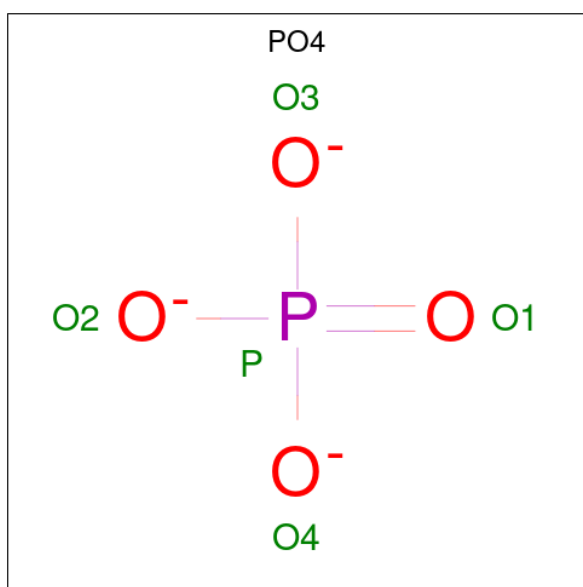
There are 4 unique types of molecules in this entry. The entry contains 11625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

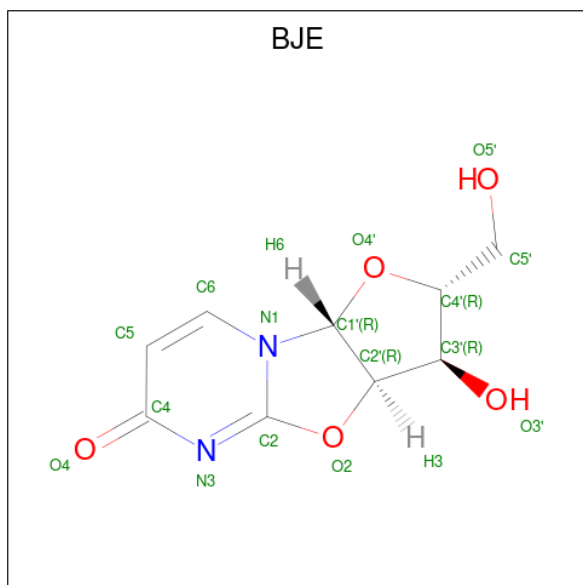
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1886	1180	332	362	12			
1	C	243	Total	C	N	O	S	0	0	0
			1824	1143	322	347	12			
1	D	241	Total	C	N	O	S	0	0	0
			1806	1132	318	344	12			
1	F	240	Total	C	N	O	S	0	0	0
			1800	1128	318	343	11			
1	E	241	Total	C	N	O	S	0	0	0
			1807	1132	319	345	11			
1	B	242	Total	C	N	O	S	0	0	0
			1814	1137	320	346	11			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is 2,2'-Anhydro-(1-beta-D-ribofuranosyl)uracil (CCD ID: BJE) (formula: $C_9H_{10}N_2O_5$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	122	Total O 122 122	0	0
4	C	109	Total O 109 109	0	0
4	D	82	Total O 82 82	0	0
4	F	95	Total O 95 95	0	0

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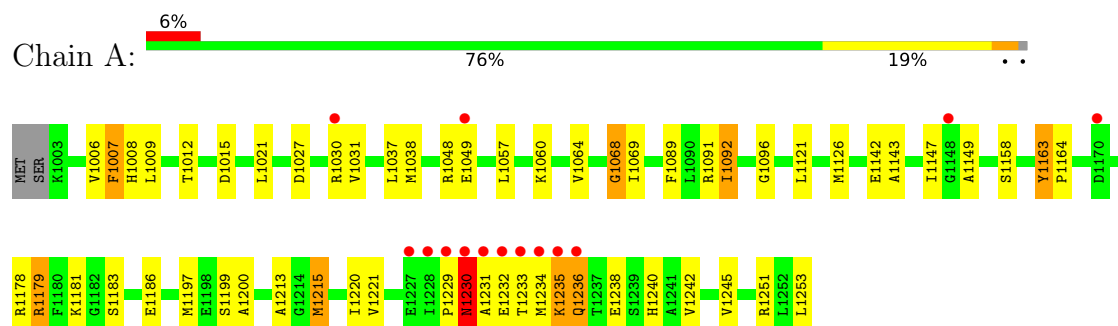
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	117	Total	O	0	0
			117	117		
4	B	116	Total	O	0	0
			116	116		

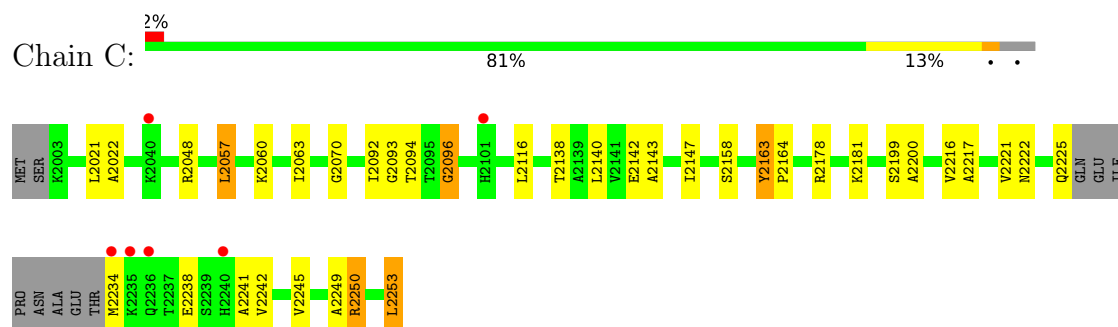
3 Residue-property plots [i](#)

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.

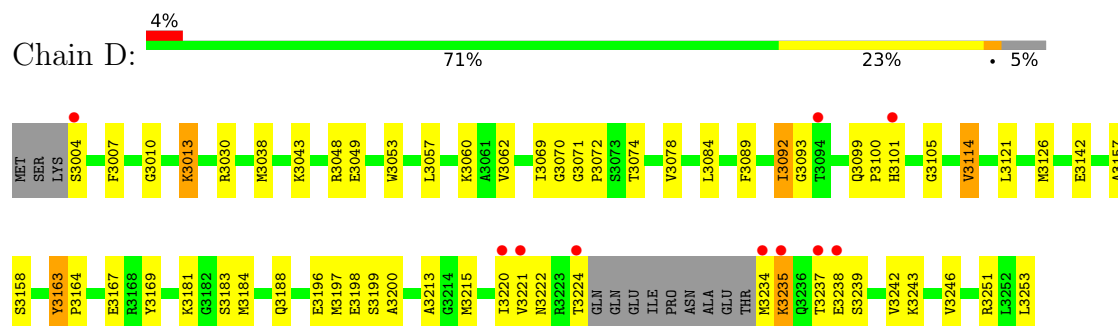
- Molecule 1: Uridine phosphorylase



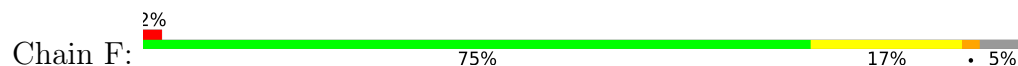
- Molecule 1: Uridine phosphorylase

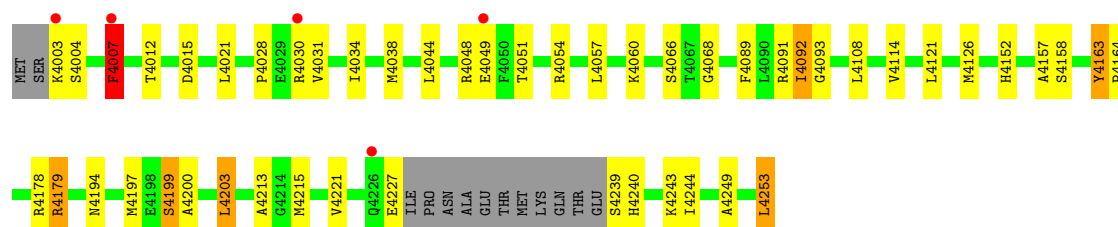


- Molecule 1: Uridine phosphorylase

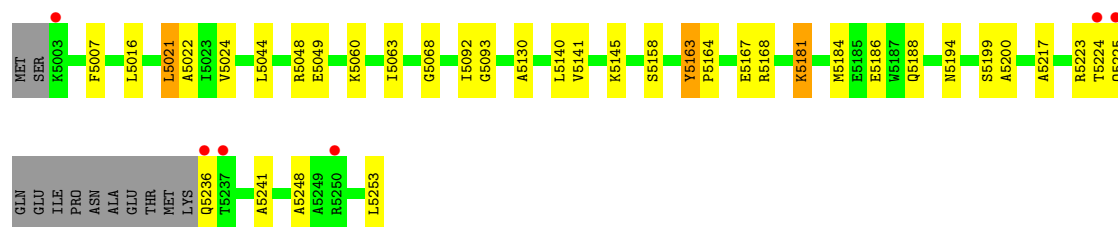
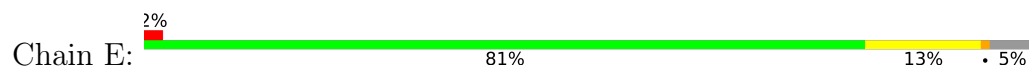


- Molecule 1: Uridine phosphorylase

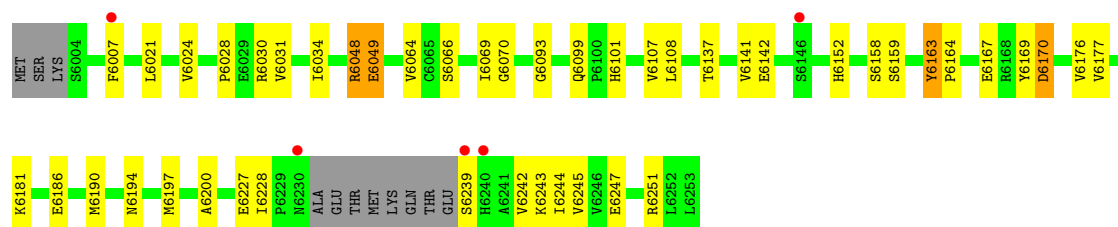
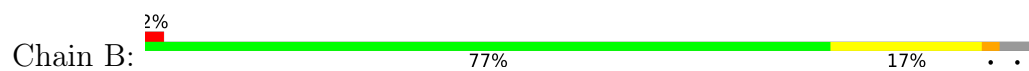




• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.88Å 124.07Å 134.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.11 28.75 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.75-2.11) 98.8 (28.75-2.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.219 0.180 , 0.218	Depositor DCC
R_{free} test set	4192 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11625	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/1916	1.03	10/2595 (0.4%)
1	B	0.51	0/1843	0.98	7/2497 (0.3%)
1	C	0.49	0/1852	0.95	3/2505 (0.1%)
1	D	0.46	0/1834	0.96	6/2482 (0.2%)
1	E	0.49	0/1835	1.00	4/2484 (0.2%)
1	F	0.49	0/1828	0.97	4/2474 (0.2%)
All	All	0.49	0/11108	0.98	34/15037 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6024	VAL	N-CA-C	7.79	115.86	108.15
1	E	5199	SER	N-CA-C	7.30	119.24	111.28
1	D	3007	PHE	N-CA-C	7.22	119.15	111.28
1	A	1236	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	D	3199	SER	N-CA-C	6.66	118.54	111.28
1	A	1199	SER	N-CA-C	6.65	118.53	111.28
1	C	2199	SER	N-CA-C	6.55	118.42	111.28
1	F	4007	PHE	N-CA-C	6.32	118.17	111.28
1	A	1230	ASN	CA-CB-CG	6.28	118.88	112.60
1	D	3070	GLY	N-CA-C	6.19	119.23	112.29
1	B	6007	PHE	N-CA-C	6.10	118.89	111.82
1	E	5007	PHE	N-CA-C	6.08	118.87	111.82
1	C	2096	GLY	N-CA-C	-6.04	103.36	112.41
1	A	1231	ALA	O-C-N	5.96	127.98	121.85
1	F	4199	SER	N-CA-C	5.89	117.70	111.28
1	D	3197	MET	N-CA-C	5.68	120.02	112.30
1	B	6070	GLY	N-CA-C	5.58	118.53	112.29
1	C	2070	GLY	N-CA-C	5.56	119.68	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6194	ASN	N-CA-C	5.56	115.88	108.38
1	A	1236	GLN	CG-CD-NE2	5.53	124.70	116.40
1	A	1231	ALA	N-CA-C	-5.37	106.21	114.16
1	B	6197	MET	N-CA-C	5.32	119.53	112.30
1	F	4194	ASN	N-CA-C	5.30	115.53	108.38
1	E	5194	ASN	N-CA-C	5.28	115.50	108.38
1	F	4197	MET	N-CA-C	5.26	119.46	112.30
1	A	1007	PHE	N-CA-C	5.26	117.09	111.36
1	D	3183	SER	N-CA-C	5.25	117.08	111.36
1	B	6159	SER	N-CA-C	5.25	118.62	110.17
1	E	5130	ALA	N-CA-C	-5.14	101.90	109.62
1	A	1068	GLY	N-CA-C	-5.14	104.10	112.83
1	A	1232	GLU	CB-CA-C	-5.12	102.70	111.46
1	D	3114	VAL	N-CA-C	-5.07	101.04	108.54
1	B	6048	ARG	CB-CA-C	-5.04	110.74	116.54
1	A	1197	MET	N-CA-C	5.00	120.47	113.02

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	1886	0	1900	44	0
1	B	1814	0	1825	32	0
1	C	1824	0	1843	27	0
1	D	1806	0	1822	47	0
1	E	1807	0	1821	24	0
1	F	1800	0	1814	35	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	B	16	0	0	1	0
3	D	16	0	0	2	0
4	A	122	0	0	2	0
4	B	116	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	109	0	0	1	0
4	D	82	0	0	0	0
4	E	117	0	0	1	0
4	F	95	0	0	1	0
All	All	11625	0	11025	193	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 9.

All (193) 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:A:1229:PRO:HB2	1:A:1233:THR:HG22	1.21	1.13
1:D:3049:GLU:HG2	1:B:6049:GLU:HG2	1.27	1.08
1:D:3100:PRO:HG3	1:D:3224:THR:HG21	1.52	0.92
1:A:1049:GLU:HB2	1:F:4049:GLU:CD	1.97	0.89
1:F:4091:ARG:HB3	1:F:4215:MET:HG3	1.53	0.89
1:A:1229:PRO:HB2	1:A:1233:THR:CG2	2.03	0.87
1:A:1229:PRO:CB	1:A:1233:THR:HG22	2.04	0.85
1:D:3049:GLU:CG	1:B:6049:GLU:HG2	2.06	0.83
1:D:3234:MET:HG3	1:D:3235:LYS:H	1.43	0.83
1:D:3049:GLU:HG2	1:B:6049:GLU:CG	2.09	0.81
1:A:1178:ARG:HA	1:A:1181:LYS:HE2	1.68	0.75
1:C:2094:THR:HG21	1:C:2238:GLU:HG2	1.69	0.75
1:D:3196:GLU:HA	3:D:706:BJE:O2	1.87	0.74
1:D:3238:GLU:O	1:D:3242:VAL:HG23	1.91	0.70
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.74	0.69
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.74	0.69
1:B:6108:LEU:HD22	1:B:6152:HIS:HB2	1.74	0.69
1:E:5060:LYS:HD3	1:E:5253:LEU:HB3	1.75	0.69
1:A:1027:ASP:HB3	1:A:1030:ARG:HG2	1.74	0.68
1:F:4249:ALA:O	1:F:4253:LEU:HD22	1.92	0.68
1:B:6170:ASP:HB2	1:B:6227:GLU:OE1	1.94	0.68
1:E:5060:LYS:HB2	1:E:5253:LEU:HD13	1.74	0.68
1:A:1049:GLU:CD	1:F:4049:GLU:HB2	2.20	0.67
1:C:2094:THR:CG2	1:C:2238:GLU:HG2	2.26	0.66
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.77	0.66
1:D:3234:MET:HG3	1:D:3235:LYS:N	2.12	0.65
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.78	0.64
1:C:2249:ALA:O	1:C:2253:LEU:HD13	1.98	0.64
1:D:3069:ILE:HD11	1:B:6048:ARG:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5048:ARG:HB3	1:E:5049:GLU:OE1	1.97	0.63
1:A:1049:GLU:HB2	1:F:4049:GLU:OE2	1.98	0.63
1:B:6239:SER:O	1:B:6243:LYS:HG3	2.00	0.62
1:C:2048:ARG:HD2	4:C:411:HOH:O	2.00	0.61
1:A:1037:LEU:HD22	1:A:1242:VAL:HG12	1.83	0.61
1:F:4179:ARG:HD2	4:F:379:HOH:O	1.99	0.61
1:D:3092:ILE:HD13	1:D:3093:GLY:N	2.15	0.61
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.83	0.60
1:A:1049:GLU:CD	1:A:1068:GLY:HA2	2.28	0.59
1:A:1179:ARG:HD3	4:A:273:HOH:O	2.02	0.59
1:D:3060:LYS:HD2	1:D:3253:LEU:HB3	1.85	0.59
1:E:5092:ILE:HD11	1:E:5241:ALA:HB1	1.84	0.58
1:D:3105:GLY:HA2	1:D:3237:THR:OG1	2.03	0.58
1:D:3121:LEU:HD21	1:D:3126:MET:HE2	1.86	0.58
1:E:5184:MET:O	1:E:5188:GLN:HG3	2.04	0.58
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.85	0.58
1:D:3048:ARG:HB3	1:D:3049:GLU:OE1	2.03	0.57
1:A:1142:GLU:HB3	1:A:1251:ARG:NH1	2.19	0.57
1:A:1238:GLU:O	1:A:1242:VAL:HG23	2.04	0.57
1:D:3092:ILE:HD13	1:D:3092:ILE:C	2.30	0.56
1:A:1069:ILE:HD11	1:F:4048:ARG:HD3	1.86	0.56
1:E:5181:LYS:NZ	1:E:5181:LYS:HB2	2.21	0.55
1:D:3013:LYS:NZ	1:D:3013:LYS:HB3	2.22	0.54
1:C:2138:THR:O	1:C:2142:GLU:HG2	2.07	0.54
1:E:5049:GLU:HG3	1:E:5068:GLY:HA3	1.89	0.53
1:A:1027:ASP:HB3	1:A:1030:ARG:CG	2.37	0.53
1:E:5060:LYS:HE2	1:E:5253:LEU:OXT	2.08	0.53
1:B:6030:ARG:HH12	1:B:6093:GLY:HA2	1.73	0.53
1:F:4007:PHE:N	1:F:4007:PHE:CD2	2.77	0.53
1:C:2234:MET:HG3	1:C:2238:GLU:OE2	2.09	0.52
1:B:6167:GLU:HG2	1:B:6169:TYR:CE1	2.45	0.51
1:D:3163:TYR:HB2	1:D:3164:PRO:CD	2.40	0.51
1:D:3142:GLU:HB3	1:D:3251:ARG:NH1	2.25	0.51
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.93	0.51
1:F:4038:MET:HG2	1:F:4057:LEU:HD13	1.92	0.51
1:D:3089:PHE:O	1:D:3213:ALA:HA	2.10	0.50
1:F:4028:PRO:HA	1:F:4066:SER:HB3	1.93	0.50
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.94	0.50
1:F:4003:LYS:HD2	1:F:4004:SER:N	2.27	0.49
1:F:4044:LEU:HD11	1:F:4054:ARG:HB2	1.93	0.49
1:A:1220:ILE:O	1:A:1229:PRO:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2238:GLU:O	1:C:2242:VAL:HG23	2.11	0.49
1:B:6242:VAL:O	1:B:6245:VAL:HG12	2.13	0.49
1:E:5163:TYR:HB2	1:E:5164:PRO:CD	2.42	0.49
1:F:4060:LYS:HD2	1:F:4253:LEU:HB3	1.93	0.49
1:E:5223:ARG:C	1:E:5225:GLN:H	2.21	0.49
1:B:6108:LEU:CD2	1:B:6152:HIS:HB2	2.42	0.49
1:F:4179:ARG:O	1:F:4179:ARG:HG3	2.11	0.49
1:B:6099:GLN:HB3	1:B:6101:HIS:CE1	2.48	0.48
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.43	0.48
1:C:2057:LEU:HB3	1:C:2253:LEU:HD21	1.94	0.48
1:C:2093:GLY:O	1:C:2217:ALA:HA	2.13	0.48
1:D:3049:GLU:CB	1:B:6049:GLU:HG2	2.43	0.48
1:D:3221:VAL:HG22	1:D:3222:ASN:N	2.28	0.48
1:D:3100:PRO:CG	1:D:3224:THR:HG21	2.34	0.48
1:A:1048:ARG:HB3	1:F:4049:GLU:OE1	2.14	0.48
1:F:4012:THR:O	1:F:4015:ASP:HB2	2.13	0.48
1:F:4199:SER:O	1:F:4203:LEU:HB2	2.14	0.48
1:F:4163:TYR:HB2	1:F:4164:PRO:CD	2.44	0.47
1:A:1229:PRO:O	1:A:1230:ASN:C	2.57	0.47
1:C:2022:ALA:HA	1:C:2063:ILE:O	2.14	0.47
1:C:2057:LEU:HB3	1:C:2253:LEU:CD2	2.45	0.47
1:E:5021:LEU:HD13	1:E:5022:ALA:N	2.29	0.47
1:B:6048:ARG:HB3	1:B:6049:GLU:OE2	2.15	0.47
1:D:3048:ARG:HD3	1:B:6069:ILE:HD11	1.97	0.47
1:F:4092:ILE:C	1:F:4092:ILE:HD13	2.39	0.47
1:A:1143:ALA:O	1:A:1147:ILE:HD13	2.15	0.47
1:C:2222:ASN:CG	1:C:2225:GLN:HG3	2.40	0.46
1:D:3114:VAL:HB	1:D:3157:ALA:HA	1.97	0.46
1:D:3239:SER:O	1:D:3243:LYS:HG3	2.15	0.46
1:F:4121:LEU:HD21	1:F:4126:MET:HE2	1.98	0.46
1:B:6021:LEU:C	1:B:6021:LEU:HD23	2.41	0.46
1:A:1006:VAL:HG21	1:A:1009:LEU:HB2	1.96	0.46
1:F:4007:PHE:N	1:F:4007:PHE:HD2	2.14	0.46
1:C:2163:TYR:HB2	1:C:2164:PRO:CD	2.45	0.46
1:B:6176:VAL:O	1:B:6181:LYS:HE2	2.16	0.46
1:C:2178:ARG:HA	1:C:2181:LYS:HE2	1.98	0.46
1:D:3049:GLU:HB3	1:B:6049:GLU:HG2	1.98	0.46
1:F:4030:ARG:O	1:F:4034:ILE:HG13	2.16	0.45
1:C:2116:LEU:HB2	1:C:2158:SER:O	2.16	0.45
1:D:3049:GLU:HG2	1:B:6049:GLU:CB	2.46	0.45
1:F:4178:ARG:HB2	1:E:5186:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6030:ARG:O	1:B:6034:ILE:HG13	2.16	0.45
1:A:1183:SER:HA	1:A:1186:GLU:OE1	2.16	0.45
1:D:3043:LYS:HB2	1:D:3053:TRP:CZ2	2.51	0.45
1:E:5140:LEU:HD23	1:E:5248:ALA:CB	2.47	0.45
1:B:6163:TYR:HB2	1:B:6164:PRO:CD	2.47	0.45
1:A:1242:VAL:O	1:A:1245:VAL:HG12	2.16	0.45
1:F:4031:VAL:HG21	1:F:4051:THR:O	2.17	0.45
1:C:2147:ILE:O	1:C:2147:ILE:CG2	2.65	0.44
1:D:3184:MET:O	1:D:3188:GLN:HG3	2.18	0.44
1:F:4108:LEU:CD2	1:F:4152:HIS:HB2	2.47	0.44
1:B:6186:GLU:HG2	1:B:6190:MET:HE3	2.00	0.44
1:D:3234:MET:O	1:D:3235:LYS:C	2.59	0.44
1:E:5141:VAL:HG12	1:E:5145:LYS:HE3	1.99	0.44
1:A:1012:THR:O	1:A:1015:ASP:HB2	2.17	0.44
1:A:1092:ILE:CD1	1:A:1242:VAL:HG22	2.48	0.44
1:F:4092:ILE:HD13	1:F:4093:GLY:N	2.33	0.44
1:E:5093:GLY:O	1:E:5217:ALA:HA	2.17	0.44
1:A:1096:GLY:HA2	1:A:1221:VAL:O	2.18	0.44
1:C:2143:ALA:O	1:C:2147:ILE:HD13	2.18	0.44
1:D:3013:LYS:HD2	1:D:3084:LEU:HA	2.00	0.44
1:C:2221:VAL:HG22	1:C:2222:ASN:N	2.33	0.43
1:E:5168:ARG:HD2	4:E:536:HOH:O	2.18	0.43
1:C:2242:VAL:O	1:C:2245:VAL:HG12	2.18	0.43
1:B:6028:PRO:HA	1:B:6066:SER:HB3	2.00	0.43
1:A:1091:ARG:NH1	1:A:1091:ARG:HG3	2.33	0.43
1:F:4049:GLU:CD	1:F:4068:GLY:HA2	2.43	0.43
1:B:6031:VAL:HG13	1:B:6064:VAL:HG12	2.01	0.43
1:A:1229:PRO:HB2	1:A:1233:THR:CB	2.47	0.43
1:A:1021:LEU:C	1:A:1021:LEU:HD23	2.43	0.43
1:A:1049:GLU:HB2	1:F:4049:GLU:CG	2.48	0.43
1:D:3239:SER:OG	1:D:3243:LYS:HE3	2.18	0.43
1:E:5016:LEU:HG	1:E:5063:ILE:HG13	2.00	0.43
1:A:1049:GLU:OE2	1:F:4049:GLU:HB2	2.19	0.43
1:B:6251:ARG:HH11	1:B:6251:ARG:HG3	1.84	0.43
1:D:3198:GLU:OE2	3:D:706:BJE:O3'	2.37	0.42
1:A:1091:ARG:HG3	1:A:1091:ARG:HH11	1.83	0.42
1:E:5024:VAL:O	1:E:5024:VAL:HG23	2.19	0.42
1:E:5236:GLN:HA	1:E:5236:GLN:OE1	2.18	0.42
1:E:5167:GLU:HG2	1:E:5167:GLU:O	2.19	0.42
1:B:6170:ASP:HB3	4:B:410:HOH:O	2.20	0.42
1:D:3038:MET:SD	1:D:3062:VAL:HG21	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4089:PHE:O	1:F:4213:ALA:HA	2.20	0.42
1:B:6227:GLU:O	1:B:6228:ILE:HD13	2.20	0.42
1:D:3142:GLU:HB3	1:D:3251:ARG:HH12	1.84	0.42
1:D:3220:ILE:HG13	1:D:3221:VAL:HG12	2.02	0.42
1:A:1007:PHE:HD2	1:A:1008:HIS:CE1	2.37	0.41
1:C:2060:LYS:HD2	1:C:2253:LEU:HB3	2.01	0.41
1:D:3004:SER:OG	1:D:3010:GLY:HA2	2.20	0.41
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.21	0.41
1:A:1121:LEU:HD21	1:A:1126:MET:HE2	2.02	0.41
1:C:2092:ILE:HD12	1:C:2216:VAL:HG13	2.02	0.41
1:F:4114:VAL:HB	1:F:4157:ALA:HA	2.02	0.41
1:A:1236:GLN:HB3	4:A:354:HOH:O	2.20	0.41
1:C:2021:LEU:C	1:C:2021:LEU:HD23	2.46	0.41
1:B:6137:THR:O	1:B:6141:VAL:HG23	2.20	0.41
1:C:2140:LEU:HD22	1:C:2216:VAL:HB	2.02	0.41
1:D:3242:VAL:O	1:D:3246:VAL:HG23	2.21	0.41
1:F:4021:LEU:HD23	1:F:4021:LEU:C	2.46	0.41
1:A:1149:ALA:HB2	1:A:1240:HIS:NE2	2.36	0.41
1:F:4239:SER:O	1:F:4243:LYS:HG3	2.21	0.41
1:E:5163:TYR:HB2	1:E:5164:PRO:HD3	2.02	0.41
1:A:1091:ARG:HD3	1:A:1215:MET:SD	2.61	0.41
1:D:3049:GLU:HG2	1:B:6049:GLU:HB3	2.03	0.41
1:D:3071:GLY:N	1:D:3072:PRO:CD	2.84	0.41
1:D:3074:THR:O	1:D:3078:VAL:HG23	2.21	0.41
1:D:3013:LYS:CD	1:D:3084:LEU:HA	2.51	0.41
1:D:3099:GLN:HB3	1:D:3101:HIS:CE1	2.56	0.41
1:D:3181:LYS:HE3	1:D:3181:LYS:HB2	1.87	0.41
1:B:6107:VAL:HG21	1:B:6244:ILE:HD12	2.02	0.41
1:B:6177:VAL:HG22	4:B:114:HOH:O	2.20	0.41
1:C:2057:LEU:HD22	1:C:2250:ARG:HG3	2.03	0.40
1:D:3057:LEU:HB3	1:D:3253:LEU:HD11	2.02	0.40
1:A:1060:LYS:HB2	1:A:1253:LEU:HD13	2.03	0.40
1:A:1229:PRO:C	1:A:1233:THR:HG22	2.46	0.40
1:F:4240:HIS:O	1:F:4244:ILE:HG13	2.20	0.40
1:E:5022:ALA:HA	1:E:5063:ILE:O	2.21	0.40
1:E:5060:LYS:HD3	1:E:5253:LEU:CB	2.48	0.40
1:C:2096:GLY:HA2	1:C:2221:VAL:O	2.22	0.40
1:D:3167:GLU:HG2	1:D:3169:TYR:CE1	2.56	0.40
1:A:1234:MET:O	1:A:1235:LYS:C	2.65	0.40
1:C:2092:ILE:HD11	1:C:2241:ALA:HB1	2.04	0.40
3:B:707:BJE:C2'	3:B:707:BJE:O5'	2.70	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	249/253 (98%)	237 (95%)	9 (4%)	3 (1%)	10	6
1	B	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	30	28
1	C	239/253 (94%)	234 (98%)	4 (2%)	1 (0%)	30	28
1	D	237/253 (94%)	231 (98%)	4 (2%)	2 (1%)	16	12
1	E	237/253 (94%)	231 (98%)	4 (2%)	2 (1%)	16	12
1	F	236/253 (93%)	226 (96%)	8 (3%)	2 (1%)	16	12
All	All	1436/1518 (95%)	1391 (97%)	34 (2%)	11 (1%)	16	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1230	ASN
1	A	1235	LYS
1	A	1163	TYR
1	D	3163	TYR
1	D	3235	LYS
1	E	5163	TYR
1	F	4163	TYR
1	B	6163	TYR
1	C	2163	TYR
1	F	4221	VAL
1	E	5224	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	200/202 (99%)	196 (98%)	4 (2%)	48	55
1	B	192/202 (95%)	188 (98%)	4 (2%)	47	54
1	C	193/202 (96%)	190 (98%)	3 (2%)	55	63
1	D	191/202 (95%)	187 (98%)	4 (2%)	47	54
1	E	191/202 (95%)	188 (98%)	3 (2%)	55	63
1	F	190/202 (94%)	184 (97%)	6 (3%)	34	37
All	All	1157/1212 (96%)	1133 (98%)	24 (2%)	47	54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1179	ARG
1	A	1215	MET
1	A	1230	ASN
1	C	2057	LEU
1	C	2250	ARG
1	C	2253	LEU
1	D	3013	LYS
1	D	3030	ARG
1	D	3092	ILE
1	D	3215	MET
1	F	4007	PHE
1	F	4092	ILE
1	F	4179	ARG
1	F	4203	LEU
1	F	4227	GLU
1	F	4253	LEU
1	E	5021	LEU
1	E	5044	LEU
1	E	5181	LYS
1	B	6049	GLU
1	B	6142	GLU
1	B	6170	ASP
1	B	6247	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1225	GLN
1	A	1230	ASN
1	C	2099	GLN
1	C	2103	ASN
1	C	2225	GLN
1	F	4103	ASN
1	F	4225	GLN
1	F	4226	GLN
1	E	5014	ASN
1	E	5020	GLN
1	B	6017	GLN
1	B	6188	GLN
1	B	6225	GLN
1	B	6226	GLN
1	B	6230	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	F	704	-	4,4,4	1.40	0	6,6,6	0.48	0
3	BJE	D	706	-	18,18,18	2.09	6 (33%)	23,27,27	4.98	13 (56%)
2	PO4	D	703	-	4,4,4	1.40	0	6,6,6	0.45	0
2	PO4	B	705	-	4,4,4	1.56	0	6,6,6	0.46	0
3	BJE	B	707	-	18,18,18	2.03	5 (27%)	23,27,27	4.96	14 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BJE	D	706	-	-	2/2/26/26	0/3/3/3
3	BJE	B	707	-	-	0/2/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	707	BJE	C2-N3	5.75	1.41	1.30
3	D	706	BJE	C2-N3	5.38	1.40	1.30
3	D	706	BJE	C2-N1	4.32	1.41	1.34
3	B	707	BJE	C2-N1	3.99	1.40	1.34
3	D	706	BJE	C5-C4	-2.89	1.38	1.44
3	B	707	BJE	C5-C4	-2.79	1.38	1.44
3	D	706	BJE	C6-C5	2.45	1.40	1.35
3	B	707	BJE	C6-C5	2.18	1.40	1.35
3	D	706	BJE	C1'-N1	2.08	1.49	1.46
3	B	707	BJE	O2-C2'	-2.08	1.43	1.46
3	D	706	BJE	O2-C2'	-2.02	1.43	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	706	BJE	O2-C2'-C3'	13.40	129.40	110.62
3	B	707	BJE	O2-C2'-C3'	12.29	127.84	110.62
3	B	707	BJE	C2'-O2-C2	-9.94	96.41	108.67
3	B	707	BJE	N1-C2-N3	-9.79	118.54	127.09
3	D	706	BJE	N1-C2-N3	-9.21	119.05	127.09
3	D	706	BJE	C2'-O2-C2	-8.80	97.81	108.67
3	D	706	BJE	O2-C2-N3	7.94	132.70	121.24
3	B	707	BJE	O2-C2-N3	7.90	132.64	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	707	BJE	O2-C2'-C1'	-6.30	97.89	105.47
3	D	706	BJE	O4'-C1'-N1	6.26	118.53	111.94
3	B	707	BJE	O4'-C1'-N1	6.00	118.26	111.94
3	D	706	BJE	O2-C2'-C1'	-4.96	99.50	105.47
3	D	706	BJE	O2-C2-N1	-4.89	108.20	111.82
3	D	706	BJE	O4'-C1'-C2'	-4.69	98.51	106.59
3	B	707	BJE	O2-C2-N1	-4.38	108.57	111.82
3	B	707	BJE	O4'-C1'-C2'	-4.17	99.40	106.59
3	D	706	BJE	C5'-C4'-C3'	-3.59	106.62	115.10
3	D	706	BJE	C2'-C3'-C4'	-3.48	94.52	101.99
3	D	706	BJE	C2-N3-C4	3.09	119.81	116.66
3	B	707	BJE	C2-N3-C4	2.81	119.52	116.66
3	D	706	BJE	C3'-C2'-C1'	-2.74	97.56	102.81
3	B	707	BJE	C5-C4-N3	2.65	121.77	118.48
3	B	707	BJE	C2'-C3'-C4'	-2.55	96.51	101.99
3	B	707	BJE	C5'-C4'-C3'	-2.32	109.61	115.10
3	B	707	BJE	C3'-C2'-C1'	-2.28	98.45	102.81
3	D	706	BJE	C5-C4-N3	2.15	121.14	118.48
3	B	707	BJE	O4-C4-C5	-2.10	119.03	122.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	706	BJE	C3'-C4'-C5'-O5'
3	D	706	BJE	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	706	BJE	2	0
3	B	707	BJE	1	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, 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%)	-0.15	14 (5%) 30 33	7, 15, 58, 99	0
1	B	242/253 (95%)	-0.31	5 (2%) 63 66	9, 15, 36, 55	0
1	C	243/253 (96%)	-0.14	6 (2%) 58 61	8, 18, 42, 85	0
1	D	241/253 (95%)	-0.08	10 (4%) 41 44	9, 17, 48, 89	0
1	E	241/253 (95%)	-0.29	6 (2%) 58 61	7, 15, 41, 61	0
1	F	240/253 (94%)	-0.16	5 (2%) 63 66	8, 18, 41, 70	0
All	All	1458/1518 (96%)	-0.19	46 (3%) 50 53	7, 16, 43, 99	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1234	MET	7.0
1	A	1233	THR	6.5
1	A	1231	ALA	6.1
1	A	1049	GLU	5.9
1	F	4049	GLU	5.2
1	F	4007	PHE	4.8
1	A	1230	ASN	4.2
1	C	2234	MET	4.2
1	F	4003	LYS	3.7
1	D	3234	MET	3.7
1	E	5003	LYS	3.3
1	B	6239	SER	3.2
1	D	3237	THR	3.2
1	B	6230	ASN	3.2
1	E	5225	GLN	3.2
1	C	2101	HIS	3.1
1	B	6007	PHE	3.1
1	D	3224	THR	3.0
1	E	5224	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	3235	LYS	2.9
1	D	3101	HIS	2.9
1	A	1148	GLY	2.9
1	A	1228	ILE	2.8
1	A	1227	GLU	2.7
1	A	1170	ASP	2.7
1	C	2236	GLN	2.7
1	D	3220	ILE	2.7
1	A	1235	LYS	2.6
1	D	3094	THR	2.5
1	A	1229	PRO	2.5
1	D	3221	VAL	2.4
1	A	1232	GLU	2.4
1	A	1030	ARG	2.3
1	E	5250	ARG	2.3
1	D	3238	GLU	2.2
1	C	2240	HIS	2.2
1	B	6240	HIS	2.2
1	F	4226	GLN	2.2
1	C	2235	LYS	2.2
1	E	5237	THR	2.2
1	B	6146	SER	2.2
1	A	1236	GLN	2.2
1	D	3004	SER	2.1
1	C	2040	LYS	2.1
1	F	4030	ARG	2.0
1	E	5236	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BJE	D	706	16/16	0.62	0.15	20,20,20,20	0
3	BJE	B	707	16/16	0.80	0.12	20,20,20,20	0
2	PO4	D	703	5/5	0.91	0.25	20,20,20,20	0
2	PO4	F	704	5/5	0.94	0.22	20,20,20,20	0
2	PO4	B	705	5/5	0.95	0.11	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.