



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U1F
Title : Structure of e. coli uridine phosphorylase complexed to 5-(m-(benzyloxy)benzyl)acyclouridine (BBAU)
Authors : Bu, W.; Settembre, E.C.; Ealick, S.E.
Deposited on : 2004-07-15
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

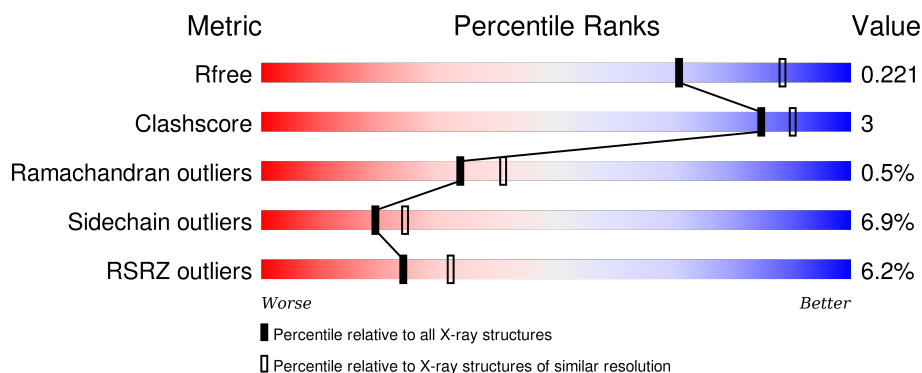
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	256	<div> <div>2%</div> <div>82% 12% • 5%</div> </div>
1	B	256	<div> <div>4%</div> <div>85% 12% • •</div> </div>
1	C	256	<div> <div>2%</div> <div>86% 11% • •</div> </div>
1	D	256	<div> <div>5%</div> <div>86% 11% •</div> </div>
1	E	256	<div> <div>7%</div> <div>80% 16% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	256	

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	K	A	1002	-	-	-	X
3	K	C	1001	-	-	-	X
3	K	E	1003	-	-	-	X
4	183	B	4300	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11915 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	243	Total	C	N	O	S	0	0	0
			1817	1139	317	350	11			
1	B	251	Total	C	N	O	S	0	0	0
			1885	1181	329	364	11			
1	C	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			
1	E	247	Total	C	N	O	S	0	0	0
			1848	1157	323	357	11			
1	F	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P12758
A	-1	SER	-	CLONING ARTIFACT	UNP P12758
A	0	HIS	-	CLONING ARTIFACT	UNP P12758
A	1	MET	-	CLONING ARTIFACT	UNP P12758
B	-2	GLY	-	CLONING ARTIFACT	UNP P12758
B	-1	SER	-	CLONING ARTIFACT	UNP P12758
B	0	HIS	-	CLONING ARTIFACT	UNP P12758
B	1	MET	-	CLONING ARTIFACT	UNP P12758
C	-2	GLY	-	CLONING ARTIFACT	UNP P12758
C	-1	SER	-	CLONING ARTIFACT	UNP P12758
C	0	HIS	-	CLONING ARTIFACT	UNP P12758
C	1	MET	-	CLONING ARTIFACT	UNP P12758
D	-2	GLY	-	CLONING ARTIFACT	UNP P12758
D	-1	SER	-	CLONING ARTIFACT	UNP P12758
D	0	HIS	-	CLONING ARTIFACT	UNP P12758
D	1	MET	-	CLONING ARTIFACT	UNP P12758
E	-2	GLY	-	CLONING ARTIFACT	UNP P12758

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	CLONING ARTIFACT	UNP P12758
E	0	HIS	-	CLONING ARTIFACT	UNP P12758
E	1	MET	-	CLONING ARTIFACT	UNP P12758
F	-2	GLY	-	CLONING ARTIFACT	UNP P12758
F	-1	SER	-	CLONING ARTIFACT	UNP P12758
F	0	HIS	-	CLONING ARTIFACT	UNP P12758
F	1	MET	-	CLONING ARTIFACT	UNP P12758

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

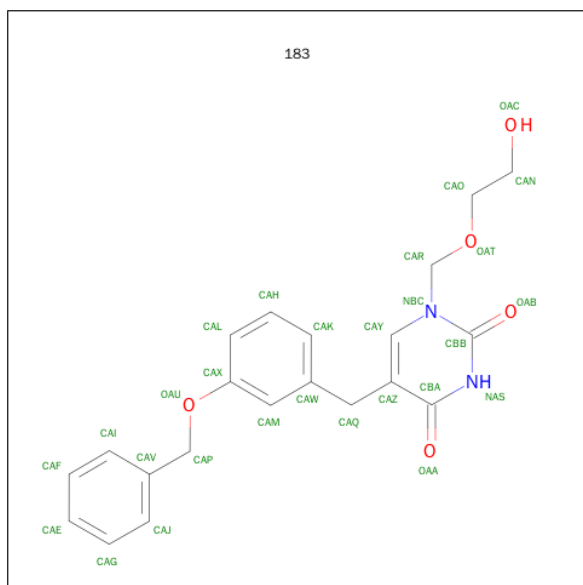


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is 1-((2-HYDROXYETHOXY)METHYL)-5-(3-(BENZYLOXY)BENZYL)PYRIDINE-2,4(1H,3H)-DIONE (three-letter code: 183) (formula: C₂₁H₂₂N₂O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 28 21 2 5	0	0
4	B	1	Total C N O 28 21 2 5	0	0
4	C	1	Total C N O 28 21 2 5	0	0
4	D	1	Total C N O 28 21 2 5	0	0
4	E	1	Total C N O 28 21 2 5	0	0
4	F	1	Total C N O 28 21 2 5	0	0

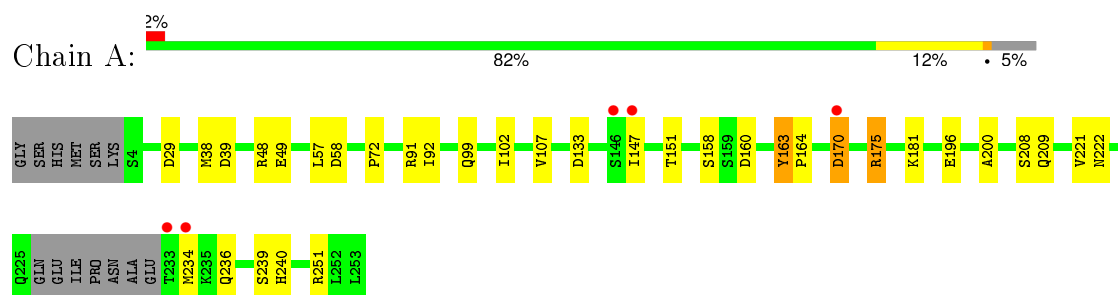
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0
5	B	81	Total 81	O 81	0	0
5	C	121	Total 121	O 121	0	0
5	D	108	Total 108	O 108	0	0
5	E	69	Total 69	O 69	0	0
5	F	54	Total 54	O 54	0	0

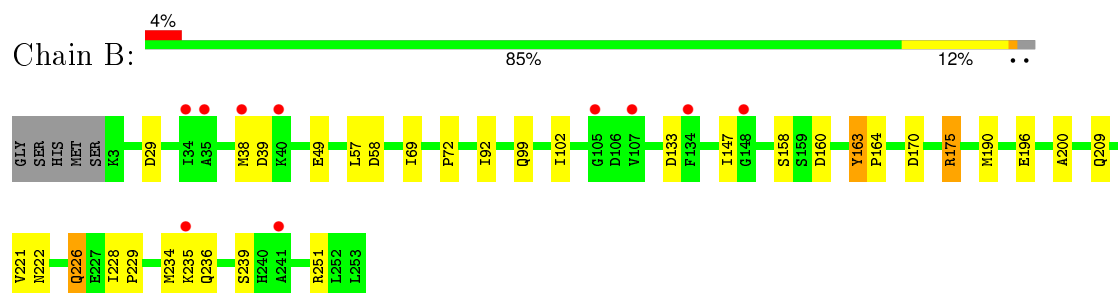
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

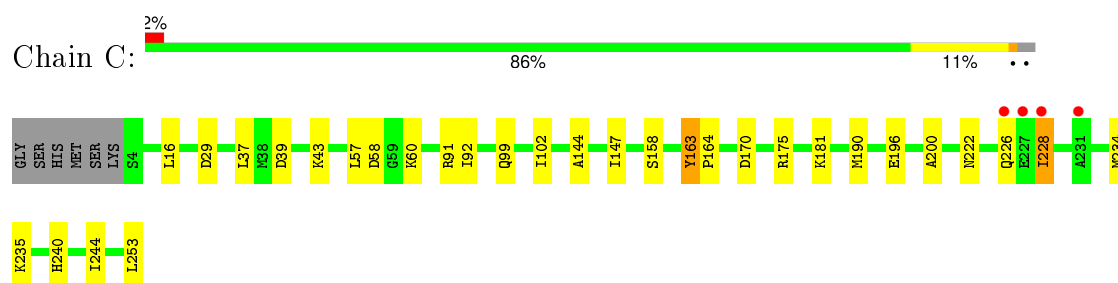
• Molecule 1: Uridine phosphorylase



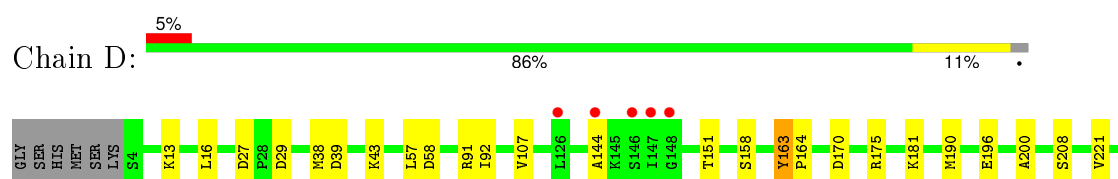
• Molecule 1: Uridine phosphorylase

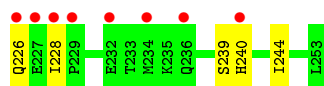


• Molecule 1: Uridine phosphorylase

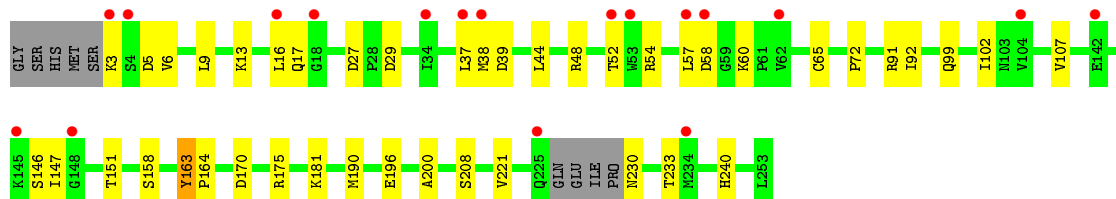
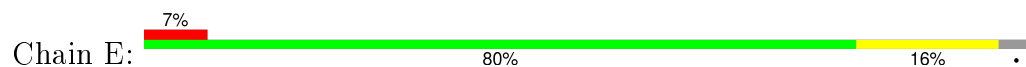


• Molecule 1: Uridine phosphorylase

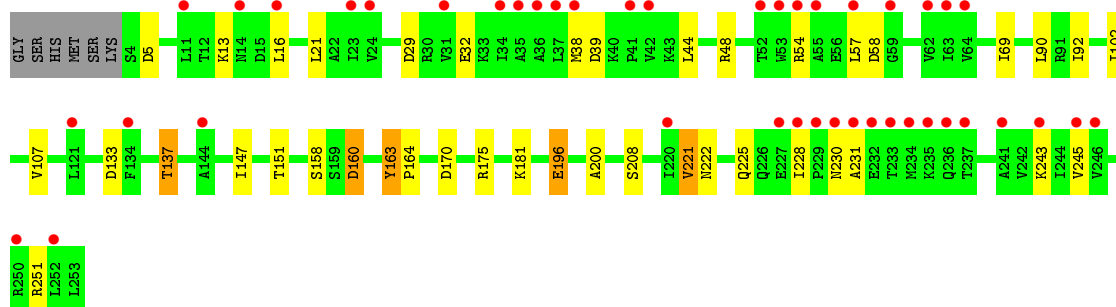
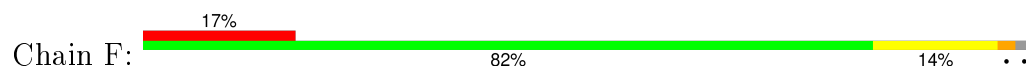




- Molecule 1: Uridine phosphorylase



- 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	91.56Å 125.81Å 141.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.30 48.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.80-2.30) 98.3 (48.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.228 0.195 , 0.221	Depositor DCC
R_{free} test set	5195 reflections (7.78%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72832 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11915	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 183, K, 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	0.31	0/1847	0.66	5/2507 (0.2%)
1	B	0.30	0/1917	0.66	5/2602 (0.2%)
1	C	0.31	0/1908	0.66	4/2591 (0.2%)
1	D	0.30	0/1908	0.66	4/2591 (0.2%)
1	E	0.29	0/1878	0.66	5/2548 (0.2%)
1	F	0.29	0/1908	0.65	6/2591 (0.2%)
All	All	0.30	0/11366	0.66	29/15430 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	170	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	170	ASP	CB-CG-OD2	5.98	123.68	118.30
1	F	29	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	58	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	58	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	170	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	29	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	58	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	58	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	29	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	58	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	29	ASP	CB-CG-OD2	5.44	123.19	118.30
1	E	29	ASP	CB-CG-OD2	5.37	123.14	118.30
1	F	5	ASP	CB-CG-OD2	5.35	123.12	118.30
1	E	58	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	170	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	29	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	39	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	170	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	39	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	39	ASP	CB-CG-OD2	5.08	122.87	118.30
1	F	133	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	5	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	39	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	39	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	39	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	133	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1817	0	1813	14	0
1	B	1885	0	1886	15	0
1	C	1876	0	1873	9	0
1	D	1876	0	1873	9	0
1	E	1848	0	1843	15	0
1	F	1876	0	1873	16	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	28	0	22	0	0
4	B	28	0	22	1	0
4	C	28	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	22	0	0
4	E	28	0	22	0	0
4	F	28	0	22	1	0
5	A	103	0	0	0	0
5	B	81	0	0	0	0
5	C	121	0	0	0	0
5	D	108	0	0	1	0
5	E	69	0	0	0	0
5	F	54	0	0	2	0
All	All	11915	0	11293	65	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 3.

All (65) 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:38:MET:HG2	1:A:57:LEU:HD13	1.80	0.64
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.84	0.59
1:B:38:MET:HG2	1:B:57:LEU:HD13	1.85	0.59
1:F:38:MET:HG2	1:F:57:LEU:HD13	1.87	0.57
1:F:44:LEU:HD11	1:F:54:ARG:HB2	1.86	0.56
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.88	0.56
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.88	0.56
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.87	0.55
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.89	0.54
1:B:99:GLN:HB2	1:B:102:ILE:HD12	1.90	0.54
1:E:52:THR:HG23	1:E:65:CYS:HB2	1.90	0.53
1:F:102:ILE:O	1:F:222:ASN:ND2	2.42	0.53
1:F:163:TYR:HB2	1:F:164:PRO:HD3	1.90	0.53
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.90	0.53
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.90	0.53
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.89	0.53
1:E:99:GLN:HB2	1:E:102:ILE:HD12	1.91	0.53
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.91	0.52
1:A:99:GLN:HB2	1:A:102:ILE:HD12	1.91	0.52
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.92	0.51
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.41	0.51
1:D:163:TYR:HB2	1:D:164:PRO:HD3	1.93	0.51
1:F:163:TYR:HB2	1:F:164:PRO:CD	2.41	0.50
1:F:137:THR:HG22	5:F:8333:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASP:HB2	5:D:6335:HOH:O	2.11	0.49
1:A:107:VAL:HG23	1:A:151:THR:HG23	1.94	0.49
1:F:222:ASN:HB3	1:F:225:GLN:HB2	1.94	0.49
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.44	0.48
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.43	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.43	0.48
1:B:222:ASN:H	1:B:226:GLN:HE21	1.61	0.48
1:E:48:ARG:HD3	1:F:69:ILE:HD11	1.95	0.48
1:A:163:TYR:HB2	1:A:164:PRO:CD	2.44	0.48
1:C:57:LEU:HB3	1:C:253:LEU:HD11	1.96	0.47
1:A:102:ILE:O	1:A:222:ASN:ND2	2.46	0.46
1:D:144:ALA:HA	1:D:244:ILE:HG12	1.98	0.46
1:E:230:ASN:HD22	1:E:233:THR:H	1.64	0.46
1:B:190:MET:HG2	1:F:208:SER:HB2	1.97	0.45
1:C:99:GLN:HB2	1:C:102:ILE:HD12	1.98	0.45
1:E:38:MET:HG2	1:E:57:LEU:HD13	1.98	0.45
1:A:48:ARG:HD3	1:B:69:ILE:HD11	1.98	0.45
1:E:44:LEU:HD11	1:E:54:ARG:HB2	1.99	0.44
1:E:6:VAL:HG21	1:E:9:LEU:HB2	2.00	0.44
1:F:196:GLU:HB2	5:F:8347:HOH:O	2.16	0.44
1:E:27:ASP:OD1	1:F:48:ARG:HG2	2.18	0.44
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.99	0.43
1:A:160:ASP:O	1:B:72:PRO:HA	2.18	0.43
1:D:107:VAL:HG23	1:D:151:THR:HG23	1.99	0.43
1:F:107:VAL:HG23	1:F:151:THR:HG23	2.00	0.43
1:F:221:VAL:HG11	4:F:8300:183:HAK	1.99	0.43
1:A:208:SER:HB2	1:C:190:MET:HG2	2.01	0.43
1:C:102:ILE:O	1:C:222:ASN:ND2	2.47	0.43
1:D:190:MET:HG2	1:E:208:SER:HB2	2.00	0.42
1:A:72:PRO:HA	1:B:160:ASP:O	2.20	0.42
1:D:208:SER:HB2	1:E:190:MET:HG2	2.01	0.42
1:E:107:VAL:HG23	1:E:151:THR:HG23	2.02	0.42
1:A:209:GLN:HA	1:B:175:ARG:HH22	1.84	0.42
1:C:228:ILE:H	1:C:228:ILE:HG13	1.58	0.41
1:B:234:MET:HG3	4:B:4300:183:HAG	2.01	0.41
1:B:228:ILE:HA	1:B:229:PRO:HD3	1.87	0.41
1:A:49:GLU:HB3	1:B:49:GLU:HB3	2.02	0.41
1:F:21:LEU:HD21	1:F:90:LEU:HD12	2.03	0.41
1:A:175:ARG:HH22	1:B:209:GLN:HA	1.86	0.41
1:E:72:PRO:HA	1:F:160:ASP:O	2.21	0.40
1:C:144:ALA:HA	1:C:244:ILE:HG12	2.04	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	239/256 (93%)	237 (99%)	1 (0%)	1 (0%)	39	48
1	B	249/256 (97%)	248 (100%)	0	1 (0%)	39	48
1	C	248/256 (97%)	244 (98%)	3 (1%)	1 (0%)	39	48
1	D	248/256 (97%)	246 (99%)	1 (0%)	1 (0%)	39	48
1	E	243/256 (95%)	240 (99%)	2 (1%)	1 (0%)	39	48
1	F	248/256 (97%)	243 (98%)	3 (1%)	2 (1%)	24	27
All	All	1475/1536 (96%)	1458 (99%)	10 (1%)	7 (0%)	34	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	231	ALA
1	A	163	TYR
1	B	163	TYR
1	C	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR

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	193/206 (94%)	180 (93%)	13 (7%)	20	26
1	B	201/206 (98%)	191 (95%)	10 (5%)	30	41
1	C	200/206 (97%)	185 (92%)	15 (8%)	17	21
1	D	200/206 (97%)	187 (94%)	13 (6%)	21	27
1	E	196/206 (95%)	181 (92%)	15 (8%)	16	20
1	F	200/206 (97%)	184 (92%)	16 (8%)	15	18
All	All	1190/1236 (96%)	1108 (93%)	82 (7%)	19	24

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	92	ILE
1	A	147	ILE
1	A	170	ASP
1	A	175	ARG
1	A	181	LYS
1	A	196	GLU
1	A	221	VAL
1	A	234	MET
1	A	236	GLN
1	A	239	SER
1	A	240	HIS
1	A	251	ARG
1	B	92	ILE
1	B	147	ILE
1	B	175	ARG
1	B	196	GLU
1	B	221	VAL
1	B	226	GLN
1	B	235	LYS
1	B	236	GLN
1	B	239	SER
1	B	251	ARG
1	C	16	LEU
1	C	37	LEU
1	C	43	LYS
1	C	60	LYS
1	C	91	ARG
1	C	92	ILE
1	C	147	ILE

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Mol	Chain	Res	Type
1	C	175	ARG
1	C	181	LYS
1	C	196	GLU
1	C	226	GLN
1	C	228	ILE
1	C	234	MET
1	C	235	LYS
1	C	240	HIS
1	D	13	LYS
1	D	16	LEU
1	D	43	LYS
1	D	91	ARG
1	D	92	ILE
1	D	175	ARG
1	D	181	LYS
1	D	196	GLU
1	D	221	VAL
1	D	226	GLN
1	D	228	ILE
1	D	239	SER
1	D	240	HIS
1	E	3	LYS
1	E	13	LYS
1	E	16	LEU
1	E	17	GLN
1	E	37	LEU
1	E	60	LYS
1	E	91	ARG
1	E	92	ILE
1	E	146	SER
1	E	147	ILE
1	E	175	ARG
1	E	181	LYS
1	E	196	GLU
1	E	221	VAL
1	E	240	HIS
1	F	13	LYS
1	F	16	LEU
1	F	32	GLU
1	F	92	ILE
1	F	137	THR
1	F	147	ILE

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Mol	Chain	Res	Type
1	F	160	ASP
1	F	175	ARG
1	F	181	LYS
1	F	196	GLU
1	F	221	VAL
1	F	228	ILE
1	F	230	ASN
1	F	243	LYS
1	F	245	VAL
1	F	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	B	240	HIS
1	C	17	GLN
1	C	47	HIS
1	C	226	GLN
1	D	226	GLN
1	E	179	HIS
1	E	230	ASN

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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	183	A	3300	-	24,30,30	3.42	18 (75%)	30,39,39	2.58	3 (10%)
2	PO4	A	4301	-	4,4,4	0.43	0	6,6,6	0.27	0
2	PO4	B	3301	-	4,4,4	0.47	0	6,6,6	0.27	0
4	183	B	4300	-	24,30,30	3.39	18 (75%)	30,39,39	2.60	3 (10%)
4	183	C	5300	-	24,30,30	3.35	18 (75%)	30,39,39	2.53	3 (10%)
2	PO4	C	6301	-	4,4,4	0.41	0	6,6,6	0.27	0
2	PO4	D	5301	-	4,4,4	0.44	0	6,6,6	0.27	0
4	183	D	6300	-	24,30,30	3.37	18 (75%)	30,39,39	2.55	3 (10%)
4	183	E	7300	-	24,30,30	3.39	18 (75%)	30,39,39	2.60	4 (13%)
2	PO4	E	8301	-	4,4,4	0.47	0	6,6,6	0.27	0
2	PO4	F	7301	-	4,4,4	0.48	0	6,6,6	0.27	0
4	183	F	8300	-	24,30,30	3.41	18 (75%)	30,39,39	2.64	3 (10%)

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	183	A	3300	-	-	0/13/14/14	0/3/3/3
2	PO4	A	4301	-	-	0/0/0/0	0/0/0/0
2	PO4	B	3301	-	-	0/0/0/0	0/0/0/0
4	183	B	4300	-	-	0/13/14/14	0/3/3/3
4	183	C	5300	-	-	0/13/14/14	0/3/3/3
2	PO4	C	6301	-	-	0/0/0/0	0/0/0/0
2	PO4	D	5301	-	-	0/0/0/0	0/0/0/0
4	183	D	6300	-	-	0/13/14/14	0/3/3/3
4	183	E	7300	-	-	0/13/14/14	0/3/3/3
2	PO4	E	8301	-	-	0/0/0/0	0/0/0/0
2	PO4	F	7301	-	-	0/0/0/0	0/0/0/0
4	183	F	8300	-	-	0/13/14/14	0/3/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4300	183	CAP-CAV	-3.87	1.41	1.50
4	D	6300	183	CAP-CAV	-3.80	1.41	1.50
4	C	5300	183	CAP-CAV	-3.79	1.41	1.50
4	F	8300	183	CAP-CAV	-3.67	1.42	1.50
4	A	3300	183	CAP-CAV	-3.64	1.42	1.50
4	E	7300	183	CAP-CAV	-3.50	1.42	1.50
4	D	6300	183	CAY-CAZ	2.50	1.43	1.37
4	C	5300	183	CAY-CAZ	2.55	1.43	1.37
4	A	3300	183	CAY-CAZ	2.56	1.43	1.37
4	E	7300	183	CAY-CAZ	2.56	1.43	1.37
4	B	4300	183	CAY-CAZ	2.63	1.43	1.37
4	F	8300	183	CAY-CAZ	2.69	1.43	1.37
4	C	5300	183	OAU-CAP	2.80	1.52	1.43
4	D	6300	183	OAU-CAP	2.81	1.52	1.43
4	B	4300	183	OAU-CAP	2.87	1.52	1.43
4	C	5300	183	CAQ-CAZ	2.88	1.57	1.52
4	D	6300	183	CAQ-CAZ	2.96	1.58	1.52
4	E	7300	183	CAQ-CAZ	2.96	1.58	1.52
4	F	8300	183	OAU-CAP	2.97	1.52	1.43
4	A	3300	183	CAQ-CAZ	2.98	1.58	1.52
4	E	7300	183	OAU-CAP	2.99	1.53	1.43
4	A	3300	183	OAU-CAP	3.03	1.53	1.43
4	F	8300	183	CAQ-CAZ	3.11	1.58	1.52
4	B	4300	183	CAQ-CAZ	3.12	1.58	1.52
4	C	5300	183	CAH-CAL	3.45	1.46	1.38
4	E	7300	183	CAF-CAE	3.45	1.46	1.38
4	C	5300	183	CAF-CAE	3.47	1.46	1.38
4	B	4300	183	CAH-CAL	3.47	1.46	1.38
4	F	8300	183	CAH-CAL	3.49	1.46	1.38
4	D	6300	183	CAH-CAL	3.49	1.46	1.38
4	A	3300	183	CAF-CAE	3.50	1.47	1.38
4	E	7300	183	CAH-CAL	3.50	1.46	1.38
4	F	8300	183	CAF-CAE	3.50	1.47	1.38
4	B	4300	183	CAF-CAE	3.52	1.47	1.38
4	D	6300	183	CAF-CAE	3.54	1.47	1.38
4	D	6300	183	CAY-NBC	3.57	1.45	1.36
4	A	3300	183	CAH-CAL	3.59	1.46	1.38
4	C	5300	183	CAY-NBC	3.62	1.45	1.36
4	E	7300	183	CAY-NBC	3.64	1.45	1.36
4	A	3300	183	CAY-NBC	3.66	1.45	1.36
4	C	5300	183	CAG-CAJ	3.67	1.46	1.38
4	F	8300	183	CAY-NBC	3.67	1.45	1.36
4	B	4300	183	CAG-CAJ	3.72	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4300	183	CAY-NBC	3.73	1.45	1.36
4	D	6300	183	CAG-CAJ	3.74	1.46	1.38
4	F	8300	183	CAG-CAJ	3.78	1.46	1.38
4	C	5300	183	CAM-CAW	3.79	1.46	1.39
4	A	3300	183	CAG-CAJ	3.81	1.46	1.38
4	E	7300	183	CAG-CAJ	3.81	1.46	1.38
4	A	3300	183	CAE-CAG	3.81	1.47	1.38
4	B	4300	183	CAE-CAG	3.82	1.47	1.38
4	E	7300	183	CAE-CAG	3.82	1.47	1.38
4	C	5300	183	CAE-CAG	3.83	1.47	1.38
4	C	5300	183	CAK-CAW	3.83	1.47	1.38
4	D	6300	183	CAK-CAW	3.84	1.47	1.38
4	D	6300	183	CAM-CAW	3.84	1.46	1.39
4	F	8300	183	CAE-CAG	3.85	1.47	1.38
4	F	8300	183	CAK-CAW	3.85	1.47	1.38
4	F	8300	183	CAJ-CAV	3.86	1.47	1.38
4	D	6300	183	CAE-CAG	3.86	1.47	1.38
4	E	7300	183	CAH-CAK	3.86	1.46	1.38
4	B	4300	183	CAM-CAW	3.86	1.46	1.39
4	C	5300	183	CAJ-CAV	3.86	1.47	1.38
4	A	3300	183	CAJ-CAV	3.87	1.47	1.38
4	F	8300	183	CAH-CAK	3.87	1.46	1.38
4	B	4300	183	CAJ-CAV	3.88	1.47	1.38
4	D	6300	183	CAF-CAI	3.88	1.46	1.38
4	B	4300	183	CAK-CAW	3.89	1.47	1.38
4	E	7300	183	CAJ-CAV	3.89	1.47	1.38
4	D	6300	183	CAJ-CAV	3.89	1.47	1.38
4	B	4300	183	CAF-CAI	3.90	1.46	1.38
4	D	6300	183	CAH-CAK	3.90	1.46	1.38
4	E	7300	183	CAK-CAW	3.91	1.47	1.38
4	C	5300	183	CAF-CAI	3.91	1.46	1.38
4	E	7300	183	CAF-CAI	3.91	1.47	1.38
4	A	3300	183	CAK-CAW	3.92	1.47	1.38
4	F	8300	183	CAM-CAW	3.93	1.46	1.39
4	F	8300	183	CAF-CAI	3.94	1.47	1.38
4	C	5300	183	CAH-CAK	3.96	1.47	1.38
4	B	4300	183	CAH-CAK	3.97	1.47	1.38
4	A	3300	183	CAF-CAI	3.97	1.47	1.38
4	A	3300	183	CAM-CAW	3.98	1.46	1.39
4	A	3300	183	CAH-CAK	3.99	1.47	1.38
4	E	7300	183	CAM-CAW	4.07	1.46	1.39
4	C	5300	183	CAL-CAX	4.08	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	8300	183	CAL-CAX	4.09	1.46	1.38
4	D	6300	183	CAL-CAX	4.10	1.46	1.38
4	E	7300	183	CAL-CAX	4.13	1.47	1.38
4	B	4300	183	CAL-CAX	4.15	1.47	1.38
4	A	3300	183	CAL-CAX	4.20	1.47	1.38
4	D	6300	183	CAI-CAV	4.35	1.48	1.38
4	B	4300	183	CAI-CAV	4.36	1.48	1.38
4	C	5300	183	CAI-CAV	4.38	1.48	1.38
4	A	3300	183	CAI-CAV	4.41	1.48	1.38
4	E	7300	183	CAI-CAV	4.49	1.48	1.38
4	B	4300	183	CAM-CAX	4.51	1.47	1.38
4	F	8300	183	CAI-CAV	4.53	1.48	1.38
4	C	5300	183	CAM-CAX	4.57	1.47	1.38
4	D	6300	183	CAM-CAX	4.71	1.47	1.38
4	F	8300	183	CAM-CAX	4.71	1.47	1.38
4	A	3300	183	CAM-CAX	4.74	1.47	1.38
4	E	7300	183	CAM-CAX	4.77	1.47	1.38
4	C	5300	183	CBA-NAS	5.62	1.43	1.33
4	E	7300	183	CBA-NAS	5.70	1.43	1.33
4	D	6300	183	CBA-NAS	5.71	1.43	1.33
4	B	4300	183	CBA-NAS	5.78	1.43	1.33
4	A	3300	183	CBA-NAS	5.85	1.44	1.33
4	F	8300	183	CBA-NAS	5.86	1.44	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	8300	183	CAZ-CBA-NAS	-3.12	121.50	125.04
4	C	5300	183	CAZ-CBA-NAS	-3.11	121.52	125.04
4	B	4300	183	CAZ-CBA-NAS	-2.92	121.73	125.04
4	A	3300	183	CAZ-CBA-NAS	-2.91	121.75	125.04
4	D	6300	183	CAZ-CBA-NAS	-2.88	121.77	125.04
4	E	7300	183	CAZ-CBA-NAS	-2.84	121.82	125.04
4	E	7300	183	OAU-CAP-CAV	2.14	115.65	109.21
4	D	6300	183	CBA-NAS-CBB	7.27	121.53	115.25
4	C	5300	183	CBA-NAS-CBB	7.28	121.54	115.25
4	E	7300	183	CBA-NAS-CBB	7.33	121.58	115.25
4	A	3300	183	CBA-NAS-CBB	7.39	121.64	115.25
4	B	4300	183	CBA-NAS-CBB	7.53	121.76	115.25
4	F	8300	183	CBA-NAS-CBB	7.61	121.83	115.25
4	C	5300	183	CAP-OAU-CAX	10.59	146.13	117.70
4	D	6300	183	CAP-OAU-CAX	10.82	146.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3300	183	CAP-OAU-CAX	10.94	147.08	117.70
4	B	4300	183	CAP-OAU-CAX	11.04	147.32	117.70
4	E	7300	183	CAP-OAU-CAX	11.15	147.64	117.70
4	F	8300	183	CAP-OAU-CAX	11.21	147.78	117.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4300	183	1	0
4	F	8300	183	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	243/256 (94%)	-0.05	5 (2%) 67 74	12, 14, 17, 21	0
1	B	251/256 (98%)	0.26	10 (3%) 42 51	12, 14, 16, 19	0
1	C	250/256 (97%)	-0.04	4 (1%) 74 80	11, 14, 20, 23	0
1	D	250/256 (97%)	0.08	13 (5%) 31 39	11, 14, 19, 24	0
1	E	247/256 (96%)	0.39	18 (7%) 18 25	13, 14, 16, 19	0
1	F	250/256 (97%)	1.00	43 (17%) 2 3	13, 14, 16, 18	0
All	All	1491/1536 (97%)	0.27	93 (6%) 24 32	11, 14, 17, 24	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	GLU	8.2
1	F	241	ALA	6.2
1	F	234	MET	5.8
1	F	243	LYS	5.7
1	E	234	MET	5.3
1	F	38	MET	5.2
1	D	228	ILE	5.2
1	F	36	ALA	4.8
1	E	3	LYS	4.8
1	F	34	ILE	4.7
1	F	229	PRO	4.7
1	F	228	ILE	4.7
1	F	35	ALA	4.7
1	F	37	LEU	4.6
1	F	230	ASN	4.6
1	F	53	TRP	4.4
1	D	229	PRO	4.4
1	F	227	GLU	4.4
1	E	4	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	57	LEU	4.3
1	C	231	ALA	4.1
1	F	23	ILE	4.0
1	D	227	GLU	4.0
1	F	236	GLN	3.8
1	C	227	GLU	3.8
1	F	62	VAL	3.7
1	B	38	MET	3.6
1	F	250	ARG	3.6
1	D	234	MET	3.5
1	E	16	LEU	3.4
1	E	225	GLN	3.4
1	F	41	PRO	3.3
1	F	245	VAL	3.3
1	B	134	PHE	3.3
1	D	232	GLU	3.2
1	F	11	LEU	3.2
1	F	252	LEU	3.2
1	F	246	VAL	3.2
1	F	31	VAL	3.2
1	E	34	ILE	3.1
1	F	63	ILE	3.1
1	F	144	ALA	3.0
1	F	42	VAL	3.0
1	A	233	THR	3.0
1	F	233	THR	3.0
1	F	16	LEU	2.9
1	C	226	GLN	2.9
1	A	234	MET	2.9
1	F	64	VAL	2.8
1	F	231	ALA	2.8
1	F	220	ILE	2.8
1	C	228	ILE	2.7
1	F	235	LYS	2.7
1	E	145	LYS	2.7
1	F	24	VAL	2.7
1	E	148	GLY	2.6
1	F	14	ASN	2.5
1	A	147	ILE	2.4
1	F	55	ALA	2.4
1	E	57	LEU	2.3
1	B	35	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	237	THR	2.3
1	B	148	GLY	2.3
1	D	146	SER	2.3
1	D	240	HIS	2.3
1	A	170	ASP	2.3
1	D	126	LEU	2.3
1	A	146	SER	2.2
1	F	134	PHE	2.2
1	E	58	ASP	2.2
1	B	107	VAL	2.2
1	D	147	ILE	2.2
1	E	104	VAL	2.2
1	F	121	LEU	2.2
1	B	40	LYS	2.2
1	F	52	THR	2.2
1	D	236	GLN	2.2
1	F	59	GLY	2.1
1	E	52	THR	2.1
1	D	226	GLN	2.1
1	B	105	GLY	2.1
1	E	53	TRP	2.1
1	B	241	ALA	2.1
1	D	144	ALA	2.1
1	E	18	GLY	2.1
1	F	54	ARG	2.1
1	B	235	LYS	2.1
1	E	38	MET	2.1
1	E	37	LEU	2.0
1	E	142	GLU	2.0
1	D	148	GLY	2.0
1	B	34	ILE	2.0
1	E	62	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	K	A	1002	1/1	0.88	0.52	45.77	69,69,69,69	0
3	K	E	1003	1/1	0.66	0.47	11.29	75,75,75,75	0
3	K	C	1001	1/1	0.93	0.27	7.36	49,49,49,49	0
4	183	B	4300	28/28	0.82	0.23	3.14	40,42,45,45	0
4	183	A	3300	28/28	0.87	0.20	1.77	38,42,49,49	0
4	183	E	7300	28/28	0.85	0.27	1.57	42,44,49,50	0
4	183	F	8300	28/28	0.79	0.29	0.80	48,49,51,51	0
2	PO4	B	3301	5/5	0.93	0.16	0.56	40,41,41,42	0
2	PO4	D	5301	5/5	0.95	0.12	0.39	42,42,43,43	0
4	183	D	6300	28/28	0.91	0.19	0.33	31,34,42,42	0
4	183	C	5300	28/28	0.93	0.16	0.21	31,33,41,41	0
2	PO4	A	4301	5/5	0.94	0.13	0.08	48,48,48,48	0
2	PO4	F	7301	5/5	0.93	0.13	-1.01	53,53,53,53	0
2	PO4	E	8301	5/5	0.96	0.10	-1.06	48,48,48,48	0
2	PO4	C	6301	5/5	0.96	0.09	-1.68	35,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.