



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TEZ
Title : COMPLEX BETWEEN DNA AND THE DNA PHOTOLYASE FROM ANA-CYSTIS NIDULANS
Authors : Essen, L.-O.; Carell, T.; Mees, A.; Klar, T.
Deposited on : 2004-05-26
Resolution : 1.80 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

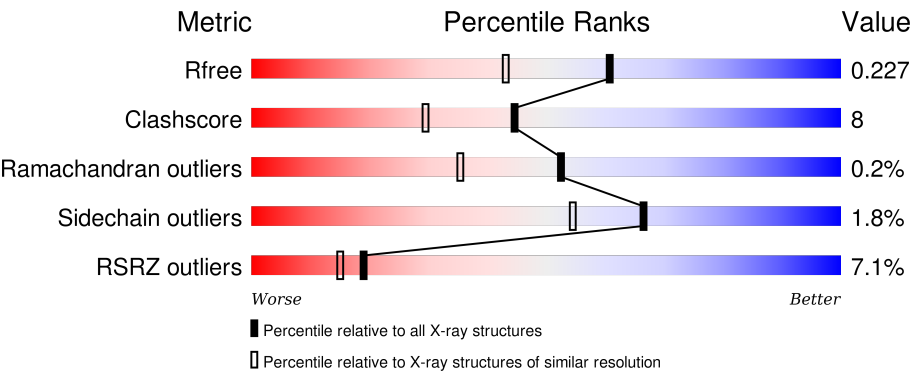
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	I	11	<div><div>45%</div><div><div></div><div>36%</div><div>27%</div><div>36%</div></div></div>
1	K	11	<div><div>36%</div><div><div></div><div>36%</div><div>27%</div><div>36%</div></div></div>
2	J	9	<div><div>44%</div><div><div></div><div>56%</div><div>44%</div></div></div>
2	L	9	<div><div>56%</div><div><div></div><div>44%</div><div>56%</div></div></div>
3	M	4	<div><div>25%</div><div><div></div><div>100%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	O	4	
4	N	5	
4	P	5	
5	A	474	
5	B	474	
5	C	474	
5	D	474	

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
7	TCP	K	12	-	-	-	X
9	HDF	A	5486	X	-	-	-
9	HDF	B	6486	X	-	-	-
9	HDF	C	7486	X	-	-	-
9	HDF	D	8486	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18206 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 DNA chain called 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	7	Total	C	N	O	P	0	0	0
			140	68	25	41	6			
1	K	7	Total	C	N	O	P	0	0	0
			140	68	25	41	6			

- Molecule 2 is a DNA chain called 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	9	Total	C	N	O	P	0	0	0
			186	87	39	51	9			
2	L	9	Total	C	N	O	P	0	0	0
			186	87	39	51	9			

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	4	Total	C	N	O	P	1	0	0
			77	38	13	23	3			
3	O	4	Total	C	N	O	P	0	0	0
			77	38	13	23	3			

- Molecule 4 is a DNA chain called 5'-D(P*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	5	Total	C	N	O	P	0	0	0
			103	48	21	29	5			
4	P	5	Total	C	N	O	P	0	0	0
			103	48	21	29	5			

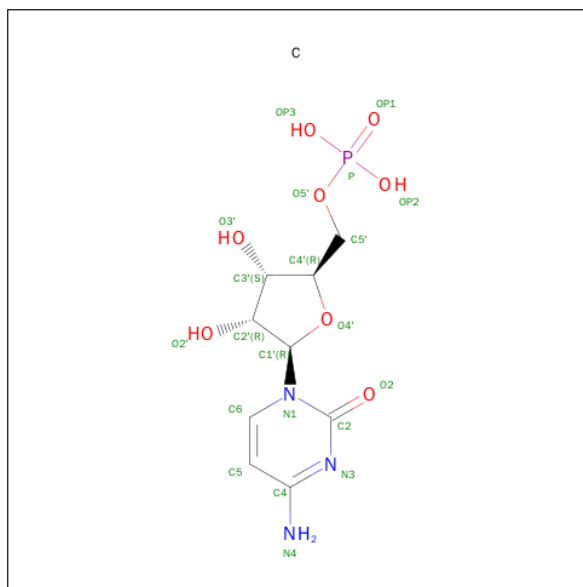
- Molecule 5 is a protein called Deoxyribodipyrimidine photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	474	Total	C	N	O	S	2	0	0
			3774	2411	674	679	10			
5	B	474	Total	C	N	O	S	6	0	0
			3782	2414	678	680	10			
5	C	474	Total	C	N	O	S	0	0	0
			3773	2409	674	680	10			
5	D	474	Total	C	N	O	S	6	0	0
			3777	2412	675	680	10			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

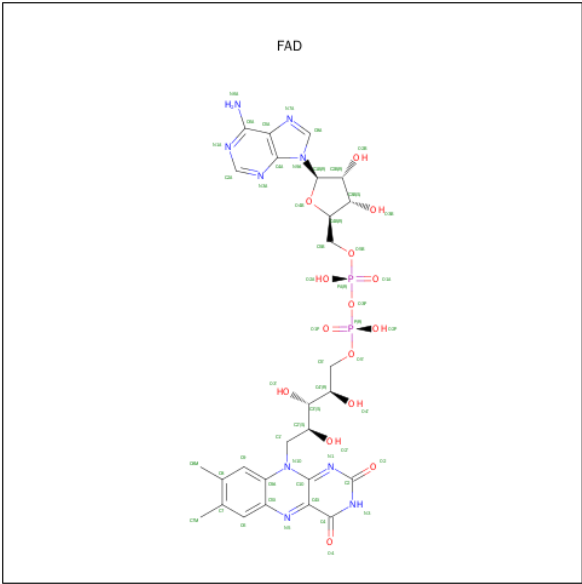
- Molecule 7 is 5'-METHYLTHYMIDINE (three-letter code: C, G, TCP) (formula: C₉H₁₄N₃O₈P, C₁₀H₁₄N₅O₈P, C₁₁H₁₆N₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	I	4	Total	C	N	O	P	0	0
			78	39	13	23	3		
7	K	4	Total	C	N	O	P	0	0
			78	39	13	23	3		

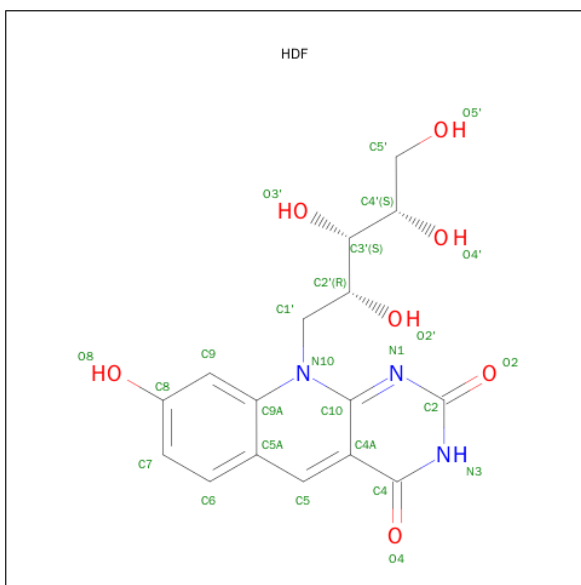
- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 9 is 8-HYDROXY-10-(D-RIBO-2,3,4,5-TETRAHYDROXYPENTYL)-5-DEAZAI SOALLOXAZINE (three-letter code: HDF) (formula: C₁₆H₁₇N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			26	16	3	7		
9	B	1	Total	C	N	O	0	0
			26	16	3	7		
9	C	1	Total	C	N	O	0	0
			26	16	3	7		
9	D	1	Total	C	N	O	0	0
			26	16	3	7		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	409	Total	O	0	0
			409	409		
10	B	404	Total	O	0	0
			404	404		
10	C	374	Total	O	0	0
			374	374		
10	D	360	Total	O	0	0
			360	360		
10	I	10	Total	O	0	0
			10	10		
10	J	11	Total	O	0	0
			11	11		
10	K	8	Total	O	0	0
			8	8		
10	L	9	Total	O	0	0
			9	9		

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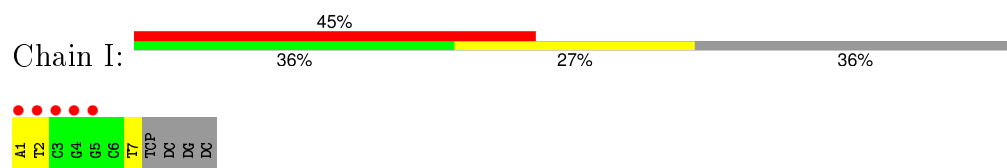
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	14	Total 14	O 14	0	0
10	N	10	Total 10	O 10	0	0
10	P	5	Total 5	O 5	0	0

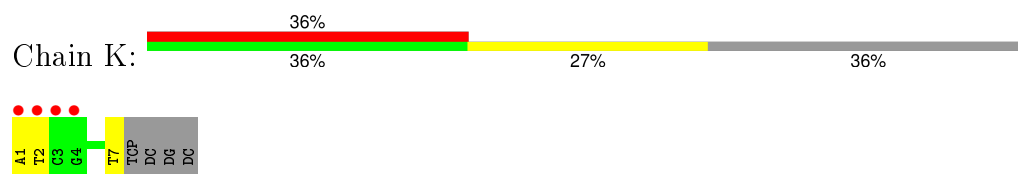
3 Residue-property plots

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.

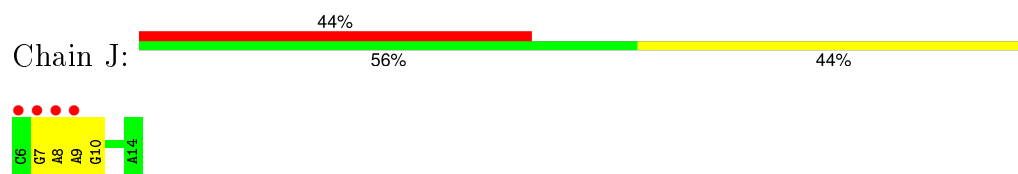
- Molecule 1: 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'



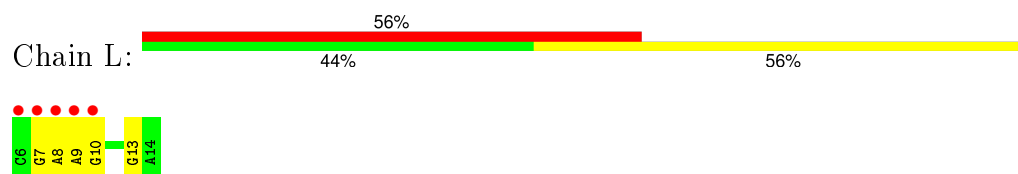
- Molecule 1: 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'



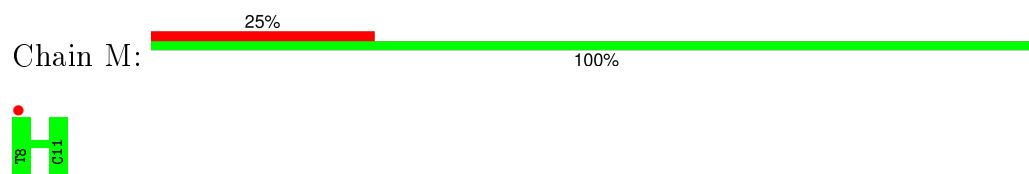
- Molecule 2: 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'



- Molecule 2: 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'



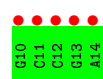
- Molecule 3: 5'-D(*TP*CP*GP*C)-3'



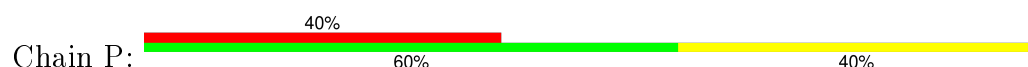
- Molecule 3: 5'-D(*TP*CP*GP*C)-3'



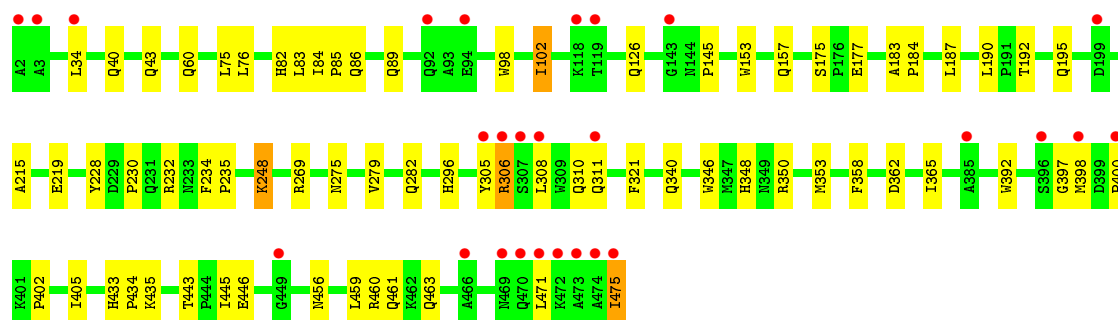
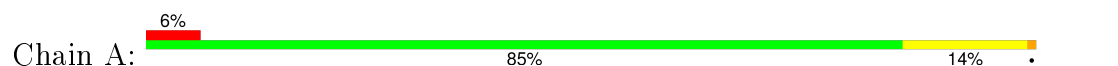
• Molecule 4: 5'-D(P*GP*CP*CP*GP*A)-3'



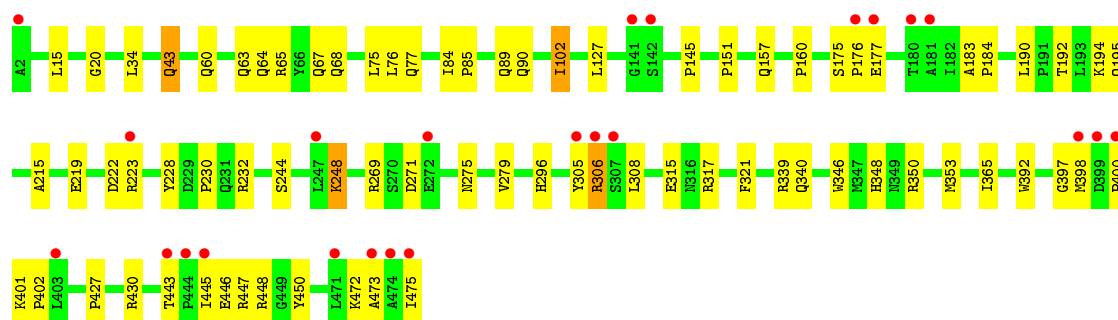
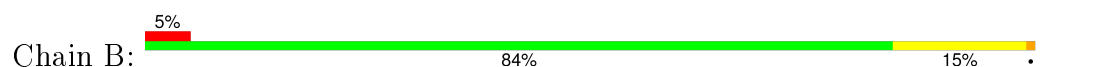
• Molecule 4: 5'-D(P*GP*CP*CP*GP*A)-3'



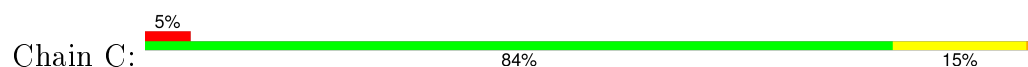
• Molecule 5: Deoxyribodipyrimidine photolyase

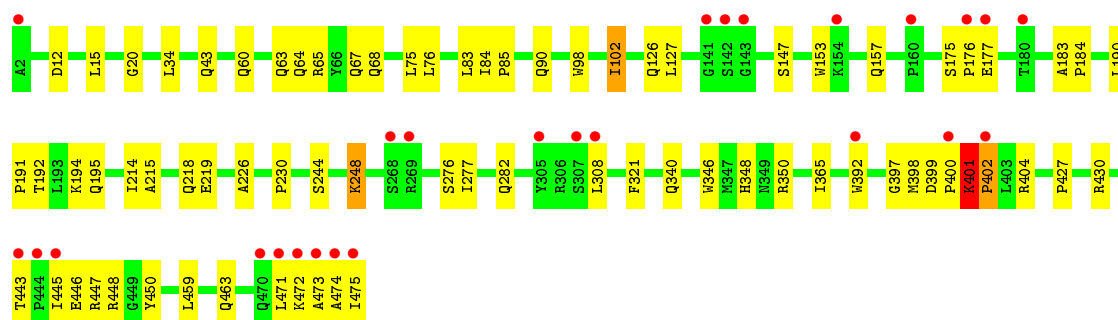


• Molecule 5: Deoxyribodipyrimidine photolyase

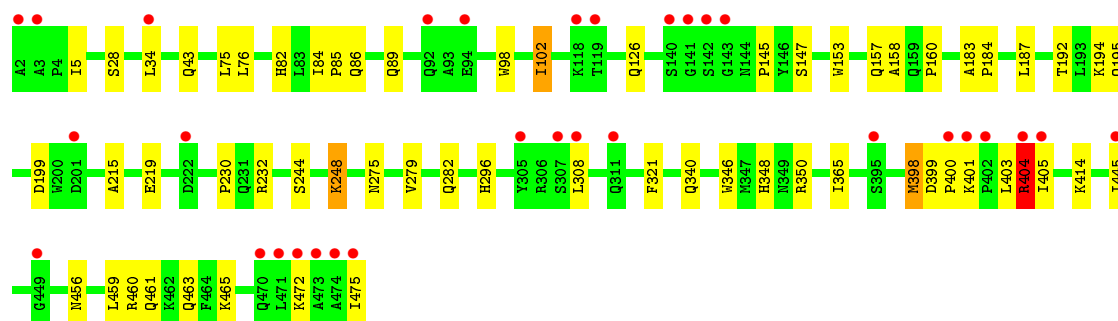
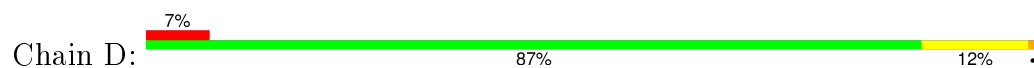


• Molecule 5: Deoxyribodipyrimidine photolyase





• Molecule 5: Deoxyribodipyrimidine photolyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.81Å 88.50Å 161.62Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.92 – 1.80 29.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.92-1.80) 96.3 (29.92-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.226 0.207 , 0.227	Depositor DCC
R_{free} test set	7425 reflections (3.40%)	DCC
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.2	EDS
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 218105 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18206	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: HDF, MG, FAD, TCP

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	I	0.25	0/156	0.67	0/239
1	K	0.25	0/156	0.68	0/239
2	J	0.42	0/209	0.72	0/320
2	L	0.43	0/209	0.72	0/320
3	M	0.38	0/85	0.85	0/129
3	O	0.34	0/85	0.82	0/129
4	N	0.54	0/115	0.76	0/175
4	P	0.52	0/115	0.76	0/175
5	A	0.32	0/3883	0.54	0/5292
5	B	0.32	0/3891	0.55	0/5302
5	C	0.32	0/3882	0.55	0/5292
5	D	0.32	0/3886	0.56	0/5296
All	All	0.32	0/16672	0.57	0/22908

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	I	140	0	80	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	140	0	80	7	0
2	J	186	0	100	5	0
2	L	186	0	100	5	0
3	M	77	0	47	0	0
3	O	77	0	47	1	0
4	N	103	0	56	0	0
4	P	103	0	56	1	0
5	A	3774	0	3681	60	0
5	B	3782	0	3694	61	0
5	C	3773	0	3674	66	0
5	D	3777	0	3685	56	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	I	78	0	48	6	0
7	K	78	0	48	6	0
8	A	53	0	31	0	0
8	B	53	0	31	1	0
8	C	53	0	31	1	0
8	D	53	0	31	1	0
9	A	26	0	15	0	0
9	B	26	0	16	0	0
9	C	26	0	15	0	0
9	D	26	0	15	0	0
10	A	409	0	0	5	0
10	B	404	0	0	7	0
10	C	374	0	0	8	0
10	D	360	0	0	10	0
10	I	10	0	0	0	0
10	J	11	0	0	0	0
10	K	8	0	0	0	0
10	L	9	0	0	0	0
10	M	14	0	0	0	0
10	N	10	0	0	0	0
10	P	5	0	0	0	0
All	All	18206	0	15581	255	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 8.

All (255) 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)
5:C:401:LYS:HB2	5:C:402:PRO:HD2	1.33	1.07
5:C:401:LYS:HG2	5:C:404:ARG:HH21	1.29	0.98
5:C:401:LYS:HG2	5:C:404:ARG:NH2	1.88	0.88
5:D:199:ASP:HB2	10:D:8744:HOH:O	1.75	0.85
5:C:226:ALA:HA	10:C:7764:HOH:O	1.78	0.84
1:K:7:DT:H72	7:K:12:TCP:H72	1.61	0.82
5:D:403:LEU:O	5:D:404:ARG:HB2	1.79	0.82
5:A:306:ARG:NH2	5:A:400:PRO:HG3	1.94	0.82
5:C:277:ILE:HG13	10:C:7764:HOH:O	1.80	0.81
1:I:7:DT:H72	7:I:12:TCP:H72	1.63	0.80
5:C:401:LYS:CG	5:C:404:ARG:HH21	1.98	0.77
1:I:1:DA:H2"	1:I:2:DT:C5	2.23	0.74
5:A:86:GLN:HE21	5:C:195:GLN:HG2	1.54	0.73
5:A:459:LEU:O	5:A:463:GLN:HG3	1.89	0.72
2:J:9:DA:C2	5:A:402:PRO:HD3	2.25	0.72
1:K:1:DA:H2"	1:K:2:DT:C5	2.25	0.71
5:B:60:GLN:NE2	10:B:9389:HOH:O	2.25	0.70
5:A:84:ILE:HB	5:A:85:PRO:HD3	1.74	0.70
5:B:195:GLN:HG2	5:D:86:GLN:HE21	1.55	0.69
5:D:84:ILE:HB	5:D:85:PRO:HD3	1.75	0.69
5:A:269:ARG:NH2	5:B:219:GLU:HA	2.09	0.68
5:B:64:GLN:O	5:B:68:GLN:HG3	1.94	0.68
5:B:306:ARG:NH2	5:B:400:PRO:HG3	2.09	0.67
5:A:34:LEU:CD1	5:A:76:LEU:HD13	2.25	0.67
5:C:401:LYS:HB2	5:C:402:PRO:CD	2.20	0.66
5:D:34:LEU:CD1	5:D:76:LEU:HD13	2.26	0.66
5:D:404:ARG:NH2	5:D:465:LYS:NZ	2.44	0.66
5:A:102:ILE:HD13	5:A:102:ILE:H	1.62	0.65
5:A:215:ALA:O	5:A:219:GLU:HG3	1.97	0.65
5:C:192:THR:OG1	5:C:195:GLN:HG3	1.96	0.64
5:D:102:ILE:HD13	5:D:102:ILE:H	1.63	0.64
5:C:471:LEU:HD12	10:C:7770:HOH:O	1.96	0.64
5:D:215:ALA:O	5:D:219:GLU:HG3	1.98	0.64
5:B:102:ILE:HD13	5:B:102:ILE:H	1.62	0.63
5:D:400:PRO:O	5:D:401:LYS:HG3	1.97	0.63
5:B:77:GLN:NE2	10:B:9386:HOH:O	2.32	0.62
5:C:84:ILE:HB	5:C:85:PRO:HD3	1.80	0.62
5:C:102:ILE:H	5:C:102:ILE:HD13	1.65	0.62
5:B:84:ILE:HB	5:B:85:PRO:HD3	1.81	0.62
5:B:215:ALA:O	5:B:219:GLU:HG3	1.99	0.61
5:C:215:ALA:O	5:C:219:GLU:HG3	2.00	0.61
7:I:12:TCP:H71	5:A:392:TRP:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:228:TYR:CE2	5:A:232:ARG:HD2	2.36	0.61
5:C:392:TRP:O	5:C:404:ARG:NH1	2.34	0.60
5:D:348:HIS:CD2	5:D:350:ARG:H	2.21	0.59
5:D:403:LEU:O	5:D:404:ARG:CB	2.47	0.59
5:B:192:THR:OG1	5:B:195:GLN:HG3	2.02	0.59
5:C:348:HIS:CD2	5:C:350:ARG:H	2.20	0.58
5:A:275:ASN:O	5:A:279:VAL:HG23	2.03	0.58
5:B:60:GLN:HG2	5:B:190:LEU:HD23	1.84	0.58
5:A:348:HIS:CD2	5:A:350:ARG:H	2.20	0.58
5:C:348:HIS:HD2	5:C:350:ARG:H	1.51	0.58
5:D:399:ASP:N	5:D:400:PRO:HD3	2.19	0.58
5:C:60:GLN:HG2	5:C:190:LEU:HD23	1.86	0.57
5:B:160:PRO:HG2	10:B:9119:HOH:O	2.04	0.57
5:C:399:ASP:N	5:C:400:PRO:HD3	2.19	0.57
5:B:348:HIS:CD2	5:B:350:ARG:H	2.21	0.57
5:A:269:ARG:HH21	5:B:219:GLU:HA	1.67	0.57
5:D:348:HIS:HD2	5:D:350:ARG:H	1.51	0.57
5:C:276:SER:HB2	10:C:7764:HOH:O	2.03	0.57
5:A:192:THR:OG1	5:A:195:GLN:HG3	2.05	0.57
5:C:34:LEU:CD1	5:C:76:LEU:HD13	2.35	0.56
5:B:348:HIS:HD2	5:B:350:ARG:H	1.53	0.56
5:D:192:THR:OG1	5:D:195:GLN:HG3	2.05	0.56
5:C:321:PHE:HB2	5:C:365:ILE:HD13	1.86	0.56
5:C:248:LYS:HD3	5:C:248:LYS:C	2.26	0.56
7:K:12:TCP:H71	5:B:392:TRP:CD2	2.40	0.56
5:C:400:PRO:O	5:C:401:LYS:HB3	2.06	0.56
5:D:405:ILE:HD12	5:D:461:GLN:HG3	1.86	0.56
5:B:427:PRO:HA	5:B:430:ARG:NE	2.21	0.55
5:C:427:PRO:HA	5:C:430:ARG:NE	2.22	0.55
5:B:248:LYS:C	5:B:248:LYS:HD3	2.27	0.55
5:C:15:LEU:HD22	5:C:65:ARG:HB3	1.89	0.54
5:A:43:GLN:NE2	5:C:43:GLN:O	2.40	0.54
5:A:305:TYR:CE1	5:A:398:MET:HG2	2.42	0.54
5:A:348:HIS:HD2	5:A:350:ARG:H	1.54	0.54
5:D:147:SER:O	5:D:399:ASP:N	2.40	0.54
5:C:401:LYS:CB	5:C:402:PRO:HD2	2.17	0.54
5:A:306:ARG:CZ	5:A:400:PRO:HG3	2.38	0.53
5:B:308:LEU:HD23	5:B:308:LEU:C	2.29	0.53
5:C:401:LYS:CD	5:C:404:ARG:HH21	2.21	0.53
5:D:321:PHE:HB2	5:D:365:ILE:HD13	1.91	0.53
2:L:9:DA:C2	5:B:402:PRO:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:472:LYS:O	5:D:475:ILE:HG22	2.09	0.53
5:C:308:LEU:HD23	5:C:308:LEU:C	2.30	0.52
5:D:160:PRO:HG2	10:D:8603:HOH:O	2.08	0.52
5:B:228:TYR:CE2	5:B:232:ARG:HD2	2.44	0.52
5:B:34:LEU:CD1	5:B:76:LEU:HD13	2.39	0.52
5:B:75:LEU:C	5:B:76:LEU:HD12	2.30	0.52
5:A:321:PHE:HB2	5:A:365:ILE:HD13	1.92	0.52
5:D:232:ARG:HD2	10:D:8648:HOH:O	2.10	0.52
5:D:404:ARG:NH2	5:D:465:LYS:HZ3	2.07	0.51
5:D:248:LYS:C	5:D:248:LYS:HD3	2.29	0.51
5:C:447:ARG:HB2	5:C:450:TYR:HB3	1.91	0.51
5:C:473:ALA:C	5:C:475:ILE:H	2.14	0.51
5:C:75:LEU:C	5:C:76:LEU:HD12	2.31	0.51
5:A:306:ARG:HB2	5:A:397:GLY:O	2.09	0.51
5:A:86:GLN:HE21	5:C:195:GLN:CG	2.21	0.51
7:I:12:TCP:H71	5:A:392:TRP:CE2	2.45	0.51
5:C:64:GLN:O	5:C:68:GLN:HG3	2.11	0.50
5:B:447:ARG:HB2	5:B:450:TYR:HB3	1.92	0.50
5:C:445:ILE:HD12	5:C:446:GLU:N	2.26	0.50
5:D:34:LEU:HD21	5:D:84:ILE:CD1	2.42	0.49
5:D:459:LEU:HG	5:D:463:GLN:HE21	1.76	0.49
5:A:445:ILE:HG13	10:A:9409:HOH:O	2.11	0.49
5:B:445:ILE:HD12	5:B:446:GLU:N	2.27	0.49
5:A:40:GLN:HG2	10:A:9283:HOH:O	2.12	0.49
5:A:269:ARG:NH2	5:B:219:GLU:HG2	2.27	0.49
5:D:308:LEU:C	5:D:308:LEU:HD23	2.32	0.49
10:A:9218:HOH:O	5:B:269:ARG:HG2	2.12	0.49
5:A:34:LEU:HD21	5:A:84:ILE:CD1	2.43	0.49
5:A:98:TRP:CE2	5:A:126:GLN:HG2	2.47	0.49
5:B:43:GLN:O	5:D:43:GLN:NE2	2.42	0.49
5:B:401:LYS:HE3	10:B:9267:HOH:O	2.12	0.49
5:B:306:ARG:HB2	5:B:397:GLY:O	2.13	0.49
5:A:175:SER:OG	5:A:177:GLU:HG2	2.13	0.49
7:K:12:TCP:H71	5:B:392:TRP:CE2	2.47	0.49
5:D:405:ILE:CD1	5:D:461:GLN:HG3	2.41	0.49
5:A:340:GLN:HG2	5:A:346:TRP:O	2.12	0.48
7:K:12:TCP:C6	5:B:353:MET:SD	3.01	0.48
1:K:7:DT:H2''	7:K:12:TCP:O5'	2.12	0.48
7:I:12:TCP:C6	5:A:353:MET:SD	3.02	0.48
5:D:85:PRO:O	5:D:89:GLN:HG3	2.14	0.48
5:A:248:LYS:C	5:A:248:LYS:HD3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:75:LEU:C	5:D:76:LEU:HD12	2.34	0.48
5:D:340:GLN:HG2	5:D:346:TRP:O	2.13	0.48
5:B:321:PHE:HB2	5:B:365:ILE:HD13	1.95	0.48
5:D:414:LYS:HG3	10:D:8833:HOH:O	2.13	0.48
1:K:7:DT:H72	7:K:12:TCP:C5M	2.39	0.48
2:L:7:DG:H1'	2:L:8:DA:O5'	2.14	0.48
1:I:7:DT:H2''	7:I:12:TCP:O5'	2.14	0.47
5:B:60:GLN:HG2	5:B:190:LEU:CD2	2.44	0.47
5:A:308:LEU:C	5:A:308:LEU:HD23	2.33	0.47
1:I:1:DA:H2''	1:I:2:DT:C6	2.49	0.47
5:B:60:GLN:O	5:B:64:GLN:HG3	2.14	0.47
5:D:183:ALA:N	5:D:184:PRO:HD2	2.28	0.47
5:C:397:GLY:O	5:C:400:PRO:HG3	2.15	0.47
5:C:60:GLN:HG2	5:C:190:LEU:CD2	2.44	0.47
5:A:75:LEU:C	5:A:76:LEU:HD12	2.35	0.47
5:D:404:ARG:HH21	5:D:465:LYS:HZ3	1.63	0.47
5:B:472:LYS:O	5:B:475:ILE:HG22	2.14	0.47
5:D:153:TRP:CH2	5:D:282:GLN:HG2	2.50	0.47
5:B:427:PRO:HB3	5:B:430:ARG:CZ	2.44	0.47
5:D:275:ASN:O	5:D:279:VAL:HG23	2.15	0.47
5:B:43:GLN:HA	5:B:43:GLN:OE1	2.14	0.47
5:B:222:ASP:O	5:B:223:ARG:HD3	2.16	0.46
5:C:472:LYS:O	5:C:475:ILE:HG22	2.15	0.46
5:C:153:TRP:CH2	5:C:282:GLN:HG2	2.50	0.46
5:B:176:PRO:HD2	5:B:177:GLU:OE2	2.16	0.46
5:D:404:ARG:NH2	5:D:465:LYS:HZ1	2.14	0.46
5:B:339:ARG:HD3	10:B:9357:HOH:O	2.16	0.46
5:A:183:ALA:HB3	5:A:184:PRO:HD3	1.97	0.46
5:D:194:LYS:NZ	10:D:8744:HOH:O	2.48	0.46
5:B:63:GLN:O	5:B:67:GLN:HG3	2.15	0.46
5:D:98:TRP:CE2	5:D:126:GLN:HG2	2.50	0.46
5:A:82:HIS:ND1	5:C:194:LYS:NZ	2.51	0.46
5:A:145:PRO:HB3	5:A:296:HIS:CD2	2.51	0.46
5:C:20:GLY:HA2	5:C:127:LEU:HD12	1.97	0.46
5:D:445:ILE:HG13	10:D:8837:HOH:O	2.16	0.46
5:B:15:LEU:HD22	5:B:65:ARG:HB3	1.97	0.46
1:K:1:DA:H2''	1:K:2:DT:C6	2.50	0.45
1:K:1:DA:H2''	1:K:2:DT:H72	1.99	0.45
5:A:153:TRP:CH2	5:A:282:GLN:HG2	2.51	0.45
5:C:401:LYS:CG	5:C:404:ARG:NH2	2.67	0.45
2:J:7:DG:H1'	2:J:8:DA:O5'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:305:TYR:CD1	5:A:398:MET:HG2	2.51	0.45
5:A:177:GLU:CD	5:A:177:GLU:H	2.20	0.45
5:A:311:GLN:CD	5:A:475:ILE:HD11	2.36	0.45
5:C:443:THR:HG23	10:C:7767:HOH:O	2.16	0.45
5:C:401:LYS:HD2	5:C:404:ARG:HE	1.80	0.45
5:B:183:ALA:HB3	5:B:184:PRO:HD3	1.97	0.45
5:D:404:ARG:NH1	5:D:461:GLN:OE1	2.49	0.45
5:A:348:HIS:HE1	10:A:9025:HOH:O	2.00	0.45
5:D:404:ARG:HD3	5:D:405:ILE:N	2.31	0.44
1:I:1:DA:H2"	1:I:2:DT:H72	1.98	0.44
5:A:234:PHE:HA	5:A:235:PRO:HD2	1.94	0.44
5:B:175:SER:OG	5:B:177:GLU:HG2	2.17	0.44
5:C:340:GLN:HG2	5:C:346:TRP:O	2.16	0.44
5:C:63:GLN:O	5:C:67:GLN:HG3	2.18	0.44
5:A:435:LYS:HE3	5:A:435:LYS:HB2	1.85	0.44
2:J:8:DA:H2"	5:A:402:PRO:HG3	1.99	0.44
5:B:306:ARG:CZ	5:B:400:PRO:HG3	2.48	0.44
5:B:177:GLU:H	5:B:177:GLU:CD	2.21	0.44
5:C:98:TRP:CE2	5:C:126:GLN:HG2	2.52	0.44
5:C:244:SER:HB3	8:C:7485:FAD:C5'	2.47	0.43
2:J:7:DG:H2"	2:J:8:DA:O5'	2.18	0.43
5:D:456:ASN:O	5:D:460:ARG:HG2	2.18	0.43
5:C:176:PRO:HD2	5:C:177:GLU:OE2	2.18	0.43
5:C:401:LYS:HB3	5:C:401:LYS:NZ	2.33	0.43
5:C:459:LEU:O	5:C:463:GLN:HG3	2.18	0.43
5:B:194:LYS:NZ	5:D:82:HIS:ND1	2.53	0.43
1:I:1:DA:H2"	1:I:2:DT:C7	2.48	0.43
5:B:473:ALA:C	5:B:475:ILE:H	2.22	0.43
5:D:404:ARG:HH22	5:D:465:LYS:HZ1	1.67	0.43
5:B:64:GLN:HB3	10:B:9210:HOH:O	2.18	0.43
5:D:244:SER:HB3	8:D:8485:FAD:C5'	2.48	0.43
5:B:340:GLN:HG2	5:B:346:TRP:O	2.17	0.43
5:A:471:LEU:O	5:A:475:ILE:HB	2.19	0.43
5:A:405:ILE:HG21	5:A:461:GLN:HG3	2.00	0.43
5:C:64:GLN:HB3	10:C:7727:HOH:O	2.17	0.43
5:B:315:GLU:HG2	5:B:317:ARG:HG3	2.01	0.43
5:C:401:LYS:CG	5:C:404:ARG:HE	2.32	0.43
5:B:275:ASN:O	5:B:279:VAL:HG23	2.19	0.43
5:D:158:ALA:HB3	10:D:8776:HOH:O	2.19	0.43
5:C:83:LEU:HD22	10:C:7779:HOH:O	2.18	0.43
5:B:305:TYR:CD1	5:B:398:MET:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:DA:H2''	1:K:2:DT:C7	2.49	0.43
5:B:244:SER:HB3	8:B:6485:FAD:C5'	2.49	0.43
3:O:9:DC:H2''	3:O:10:DG:OP2	2.17	0.42
5:D:194:LYS:CD	10:D:8744:HOH:O	2.66	0.42
5:D:459:LEU:O	5:D:463:GLN:HG3	2.19	0.42
5:C:183:ALA:N	5:C:184:PRO:HD2	2.34	0.42
5:C:214:ILE:O	5:C:218:GLN:HG3	2.19	0.42
5:A:76:LEU:HD23	5:A:83:LEU:HB3	2.00	0.42
1:I:7:DT:H72	7:I:12:TCP:C5M	2.42	0.42
5:A:305:TYR:O	5:A:310:GLN:NE2	2.52	0.42
5:A:433:HIS:ND1	5:A:434:PRO:HD2	2.34	0.42
5:A:60:GLN:HG2	5:A:190:LEU:HD23	2.01	0.42
2:L:9:DA:H2''	2:L:10:DG:O5'	2.19	0.42
5:D:5:ILE:HD12	5:D:28:SER:HB3	2.02	0.42
2:L:13:DG:C5'	5:B:151:PRO:HG2	2.49	0.42
5:D:219:GLU:HG3	10:D:8642:HOH:O	2.19	0.42
5:A:85:PRO:O	5:A:89:GLN:HG3	2.20	0.42
5:A:475:ILE:OXT	5:A:475:ILE:HG23	2.19	0.42
5:A:471:LEU:HD11	5:A:475:ILE:HD12	2.02	0.42
5:D:187:LEU:HD12	5:D:187:LEU:HA	1.95	0.42
5:C:147:SER:O	5:C:399:ASP:N	2.50	0.42
5:D:404:ARG:HD3	5:D:405:ILE:H	1.84	0.42
5:D:34:LEU:HD21	5:D:84:ILE:HD12	2.00	0.42
5:C:34:LEU:HD21	5:C:84:ILE:CD1	2.49	0.42
4:P:11:DC:H2''	4:P:12:DC:C5	2.55	0.42
5:C:447:ARG:O	5:C:448:ARG:C	2.58	0.42
5:C:392:TRP:HD1	10:C:7668:HOH:O	2.03	0.41
2:L:7:DG:H2''	2:L:8:DA:O5'	2.20	0.41
5:A:219:GLU:HG3	10:A:9159:HOH:O	2.20	0.41
5:C:427:PRO:HB3	5:C:430:ARG:CZ	2.50	0.41
5:A:306:ARG:HH22	5:A:308:LEU:HD13	1.85	0.41
5:B:85:PRO:O	5:B:89:GLN:HG3	2.21	0.41
5:C:177:GLU:H	5:C:177:GLU:CD	2.23	0.41
5:C:12:ASP:OD1	5:C:12:ASP:N	2.54	0.41
5:C:34:LEU:HD21	5:C:84:ILE:HD12	2.03	0.41
5:B:447:ARG:O	5:B:448:ARG:C	2.59	0.41
5:D:398:MET:HE2	5:D:398:MET:HA	2.03	0.41
5:A:443:THR:OG1	5:A:446:GLU:HG3	2.21	0.41
5:A:456:ASN:O	5:A:460:ARG:HG2	2.21	0.41
5:C:190:LEU:HD12	5:C:191:PRO:HD2	2.03	0.40
2:J:9:DA:H2''	2:J:10:DG:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:20:GLY:HA2	5:B:127:LEU:HD12	2.03	0.40
5:B:145:PRO:HB3	5:B:296:HIS:CD2	2.56	0.40
5:D:145:PRO:HB3	5:D:296:HIS:CD2	2.55	0.40
5:D:126:GLN:NE2	10:D:8518:HOH:O	2.55	0.40
5:A:187:LEU:HA	5:A:187:LEU:HD12	1.96	0.40
5:C:175:SER:OG	5:C:177:GLU:HG2	2.22	0.40
5:A:358:PHE:O	5:A:362:ASP:HB2	2.22	0.40
5:B:443:THR:HG23	10:B:9276:HOH:O	2.21	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	
5	A	472/474 (100%)	457 (97%)	15 (3%)	0	100	100
5	B	472/474 (100%)	458 (97%)	14 (3%)	0	100	100
5	C	472/474 (100%)	454 (96%)	15 (3%)	3 (1%)	30	14
5	D	472/474 (100%)	453 (96%)	18 (4%)	1 (0%)	52	35
All	All	1888/1896 (100%)	1822 (96%)	62 (3%)	4 (0%)	52	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	404	ARG
5	C	474	ALA
5	C	402	PRO
5	C	401	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	383/385 (100%)	377 (98%)	6 (2%)	70	59
5	B	385/385 (100%)	377 (98%)	8 (2%)	61	47
5	C	383/385 (100%)	376 (98%)	7 (2%)	66	54
5	D	384/385 (100%)	378 (98%)	6 (2%)	70	59
All	All	1535/1540 (100%)	1508 (98%)	27 (2%)	66	54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	102	ILE
5	A	157	GLN
5	A	230	PRO
5	A	248	LYS
5	A	306	ARG
5	A	475	ILE
5	B	43	GLN
5	B	90	GLN
5	B	102	ILE
5	B	157	GLN
5	B	230	PRO
5	B	248	LYS
5	B	271	ASP
5	B	306	ARG
5	C	90	GLN
5	C	102	ILE
5	C	157	GLN
5	C	230	PRO
5	C	248	LYS
5	C	398	MET
5	C	401	LYS
5	D	102	ILE
5	D	157	GLN
5	D	230	PRO

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Mol	Chain	Res	Type
5	D	248	LYS
5	D	398	MET
5	D	404	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	63	GLN
5	A	77	GLN
5	A	86	GLN
5	A	112	GLN
5	A	126	GLN
5	A	157	GLN
5	A	310	GLN
5	A	328	GLN
5	A	348	HIS
5	A	372	GLN
5	A	376	GLN
5	A	386	ASN
5	A	461	GLN
5	A	463	GLN
5	B	60	GLN
5	B	63	GLN
5	B	77	GLN
5	B	90	GLN
5	B	112	GLN
5	B	126	GLN
5	B	157	GLN
5	B	218	GLN
5	B	259	GLN
5	B	348	HIS
5	B	372	GLN
5	B	376	GLN
5	B	386	ASN
5	B	461	GLN
5	C	63	GLN
5	C	77	GLN
5	C	90	GLN
5	C	112	GLN
5	C	126	GLN
5	C	157	GLN
5	C	348	HIS

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Mol	Chain	Res	Type
5	C	372	GLN
5	C	376	GLN
5	C	386	ASN
5	C	461	GLN
5	D	63	GLN
5	D	77	GLN
5	D	86	GLN
5	D	126	GLN
5	D	157	GLN
5	D	328	GLN
5	D	348	HIS
5	D	372	GLN
5	D	376	GLN
5	D	386	ASN
5	D	463	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
8	FAD	A	5485	-	48,58,58	1.35	5 (10%)	54,89,89	2.04	7 (12%)
9	HDF	A	5486	-	25,28,28	4.30	13 (52%)	28,41,41	3.87	18 (64%)
8	FAD	B	6485	-	48,58,58	1.39	6 (12%)	54,89,89	2.04	9 (16%)
9	HDF	B	6486	-	25,28,28	4.29	14 (56%)	28,41,41	3.88	18 (64%)
8	FAD	C	7485	-	48,58,58	1.33	7 (14%)	54,89,89	2.03	7 (12%)
9	HDF	C	7486	-	25,28,28	4.37	14 (56%)	28,41,41	3.87	18 (64%)
8	FAD	D	8485	-	48,58,58	1.42	7 (14%)	54,89,89	1.98	8 (14%)
9	HDF	D	8486	-	25,28,28	4.33	14 (56%)	28,41,41	3.86	18 (64%)
7	TCP	I	12	1	14,19,19	1.21	3 (21%)	17,27,27	4.10	3 (17%)
7	C	I	13	-	12,20,22	0.69	0	18,28,33	0.82	1 (5%)
7	G	I	14	-	16,24,26	1.10	1 (6%)	20,35,40	2.58	3 (15%)
7	C	I	15	-	12,20,22	0.69	0	18,28,33	0.92	1 (5%)
7	TCP	K	12	1	14,19,19	1.19	3 (21%)	17,27,27	4.12	3 (17%)
7	C	K	13	2	12,20,22	0.68	0	18,28,33	0.83	1 (5%)
7	G	K	14	-	16,24,26	1.10	1 (6%)	20,35,40	2.59	3 (15%)
7	C	K	15	-	12,20,22	0.70	0	18,28,33	0.92	1 (5%)

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
8	FAD	A	5485	-	-	0/30/50/50	0/6/6/6
9	HDF	A	5486	-	2/2/3/3	0/14/14/14	0/3/3/3
8	FAD	B	6485	-	-	0/30/50/50	0/6/6/6
9	HDF	B	6486	-	2/2/3/3	0/14/14/14	0/3/3/3
8	FAD	C	7485	-	-	0/30/50/50	0/6/6/6
9	HDF	C	7486	-	2/2/3/3	0/14/14/14	0/3/3/3
8	FAD	D	8485	-	-	0/30/50/50	0/6/6/6
9	HDF	D	8486	-	2/2/3/3	0/14/14/14	0/3/3/3
7	TCP	I	12	1	-	0/3/19/19	0/2/2/2
7	C	I	13	-	-	0/3/21/26	0/2/2/2
7	G	I	14	-	-	0/3/21/26	0/3/3/3
7	C	I	15	-	-	0/3/21/26	0/2/2/2
7	TCP	K	12	1	-	0/3/19/19	0/2/2/2
7	C	K	13	2	-	0/3/21/26	0/2/2/2
7	G	K	14	-	-	0/3/21/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	C	K	15	-	-	0/3/21/26	0/2/2/2

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	8486	HDF	C5-C4A	-9.09	1.39	1.53
9	C	7486	HDF	C5-C4A	-9.05	1.39	1.53
9	A	5486	HDF	C5-C4A	-8.94	1.40	1.53
9	B	6486	HDF	C5-C4A	-8.69	1.40	1.53
9	C	7486	HDF	C4A-C10	-8.56	1.43	1.54
9	B	6486	HDF	C4A-C10	-8.48	1.43	1.54
9	D	8486	HDF	C4A-C10	-8.40	1.43	1.54
9	A	5486	HDF	C4A-C10	-8.27	1.43	1.54
9	D	8486	HDF	C9-C8	-8.25	1.36	1.51
9	A	5486	HDF	C9-C8	-8.15	1.36	1.51
9	C	7486	HDF	C9-C8	-8.03	1.36	1.51
9	B	6486	HDF	C9-C8	-7.97	1.36	1.51
9	A	5486	HDF	C6-C5A	-6.94	1.37	1.53
9	D	8486	HDF	C6-C5A	-6.87	1.37	1.53
9	C	7486	HDF	C9-C9A	-6.75	1.37	1.53
9	B	6486	HDF	C9-C9A	-6.69	1.37	1.53
9	C	7486	HDF	C6-C5A	-6.61	1.38	1.53
9	B	6486	HDF	C6-C5A	-6.53	1.38	1.53
9	A	5486	HDF	C9-C9A	-6.50	1.38	1.53
9	D	8486	HDF	C9-C9A	-6.40	1.38	1.53
9	C	7486	HDF	C5A-C9A	-6.01	1.42	1.53
9	B	6486	HDF	C5A-C9A	-5.83	1.42	1.53
9	A	5486	HDF	C5A-C9A	-5.73	1.42	1.53
9	B	6486	HDF	C5-C5A	-5.70	1.38	1.53
9	D	8486	HDF	C5A-C9A	-5.69	1.42	1.53
9	C	7486	HDF	C5-C5A	-5.66	1.38	1.53
9	D	8486	HDF	C5-C5A	-5.49	1.39	1.53
9	A	5486	HDF	C5-C5A	-5.46	1.39	1.53
9	B	6486	HDF	C7-C6	-5.15	1.39	1.52
9	C	7486	HDF	C7-C6	-5.09	1.39	1.52
9	A	5486	HDF	C7-C6	-5.06	1.39	1.52
9	D	8486	HDF	C7-C6	-4.96	1.39	1.52
9	A	5486	HDF	C7-C8	-4.00	1.40	1.51
9	C	7486	HDF	C7-C8	-3.93	1.40	1.51
9	D	8486	HDF	C7-C8	-3.91	1.40	1.51
9	B	6486	HDF	C7-C8	-3.87	1.40	1.51
9	C	7486	HDF	C9A-N10	-3.86	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	8486	HDF	C9A-N10	-3.81	1.40	1.48
9	A	5486	HDF	C9A-N10	-3.79	1.40	1.48
9	B	6486	HDF	C9A-N10	-3.75	1.40	1.48
9	D	8486	HDF	C4A-C4	-3.58	1.45	1.51
9	C	7486	HDF	C4A-C4	-3.56	1.45	1.51
9	A	5486	HDF	C4A-C4	-3.54	1.46	1.51
9	B	6486	HDF	C1'-C2'	-3.52	1.47	1.52
9	D	8486	HDF	C1'-C2'	-3.44	1.47	1.52
9	C	7486	HDF	C1'-C2'	-3.37	1.47	1.52
9	A	5486	HDF	C1'-C2'	-3.31	1.47	1.52
9	B	6486	HDF	C4A-C4	-3.16	1.46	1.51
9	C	7486	HDF	O8-C8	-2.36	1.36	1.43
9	D	8486	HDF	O8-C8	-2.32	1.36	1.43
9	A	5486	HDF	O8-C8	-2.27	1.36	1.43
9	B	6486	HDF	O8-C8	-2.22	1.36	1.43
7	I	12	TCP	C6-C5	-2.11	1.34	1.40
7	K	12	TCP	C6-C5	-2.05	1.34	1.40
8	D	8485	FAD	C2A-N1A	2.05	1.37	1.33
8	C	7485	FAD	C2A-N3A	2.06	1.35	1.32
8	D	8485	FAD	C2A-N3A	2.10	1.35	1.32
8	B	6485	FAD	C2A-N3A	2.11	1.35	1.32
8	C	7485	FAD	C2A-N1A	2.12	1.37	1.33
9	D	8486	HDF	C4-N3	2.17	1.41	1.37
8	D	8485	FAD	O4B-C1B	2.20	1.44	1.41
9	B	6486	HDF	C4-N3	2.26	1.41	1.37
7	I	12	TCP	C6-N1	2.30	1.38	1.35
8	B	6485	FAD	C5X-N5	2.30	1.39	1.35
8	A	5485	FAD	C5X-N5	2.36	1.39	1.35
8	C	7485	FAD	C5X-N5	2.37	1.39	1.35
7	K	12	TCP	C6-N1	2.40	1.38	1.35
8	C	7485	FAD	O4B-C1B	2.47	1.44	1.41
8	C	7485	FAD	C9A-N10	2.51	1.42	1.38
8	A	5485	FAD	O4B-C1B	2.52	1.44	1.41
9	C	7486	HDF	C4-N3	2.56	1.41	1.37
8	D	8485	FAD	C5X-N5	2.69	1.39	1.35
8	B	6485	FAD	O4B-C1B	2.90	1.44	1.41
7	K	12	TCP	C4-N3	2.93	1.38	1.33
8	C	7485	FAD	C4-N3	2.94	1.38	1.33
8	B	6485	FAD	C4-N3	3.01	1.38	1.33
7	I	12	TCP	C4-N3	3.03	1.38	1.33
8	A	5485	FAD	C4-N3	3.06	1.38	1.33
8	B	6485	FAD	C9A-N10	3.08	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	5485	FAD	C9A-N10	3.16	1.43	1.38
7	I	14	G	C6-N1	3.50	1.39	1.33
7	K	14	G	C6-N1	3.53	1.39	1.33
8	D	8485	FAD	C4-N3	3.54	1.39	1.33
8	D	8485	FAD	C9A-N10	3.59	1.43	1.38
8	C	7485	FAD	C4X-N5	3.89	1.39	1.33
8	A	5485	FAD	C4X-N5	4.35	1.40	1.33
8	B	6485	FAD	C4X-N5	4.42	1.40	1.33
8	D	8485	FAD	C4X-N5	4.43	1.40	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	12	TCP	C5-C4-N3	-8.94	115.18	125.14
7	I	12	TCP	C5-C4-N3	-8.91	115.22	125.14
7	K	14	G	C5-C6-N1	-8.80	111.55	123.59
7	I	14	G	C5-C6-N1	-8.78	111.58	123.59
8	C	7485	FAD	C4X-C4-N3	-4.85	116.96	123.59
8	A	5485	FAD	C4X-C4-N3	-4.75	117.10	123.59
8	B	6485	FAD	C4X-C4-N3	-4.68	117.19	123.59
8	D	8485	FAD	N3A-C2A-N1A	-4.65	125.34	128.89
8	A	5485	FAD	N3A-C2A-N1A	-4.63	125.35	128.89
8	B	6485	FAD	N3A-C2A-N1A	-4.63	125.35	128.89
8	D	8485	FAD	C4X-C4-N3	-4.61	117.28	123.59
8	C	7485	FAD	N3A-C2A-N1A	-4.57	125.39	128.89
8	A	5485	FAD	C4-C4X-C10	-3.30	117.83	119.94
8	D	8485	FAD	C4-C4X-C10	-3.09	117.97	119.94
8	C	7485	FAD	C4-C4X-C10	-2.85	118.12	119.94
8	B	6485	FAD	C4-C4X-C10	-2.80	118.15	119.94
7	K	14	G	N3-C2-N1	-2.32	123.92	127.44
8	D	8485	FAD	C4X-C10-N10	-2.30	119.16	120.52
8	B	6485	FAD	C4X-C10-N10	-2.30	119.16	120.52
7	I	14	G	N3-C2-N1	-2.25	124.01	127.44
8	A	5485	FAD	C4X-C10-N10	-2.15	119.25	120.52
8	D	8485	FAD	C9A-C5X-N5	-2.05	119.32	122.36
8	B	6485	FAD	C9A-C5X-N5	-2.01	119.38	122.36
8	C	7485	FAD	C4X-C10-N10	-2.00	119.34	120.52
8	B	6485	FAD	C1'-N10-C9A	2.01	121.12	118.86
7	K	12	TCP	C5M-C5-C6	2.14	122.93	118.62
7	I	12	TCP	C5M-C5-C6	2.16	122.96	118.62
8	B	6485	FAD	C4-C4X-N5	2.24	121.44	118.72
9	D	8486	HDF	O2'-C2'-C1'	2.38	116.08	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	8485	FAD	C4-C4X-N5	2.42	121.65	118.72
9	A	5486	HDF	O2'-C2'-C1'	2.43	116.19	110.45
8	A	5485	FAD	C4-C4X-N5	2.44	121.68	118.72
8	C	7485	FAD	C4-C4X-N5	2.52	121.78	118.72
9	C	7486	HDF	O2'-C2'-C1'	2.53	116.44	110.45
9	B	6486	HDF	O2'-C2'-C1'	2.64	116.68	110.45
9	C	7486	HDF	C9-C9A-N10	2.82	118.79	113.03
9	B	6486	HDF	C9-C9A-N10	2.84	118.82	113.03
9	A	5486	HDF	O3'-C3'-C2'	2.88	116.02	108.75
9	D	8486	HDF	O3'-C3'-C2'	2.92	116.12	108.75
9	D	8486	HDF	C9-C9A-N10	2.94	119.03	113.03
9	A	5486	HDF	C9-C9A-N10	2.94	119.03	113.03
9	B	6486	HDF	C4A-C5-C5A	2.98	120.15	110.08
9	C	7486	HDF	C4A-C5-C5A	2.99	120.18	110.08
9	A	5486	HDF	C4A-C5-C5A	2.99	120.20	110.08
9	D	8486	HDF	C4A-C5-C5A	3.03	120.30	110.08
9	B	6486	HDF	C7-C6-C5A	3.09	119.55	112.28
9	B	6486	HDF	O3'-C3'-C2'	3.11	116.60	108.75
9	C	7486	HDF	O4-C4-C4A	3.12	127.74	121.88
9	C	7486	HDF	C5-C4A-C4	3.12	117.02	110.89
7	I	13	C	C2-N3-C4	3.12	120.02	115.61
7	I	15	C	C2-N3-C4	3.13	120.03	115.61
7	K	13	C	C2-N3-C4	3.14	120.04	115.61
9	D	8486	HDF	C7-C6-C5A	3.14	119.67	112.28
7	K	15	C	C2-N3-C4	3.15	120.06	115.61
9	D	8486	HDF	C5-C4A-C4	3.16	117.11	110.89
9	A	5486	HDF	C7-C6-C5A	3.16	119.72	112.28
9	C	7486	HDF	C7-C6-C5A	3.18	119.75	112.28
9	C	7486	HDF	O3'-C3'-C2'	3.18	116.76	108.75
9	A	5486	HDF	C5-C4A-C4	3.18	117.15	110.89
9	D	8486	HDF	O4-C4-C4A	3.22	127.94	121.88
8	A	5485	FAD	C4X-N5-C5X	3.23	120.48	116.76
9	B	6486	HDF	C5-C4A-C4	3.23	117.24	110.89
9	B	6486	HDF	O4-C4-C4A	3.40	128.28	121.88
9	A	5486	HDF	O4-C4-C4A	3.42	128.31	121.88
8	B	6485	FAD	C4X-N5-C5X	3.51	120.80	116.76
9	B	6486	HDF	C5-C5A-C6	3.57	119.75	112.68
9	A	5486	HDF	C5-C5A-C6	3.60	119.81	112.68
8	D	8485	FAD	C4X-N5-C5X	3.60	120.90	116.76
8	C	7485	FAD	C4X-N5-C5X	3.61	120.91	116.76
9	D	8486	HDF	C5-C5A-C6	3.64	119.89	112.68
9	C	7486	HDF	C5-C5A-C6	3.65	119.91	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	5486	HDF	O8-C8-C7	3.66	120.40	110.05
9	A	5486	HDF	C8-C9-C9A	3.67	120.44	112.96
9	B	6486	HDF	C8-C9-C9A	3.70	120.49	112.96
9	D	8486	HDF	C8-C9-C9A	3.70	120.51	112.96
9	B	6486	HDF	O8-C8-C7	3.71	120.55	110.05
9	C	7486	HDF	O8-C8-C7	3.71	120.56	110.05
9	D	8486	HDF	O8-C8-C7	3.75	120.66	110.05
9	C	7486	HDF	C8-C9-C9A	3.76	120.62	112.96
9	C	7486	HDF	C6-C7-C8	3.80	118.63	111.59
9	B	6486	HDF	C6-C7-C8	3.96	118.91	111.59
9	D	8486	HDF	C6-C7-C8	3.96	118.91	111.59
9	A	5486	HDF	C6-C7-C8	3.97	118.94	111.59
9	D	8486	HDF	O8-C8-C9	4.05	117.92	109.86
9	A	5486	HDF	C1'-C2'-C3'	4.09	121.52	109.82
9	C	7486	HDF	O8-C8-C9	4.10	118.01	109.86
9	C	7486	HDF	C1'-C2'-C3'	4.11	121.58	109.82
9	B	6486	HDF	O8-C8-C9	4.12	118.05	109.86
9	B	6486	HDF	C1'-C2'-C3'	4.14	121.64	109.82
9	D	8486	HDF	C1'-C2'-C3'	4.14	121.65	109.82
9	A	5486	HDF	O8-C8-C9	4.19	118.20	109.86
9	A	5486	HDF	C5A-C9A-N10	5.68	122.45	110.12
9	D	8486	HDF	C5A-C9A-N10	5.68	122.46	110.12
9	B	6486	HDF	C5A-C9A-N10	5.72	122.54	110.12
9	C	7486	HDF	C5A-C9A-N10	5.76	122.63	110.12
9	C	7486	HDF	C5-C5A-C9A	6.35	119.11	109.94
9	D	8486	HDF	C5-C5A-C9A	6.37	119.14	109.94
9	A	5486	HDF	C5-C5A-C9A	6.42	119.21	109.94
9	B	6486	HDF	C5-C5A-C9A	6.44	119.24	109.94
7	I	14	G	C6-N1-C2	6.59	125.08	115.94
7	K	14	G	C6-N1-C2	6.61	125.11	115.94
9	C	7486	HDF	C6-C5A-C9A	7.04	120.97	110.23
9	A	5486	HDF	C6-C5A-C9A	7.04	120.97	110.23
9	D	8486	HDF	C6-C5A-C9A	7.05	120.97	110.23
9	B	6486	HDF	C6-C5A-C9A	7.07	121.00	110.23
9	B	6486	HDF	C5-C4A-C10	7.63	118.76	107.89
9	A	5486	HDF	C5-C4A-C10	7.66	118.80	107.89
9	D	8486	HDF	C5-C4A-C10	7.72	118.88	107.89
9	C	7486	HDF	C5-C4A-C10	7.73	118.89	107.89
9	A	5486	HDF	C9-C8-C7	8.53	121.40	110.52
9	B	6486	HDF	C9-C8-C7	8.54	121.40	110.52
9	D	8486	HDF	C9-C8-C7	8.55	121.42	110.52
9	C	7486	HDF	C9-C8-C7	8.56	121.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	8485	FAD	C4-N3-C2	10.18	124.05	115.25
8	C	7485	FAD	C4-N3-C2	10.51	124.33	115.25
8	B	6485	FAD	C4-N3-C2	10.66	124.46	115.25
8	A	5485	FAD	C4-N3-C2	10.77	124.56	115.25
7	I	12	TCP	C4-N3-C2	13.89	127.25	115.25
7	K	12	TCP	C4-N3-C2	13.93	127.29	115.25

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	D	8486	HDF	C4'
9	D	8486	HDF	C2'
9	B	6486	HDF	C4'
9	B	6486	HDF	C2'
9	A	5486	HDF	C4'
9	A	5486	HDF	C2'
9	C	7486	HDF	C4'
9	C	7486	HDF	C2'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	6485	FAD	1	0
8	C	7485	FAD	1	0
8	D	8485	FAD	1	0
7	I	12	TCP	6	0
7	K	12	TCP	6	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	I	7/11 (63%)	3.02	5 (71%) 0 0	41, 52, 58, 60	7 (100%)
1	K	7/11 (63%)	3.24	4 (57%) 0 0	42, 52, 60, 60	7 (100%)
2	J	9/9 (100%)	2.11	4 (44%) 0 0	37, 48, 62, 63	9 (100%)
2	L	9/9 (100%)	2.63	5 (55%) 0 0	42, 50, 62, 64	9 (100%)
3	M	4/4 (100%)	1.93	1 (25%) 1 0	39, 47, 48, 51	4 (100%)
3	O	4/4 (100%)	3.51	4 (100%) 0 0	47, 52, 55, 56	4 (100%)
4	N	5/5 (100%)	4.25	5 (100%) 0 0	51, 53, 56, 59	5 (100%)
4	P	5/5 (100%)	2.47	2 (40%) 0 0	43, 47, 55, 60	5 (100%)
5	A	474/474 (100%)	0.38	27 (5%) 27 22	15, 27, 48, 63	1 (0%)
5	B	474/474 (100%)	0.29	24 (5%) 32 26	14, 26, 47, 65	2 (0%)
5	C	474/474 (100%)	0.31	26 (5%) 29 23	14, 25, 48, 65	0
5	D	474/474 (100%)	0.39	31 (6%) 22 18	16, 27, 48, 63	2 (0%)
All	All	1946/1954 (99%)	0.41	138 (7%) 19 15	14, 27, 50, 65	55 (2%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	2	ALA	9.8
5	C	475	ILE	8.8
5	B	475	ILE	8.8
5	D	2	ALA	8.6
5	D	475	ILE	7.3
5	A	475	ILE	7.3
2	J	6	DC	6.5
5	C	2	ALA	6.4
5	C	473	ALA	6.3
4	N	10	DG	6.1
5	B	2	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	K	1	DA	6.0
5	B	473	ALA	6.0
5	A	474	ALA	5.6
5	B	305	TYR	5.5
5	A	305	TYR	5.5
4	N	11	DC	5.5
2	L	6	DC	5.4
1	K	2	DT	5.4
5	C	474	ALA	5.2
5	D	305	TYR	5.2
5	D	3	ALA	5.0
2	L	7	DG	4.9
4	P	10	DG	4.9
5	B	474	ALA	4.9
1	I	3	DC	4.8
5	A	307	SER	4.8
5	C	445	ILE	4.7
1	I	1	DA	4.6
5	D	473	ALA	4.6
5	A	398	MET	4.5
5	A	471	LEU	4.5
1	I	2	DT	4.5
5	D	471	LEU	4.5
5	A	3	ALA	4.5
3	O	8	DT	4.5
2	L	9	DA	4.2
5	D	474	ALA	4.1
5	A	308	LEU	4.1
5	D	307	SER	4.1
5	C	269	ARG	4.1
3	O	11	DC	4.0
1	K	3	DC	4.0
2	J	7	DG	3.9
5	B	445	ILE	3.9
5	C	141	GLY	3.8
3	M	8	DT	3.8
5	D	404	ARG	3.8
5	C	402	PRO	3.7
5	A	473	ALA	3.7
1	K	4	DG	3.6
5	C	471	LEU	3.6
4	P	11	DC	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	8	DA	3.5
4	N	14	DA	3.5
4	N	13	DG	3.4
2	L	8	DA	3.4
5	B	398	MET	3.3
1	I	4	DG	3.3
5	C	177	GLU	3.2
3	O	9	DC	3.1
5	B	471	LEU	3.1
5	D	142	SER	3.1
5	A	466	ALA	3.1
5	C	307	SER	3.1
5	B	141	GLY	3.1
5	A	143	GLY	3.0
5	B	177	GLU	3.0
5	C	142	SER	3.0
5	A	311	GLN	3.0
5	D	449	GLY	3.0
5	C	268	SER	3.0
5	B	400	PRO	2.9
5	D	311	GLN	2.9
5	B	272	GLU	2.9
5	D	472	LYS	2.9
5	A	118	LYS	2.8
5	D	445	ILE	2.8
5	D	140	SER	2.8
5	D	405	ILE	2.8
4	N	12	DC	2.8
5	A	94	GLU	2.7
5	D	308	LEU	2.7
5	A	34	LEU	2.7
5	A	396	SER	2.7
5	D	94	GLU	2.6
5	C	392	TRP	2.6
5	D	400	PRO	2.6
5	D	402	PRO	2.5
5	C	470	GLN	2.5
5	C	154	LYS	2.4
5	D	395	SER	2.4
2	L	10	DG	2.4
5	D	143	GLY	2.4
5	A	119	THR	2.4

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Mol	Chain	Res	Type	RSRZ
5	A	306	ARG	2.4
5	A	470	GLN	2.4
5	D	222	ASP	2.4
3	O	10	DG	2.4
5	B	307	SER	2.4
5	A	469	ASN	2.4
5	C	143	GLY	2.4
5	A	400	PRO	2.4
5	D	470	GLN	2.3
5	A	199	ASP	2.3
5	B	223	ARG	2.3
5	C	176	PRO	2.3
5	C	444	PRO	2.3
5	A	449	GLY	2.3
5	D	34	LEU	2.3
5	B	180	THR	2.3
5	B	443	THR	2.3
5	C	472	LYS	2.2
1	I	5	DG	2.2
5	B	306	ARG	2.2
2	J	9	DA	2.2
5	B	181	ALA	2.2
5	C	400	PRO	2.2
5	C	443	THR	2.2
5	D	119	THR	2.2
5	D	141	GLY	2.2
5	C	180	THR	2.2
5	A	472	LYS	2.1
5	B	403	LEU	2.1
5	C	160	PRO	2.1
5	D	201	ASP	2.1
5	D	401	LYS	2.1
5	B	176	PRO	2.1
5	B	399	ASP	2.1
5	D	118	LYS	2.1
5	A	92	GLN	2.1
5	B	247	LEU	2.0
5	D	92	GLN	2.0
5	A	385	ALA	2.0
5	B	142	SER	2.0
5	C	305	TYR	2.0
5	C	308	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
5	B	444	PRO	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. 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
7	TCP	K	12	18/18	0.78	0.22	2.84	33,35,39,42	18
7	TCP	I	12	18/18	0.90	0.15	0.65	32,34,37,40	18
9	HDF	C	7486	26/26	0.92	0.13	0.61	12,16,19,23	0
9	HDF	D	8486	26/26	0.93	0.13	0.46	14,18,24,30	0
9	HDF	B	6486	26/26	0.93	0.13	0.45	12,16,19,25	0
9	HDF	A	5486	26/26	0.92	0.13	0.44	13,18,25,29	0
8	FAD	A	5485	53/53	0.97	0.14	0.43	13,16,18,19	0
7	C	K	13	19/21	0.88	0.21	0.32	35,44,53,53	19
8	FAD	C	7485	53/53	0.97	0.13	0.28	12,16,19,19	0
7	G	K	14	22/24	0.88	0.23	0.28	26,42,50,51	22
7	C	I	13	19/21	0.92	0.18	0.12	35,43,52,55	19
8	FAD	B	6485	53/53	0.98	0.13	0.05	11,16,19,20	0
7	G	I	14	22/24	0.90	0.20	0.04	26,41,46,47	22
8	FAD	D	8485	53/53	0.98	0.12	-0.00	12,16,19,21	0
7	C	K	15	19/21	0.85	0.24	-	35,49,51,54	19
7	C	I	15	19/21	0.85	0.26	-	40,50,51,55	19
6	MG	A	9002	1/1	0.87	0.21	-	50,50,50,50	0
6	MG	B	9001	1/1	0.93	0.14	-	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.