Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:30 PM GMT

PDB ID	:	4IEM
Title	:	Human apurinic/apyrimidinic endonuclease (APE1) with product DNA and Mg2+
Authors	:	Tsutakawa, S.E.; Mol, C.D.; Arvai, A.S.; Tainer, J.A.
Deposited on	:	2012-12-13
Resolution	:	2.39 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

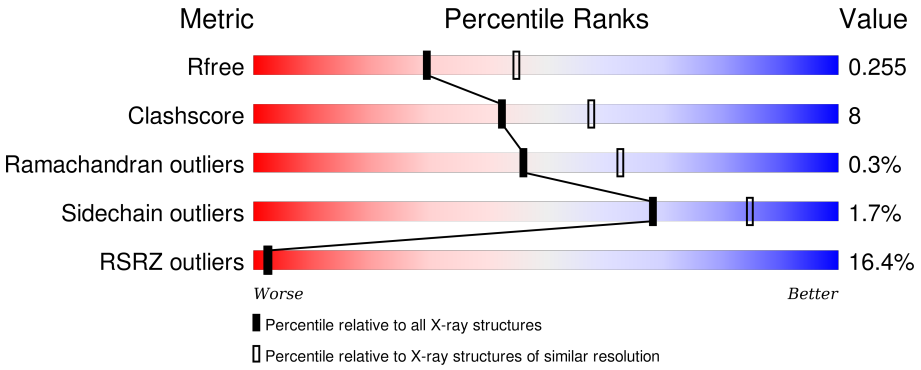
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	A	317	8% 80% 8% 12%
1	B	317	35% 59% 27% • 13%
1	C	317	5% 79% 9% 12%
1	D	317	12% 71% 15% • 13%
2	E	5	40% 60%

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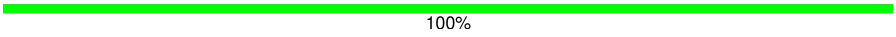
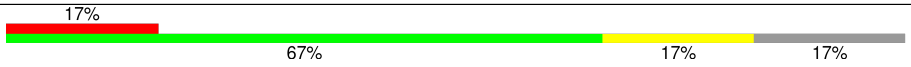
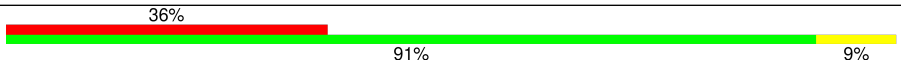
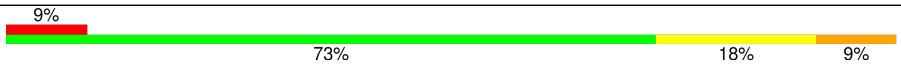
Mol	Chain	Length	Quality of chain
2	H	5	
2	K	5	
2	N	5	
3	F	6	
3	I	6	
3	L	6	
3	O	6	
4	G	11	
4	J	11	
4	M	11	
4	P	11	

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
6	NA	A	504	-	-	-	X
6	NA	B	402	-	-	-	X
6	NA	B	403	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20539 atoms, of which 9721 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 DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	H	N	O	S	0	1	0
			4420	1416	2203	385	407	9			
1	B	275	Total	C	H	N	O	S	0	3	0
			4404	1410	2195	384	406	9			
1	C	278	Total	C	H	N	O	S	0	0	0
			4399	1411	2190	382	407	9			
1	D	276	Total	C	H	N	O	S	0	0	0
			4378	1404	2180	380	405	9			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	5	Total	C	H	N	O	P	0	0	0
			155	48	57	18	28	4			
2	H	5	Total	C	H	N	O	P	0	0	0
			155	48	57	18	28	4			
2	K	5	Total	C	H	N	O	P	0	0	0
			155	48	57	18	28	4			
2	N	5	Total	C	H	N	O	P	0	0	0
			155	48	57	18	28	4			

- Molecule 3 is a DNA chain called DNA (5'-D(P*(3DR)P*GP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	6	Total	C	H	N	O	P	0	0	0
			181	54	65	20	36	6			
3	I	5	Total	C	H	N	O	P	0	0	0
			121	35	42	12	27	5			
3	L	6	Total	C	H	N	O	P	0	0	0
			181	54	65	20	36	6			
3	O	6	Total	C	H	N	O	P	0	0	0
			151	44	53	15	33	6			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	11	Total	C	H	N	O	P	0	0	0
			349	107	125	43	64	10			
4	J	11	Total	C	H	N	O	P	0	0	0
			349	107	125	43	64	10			
4	M	11	Total	C	H	N	O	P	0	0	0
			349	107	125	43	64	10			
4	P	11	Total	C	H	N	O	P	0	0	0
			349	107	125	43	64	10			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	3	Total	Mg	0	0
			3	3		
5	D	1	Total	Mg	0	0
			1	1		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		
6	B	3	Total	Na	0	0
			3	3		
6	A	2	Total	Na	0	0
			2	2		
6	N	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

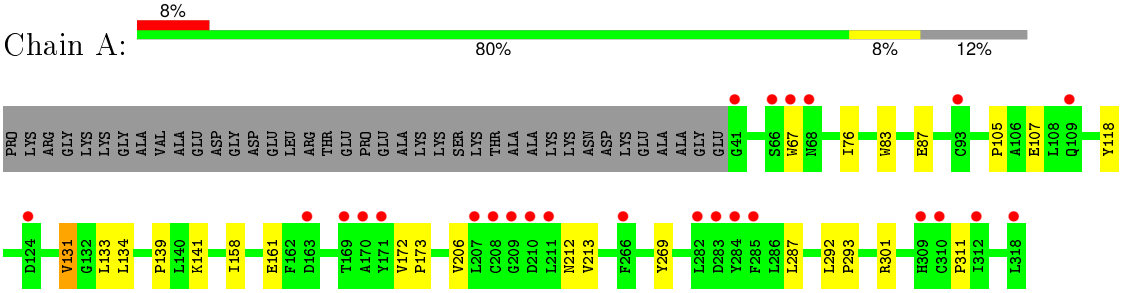
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	19	Total O 19 19	0	0
7	C	72	Total O 72 72	0	0
7	D	39	Total O 39 39	0	0
7	E	5	Total O 5 5	0	0
7	F	9	Total O 9 9	0	0
7	G	8	Total O 8 8	0	0
7	H	3	Total O 3 3	0	0
7	I	2	Total O 2 2	0	0
7	J	5	Total O 5 5	0	0
7	K	8	Total O 8 8	0	0
7	L	5	Total O 5 5	0	0
7	M	10	Total O 10 10	0	0
7	N	3	Total O 3 3	0	0
7	O	6	Total O 6 6	0	0
7	P	8	Total O 8 8	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.

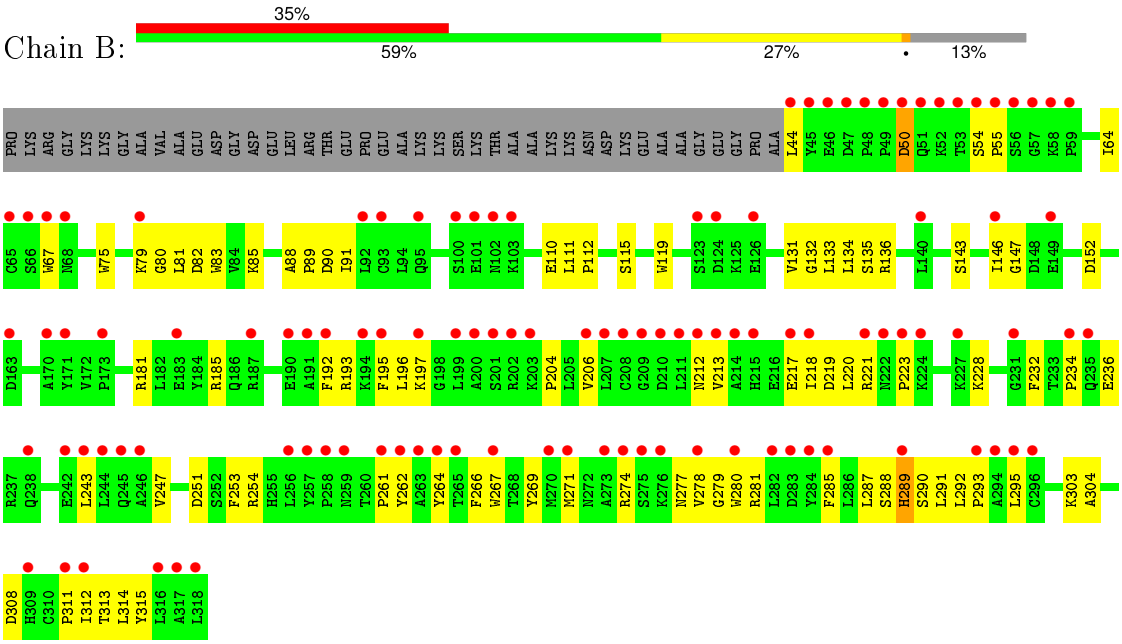
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain A:



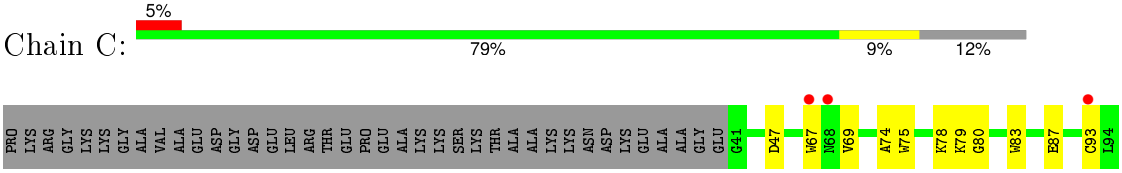
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

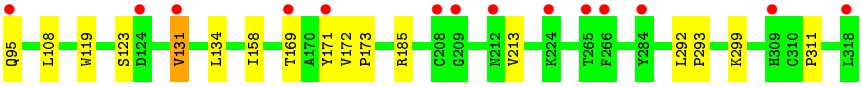
Chain B:



- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

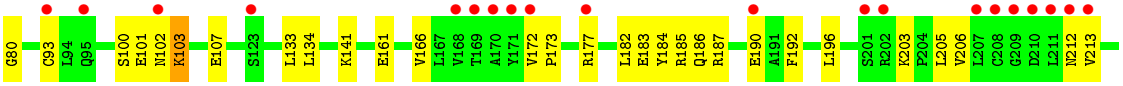
Chain C:

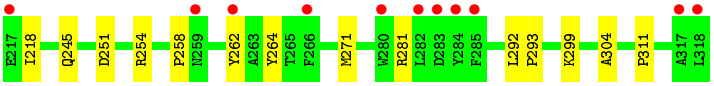




• Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain D:



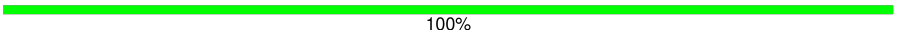


• Molecule 2: DNA (5'-D(*GP*CP*TP*AP*C)-3')

Chain E:

• Molecule 2: DNA (5'-D(*GP*CP*TP*AP*C)-3')

Chain H:



There are no outlier residues recorded for this chain.

• Molecule 2: DNA (5'-D(*GP*CP*TP*AP*C)-3')

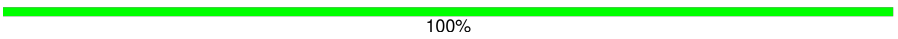
Chain K:

• Molecule 2: DNA (5'-D(*GP*CP*TP*AP*C)-3')

Chain N:

• Molecule 3: DNA (5'-D(P*(3DR)P*GP*AP*TP*CP*G)-3')

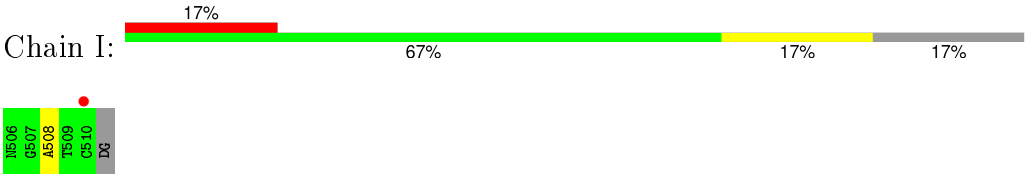
Chain F:



There are no outlier residues recorded for this chain.

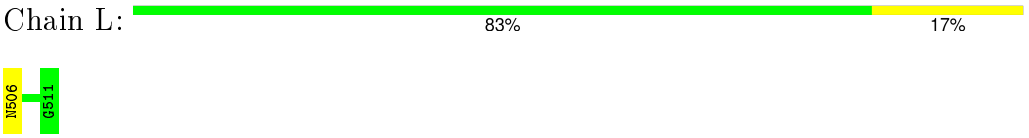
• Molecule 3: DNA (5'-D(P*(3DR)P*GP*AP*TP*CP*G)-3')

Chain I:



• Molecule 3: DNA (5'-D(P*(3DR)P*GP*AP*TP*CP*G)-3')

Chain L:



• Molecule 3: DNA (5'-D(P*(3DR)P*GP*AP*TP*CP*G)-3')

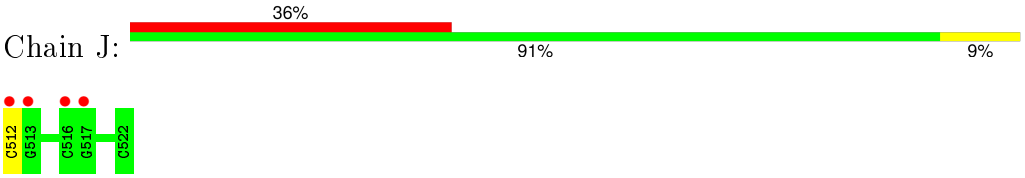
Chain O:

• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

Chain G:

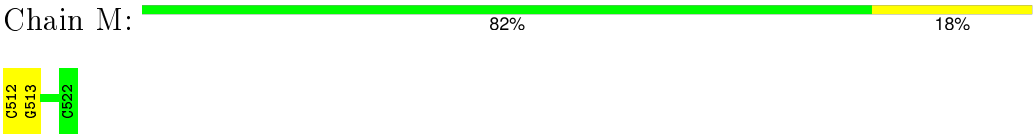
• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

Chain J:



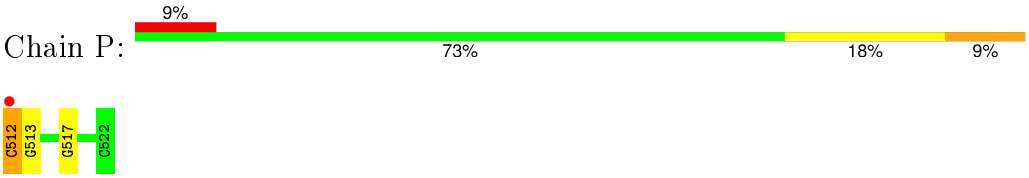
• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

Chain M:



• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.64Å 74.09Å 112.14Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	29.64 – 2.39 29.64 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.64-2.39) 85.8 (29.64-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.62 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.246 0.221 , 0.255	Depositor DCC
R_{free} test set	2871 reflections (5.59%)	DCC
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 56721 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20539	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: NA, MG, 3DR

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	0.25	0/2279	0.45	0/3089
1	B	0.28	0/2275	0.46	0/3083
1	C	0.25	0/2268	0.46	0/3075
1	D	0.24	0/2256	0.45	0/3058
2	E	0.51	0/109	1.23	1/166 (0.6%)
2	H	0.44	0/109	1.14	0/166
2	K	0.50	0/109	1.06	0/166
2	N	0.47	0/109	1.08	0/166
3	F	0.49	0/116	1.10	0/177
3	I	0.50	0/74	1.19	0/113
3	L	0.49	0/116	1.07	0/177
3	O	0.51	0/95	1.02	0/145
4	G	0.55	0/251	1.09	0/386
4	J	0.47	0/251	0.99	0/386
4	M	0.48	0/251	1.08	0/386
4	P	0.51	0/251	1.46	4/386 (1.0%)
All	All	0.31	0/10919	0.64	5/15125 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	512	DC	O4'-C1'-N1	13.75	117.62	108.00
4	P	512	DC	O4'-C1'-C2'	-8.59	99.03	105.90
4	P	512	DC	C1'-O4'-C4'	-8.18	101.92	110.10
4	P	512	DC	C3'-C2'-C1'	-8.11	92.77	102.50
2	E	501	DG	O4'-C1'-N9	5.20	111.64	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2217	2203	2197	16	0
1	B	2209	2195	2182	86	0
1	C	2209	2190	2184	18	0
1	D	2198	2180	2174	37	0
2	E	98	57	57	1	0
2	H	98	57	57	0	0
2	K	98	57	57	2	0
2	N	98	57	57	5	0
3	F	116	65	65	0	0
3	I	79	42	42	1	0
3	L	116	65	65	1	0
3	O	98	53	53	2	0
4	G	224	125	125	3	0
4	J	224	125	125	3	0
4	M	224	125	125	2	0
4	P	224	125	125	2	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	N	1	0	0	0	0
7	A	70	0	0	0	0
7	B	19	0	0	0	0
7	C	72	0	0	0	0
7	D	39	0	0	1	0
7	E	5	0	0	0	0
7	F	9	0	0	0	0
7	G	8	0	0	0	0
7	H	3	0	0	0	0
7	I	2	0	0	0	0
7	J	5	0	0	0	0
7	K	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	5	0	0	0	0
7	M	10	0	0	0	0
7	N	3	0	0	0	0
7	O	6	0	0	0	0
7	P	8	0	0	0	0
All	All	10818	9721	9690	168	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 (168) 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:C:83:TRP:CH2	1:C:87:GLU:HG3	2.18	0.79
1:B:285:PHE:CE2	1:B:312:ILE:HD12	2.19	0.78
1:C:69:VAL:HG13	1:C:75:TRP:CG	2.21	0.75
1:B:206:VAL:HG13	1:B:287:LEU:CD2	2.21	0.70
1:B:204:PRO:HB3	1:B:291:LEU:HD11	1.73	0.70
1:B:64:ILE:HG23	1:B:91:ILE:HD11	1.72	0.70
1:D:177:ARG:HE	2:N:505:DC:N4	1.89	0.69
4:P:512:DC:H4'	4:P:513:DG:H5'	1.74	0.69
1:D:141:LYS:HE3	1:D:161:GLU:CD	2.14	0.68
1:D:101:GLU:OE1	1:D:101:GLU:N	2.28	0.67
1:B:54:SER:HB2	1:B:55:PRO:HD2	1.76	0.66
1:B:206:VAL:HG13	1:B:287:LEU:HD21	1.79	0.63
1:B:287:LEU:HD12	1:B:295:LEU:HD21	1.79	0.63
1:B:292:LEU:N	1:B:293:PRO:CD	2.61	0.63
1:B:204:PRO:CB	1:B:291:LEU:HD11	2.30	0.61
1:B:292:LEU:N	1:B:293:PRO:HD2	2.14	0.61
1:A:83:TRP:CH2	1:A:87:GLU:HG3	2.36	0.60
1:B:291:LEU:N	1:B:291:LEU:HD12	2.16	0.60
1:B:289:HIS:HA	1:B:292:LEU:HD13	1.83	0.59
1:A:107:GLU:N	1:A:107:GLU:OE1	2.35	0.58
1:D:187:ARG:HA	1:D:190:GLU:OE1	2.04	0.58
1:C:69:VAL:HG13	1:C:75:TRP:CB	2.33	0.58
1:B:218:ILE:HD13	1:B:254:ARG:CZ	2.34	0.58
1:B:264:TYR:HB2	1:B:267:TRP:CZ2	2.39	0.58
1:C:185:ARG:NH2	1:C:213:VAL:HG22	2.19	0.57
3:O:510:DC:H4'	3:O:511:DG:OP1	2.05	0.57
1:B:90:ASP:HA	1:B:136:ARG:NH1	2.20	0.56
1:B:64:ILE:HG23	1:B:91:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG22	1:D:75:TRP:CG	2.41	0.56
1:B:217:GLU:HG2	1:B:223:PRO:HG2	1.88	0.56
1:A:172:VAL:HG13	1:A:173:PRO:HD2	1.88	0.55
1:A:133:LEU:C	1:A:134:LEU:HD23	2.26	0.55
1:B:64:ILE:CG2	1:B:91:ILE:HD11	2.37	0.55
1:B:185:ARG:HH22	1:B:213:VAL:HG23	1.73	0.54
1:B:219:ASP:OD1	1:B:281:ARG:NH2	2.41	0.54
1:D:172:VAL:HG13	1:D:173:PRO:HD2	1.90	0.54
1:B:228:LYS:HE3	4:J:512:DC:H3'	1.88	0.54
4:M:512:DC:H2"	4:M:513:DG:C8	2.43	0.53
1:B:146:ILE:HG23	1:B:195:PHE:CG	2.42	0.53
1:B:206:VAL:HG22	1:B:287:LEU:HD22	1.91	0.53
1:B:54:SER:CB	1:B:55:PRO:HD2	2.38	0.53
1:A:83:TRP:CZ2	1:A:87:GLU:HG3	2.44	0.53
1:B:251:ASP:OD2	1:B:281:ARG:NH1	2.41	0.53
1:D:133:LEU:C	1:D:134:LEU:HD23	2.29	0.53
1:B:67:TRP:CD2	1:B:311:PRO:HG3	2.43	0.52
1:B:91:ILE:HG22	1:B:135:SER:HB2	1.91	0.52
1:B:228:LYS:CE	4:J:512:DC:H3'	2.38	0.52
1:D:76:ILE:HG21	1:D:107:GLU:HG3	1.92	0.52
1:B:221:ARG:C	1:B:223:PRO:HD3	2.30	0.52
1:B:91:ILE:HG22	1:B:135:SER:CB	2.40	0.52
1:B:285:PHE:CZ	1:B:312:ILE:HD12	2.44	0.52
4:G:518:DG:C2	4:G:519:DT:C2	2.98	0.52
1:C:93:CYS:HB3	1:C:169:THR:OG1	2.10	0.52
1:A:67:TRP:CD2	1:A:311:PRO:HG3	2.45	0.51
1:D:50:ASP:OD2	1:D:299:LYS:HE2	2.10	0.51
1:B:64:ILE:HD13	1:B:91:ILE:HD11	1.92	0.51
1:D:141:LYS:HG2	1:D:161:GLU:HB3	1.93	0.51
1:B:75:TRP:CE2	1:B:80:GLY:HA3	2.45	0.51
1:B:88:ALA:N	1:B:89:PRO:HD3	2.26	0.51
1:B:64:ILE:CG1	1:B:91:ILE:HD11	2.41	0.50
1:B:193:ARG:HG3	1:B:243:LEU:HD12	1.92	0.50
1:D:75:TRP:CE2	1:D:80:GLY:HA3	2.47	0.49
1:D:177:ARG:NE	2:N:505:DC:N4	2.59	0.49
1:B:146:ILE:HG23	1:B:195:PHE:CB	2.43	0.49
1:D:100:SER:OG	1:D:103:LYS:NZ	2.46	0.49
1:A:67:TRP:CE3	1:A:311:PRO:HG3	2.47	0.49
1:B:269:TYR:CE2	1:B:308:ASP:HB3	2.48	0.49
2:K:504:DA:H2"	2:K:505:DC:O5'	2.13	0.49
1:B:267:TRP:CE3	1:B:274:ARG:CZ	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:HD21	1:B:232:PHE:CE1	2.48	0.49
1:C:108:LEU:HD21	1:C:119:TRP:CZ2	2.49	0.48
1:B:119:TRP:CH2	1:B:134:LEU:HD11	2.49	0.48
1:B:44:LEU:HD22	1:B:277:ASN:HB2	1.94	0.48
1:B:185:ARG:NH1	1:B:236:GLU:OE2	2.47	0.48
1:D:54:SER:HB2	1:D:55:PRO:HD2	1.95	0.48
1:B:146:ILE:HG23	1:B:195:PHE:HB2	1.96	0.48
1:D:251:ASP:CG	1:D:281:ARG:HH12	2.18	0.47
1:C:75:TRP:CE2	1:C:80:GLY:HA3	2.50	0.47
1:B:285:PHE:CD2	1:B:314:LEU:HB2	2.50	0.47
1:B:266:PHE:C	1:B:267:TRP:CE3	2.88	0.47
1:B:278:VAL:HG12	1:B:278:VAL:O	2.14	0.47
1:B:220:LEU:CD2	1:B:232:PHE:CE1	2.97	0.47
1:D:102:ASN:OD1	1:D:103:LYS:N	2.48	0.46
1:B:136:ARG:HB2	1:B:136:ARG:NH1	2.30	0.46
1:B:185:ARG:HH22	1:B:213:VAL:CG2	2.28	0.46
1:D:69:VAL:HG22	1:D:75:TRP:CD1	2.50	0.46
1:B:64:ILE:HG22	1:B:285:PHE:CE1	2.50	0.46
1:C:134:LEU:HD12	1:C:134:LEU:N	2.31	0.46
1:D:192:PHE:CE2	1:D:196:LEU:HD11	2.51	0.46
1:D:182:LEU:O	1:D:186:GLN:HG3	2.16	0.46
1:D:43:ALA:HB1	1:D:262:TYR:CZ	2.50	0.46
1:C:292:LEU:N	1:C:293:PRO:CD	2.79	0.46
1:B:64:ILE:HD12	1:B:314:LEU:HD23	1.98	0.45
1:B:271:MET:HE3	3:I:508:DA:O4'	2.16	0.45
1:B:85:LYS:HE2	1:B:110:GLU:O	2.17	0.45
1:D:205:LEU:HD23	1:D:206:VAL:N	2.32	0.45
1:C:185:ARG:HH22	1:C:213:VAL:HG22	1.81	0.45
1:B:228:LYS:NZ	4:J:512:DC:H3'	2.32	0.45
1:B:196:LEU:HD12	1:B:243:LEU:HD11	1.97	0.45
1:D:205:LEU:HD23	1:D:205:LEU:C	2.37	0.45
1:B:146:ILE:HD12	1:B:195:PHE:CD2	2.52	0.45
1:D:185:ARG:HH22	1:D:213:VAL:HG22	1.81	0.45
2:K:505:DC:H3'	3:L:506:3DR:OP3	2.17	0.45
1:C:78:LYS:O	1:C:79:LYS:HB2	2.17	0.45
1:A:292:LEU:N	1:A:293:PRO:CD	2.80	0.44
1:B:90:ASP:HA	1:B:136:ARG:HH12	1.81	0.44
1:C:74:ALA:O	1:C:78:LYS:HG3	2.18	0.44
1:B:83:TRP:NE1	1:B:304:ALA:HB2	2.32	0.44
1:B:50:ASP:N	1:B:50:ASP:OD1	2.50	0.44
1:B:288:SER:O	1:B:290:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:512:DC:C2'	4:M:513:DG:C8	3.01	0.44
1:B:134:LEU:N	1:B:134:LEU:HD12	2.32	0.44
1:D:69:VAL:HG22	1:D:75:TRP:CD2	2.53	0.43
1:D:54:SER:CB	1:D:55:PRO:HD2	2.48	0.43
1:B:253:PHE:C	1:B:253:PHE:CD2	2.91	0.43
1:B:292:LEU:HD12	1:B:292:LEU:N	2.33	0.43
1:C:67:TRP:CD2	1:C:311:PRO:HG3	2.52	0.43
1:A:206:VAL:HG22	1:A:287:LEU:HD22	1.99	0.43
1:B:81:LEU:HD22	1:B:111:LEU:HD11	2.00	0.43
1:D:304:ALA:HB3	1:D:311:PRO:CD	2.48	0.43
1:A:76:ILE:HD12	1:A:105:PRO:HG2	2.01	0.43
1:D:183:GLU:CG	1:D:184:TYR:N	2.81	0.43
1:D:166:VAL:HG23	1:D:203:LYS:HB3	2.00	0.43
1:D:262:TYR:HA	1:D:264:TYR:CZ	2.53	0.42
1:B:50:ASP:OD2	1:B:315:TYR:OH	2.31	0.42
1:A:131:VAL:HG12	1:A:158:ILE:CD1	2.49	0.42
1:B:54:SER:CB	1:B:55:PRO:CD	2.98	0.42
1:B:146:ILE:HG22	1:B:147:GLY:H	1.84	0.42
4:G:512:DC:H2'	4:G:513:DG:C8	2.55	0.42
1:B:292:LEU:N	1:B:292:LEU:CD1	2.83	0.42
1:B:133:LEU:C	1:B:134:LEU:HD12	2.40	0.42
1:D:292:LEU:N	1:D:293:PRO:CD	2.83	0.42
1:B:110:GLU:C	1:B:112:PRO:HD3	2.40	0.42
1:B:267:TRP:CE3	1:B:274:ARG:NH2	2.88	0.42
1:B:217:GLU:HG2	1:B:223:PRO:CG	2.50	0.42
1:B:304:ALA:HB3	1:B:311:PRO:CD	2.50	0.42
1:C:131:VAL:HG12	1:C:158:ILE:CD1	2.50	0.42
2:E:504:DA:H2"	2:E:505:DC:O5'	2.20	0.42
1:B:251:ASP:C	1:B:251:ASP:OD1	2.59	0.41
1:D:212:ASN:ND2	7:D:519:HOH:O	2.52	0.41
2:N:501:DG:O6	4:P:517:DG:H2"	2.20	0.41
1:A:118:TYR:OH	1:A:139:PRO:HD2	2.21	0.41
1:A:269:TYR:CE2	4:G:519:DT:H4'	2.55	0.41
1:D:254:ARG:HA	1:D:254:ARG:HD3	1.83	0.41
1:B:146:ILE:O	1:B:152:ASP:OD2	2.38	0.41
1:B:64:ILE:O	1:B:313:THR:HA	2.21	0.41
1:A:87:GLU:OE2	1:A:301:ARG:NH2	2.53	0.41
1:B:261:PRO:HB2	1:B:262:TYR:CD2	2.56	0.41
1:B:279:GLY:C	1:B:280:TRP:CD1	2.94	0.41
1:B:131:VAL:CG1	1:B:132:GLY:N	2.84	0.41
1:B:79:LYS:HD2	1:B:82:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:HA	1:C:173:PRO:HD3	1.97	0.41
1:B:64:ILE:CD1	1:B:91:ILE:HD11	2.51	0.41
1:D:177:ARG:HE	2:N:505:DC:H41	1.68	0.41
1:B:67:TRP:CE3	1:B:311:PRO:HG3	2.56	0.41
1:C:47:ASP:OD2	1:C:299:LYS:HE3	2.21	0.41
1:B:64:ILE:CG2	1:B:285:PHE:CE1	3.04	0.41
2:N:505:DC:H3'	3:O:506:3DR:OP3	2.20	0.41
1:B:146:ILE:HD11	1:B:192:PHE:CD1	2.56	0.41
1:D:183:GLU:HG2	1:D:184:TYR:N	2.34	0.41
1:C:95:GLN:HB3	1:C:171:TYR:HB2	2.02	0.41
1:D:218:ILE:O	1:D:218:ILE:HG12	2.21	0.41
1:D:251:ASP:OD1	1:D:281:ARG:NH1	2.54	0.40
1:A:134:LEU:HD23	1:A:134:LEU:N	2.37	0.40
1:B:197:LYS:HD3	1:B:247:VAL:HA	2.03	0.40
1:D:93:CYS:SG	1:D:133:LEU:HD13	2.62	0.40
1:C:69:VAL:CG1	1:C:75:TRP:CB	2.97	0.40
1:A:141:LYS:HB3	1:A:161:GLU:HB3	2.03	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	277/317 (87%)	271 (98%)	6 (2%)	0	100	100
1	B	276/317 (87%)	252 (91%)	22 (8%)	2 (1%)	26	38
1	C	276/317 (87%)	268 (97%)	8 (3%)	0	100	100
1	D	274/317 (86%)	263 (96%)	10 (4%)	1 (0%)	39	56
All	All	1103/1268 (87%)	1054 (96%)	46 (4%)	3 (0%)	46	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	HIS
1	D	271	MET
1	B	234	PRO

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	238/265 (90%)	235 (99%)	3 (1%)	76 89
1	B	238/265 (90%)	232 (98%)	6 (2%)	55 76
1	C	237/265 (89%)	235 (99%)	2 (1%)	86 94
1	D	236/265 (89%)	231 (98%)	5 (2%)	61 80
All	All	949/1060 (90%)	933 (98%)	16 (2%)	68 85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	VAL
1	A	212	ASN
1	A	213	VAL
1	B	50	ASP
1	B	115	SER
1	B	143	SER
1	B	181	ARG
1	B	212	ASN
1	B	303	LYS
1	C	123	SER
1	C	131	VAL
1	D	56	SER
1	D	69	VAL
1	D	103	LYS
1	D	245	GLN
1	D	258	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	HIS
1	B	186	GLN
1	B	255	HIS
1	D	289	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	3DR	F	506	3,5	12,12,12	1.66	3 (25%)	14,17,17	0.87	0
3	3DR	I	506	3,5	12,12,12	1.77	4 (33%)	14,17,17	0.78	0
3	3DR	L	506	3,5	12,12,12	1.76	4 (33%)	14,17,17	0.87	0
3	3DR	O	506	3,5	12,12,12	1.69	3 (25%)	14,17,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3DR	F	506	3,5	-	0/6/16/16	0/1/1/1
3	3DR	I	506	3,5	-	0/6/16/16	0/1/1/1
3	3DR	L	506	3,5	-	0/6/16/16	0/1/1/1
3	3DR	O	506	3,5	-	0/6/16/16	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	506	3DR	C2'-C3'	-3.27	1.46	1.52
3	I	506	3DR	C2'-C3'	-3.27	1.46	1.52
3	O	506	3DR	C2'-C3'	-3.15	1.47	1.52
3	F	506	3DR	C2'-C3'	-3.10	1.47	1.52
3	O	506	3DR	O4'-C4'	-3.06	1.38	1.44
3	L	506	3DR	O4'-C4'	-3.03	1.39	1.44
3	I	506	3DR	O4'-C4'	-3.00	1.39	1.44
3	F	506	3DR	O4'-C4'	-2.95	1.39	1.44
3	I	506	3DR	O3'-C3'	-2.62	1.37	1.43
3	L	506	3DR	O3'-C3'	-2.57	1.37	1.43
3	O	506	3DR	O3'-C3'	-2.43	1.37	1.43
3	F	506	3DR	O3'-C3'	-2.39	1.38	1.43
3	L	506	3DR	C3'-C4'	-2.09	1.47	1.53
3	I	506	3DR	C3'-C4'	-2.07	1.47	1.53

There are no bond angle outliers.

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
3	L	506	3DR	1	0
3	O	506	3DR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	278/317 (87%)	0.39	25 (8%) 12 11	24, 36, 54, 76	0
1	B	275/317 (86%)	1.82	110 (40%) 0 0	36, 68, 88, 100	0
1	C	278/317 (87%)	0.29	17 (6%) 25 25	20, 36, 58, 70	0
1	D	276/317 (87%)	0.81	37 (13%) 4 4	29, 52, 73, 81	0
2	E	5/5 (100%)	-0.34	0 100 100	38, 43, 44, 45	0
2	H	5/5 (100%)	-0.04	0 100 100	51, 58, 59, 63	0
2	K	5/5 (100%)	-0.04	0 100 100	41, 41, 48, 50	0
2	N	5/5 (100%)	0.04	0 100 100	52, 53, 56, 57	0
3	F	5/6 (83%)	-0.04	0 100 100	32, 34, 47, 51	0
3	I	4/6 (66%)	1.34	1 (25%) 1 1	68, 71, 71, 106	0
3	L	5/6 (83%)	-0.18	0 100 100	34, 35, 45, 52	0
3	O	5/6 (83%)	0.16	0 100 100	55, 55, 77, 101	0
4	G	11/11 (100%)	-0.13	0 100 100	38, 48, 61, 62	0
4	J	11/11 (100%)	1.07	4 (36%) 0 0	55, 70, 89, 98	0
4	M	11/11 (100%)	-0.18	0 100 100	41, 46, 60, 65	0
4	P	11/11 (100%)	0.25	1 (9%) 11 11	44, 50, 85, 87	0
All	All	1190/1356 (87%)	0.78	195 (16%) 2 2	20, 46, 81, 106	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLY	7.9
1	B	294	ALA	7.7
1	B	208	CYS	7.0
1	B	209	GLY	6.8
1	B	44	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	58	LYS	5.5
1	B	200	ALA	5.4
1	B	282	LEU	5.4
1	B	201	SER	5.4
1	B	49	PRO	5.1
1	B	318	LEU	5.0
1	B	202	ARG	5.0
1	B	53	THR	4.9
1	D	208	CYS	4.8
1	D	123	SER	4.7
1	D	209	GLY	4.7
1	B	199	LEU	4.6
1	B	221	ARG	4.5
1	B	263	ALA	4.4
1	B	224	LYS	4.4
1	B	140	LEU	4.3
1	B	55	PRO	4.3
1	D	210	ASP	4.2
1	B	66	SER	4.2
1	A	208	CYS	4.2
1	C	208	CYS	4.2
1	B	212	ASN	4.2
1	B	258	PRO	4.1
1	B	243	LEU	4.0
1	B	170	ALA	4.0
1	B	271	MET	4.0
1	B	93	CYS	4.0
1	B	210	ASP	4.0
1	A	209	GLY	3.9
1	B	65	CYS	3.9
1	B	56	SER	3.9
1	D	211	LEU	3.9
1	B	227	LYS	3.8
1	B	242	GLU	3.8
1	B	264	TYR	3.8
1	B	48	PRO	3.8
1	D	282	LEU	3.7
1	D	44	LEU	3.7
1	B	274	ARG	3.7
1	B	276	LYS	3.7
1	A	93	CYS	3.6
1	B	312	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	59	PRO	3.6
1	B	211	LEU	3.5
1	C	318	LEU	3.5
1	B	317	ALA	3.5
1	A	124	ASP	3.4
1	D	283	ASP	3.4
1	B	52	LYS	3.4
1	B	214	ALA	3.4
1	B	285	PHE	3.3
1	D	43	ALA	3.3
1	D	170	ALA	3.3
1	B	54	SER	3.3
1	B	213	VAL	3.3
1	B	194	LYS	3.2
1	D	285	PHE	3.2
1	B	45	TYR	3.2
1	A	318	LEU	3.2
1	B	270	MET	3.2
1	B	283	ASP	3.2
1	B	293	PRO	3.2
1	B	67	TRP	3.1
1	B	278	VAL	3.1
1	B	46	GLU	3.1
1	D	172	VAL	3.1
1	B	280	TRP	3.1
1	B	284	TYR	3.1
1	B	309	HIS	3.1
1	B	149	GLU	3.0
1	D	212	ASN	3.0
1	B	265	THR	3.0
1	B	68	ASN	3.0
1	B	103	LYS	3.0
1	B	100	SER	3.0
1	B	238	GLN	2.9
1	C	171	TYR	2.9
1	D	169	THR	2.9
1	B	197	LYS	2.9
1	D	317	ALA	2.9
1	B	262	TYR	2.9
1	A	169	THR	2.9
1	B	218	ILE	2.9
1	B	289	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
3	I	510	DC	2.9
1	B	316	LEU	2.9
1	D	207	LEU	2.9
1	B	246	ALA	2.8
1	B	124	ASP	2.8
1	B	207	LEU	2.8
1	A	283	ASP	2.8
1	B	47	ASP	2.8
1	B	223	PRO	2.8
4	J	513	DG	2.8
1	A	68	ASN	2.8
1	B	257	TYR	2.8
1	B	295	LEU	2.7
1	B	261	PRO	2.7
1	A	170	ALA	2.7
1	B	191	ALA	2.7
1	D	102	ASN	2.6
1	B	187	ARG	2.6
1	B	296	CYS	2.6
1	D	284	TYR	2.6
1	A	210	ASP	2.6
1	A	109	GLN	2.6
1	D	177	ARG	2.6
4	J	517	DG	2.6
1	B	92	LEU	2.6
1	D	318	LEU	2.6
1	B	50	ASP	2.5
1	D	171	TYR	2.5
1	C	124	ASP	2.5
1	D	49	PRO	2.5
1	D	262	TYR	2.5
1	B	273	ALA	2.5
1	B	101	GLU	2.5
1	A	66	SER	2.5
1	C	224	LYS	2.5
1	C	209	GLY	2.5
1	A	171	TYR	2.5
1	B	275	SER	2.4
1	B	217	GLU	2.4
1	C	67	TRP	2.4
1	A	312	ILE	2.4
1	A	266	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	2.4
1	D	58	LYS	2.4
1	A	285	PHE	2.4
1	C	93	CYS	2.4
1	D	93	CYS	2.4
1	D	213	VAL	2.4
1	A	41	GLY	2.4
1	B	259	ASN	2.4
1	B	163	ASP	2.4
1	A	163	ASP	2.4
1	B	195	PHE	2.4
1	A	309	HIS	2.4
1	C	309	HIS	2.3
1	B	311	PRO	2.3
1	B	123	SER	2.3
1	B	245	GLN	2.3
1	D	266	PHE	2.3
1	D	280	TRP	2.3
1	A	211	LEU	2.3
1	B	192	PHE	2.3
1	A	207	LEU	2.3
1	D	202	ARG	2.3
1	B	235	GLN	2.3
1	C	266	PHE	2.3
1	D	95	GLN	2.3
1	B	215	HIS	2.3
1	B	267	TRP	2.3
4	P	512	DC	2.3
1	D	217	GLU	2.2
1	B	95	GLN	2.2
1	C	95	GLN	2.2
1	B	234	PRO	2.2
1	C	284	TYR	2.2
1	B	190	GLU	2.2
1	B	171	TYR	2.2
1	B	244	LEU	2.2
1	C	265	THR	2.2
1	A	67	TRP	2.1
1	D	45	TYR	2.1
1	B	222	ASN	2.1
1	C	68	ASN	2.1
1	D	168	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	J	516	DC	2.1
1	B	51	GLN	2.1
1	A	282	LEU	2.1
1	B	102	ASN	2.1
1	B	146	ILE	2.1
4	J	512	DC	2.1
1	B	79	LYS	2.1
1	C	131	VAL	2.1
1	C	169	THR	2.0
1	C	212	ASN	2.0
1	D	259	ASN	2.0
1	B	256	LEU	2.0
1	B	203	LYS	2.0
1	D	68	ASN	2.0
1	B	183	GLU	2.0
1	D	190	GLU	2.0
1	B	173	PRO	2.0
1	B	231	GLY	2.0
1	B	206	VAL	2.0
1	D	201	SER	2.0
1	A	284	TYR	2.0
1	A	310	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	3DR	O	506	12/12	0.95	0.25	-	40,56,71,71	0
3	3DR	I	506	12/12	0.95	0.30	-	42,62,75,78	0
3	3DR	L	506	12/12	0.97	0.25	-	25,36,49,49	0
3	3DR	F	506	12/12	0.99	0.22	-	21,35,44,47	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NA	A	504	1/1	0.43	0.31	20.60	50,50,50,50	0
6	NA	B	403	1/1	0.97	0.52	5.61	79,79,79,79	0
6	NA	B	402	1/1	0.02	0.48	3.36	81,81,81,81	0
5	MG	A	501	1/1	0.44	0.19	0.98	55,55,55,55	0
5	MG	A	503	1/1	0.94	0.14	0.36	38,38,38,38	0
5	MG	C	402	1/1	0.96	0.11	-1.22	48,48,48,48	0
6	NA	B	404	1/1	0.93	0.15	-1.45	72,72,72,72	0
5	MG	D	401	1/1	0.40	0.17	-1.63	61,61,61,61	0
5	MG	A	502	1/1	0.93	0.13	-2.27	42,42,42,42	0
5	MG	B	401	1/1	0.92	0.08	-3.20	61,61,61,61	0
5	MG	C	401	1/1	0.92	0.10	-4.39	49,49,49,49	0
6	NA	F	601	1/1	0.86	0.16	-	64,64,64,64	0
6	NA	D	402	1/1	0.72	0.25	-	78,78,78,78	0
6	NA	E	601	1/1	0.93	0.12	-	56,56,56,56	0
6	NA	A	505	1/1	0.95	0.23	-	55,55,55,55	0
6	NA	N	601	1/1	0.90	0.18	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.