Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 10:54 PM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

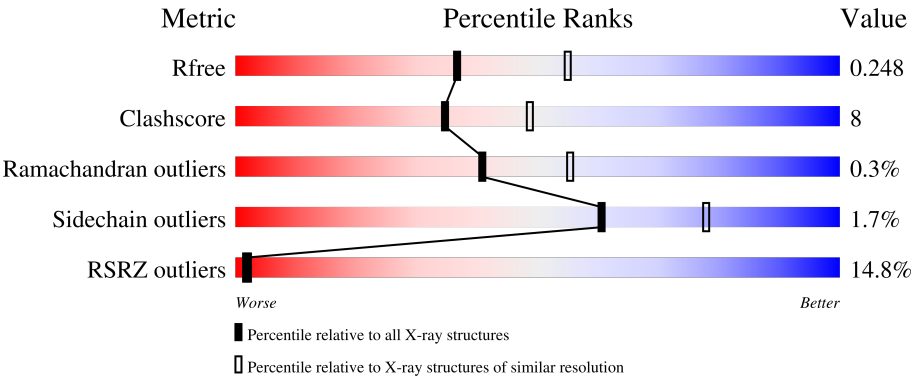
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	7% 80% 8% 12%
1	B	317	32% 59% 27% • 13%
1	C	317	4% 79% 9% 12%
1	D	317	10% 71% 15% • 13%
2	E	5	40% 60%

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Mol	Chain	Length	Quality of chain
2	H	5	100%
2	K	5	60% 40%
2	N	5	60% 40%
3	F	6	83% 17%
3	I	6	17% 50% 33% 17%
3	L	6	83% 17%
3	O	6	50% 33% 17%
4	G	11	64% 36%
4	J	11	27% 91% 9%
4	M	11	82% 18%
4	P	11	9% 73% 18% 9%

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	B	402	-	-	-	X

2 Entry composition (i)

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 349	C 107	H 125	N 43	O 64	P 10	0	0	0
4	J	11	Total 349	C 107	H 125	N 43	O 64	P 10	0	0	0
4	M	11	Total 349	C 107	H 125	N 43	O 64	P 10	0	0	0
4	P	11	Total 349	C 107	H 125	N 43	O 64	P 10	0	0	0

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

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

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

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

- Molecule 7 is water.

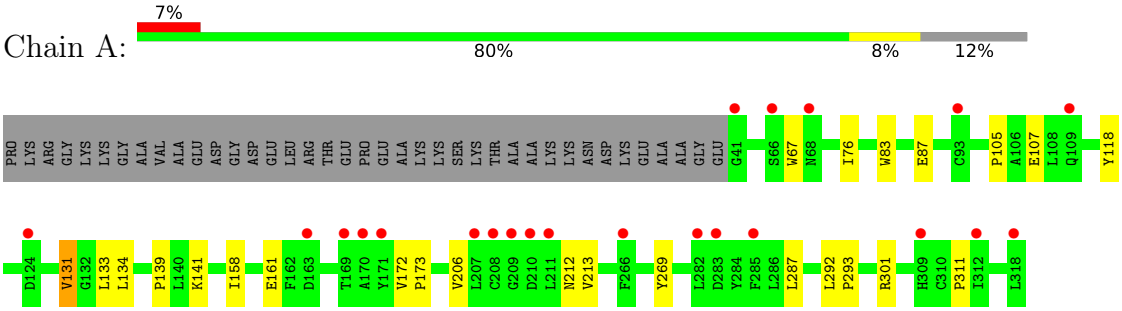
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	E	5	Total O 5 5	0	0
7	F	9	Total O 9 9	0	0
7	G	8	Total O 8 8	0	0
7	B	19	Total O 19 19	0	0
7	H	3	Total O 3 3	0	0
7	I	2	Total O 2 2	0	0
7	J	5	Total O 5 5	0	0
7	C	72	Total O 72 72	0	0
7	K	8	Total O 8 8	0	0
7	L	5	Total O 5 5	0	0
7	M	10	Total O 10 10	0	0
7	D	39	Total O 39 39	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

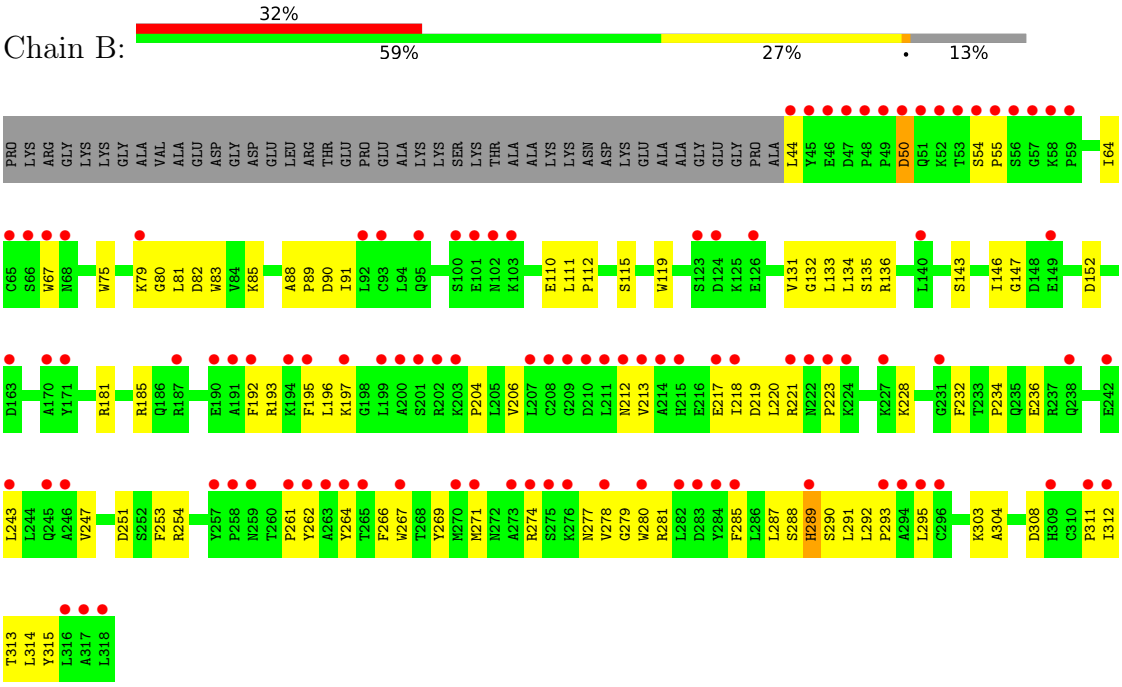
• Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain A:



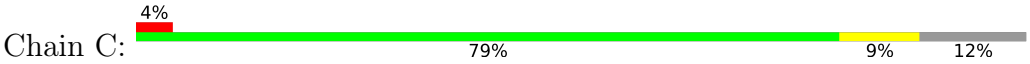
• Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

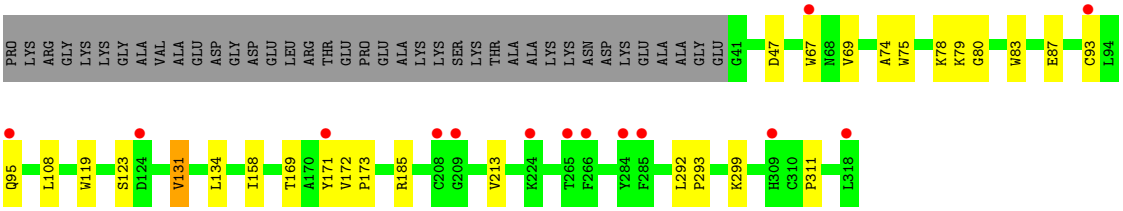
Chain B:



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

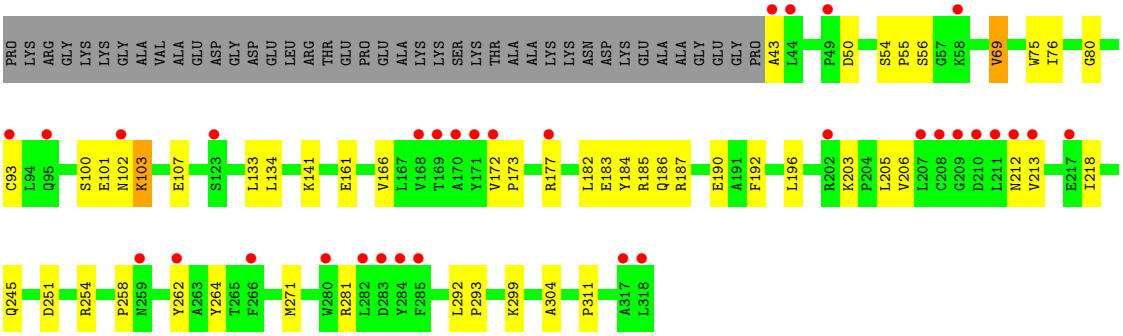
Chain C:





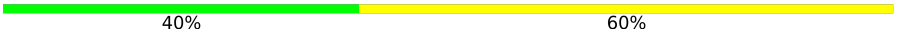
• Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain D:



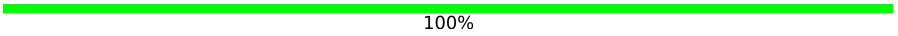
• Molecule 2: DNA (5'-D(*GP*CP*TP*AP*C)-3')

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')

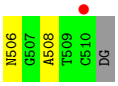
Chain N:

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

Chain F:

• 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')

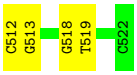
Chain L:

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

Chain O:

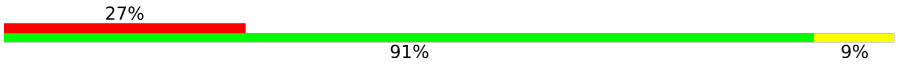
• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

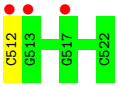
Chain G:



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

Chain J:



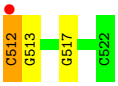


• Molecule 4: DNA (5'-D(*CP*GP*AP*TP*CP*GP*GP*TP*AP*GP*C)-3')

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]	4.18 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.208 , 0.246 0.211 , 0.248	Depositor DCC
R_{free} test set	2871 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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:N	1:D:101:GLU:OE1	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:HD12	1:B:291:LEU:N	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
1:B:146:ILE:HG23	1:B:195:PHE:CG	2.42	0.53
4:M:512:DC:H2"	4:M:513:DG:C8	2.43	0.53
1:A:83:TRP:CZ2	1:A:87:GLU:HG3	2.44	0.53
1:B:54:SER:CB	1:B:55:PRO:HD2	2.38	0.53
1:B:206:VAL:HG22	1:B:287:LEU:HD22	1.91	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
4:G:518:DG:C2	4:G:519:DT:C2	2.98	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
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: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:D:177:ARG:NE	2:N:505:DC:N4	2.59	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:220:LEU:HD21	1:B:232:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:TRP:CE3	1:B:274:ARG:CZ	2.96	0.49
1:C:108:LEU:HD21	1:C:119:TRP:CZ2	2.49	0.48
1:B:44:LEU:HD22	1:B:277:ASN:HB2	1.94	0.48
1:B:119:TRP:CH2	1:B:134:LEU:HD11	2.49	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:266:PHE:C	1:B:267:TRP:CE3	2.88	0.47
1:B:285:PHE:CD2	1:B:314:LEU:HB2	2.50	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:NH1	1:B:136:ARG:HB2	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:182:LEU:O	1:D:186:GLN:HG3	2.16	0.46
1:D:192:PHE:CE2	1:D:196:LEU:HD11	2.51	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:B:196:LEU:HD12	1:B:243:LEU:HD11	1.97	0.45
1:B:228:LYS:NZ	4:J:512:DC:H3'	2.32	0.45
1:C:185:ARG:HH22	1:C:213:VAL:HG22	1.81	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
1:C:78:LYS:O	1:C:79:LYS:HB2	2.17	0.45
2:K:505:DC:H3'	3:L:506:3DR:OP3	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:50:ASP:N	1:B:50:ASP:OD1	2.50	0.44
1:B:83:TRP:NE1	1:B:304:ALA:HB2	2.32	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)
1:B:134:LEU:HD12	1:B:134:LEU:N	2.32	0.44
4:M:512:DC:C2'	4:M:513:DG:C8	3.01	0.44
1:B:253:PHE:CD2	1:B:253:PHE:C	2.91	0.43
1:D:54:SER:CB	1:D:55:PRO:HD2	2.48	0.43
1:D:69:VAL:HG22	1:D:75:TRP:CD2	2.53	0.43
1:A:206:VAL:HG22	1:A:287:LEU:HD22	1.99	0.43
1:B:292:LEU:N	1:B:292:LEU:HD12	2.33	0.43
1:C:67:TRP:CD2	1:C:311:PRO:HG3	2.52	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:A:131:VAL:HG12	1:A:158:ILE:CD1	2.49	0.42
1:B:50:ASP:OD2	1:B:315:TYR:OH	2.31	0.42
1:D:262:TYR:HA	1:D:264:TYR:CZ	2.53	0.42
4:G:512:DC:H2'	4:G:513:DG:C8	2.55	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
1:B:133:LEU:C	1:B:134:LEU:HD12	2.40	0.42
1:B:292:LEU:N	1:B:292:LEU:CD1	2.83	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:217:GLU:HG2	1:B:223:PRO:CG	2.50	0.42
1:B:267:TRP:CE3	1:B:274:ARG:NH2	2.88	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:OD1	1:B:251:ASP:C	2.59	0.41
1:D:212:ASN:ND2	7:D:519:HOH:O	2.52	0.41
1:A:118:TYR:OH	1:A:139:PRO:HD2	2.21	0.41
2:N:501:DG:O6	4:P:517:DG:H2"	2.20	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:A:87:GLU:OE2	1:A:301:ARG:NH2	2.53	0.41
1:B:64:ILE:O	1:B:313:THR:HA	2.21	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: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:D:177:ARG:HE	2:N:505:DC:H41	1.68	0.41
1:B:64:ILE:CG2	1:B:285:PHE:CE1	3.04	0.41
1:B:146:ILE:HD11	1:B:192:PHE:CD1	2.56	0.41
1:C:95:GLN:HB3	1:C:171:TYR:HB2	2.02	0.41
1:D:183:GLU:HG2	1:D:184:TYR:N	2.34	0.41
1:D:218:ILE:HG12	1:D:218:ILE:O	2.21	0.41
2:N:505:DC:H3'	3:O:506:3DR:OP3	2.20	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:A:141:LYS:HB3	1:A:161:GLU:HB3	2.03	0.40
1:C:69:VAL:CG1	1:C:75:TRP:CB	2.97	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%)	22	32
1	C	276/317 (87%)	268 (97%)	8 (3%)	0	100	100
1	D	274/317 (86%)	263 (96%)	10 (4%)	1 (0%)	34	48
All	All	1103/1268 (87%)	1054 (96%)	46 (4%)	3 (0%)	41	55

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%)	69	84
1	B	238/265 (90%)	232 (98%)	6 (2%)	47	67
1	C	237/265 (89%)	235 (99%)	2 (1%)	81	91
1	D	236/265 (89%)	231 (98%)	5 (2%)	53	72
All	All	949/1060 (90%)	933 (98%)	16 (2%)	60	78

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

Sometimes 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	5,3	12,12,12	1.73	3 (25%)	16,17,17	1.03	1 (6%)
3	3DR	I	506	5,3	12,12,12	1.84	4 (33%)	16,17,17	0.94	0
3	3DR	L	506	5,3	12,12,12	1.83	4 (33%)	16,17,17	0.99	0
3	3DR	O	506	5,3	12,12,12	1.76	3 (25%)	16,17,17	1.05	1 (6%)

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	5,3	-	3/6/16/16	0/1/1/1
3	3DR	I	506	5,3	-	2/6/16/16	0/1/1/1
3	3DR	L	506	5,3	-	3/6/16/16	0/1/1/1
3	3DR	O	506	5,3	-	2/6/16/16	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	506	3DR	O4'-C4'	-3.34	1.38	1.44
3	L	506	3DR	O4'-C4'	-3.30	1.39	1.44
3	I	506	3DR	O4'-C4'	-3.27	1.39	1.44
3	L	506	3DR	C2'-C3'	-3.24	1.46	1.52
3	I	506	3DR	C2'-C3'	-3.23	1.46	1.52
3	F	506	3DR	O4'-C4'	-3.22	1.39	1.44
3	O	506	3DR	C2'-C3'	-3.12	1.47	1.52
3	F	506	3DR	C2'-C3'	-3.07	1.47	1.52
3	I	506	3DR	O3'-C3'	-2.77	1.37	1.43
3	L	506	3DR	O3'-C3'	-2.72	1.37	1.43
3	O	506	3DR	O3'-C3'	-2.57	1.37	1.43
3	F	506	3DR	O3'-C3'	-2.53	1.38	1.43
3	L	506	3DR	C3'-C4'	-2.15	1.47	1.53
3	I	506	3DR	C3'-C4'	-2.13	1.47	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	506	3DR	O4'-C4'-C3'	2.02	106.70	103.73
3	F	506	3DR	P-O5'-C5'	2.02	123.85	118.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	506	3DR	C3'-C4'-C5'-O5'
3	O	506	3DR	C3'-C4'-C5'-O5'
3	I	506	3DR	C3'-C4'-C5'-O5'
3	L	506	3DR	C3'-C4'-C5'-O5'
3	F	506	3DR	O4'-C4'-C5'-O5'
3	O	506	3DR	O4'-C4'-C5'-O5'
3	F	506	3DR	C5'-O5'-P-OP1
3	I	506	3DR	O4'-C4'-C5'-O5'
3	L	506	3DR	O4'-C4'-C5'-O5'
3	L	506	3DR	C5'-O5'-P-OP1

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 monosaccharides 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 (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, 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%)	0.33	22 (7%) 12 11	24, 36, 54, 76	0
1	B	275/317 (86%)	1.71	102 (37%) 0 0	36, 68, 88, 100	0
1	C	278/317 (87%)	0.25	14 (5%) 28 27	20, 36, 58, 70	0
1	D	276/317 (87%)	0.74	33 (11%) 4 3	29, 52, 73, 81	0
2	E	5/5 (100%)	-0.39	0 100 100	38, 43, 44, 45	0
2	H	5/5 (100%)	-0.09	0 100 100	51, 58, 59, 63	0
2	K	5/5 (100%)	-0.07	0 100 100	41, 41, 48, 50	0
2	N	5/5 (100%)	0.01	0 100 100	52, 53, 56, 57	0
3	F	5/6 (83%)	-0.08	0 100 100	32, 34, 47, 51	0
3	I	4/6 (66%)	1.27	1 (25%) 0 0	68, 71, 71, 106	0
3	L	5/6 (83%)	-0.26	0 100 100	34, 35, 45, 52	0
3	O	5/6 (83%)	0.14	0 100 100	55, 55, 77, 101	0
4	G	11/11 (100%)	-0.17	0 100 100	38, 48, 61, 62	0
4	J	11/11 (100%)	0.99	3 (27%) 0 0	55, 70, 89, 98	0
4	M	11/11 (100%)	-0.24	0 100 100	41, 46, 60, 65	0
4	P	11/11 (100%)	0.20	1 (9%) 9 8	44, 50, 85, 87	0
All	All	1190/1356 (87%)	0.71	176 (14%) 2 2	20, 46, 81, 106	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLY	7.9
1	B	294	ALA	7.3
1	B	208	CYS	6.7
1	B	209	GLY	6.5
1	B	44	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	58	LYS	5.6
1	B	200	ALA	5.4
1	B	201	SER	5.4
1	B	282	LEU	5.2
1	B	202	ARG	5.1
1	B	53	THR	4.8
1	B	49	PRO	4.7
1	B	318	LEU	4.7
1	B	224	LYS	4.6
1	D	123	SER	4.6
1	D	208	CYS	4.5
1	B	199	LEU	4.5
1	B	221	ARG	4.5
1	D	209	GLY	4.3
1	B	263	ALA	4.2
1	B	258	PRO	4.1
1	C	208	CYS	4.1
1	B	55	PRO	4.1
1	B	212	ASN	4.0
1	D	210	ASP	4.0
1	A	208	CYS	4.0
1	B	140	LEU	4.0
1	B	66	SER	3.9
1	B	170	ALA	3.9
1	B	210	ASP	3.8
1	A	209	GLY	3.8
1	B	227	LYS	3.8
1	B	56	SER	3.7
1	B	243	LEU	3.7
1	B	271	MET	3.7
1	B	242	GLU	3.7
1	B	264	TYR	3.7
1	B	93	CYS	3.6
1	D	211	LEU	3.6
1	B	65	CYS	3.6
1	C	318	LEU	3.6
1	B	59	PRO	3.6
1	D	282	LEU	3.5
1	B	276	LYS	3.5
1	B	48	PRO	3.5
1	A	318	LEU	3.4
1	B	211	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	LYS	3.4
1	D	44	LEU	3.4
1	A	93	CYS	3.4
1	B	312	ILE	3.4
1	A	124	ASP	3.3
1	B	317	ALA	3.3
1	B	52	LYS	3.3
1	B	274	ARG	3.3
1	B	54	SER	3.2
1	D	283	ASP	3.2
1	B	214	ALA	3.2
1	D	170	ALA	3.2
1	B	285	PHE	3.1
1	B	213	VAL	3.1
1	B	100	SER	3.1
1	B	103	LYS	3.1
1	B	149	GLU	3.1
1	B	218	ILE	3.1
1	D	285	PHE	3.1
1	B	283	ASP	3.0
1	B	197	LYS	3.0
1	B	67	TRP	3.0
1	B	280	TRP	3.0
1	B	309	HIS	3.0
1	B	284	TYR	2.9
1	B	45	TYR	2.9
1	B	46	GLU	2.9
1	B	265	THR	2.9
1	B	223	PRO	2.9
1	D	172	VAL	2.9
1	B	246	ALA	2.9
1	B	278	VAL	2.9
1	B	316	LEU	2.9
1	D	43	ALA	2.9
4	J	513	DG	2.8
1	C	171	TYR	2.8
1	D	212	ASN	2.8
1	D	207	LEU	2.8
3	I	510	DC	2.8
1	B	68	ASN	2.8
1	D	169	THR	2.8
1	B	191	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	2.8
1	B	270	MET	2.8
1	B	262	TYR	2.8
1	B	293	PRO	2.7
1	B	257	TYR	2.7
1	B	187	ARG	2.7
1	D	102	ASN	2.7
1	A	169	THR	2.7
1	B	289	HIS	2.7
1	B	261	PRO	2.6
1	A	283	ASP	2.6
1	A	68	ASN	2.6
1	A	109	GLN	2.6
1	B	217	GLU	2.6
1	B	47	ASP	2.6
1	B	124	ASP	2.6
1	B	238	GLN	2.6
1	A	170	ALA	2.6
1	D	317	ALA	2.6
1	D	177	ARG	2.5
1	A	210	ASP	2.5
1	B	295	LEU	2.5
4	J	517	DG	2.5
1	B	101	GLU	2.5
1	B	296	CYS	2.5
1	D	318	LEU	2.5
1	A	266	PHE	2.5
1	D	284	TYR	2.5
1	B	126	GLU	2.4
1	C	224	LYS	2.4
1	B	259	ASN	2.4
1	A	171	TYR	2.4
1	D	171	TYR	2.4
1	C	209	GLY	2.4
1	D	49	PRO	2.4
1	A	285	PHE	2.4
1	C	67	TRP	2.4
1	D	266	PHE	2.4
1	A	66	SER	2.4
1	C	93	CYS	2.4
1	C	124	ASP	2.3
1	B	190	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	50	ASP	2.3
1	B	92	LEU	2.3
1	D	58	LYS	2.3
1	D	262	TYR	2.3
1	B	245	GLN	2.3
1	A	312	ILE	2.3
1	A	309	HIS	2.3
1	D	202	ARG	2.3
1	B	275	SER	2.3
1	D	280	TRP	2.2
1	D	217	GLU	2.2
1	A	41	GLY	2.2
1	A	211	LEU	2.2
1	A	163	ASP	2.2
1	D	213	VAL	2.2
1	B	195	PHE	2.2
1	C	284	TYR	2.2
1	B	311	PRO	2.2
1	D	93	CYS	2.2
1	A	207	LEU	2.2
1	B	273	ALA	2.2
1	D	95	GLN	2.2
1	C	95	GLN	2.2
1	C	309	HIS	2.2
1	D	259	ASN	2.1
1	B	215	HIS	2.1
4	P	512	DC	2.1
1	B	102	ASN	2.1
4	J	512	DC	2.1
1	B	203	LYS	2.1
1	D	168	VAL	2.1
1	B	192	PHE	2.1
1	C	266	PHE	2.1
1	B	123	SER	2.1
1	B	95	GLN	2.1
1	C	265	THR	2.1
1	A	282	LEU	2.1
1	B	163	ASP	2.1
1	B	231	GLY	2.1
1	B	267	TRP	2.1
1	B	171	TYR	2.0
1	C	285	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	79	LYS	2.0
1	B	222	ASN	2.0
1	B	51	GLN	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. 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	B-factors(Å^2)	Q<0.9
3	3DR	I	506	12/12	0.95	0.30	42,62,75,78	0
3	3DR	O	506	12/12	0.95	0.25	40,56,71,71	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
6	NA	B	402	1/1	0.01	0.47	81,81,81,81	0
5	MG	D	401	1/1	0.41	0.17	61,61,61,61	0
6	NA	A	504	1/1	0.42	0.31	50,50,50,50	0
5	MG	A	501	1/1	0.44	0.19	55,55,55,55	0
6	NA	D	402	1/1	0.74	0.23	78,78,78,78	0
6	NA	F	601	1/1	0.86	0.16	64,64,64,64	0
6	NA	N	601	1/1	0.89	0.19	56,56,56,56	0
6	NA	B	404	1/1	0.92	0.16	72,72,72,72	0
5	MG	B	401	1/1	0.92	0.08	61,61,61,61	0
5	MG	C	401	1/1	0.92	0.11	49,49,49,49	0
6	NA	E	601	1/1	0.93	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	502	1/1	0.93	0.14	42,42,42,42	0
5	MG	A	503	1/1	0.93	0.13	38,38,38,38	0
6	NA	A	505	1/1	0.95	0.25	55,55,55,55	0
5	MG	C	402	1/1	0.96	0.11	48,48,48,48	0
6	NA	B	403	1/1	0.98	0.54	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.