Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:36 PM GMT

PDB ID	:	3U8U
Title	:	Crystal structure of Human Apurinic/Apyridinimic Endonuclease, Ape1 in a new crystal form
Authors	:	Agarwal, R.; Naidu, M.D.
Deposited on	:	2011-10-17
Resolution	:	2.15 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:

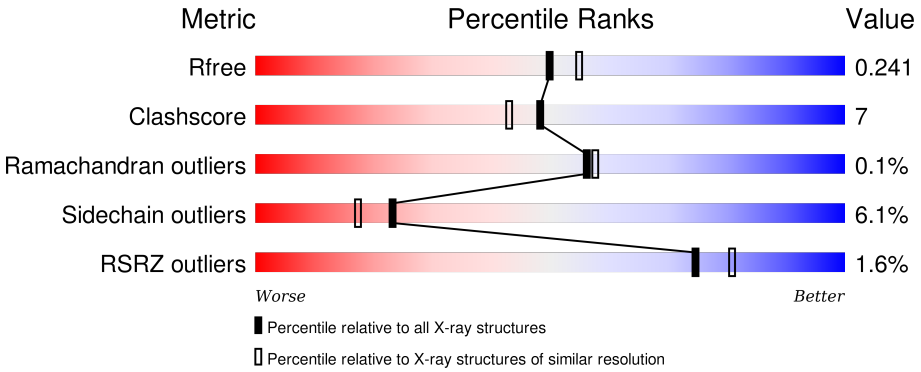
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	318	2% 72% 13% • 14%
1	B	318	2% 73% 11% • 14%
1	C	318	% 74% 11% • 14%
1	D	318	2% 73% 10% • 15%
1	E	318	% 73% 10% • 15%

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Mol	Chain	Length	Quality of chain
1	F	318	2% 72% 13% 14%

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
2	MG	A	319	-	-	-	X
2	MG	D	319	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13631 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2162	1383	371	399	9			
1	B	275	Total	C	N	O	S	0	0	0
			2143	1374	366	394	9			
1	C	275	Total	C	N	O	S	0	0	0
			2147	1375	367	396	9			
1	D	269	Total	C	N	O	S	0	0	0
			2080	1331	356	386	7			
1	E	271	Total	C	N	O	S	0	0	0
			2110	1351	364	386	9			
1	F	275	Total	C	N	O	S	0	0	0
			2144	1371	370	394	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is water.

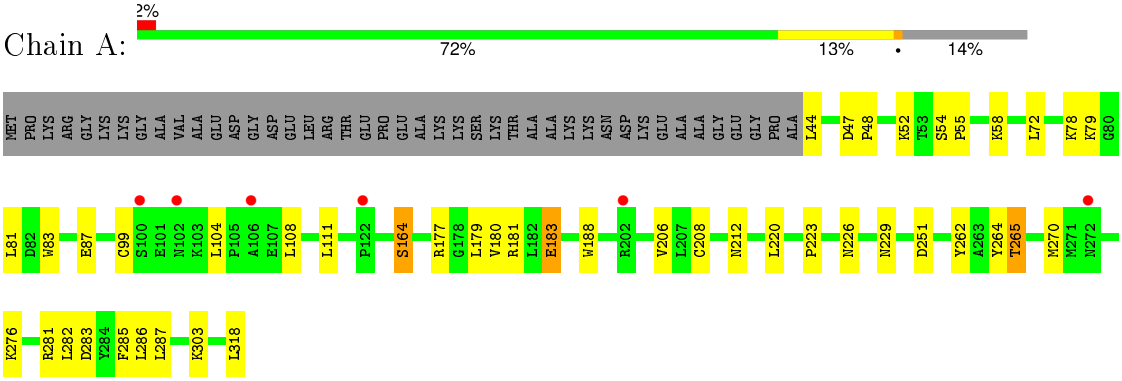
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	173	Total O 173 173	0	0
4	B	157	Total O 157 157	0	0
4	C	97	Total O 97 97	0	0
4	D	134	Total O 134 134	0	0
4	E	146	Total O 146 146	0	0
4	F	128	Total O 128 128	0	0

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.

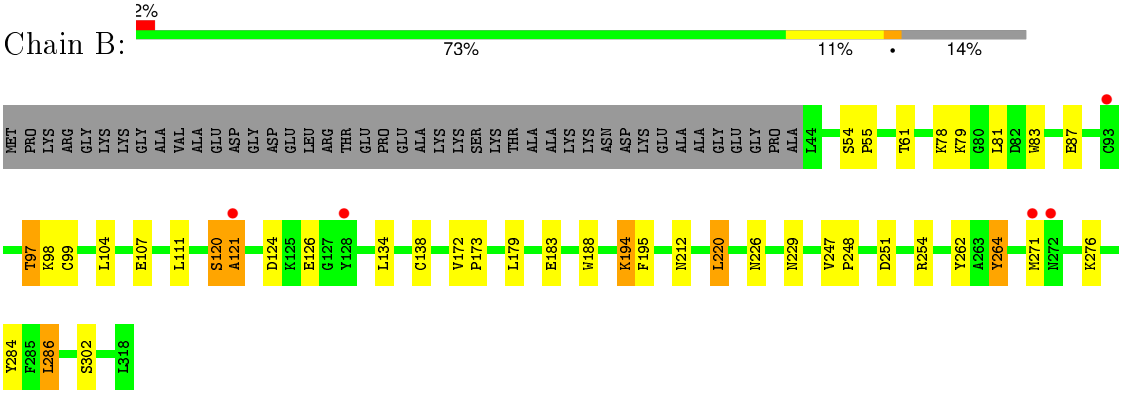
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain A:



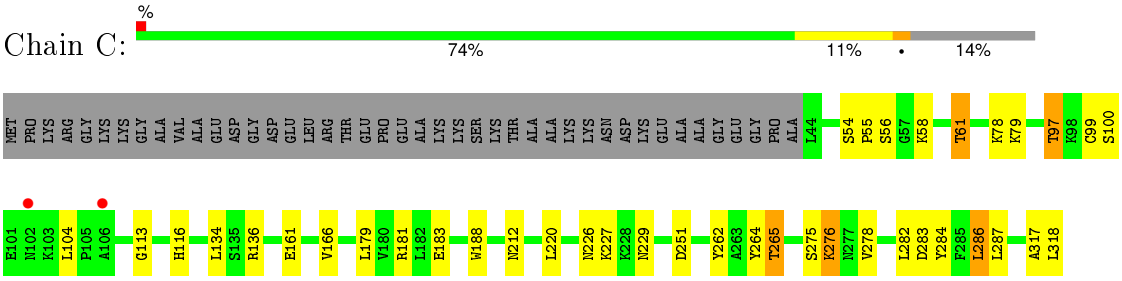
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain B:



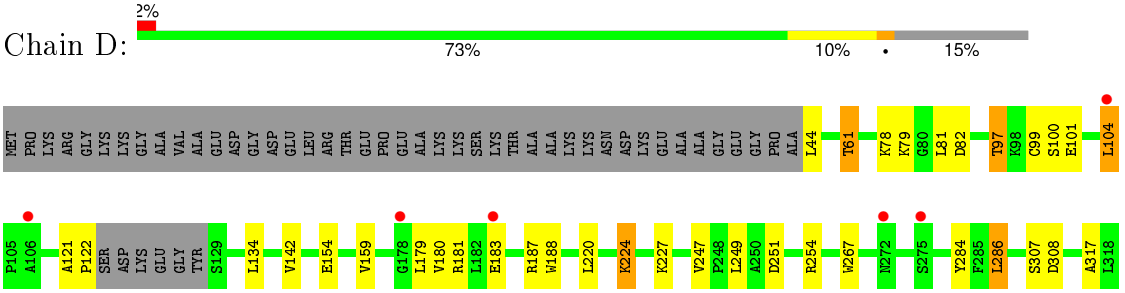
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain C:



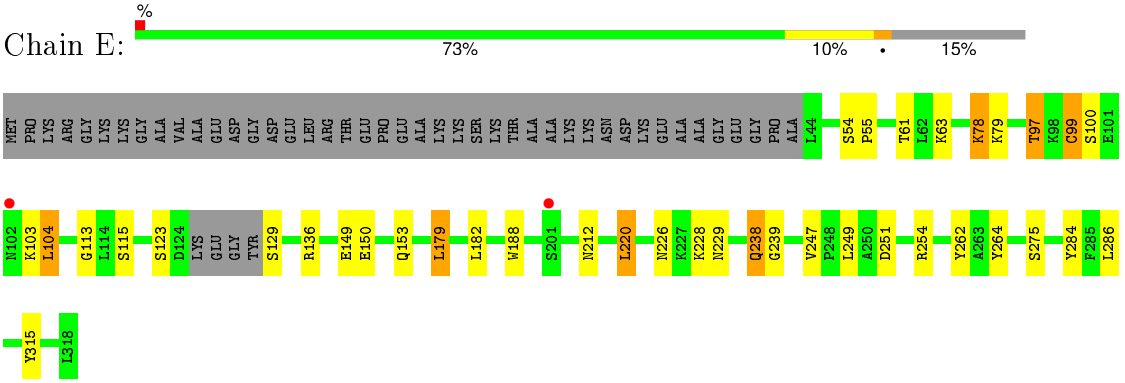
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain D:



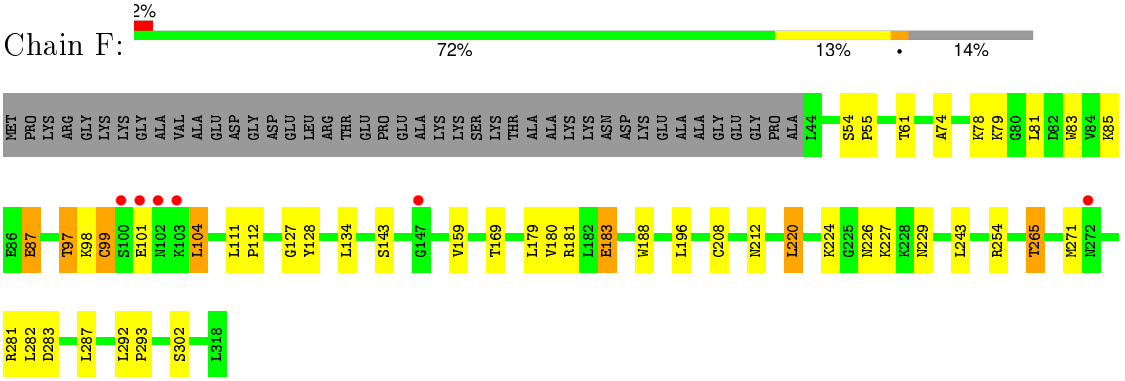
• Molecule 1: DNA-(apurinic or apyrimidinic site) lyase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.84Å 97.28Å 132.15Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	40.71 – 2.15 40.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.71-2.15) 99.3 (40.70-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.243 0.197 , 0.241	Depositor DCC
R_{free} test set	6601 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	EDS
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.013 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 131120 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13631	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.82 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2799e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, CL

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	0.61	0/2220	0.61	1/3016 (0.0%)
1	B	0.64	2/2201 (0.1%)	0.61	0/2993
1	C	0.60	0/2205	0.61	0/2999
1	D	0.65	0/2136	0.60	0/2911
1	E	0.58	0/2166	0.59	0/2944
1	F	0.63	1/2202 (0.0%)	0.62	2/2995 (0.1%)
All	All	0.62	3/13130 (0.0%)	0.61	3/17858 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	TYR	CD2-CE2	-5.22	1.31	1.39
1	B	264	TYR	CD1-CE1	-5.16	1.31	1.39
1	F	128	TYR	CD1-CE1	-5.09	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	281	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	281	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	F	281	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2162	0	2106	37	0
1	B	2143	0	2076	31	0
1	C	2147	0	2077	27	0
1	D	2080	0	1983	28	0
1	E	2110	0	2051	21	0
1	F	2144	0	2071	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	A	173	0	0	3	0
4	B	157	0	0	2	0
4	C	97	0	0	2	0
4	D	134	0	0	7	0
4	E	146	0	0	1	0
4	F	128	0	0	4	0
All	All	13631	0	12364	183	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 7.

All (183) 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:B:83:TRP:CH2	1:B:87:GLU:HG3	1.81	1.16
1:F:83:TRP:CH2	1:F:87:GLU:HG3	1.84	1.13
1:C:97:THR:HG21	4:C:349:HOH:O	1.50	1.09
1:D:97:THR:HG21	4:D:586:HOH:O	1.52	1.07
1:A:265:THR:HG23	1:A:283:ASP:OD2	1.57	1.02
1:A:83:TRP:CH2	1:A:87:GLU:HG3	1.94	1.01
1:F:265:THR:HG23	1:F:283:ASP:OD2	1.65	0.95
1:D:224:LYS:HE2	4:D:594:HOH:O	1.66	0.94
1:B:97:THR:HG21	4:B:734:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:THR:HG21	4:E:372:HOH:O	1.69	0.90
1:C:265:THR:HG23	1:C:283:ASP:OD2	1.72	0.90
1:A:265:THR:CG2	1:A:283:ASP:OD2	2.23	0.87
1:A:83:TRP:CZ3	1:A:87:GLU:HG3	2.10	0.87
1:D:121:ALA:HB1	1:D:122:PRO:HD2	1.57	0.86
1:B:83:TRP:CH2	1:B:87:GLU:CG	2.60	0.85
1:F:83:TRP:CH2	1:F:87:GLU:CG	2.60	0.85
1:A:83:TRP:CH2	1:A:87:GLU:CG	2.58	0.84
1:A:265:THR:HG21	1:A:283:ASP:H	1.41	0.84
1:D:99:CYS:O	1:D:121:ALA:HB2	1.79	0.83
1:F:265:THR:CG2	1:F:283:ASP:OD2	2.27	0.82
1:B:138:CYS:SG	4:B:701:HOH:O	2.38	0.81
1:D:227:LYS:CB	4:D:523:HOH:O	2.27	0.81
1:F:226:ASN:HD22	1:F:229:ASN:HD22	1.29	0.81
1:C:226:ASN:ND2	1:C:229:ASN:HD22	1.78	0.80
1:B:83:TRP:CZ3	1:B:87:GLU:HG3	2.16	0.79
1:E:226:ASN:ND2	1:E:229:ASN:HD22	1.80	0.79
1:A:183:GLU:CD	1:A:183:GLU:H	1.87	0.78
1:D:224:LYS:HE3	4:D:760:HOH:O	1.82	0.78
1:C:265:THR:CG2	1:C:283:ASP:OD2	2.33	0.76
1:B:226:ASN:HD22	1:B:229:ASN:HD22	1.34	0.75
1:D:44:LEU:N	4:D:672:HOH:O	2.22	0.73
1:F:97:THR:HG21	4:F:402:HOH:O	1.88	0.72
1:F:265:THR:HG21	1:F:283:ASP:H	1.56	0.71
1:B:226:ASN:ND2	1:B:229:ASN:HD22	1.89	0.71
1:A:220:LEU:HD21	1:A:223:PRO:HB3	1.71	0.70
1:F:101:GLU:CB	4:F:861:HOH:O	2.39	0.70
1:E:226:ASN:HD22	1:E:229:ASN:HD22	1.39	0.70
1:C:276:LYS:HB3	1:C:278:VAL:HG23	1.74	0.69
1:F:196:LEU:HD12	1:F:243:LEU:HD11	1.75	0.69
1:B:120:SER:O	1:B:121:ALA:HB3	1.93	0.69
1:C:265:THR:HG21	1:C:283:ASP:HB2	1.75	0.68
1:C:226:ASN:HD22	1:C:229:ASN:HD22	1.40	0.68
1:A:265:THR:HG21	1:A:283:ASP:N	2.08	0.67
1:F:226:ASN:ND2	1:F:229:ASN:HD22	1.92	0.67
1:B:97:THR:HG22	1:B:99:CYS:H	1.60	0.66
1:F:97:THR:HG22	1:F:99:CYS:H	1.61	0.65
1:A:220:LEU:HD11	1:A:223:PRO:HA	1.80	0.64
1:E:97:THR:HG22	1:E:99:CYS:H	1.63	0.63
1:D:187:ARG:HD2	4:D:637:HOH:O	1.99	0.63
1:E:238:GLN:HG3	1:E:239:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:HG21	1:C:318:LEU:H	1.64	0.62
1:B:97:THR:HG22	1:B:99:CYS:N	2.14	0.61
1:F:83:TRP:CZ3	1:F:87:GLU:HG3	2.34	0.60
1:B:78:LYS:O	1:B:79:LYS:HB2	2.00	0.60
1:A:183:GLU:CD	1:A:183:GLU:N	2.55	0.60
1:D:97:THR:HG22	1:D:99:CYS:H	1.65	0.60
1:F:98:LYS:HB3	1:F:127:GLY:HA2	1.83	0.60
1:A:72:LEU:HD12	1:A:99:CYS:SG	2.41	0.60
1:A:226:ASN:ND2	1:A:229:ASN:HD22	2.00	0.60
1:B:120:SER:O	1:B:121:ALA:CB	2.50	0.59
1:A:265:THR:HG22	1:A:282:LEU:H	1.66	0.59
1:A:164:SER:HB3	4:A:330:HOH:O	2.03	0.58
1:F:265:THR:HG21	1:F:283:ASP:N	2.18	0.58
1:B:97:THR:HG23	1:B:99:CYS:HB3	1.86	0.58
1:A:44:LEU:N	4:A:338:HOH:O	2.36	0.58
1:B:54:SER:HB2	1:B:55:PRO:HD2	1.86	0.56
1:B:98:LYS:HA	1:B:126:GLU:O	2.06	0.56
1:E:97:THR:CG2	1:E:99:CYS:H	2.18	0.56
1:C:265:THR:HG21	1:C:283:ASP:CB	2.35	0.56
1:A:78:LYS:O	1:A:79:LYS:HB2	2.06	0.56
1:C:284:TYR:HB3	1:C:286:LEU:HD13	1.87	0.56
1:D:97:THR:HG22	1:D:99:CYS:N	2.21	0.55
1:F:265:THR:HG22	1:F:282:LEU:H	1.70	0.55
1:F:97:THR:HG22	1:F:99:CYS:N	2.22	0.55
1:C:265:THR:HG21	1:C:283:ASP:H	1.71	0.54
1:A:226:ASN:HD22	1:A:229:ASN:HD22	1.54	0.54
1:B:54:SER:HB2	1:B:55:PRO:CD	2.38	0.54
1:C:61:THR:CG2	1:C:318:LEU:H	2.20	0.54
1:C:116:HIS:ND1	4:C:593:HOH:O	2.32	0.53
1:F:74:ALA:O	1:F:78:LYS:HG3	2.08	0.53
1:E:63:LYS:HE3	1:E:315:TYR:OH	2.08	0.53
1:D:121:ALA:HB1	1:D:122:PRO:CD	2.34	0.53
1:A:54:SER:HB2	1:A:55:PRO:CD	2.40	0.52
1:C:134:LEU:HD12	1:C:134:LEU:N	2.25	0.52
1:F:101:GLU:HA	1:F:104:LEU:CD2	2.41	0.51
1:F:83:TRP:CZ2	1:F:87:GLU:CG	2.94	0.50
1:D:122:PRO:HB3	1:D:154:GLU:HA	1.92	0.50
1:F:83:TRP:CZ2	1:F:87:GLU:HG2	2.47	0.50
1:A:72:LEU:HD13	1:A:108:LEU:CD1	2.42	0.50
1:A:54:SER:HB2	1:A:55:PRO:HD2	1.92	0.50
1:A:206:VAL:HG22	1:A:287:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LYS:O	1:E:79:LYS:HB2	2.10	0.49
1:A:262:TYR:HA	1:A:264:TYR:CZ	2.47	0.49
1:C:265:THR:HG21	1:C:283:ASP:N	2.27	0.49
1:E:284:TYR:HB3	1:E:286:LEU:HD13	1.94	0.49
1:D:78:LYS:O	1:D:79:LYS:HB2	2.12	0.49
1:F:265:THR:CG2	1:F:282:LEU:H	2.25	0.49
1:A:83:TRP:CZ3	1:A:87:GLU:CG	2.86	0.48
1:C:113:GLY:O	1:C:136:ARG:HG3	2.12	0.48
1:A:265:THR:CG2	1:A:282:LEU:H	2.27	0.48
1:C:251:ASP:HA	1:C:286:LEU:HD12	1.95	0.48
1:C:161:GLU:HG3	1:C:166:VAL:HG22	1.96	0.48
1:A:177:ARG:O	1:A:180:VAL:HG22	2.15	0.47
1:E:149:GLU:O	1:E:153:GLN:NE2	2.28	0.47
1:E:63:LYS:HE3	1:E:315:TYR:CZ	2.49	0.47
1:D:101:GLU:HA	1:D:104:LEU:HD22	1.97	0.47
1:D:97:THR:HG23	1:D:99:CYS:HB3	1.96	0.47
1:A:251:ASP:HA	1:A:286:LEU:CD2	2.44	0.47
1:D:134:LEU:HD12	1:D:134:LEU:N	2.30	0.46
1:B:284:TYR:HB3	1:B:286:LEU:HD13	1.97	0.46
1:F:183:GLU:CD	1:F:183:GLU:H	2.19	0.46
1:A:270:MET:HE3	1:A:270:MET:HB3	1.79	0.46
1:D:251:ASP:HA	1:D:286:LEU:HD12	1.97	0.46
1:F:143:SER:HB2	1:F:159:VAL:HB	1.97	0.46
1:C:265:THR:HG22	1:C:282:LEU:H	1.81	0.46
1:E:100:SER:O	1:E:104:LEU:HD13	2.16	0.45
1:E:188:TRP:CD1	1:E:188:TRP:C	2.89	0.45
1:C:54:SER:HB2	1:C:55:PRO:HD2	1.99	0.45
1:F:81:LEU:O	1:F:85:LYS:HG3	2.16	0.45
1:C:78:LYS:O	1:C:79:LYS:HB2	2.17	0.45
1:B:83:TRP:CZ2	1:B:87:GLU:CG	3.00	0.45
1:B:262:TYR:HA	1:B:264:TYR:CZ	2.52	0.45
1:B:172:VAL:HG13	1:B:173:PRO:HD2	1.98	0.45
1:E:54:SER:HB2	1:E:55:PRO:HD2	1.98	0.45
1:E:251:ASP:HA	1:E:286:LEU:HD12	1.99	0.45
1:C:188:TRP:CD1	1:C:188:TRP:C	2.89	0.45
1:B:194:LYS:HG3	1:B:195:PHE:N	2.31	0.45
1:A:83:TRP:CH2	1:A:87:GLU:HG2	2.47	0.44
1:E:254:ARG:HD3	1:E:254:ARG:HA	1.79	0.44
1:C:61:THR:HB	1:C:317:ALA:HA	1.99	0.44
1:F:180:VAL:HG12	1:F:180:VAL:O	2.17	0.44
1:B:81:LEU:HD22	1:B:111:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:LEU:N	1:F:293:PRO:CD	2.81	0.44
1:D:61:THR:HB	1:D:317:ALA:HA	2.00	0.43
1:F:54:SER:HB2	1:F:55:PRO:HD2	1.99	0.43
1:C:265:THR:CG2	1:C:283:ASP:HB2	2.45	0.43
1:B:220:LEU:HD12	1:B:220:LEU:N	2.34	0.43
1:A:188:TRP:C	1:A:188:TRP:CD1	2.91	0.43
1:B:271:MET:O	1:B:276:LYS:NZ	2.45	0.42
1:A:52:LYS:HE3	4:A:420:HOH:O	2.19	0.42
1:D:247:VAL:HB	1:D:249:LEU:HG	2.00	0.42
1:A:220:LEU:H	1:A:220:LEU:HD23	1.84	0.42
1:D:79:LYS:HD2	1:D:82:ASP:OD2	2.20	0.42
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.92	0.42
1:F:188:TRP:C	1:F:188:TRP:CD1	2.93	0.42
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.91	0.42
1:E:113:GLY:O	1:E:136:ARG:HG2	2.19	0.42
1:F:101:GLU:O	1:F:104:LEU:HD22	2.20	0.42
1:F:111:LEU:HD12	1:F:112:PRO:HD2	2.02	0.42
1:F:227:LYS:HD2	4:F:384:HOH:O	2.19	0.42
1:F:101:GLU:HA	1:F:104:LEU:HD22	2.02	0.42
1:B:188:TRP:C	1:B:188:TRP:CD1	2.93	0.42
1:A:208:CYS:HB3	1:A:285:PHE:CD1	2.55	0.42
1:F:254:ARG:HD3	1:F:254:ARG:HA	1.88	0.42
1:B:97:THR:CG2	1:B:99:CYS:HB3	2.50	0.42
1:D:81:LEU:HA	1:D:81:LEU:HD23	1.66	0.42
1:D:224:LYS:CE	4:D:594:HOH:O	2.42	0.41
1:D:307:SER:OG	1:D:308:ASP:N	2.53	0.41
1:F:224:LYS:HE2	1:F:224:LYS:HB2	1.89	0.41
1:F:224:LYS:HE2	4:F:373:HOH:O	2.20	0.41
1:C:97:THR:HG22	1:C:99:CYS:H	1.85	0.41
1:E:220:LEU:HD12	1:E:220:LEU:H	1.84	0.41
1:D:254:ARG:HA	1:D:254:ARG:HD3	1.71	0.41
1:C:58:LYS:HB2	1:C:58:LYS:HE2	1.74	0.41
1:F:169:THR:HA	1:F:208:CYS:O	2.21	0.41
1:A:72:LEU:HD13	1:A:108:LEU:HD11	2.02	0.41
1:A:81:LEU:HD22	1:A:111:LEU:HD13	2.02	0.41
1:D:284:TYR:HB3	1:D:286:LEU:HD13	2.03	0.41
1:E:179:LEU:HG	1:E:182:LEU:HD22	2.01	0.41
1:B:247:VAL:N	1:B:248:PRO:HA	2.36	0.41
1:B:134:LEU:HD12	1:B:134:LEU:N	2.36	0.41
1:F:79:LYS:HA	1:F:79:LYS:HD2	1.93	0.41
1:E:247:VAL:HB	1:E:249:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:HA	1:B:254:ARG:HD3	1.86	0.40
1:A:47:ASP:HA	1:A:48:PRO:HD3	1.91	0.40
1:D:100:SER:HB3	1:D:121:ALA:HB3	2.04	0.40
1:B:251:ASP:HA	1:B:286:LEU:HD12	2.02	0.40
1:F:111:LEU:HA	1:F:112:PRO:HD3	1.95	0.40
1:C:262:TYR:HA	1:C:264:TYR:CZ	2.56	0.40
1:F:220:LEU:N	1:F:220:LEU:HD12	2.36	0.40
1:E:262:TYR:HA	1:E:264:TYR:CZ	2.56	0.40
1:D:142:VAL:HA	1:D:159:VAL:O	2.21	0.40
1:D:188:TRP:CD1	1:D:188:TRP:C	2.95	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	273/318 (86%)	269 (98%)	4 (2%)	0	100	100
1	B	273/318 (86%)	268 (98%)	4 (2%)	1 (0%)	39	34
1	C	273/318 (86%)	265 (97%)	8 (3%)	0	100	100
1	D	265/318 (83%)	260 (98%)	5 (2%)	0	100	100
1	E	267/318 (84%)	260 (97%)	7 (3%)	0	100	100
1	F	273/318 (86%)	265 (97%)	8 (3%)	0	100	100
All	All	1624/1908 (85%)	1587 (98%)	36 (2%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	ALA

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	228/266 (86%)	218 (96%)	10 (4%)	35	31
1	B	223/266 (84%)	210 (94%)	13 (6%)	25	19
1	C	224/266 (84%)	208 (93%)	16 (7%)	18	12
1	D	214/266 (80%)	203 (95%)	11 (5%)	29	24
1	E	221/266 (83%)	205 (93%)	16 (7%)	18	12
1	F	223/266 (84%)	208 (93%)	15 (7%)	20	13
All	All	1333/1596 (84%)	1252 (94%)	81 (6%)	23	17

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	104	LEU
1	A	164	SER
1	A	179	LEU
1	A	181	ARG
1	A	183	GLU
1	A	212	ASN
1	A	265	THR
1	A	276	LYS
1	A	303	LYS
1	B	61	THR
1	B	97	THR
1	B	104	LEU
1	B	107	GLU
1	B	120	SER
1	B	124	ASP
1	B	179	LEU
1	B	183	GLU
1	B	194	LYS
1	B	212	ASN
1	B	220	LEU
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	302	SER
1	C	56	SER
1	C	61	THR
1	C	97	THR
1	C	100	SER
1	C	104	LEU
1	C	179	LEU
1	C	181	ARG
1	C	183	GLU
1	C	212	ASN
1	C	220	LEU
1	C	227	LYS
1	C	265	THR
1	C	275	SER
1	C	276	LYS
1	C	286	LEU
1	C	287	LEU
1	D	61	THR
1	D	97	THR
1	D	104	LEU
1	D	179	LEU
1	D	180	VAL
1	D	181	ARG
1	D	183	GLU
1	D	220	LEU
1	D	224	LYS
1	D	267	TRP
1	D	286	LEU
1	E	61	THR
1	E	78	LYS
1	E	97	THR
1	E	99	CYS
1	E	103	LYS
1	E	104	LEU
1	E	115	SER
1	E	123	SER
1	E	129	SER
1	E	150	GLU
1	E	179	LEU
1	E	212	ASN
1	E	220	LEU
1	E	228	LYS

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Mol	Chain	Res	Type
1	E	238	GLN
1	E	275	SER
1	F	61	THR
1	F	87	GLU
1	F	97	THR
1	F	99	CYS
1	F	104	LEU
1	F	134	LEU
1	F	179	LEU
1	F	181	ARG
1	F	183	GLU
1	F	212	ASN
1	F	220	LEU
1	F	265	THR
1	F	271	MET
1	F	287	LEU
1	F	302	SER

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

Mol	Chain	Res	Type
1	A	116	HIS
1	A	212	ASN
1	A	226	ASN
1	B	116	HIS
1	B	212	ASN
1	B	226	ASN
1	C	212	ASN
1	C	226	ASN
1	D	116	HIS
1	D	212	ASN
1	D	226	ASN
1	E	212	ASN
1	E	226	ASN
1	F	212	ASN
1	F	226	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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	275/318 (86%)	-0.18	6 (2%)	65	73	19, 28, 45, 65	0
1	B	275/318 (86%)	-0.10	5 (1%)	71	79	19, 31, 48, 60	0
1	C	275/318 (86%)	-0.12	2 (0%)	89	91	21, 32, 49, 66	0
1	D	269/318 (84%)	-0.03	6 (2%)	65	73	20, 32, 51, 63	0
1	E	271/318 (85%)	-0.10	2 (0%)	89	91	18, 31, 47, 54	0
1	F	275/318 (86%)	-0.09	6 (2%)	65	73	19, 32, 51, 64	0
All	All	1640/1908 (85%)	-0.10	27 (1%)	74	81	18, 31, 49, 66	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	MET	3.9
1	B	128	TYR	3.5
1	F	100	SER	3.4
1	A	202	ARG	3.1
1	F	101	GLU	2.9
1	F	102	ASN	2.9
1	D	106	ALA	2.8
1	F	147	GLY	2.7
1	D	272	ASN	2.7
1	A	106	ALA	2.6
1	D	178	GLY	2.6
1	C	106	ALA	2.6
1	D	183	GLU	2.5
1	D	275	SER	2.5
1	C	102	ASN	2.4
1	A	100	SER	2.4
1	B	272	ASN	2.3
1	A	122	PRO	2.3
1	A	102	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	121	ALA	2.2
1	E	201	SER	2.2
1	E	102	ASN	2.2
1	D	104	LEU	2.1
1	B	93	CYS	2.1
1	F	272	ASN	2.1
1	F	103	LYS	2.1
1	A	272	ASN	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, 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
2	MG	D	319	1/1	0.92	0.17	2.14	46,46,46,46	0
2	MG	A	319	1/1	0.80	0.12	2.13	31,31,31,31	0
2	MG	E	319	1/1	0.96	0.09	-0.59	23,23,23,23	0
3	CL	C	320	1/1	0.99	0.08	-0.93	34,34,34,34	0
3	CL	B	320	1/1	0.99	0.05	-1.02	45,45,45,45	0
2	MG	C	319	1/1	0.95	0.05	-1.22	33,33,33,33	0
3	CL	F	320	1/1	0.98	0.08	-1.28	40,40,40,40	0
2	MG	B	319	1/1	0.87	0.07	-1.45	37,37,37,37	0
3	CL	A	320	1/1	0.99	0.05	-2.71	36,36,36,36	0
2	MG	F	319	1/1	0.95	0.09	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.