Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:15 AM GMT

PDB ID	:	2GB7
Title	:	Metal-depleted Ecl18kI in complex with uncleaved, modified DNA
Authors	:	Bochtler, M.; Szczepanowski, R.H.; Tamulaitis, G.; Grazulis, S.; Czapinska, H.; Manakova, E.; Siksnys, V.
Deposited on	:	2006-03-10
Resolution	:	1.70 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:

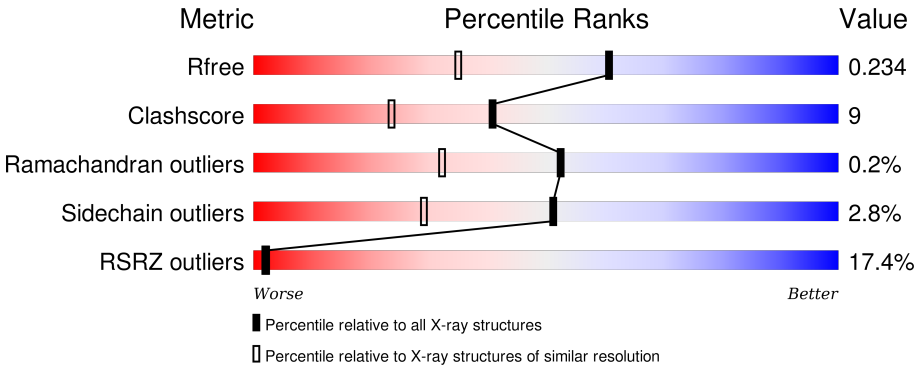
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	E	9	67% 33%
1	G	9	56% 44%
2	F	9	44% 56%
2	H	9	89% 11%
3	A	305	23% 82% 14% .

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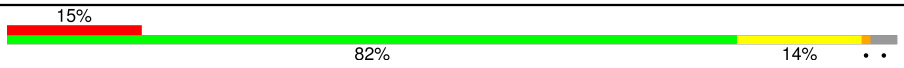
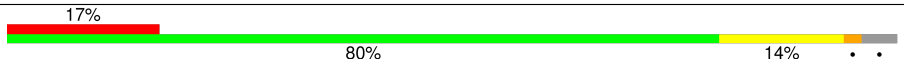
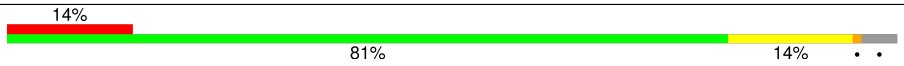
Mol	Chain	Length	Quality of chain
3	B	305	
3	C	305	
3	D	305	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA STRAND 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	9	Total	C	N	O	P	0	9	0
			364	172	74	102	16			
1	G	9	Total	C	N	O	P	0	9	0
			364	172	74	102	16			

- Molecule 2 is a DNA chain called DNA STRAND 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	9	Total	C	N	O	P	0	9	0
			362	172	68	106	16			
2	H	9	Total	C	N	O	P	0	9	0
			362	172	68	106	16			

- Molecule 3 is a protein called R.Ecl18kI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	293	Total	C	N	O	S	53	0	0
			2421	1537	404	467	13			
3	B	295	Total	C	N	O	S	26	0	0
			2441	1552	405	471	13			
3	C	293	Total	C	N	O	S	30	0	0
			2421	1542	400	466	13			
3	D	292	Total	C	N	O	S	10	0	0
			2412	1537	398	464	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	GLN	ARG	ENGINEERED	UNP O87963
B	277	GLN	ARG	ENGINEERED	UNP O87963
C	277	GLN	ARG	ENGINEERED	UNP O87963
D	277	GLN	ARG	ENGINEERED	UNP O87963

- Molecule 4 is water.

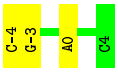
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	B	144	Total O 144 144	0	0
4	C	128	Total O 128 128	0	0
4	D	148	Total O 148 148	0	0
4	E	20	Total O 20 20	0	0
4	F	26	Total O 26 26	0	0
4	G	24	Total O 24 24	0	0
4	H	29	Total O 29 29	0	0

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.

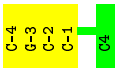
- Molecule 1: DNA STRAND 1

Chain E:



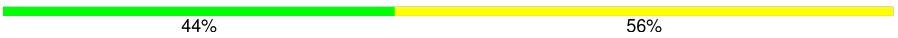
- Molecule 1: DNA STRAND 1

Chain G:



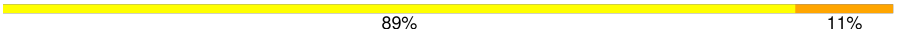
- Molecule 2: DNA STRAND 2

Chain F:



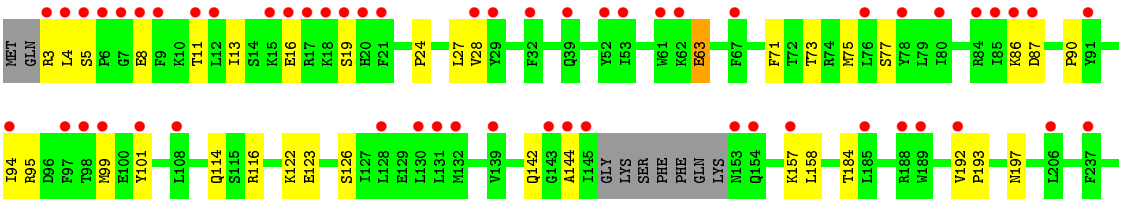
- Molecule 2: DNA STRAND 2

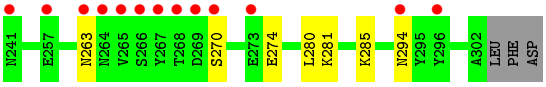
Chain H:



- Molecule 3: R.Ecl18kI

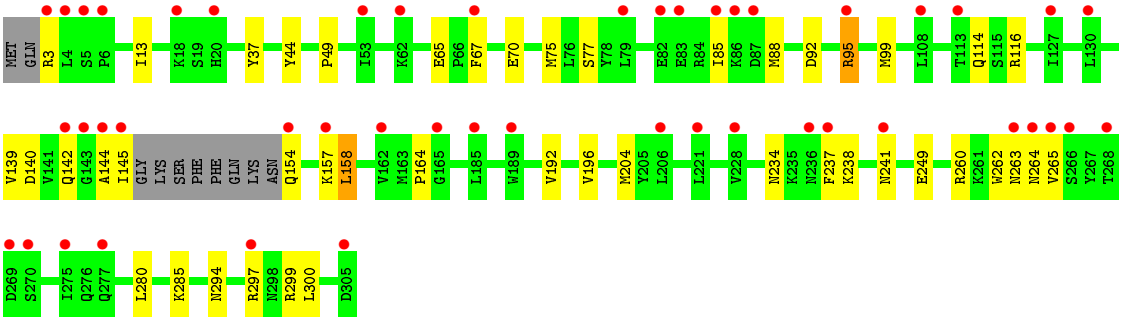
Chain A:





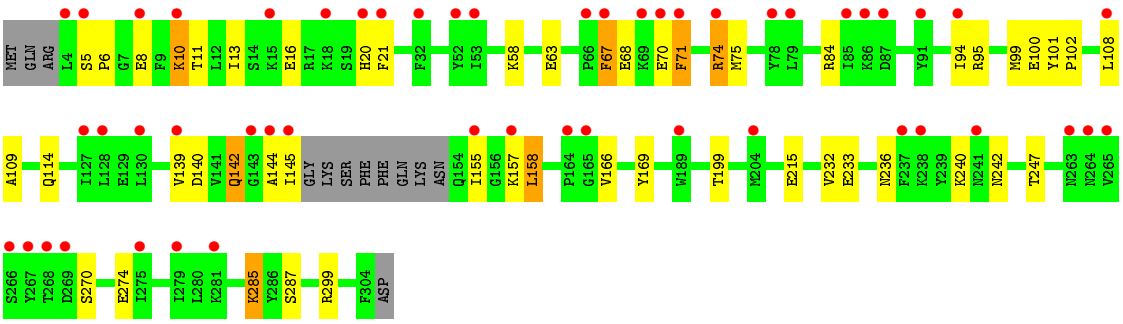
• Molecule 3: R.Ecl18kI

Chain B:



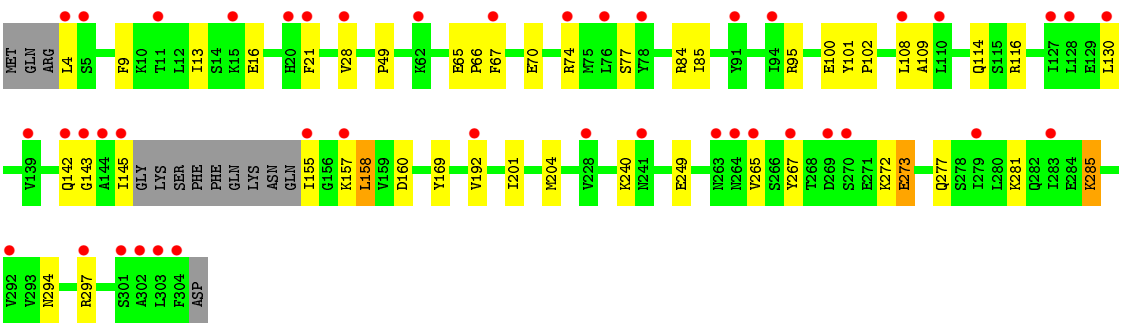
• Molecule 3: R.Ecl18kI

Chain C:



• Molecule 3: R.Ecl18kI

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.70Å 96.74Å 192.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.98 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-1.70) 96.8 (19.98-1.69)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.51 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.236 0.206 , 0.234	Depositor DCC
R_{free} test set	7777 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 157802 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

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	E	0.31	0/408	0.68	0/626
1	G	0.33	0/408	0.75	0/626
2	F	0.31	0/404	0.80	0/620
2	H	0.35	0/404	0.71	0/620
3	A	0.57	0/2468	0.67	0/3330
3	B	0.60	0/2489	0.71	0/3357
3	C	0.59	0/2469	0.71	0/3332
3	D	0.59	0/2460	0.72	0/3320
All	All	0.56	0/11510	0.71	0/15831

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
3	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	241	ASN	Peptide
2	H	-1[A]	DC	Sidechain

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	E	364	0	185	9	0
1	G	364	0	189	8	0
2	F	362	0	194	15	0
2	H	362	0	195	13	0
3	A	2421	0	2387	31	0
3	B	2441	0	2405	47	0
3	C	2421	0	2388	54	0
3	D	2412	0	2380	35	0
4	A	83	0	0	2	0
4	B	144	0	0	10	0
4	C	128	0	0	10	0
4	D	148	0	0	6	0
4	E	20	0	0	3	0
4	F	26	0	0	1	0
4	G	24	0	0	3	0
4	H	29	0	0	1	0
All	All	11749	0	10323	184	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 9.

All (184) 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)
3:C:67:PHE:HD1	3:C:67:PHE:C	1.48	1.16
1:G:-3[A]:DG:H5"	3:C:157:LYS:HB2	1.32	1.05
3:C:63:GLU:HG3	4:C:418:HOH:O	1.57	1.04
3:B:77:SER:HB2	4:B:363:HOH:O	1.61	0.97
3:C:67:PHE:C	3:C:67:PHE:CD1	2.27	0.96
3:A:27:LEU:HD11	3:A:63:GLU:HG2	1.50	0.91
1:G:-3[A]:DG:C5'	3:C:157:LYS:HB2	2.00	0.90
3:C:16:GLU:HB2	4:C:403:HOH:O	1.72	0.88
2:H:-3[B]:DC:H5"	3:C:157:LYS:HB2	1.56	0.85
3:D:21:PHE:CE1	3:D:67:PHE:HD2	1.94	0.85
3:D:160:ASP:HB3	4:D:401:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:PHE:CE1	3:C:67:PHE:CZ	2.66	0.83
3:B:140:ASP:HB3	3:B:145:ILE:HD11	1.59	0.82
3:D:240:LYS:HD3	4:D:410:HOH:O	1.78	0.81
2:F:-3[B]:DC:H5"	3:A:157:LYS:HB2	1.62	0.81
3:C:21:PHE:CE1	3:C:67:PHE:CE1	2.70	0.80
3:C:21:PHE:CD1	3:C:67:PHE:CZ	2.70	0.79
3:C:67:PHE:HD1	3:C:68:GLU:N	1.80	0.77
3:A:3:ARG:HG2	3:A:4:LEU:H	1.50	0.77
3:A:27:LEU:CD1	3:A:63:GLU:HG2	2.15	0.77
3:B:196:VAL:HG23	3:B:204:MET:HE3	1.70	0.74
3:B:70:GLU:HG3	4:B:374:HOH:O	1.87	0.74
1:E:-4[A]:DC:H2"	1:E:-3[A]:DG:OP2	1.86	0.74
3:C:67:PHE:CD1	3:C:68:GLU:N	2.54	0.74
4:G:19:HOH:O	3:D:157:LYS:HG3	1.88	0.73
3:C:13:ILE:HD13	3:C:75:MET:CE	2.19	0.72
3:A:197:ASN:HB3	4:B:387:HOH:O	1.90	0.71
3:A:63:GLU:HG3	3:A:63:GLU:O	1.90	0.70
3:C:67:PHE:HD1	3:C:67:PHE:O	1.74	0.69
3:C:13:ILE:HD13	3:C:75:MET:HE3	1.75	0.68
3:A:270:SER:O	3:A:274:GLU:HG2	1.94	0.67
1:E:-4[B]:DC:H2"	1:E:-3[B]:DG:OP2	1.93	0.67
3:D:21:PHE:CE1	3:D:67:PHE:CD2	2.82	0.66
3:D:158:LEU:HD11	3:D:192:VAL:HG22	1.77	0.66
3:C:95:ARG:O	3:C:99:MET:HG3	1.96	0.66
3:A:94:ILE:HD12	3:B:85:ILE:HD13	1.77	0.65
1:E:0[A]:DA:C2	4:E:162:HOH:O	2.48	0.65
2:F:-3[A]:DC:H5"	3:B:157:LYS:HB2	1.79	0.65
3:B:196:VAL:CG2	3:B:204:MET:HE3	2.27	0.64
2:H:0[A]:DT:H72	4:D:348:HOH:O	1.97	0.64
3:B:294:ASN:HA	3:B:297:ARG:HG2	1.79	0.64
3:B:237:PHE:CD2	3:B:238:LYS:HG2	2.33	0.63
3:D:273:GLU:O	3:D:277:GLN:HG3	1.98	0.63
3:A:144:ALA:O	3:A:285:LYS:HD3	1.99	0.63
3:C:75:MET:HE1	4:C:403:HOH:O	1.99	0.62
3:A:77:SER:HB2	4:A:339:HOH:O	2.00	0.62
3:D:84:ARG:NH2	3:D:100:GLU:HG3	2.16	0.61
3:D:77:SER:HB2	4:D:358:HOH:O	2.01	0.60
3:A:90:PRO:HB2	3:B:85:ILE:HG22	1.82	0.60
3:B:85:ILE:O	3:B:85:ILE:HG22	2.00	0.60
3:C:144:ALA:HA	3:C:285:LYS:HE2	1.83	0.59
1:G:-4[B]:DC:H4'	4:G:19:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:PHE:CZ	3:C:67:PHE:CE1	2.90	0.58
3:B:13:ILE:HG12	3:B:75:MET:HE2	1.85	0.58
3:C:20:HIS:O	3:C:67:PHE:CZ	2.55	0.58
3:B:13:ILE:HA	3:B:75:MET:HE1	1.87	0.57
3:A:94:ILE:CD1	3:B:85:ILE:HD13	2.34	0.56
3:B:234:ASN:HB2	4:B:448:HOH:O	2.05	0.56
3:D:265:VAL:HB	4:D:434:HOH:O	2.05	0.55
3:A:3:ARG:O	3:A:4:LEU:HG	2.06	0.55
3:C:155:ILE:HD11	3:C:169:TYR:CE2	2.41	0.55
3:A:3:ARG:CG	3:A:4:LEU:H	2.18	0.55
3:B:95:ARG:O	3:B:99:MET:HG3	2.06	0.55
3:B:158:LEU:C	3:B:158:LEU:HD23	2.26	0.55
3:D:142:GLN:HG3	3:D:143:GLY:N	2.21	0.55
3:C:67:PHE:O	3:C:67:PHE:CD1	2.54	0.54
3:D:142:GLN:HG2	3:D:160:ASP:HA	1.88	0.54
3:C:13:ILE:HD13	3:C:75:MET:HE2	1.89	0.54
3:C:11:THR:C	4:C:427:HOH:O	2.45	0.54
3:B:85:ILE:CG2	3:B:85:ILE:O	2.55	0.54
2:H:0[B]:DT:H72	4:C:412:HOH:O	2.07	0.53
3:D:84:ARG:NH2	3:D:100:GLU:CG	2.71	0.53
3:C:75:MET:HA	4:C:366:HOH:O	2.08	0.53
3:C:139:VAL:O	3:C:299:ARG:NH1	2.42	0.53
3:A:86:LYS:O	3:A:87:ASP:HB2	2.08	0.53
3:C:70:GLU:HG3	4:C:415:HOH:O	2.08	0.52
3:B:67:PHE:HA	3:B:70:GLU:HG2	1.91	0.51
2:F:2[A]:DG:O4'	3:A:114:GLN:HG3	2.11	0.51
3:B:234:ASN:CG	4:B:448:HOH:O	2.49	0.51
1:G:-3[B]:DG:H5"	3:D:157:LYS:HB2	1.92	0.50
3:D:142:GLN:HG3	3:D:143:GLY:H	1.76	0.50
1:E:0[A]:DA:H2	4:E:162:HOH:O	1.90	0.50
3:D:70:GLU:HG3	3:D:74:ARG:HH12	1.76	0.50
1:E:0[B]:DA:H2'	1:E:0[B]:DA:N3	2.27	0.50
2:F:-3[A]:DC:H5"	3:B:157:LYS:CB	2.41	0.50
3:C:236:ASN:O	3:C:240:LYS:HE2	2.11	0.50
3:D:155:ILE:HD11	3:D:169:TYR:CE2	2.47	0.50
3:B:234:ASN:HB2	4:B:382:HOH:O	2.12	0.50
3:A:3:ARG:HG2	3:A:4:LEU:N	2.24	0.50
3:B:13:ILE:CG1	3:B:75:MET:HE2	2.42	0.49
3:B:234:ASN:CB	4:B:448:HOH:O	2.60	0.49
3:C:20:HIS:O	3:C:67:PHE:CE2	2.65	0.49
3:D:84:ARG:CZ	3:D:100:GLU:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:VAL:HG22	3:C:247:THR:HG21	1.94	0.49
3:B:237:PHE:HD2	3:B:238:LYS:HG2	1.77	0.49
3:B:280:LEU:HD21	3:B:300:LEU:HD21	1.95	0.48
2:H:-2[A]:DC:H2'	2:H:-1[A]:DC:C6	2.47	0.48
3:C:84:ARG:CZ	3:C:100:GLU:OE2	2.62	0.48
1:E:-4[A]:DC:O2	2:F:4[A]:DG:N2	2.37	0.48
3:C:71:PHE:C	3:C:71:PHE:CD2	2.87	0.48
3:B:88:MET:HE1	3:B:92:ASP:O	2.14	0.48
3:C:13:ILE:HD12	3:C:108:LEU:HD13	1.96	0.47
3:B:144:ALA:HA	3:B:285:LYS:HG2	1.97	0.47
2:F:2[B]:DG:O4'	3:B:114:GLN:HG3	2.13	0.47
3:C:199:THR:HG21	4:C:426:HOH:O	2.13	0.47
2:F:3[A]:DC:H2"	2:F:4[A]:DG:C8	2.49	0.47
3:B:294:ASN:OD1	4:B:412:HOH:O	2.20	0.47
2:H:2[B]:DG:N3	3:D:114:GLN:HB3	2.30	0.47
2:F:0[A]:DT:H3'	3:B:116:ARG:HB3	1.97	0.47
3:D:201:ILE:HD13	3:D:204:MET:CE	2.45	0.47
3:B:234:ASN:ND2	4:B:448:HOH:O	2.47	0.47
1:G:-4[A]:DC:H1'	1:G:-3[A]:DG:C8	2.49	0.46
3:A:13:ILE:HA	3:A:75:MET:CE	2.45	0.46
3:A:16:GLU:HB3	3:A:71:PHE:HE1	1.80	0.46
3:C:270:SER:O	3:C:274:GLU:HG3	2.14	0.46
2:F:-3[B]:DC:C5'	3:A:157:LYS:HB2	2.41	0.46
3:D:70:GLU:HB3	4:D:435:HOH:O	2.15	0.45
3:C:101:TYR:N	3:C:102:PRO:CD	2.79	0.45
1:E:0[A]:DA:OP1	3:A:184:THR:HG23	2.16	0.45
3:D:294:ASN:HA	3:D:297:ARG:HG2	1.98	0.45
3:C:94:ILE:HD12	3:D:85:ILE:HD13	1.97	0.45
2:F:0[B]:DT:OP2	2:F:0[B]:DT:H4'	2.16	0.45
3:D:9:PHE:O	3:D:13:ILE:HG13	2.16	0.45
3:A:95:ARG:O	3:A:99:MET:HG3	2.17	0.45
1:G:-2[B]:DC:H2'	1:G:-1[B]:DC:C6	2.52	0.45
4:E:307:HOH:O	2:F:3[B]:DC:H5	1.99	0.45
3:B:237:PHE:CE2	3:B:238:LYS:HE3	2.52	0.44
2:H:-4[A]:DG:H2"	2:H:-3[A]:DC:OP2	2.16	0.44
3:B:139:VAL:O	3:B:299:ARG:NH1	2.49	0.44
1:G:-4[B]:DC:H1'	1:G:-3[B]:DG:C8	2.53	0.44
4:G:8:HOH:O	2:H:0[A]:DT:H6	1.99	0.44
3:C:140:ASP:OD2	3:C:166:VAL:HG22	2.17	0.44
2:H:3[A]:DC:H2"	2:H:4[A]:DG:C8	2.52	0.44
3:D:101:TYR:N	3:D:102:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:-4[B]:DC:O2	2:F:4[B]:DG:N2	2.43	0.44
4:H:14:HOH:O	3:C:10:LYS:HE3	2.16	0.44
3:A:24:PRO:HB3	3:A:123:GLU:HG3	1.98	0.44
3:B:164:PRO:HG3	3:B:262:TRP:CD2	2.52	0.43
1:E:0[A]:DA:H2'	1:E:0[A]:DA:N3	2.34	0.43
2:H:2[A]:DG:O4'	3:C:114:GLN:HG3	2.18	0.43
3:C:21:PHE:CZ	3:C:67:PHE:CZ	3.07	0.43
3:D:155:ILE:HD11	3:D:169:TYR:CD2	2.54	0.43
3:C:84:ARG:NH2	3:C:100:GLU:OE2	2.52	0.43
3:B:260:ARG:HA	3:B:263:ASN:HD22	1.82	0.43
3:C:75:MET:CE	4:C:403:HOH:O	2.63	0.43
2:H:0[A]:DT:H3'	3:D:116:ARG:HB3	2.00	0.43
3:C:5:SER:OG	3:C:8:GLU:HG3	2.19	0.43
3:B:196:VAL:CG2	3:B:204:MET:CE	2.96	0.42
3:A:90:PRO:HG3	3:B:88:MET:O	2.19	0.42
3:C:142:GLN:NE2	3:C:155:ILE:HG22	2.34	0.42
3:C:58:LYS:HE3	3:C:58:LYS:HB3	1.66	0.42
2:H:2[B]:DG:O4'	3:D:114:GLN:HG3	2.20	0.42
3:D:49:PRO:HD2	3:D:249:GLU:HG3	2.02	0.42
3:A:27:LEU:HD11	3:A:63:GLU:CG	2.36	0.42
3:D:28:VAL:HG12	3:D:130:LEU:HD12	2.02	0.42
3:B:196:VAL:HG23	3:B:204:MET:CE	2.46	0.42
3:A:73:THR:HG21	3:B:99:MET:HG2	2.02	0.42
3:A:294:ASN:HB2	4:A:369:HOH:O	2.18	0.42
3:A:28:VAL:HG21	3:A:126:SER:HB2	2.02	0.42
3:C:215:GLU:OE1	3:C:242:ASN:ND2	2.52	0.42
3:A:5:SER:OG	3:A:8:GLU:HB2	2.19	0.42
3:B:65:GLU:HG3	4:B:442:HOH:O	2.19	0.42
3:C:158:LEU:C	3:C:158:LEU:HD23	2.39	0.42
3:B:262:TRP:O	3:B:265:VAL:HG12	2.19	0.42
2:H:0[A]:DT:OP2	2:H:1[A]:DG:H2'	2.20	0.42
2:H:3[B]:DC:H2"	2:H:4[B]:DG:C8	2.54	0.42
2:F:2[B]:DG:N3	3:B:114:GLN:HB3	2.35	0.41
3:D:267:TYR:O	3:D:272:LYS:HE3	2.21	0.41
3:D:281:LYS:HG3	3:D:285:LYS:NZ	2.35	0.41
3:C:67:PHE:HD1	3:C:68:GLU:CA	2.33	0.41
3:C:5:SER:HB2	3:C:6:PRO:HD2	2.02	0.41
2:F:-3[B]:DC:N4	4:F:218:HOH:O	2.53	0.41
3:B:158:LEU:HD11	3:B:192:VAL:HG22	2.02	0.41
3:B:37:TYR:HE1	3:B:44:TYR:HH	1.66	0.41
3:C:67:PHE:CD1	3:C:68:GLU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:13:ILE:HD13	3:D:108:LEU:HA	2.03	0.41
1:G:-3[A]:DG:H5'	3:C:157:LYS:HB2	1.95	0.40
3:C:74:ARG:C	4:C:366:HOH:O	2.58	0.40
3:B:49:PRO:HD2	3:B:249:GLU:HG3	2.04	0.40
3:A:192:VAL:HB	3:A:193:PRO:HD3	2.04	0.40
3:B:280:LEU:CD2	3:B:300:LEU:HD21	2.51	0.40
2:F:0[B]:DT:H3'	3:A:116:ARG:HB3	2.03	0.40
3:C:109:ALA:CB	3:D:109:ALA:HB3	2.52	0.40
3:D:65:GLU:N	3:D:66:PRO:HD2	2.37	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
3	A	289/305 (95%)	283 (98%)	5 (2%)	1 (0%)	46 26
3	B	291/305 (95%)	285 (98%)	6 (2%)	0	100 100
3	C	289/305 (95%)	284 (98%)	4 (1%)	1 (0%)	46 26
3	D	288/305 (94%)	285 (99%)	3 (1%)	0	100 100
All	All	1157/1220 (95%)	1137 (98%)	18 (2%)	2 (0%)	52 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	74	ARG
3	A	101	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	272/283 (96%)	263 (97%)	9 (3%)	45 22
3	B	274/283 (97%)	268 (98%)	6 (2%)	60 39
3	C	272/283 (96%)	263 (97%)	9 (3%)	45 22
3	D	271/283 (96%)	264 (97%)	7 (3%)	54 32
All	All	1089/1132 (96%)	1058 (97%)	31 (3%)	51 29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	THR
3	A	19	SER
3	A	63	GLU
3	A	122	LYS
3	A	142	GLN
3	A	158	LEU
3	A	263	ASN
3	A	280	LEU
3	A	281	LYS
3	B	3	ARG
3	B	95	ARG
3	B	142	GLN
3	B	154	GLN
3	B	158	LEU
3	B	264	ASN
3	C	10	LYS
3	C	67	PHE
3	C	71	PHE
3	C	142	GLN
3	C	145	ILE
3	C	158	LEU
3	C	233	GLU
3	C	285	LYS
3	C	287	SER

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Mol	Chain	Res	Type
3	D	4	LEU
3	D	16	GLU
3	D	95	ARG
3	D	145	ILE
3	D	158	LEU
3	D	273	GLU
3	D	285	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	190	GLN
3	A	263	ASN
3	A	276	GLN
3	B	197	ASN
3	B	263	ASN
3	B	264	ASN
3	C	142	GLN
3	C	276	GLN
3	D	263	ASN
3	D	277	GLN

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

There are no ligands in this entry.

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	E	9/9 (100%)	0.31	0 100 100	12, 15, 23, 33	0
1	G	9/9 (100%)	0.18	0 100 100	7, 11, 19, 23	0
2	F	9/9 (100%)	0.41	0 100 100	9, 14, 28, 31	0
2	H	9/9 (100%)	0.13	0 100 100	7, 9, 19, 23	0
3	A	293/305 (96%)	1.24	69 (23%) 1 1	8, 24, 42, 53	19 (6%)
3	B	295/305 (96%)	0.93	47 (15%) 3 3	7, 15, 29, 47	19 (6%)
3	C	293/305 (96%)	1.05	51 (17%) 2 2	7, 15, 32, 40	26 (8%)
3	D	292/305 (95%)	0.89	43 (14%) 3 4	5, 15, 31, 51	17 (5%)
All	All	1209/1256 (96%)	1.00	210 (17%) 2 2	5, 17, 36, 53	81 (6%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	4	LEU	8.8
3	C	78	TYR	8.3
3	C	66	PRO	7.3
3	C	67	PHE	5.9
3	A	67	PHE	5.9
3	A	153	ASN	5.8
3	B	144	ALA	5.8
3	B	264	ASN	5.8
3	B	143	GLY	5.7
3	D	302	ALA	5.7
3	B	265	VAL	5.7
3	A	264	ASN	5.7
3	C	266	SER	5.6
3	A	78	TYR	5.6
3	C	264	ASN	5.3
3	D	67	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
3	D	157	LYS	5.3
3	A	265	VAL	5.1
3	C	268	THR	5.1
3	A	266	SER	5.0
3	A	20	HIS	4.9
3	C	74	ARG	4.9
3	C	241	ASN	4.8
3	B	86	LYS	4.7
3	D	143	GLY	4.6
3	B	83	GLU	4.6
3	A	94	ILE	4.5
3	A	267	TYR	4.5
3	B	145	ILE	4.4
3	B	18	LYS	4.4
3	A	270	SER	4.3
3	D	4	LEU	4.3
3	C	4	LEU	4.3
3	A	130	LEU	4.2
3	D	91	TYR	4.2
3	D	108	LEU	4.1
3	A	131	LEU	4.1
3	C	263	ASN	4.0
3	C	85	ILE	3.9
3	C	155	ILE	3.9
3	A	269	ASP	3.9
3	C	70	GLU	3.8
3	A	91	TYR	3.8
3	B	266	SER	3.6
3	C	237	PHE	3.6
3	A	87	ASP	3.6
3	C	269	ASP	3.6
3	A	11	THR	3.6
3	B	4	LEU	3.6
3	D	127	ILE	3.6
3	A	145	ILE	3.6
3	A	268	THR	3.5
3	D	78	TYR	3.5
3	B	268	THR	3.5
3	C	18	LYS	3.5
3	D	145	ILE	3.5
3	A	263	ASN	3.4
3	A	21	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	76	LEU	3.4
3	D	264	ASN	3.4
3	C	145	ILE	3.4
3	A	5	SER	3.4
3	B	87	ASP	3.3
3	B	305	ASP	3.3
3	B	85	ILE	3.3
3	C	157	LYS	3.3
3	D	20	HIS	3.3
3	A	7	GLY	3.2
3	D	265	VAL	3.2
3	C	20	HIS	3.2
3	D	155	ILE	3.2
3	A	3	ARG	3.2
3	A	154	GLN	3.2
3	A	157	LYS	3.2
3	B	154	GLN	3.2
3	C	79	LEU	3.2
3	B	241	ASN	3.2
3	A	61	TRP	3.1
3	C	265	VAL	3.1
3	A	85	ILE	3.1
3	D	15	LYS	3.1
3	B	5	SER	3.1
3	A	108	LEU	3.1
3	B	130	LEU	3.0
3	C	165	GLY	3.0
3	B	3	ARG	3.0
3	B	228	VAL	3.0
3	D	28	VAL	3.0
3	D	21	PHE	3.0
3	D	301	SER	3.0
3	B	127	ILE	3.0
3	B	82	GLU	3.0
3	B	277	GLN	3.0
3	A	84	ARG	3.0
3	C	87	ASP	2.9
3	A	192	VAL	2.9
3	A	185	LEU	2.9
3	A	86	LYS	2.9
3	D	5	SER	2.9
3	D	11	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	269	ASP	2.9
3	D	142	GLN	2.8
3	A	128	LEU	2.8
3	B	237	PHE	2.8
3	A	99	MET	2.8
3	A	53	ILE	2.8
3	C	189	TRP	2.8
3	A	62	LYS	2.8
3	C	69	LYS	2.8
3	B	157	LYS	2.8
3	D	270	SER	2.8
3	A	28	VAL	2.8
3	A	18	LYS	2.7
3	D	267	TYR	2.7
3	B	6	PRO	2.7
3	A	19	SER	2.7
3	D	303	LEU	2.7
3	A	294	ASN	2.7
3	C	53	ILE	2.6
3	A	101	TYR	2.6
3	D	139	VAL	2.6
3	C	144	ALA	2.6
3	A	237	PHE	2.6
3	D	74	ARG	2.6
3	B	79	LEU	2.6
3	B	142	GLN	2.6
3	D	62	LYS	2.5
3	C	71	PHE	2.5
3	C	143	GLY	2.5
3	D	263	ASN	2.5
3	D	279	ILE	2.5
3	A	143	GLY	2.5
3	B	95	ARG	2.5
3	B	189	TRP	2.5
3	A	97	PHE	2.5
3	A	29	TYR	2.5
3	D	192	VAL	2.5
3	B	269	ASP	2.5
3	A	15	LYS	2.5
3	A	16	GLU	2.5
3	A	32	PHE	2.5
3	B	62	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	67	PHE	2.5
3	C	267	TYR	2.4
3	C	275	ILE	2.4
3	D	130	LEU	2.4
3	C	32	PHE	2.4
3	D	304	PHE	2.4
3	D	241	ASN	2.4
3	D	292	VAL	2.4
3	C	204	MET	2.4
3	C	15	LYS	2.4
3	A	206	LEU	2.4
3	B	206	LEU	2.4
3	C	279	ILE	2.4
3	B	165	GLY	2.4
3	A	132	MET	2.4
3	A	241	ASN	2.4
3	B	236	ASN	2.4
3	B	185	LEU	2.3
3	D	94	ILE	2.3
3	A	144	ALA	2.3
3	C	281	LYS	2.3
3	A	98	THR	2.3
3	A	12	LEU	2.3
3	B	275	ILE	2.3
3	D	144	ALA	2.3
3	A	9	PHE	2.3
3	A	139	VAL	2.3
3	C	94	ILE	2.3
3	C	164	PRO	2.3
3	A	273	GLU	2.2
3	C	130	LEU	2.2
3	D	110	LEU	2.2
3	C	139	VAL	2.2
3	B	20	HIS	2.2
3	B	113	THR	2.2
3	B	108	LEU	2.2
3	B	53	ILE	2.2
3	C	91	TYR	2.2
3	C	21	PHE	2.2
3	C	10	LYS	2.2
3	A	52	TYR	2.2
3	C	52	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	B	297	ARG	2.2
3	C	86	LYS	2.2
3	A	80	ILE	2.2
3	D	283	ILE	2.2
3	A	17	ARG	2.1
3	B	270	SER	2.1
3	C	128	LEU	2.1
3	A	8	GLU	2.1
3	B	263	ASN	2.1
3	A	296	TYR	2.1
3	A	188	ARG	2.1
3	A	6	PRO	2.1
3	B	221	LEU	2.1
3	C	8	GLU	2.1
3	D	128	LEU	2.1
3	C	238	LYS	2.1
3	B	162	VAL	2.1
3	D	76	LEU	2.1
3	D	297	ARG	2.1
3	D	228	VAL	2.0
3	A	39	GLN	2.0
3	A	189	TRP	2.0
3	A	257	GLU	2.0
3	C	127	ILE	2.0
3	C	5	SER	2.0
3	C	108	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.