Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 06:16 PM EDT

PDB ID	:	8D29
Title	:	Crystal structure of theophylline aptamer - apo form
Authors	:	Menichelli, E.; Spraggon, G.
Deposited on	:	2022-05-28
Resolution	:	1.81 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:

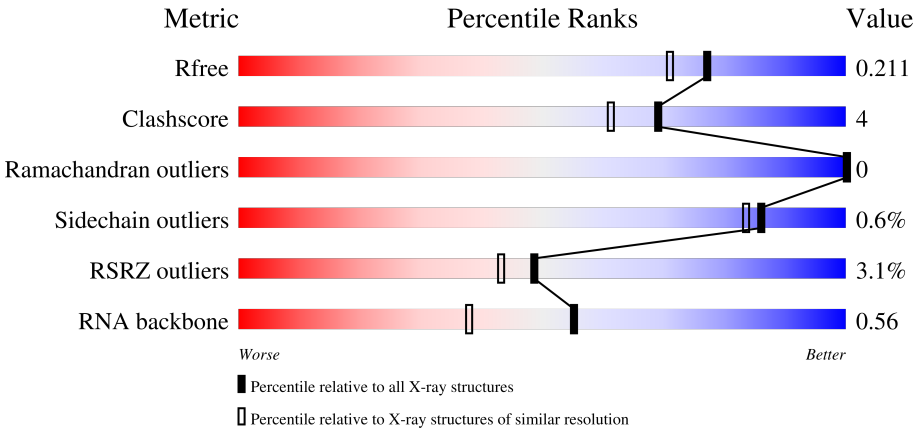
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)
RNA backbone	3102	1047 (2.40-1.24)

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	229	92% 5%
1	D	229	94%
1	G	229	93% 5%
1	H	229	2% 92%

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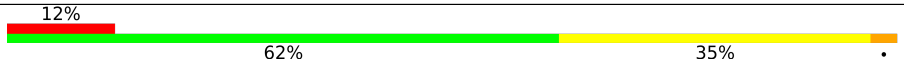
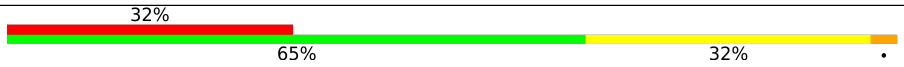
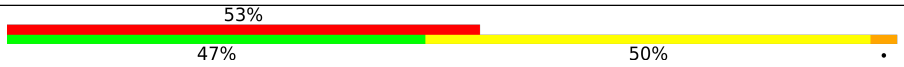
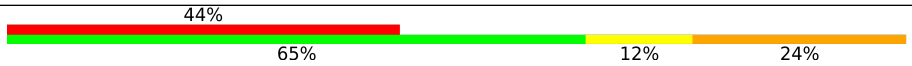
Mol	Chain	Length	Quality of chain
2	B	214	
2	E	214	
2	I	214	
2	L	214	
3	C	34	
3	F	34	
3	J	34	
3	R	34	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18122 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	2	0
			1669	1052	285	326	6			
1	D	224	Total	C	N	O	S	0	2	0
			1675	1054	285	330	6			
1	G	218	Total	C	N	O	S	0	2	0
			1630	1029	275	319	7			
1	H	220	Total	C	N	O	S	0	3	0
			1656	1045	283	322	6			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	2	2	0
			1635	1022	274	332	7			
2	E	213	Total	C	N	O	S	2	2	0
			1635	1021	273	334	7			
2	I	213	Total	C	N	O	S	2	1	0
			1636	1022	274	334	6			
2	L	214	Total	C	N	O	S	2	2	0
			1645	1027	275	335	8			

- Molecule 3 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	34	Total	C	N	O	P	0	0	0
			723	324	134	232	33			
3	F	34	Total	C	N	O	P	60	0	0
			723	324	134	232	33			
3	J	34	Total	C	N	O	P	60	0	0
			723	324	134	232	33			
3	R	34	Total	C	N	O	P	0	0	0
			723	324	134	232	33			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	H	1	Total K 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Na 1 1	0	0

- Molecule 6 is water.

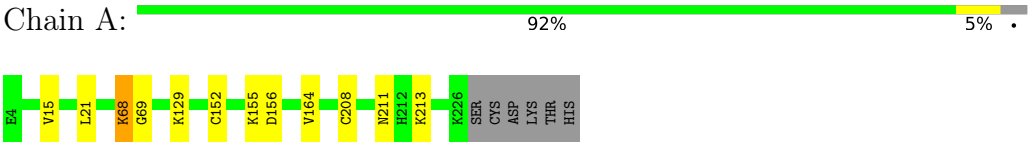
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	299	Total O 299 299	0	0
6	B	208	Total O 208 208	0	0
6	C	42	Total O 42 42	0	0
6	D	313	Total O 313 313	0	0
6	E	208	Total O 208 208	0	0
6	F	27	Total O 27 27	0	0
6	G	267	Total O 267 267	0	0
6	H	266	Total O 266 266	0	0
6	I	180	Total O 180 180	0	0
6	J	17	Total O 17 17	0	0
6	L	197	Total O 197 197	0	0
6	R	19	Total O 19 19	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.

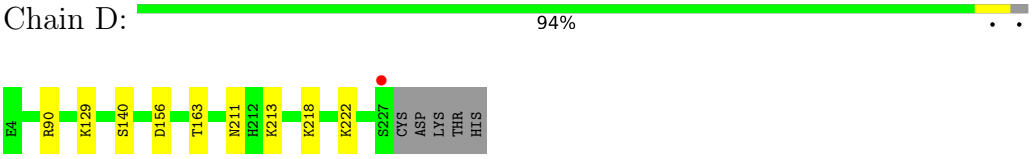
• Molecule 1: Fab heavy chain

Chain A:



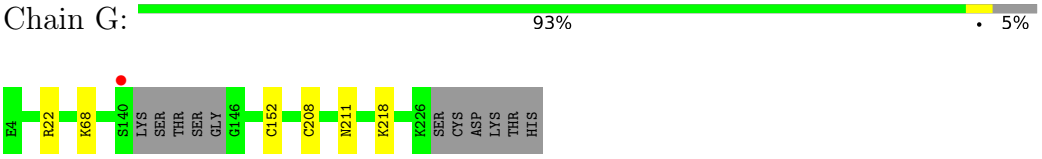
• Molecule 1: Fab heavy chain

Chain D:



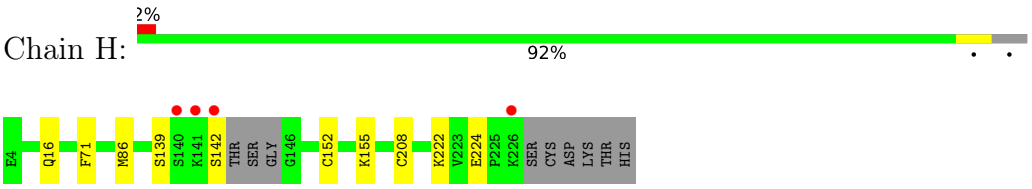
• Molecule 1: Fab heavy chain

Chain G:



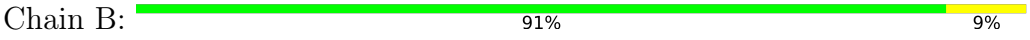
• Molecule 1: Fab heavy chain

Chain H:



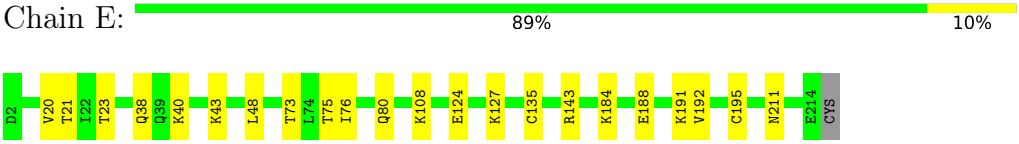
• Molecule 2: Fab light chain

Chain B:



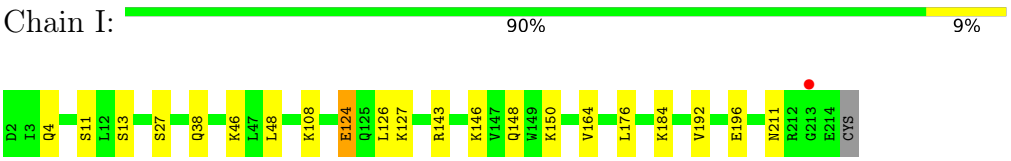
• Molecule 2: Fab light chain

Chain E:



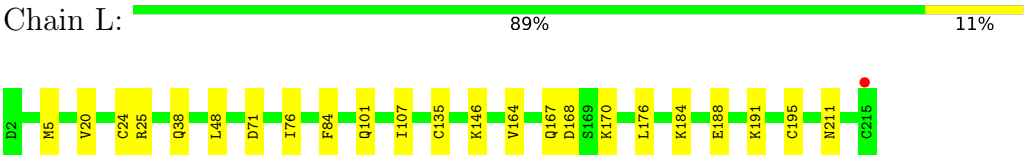
• Molecule 2: Fab light chain

Chain I:



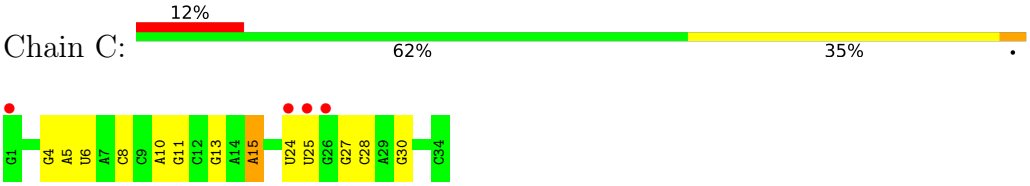
• Molecule 2: Fab light chain

Chain L:



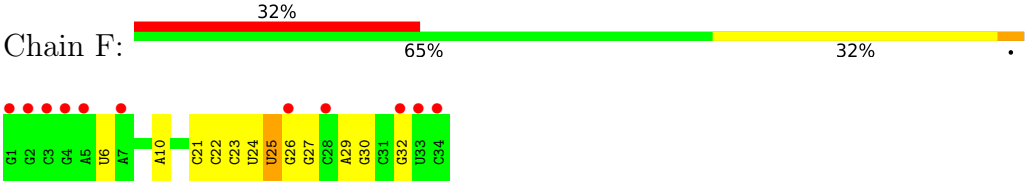
• Molecule 3: RNA (34-MER)

Chain C:



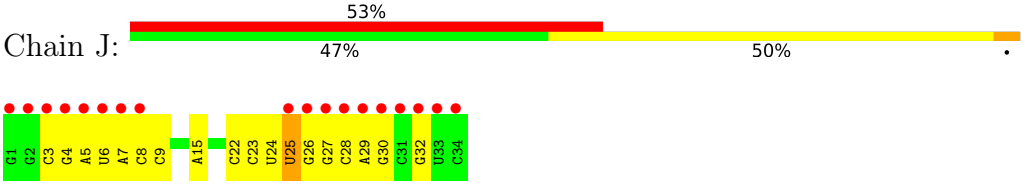
• Molecule 3: RNA (34-MER)

Chain F:



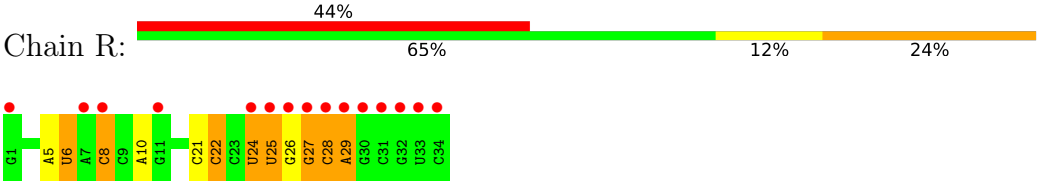
• Molecule 3: RNA (34-MER)

Chain J:



• Molecule 3: RNA (34-MER)

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.15Å 92.85Å 93.64Å 97.34° 90.32° 106.92°	Depositor
Resolution (Å)	68.66 – 1.81 68.66 – 1.81	Depositor EDS
% Data completeness (in resolution range)	93.7 (68.66-1.81) 93.7 (68.66-1.81)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.175 , 0.211 0.175 , 0.211	Depositor DCC
R_{free} test set	10352 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18122	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 30.18 % 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 1.3671e-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, 0.333 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: K, NA

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	0.48	0/1716	0.64	0/2336
1	D	0.46	0/1722	0.66	0/2345
1	G	0.49	0/1676	0.66	0/2283
1	H	0.41	0/1705	0.62	0/2319
2	B	0.87	0/1676	0.70	0/2275
2	E	0.42	0/1676	0.62	0/2276
2	I	0.41	0/1674	0.62	0/2272
2	L	0.42	0/1686	0.62	0/2288
3	C	0.32	0/808	0.78	1/1258 (0.1%)
3	F	0.30	0/808	0.79	1/1258 (0.1%)
3	J	0.27	0/808	0.77	1/1258 (0.1%)
3	R	0.34	0/808	0.85	0/1258
All	All	0.48	0/16763	0.68	3/23426 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	15	A	O4'-C1'-N9	-6.81	102.75	108.20
3	F	25	U	C2'-C3'-O3'	6.27	123.73	113.70
3	J	15	A	O4'-C1'-N9	-5.05	104.16	108.20

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	1669	0	1634	7	0
1	D	1675	0	1631	7	0
1	G	1630	0	1581	4	0
1	H	1656	0	1623	7	0
2	B	1635	0	1589	20	0
2	E	1635	0	1581	15	0
2	I	1636	0	1588	15	0
2	L	1645	0	1600	15	0
3	C	723	0	372	2	0
3	F	723	0	372	1	0
3	J	723	0	372	9	0
3	R	723	0	372	9	0
4	A	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
5	G	1	0	0	0	0
6	A	299	0	0	0	0
6	B	208	0	0	1	0
6	C	42	0	0	0	0
6	D	313	0	0	2	0
6	E	208	0	0	4	0
6	F	27	0	0	0	0
6	G	267	0	0	2	0
6	H	266	0	0	0	0
6	I	180	0	0	2	0
6	J	17	0	0	0	0
6	L	197	0	0	3	0
6	R	19	0	0	0	0
All	All	18122	0	14315	110	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 4.

All (110) 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:D:90:ARG:NH1	6:D:401:HOH:O	1.56	1.37
2:B:148:GLN:NE2	2:B:155:LEU:HD12	1.53	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLN:HE21	2:B:155:LEU:HD12	1.05	1.11
2:B:189:LYS:HE3	2:B:189:LYS:HA	1.41	1.02
2:I:150:LYS:NZ	2:I:196:GLU:OE1	2.00	0.95
3:J:9:C:H42	3:J:26:G:H1	1.14	0.91
2:I:146:LYS:HE3	2:I:148:GLN:OE1	1.74	0.86
1:G:218:LYS:NZ	6:G:401:HOH:O	2.21	0.74
2:B:192:VAL:HG22	2:B:211:ASN:OD1	1.92	0.69
2:E:127:LYS:HA	2:E:127:LYS:HE2	1.78	0.65
2:L:184:LYS:O	2:L:188:GLU:HG3	1.96	0.65
3:R:24:U:H4'	3:R:25:U:OP1	1.95	0.65
2:B:148:GLN:NE2	2:B:155:LEU:CD1	2.47	0.61
2:E:184:LYS:HE2	2:E:188:GLU:OE2	2.01	0.61
2:B:148:GLN:CD	2:B:155:LEU:HD12	2.20	0.61
2:E:127:LYS:HA	2:E:127:LYS:CE	2.32	0.60
3:R:26:G:H2'	3:R:27:G:H5"	1.83	0.60
2:I:146:LYS:CE	2:I:148:GLN:OE1	2.48	0.59
2:B:171:ASP:O	2:B:173:THR:HG23	2.03	0.59
2:E:80:GLN:NE2	6:E:402:HOH:O	2.35	0.59
2:I:13:SER:OG	2:I:108:LYS:HE3	2.02	0.58
2:I:13:SER:OG	2:I:108:LYS:CE	2.51	0.58
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.85	0.58
2:L:168:ASP:OD2	2:L:170:LYS:HE3	2.04	0.58
3:J:8:C:H42	3:J:27:G:H1	1.52	0.57
2:L:25:ARG:HG2	2:L:71:ASP:OD1	2.04	0.57
3:J:25:U:H6	3:J:25:U:O5'	1.87	0.57
2:B:146:LYS:HE2	2:B:148:GLN:HB2	1.86	0.57
2:I:124:GLU:HA	2:I:127:LYS:HD2	1.86	0.57
2:E:73:THR:HG23	6:E:551:HOH:O	2.04	0.57
1:D:218:LYS:HE3	1:H:16:GLN:HG3	1.88	0.56
2:B:189:LYS:HA	2:B:189:LYS:CE	2.22	0.55
3:F:21:C:H6	3:F:21:C:O5'	1.90	0.54
2:B:181:THR:O	2:B:182:LEU:HD23	2.08	0.53
2:L:135:CYS:SG	2:L:195[B]:CYS:SG	3.02	0.53
2:B:148:GLN:CG	2:B:155:LEU:CD1	2.87	0.53
1:A:152:CYS:SG	1:A:208[B]:CYS:HB3	2.49	0.52
2:B:168:ASP:HB3	2:B:171:ASP:OD1	2.09	0.52
3:J:3:C:H2'	3:J:4:G:H8	1.73	0.52
2:E:40:LYS:NZ	6:E:405:HOH:O	2.44	0.51
1:G:22:ARG:HD2	6:G:414:HOH:O	2.10	0.51
1:H:222:LYS:HE2	1:H:224:GLU:HG2	1.93	0.51
2:L:107:ILE:HD12	2:L:167:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:THR:HG22	2:E:73:THR:HG22	1.93	0.50
3:J:5:A:O5'	3:J:5:A:H8	1.95	0.50
1:H:155:LYS:HE3	6:L:405:HOH:O	2.11	0.50
2:L:191:LYS:HE2	2:L:211:ASN:HB3	1.94	0.49
2:E:191:LYS:HG2	2:E:192:VAL:HG23	1.95	0.49
3:R:25:U:H2'	3:R:26:G:C8	2.47	0.49
2:I:11:SER:HB2	6:I:315:HOH:O	2.13	0.49
2:L:164:VAL:HG22	2:L:176:LEU:HD12	1.94	0.49
3:J:4:G:H2'	3:J:5:A:C8	2.48	0.48
2:E:40:LYS:HB2	2:E:43:LYS:HD3	1.95	0.48
1:H:139:SER:O	1:H:142:SER:OG	2.17	0.48
1:D:211:ASN:OD1	1:D:218:LYS:HG2	2.13	0.48
3:J:3:C:H2'	3:J:4:G:C8	2.48	0.48
2:I:38:GLN:HB2	2:I:48:LEU:HD11	1.96	0.48
2:E:20:VAL:HG22	2:E:76:ILE:HB	1.96	0.47
1:H:152:CYS:SG	1:H:208[B]:CYS:HB3	2.53	0.47
2:E:135:CYS:SG	2:E:195[B]:CYS:SG	3.06	0.47
2:I:4:GLN:HB2	2:I:27:SER:HB3	1.96	0.47
2:L:101:GLN:HB2	6:L:431:HOH:O	2.14	0.47
2:I:126:LEU:O	2:I:184:LYS:HE3	2.15	0.47
1:G:152:CYS:SG	1:G:208[B]:CYS:HB3	2.53	0.47
1:A:129:LYS:HD3	1:A:156:ASP:O	2.15	0.47
1:A:211:ASN:HD21	1:A:213:LYS:NZ	2.12	0.47
1:D:222:LYS:HD3	6:D:529:HOH:O	2.15	0.46
2:B:189:LYS:N	2:B:189:LYS:HD2	2.31	0.46
2:I:108:LYS:NZ	6:I:309:HOH:O	2.48	0.46
3:C:13:G:H2'	3:C:15:A:H62	1.81	0.46
1:D:211:ASN:HD21	1:D:213:LYS:CE	2.29	0.45
6:E:578:HOH:O	2:I:46:LYS:HE3	2.15	0.45
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.97	0.45
2:I:13:SER:OG	2:I:108:LYS:HE2	2.15	0.45
1:H:71:PHE:CE1	1:H:86:MET:HB3	2.51	0.45
2:B:148:GLN:CG	2:B:155:LEU:HD12	2.46	0.45
2:B:189:LYS:HE3	2:B:189:LYS:CA	2.22	0.45
2:E:38:GLN:HB2	2:E:48:LEU:HD11	1.99	0.45
2:L:5:MET:HB3	2:L:24:CYS:SG	2.58	0.44
1:A:155:LYS:HE3	6:B:452:HOH:O	2.18	0.44
3:J:27:G:H2'	3:J:28:C:C6	2.53	0.44
3:R:27:G:H2'	3:R:28:C:C6	2.52	0.44
1:H:152:CYS:SG	1:H:208[B]:CYS:CB	3.06	0.44
2:E:124:GLU:OE1	2:E:124:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:168:ASP:CG	2:L:170:LYS:HE3	2.38	0.43
2:E:192:VAL:HG22	2:E:211:ASN:OD1	2.18	0.43
1:A:164:VAL:HG13	1:A:208[B]:CYS:SG	2.59	0.43
1:G:152:CYS:SG	1:G:208[B]:CYS:CB	3.07	0.43
2:L:146:LYS:NZ	6:L:306:HOH:O	2.52	0.43
3:J:25:U:O5'	3:J:25:U:C6	2.71	0.43
2:B:126:LEU:O	2:B:184:LYS:HD2	2.19	0.42
3:R:5:A:H2'	3:R:6:U:O4'	2.18	0.42
2:B:121:PRO:HD3	2:B:133:VAL:HG22	2.01	0.42
2:L:168:ASP:OD1	2:L:170:LYS:HE3	2.19	0.42
2:L:84:PHE:CG	2:L:107:ILE:HG13	2.55	0.42
3:R:6:U:H3	3:R:29:A:N6	2.17	0.42
3:C:4:G:H2'	3:C:5:A:C8	2.55	0.42
3:R:6:U:H3	3:R:29:A:H61	1.66	0.42
1:D:129:LYS:HD3	1:D:156:ASP:O	2.20	0.41
3:R:8:C:H6	3:R:8:C:O5'	2.02	0.41
1:A:15:VAL:HG11	1:A:21:LEU:HD13	2.02	0.41
2:B:171:ASP:OD1	2:B:171:ASP:C	2.59	0.41
2:L:20:VAL:HG22	2:L:76:ILE:HB	2.03	0.41
3:R:21:C:H2'	3:R:22:C:O4'	2.21	0.41
2:E:21:THR:HG22	2:E:75:THR:OG1	2.21	0.41
2:I:192:VAL:HG22	2:I:211:ASN:OD1	2.20	0.41
1:A:68:LYS:HD2	1:A:69:GLY:N	2.37	0.40
1:D:163:THR:OG1	1:D:211:ASN:HB3	2.21	0.40
2:I:164:VAL:HG22	2:I:176:LEU:HD12	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	223/229 (97%)	218 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	224/229 (98%)	219 (98%)	5 (2%)	0	100	100
1	G	216/229 (94%)	212 (98%)	4 (2%)	0	100	100
1	H	219/229 (96%)	213 (97%)	6 (3%)	0	100	100
2	B	213/214 (100%)	209 (98%)	4 (2%)	0	100	100
2	E	213/214 (100%)	210 (99%)	3 (1%)	0	100	100
2	I	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	L	214/214 (100%)	210 (98%)	4 (2%)	0	100	100
All	All	1734/1772 (98%)	1697 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/190 (97%)	184 (100%)	1 (0%)	88	87
1	D	186/190 (98%)	185 (100%)	1 (0%)	88	87
1	G	180/190 (95%)	178 (99%)	2 (1%)	73	67
1	H	184/190 (97%)	184 (100%)	0	100	100
2	B	189/189 (100%)	188 (100%)	1 (0%)	88	87
2	E	189/189 (100%)	187 (99%)	2 (1%)	73	67
2	I	189/189 (100%)	187 (99%)	2 (1%)	73	67
2	L	191/189 (101%)	191 (100%)	0	100	100
All	All	1493/1516 (98%)	1484 (99%)	9 (1%)	86	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
2	B	170	LYS

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Mol	Chain	Res	Type
1	D	140	SER
2	E	108	LYS
2	E	143	ARG
1	G	68	LYS
1	G	211	ASN
2	I	124	GLU
2	I	143	ARG

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	211	ASN
2	B	4	GLN
1	D	6	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	33/34 (97%)	9 (27%)	0
3	F	33/34 (97%)	11 (33%)	1 (3%)
3	J	33/34 (97%)	9 (27%)	0
3	R	33/34 (97%)	9 (27%)	1 (3%)
All	All	132/136 (97%)	38 (28%)	2 (1%)

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	6	U
3	C	8	C
3	C	10	A
3	C	11	G
3	C	24	U
3	C	25	U
3	C	27	G
3	C	28	C
3	C	30	G
3	F	6	U
3	F	10	A
3	F	22	C

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Mol	Chain	Res	Type
3	F	23	C
3	F	24	U
3	F	25	U
3	F	26	G
3	F	27	G
3	F	29	A
3	F	30	G
3	F	32	G
3	J	6	U
3	J	7	A
3	J	22	C
3	J	23	C
3	J	24	U
3	J	25	U
3	J	29	A
3	J	30	G
3	J	32	G
3	R	6	U
3	R	8	C
3	R	10	A
3	R	22	C
3	R	24	U
3	R	25	U
3	R	27	G
3	R	28	C
3	R	29	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	F	25	U
3	R	24	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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	223/229 (97%)	-0.46	0 100 100	10, 17, 34, 57	0
1	D	224/229 (97%)	-0.42	1 (0%) 92 91	11, 18, 37, 82	0
1	G	218/229 (95%)	-0.45	1 (0%) 91 89	12, 20, 36, 77	0
1	H	220/229 (96%)	-0.38	4 (1%) 68 64	11, 19, 40, 88	0
2	B	213/214 (99%)	-0.53	1 (0%) 91 89	12, 23, 43, 73	2 (0%)
2	E	213/214 (99%)	-0.56	0 100 100	12, 24, 42, 66	2 (0%)
2	I	213/214 (99%)	-0.45	1 (0%) 91 89	14, 27, 52, 82	2 (0%)
2	L	214/214 (100%)	-0.55	1 (0%) 91 89	13, 24, 46, 77	2 (0%)
3	C	34/34 (100%)	0.65	4 (11%) 4 3	19, 83, 123, 136	0
3	F	31/34 (91%)	1.35	11 (35%) 0 0	20, 119, 148, 161	0
3	J	31/34 (91%)	2.16	18 (58%) 0 0	21, 134, 188, 190	0
3	R	34/34 (100%)	1.47	15 (44%) 0 0	25, 115, 149, 157	0
All	All	1868/1908 (97%)	-0.35	57 (3%) 49 43	10, 22, 77, 190	8 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	7	A	6.5
1	H	140	SER	6.1
3	J	5	A	5.5
3	J	4	G	5.2
3	J	6	U	5.1
2	I	213	GLY	4.8
3	J	29	A	4.6
3	R	29	A	4.4
3	F	4	G	4.0
3	J	30	G	4.0
3	J	32	G	3.9

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Mol	Chain	Res	Type	RSRZ
3	F	5	A	3.8
3	R	28	C	3.8
3	R	24	U	3.7
3	F	1	G	3.7
1	H	141	LYS	3.6
3	J	3	C	3.6
1	G	140	SER	3.6
3	J	27	G	3.5
3	R	31	C	3.5
3	J	25	U	3.4
3	J	26	G	3.4
3	R	26	G	3.4
3	R	34	C	3.4
1	H	226	LYS	3.2
3	F	2	G	3.2
3	F	32	G	3.2
3	R	27	G	3.1
2	L	215	CYS	3.0
3	C	24	U	3.0
3	J	34	C	2.9
3	J	8	C	2.9
3	J	31	C	2.9
3	R	25	U	2.9
3	F	3	C	2.9
3	J	33	U	2.8
3	J	1	G	2.7
3	J	28	C	2.7
3	R	30	G	2.7
1	H	142	SER	2.7
2	B	213	GLY	2.6
3	J	2	G	2.6
3	R	32	G	2.6
3	F	7	A	2.6
3	F	34	C	2.5
1	D	227	SER	2.5
3	C	26	G	2.5
3	R	1	G	2.4
3	R	8	C	2.4
3	F	26	G	2.3
3	F	33	U	2.3
3	R	33	U	2.3
3	R	11	G	2.2

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Mol	Chain	Res	Type	RSRZ
3	R	7	A	2.2
3	F	28	C	2.2
3	C	1	G	2.1
3	C	25	U	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 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
4	K	H	301	1/1	0.93	0.16	22,22,22,22	1
5	NA	G	301	1/1	0.93	0.13	31,31,31,31	1
4	K	A	302	1/1	0.98	0.07	14,14,14,14	1
4	K	D	301	1/1	0.98	0.13	21,21,21,21	1
4	K	A	301	1/1	0.99	0.08	20,20,20,20	1
4	K	E	301	1/1	0.99	0.12	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.