



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2021 – 04:11 PM JST

PDB ID : 7EL1
Title : Structure of a protein from bacteria
Authors : Liu, H.; Zhu, Y.; Huang, Z.
Deposited on : 2021-04-07
Resolution : 2.22 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 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	:	2.22
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)	:	2.22

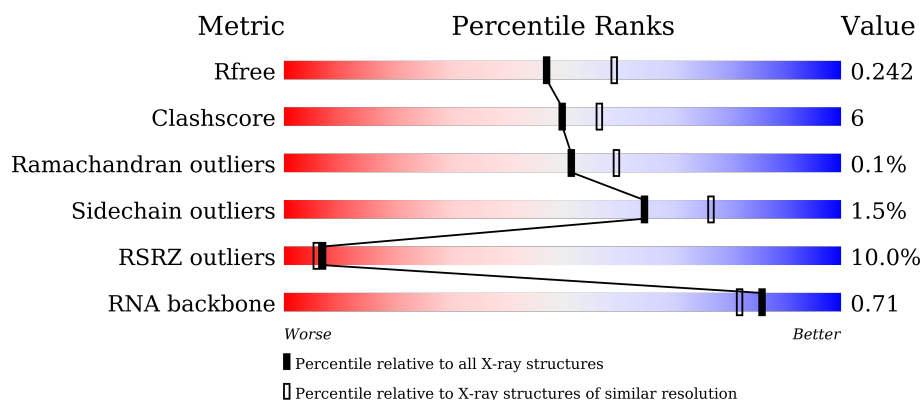
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)
RNA backbone	3102	1049 (2.64-1.80)

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 $\leq 5\%$. 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	1053	<div> <div>11%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
2	B	73	<div> <div>11%</div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
3	C	28	<div> <div>89%</div> <div>7%</div> <div>•</div> </div>
4	D	8	<div> <div>88%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	100	<div><div></div><div>4%</div><div></div><div>79%</div><div></div><div>17%</div><div></div><div>• •</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11628 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 CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1033	Total	C	N	O	S	0	0	0
			8413	5349	1466	1586	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ASN	engineered mutation	UNP J7RUA5
A	946	ALA	CYS	engineered mutation	UNP J7RUA5

- Molecule 2 is a RNA chain called RNA (73-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	P	0	0	0
			1545	689	279	504	73			

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			561	270	99	165	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			164	80	31	46	7			

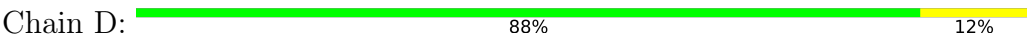
- Molecule 5 is a protein called 100AA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	98	Total	C	N	O	S	0	0	0
			819	526	134	157	2			

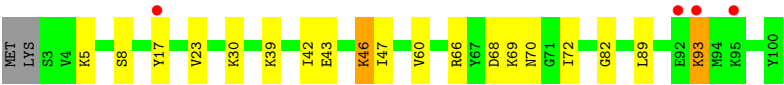
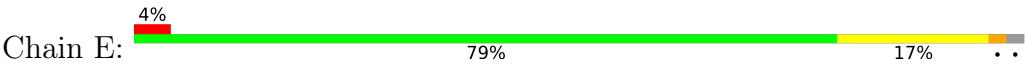
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	35	Total	O	0	0
			35	35		
6	C	5	Total	O	0	0
			5	5		
6	D	9	Total	O	0	0
			9	9		
6	E	4	Total	O	0	0
			4	4		

● Molecule 4: DNA (5'-D(*TP*TP*GP*AP*AP*TP*AP*G)-3')



● Molecule 5: 100AA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	330.58Å 105.22Å 68.55Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.22 44.37 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.22) 99.8 (44.37-2.22)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.22Å)	Xtriage
Refinement program	PHENIX v1.11	Depositor
R, R_{free}	0.213 , 0.242 0.213 , 0.242	Depositor DCC
R_{free} test set	5675 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11628	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.47	1/8559 (0.0%)	0.64	5/11529 (0.0%)
2	B	0.71	1/1729 (0.1%)	1.15	3/2692 (0.1%)
3	C	1.02	0/627	1.18	2/963 (0.2%)
4	D	1.26	0/184	1.35	2/283 (0.7%)
5	E	0.51	0/836	0.73	1/1120 (0.1%)
All	All	0.57	2/11935 (0.0%)	0.80	13/16587 (0.1%)

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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-9.19	1.50	1.61
1	A	308	GLU	CB-CG	5.27	1.62	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	G	O5'-P-OP2	-14.63	92.53	105.70
5	E	46	LYS	CD-CE-NZ	-12.60	82.72	111.70
1	A	878	LYS	CD-CE-NZ	-10.50	87.55	111.70
4	D	4	DA	O4'-C1'-N9	8.57	114.00	108.00
1	A	208	ARG	NE-CZ-NH2	7.01	123.80	120.30
3	C	13	DA	O4'-C1'-N9	5.99	112.19	108.00
1	A	116	ARG	NE-CZ-NH1	-5.75	117.43	120.30
3	C	14	DG	O4'-C4'-C3'	-5.65	102.24	104.50
4	D	4	DA	C1'-O4'-C4'	-5.43	104.67	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	208	ARG	CG-CD-NE	5.22	122.77	111.80
2	B	70	G	C2-N3-C4	5.19	114.50	111.90
2	B	62	A	P-O3'-C3'	5.10	125.82	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ARG	Peptide

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	8413	0	8422	113	0
2	B	1545	0	773	6	0
3	C	561	0	317	2	0
4	D	164	0	93	0	0
5	E	819	0	801	11	0
6	A	73	0	0	2	0
6	B	35	0	0	0	0
6	C	5	0	0	0	0
6	D	9	0	0	0	0
6	E	4	0	0	1	0
All	All	11628	0	10406	126	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 6.

All (126) 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:A:520:LEU:O	1:A:524:ILE:HD12	1.55	1.06
1:A:134:THR:HG22	1:A:170:ARG:HH11	1.28	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:LEU:HD13	1:A:524:ILE:HD11	1.48	0.95
1:A:521:ILE:HA	1:A:524:ILE:CD1	1.97	0.94
1:A:504:ARG:HA	1:A:504:ARG:HH21	1.36	0.88
1:A:861:THR:HG23	1:A:863:ASN:H	1.40	0.87
1:A:504:ARG:HH22	1:A:507:GLU:HB3	1.40	0.86
1:A:521:ILE:HA	1:A:524:ILE:HD12	1.57	0.85
1:A:657:MET:CE	1:A:673:VAL:HG12	2.11	0.81
1:A:504:ARG:HH22	1:A:507:GLU:CB	1.95	0.80
1:A:657:MET:HE1	1:A:673:VAL:HG12	1.63	0.79
1:A:690:PHE:HB3	1:A:694:ARG:HH22	1.48	0.79
1:A:499:ARG:O	1:A:503:GLU:HG2	1.83	0.77
1:A:303:ILE:HD11	1:A:305:VAL:HG22	1.67	0.76
1:A:134:THR:HG22	1:A:170:ARG:NH1	2.01	0.75
1:A:521:ILE:HA	1:A:524:ILE:HD13	1.67	0.75
5:E:30:LYS:HD3	5:E:60:VAL:HG12	1.69	0.75
1:A:502:ASN:HA	1:A:505:ILE:HG13	1.70	0.73
1:A:272:ASN:HD22	1:A:273:GLU:N	1.89	0.71
1:A:92:ARG:HD2	1:A:179:GLU:OE2	1.89	0.71
1:A:504:ARG:HA	1:A:504:ARG:NH2	2.05	0.71
1:A:595:SER:HB3	5:E:8:SER:HB3	1.77	0.66
1:A:690:PHE:HB3	1:A:694:ARG:NH2	2.10	0.66
1:A:521:ILE:CA	1:A:524:ILE:HD12	2.25	0.66
1:A:520:LEU:C	1:A:524:ILE:HD12	2.16	0.65
1:A:653:THR:O	1:A:657:MET:HG2	1.96	0.64
5:E:47:ILE:HD11	5:E:82:GLY:HA2	1.80	0.64
1:A:303:ILE:CD1	1:A:305:VAL:HG22	2.28	0.64
1:A:360:SER:O	1:A:364:ILE:HG12	1.98	0.64
1:A:328:VAL:HG11	1:A:352:ALA:HB2	1.80	0.64
1:A:64:ILE:HD11	1:A:114:LYS:HB2	1.79	0.63
1:A:685:ARG:HH11	1:A:694:ARG:NH1	1.97	0.62
1:A:520:LEU:O	1:A:524:ILE:CD1	2.40	0.62
1:A:857:TYR:O	1:A:861:THR:HG22	1.98	0.62
1:A:40:ASN:HD21	1:A:485:LYS:HB2	1.64	0.62
1:A:265:LEU:O	1:A:274:LYS:NZ	2.28	0.61
1:A:867:LYS:NZ	2:B:45:C:O2	2.33	0.60
1:A:1044:LYS:NZ	6:A:1101:HOH:O	2.33	0.60
1:A:685:ARG:NH2	1:A:704:ASP:OD1	2.34	0.59
1:A:131:GLU:OE1	1:A:132:LEU:HD23	2.02	0.59
1:A:504:ARG:NH2	1:A:507:GLU:HB3	2.14	0.59
1:A:525:LYS:O	1:A:529:MET:HG2	2.03	0.59
1:A:612:ALA:HA	1:A:618:ILE:HG22	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LYS:HA	1:A:342:ILE:HG22	1.84	0.58
1:A:92:ARG:HD3	1:A:112:LEU:HG	1.87	0.57
1:A:685:ARG:HB3	1:A:690:PHE:HB2	1.86	0.57
1:A:680:PHE:O	1:A:683:PHE:HB3	2.04	0.56
1:A:690:PHE:C	1:A:694:ARG:HH22	2.09	0.56
1:A:936:LYS:HD2	1:A:941:GLU:OE1	2.05	0.56
1:A:13:ILE:HD12	1:A:449:VAL:HG11	1.88	0.56
1:A:561:ARG:HB2	1:A:686:ARG:NH1	2.22	0.55
1:A:685:ARG:HH11	1:A:694:ARG:CZ	2.21	0.54
1:A:526:LEU:HD23	1:A:529:MET:SD	2.48	0.54
1:A:867:LYS:HD2	2:B:46:U:H1'	1.89	0.54
5:E:66:ARG:HD2	5:E:68:ASP:OD2	2.07	0.54
5:E:70:ASN:OD1	5:E:72:ILE:N	2.41	0.53
1:A:277:TYR:CD1	1:A:409:HIS:CD2	2.96	0.53
1:A:303:ILE:C	1:A:303:ILE:HD12	2.29	0.53
1:A:649:THR:O	1:A:654:ARG:NH1	2.42	0.52
1:A:691:LYS:O	1:A:694:ARG:CZ	2.57	0.52
1:A:681:THR:O	1:A:685:ARG:HG3	2.08	0.52
1:A:519:TYR:O	1:A:523:LYS:HG3	2.11	0.51
1:A:502:ASN:HA	1:A:505:ILE:CG1	2.38	0.51
1:A:864:TYR:CE2	6:A:1138:HOH:O	2.62	0.50
1:A:287:VAL:HG23	1:A:302:GLU:HG3	1.93	0.50
5:E:39:LYS:O	5:E:43:GLU:HG3	2.12	0.50
1:A:362:GLU:H	1:A:362:GLU:CD	2.15	0.50
1:A:718:TRP:CD1	1:A:753:ILE:HD11	2.46	0.50
1:A:21:ILE:HD13	1:A:710:ASN:OD1	2.11	0.49
1:A:303:ILE:HD13	1:A:305:VAL:HG13	1.94	0.49
1:A:683:PHE:CZ	1:A:687:LYS:HE2	2.47	0.49
1:A:498:ASN:O	1:A:502:ASN:HB2	2.12	0.49
1:A:657:MET:HE3	1:A:673:VAL:HG12	1.90	0.49
1:A:505:ILE:HD12	1:A:506:GLU:N	2.28	0.49
1:A:502:ASN:HD22	1:A:505:ILE:HD11	1.78	0.49
1:A:805:LEU:HD12	1:A:816:LEU:HD23	1.93	0.49
2:B:23:U:H2'	2:B:24:U:C6	2.47	0.49
1:A:351:ILE:HD11	1:A:375:LEU:HD11	1.94	0.48
1:A:277:TYR:CD1	1:A:409:HIS:HD2	2.32	0.48
2:B:12:G:H2'	2:B:13:C:C6	2.48	0.48
1:A:127:ASP:OD1	1:A:127:ASP:N	2.46	0.48
1:A:690:PHE:CB	1:A:694:ARG:HH22	2.22	0.48
1:A:680:PHE:CZ	1:A:684:LEU:HD11	2.48	0.48
1:A:829:MET:O	1:A:832:HIS:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:VAL:HG22	6:E:203:HOH:O	2.13	0.48
1:A:5:TYR:CE2	1:A:471:PRO:HB3	2.49	0.47
1:A:273:GLU:HG3	1:A:274:LYS:HG2	1.97	0.47
1:A:40:ASN:ND2	1:A:485:LYS:HB2	2.28	0.47
1:A:24:GLU:HG2	1:A:25:THR:H	1.79	0.46
1:A:924:LYS:NZ	1:A:955:LYS:O	2.44	0.46
1:A:430:LEU:HD21	1:A:440:LEU:HD13	1.98	0.46
1:A:255:LEU:HD23	1:A:404:LEU:HD21	1.97	0.46
1:A:361:SER:O	1:A:365:GLN:HG3	2.16	0.46
1:A:64:ILE:HD11	1:A:114:LYS:CB	2.44	0.45
1:A:570:ASN:HA	1:A:622:LYS:HD3	1.99	0.45
1:A:969:ASN:OD1	1:A:980:ARG:HD2	2.17	0.44
1:A:502:ASN:ND2	1:A:505:ILE:HD11	2.32	0.44
1:A:536:TYR:CD2	1:A:575:VAL:HG11	2.52	0.44
1:A:891:LEU:HD21	2:B:56:A:H4'	2.00	0.44
1:A:42:GLU:HA	1:A:45:GLU:HB2	2.01	0.43
1:A:440:LEU:HD22	1:A:659:LEU:HD13	2.00	0.43
1:A:683:PHE:HD2	1:A:684:LEU:HD12	1.84	0.43
1:A:272:ASN:ND2	1:A:274:LYS:H	2.16	0.43
1:A:482:LYS:HD3	1:A:482:LYS:HA	1.86	0.43
1:A:582:LYS:HE3	1:A:596:ASP:O	2.18	0.43
1:A:481:GLU:O	1:A:482:LYS:HG2	2.18	0.43
1:A:303:ILE:CD1	1:A:303:ILE:C	2.87	0.43
1:A:408:TRP:HB3	1:A:409:HIS:CD2	2.54	0.42
1:A:582:LYS:HB2	1:A:582:LYS:HE2	1.74	0.42
1:A:445:ILE:HD12	1:A:445:ILE:HA	1.84	0.42
2:B:62:A:H4'	2:B:63:A:O5'	2.19	0.42
5:E:5:LYS:HG2	5:E:23:VAL:HG22	2.00	0.42
1:A:526:LEU:HA	1:A:529:MET:CG	2.49	0.42
5:E:17:TYR:CD1	5:E:42:ILE:HG13	2.54	0.42
1:A:40:ASN:HD21	1:A:485:LYS:CB	2.31	0.41
1:A:527:HIS:CE1	1:A:543:LEU:HG	2.56	0.41
1:A:502:ASN:HD22	1:A:505:ILE:CG1	2.33	0.41
1:A:135:LYS:HG3	3:C:13:DA:H5''	2.02	0.41
1:A:24:GLU:HG2	1:A:25:THR:N	2.35	0.41
1:A:148:LYS:NZ	1:A:156:GLU:OE1	2.38	0.41
1:A:342:ILE:HG21	1:A:342:ILE:HD13	1.85	0.41
5:E:89:LEU:O	5:E:93:LYS:NZ	2.52	0.41
1:A:353:LYS:O	1:A:357:ILE:HG12	2.21	0.41
5:E:69:LYS:HB3	5:E:69:LYS:HE2	1.79	0.41
1:A:315:VAL:HG12	3:C:24:DT:H2''	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:LYS:HB2	1:A:940:TYR:CE1	2.56	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	1029/1053 (98%)	992 (96%)	36 (4%)	1 (0%)	51	60
5	E	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
All	All	1125/1153 (98%)	1086 (96%)	38 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	LYS

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	911/970 (94%)	898 (99%)	13 (1%)	67	78
5	E	91/94 (97%)	89 (98%)	2 (2%)	52	64
All	All	1002/1064 (94%)	987 (98%)	15 (2%)	65	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ASP
1	A	193	LEU
1	A	208	ARG
1	A	232	MET
1	A	272	ASN
1	A	320	LYS
1	A	339	LYS
1	A	387	LYS
1	A	419	ASN
1	A	551	PHE
1	A	567	ASN
1	A	617	ARG
1	A	849	ASP
5	E	46	LYS
5	E	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	272	ASN
1	A	377	GLN
1	A	433	GLN
1	A	502	ASN
1	A	557	HIS
1	A	567	ASN
1	A	570	ASN
1	A	700	HIS
1	A	835	GLN
1	A	885	ASN
1	A	985	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/73 (97%)	6 (8%)	1 (1%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	38	A
2	B	39	C
2	B	55	A
2	B	57	G
2	B	63	A
2	B	65	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	62	A

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 [i](#)

There are no ligands in this entry.

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, 95th 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	1033/1053 (98%)	0.80	112 (10%) 5 4	36, 65, 103, 146	0
2	B	73/73 (100%)	0.85	8 (10%) 5 4	42, 54, 112, 120	0
3	C	28/28 (100%)	0.12	0 100 100	46, 56, 82, 83	0
4	D	8/8 (100%)	-0.08	0 100 100	41, 45, 50, 52	0
5	E	98/100 (98%)	0.67	4 (4%) 37 35	53, 69, 81, 82	0
All	All	1240/1262 (98%)	0.77	124 (10%) 7 6	36, 65, 101, 146	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	GLY	16.6
1	A	492	ASN	11.1
1	A	615	LYS	9.8
1	A	505	ILE	8.9
1	A	494	MET	8.9
1	A	617	ARG	8.0
1	A	122	ASN	7.6
1	A	124	VAL	7.4
1	A	498	ASN	7.4
2	B	35	G	7.4
1	A	501	THR	7.3
1	A	551	PHE	7.3
2	B	36	A	7.2
2	B	37	A	7.2
1	A	125	GLU	7.0
1	A	692	LYS	6.9
1	A	499	ARG	6.6
1	A	548	ASN	6.4
1	A	481	GLU	6.2
2	B	38	A	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	432	GLN	6.0
1	A	500	GLN	6.0
1	A	495	GLN	5.8
1	A	426	LYS	5.7
1	A	496	LYS	5.6
1	A	516	ASN	5.6
1	A	512	THR	5.6
1	A	489	LYS	5.5
1	A	130	ASN	5.5
2	B	39	C	5.4
1	A	508	ILE	5.3
2	B	34	G	5.3
1	A	691	LYS	5.1
1	A	647	VAL	5.0
1	A	757	PRO	5.0
1	A	127	ASP	5.0
1	A	497	ARG	4.9
1	A	507	GLU	4.7
1	A	722	ASP	4.6
1	A	490	MET	4.6
1	A	128	THR	4.5
1	A	550	PRO	4.4
1	A	123	GLU	4.4
1	A	485	LYS	4.3
1	A	511	THR	4.2
1	A	504	ARG	4.0
1	A	713	PHE	4.0
1	A	765	ASP	3.9
1	A	721	LEU	3.8
2	B	40	A	3.8
1	A	502	ASN	3.8
1	A	503	GLU	3.7
1	A	24	GLU	3.7
1	A	549	ASN	3.6
1	A	484	SER	3.6
1	A	129	GLY	3.6
1	A	763	ILE	3.5
1	A	686	ARG	3.5
1	A	545	ASP	3.3
1	A	715	PHE	3.3
1	A	524	ILE	3.3
1	A	519	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	694	ARG	3.2
1	A	720	LYS	3.2
1	A	440	LEU	3.2
1	A	126	GLU	3.2
1	A	616	GLY	3.2
1	A	613	LYS	3.1
1	A	513	GLY	3.1
1	A	749	GLU	3.1
1	A	80	HIS	3.1
1	A	753	ILE	3.1
1	A	430	LEU	3.1
1	A	693	GLU	3.1
1	A	514	LYS	3.0
1	A	1006	GLU	3.0
1	A	3	ARG	3.0
1	A	509	ILE	3.0
1	A	1009	ASN	3.0
1	A	585	ASN	2.9
1	A	680	PHE	2.9
1	A	745	GLU	2.9
1	A	23	TYR	2.9
1	A	561	ARG	2.9
1	A	758	HIS	2.8
1	A	427	LYS	2.8
2	B	41	G	2.7
1	A	543	LEU	2.7
1	A	486	ASP	2.7
1	A	491	ILE	2.7
1	A	483	ASN	2.7
1	A	762	HIS	2.7
1	A	515	GLU	2.6
1	A	565	PHE	2.6
1	A	849	ASP	2.5
1	A	431	SER	2.4
1	A	446	LEU	2.4
1	A	520	LEU	2.4
1	A	689	LYS	2.4
1	A	308	GLU	2.4
1	A	716	LYS	2.3
1	A	569	PHE	2.3
1	A	683	PHE	2.3
1	A	541	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	506	GLU	2.3
1	A	429	ASP	2.3
1	A	488	GLN	2.3
1	A	421	LEU	2.3
5	E	93	LYS	2.2
1	A	795	ASP	2.2
1	A	527	HIS	2.2
5	E	95	LYS	2.2
1	A	423	LEU	2.2
1	A	649	THR	2.2
1	A	493	GLU	2.1
1	A	544	GLU	2.1
5	E	92	GLU	2.1
1	A	690	PHE	2.1
1	A	552	ASN	2.0
1	A	425	PRO	2.0
1	A	723	LYS	2.0
1	A	428	VAL	2.0
5	E	17	TYR	2.0
1	A	644	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.