Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:40 AM EDT

PDB ID	:	6QF6
Title	:	Structure of an E.coli expressed anti-Mcl1 scFv
Authors	:	Luptak, J.
Deposited on	:	2019-01-09
Resolution	:	2.59 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:

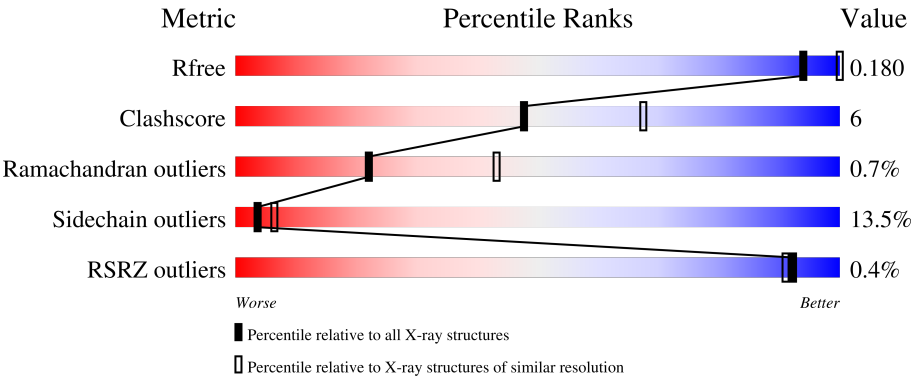
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	247	67% 22% • 9%
1	B	247	65% 25% • 8%
1	C	247	71% 18% • 8%
1	D	247	77% 14% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7034 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 E.coli expressed scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1691	1057	289	339	6			
1	B	228	Total	C	N	O	S	0	0	0
			1707	1067	292	342	6			
1	C	227	Total	C	N	O	S	0	0	0
			1698	1062	290	340	6			
1	D	228	Total	C	N	O	S	0	0	0
			1707	1067	292	342	6			

- Molecule 2 is water.

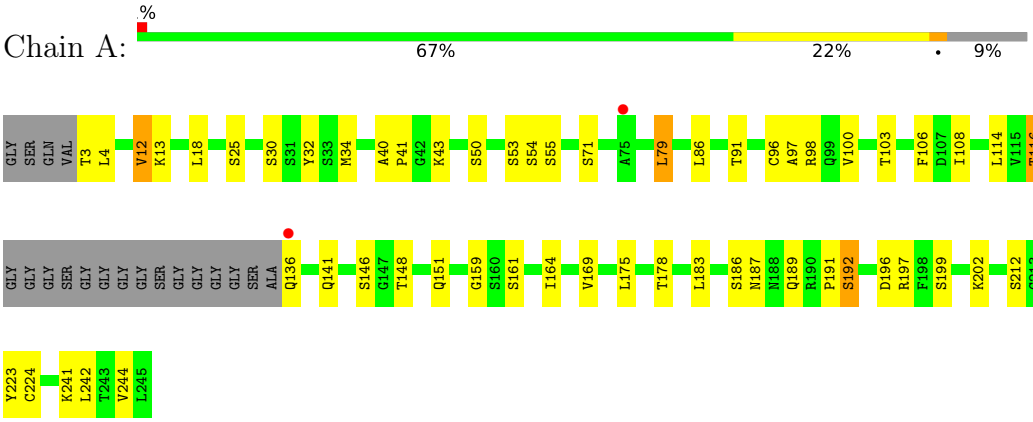
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total	O	0	0
			62	62		
2	B	48	Total	O	0	0
			48	48		
2	C	64	Total	O	0	0
			64	64		
2	D	57	Total	O	0	0
			57	57		

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.

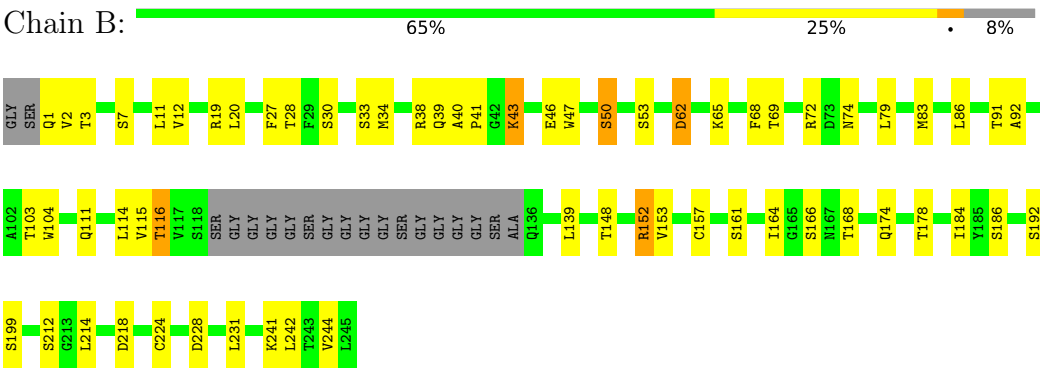
• Molecule 1: E.coli expressed scFv

Chain A:



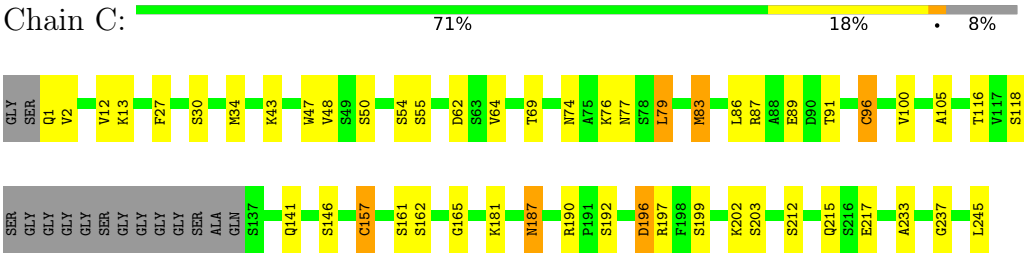
• Molecule 1: E.coli expressed scFv

Chain B:



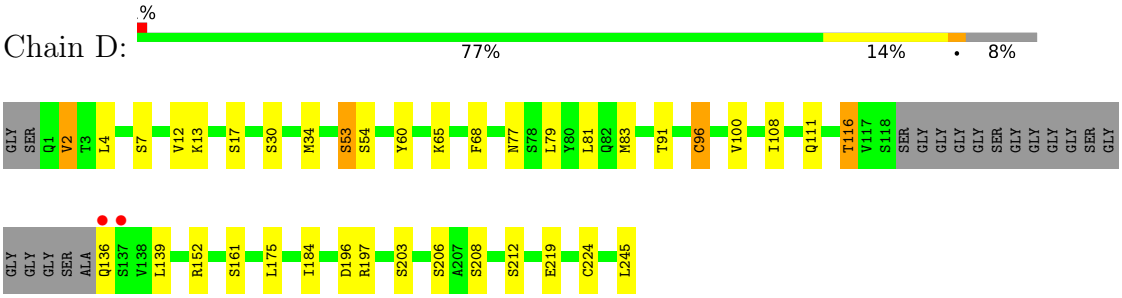
• Molecule 1: E.coli expressed scFv

Chain C:



• Molecule 1: E.coli expressed scFv

Chain D:


%
77%
14%
8%
GLY SER Q1 V2 T3 L4 S7 V12 K13 S17 S30 M34 S53 S54 Y60 K65 F68 N77 S78 L79 Y80 L81 Q82 M83 T91 C96 V100 I108 Q111 T116 V117 S118 SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY
GLY GLY GLY SER ALA Q136 S137 V138 L139 R152 S161 L175 I184 D196 R197 S203 S206 A207 S208 S212 E219 C224 L245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.18Å 180.18Å 88.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.40 – 2.59 39.18 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (127.40-2.59) 51.3 (39.18-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.181 , 0.262 0.198 , 0.180	Depositor DCC
R_{free} test set	1243 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.55	0/1729	0.76	0/2350
1	B	0.53	0/1745	0.75	0/2372
1	C	0.50	0/1736	0.75	0/2360
1	D	0.50	0/1745	0.76	1/2372 (0.0%)
All	All	0.52	0/6955	0.76	1/9454 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	53	SER	C-N-CA	6.00	136.71	121.70

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	1691	0	1622	25	0
1	B	1707	0	1642	24	0
1	C	1698	0	1634	22	0
1	D	1707	0	1642	11	0
2	A	62	0	0	0	0
2	B	48	0	0	0	0
2	C	64	0	0	0	0
2	D	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7034	0	6540	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLN:HG3	1:C:157:CYS:HB2	1.67	0.77
1:C:47:TRP:CZ3	1:C:233:ALA:HB1	2.21	0.76
1:C:161:SER:HA	1:C:165:GLY:HA3	1.69	0.73
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.73	0.69
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.75	0.69
1:B:218:ASP:O	1:B:242:LEU:HD23	1.93	0.68
1:B:40:ALA:HB3	1:B:43:LYS:HB2	1.75	0.68
1:C:187:ASN:OD1	1:C:202:LYS:HD3	1.94	0.67
1:C:12:VAL:HG21	1:C:86:LEU:HD13	1.77	0.65
1:A:40:ALA:HB1	1:A:41:PRO:HD2	1.79	0.63
1:A:40:ALA:HB1	1:A:41:PRO:CD	2.30	0.60
1:A:164:ILE:HD13	1:A:169:VAL:HG11	1.84	0.59
1:D:197:ARG:HB3	1:D:212:SER:O	2.03	0.58
1:B:34:MET:HB3	1:B:79:LEU:HD22	1.86	0.57
1:A:189:GLN:HE22	1:C:190:ARG:H	1.51	0.57
1:D:60:TYR:HB2	1:D:65:LYS:HD2	1.87	0.56
1:A:4:LEU:HD12	1:A:108:ILE:HG22	1.88	0.55
1:A:197:ARG:HB3	1:A:212:SER:O	2.06	0.55
1:A:97:ALA:HB1	1:A:106:PHE:HB3	1.89	0.54
1:A:159:GLY:HA3	1:A:164:ILE:HG13	1.90	0.54
1:A:3:THR:N	1:A:25:SER:HG	2.06	0.53
1:A:12:VAL:HG11	1:A:86:LEU:HD13	1.89	0.53
1:D:68:PHE:HB3	1:D:81:LEU:HD11	1.89	0.53
1:B:168:THR:HB	1:B:186:SER:HA	1.91	0.53
1:A:148:THR:H	1:A:151:GLN:NE2	2.08	0.52
1:B:40:ALA:HB1	1:B:41:PRO:HD2	1.91	0.52
1:A:30:SER:O	1:A:53:SER:HB2	2.10	0.51
1:A:187:ASN:OD1	1:A:202:LYS:HD3	2.10	0.51
1:C:12:VAL:HG21	1:C:86:LEU:CD1	2.40	0.51
1:C:215:GLN:HB3	1:C:217:GLU:HG2	1.93	0.50
1:A:214:LEU:HD21	1:A:242:LEU:HD21	1.94	0.50
1:C:197:ARG:HB3	1:C:212:SER:O	2.11	0.50
1:C:47:TRP:CZ3	1:C:233:ALA:CB	2.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:MET:HE1	1:B:115:VAL:HG11	1.94	0.49
1:B:39:GLN:HE22	1:B:174:GLN:HE22	1.61	0.49
1:C:30:SER:HB3	1:C:74:ASN:HB3	1.94	0.49
1:D:17:SER:HA	1:D:83:MET:O	2.13	0.49
1:B:100:VAL:HG23	1:B:103:THR:OG1	2.12	0.48
1:A:148:THR:O	1:A:151:GLN:HG2	2.13	0.48
1:B:228:ASP:HB3	1:B:231:LEU:HB2	1.95	0.48
1:B:62:ASP:HA	1:B:65:LYS:HD2	1.95	0.48
1:B:214:LEU:HD13	1:B:244:VAL:HG13	1.94	0.48
1:B:161:SER:O	1:B:166:SER:HB2	2.15	0.47
1:A:141:GLN:HE22	1:A:223:TYR:HA	1.80	0.47
1:B:47:TRP:HZ2	1:B:50:SER:HB3	1.79	0.46
1:D:79:LEU:HD23	1:D:96:CYS:SG	2.55	0.46
1:B:197:ARG:HB3	1:B:212:SER:O	2.16	0.45
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.99	0.45
1:B:68:PHE:CE1	1:B:83:MET:HB3	2.52	0.44
1:A:183:LEU:O	1:A:191:PRO:HD2	2.17	0.44
1:D:4:LEU:HD13	1:D:96:CYS:HB3	2.00	0.44
1:B:152:ARG:HA	1:B:212:SER:HA	2.00	0.44
1:C:2:VAL:HG13	1:C:27:PHE:CD1	2.54	0.43
1:C:34:MET:HB3	1:C:79:LEU:HD22	2.00	0.43
1:C:87:ARG:HD3	1:C:89:GLU:OE2	2.19	0.43
1:B:2:VAL:HG23	1:B:27:PHE:CD1	2.54	0.42
1:B:30:SER:HB3	1:B:74:ASN:HB3	2.01	0.42
1:C:100:VAL:HG22	1:C:105:ALA:O	2.20	0.42
1:D:152:ARG:HG3	1:D:212:SER:HA	2.01	0.42
1:D:139:LEU:HD23	1:D:139:LEU:HA	1.93	0.42
1:A:100:VAL:HG23	1:A:103:THR:H	1.85	0.42
1:C:34:MET:O	1:C:50:SER:HA	2.19	0.42
1:B:91:THR:HG23	1:B:116:THR:HA	2.01	0.42
1:D:2:VAL:HG12	1:D:108:ILE:HG21	2.01	0.42
1:A:12:VAL:HG12	1:A:117:VAL:HG22	2.01	0.41
1:A:100:VAL:HG21	1:A:103:THR:OG1	2.19	0.41
1:B:20:LEU:HD21	1:B:83:MET:HE2	2.02	0.41
1:C:79:LEU:HD23	1:C:96:CYS:SG	2.60	0.41
1:C:83:MET:HB2	1:C:86:LEU:HD21	2.02	0.41
1:B:139:LEU:HD21	1:B:164:ILE:HD11	2.03	0.41
1:C:91:THR:OG1	1:C:116:THR:HA	2.20	0.41
1:C:47:TRP:CE3	1:C:233:ALA:HB1	2.55	0.41
1:A:91:THR:HG23	1:A:116:THR:HA	2.03	0.41
1:B:79:LEU:HD23	1:B:96:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:HG23	1:D:116:THR:HA	2.03	0.41
1:B:91:THR:O	1:B:92:ALA:HB2	2.21	0.40
1:A:32:TYR:CE2	1:A:98:ARG:NH1	2.89	0.40
1:C:48:VAL:HG13	1:C:64:VAL:HG11	2.04	0.40
1:B:53:SER:HA	1:B:72:ARG:CZ	2.52	0.40
1:A:214:LEU:HD13	1:A:244:VAL:HG13	2.03	0.40
1:C:141:GLN:OE1	1:C:237:GLY:HA3	2.21	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	222/247 (90%)	198 (89%)	23 (10%)	1 (0%)	29	52
1	B	224/247 (91%)	204 (91%)	18 (8%)	2 (1%)	17	35
1	C	223/247 (90%)	206 (92%)	15 (7%)	2 (1%)	17	35
1	D	224/247 (91%)	212 (95%)	11 (5%)	1 (0%)	34	57
All	All	893/988 (90%)	820 (92%)	67 (8%)	6 (1%)	22	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	SER
1	B	196	ASP
1	C	196	ASP
1	D	2	VAL
1	C	187	ASN
1	B	101	GLY

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	184/191 (96%)	159 (86%)	25 (14%)	3 6
1	B	186/191 (97%)	155 (83%)	31 (17%)	2 3
1	C	185/191 (97%)	163 (88%)	22 (12%)	5 9
1	D	186/191 (97%)	164 (88%)	22 (12%)	5 9
All	All	741/764 (97%)	641 (86%)	100 (14%)	4 6

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	LYS
1	A	18	LEU
1	A	50	SER
1	A	54	SER
1	A	55	SER
1	A	71	SER
1	A	79	LEU
1	A	96	CYS
1	A	114	LEU
1	A	116	THR
1	A	118	SER
1	A	136	GLN
1	A	146	SER
1	A	161	SER
1	A	175	LEU
1	A	178	THR
1	A	186	SER
1	A	192	SER
1	A	196	ASP
1	A	199	SER
1	A	214	LEU
1	A	221	ASP
1	A	224	CYS

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Mol	Chain	Res	Type
1	A	241	LYS
1	B	1	GLN
1	B	3	THR
1	B	7	SER
1	B	11	LEU
1	B	12	VAL
1	B	19	ARG
1	B	28	THR
1	B	33	SER
1	B	38	ARG
1	B	43	LYS
1	B	46	GLU
1	B	50	SER
1	B	62	ASP
1	B	69	THR
1	B	86	LEU
1	B	96	CYS
1	B	100	VAL
1	B	104	TRP
1	B	111	GLN
1	B	114	LEU
1	B	116	THR
1	B	148	THR
1	B	152	ARG
1	B	153	VAL
1	B	157	CYS
1	B	178	THR
1	B	184	ILE
1	B	192	SER
1	B	199	SER
1	B	224	CYS
1	B	241	LYS
1	C	1	GLN
1	C	13	LYS
1	C	43	LYS
1	C	54	SER
1	C	55	SER
1	C	62	ASP
1	C	69	THR
1	C	76	LYS
1	C	77	ASN
1	C	79	LEU

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Mol	Chain	Res	Type
1	C	83	MET
1	C	96	CYS
1	C	118	SER
1	C	146	SER
1	C	157	CYS
1	C	162	SER
1	C	181	LYS
1	C	192	SER
1	C	196	ASP
1	C	199	SER
1	C	203	SER
1	C	245	LEU
1	D	7	SER
1	D	12	VAL
1	D	13	LYS
1	D	30	SER
1	D	53	SER
1	D	54	SER
1	D	77	ASN
1	D	96	CYS
1	D	100	VAL
1	D	111	GLN
1	D	116	THR
1	D	136	GLN
1	D	161	SER
1	D	175	LEU
1	D	184	ILE
1	D	196	ASP
1	D	203	SER
1	D	206	SER
1	D	208	SER
1	D	219	GLU
1	D	224	CYS
1	D	245	LEU

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	151	GLN
1	A	173	GLN
1	A	189	GLN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	232	ASN
1	B	39	GLN
1	B	174	GLN
1	B	215	GLN
1	C	167	ASN
1	D	99	GLN
1	D	151	GLN
1	D	170	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 monosaccharides 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	A	226/247 (91%)	-0.45	2 (0%) 84 82	15, 31, 54, 86	0
1	B	228/247 (92%)	-0.37	0 100 100	8, 37, 57, 78	0
1	C	227/247 (91%)	-0.44	0 100 100	13, 35, 54, 75	0
1	D	228/247 (92%)	-0.40	2 (0%) 84 82	20, 38, 59, 82	0
All	All	909/988 (92%)	-0.42	4 (0%) 92 91	8, 35, 57, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	GLN	4.3
1	A	136	GLN	3.1
1	D	137	SER	2.5
1	A	75	ALA	2.3

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.