Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:52 pm BST

PDB ID	:	6BVA
Title	:	Ubiquitin Variant (UbV.Fl10.1) bound to a human Skp1-Fbl10 fragment complex.
Authors	:	Manczyk, N.; Sicheri, F.
Deposited on	:	2017-12-12
Resolution	:	2.66 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

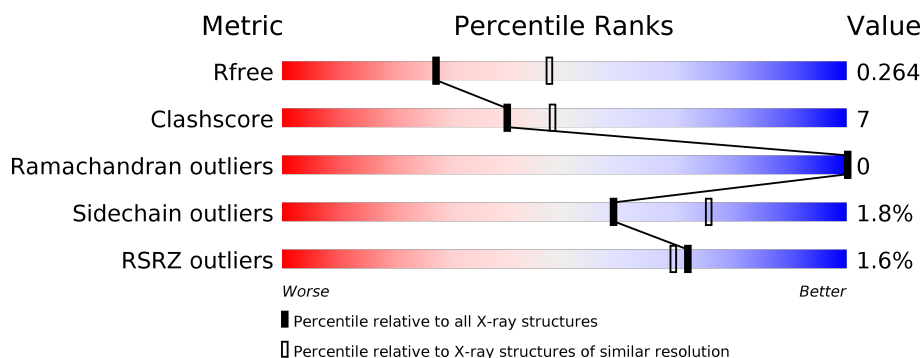|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.66 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	C	165	% / 81% 11% 8%
1	D	165	2% / 74% 17% 9%
2	E	47	4% / 72% 11% • 15%
2	F	47	68% 17% 15%
3	A	86	2% / 81% 19%
3	B	86	77% 16% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4111 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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	150	Total 1054	C 673	N 173	O 203	S 5	0	0	0
1	C	152	Total 1089	C 700	N 182	O 201	S 6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P63208
D	0	ALA	-	expression tag	UNP P63208
C	-1	GLY	-	expression tag	UNP P63208
C	0	ALA	-	expression tag	UNP P63208

- Molecule 2 is a protein called Lysine-specific demethylase 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	40	Total 307	C 199	N 52	O 51	S 5	0	0	0
2	F	40	Total 329	C 211	N 59	O 53	S 6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1058	GLY	-	expression tag	UNP Q8NHM5
E	1059	ALA	-	expression tag	UNP Q8NHM5
F	1058	GLY	-	expression tag	UNP Q8NHM5
F	1059	ALA	-	expression tag	UNP Q8NHM5

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	81	Total	C	N	O	S	0	0	0
			612	396	109	106	1			
3	A	86	Total	C	N	O	S	0	0	0
			680	429	123	127	1			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P0CG47
B	-1	SER	-	expression tag	UNP P0CG47
B	8	PHE	LEU	engineered mutation	UNP P0CG47
B	9	ARG	THR	engineered mutation	UNP P0CG47
B	10	ASP	GLY	engineered mutation	UNP P0CG47
B	11	ARG	LYS	engineered mutation	UNP P0CG47
B	11a	LEU	-	insertion	UNP P0CG47
B	11b	ARG	-	insertion	UNP P0CG47
B	11c	ASN	-	insertion	UNP P0CG47
B	11d	LEU	-	insertion	UNP P0CG47
B	11e	LEU	-	insertion	UNP P0CG47
B	11f	PRO	-	insertion	UNP P0CG47
B	11g	GLN	-	insertion	UNP P0CG47
B	42	VAL	ARG	engineered mutation	UNP P0CG47
B	46	SER	ALA	engineered mutation	UNP P0CG47
B	47	ARG	GLY	engineered mutation	UNP P0CG47
B	49	ARG	GLN	engineered mutation	UNP P0CG47
B	68	ARG	HIS	engineered mutation	UNP P0CG47
B	72	VAL	ARG	engineered mutation	UNP P0CG47
B	73	PHE	LEU	engineered mutation	UNP P0CG47
B	74	GLY	ARG	engineered mutation	UNP P0CG47
B	75	ARG	GLY	engineered mutation	UNP P0CG47
B	76	ARG	GLY	engineered mutation	UNP P0CG47
A	-2	GLY	-	expression tag	UNP P0CG47
A	-1	SER	-	expression tag	UNP P0CG47
A	8	PHE	LEU	engineered mutation	UNP P0CG47
A	9	ARG	THR	engineered mutation	UNP P0CG47
A	10	ASP	GLY	engineered mutation	UNP P0CG47
A	11	ARG	LYS	engineered mutation	UNP P0CG47
A	11a	LEU	-	insertion	UNP P0CG47
A	11b	ARG	-	insertion	UNP P0CG47
A	11c	ASN	-	insertion	UNP P0CG47
A	11d	LEU	-	insertion	UNP P0CG47
A	11e	LEU	-	insertion	UNP P0CG47
A	11f	PRO	-	insertion	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11g	GLN	-	insertion	UNP P0CG47
A	42	VAL	ARG	engineered mutation	UNP P0CG47
A	46	SER	ALA	engineered mutation	UNP P0CG47
A	47	ARG	GLY	engineered mutation	UNP P0CG47
A	49	ARG	GLN	engineered mutation	UNP P0CG47
A	68	ARG	HIS	engineered mutation	UNP P0CG47
A	72	VAL	ARG	engineered mutation	UNP P0CG47
A	73	PHE	LEU	engineered mutation	UNP P0CG47
A	74	GLY	ARG	engineered mutation	UNP P0CG47
A	75	ARG	GLY	engineered mutation	UNP P0CG47
A	76	ARG	GLY	engineered mutation	UNP P0CG47

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total 4	O 4	0	0
4	E	1	Total 1	O 1	0	0
4	B	8	Total 8	O 8	0	0
4	A	14	Total 14	O 14	0	0
4	C	11	Total 11	O 11	0	0
4	F	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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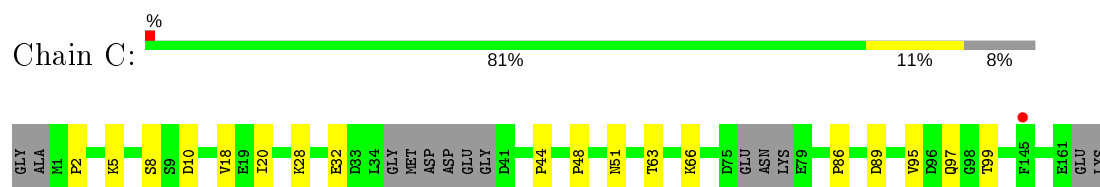 of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
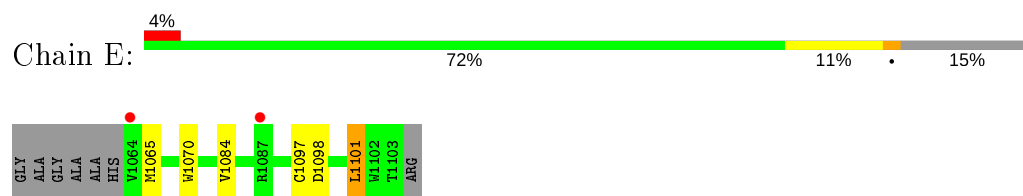
- Molecule 1: S-phase kinase-associated protein 1
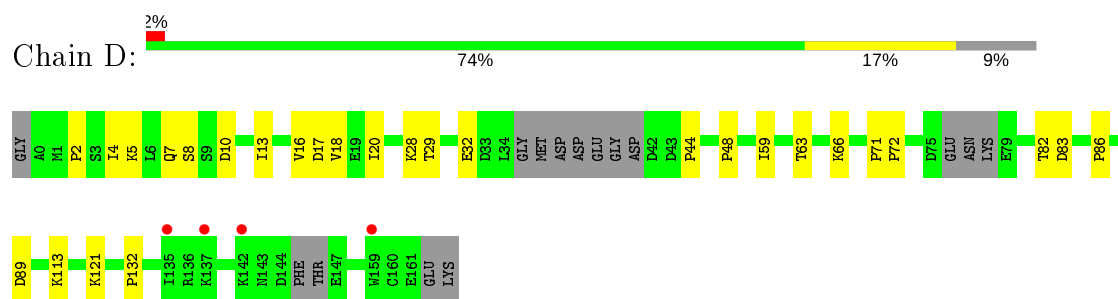
Chain D:

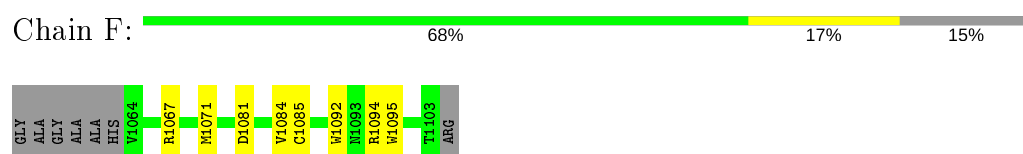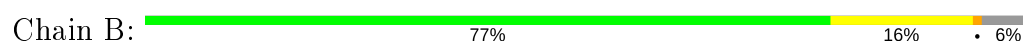- Molecule 1: S-phase kinase-associated protein 1

Chain C:

- Molecule 2: Lysine-specific demethylase 2B
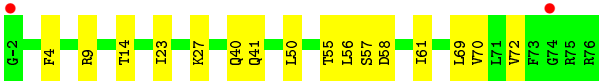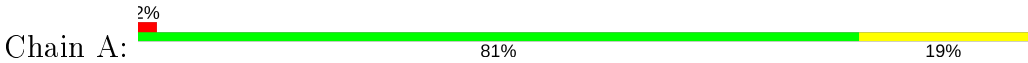
Chain E:

- Molecule 2: Lysine-specific demethylase 2B

Chain F:

- Molecule 3: Polyubiquitin-B

Chain B:

- Molecule 3: Polyubiquitin-B

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.36Å 81.79Å 128.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.66 47.46 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.46-2.66) 99.1 (47.46-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$<I/\sigma(I)>$ [1]	2.14 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.216 , 0.263 0.216 , 0.264	Depositor DCC
R_{free} test set	1070 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.6	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4111	wwPDB-VP
Average B, all atoms (Å^2)	69.0	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 44.36 % 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 1.5434e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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	C	0.32	0/1110	0.50	0/1521
1	D	0.32	0/1071	0.51	0/1468
2	E	0.27	0/318	0.54	0/437
2	F	0.29	0/340	0.48	0/464
3	A	0.37	0/688	0.63	0/929
3	B	0.38	0/620	0.62	1/842 (0.1%)
All	All	0.33	0/4147	0.55	1/5661 (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})
3	B	68	ARG	NE-CZ-NH1	-5.78	117.41	120.30

There are no chirality outliers.

There are no planarity outliers.

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	C	1089	0	1004	11	0
1	D	1054	0	953	20	0
2	E	307	0	245	3	0
2	F	329	0	290	6	0
3	A	680	0	690	10	0
3	B	612	0	613	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	0	0	0
4	B	8	0	0	0	0
4	C	11	0	0	0	0
4	D	4	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
All	All	4111	0	3795	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (55) 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:86:PRO:HG2	1:C:89:ASP:OD2	1.89	0.72
1:C:28:LYS:NZ	1:C:32:GLU:OE1	2.25	0.70
1:D:17:ASP:HB2	1:D:20:ILE:HD12	1.76	0.67
1:D:7:GLN:HG3	1:D:13:ILE:HD13	1.78	0.65
1:D:132:PRO:HD3	2:E:1084:VAL:HG13	1.77	0.65
1:D:4:ILE:HG23	1:D:16:VAL:HG23	1.83	0.59
1:D:28:LYS:NZ	1:D:32:GLU:OE2	2.37	0.58
3:A:23:ILE:HG12	3:A:50:LEU:HB3	1.87	0.56
1:D:59:ILE:O	1:D:63:THR:HG23	2.07	0.55
1:D:86:PRO:HG2	1:D:89:ASP:OD2	2.06	0.55
3:B:36:ILE:O	3:B:41:GLN:NE2	2.40	0.55
1:D:2:PRO:O	1:D:18:VAL:HG23	2.07	0.55
1:C:5:LYS:HB3	1:C:44:PRO:HB3	1.89	0.54
3:A:56:LEU:HB3	3:A:61:ILE:HB	1.89	0.54
1:D:82:THR:HG23	1:D:121:LYS:HB3	1.90	0.53
3:B:23:ILE:HG12	3:B:50:LEU:HB3	1.90	0.53
2:F:1067:ARG:HB2	2:F:1095:TRP:CZ2	2.44	0.53
1:D:48:PRO:HG3	3:B:70:VAL:HG21	1.92	0.52
1:D:20:ILE:HD13	1:D:63:THR:HG22	1.92	0.50
1:C:10:ASP:OD1	1:C:51:ASN:HB2	2.11	0.50
2:E:1065:MET:HE3	2:E:1070:TRP:HE1	1.77	0.50
3:B:43:LEU:HD23	3:B:69:LEU:HB2	1.94	0.49
3:A:70:VAL:HG21	1:C:48:PRO:HG3	1.95	0.49
2:F:1067:ARG:O	2:F:1071:MET:HG2	2.13	0.48
2:E:1098:ASP:HB3	2:E:1101:LEU:HD12	1.94	0.48
1:D:71:PRO:HB2	1:D:113:LYS:HD3	1.96	0.48
1:D:72:PRO:O	1:D:113:LYS:NZ	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1067:ARG:HB2	2:F:1095:TRP:CE2	2.49	0.48
3:A:4:PHE:CE2	3:A:14:THR:HG22	2.49	0.47
3:A:9:ARG:HG2	3:A:9:ARG:HH11	1.79	0.47
3:B:45:PHE:HB2	3:B:67:LEU:HD22	1.95	0.47
1:C:95:VAL:CG1	1:C:99:THR:HB	2.44	0.47
3:A:55:THR:HG22	3:A:58:ASP:CG	2.34	0.46
1:D:8:SER:OG	1:D:10:ASP:OD1	2.15	0.45
3:A:55:THR:HG22	3:A:58:ASP:OD2	2.16	0.45
1:C:95:VAL:HG13	1:C:99:THR:HB	1.98	0.45
3:B:37:PRO:HG2	3:B:40:GLN:OE1	2.17	0.45
3:B:9:ARG:HH11	3:B:9:ARG:HG2	1.81	0.45
3:A:40:GLN:HB3	3:A:72:VAL:O	2.18	0.44
1:D:29:THR:HG22	3:B:68:ARG:HH12	1.83	0.44
1:D:2:PRO:HB2	1:D:18:VAL:HG21	1.99	0.44
1:D:28:LYS:O	1:D:32:GLU:HG3	2.18	0.43
2:F:1085:CYS:HB3	2:F:1092:TRP:CE3	2.53	0.43
1:D:83:ASP:OD2	1:D:83:ASP:N	2.43	0.43
1:C:28:LYS:O	1:C:32:GLU:HG3	2.19	0.43
3:A:23:ILE:O	3:A:27:LYS:HG3	2.20	0.42
1:C:20:ILE:CD1	1:C:63:THR:HA	2.50	0.42
3:B:1:MET:HG3	3:B:17:VAL:HG23	2.02	0.41
1:C:2:PRO:O	1:C:18:VAL:HG23	2.18	0.41
2:F:1081:ASP:O	2:F:1084:VAL:HG22	2.20	0.41
3:A:41:GLN:HB3	3:A:69:LEU:HD11	2.02	0.41
1:C:66:LYS:HB3	1:C:66:LYS:HE3	1.78	0.41
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.91	0.41
1:D:5:LYS:HB3	1:D:44:PRO:HB3	2.03	0.41
2:F:1067:ARG:HD3	2:F:1095:TRP:CD1	2.57	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	C	146/165 (88%)	139 (95%)	7 (5%)	0	100	100
1	D	142/165 (86%)	136 (96%)	6 (4%)	0	100	100
2	E	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
2	F	38/47 (81%)	38 (100%)	0	0	100	100
3	A	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
3	B	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
All	All	527/596 (88%)	508 (96%)	19 (4%)	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	C	105/150 (70%)	103 (98%)	2 (2%)	57	74
1	D	100/150 (67%)	99 (99%)	1 (1%)	76	86
2	E	27/41 (66%)	25 (93%)	2 (7%)	13	21
2	F	33/41 (80%)	32 (97%)	1 (3%)	41	59
3	A	74/80 (92%)	73 (99%)	1 (1%)	67	81
3	B	61/80 (76%)	61 (100%)	0	100	100
All	All	400/542 (74%)	393 (98%)	7 (2%)	59	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	66	LYS
2	E	1097	CYS
2	E	1101	LEU
3	A	57	SER
1	C	8	SER
1	C	97	GLN
2	F	1094	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	7	GLN
1	D	97	GLN
3	A	41	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	C	152/165 (92%)	-0.22	1 (0%)	87	87	30, 55, 109, 136	0
1	D	150/165 (90%)	-0.09	4 (2%)	54	50	35, 68, 151, 183	0
2	E	40/47 (85%)	0.49	2 (5%)	28	25	59, 104, 141, 151	0
2	F	40/47 (85%)	0.11	0	100	100	52, 75, 97, 122	0
3	A	86/86 (100%)	-0.14	2 (2%)	60	56	30, 52, 82, 141	0
3	B	81/86 (94%)	-0.26	0	100	100	42, 68, 106, 115	0
All	All	549/596 (92%)	-0.10	9 (1%)	72	69	30, 66, 125, 183	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1064	VAL	3.3
2	E	1087	ARG	3.3
3	A	-2	GLY	3.0
1	C	145	PHE	2.9
1	D	137	LYS	2.7
1	D	159	TRP	2.5
3	A	74	GLY	2.2
1	D	142	LYS	2.1
1	D	135	ILE	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.