



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2016 – 04:30 PM EDT

PDB ID : 5ECJ
Title : Crystal structure of monobody Mb(S4) bound to Prdm14 in complex with Mtgr1
Authors : Gupta, A.; Koide, S.
Deposited on : 2015-10-20
Resolution : 3.05 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
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) : rb-20027257

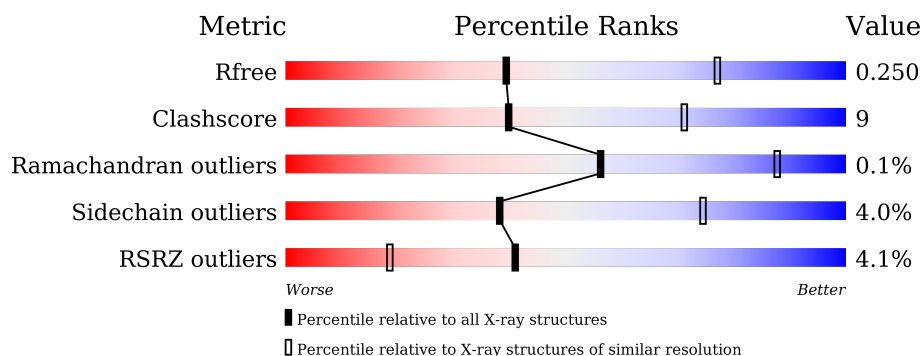
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 $\leq 5\%$. 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	309	<div> <div>2%</div> <div>64%</div> <div>20%</div> <div>•</div> <div>15%</div> </div>
1	B	309	<div> <div>6%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>15%</div> </div>
2	E	95	<div> <div>79%</div> <div>16%</div> <div>••</div> </div>
2	F	95	<div> <div>7%</div> <div>68%</div> <div>27%</div> <div>••</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5480 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 PR domain zinc finger protein 14,Protein CBFA2T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2045	1306	358	370	11			
1	B	263	Total	C	N	O	S	0	0	0
			2045	1306	354	374	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP E9Q3T6
A	0	SER	-	expression tag	UNP E9Q3T6
A	191	GLY	-	linker	UNP E9Q3T6
A	192	SER	-	linker	UNP E9Q3T6
A	193	SER	-	linker	UNP E9Q3T6
A	194	GLY	-	linker	UNP E9Q3T6
A	195	SER	-	linker	UNP E9Q3T6
A	196	SER	-	linker	UNP E9Q3T6
A	197	GLY	-	linker	UNP E9Q3T6
A	198	SER	-	linker	UNP E9Q3T6
A	301	LYS	HIS	engineered mutation	UNP O70374
B	-1	GLY	-	expression tag	UNP E9Q3T6
B	0	SER	-	expression tag	UNP E9Q3T6
B	191	GLY	-	linker	UNP E9Q3T6
B	192	SER	-	linker	UNP E9Q3T6
B	193	SER	-	linker	UNP E9Q3T6
B	194	GLY	-	linker	UNP E9Q3T6
B	195	SER	-	linker	UNP E9Q3T6
B	196	SER	-	linker	UNP E9Q3T6
B	197	GLY	-	linker	UNP E9Q3T6
B	198	SER	-	linker	UNP E9Q3T6
B	301	LYS	HIS	engineered mutation	UNP O70374

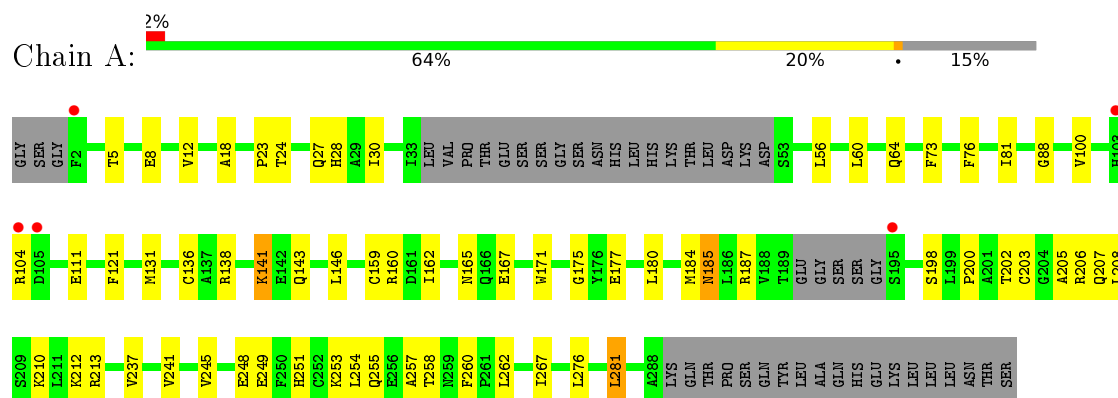
- Molecule 2 is a protein called Monobody Mb(S4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	93	Total 688	C 448	N 105	O 135	0	0	0
2	E	93	Total 702	C 459	N 105	O 138	0	0	0

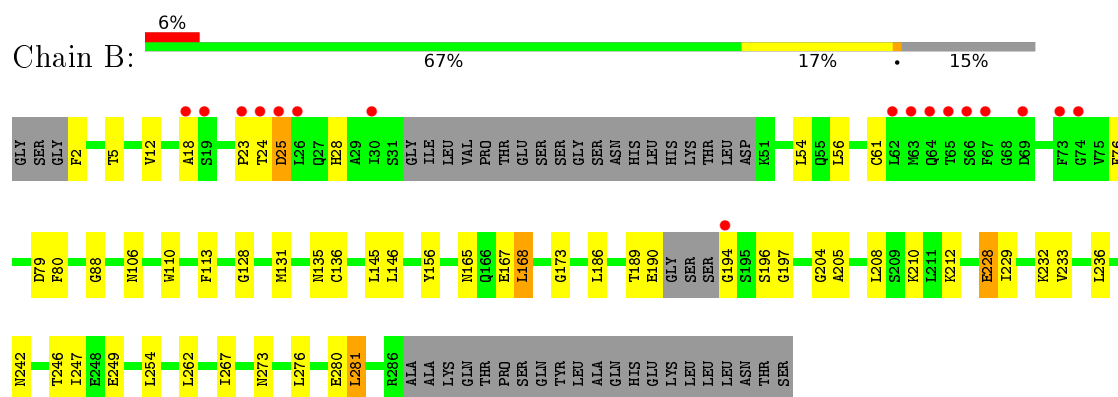
3 Residue-property plots [i](#)

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.

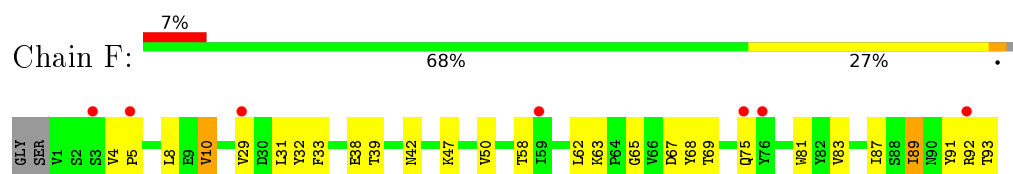
- Molecule 1: PR domain zinc finger protein 14,Protein CBFA2T2



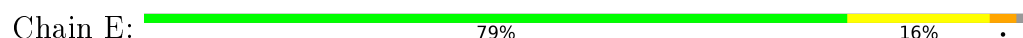
- Molecule 1: PR domain zinc finger protein 14,Protein CBFA2T2



- Molecule 2: Monobody Mb(S4)



- Molecule 2: Monobody Mb(S4)





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.81Å 106.81Å 180.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.76 – 3.05 47.77 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.76-3.05) 100.0 (47.77-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.189 , 0.250 0.190 , 0.250	Depositor DCC
R_{free} test set	1724 reflections (8.38%)	DCC
Wilson B-factor (Å ²)	106.1	Xtrriage
Anisotropy	0.328	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5480	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 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	A	0.33	0/2093	0.54	0/2835
1	B	0.29	0/2093	0.50	0/2837
2	E	0.36	0/723	0.60	1/998 (0.1%)
2	F	0.31	0/708	0.53	0/978
All	All	0.32	0/5617	0.53	1/7648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	18	LEU	CA-CB-CG	6.40	130.03	115.30

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	2045	0	1963	36	0
1	B	2045	0	1950	36	0
2	E	702	0	686	8	0
2	F	688	0	666	17	0
All	All	5480	0	5265	95	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 (95) 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:B:189:THR:HG1	1:B:194:GLY:N	1.77	0.83
2:E:35:THR:HB	2:E:71:THR:HG22	1.62	0.82
1:B:23:PRO:HB3	1:B:165:ASN:HB3	1.67	0.76
1:B:205:ALA:O	1:B:210:LYS:NZ	2.18	0.76
1:A:184:MET:O	1:A:200:PRO:HD3	1.86	0.75
1:A:254:LEU:HD12	1:A:262:LEU:HD21	1.69	0.75
1:B:25:ASP:N	1:B:25:ASP:OD1	2.20	0.73
1:B:186:LEU:HD22	1:B:196:SER:HA	1.73	0.71
2:E:14:THR:HG23	2:E:16:THR:H	1.56	0.70
2:E:38:GLU:OE1	2:E:63:LYS:NZ	2.26	0.69
1:B:189:THR:OG1	1:B:194:GLY:N	2.26	0.68
1:B:113:PHE:CD1	1:B:197:GLY:HA3	2.28	0.68
1:A:205:ALA:O	1:A:210:LYS:HE2	1.93	0.68
1:B:18:ALA:HA	1:B:24:THR:HG22	1.77	0.66
1:A:251:HIS:HB2	1:A:267:ILE:HD11	1.78	0.64
1:A:23:PRO:HB3	1:A:165:ASN:HB3	1.81	0.62
2:E:67:ASP:HB3	2:E:92:ARG:HB3	1.83	0.60
1:B:28:HIS:CD2	1:B:135:ASN:HB3	2.36	0.60
2:F:67:ASP:HB3	2:F:92:ARG:HG3	1.84	0.59
1:A:81:ILE:HB	1:A:162:ILE:HB	1.85	0.59
1:A:206:ARG:O	1:A:210:LYS:HG3	2.03	0.58
2:E:39:THR:HG22	2:E:69:THR:OG1	2.04	0.57
1:A:12:VAL:HG12	1:A:212:LYS:HE2	1.86	0.57
2:F:38:GLU:OE2	2:F:63:LYS:NZ	2.36	0.56
1:B:88:GLY:HA2	1:B:131:MET:HE1	1.88	0.56
1:A:88:GLY:HA2	1:A:131:MET:SD	2.46	0.56
2:F:65:GLY:N	2:F:93:THR:OG1	2.34	0.55
1:A:104:ARG:O	1:A:207:GLN:NE2	2.38	0.55
1:A:18:ALA:HA	1:A:24:THR:HG22	1.89	0.55
1:A:12:VAL:HG21	1:A:281:LEU:HG	1.87	0.55
1:A:258:THR:HG23	1:A:260:PHE:HB3	1.89	0.54
1:B:110:TRP:HE1	1:B:156:TYR:HH	1.55	0.54
1:B:146:LEU:HD22	1:B:173:GLY:HA2	1.89	0.53
2:F:8:LEU:H	2:F:87:ILE:HD13	1.72	0.53
1:B:106:ASN:ND2	1:B:204:GLY:O	2.31	0.53
1:A:27:GLN:HB2	1:A:138:ARG:NH1	2.24	0.53
1:A:185:ASN:ND2	1:A:198:SER:O	2.41	0.53
1:A:255:GLN:HE21	1:A:262:LEU:H	1.57	0.52
1:B:145:LEU:HD11	1:B:168:LEU:HD13	1.90	0.52
2:F:33:PHE:CD1	2:F:47:LYS:HE3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:VAL:HG11	2:F:91:TYR:CD1	2.46	0.51
1:A:56:LEU:HD21	1:A:60:LEU:O	2.12	0.50
1:A:208:LEU:HD13	1:A:276:LEU:HB3	1.92	0.50
2:F:39:THR:HG22	2:F:69:THR:OG1	2.12	0.49
1:A:251:HIS:CB	1:A:267:ILE:HD11	2.42	0.49
1:A:248:GLU:H	1:A:248:GLU:CD	2.17	0.48
1:A:237:VAL:O	1:A:241:VAL:HG23	2.13	0.48
1:A:251:HIS:CG	1:A:267:ILE:HD11	2.49	0.48
1:B:56:LEU:HD21	1:B:61:CYS:HA	1.96	0.47
2:F:29:VAL:HG11	2:F:32:TYR:OH	2.14	0.47
1:B:54:LEU:HA	1:B:128:GLY:O	2.14	0.47
2:F:31:LEU:HB2	2:F:75:GLN:HG2	1.97	0.47
1:B:229:ILE:O	1:B:233:VAL:HG23	2.14	0.47
1:B:113:PHE:CE1	1:B:197:GLY:HA3	2.49	0.46
1:A:76:PHE:CE2	1:A:167:GLU:HB2	2.51	0.46
1:B:208:LEU:HD13	1:B:276:LEU:HB3	1.98	0.46
2:F:32:TYR:HB2	2:F:50:VAL:HG12	1.98	0.46
1:B:228:GLU:O	1:B:232:LYS:HD3	2.16	0.46
1:A:28:HIS:ND1	1:A:136:CYS:HB2	2.32	0.45
1:B:273:ASN:O	1:B:276:LEU:HB2	2.17	0.45
1:A:177:GLU:HG3	1:B:228:GLU:OE2	2.17	0.45
1:A:251:HIS:CD2	1:A:267:ILE:HD11	2.52	0.44
2:E:34:ILE:HD11	2:E:50:VAL:HG22	1.99	0.44
1:B:212:LYS:NZ	1:B:280:GLU:OE2	2.31	0.44
1:A:141:LYS:HE3	1:A:141:LYS:HA	1.98	0.44
1:A:175:GLY:HA2	1:A:187:ARG:HB3	2.00	0.44
1:A:64:GLN:HB2	1:A:73:PHE:CE1	2.52	0.44
1:B:28:HIS:CG	1:B:135:ASN:HB3	2.53	0.44
1:B:12:VAL:HG21	1:B:281:LEU:HG	1.99	0.44
2:F:29:VAL:HG11	2:F:32:TYR:CZ	2.53	0.44
1:B:2:PHE:HB2	1:B:242:ASN:O	2.17	0.44
1:B:247:ILE:HG22	1:B:267:ILE:HG23	2.00	0.44
2:F:4:VAL:HG22	2:F:5:PRO:O	2.18	0.44
1:B:25:ASP:HB3	1:B:76:PHE:HZ	1.83	0.43
1:A:5:THR:HG23	1:A:8:GLU:H	1.83	0.43
2:E:14:THR:HG22	2:E:17:SER:OG	2.18	0.43
1:B:76:PHE:CE2	1:B:167:GLU:HB2	2.53	0.43
1:B:246:THR:HG23	1:B:249:GLU:H	1.82	0.42
1:B:12:VAL:HG12	1:B:212:LYS:HE2	2.01	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.84	0.42
2:F:8:LEU:H	2:F:87:ILE:CD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD23	1:B:262:LEU:HD11	2.02	0.42
2:F:81:TRP:N	1:B:80:PHE:O	2.49	0.42
1:A:253:LYS:NZ	1:A:257:ALA:HB2	2.34	0.41
2:F:89:ILE:HA	2:F:89:ILE:HD13	1.75	0.41
1:A:143:GLN:O	1:A:160:ARG:NH2	2.53	0.41
1:A:245:VAL:HG22	1:A:249:GLU:OE2	2.20	0.41
1:A:111:GLU:HG3	1:A:121:PHE:CE2	2.56	0.41
1:B:189:THR:HB	1:B:190:GLU:H	1.74	0.41
1:B:28:HIS:ND1	1:B:136:CYS:HB2	2.35	0.41
2:F:62:LEU:HB3	2:F:68:TYR:CE1	2.55	0.41
2:F:42:ASN:N	2:F:42:ASN:OD1	2.50	0.41
1:A:146:LEU:HG	1:A:159:CYS:HB3	2.03	0.41
2:E:89:ILE:HA	2:E:89:ILE:HD12	1.96	0.40
1:A:171:TRP:NE1	1:A:213:ARG:HG2	2.36	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	257/309 (83%)	244 (95%)	12 (5%)	1 (0%)	39	74
1	B	257/309 (83%)	248 (96%)	9 (4%)	0	100	100
2	E	91/95 (96%)	87 (96%)	4 (4%)	0	100	100
2	F	91/95 (96%)	88 (97%)	3 (3%)	0	100	100
All	All	696/808 (86%)	667 (96%)	28 (4%)	1 (0%)	56	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ILE

5.3.2 Protein sidechains ⓘ

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	215/267 (80%)	208 (97%)	7 (3%)	45	79
1	B	216/267 (81%)	210 (97%)	6 (3%)	51	82
2	E	77/80 (96%)	71 (92%)	6 (8%)	16	47
2	F	74/80 (92%)	70 (95%)	4 (5%)	27	62
All	All	582/694 (84%)	559 (96%)	23 (4%)	38	74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	VAL
1	A	141	LYS
1	A	180	LEU
1	A	185	ASN
1	A	202	THR
1	A	203	CYS
1	A	281	LEU
2	F	10	VAL
2	F	58	THR
2	F	83	VAL
2	F	89	ILE
1	B	5	THR
1	B	25	ASP
1	B	79	ASP
1	B	168	LEU
1	B	228	GLU
1	B	281	LEU
2	E	18	LEU
2	E	35	THR
2	E	49	THR
2	E	71	THR
2	E	83	VAL
2	E	93	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates 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	263/309 (85%)	-0.05	5 (1%) 70 45	68, 113, 165, 226	0
1	B	263/309 (85%)	0.09	17 (6%) 22 8	82, 119, 181, 228	0
2	E	93/95 (97%)	-0.18	0 100 100	76, 103, 133, 184	0
2	F	93/95 (97%)	0.26	7 (7%) 17 6	91, 128, 175, 201	0
All	All	712/808 (88%)	0.02	29 (4%) 41 18	68, 115, 175, 228	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	LEU	5.2
1	B	25	ASP	4.1
1	B	69	ASP	4.1
1	B	73	PHE	3.8
1	B	63	MET	3.8
1	B	67	PHE	3.6
2	F	3	SER	3.6
1	B	65	THR	3.4
2	F	76	TYR	3.4
1	B	26	LEU	3.2
2	F	29	VAL	3.1
1	B	64	GLN	2.9
1	B	66	SER	2.9
1	B	23	PRO	2.8
1	B	74	GLY	2.8
1	A	103	HIS	2.7
2	F	75	GLN	2.5
2	F	5	PRO	2.5
1	A	105	ASP	2.5
1	B	19	SER	2.5
1	B	18	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	30	ILE	2.2
1	B	194	GLY	2.2
1	A	2	PHE	2.2
1	B	24	THR	2.1
1	A	195	SER	2.1
2	F	92	ARG	2.1
2	F	59	ILE	2.1
1	A	104	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 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.