



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:45 pm GMT

PDB ID : 7AHZ
Title : Crystal structure of Western clawed frog MDM2 RING domain homodimer bound to UbcH5B-Ub
Authors : Magnussen, H.M.; Huang, D.T.
Deposited on : 2020-09-25
Resolution : 1.82 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

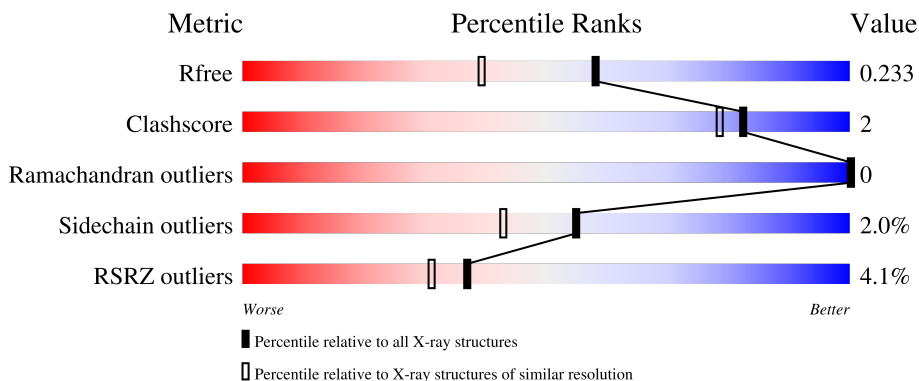
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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)

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	AAA	71	 69% 8% 21%
1	DDD	71	 69% 10% 21%
1	GGG	71	 75% 8% 15%
1	JJJ	71	 66% 14% 20%
2	BBB	147	 97%

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Mol	Chain	Length	Quality of chain
2	EEE	147	<p>3% 92% 6% ..</p>
2	HHH	147	<p>% 95% . ..</p>
2	KKK	147	<p>5% 95% 5% .</p>
3	CCC	81	<p>% 94% . .</p>
3	FFF	81	<p>% 89% 5% . 5%</p>
3	III	81	<p>93% . 5%</p>
3	LLL	81	<p>32% 89% 6% 5%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18139 atoms, of which 8971 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 E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	56	Total 890	C 273	H 457	N 79	O 72	S 9	27	0	0
1	DDD	56	Total 905	C 276	H 466	N 82	O 72	S 9	26	0	0
1	GGG	60	Total 952	C 291	H 489	N 85	O 78	S 9	29	0	0
1	JJJ	57	Total 900	C 276	H 460	N 82	O 73	S 9	27	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	412	GLY	-	expression tag	UNP Q6P3Q9
AAA	413	SER	-	expression tag	UNP Q6P3Q9
DDD	412	GLY	-	expression tag	UNP Q6P3Q9
DDD	413	SER	-	expression tag	UNP Q6P3Q9
GGG	412	GLY	-	expression tag	UNP Q6P3Q9
GGG	413	SER	-	expression tag	UNP Q6P3Q9
JJJ	412	GLY	-	expression tag	UNP Q6P3Q9
JJJ	413	SER	-	expression tag	UNP Q6P3Q9

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2D 2 (UBC4/5 homolog, yeast).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	BBB	146	Total 2360	C 759	H 1177	N 205	O 213	S 6	60	1	0
2	EEE	146	Total 2319	C 749	H 1156	N 199	O 209	S 6	63	0	0
2	HHH	146	Total 2374	C 764	H 1186	N 209	O 209	S 6	65	2	0
2	KKK	146	Total 2266	C 735	H 1132	N 194	O 199	S 6	70	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	22	ARG	SER	engineered mutation	UNP Q28EY6
BBB	85	LYS	CYS	engineered mutation	UNP Q28EY6
EEE	22	ARG	SER	engineered mutation	UNP Q28EY6
EEE	85	LYS	CYS	engineered mutation	UNP Q28EY6
HHH	22	ARG	SER	engineered mutation	UNP Q28EY6
HHH	85	LYS	CYS	engineered mutation	UNP Q28EY6
KKK	22	ARG	SER	engineered mutation	UNP Q28EY6
KKK	85	LYS	CYS	engineered mutation	UNP Q28EY6

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	CCC	78	1241	381	634	107	118	1	31	0	0
3	FFF	77	1229	378	630	106	114	1	32	0	0
3	III	77	1240	381	633	106	119	1	30	0	0
3	LLL	77	1098	345	551	97	104	1	39	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-4	GLY	-	expression tag	UNP P0CG47
CCC	-3	SER	-	expression tag	UNP P0CG47
CCC	0	SER	-	insertion	UNP P0CG47
FFF	-4	GLY	-	expression tag	UNP P0CG47
FFF	-3	SER	-	expression tag	UNP P0CG47
FFF	0	SER	-	insertion	UNP P0CG47
III	-4	GLY	-	expression tag	UNP P0CG47
III	-3	SER	-	expression tag	UNP P0CG47
III	0	SER	-	insertion	UNP P0CG47
LLL	-4	GLY	-	expression tag	UNP P0CG47
LLL	-3	SER	-	expression tag	UNP P0CG47
LLL	0	SER	-	insertion	UNP P0CG47

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total 2	Zn 2	0	0
4	DDD	2	Total 2	Zn 2	0	0
4	GGG	2	Total 2	Zn 2	0	0
4	JJJ	2	Total 2	Zn 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HHH	1	Total 1	Cl 1	0	0

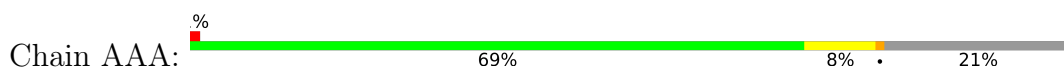
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	23	Total 23	O 23	0	0
6	BBB	51	Total 51	O 51	0	0
6	CCC	37	Total 37	O 37	0	0
6	DDD	18	Total 18	O 18	0	0
6	EEE	40	Total 40	O 40	0	0
6	FFF	30	Total 30	O 30	0	0
6	GGG	13	Total 13	O 13	0	0
6	HHH	51	Total 51	O 51	0	0
6	III	44	Total 44	O 44	0	0
6	JJJ	16	Total 16	O 16	0	0
6	KKK	28	Total 28	O 28	0	0
6	LLL	5	Total 5	O 5	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.

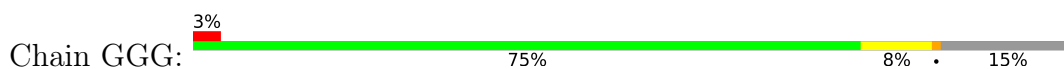
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



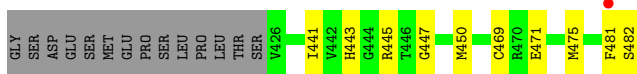
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



- Molecule 1: E3 ubiquitin-protein ligase Mdm2



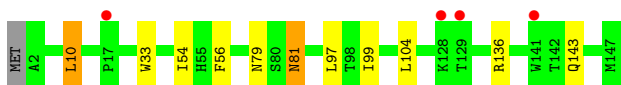
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



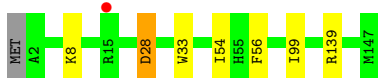
- Molecule 2: Ubiquitin-conjugating enzyme E2D 2 (UBC4/5 homolog, yeast)



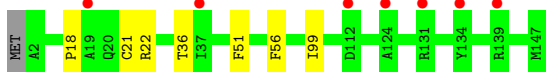
- Molecule 2: Ubiquitin-conjugating enzyme E2D 2 (UBC4/5 homolog, yeast)



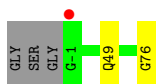
- Molecule 2: Ubiquitin-conjugating enzyme E2D 2 (UBC4/5 homolog, yeast)



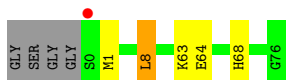
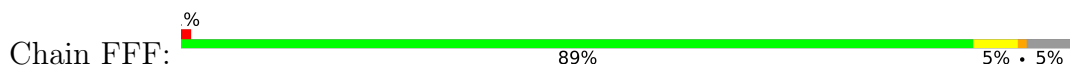
- Molecule 2: Ubiquitin-conjugating enzyme E2D 2 (UBC4/5 homolog, yeast)



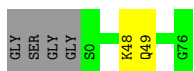
- Molecule 3: Polyubiquitin-B



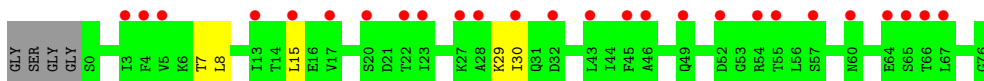
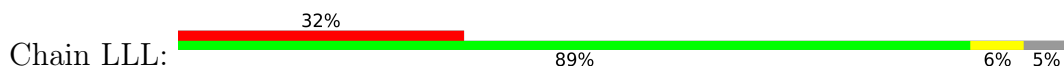
- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.03Å 153.15Å 82.08Å 90.00° 107.01° 90.00°	Depositor
Resolution (Å)	52.62 – 1.82 52.62 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.0 (52.62-1.82) 98.0 (52.62-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.82Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.195 , 0.231 0.203 , 0.233	Depositor DCC
R_{free} test set	5516 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18139	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN

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	AAA	0.68	0/442	0.83	0/594
1	DDD	0.64	0/448	0.82	0/601
1	GGG	0.70	0/472	0.82	0/636
1	JJJ	0.66	0/449	0.81	0/604
2	BBB	0.61	0/1222	0.77	0/1664
2	EEE	0.64	0/1199	0.76	0/1635
2	HHH	0.65	0/1232	0.77	0/1678
2	KKK	0.63	0/1173	0.75	0/1604
3	CCC	0.64	0/613	0.80	0/824
3	FFF	0.66	0/605	0.83	0/814
3	III	0.64	0/613	0.82	0/824
3	LLL	0.69	0/553	0.84	0/751
All	All	0.65	0/9021	0.79	0/12229

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	433	457	446	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	439	466	457	3	0
1	GGG	463	489	478	5	0
1	JJJ	440	460	448	7	0
2	BBB	1183	1177	1171	4	0
2	EEE	1163	1156	1143	9	0
2	HHH	1188	1186	1177	6	0
2	KKK	1134	1132	1104	5	0
3	CCC	607	634	633	1	0
3	FFF	599	630	625	4	0
3	III	607	633	634	1	0
3	LLL	547	551	521	3	0
4	AAA	2	0	0	0	0
4	DDD	2	0	0	0	0
4	GGG	2	0	0	0	0
4	JJJ	2	0	0	0	0
5	HHH	1	0	0	0	0
6	AAA	23	0	0	1	0
6	BBB	51	0	0	0	0
6	CCC	37	0	0	0	0
6	DDD	18	0	0	0	0
6	EEE	40	0	0	1	0
6	FFF	30	0	0	0	0
6	GGG	13	0	0	0	0
6	HHH	51	0	0	1	0
6	III	44	0	0	1	0
6	JJJ	16	0	0	0	0
6	KKK	28	0	0	0	0
6	LLL	5	0	0	0	0
All	All	9168	8971	8837	44	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 2.

All (44) 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:DDD:453:TYR:CE2	1:DDD:457:LYS:HD2	2.21	0.75
2:EEE:81:ASN:C	2:EEE:81:ASN:HD22	2.00	0.64
2:EEE:79:ASN:OD1	2:EEE:81:ASN:ND2	2.32	0.62
1:JJJ:475:MET:HE3	1:JJJ:475:MET:HA	1.90	0.53
2:KKK:36:THR:HG22	2:KKK:51:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HHH:8:LYS:NZ	6:HHH:302:HOH:O	2.45	0.49
1:GGG:458:LYS:HE3	1:GGG:462:ARG:NH2	2.28	0.48
2:EEE:136:ARG:HG3	6:EEE:232:HOH:O	2.13	0.48
1:GGG:425:SER:HB2	1:JJJ:481:PHE:CE2	2.49	0.48
3:LLL:7:THR:HG22	3:LLL:8:LEU:H	1.78	0.48
1:AAA:427:GLU:HG2	6:AAA:617:HOH:O	2.14	0.47
3:FFF:1:MET:HB2	3:FFF:63:LYS:HD3	1.97	0.47
2:KKK:18:PRO:O	2:KKK:22:ARG:NH1	2.48	0.46
2:HHH:56:PHE:CZ	2:HHH:99:ILE:HG13	2.51	0.46
1:AAA:456:ALA:HB1	1:AAA:476:ILE:HD12	1.98	0.45
2:EEE:56:PHE:CZ	2:EEE:99:ILE:HG13	2.52	0.45
2:BBB:56:PHE:CZ	2:BBB:99:ILE:HG13	2.53	0.44
2:EEE:33:TRP:HB2	2:EEE:54:ILE:HB	1.99	0.44
2:HHH:33:TRP:HB2	2:HHH:54:ILE:HB	2.00	0.44
1:JJJ:441:ILE:O	1:JJJ:447:GLY:HA2	2.17	0.44
2:EEE:97:LEU:HD23	3:FFF:8:LEU:HD21	2.00	0.43
1:GGG:450:MET:HG2	1:JJJ:482:SER:HB2	2.00	0.43
1:GGG:475:MET:SD	1:JJJ:445:ARG:NH1	2.80	0.43
3:FFF:63:LYS:HG3	3:FFF:64:GLU:HG3	2.00	0.43
2:BBB:22:ARG:HA	2:BBB:22:ARG:HD3	1.92	0.42
1:GGG:425:SER:CB	1:JJJ:481:PHE:CE2	3.02	0.42
2:HHH:28:ASP:N	2:HHH:28:ASP:OD1	2.52	0.42
3:III:48:LYS:NZ	6:III:101:HOH:O	2.44	0.42
3:LLL:15:LEU:HD22	3:LLL:29:LYS:HB3	2.01	0.42
2:BBB:56:PHE:HZ	2:BBB:99:ILE:HG13	1.85	0.42
2:EEE:56:PHE:HZ	2:EEE:99:ILE:HG13	1.85	0.41
2:EEE:10:LEU:HD23	2:EEE:10:LEU:HA	1.89	0.41
1:JJJ:469:CYS:SG	1:JJJ:471:GLU:HG2	2.60	0.41
2:KKK:99:ILE:HD13	2:KKK:99:ILE:HA	1.93	0.41
1:AAA:441:ILE:O	1:AAA:447:GLY:HA2	2.20	0.41
2:EEE:104:LEU:HD21	3:FFF:68:HIS:CB	2.50	0.41
1:DDD:441:ILE:O	1:DDD:447:GLY:HA2	2.21	0.41
2:KKK:18:PRO:HB2	2:KKK:21:CYS:O	2.21	0.41
3:LLL:15:LEU:HD11	3:LLL:30:ILE:HG13	2.02	0.41
1:DDD:453:TYR:CZ	1:DDD:457:LYS:HD2	2.55	0.40
2:HHH:99:ILE:HD13	2:HHH:99:ILE:HA	1.91	0.40
2:BBB:117:ASP:O	3:CCC:76:GLY:HA2	2.22	0.40
2:KKK:56:PHE:CZ	2:KKK:99:ILE:HG13	2.57	0.40
2:HHH:56:PHE:HZ	2:HHH:99:ILE:HG13	1.86	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	AAA	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	DDD	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	GGG	58/71 (82%)	55 (95%)	3 (5%)	0	100	100
1	JJJ	55/71 (78%)	52 (94%)	3 (6%)	0	100	100
2	BBB	145/147 (99%)	143 (99%)	2 (1%)	0	100	100
2	EEE	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
2	HHH	146/147 (99%)	144 (99%)	2 (1%)	0	100	100
2	KKK	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
3	CCC	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
3	FFF	75/81 (93%)	75 (100%)	0	0	100	100
3	III	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
3	LLL	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
All	All	1102/1196 (92%)	1076 (98%)	26 (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	AAA	50/65 (77%)	47 (94%)	3 (6%)	19	6
1	DDD	51/65 (78%)	48 (94%)	3 (6%)	19	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GGG	54/65 (83%)	51 (94%)	3 (6%)	21	8
1	JJJ	50/65 (77%)	48 (96%)	2 (4%)	31	16
2	BBB	131/131 (100%)	131 (100%)	0	100	100
2	EEE	127/131 (97%)	124 (98%)	3 (2%)	49	35
2	HHH	131/131 (100%)	129 (98%)	2 (2%)	65	55
2	KKK	120/131 (92%)	120 (100%)	0	100	100
3	CCC	68/70 (97%)	67 (98%)	1 (2%)	65	55
3	FFF	66/70 (94%)	65 (98%)	1 (2%)	65	55
3	III	69/70 (99%)	68 (99%)	1 (1%)	67	58
3	LLL	52/70 (74%)	52 (100%)	0	100	100
All	All	969/1064 (91%)	950 (98%)	19 (2%)	55	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	427	GLU
1	AAA	443	HIS
1	AAA	450	MET
3	CCC	49	GLN
1	DDD	443	HIS
1	DDD	450	MET
1	DDD	482	SER
2	EEE	10	LEU
2	EEE	81	ASN
2	EEE	143	GLN
3	FFF	8	LEU
1	GGG	443	HIS
1	GGG	450	MET
1	GGG	482	SER
2	HHH	28	ASP
2	HHH	139	ARG
3	III	49	GLN
1	JJJ	443	HIS
1	JJJ	450	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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 [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	AAA	56/71 (78%)	0.46	1 (1%) 68 64	31, 38, 58, 74	0
1	DDD	56/71 (78%)	0.30	0 100 100	34, 41, 60, 70	0
1	GGG	60/71 (84%)	0.31	2 (3%) 46 40	33, 47, 76, 91	0
1	JJJ	57/71 (80%)	0.40	1 (1%) 68 64	34, 44, 62, 86	0
2	BBB	146/147 (99%)	0.15	2 (1%) 75 72	36, 52, 76, 84	0
2	EEE	146/147 (99%)	0.40	4 (2%) 54 49	38, 55, 83, 101	0
2	HHH	146/147 (99%)	0.11	1 (0%) 87 86	32, 46, 69, 99	0
2	KKK	146/147 (99%)	0.43	7 (4%) 30 25	37, 59, 88, 100	0
3	CCC	78/81 (96%)	0.05	1 (1%) 77 74	34, 45, 67, 78	0
3	FFF	77/81 (95%)	0.12	1 (1%) 77 74	37, 48, 69, 83	0
3	III	77/81 (95%)	0.03	0 100 100	30, 42, 58, 68	1 (1%)
3	LLL	77/81 (95%)	1.47	26 (33%) 0 0	53, 71, 91, 97	0
All	All	1122/1196 (93%)	0.33	46 (4%) 37 31	30, 50, 80, 101	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	LLL	17	VAL	5.1
3	LLL	23	ILE	4.9
3	LLL	20	SER	4.2
3	LLL	45	PHE	4.1
1	GGG	423	LEU	3.9
3	LLL	65	SER	3.8
3	LLL	55	THR	3.5
2	KKK	19	ALA	3.4
2	EEE	128	LYS	3.3
3	LLL	15	LEU	3.3
3	LLL	27	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	LLL	28	ALA	3.2
3	LLL	3	ILE	3.1
3	LLL	30	ILE	2.9
2	KKK	124	ALA	2.9
3	LLL	54	ARG	2.9
3	CCC	-1	GLY	2.8
3	LLL	52	ASP	2.8
3	LLL	46	ALA	2.8
2	KKK	134	TYR	2.7
3	LLL	13	ILE	2.7
3	LLL	22	THR	2.7
3	LLL	43	LEU	2.5
3	LLL	64	GLU	2.5
3	LLL	32	ASP	2.5
2	EEE	129	THR	2.5
3	LLL	49	GLN	2.4
3	LLL	67	LEU	2.3
2	KKK	131	ARG	2.3
2	KKK	112	ASP	2.3
2	KKK	37	ILE	2.3
2	KKK	139	ARG	2.3
3	LLL	66	THR	2.2
3	LLL	60	ASN	2.2
2	EEE	17	PRO	2.2
2	BBB	147	MET	2.2
1	JJJ	481	PHE	2.2
2	EEE	141	TRP	2.1
3	LLL	4	PHE	2.1
3	FFF	0	SER	2.1
1	AAA	481	PHE	2.1
3	LLL	5	VAL	2.1
2	HHH	15	ARG	2.1
2	BBB	132	GLU	2.1
3	LLL	57	SER	2.1
1	GGG	455	CYS	2.0

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 [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, 95th 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	ZN	AAA	501	1/1	0.99	0.17	35,35,35,35	0
4	ZN	JJJ	501	1/1	0.99	0.17	37,37,37,37	0
4	ZN	JJJ	502	1/1	0.99	0.17	43,43,43,43	0
5	CL	HHH	201	1/1	0.99	0.14	39,39,39,39	0
4	ZN	GGG	501	1/1	1.00	0.11	49,49,49,49	0
4	ZN	GGG	502	1/1	1.00	0.17	35,35,35,35	0
4	ZN	AAA	502	1/1	1.00	0.18	33,33,33,33	0
4	ZN	DDD	501	1/1	1.00	0.16	40,40,40,40	0
4	ZN	DDD	502	1/1	1.00	0.18	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.