



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2017 – 11:07 PM EDT

PDB ID : 5MW9
Title : Complex between the Leucine Zipper (LZ) and Centrosomin-motif 2 (CM2) domains of Drosophila melanogaster Centrosomin (Cnn) - L535E mutant form
Authors : Feng, Z.; Johnson, S.; Raff, J.W.; Lea, S.M.
Deposited on : 2017-01-18
Resolution : 2.20 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029077

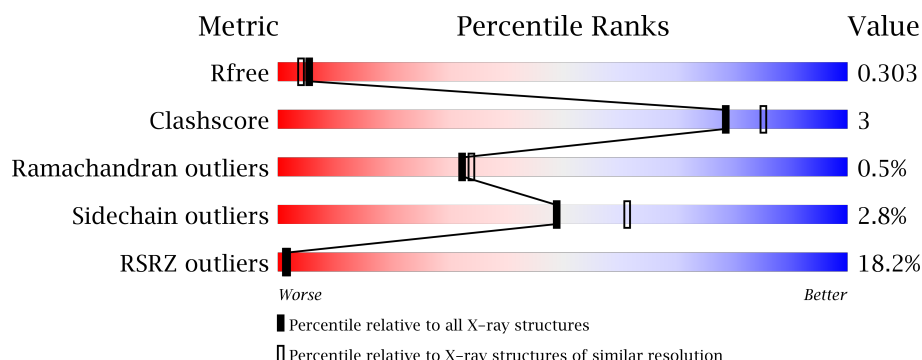
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



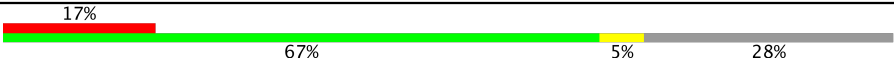
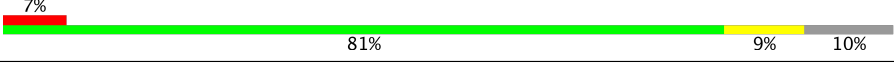
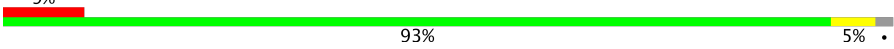
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	70	<div> <div>14%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	70	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>11%</div> </div> </div>
1	E	70	<div> <div>21%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>13%</div> </div> </div>
1	F	70	<div> <div>29%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div> </div>
2	C	58	<div> <div>24%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	58	
2	G	58	
2	H	58	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3729 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 Centrosomin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			546	333	109	101	3			
1	B	62	Total	C	N	O	S	0	0	0
			504	310	100	92	2			
1	E	61	Total	C	N	O	S	0	0	0
			507	312	102	91	2			
1	F	64	Total	C	N	O	S	0	0	0
			532	326	106	97	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1079	GLY	-	expression tag	UNP P54623
A	1080	GLY	-	expression tag	UNP P54623
A	1081	SER	-	expression tag	UNP P54623
B	1079	GLY	-	expression tag	UNP P54623
B	1080	GLY	-	expression tag	UNP P54623
B	1081	SER	-	expression tag	UNP P54623
E	1079	GLY	-	expression tag	UNP P54623
E	1080	GLY	-	expression tag	UNP P54623
E	1081	SER	-	expression tag	UNP P54623
F	1079	GLY	-	expression tag	UNP P54623
F	1080	GLY	-	expression tag	UNP P54623
F	1081	SER	-	expression tag	UNP P54623

- Molecule 2 is a protein called Centrosomin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	46	Total	C	N	O	S	0	0	0
			366	228	65	71	2			
2	D	42	Total	C	N	O	S	0	0	0
			334	207	58	67	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	57	Total	C	N	O	S	0	0	0
			449	277	79	90	3			
2	G	52	Total	C	N	O	S	0	0	0
			412	254	73	83	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	487	GLY	-	expression tag	UNP P54623
C	488	PRO	-	expression tag	UNP P54623
C	489	MET	-	expression tag	UNP P54623
C	522	ILE	VAL	conflict	UNP P54623
C	535	GLU	LEU	engineered mutation	UNP P54623
D	487	GLY	-	expression tag	UNP P54623
D	488	PRO	-	expression tag	UNP P54623
D	489	MET	-	expression tag	UNP P54623
D	522	ILE	VAL	conflict	UNP P54623
D	535	GLU	LEU	engineered mutation	UNP P54623
H	487	GLY	-	expression tag	UNP P54623
H	488	PRO	-	expression tag	UNP P54623
H	489	MET	-	expression tag	UNP P54623
H	522	ILE	VAL	conflict	UNP P54623
H	535	GLU	LEU	engineered mutation	UNP P54623
G	487	GLY	-	expression tag	UNP P54623
G	488	PRO	-	expression tag	UNP P54623
G	489	MET	-	expression tag	UNP P54623
G	522	ILE	VAL	conflict	UNP P54623
G	535	GLU	LEU	engineered mutation	UNP P54623

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		

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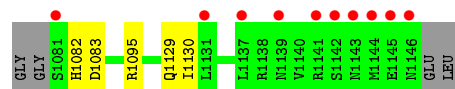
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	25	Total 25	O 25	0	0
4	H	7	Total 7	O 7	0	0
4	G	13	Total 13	O 13	0	0

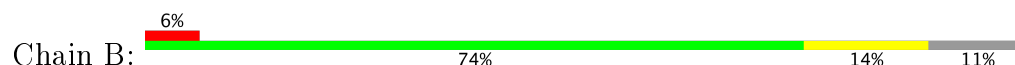
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

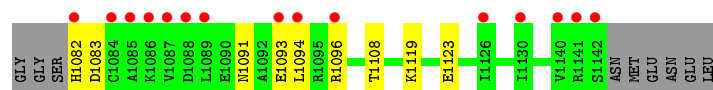
• Molecule 1: Centrosomin



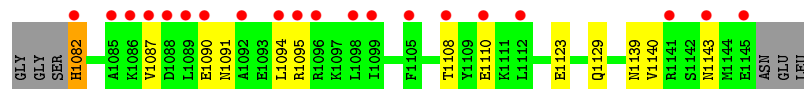
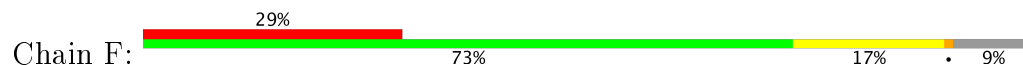
• Molecule 1: Centrosomin



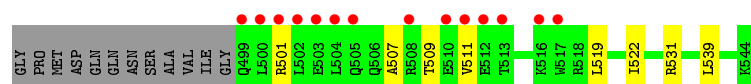
• Molecule 1: Centrosomin



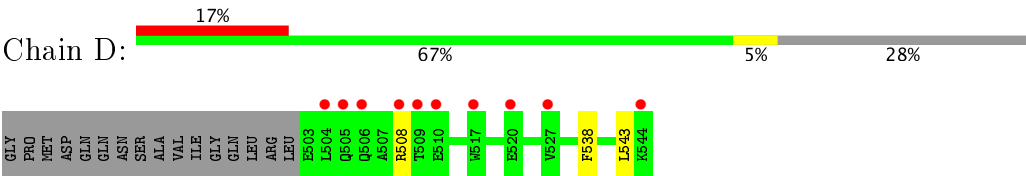
• Molecule 1: Centrosomin



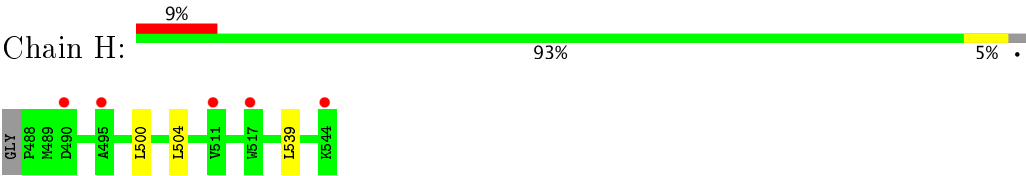
• Molecule 2: Centrosomin



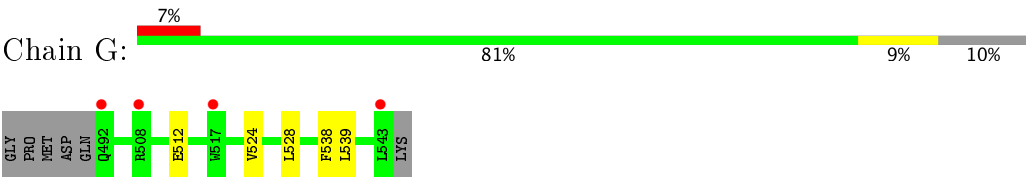
• Molecule 2: Centrosomin



● Molecule 2: Centrosomin



● Molecule 2: Centrosomin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	275.79 Å 43.00 Å 48.35 Å 90.00° 96.57° 90.00°	Depositor
Resolution (Å)	31.35 – 2.20 31.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (31.35-2.20) 96.0 (31.35-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.258 , 0.302 0.260 , 0.303	Depositor DCC
R_{free} test set	1240 reflections (4.45%)	DCC
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3729	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.64% 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: 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	A	0.24	0/549	0.35	0/730
1	B	0.24	0/507	0.35	0/674
1	E	0.23	0/510	0.32	0/678
1	F	0.23	0/535	0.36	0/711
2	C	0.23	0/368	0.35	0/496
2	D	0.22	0/336	0.33	0/453
2	G	0.23	0/414	0.33	0/559
2	H	0.23	0/452	0.35	0/609
All	All	0.23	0/3671	0.34	0/4910

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	A	546	0	567	3	0
1	B	504	0	528	7	0
1	E	507	0	535	4	0
1	F	532	0	556	9	0
2	C	366	0	367	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	334	0	330	2	0
2	G	412	0	411	5	0
2	H	449	0	447	2	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
4	A	32	0	0	0	0
4	B	25	0	0	0	0
4	G	13	0	0	1	0
4	H	7	0	0	0	0
All	All	3729	0	3741	24	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 3.

All (24) 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:1136:VAL:HG21	2:C:531:ARG:HG2	1.82	0.61
1:F:1082:HIS:HD1	1:F:1087:VAL:HG21	1.67	0.59
1:A:1095:ARG:NH2	1:B:1090:GLU:OE2	2.34	0.57
1:E:1094:LEU:HD13	1:F:1095:ARG:HB3	1.88	0.56
2:H:539:LEU:HD21	2:G:539:LEU:HD21	1.89	0.55
1:F:1140:VAL:HG21	2:G:528:LEU:HD21	1.90	0.54
1:B:1133:THR:HA	1:B:1136:VAL:HG22	1.92	0.52
1:E:1091:ASN:ND2	1:F:1091:ASN:OD1	2.37	0.51
1:E:1119:LYS:NZ	1:E:1123:GLU:OE2	2.46	0.49
1:B:1083:ASP:HB3	1:B:1086:LYS:HB3	1.96	0.48
1:B:1127:LYS:HG2	2:D:543:LEU:HD21	1.95	0.47
1:F:1140:VAL:HG22	2:G:524:VAL:HG13	1.97	0.46
2:C:507:ALA:HA	2:C:511:VAL:HG23	1.99	0.44
1:F:1139:ASN:O	1:F:1143:ASN:ND2	2.28	0.44
2:G:512:GLU:HG3	4:G:605:HOH:O	2.18	0.43
2:C:519:LEU:HA	2:C:522:ILE:HG22	1.99	0.43
1:A:1129:GLN:HG3	2:D:538:PHE:CD2	2.54	0.43
1:A:1130:ILE:HD11	2:C:539:LEU:HB3	2.01	0.42
1:E:1108:THR:HG22	1:F:1108:THR:HG22	2.01	0.42
1:F:1090:GLU:O	1:F:1094:LEU:HB2	2.19	0.42
1:B:1134:HIS:NE2	1:B:1138:ARG:HD2	2.34	0.42
1:B:1083:ASP:O	1:B:1087:VAL:HG23	2.22	0.40
2:H:500:LEU:O	2:H:504:LEU:HB2	2.20	0.40
1:F:1129:GLN:HG3	2:G:538:PHE:CD2	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	A	64/70 (91%)	62 (97%)	1 (2%)	1 (2%)	11	8
1	B	60/70 (86%)	60 (100%)	0	0	100	100
1	E	59/70 (84%)	58 (98%)	0	1 (2%)	11	7
1	F	62/70 (89%)	61 (98%)	1 (2%)	0	100	100
2	C	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
2	D	40/58 (69%)	40 (100%)	0	0	100	100
2	G	50/58 (86%)	50 (100%)	0	0	100	100
2	H	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
All	All	434/512 (85%)	428 (99%)	4 (1%)	2 (0%)	32	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1083	ASP
1	E	1083	ASP

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	60/62 (97%)	59 (98%)	1 (2%)	66	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	54/62 (87%)	53 (98%)	1 (2%)	62	76
1	E	55/62 (89%)	52 (94%)	3 (6%)	25	29
1	F	58/62 (94%)	55 (95%)	3 (5%)	27	32
2	C	40/51 (78%)	38 (95%)	2 (5%)	28	34
2	D	37/51 (72%)	36 (97%)	1 (3%)	50	62
2	G	46/51 (90%)	46 (100%)	0	100	100
2	H	50/51 (98%)	50 (100%)	0	100	100
All	All	400/452 (88%)	389 (97%)	11 (3%)	49	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1082	HIS
1	B	1082	HIS
2	C	501	ARG
2	C	509	THR
1	E	1082	HIS
1	E	1093	GLU
1	E	1096	ARG
1	F	1082	HIS
1	F	1110	GLU
1	F	1123	GLU
2	D	508	ARG

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

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

Of 2 ligands modelled in this entry, 2 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

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, 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	66/70 (94%)	0.97	10 (15%)	2 2	35, 58, 154, 188	0
1	B	62/70 (88%)	0.72	4 (6%)	20 18	39, 58, 106, 154	0
1	E	61/70 (87%)	1.48	15 (24%)	1 1	76, 100, 174, 193	0
1	F	64/70 (91%)	1.84	20 (31%)	0 0	63, 108, 168, 175	0
2	C	46/58 (79%)	1.89	14 (30%)	0 0	60, 123, 184, 233	0
2	D	42/58 (72%)	1.47	10 (23%)	1 1	59, 103, 143, 155	0
2	G	52/58 (89%)	0.75	4 (7%)	14 13	52, 70, 100, 135	0
2	H	57/58 (98%)	0.70	5 (8%)	11 9	44, 66, 114, 140	0
All	All	450/512 (87%)	1.21	82 (18%)	1 1	35, 83, 164, 233	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1089	LEU	8.4
2	D	504	LEU	8.3
2	D	544	LYS	8.2
2	C	499	GLN	7.8
1	E	1141	ARG	7.7
1	E	1085	ALA	7.5
2	C	517	TRP	7.0
1	B	1138	ARG	6.6
1	A	1081	SER	6.5
1	F	1085	ALA	6.5
1	A	1146	ASN	6.4
2	C	501	ARG	6.4
2	C	508	ARG	6.2
2	C	502	LEU	6.1
2	C	510	GLU	5.7
1	F	1094	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	1087	VAL	5.6
1	A	1142	SER	5.3
2	C	500	LEU	5.2
1	F	1145	GLU	5.0
1	E	1142	SER	4.8
1	F	1099	ILE	4.8
2	H	544	LYS	4.7
1	F	1098	LEU	4.6
1	E	1084	CYS	4.4
1	A	1145	GLU	4.3
1	F	1092	ALA	4.1
2	D	508	ARG	4.1
1	E	1086	LYS	4.1
1	F	1086	LYS	4.0
2	C	505	GLN	4.0
2	C	504	LEU	3.9
1	A	1141	ARG	3.8
2	G	517	TRP	3.7
1	F	1112	LEU	3.7
1	F	1095	ARG	3.5
1	F	1096	ARG	3.5
1	E	1094	LEU	3.5
1	F	1110	GLU	3.5
1	F	1082	HIS	3.5
1	E	1126	ILE	3.5
2	C	513	THR	3.4
2	D	505	GLN	3.4
2	D	527	VAL	3.4
1	F	1089	LEU	3.3
1	E	1082	HIS	3.1
2	D	517	TRP	3.0
1	A	1144	MET	2.9
2	D	520	GLU	2.9
1	F	1088	ASP	2.8
2	G	492	GLN	2.8
2	H	517	TRP	2.8
1	E	1096	ARG	2.7
1	F	1108	THR	2.6
2	D	506	GLN	2.6
2	C	503	GLU	2.6
2	C	512	GLU	2.6
1	B	1139	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	1141	ARG	2.5
1	A	1143	ASN	2.4
1	E	1087	VAL	2.3
2	C	511	VAL	2.3
2	H	490	ASP	2.3
1	B	1128	ASN	2.3
1	E	1093	GLU	2.2
1	A	1131	LEU	2.2
1	F	1105	PHE	2.2
1	A	1137	LEU	2.2
1	B	1137	LEU	2.2
1	F	1143	ASN	2.2
2	G	543	LEU	2.2
1	E	1140	VAL	2.1
2	H	511	VAL	2.1
1	A	1139	ASN	2.1
1	E	1088	ASP	2.1
2	H	495	ALA	2.1
2	G	508	ARG	2.0
2	C	516	LYS	2.0
2	D	510	GLU	2.0
1	E	1130	ILE	2.0
2	D	509	THR	2.0
1	F	1090	GLU	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	1201	1/1	0.98	0.10	-	67,67,67,67	0
3	ZN	F	1201	1/1	0.56	0.07	-	330,330,330,330	0

6.5 Other polymers [i](#)

There are no such residues in this entry.