



wwPDB X-ray Structure Validation Summary Report

Sep 12, 2023 – 05:56 PM EDT


PDB ID : 4OCM
Title : Crystal Structure of the Rpn8-Rpn11 MPN domain heterodimer, crystal form Ib
Authors : Pathare, G.R.; Bracher, A.
Deposited on : 2014-01-09
Resolution : 1.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.35.1
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) : 2.35.1

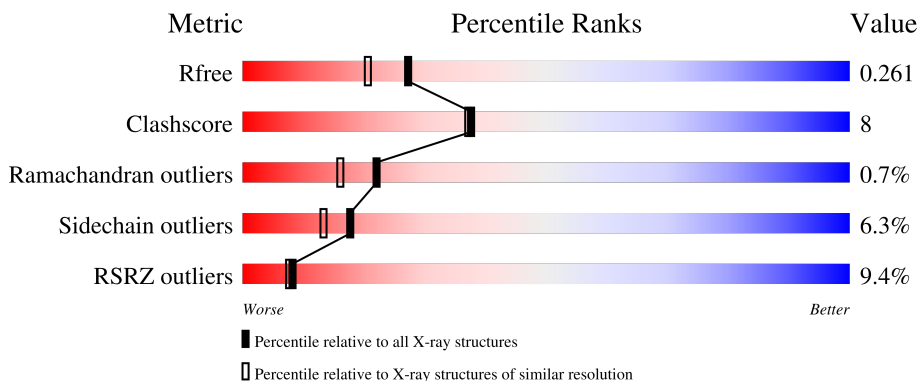
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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.



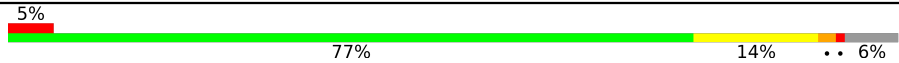
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	A	187	 7% 68% 19% • 12%
1	D	187	 7% 65% 20% •• 11%
2	B	220	 7% 64% 14% • 20%
2	E	220	 12% 71% 10% • 16%
3	C	133	 9% 78% 14% • 6%

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Mol	Chain	Length	Quality of chain
3	F	133	 <p>5% 77% 14% •• 6%</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7521 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 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1277	814	215	243	5	0	0	0
1	D	166	1299	828	218	248	5	0	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q08723
A	0	HIS	-	cloning artifact	UNP Q08723
A	177	GLY	-	SEE REMARK 999	UNP Q08723
A	178	SER	-	SEE REMARK 999	UNP Q08723
A	179	GLY	-	SEE REMARK 999	UNP Q08723
A	180	GLY	-	SEE REMARK 999	UNP Q08723
A	181	SER	-	SEE REMARK 999	UNP Q08723
A	182	GLY	-	SEE REMARK 999	UNP Q08723
A	183	GLY	-	SEE REMARK 999	UNP Q08723
A	184	SER	-	SEE REMARK 999	UNP Q08723
A	185	GLY	-	SEE REMARK 999	UNP Q08723
D	-1	GLY	-	cloning artifact	UNP Q08723
D	0	HIS	-	cloning artifact	UNP Q08723
D	177	GLY	-	SEE REMARK 999	UNP Q08723
D	178	SER	-	SEE REMARK 999	UNP Q08723
D	179	GLY	-	SEE REMARK 999	UNP Q08723
D	180	GLY	-	SEE REMARK 999	UNP Q08723
D	181	SER	-	SEE REMARK 999	UNP Q08723
D	182	GLY	-	SEE REMARK 999	UNP Q08723
D	183	GLY	-	SEE REMARK 999	UNP Q08723
D	184	SER	-	SEE REMARK 999	UNP Q08723
D	185	GLY	-	SEE REMARK 999	UNP Q08723

- Molecule 2 is a protein called 26S proteasome regulatory subunit RPN11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	177	1376	879	236	249	12	0	0	0
2	E	184	1420	903	242	263	12	0	1	0

- Molecule 3 is a protein called Nb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	125	981	615	175	187	4	0	1	0
3	F	125	969	609	173	183	4	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	E	1	1	1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	D	1	1	1	0	0

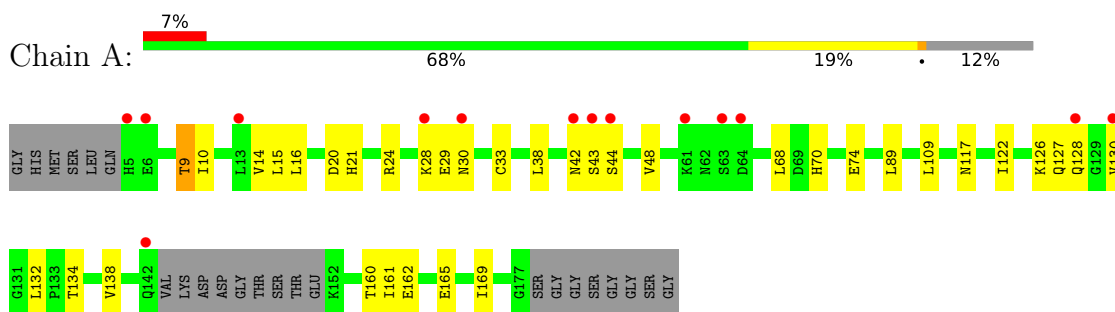
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	23	23	23	0	0
6	B	31	31	31	0	0
6	C	23	23	23	0	0
6	D	33	33	33	0	0
6	E	43	43	43	0	0
6	F	43	43	43	0	0

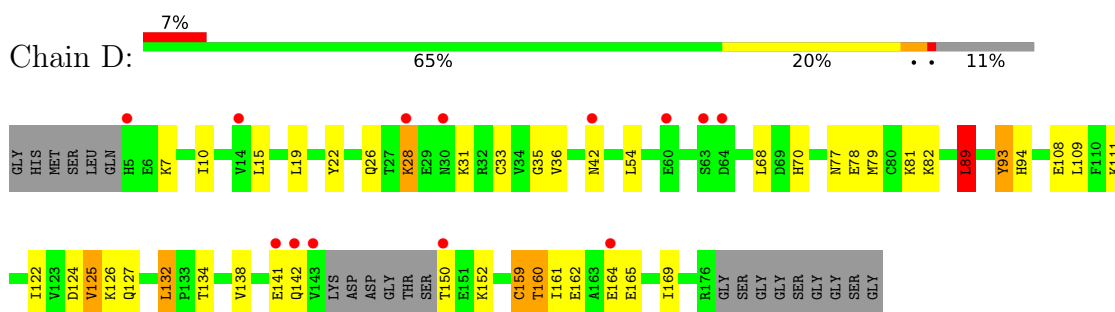
3 Residue-property plots [i](#)

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.

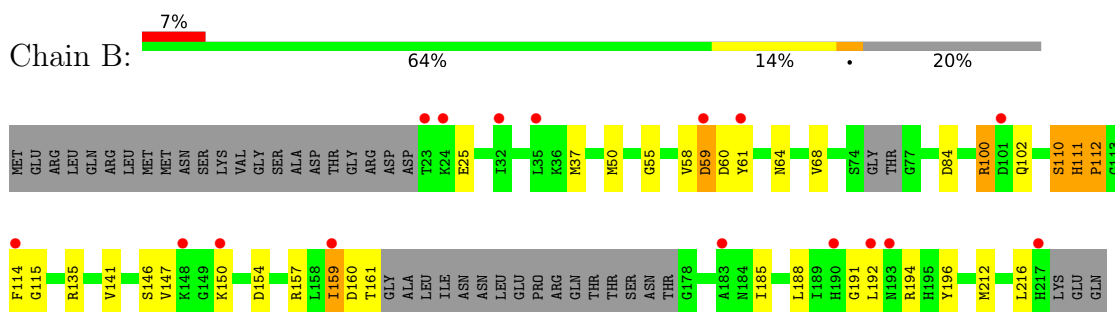
- Molecule 1: 26S proteasome regulatory subunit RPN8



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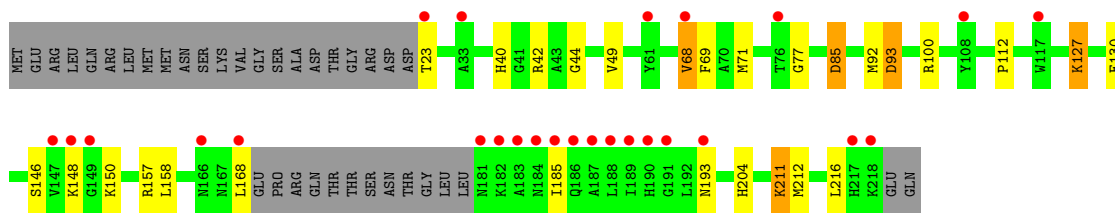


- Molecule 2: 26S proteasome regulatory subunit RPN11

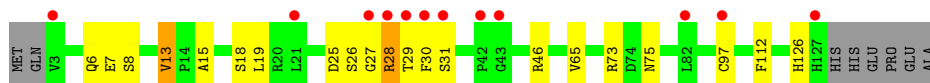
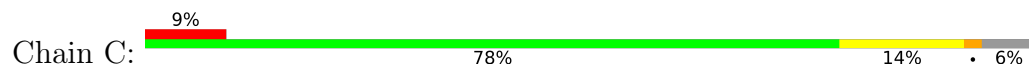


- Molecule 2: 26S proteasome regulatory subunit RPN11

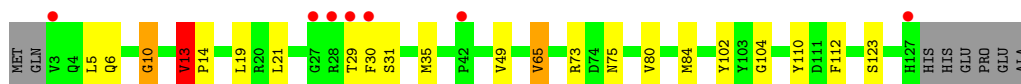
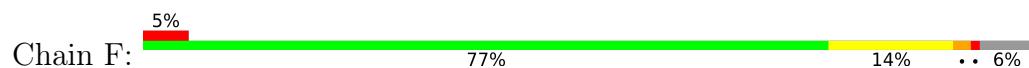




- Molecule 3: Nb1



- Molecule 3: Nb1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 44.97Å 200.04Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.99 29.71 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-1.99) 96.5 (29.71-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.262 0.214 , 0.261	Depositor DCC
R_{free} test set	3757 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7521	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.20 % 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 1.5806e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, K

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	0.86	0/1301	0.91	5/1766 (0.3%)
1	D	1.16	6/1322 (0.5%)	1.00	2/1793 (0.1%)
2	B	0.93	0/1400	0.90	2/1889 (0.1%)
2	E	1.10	2/1445 (0.1%)	1.02	5/1957 (0.3%)
3	C	0.88	0/1007	0.91	0/1365
3	F	1.26	2/995 (0.2%)	1.01	2/1349 (0.1%)
All	All	1.04	10/7470 (0.1%)	0.96	16/10119 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	CYS	CB-SG	-7.79	1.69	1.82
2	E	130	GLU	CG-CD	6.66	1.61	1.51
1	D	93	TYR	CD2-CE2	6.44	1.49	1.39
1	D	125	VAL	CB-CG1	-5.88	1.40	1.52
3	F	49	VAL	CB-CG1	5.87	1.65	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	92	MET	CG-SD-CE	-8.27	86.97	100.20
3	F	65	VAL	CG1-CB-CG2	7.26	122.51	110.90
1	A	24	ARG	NE-CZ-NH1	-7.19	116.71	120.30
2	E	68	VAL	CA-CB-CG1	6.65	120.88	110.90
2	E	68	VAL	CG1-CB-CG2	6.43	121.18	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	GLN	Peptide
2	B	110	SER	Peptide

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	1277	0	1247	17	0
1	D	1299	0	1270	34	0
2	B	1376	0	1385	29	0
2	E	1420	0	1403	13	0
3	C	981	0	917	12	0
3	F	969	0	908	15	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	0	0	0
6	B	31	0	0	1	0
6	C	23	0	0	0	0
6	D	33	0	0	4	0
6	E	43	0	0	1	0
6	F	43	0	0	0	0
All	All	7521	0	7130	111	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 8.

The worst 5 of 111 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:D:70:HIS:HE1	1:D:109:LEU:HD21	1.11	1.14
1:D:70:HIS:CE1	1:D:109:LEU:HD21	1.95	1.01
3:C:75[B]:ASN:H	3:C:75[B]:ASN:HD22	1.23	0.84
1:A:9:THR:HG23	1:A:162:GLU:HB3	1.65	0.79
3:C:75[B]:ASN:H	3:C:75[B]:ASN:ND2	1.81	0.79

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	160/187 (86%)	153 (96%)	7 (4%)	0	100	100
1	D	163/187 (87%)	157 (96%)	6 (4%)	0	100	100
2	B	171/220 (78%)	164 (96%)	4 (2%)	3 (2%)	8	3
2	E	181/220 (82%)	171 (94%)	8 (4%)	2 (1%)	14	8
3	C	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
3	F	123/133 (92%)	118 (96%)	4 (3%)	1 (1%)	19	13
All	All	922/1080 (85%)	884 (96%)	32 (4%)	6 (1%)	22	16

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	ASP
3	F	10	GLY
2	E	112	PRO
2	B	58	VAL
2	E	77	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	137/162 (85%)	127 (93%)	10 (7%)	14	9
1	D	139/162 (86%)	132 (95%)	7 (5%)	24	20
2	B	151/191 (79%)	146 (97%)	5 (3%)	38	37
2	E	154/191 (81%)	144 (94%)	10 (6%)	17	12
3	C	102/109 (94%)	92 (90%)	10 (10%)	8	4
3	F	100/109 (92%)	93 (93%)	7 (7%)	15	10
All	All	783/924 (85%)	734 (94%)	49 (6%)	18	13

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	89	LEU
2	E	93	ASP
1	D	126	LYS
2	E	23	THR
2	E	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	ASN
1	D	70	HIS
3	F	75	ASN
2	E	186	GLN
2	E	204	HIS

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 3 ligands modelled in this entry, 3 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	A	164/187 (87%)	0.61	14 (8%) 10 10	27, 45, 71, 87	0
1	D	166/187 (88%)	0.48	13 (7%) 13 12	14, 36, 62, 83	0
2	B	177/220 (80%)	0.49	16 (9%) 9 8	24, 40, 68, 73	0
2	E	184/220 (83%)	0.86	26 (14%) 2 2	15, 33, 87, 134	0
3	C	125/133 (93%)	0.61	12 (9%) 8 7	24, 40, 64, 91	0
3	F	125/133 (93%)	0.30	7 (5%) 24 23	16, 30, 56, 76	0
All	All	941/1080 (87%)	0.57	88 (9%) 8 8	14, 38, 69, 134	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	185	ILE	15.4
1	D	143	VAL	9.4
2	E	183	ALA	8.5
2	E	181	ASN	7.1
3	C	28	ARG	6.7

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 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
5	K	D	301	1/1	0.94	0.15	68,68,68,68	0
4	ZN	B	401	1/1	0.97	0.07	77,77,77,77	0
4	ZN	E	401	1/1	0.98	0.04	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.