



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:55 pm GMT

PDB ID : 4C8F
Title : mouse ZNRF3 ectodomain crystal form IV
Authors : Zebisch, M.; Jones, E.Y.
Deposited on : 2013-09-30
Resolution : 2.69 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 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

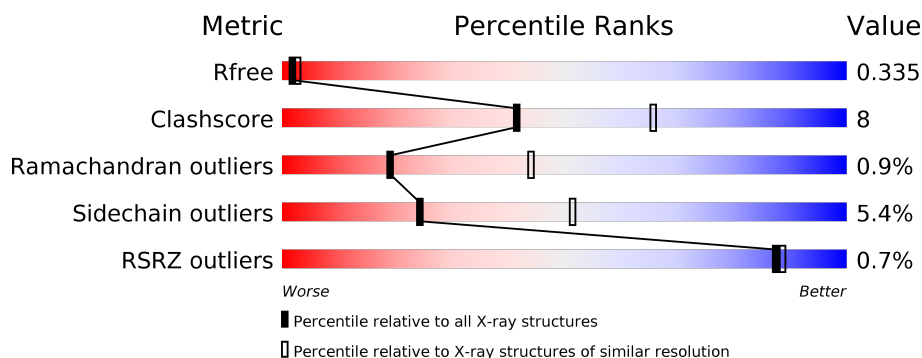
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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	165	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>16%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	165	<div> <div>58%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>
1	C	165	<div> <div>%</div> <div>68%</div> <div>16%</div> <div>16%</div> </div>
1	D	165	<div> <div>59%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4174 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 E3 UBIQUITIN-PROTEIN LIGASE ZNR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1044	660	183	197	4			
1	B	136	Total	C	N	O	S	0	0	0
			1032	651	182	195	4			
1	C	139	Total	C	N	O	S	0	0	0
			1054	665	187	198	4			
1	D	137	Total	C	N	O	S	0	0	0
			1044	660	183	197	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLU	-	expression tag	UNP Q5SSZ7
A	51	THR	-	expression tag	UNP Q5SSZ7
A	52	GLY	-	expression tag	UNP Q5SSZ7
A	206	GLY	-	expression tag	UNP Q5SSZ7
A	207	THR	-	expression tag	UNP Q5SSZ7
A	208	LYS	-	expression tag	UNP Q5SSZ7
A	209	HIS	-	expression tag	UNP Q5SSZ7
A	210	HIS	-	expression tag	UNP Q5SSZ7
A	211	HIS	-	expression tag	UNP Q5SSZ7
A	212	HIS	-	expression tag	UNP Q5SSZ7
A	213	HIS	-	expression tag	UNP Q5SSZ7
A	214	HIS	-	expression tag	UNP Q5SSZ7
B	50	GLU	-	expression tag	UNP Q5SSZ7
B	51	THR	-	expression tag	UNP Q5SSZ7
B	52	GLY	-	expression tag	UNP Q5SSZ7
B	206	GLY	-	expression tag	UNP Q5SSZ7
B	207	THR	-	expression tag	UNP Q5SSZ7
B	208	LYS	-	expression tag	UNP Q5SSZ7
B	209	HIS	-	expression tag	UNP Q5SSZ7
B	210	HIS	-	expression tag	UNP Q5SSZ7
B	211	HIS	-	expression tag	UNP Q5SSZ7

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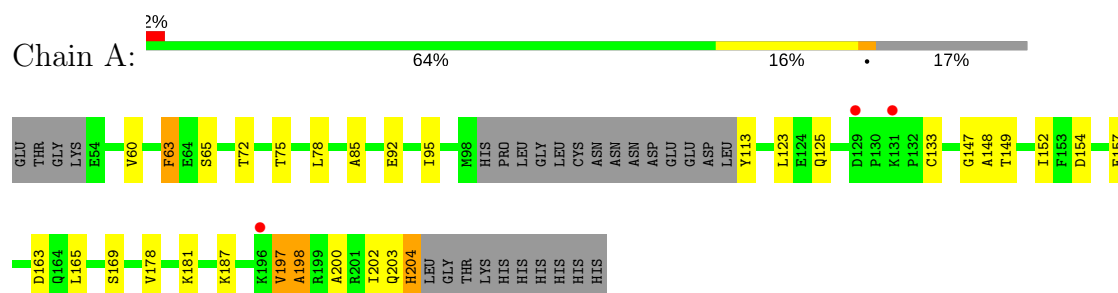
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Chain	Residue	Modelled	Actual	Comment	Reference
B	212	HIS	-	expression tag	UNP Q5SSZ7
B	213	HIS	-	expression tag	UNP Q5SSZ7
B	214	HIS	-	expression tag	UNP Q5SSZ7
C	50	GLU	-	expression tag	UNP Q5SSZ7
C	51	THR	-	expression tag	UNP Q5SSZ7
C	52	GLY	-	expression tag	UNP Q5SSZ7
C	206	GLY	-	expression tag	UNP Q5SSZ7
C	207	THR	-	expression tag	UNP Q5SSZ7
C	208	LYS	-	expression tag	UNP Q5SSZ7
C	209	HIS	-	expression tag	UNP Q5SSZ7
C	210	HIS	-	expression tag	UNP Q5SSZ7
C	211	HIS	-	expression tag	UNP Q5SSZ7
C	212	HIS	-	expression tag	UNP Q5SSZ7
C	213	HIS	-	expression tag	UNP Q5SSZ7
C	214	HIS	-	expression tag	UNP Q5SSZ7
D	50	GLU	-	expression tag	UNP Q5SSZ7
D	51	THR	-	expression tag	UNP Q5SSZ7
D	52	GLY	-	expression tag	UNP Q5SSZ7
D	206	GLY	-	expression tag	UNP Q5SSZ7
D	207	THR	-	expression tag	UNP Q5SSZ7
D	208	LYS	-	expression tag	UNP Q5SSZ7
D	209	HIS	-	expression tag	UNP Q5SSZ7
D	210	HIS	-	expression tag	UNP Q5SSZ7
D	211	HIS	-	expression tag	UNP Q5SSZ7
D	212	HIS	-	expression tag	UNP Q5SSZ7
D	213	HIS	-	expression tag	UNP Q5SSZ7
D	214	HIS	-	expression tag	UNP Q5SSZ7

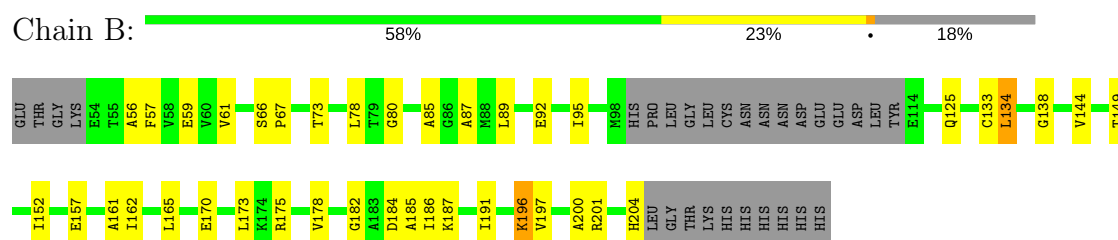
3 Residue-property plots [i](#)

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.

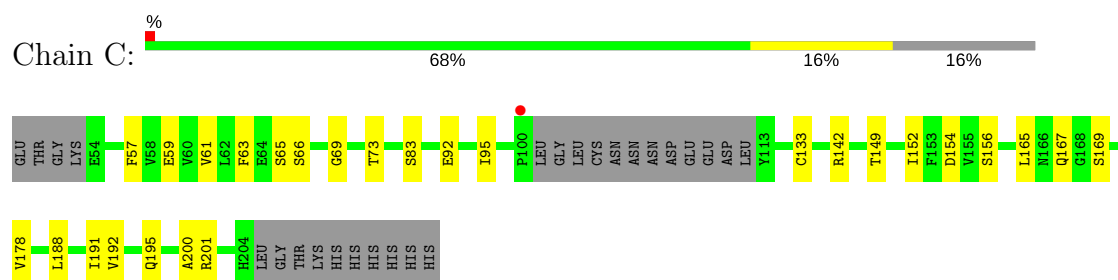
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



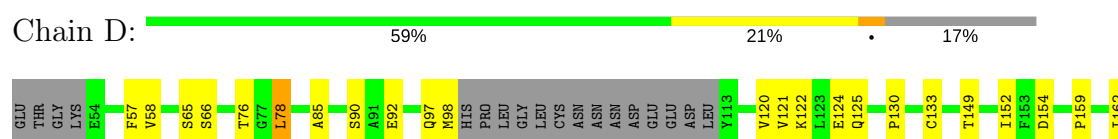
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



D163	Q164	L165	E170	D171	P172	V178	G182	A183	D184	A185	I186	K187	I191	V192	N193	I202	Q203	H204	LEU	GLY	THR	LYS	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.20Å 112.63Å 62.22Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	41.43 – 2.69 35.50 – 2.69	Depositor EDS
% Data completeness (in resolution range)	87.7 (41.43-2.69) 87.9 (35.50-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.235 , 0.341 0.237 , 0.335	Depositor DCC
R_{free} test set	922 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l 0.032 for -k,-h,-l 0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4174	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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

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	0.55	0/1061	0.79	1/1436 (0.1%)
1	B	0.56	0/1048	0.80	1/1418 (0.1%)
1	C	0.56	0/1072	0.75	0/1452
1	D	0.56	0/1061	0.79	1/1436 (0.1%)
All	All	0.56	0/4242	0.78	3/5742 (0.1%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	154	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	202	ILE	CB-CA-C	-5.16	101.28	111.60
1	B	201	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Peptide

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	1044	0	1054	12	0
1	B	1032	0	1045	20	0
1	C	1054	0	1061	14	0
1	D	1044	0	1054	21	0
All	All	4174	0	4214	64	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.

All (64) 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:85:ALA:HB2	1:D:165:LEU:O	1.83	0.78
1:B:57:PHE:CZ	1:B:59:GLU:OE2	2.38	0.75
1:B:85:ALA:HB2	1:B:165:LEU:O	1.88	0.73
1:A:95:ILE:HD11	1:A:200:ALA:HB2	1.74	0.69
1:B:196:LYS:HG2	1:B:197:VAL:HG23	1.79	0.64
1:C:95:ILE:HD11	1:C:200:ALA:HB2	1.80	0.63
1:C:92:GLU:OE1	1:C:201:ARG:NE	2.30	0.63
1:C:92:GLU:O	1:C:149:THR:HG21	1.99	0.61
1:D:90:SER:HB2	1:D:202:ILE:O	2.01	0.61
1:A:152:ILE:HD11	1:A:202:ILE:HD11	1.83	0.61
1:D:184:ASP:OD1	1:D:184:ASP:N	2.38	0.57
1:D:186:ILE:O	1:D:187:LYS:C	2.43	0.57
1:B:92:GLU:O	1:B:149:THR:HG21	2.05	0.56
1:D:154:ASP:OD1	1:D:154:ASP:C	2.46	0.54
1:C:57:PHE:CZ	1:C:59:GLU:OE2	2.62	0.53
1:B:125:GLN:HG3	1:B:157:GLU:HB3	1.91	0.52
1:D:76:THR:HG21	1:D:191:ILE:HD11	1.92	0.52
1:D:152:ILE:HA	1:D:178:VAL:O	2.09	0.52
1:B:134:LEU:HD22	1:B:138:GLY:HA3	1.91	0.52
1:C:59:GLU:OE2	1:D:203:GLN:OE1	2.28	0.52
1:B:152:ILE:HA	1:B:178:VAL:O	2.10	0.52
1:B:144:VAL:HG13	1:B:175:ARG:HG2	1.93	0.50
1:D:57:PHE:HB2	1:D:203:GLN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:MET:HG3	1:D:121:VAL:HG22	1.94	0.49
1:D:122:LYS:HA	1:D:154:ASP:HB3	1.94	0.49
1:B:187:LYS:O	1:B:191:ILE:HD12	2.13	0.49
1:B:87:ALA:HB1	1:B:89:LEU:HG	1.96	0.47
1:A:92:GLU:O	1:A:149:THR:HG21	2.15	0.47
1:B:61:VAL:HG13	1:B:73:THR:CG2	2.45	0.47
1:A:78:LEU:HD21	1:A:187:LYS:HB3	1.97	0.47
1:D:58:VAL:HB	1:D:78:LEU:HB3	1.97	0.46
1:D:182:GLY:O	1:D:185:ALA:HB3	2.15	0.46
1:C:154:ASP:OD1	1:C:156:SER:OG	2.22	0.46
1:A:85:ALA:HB2	1:A:165:LEU:O	2.16	0.46
1:B:56:ALA:N	1:B:80:GLY:O	2.42	0.46
1:A:152:ILE:HA	1:A:178:VAL:O	2.15	0.46
1:C:188:LEU:O	1:C:192:VAL:HG23	2.16	0.46
1:A:123:LEU:O	1:A:157:GLU:HB2	2.16	0.45
1:B:161:ALA:O	1:B:162:ILE:C	2.53	0.45
1:D:92:GLU:O	1:D:149:THR:HG21	2.16	0.45
1:A:60:VAL:O	1:A:75:THR:HA	2.17	0.45
1:A:197:VAL:O	1:A:198:ALA:HB2	2.16	0.45
1:B:95:ILE:HD11	1:B:200:ALA:HB2	1.99	0.45
1:A:203:GLN:O	1:A:204:HIS:HB2	2.17	0.44
1:C:61:VAL:HG13	1:C:73:THR:HG22	1.98	0.44
1:D:171:ASP:N	1:D:172:PRO:CD	2.80	0.44
1:D:97:GLN:HA	1:D:120:VAL:O	2.18	0.44
1:B:185:ALA:O	1:B:186:ILE:C	2.56	0.43
1:D:65:SER:OG	1:D:66:SER:N	2.51	0.43
1:C:65:SER:OG	1:C:66:SER:O	2.37	0.43
1:B:204:HIS:HA	1:C:69:GLY:HA3	2.00	0.43
1:A:63:PHE:C	1:A:63:PHE:CD1	2.92	0.43
1:C:152:ILE:HA	1:C:178:VAL:O	2.18	0.43
1:B:66:SER:O	1:B:67:PRO:C	2.57	0.42
1:B:134:LEU:CD2	1:B:138:GLY:HA3	2.49	0.42
1:A:147:GLY:O	1:A:148:ALA:C	2.59	0.42
1:D:203:GLN:O	1:D:204:HIS:HB2	2.19	0.42
1:D:159:PRO:O	1:D:162:ILE:HD12	2.19	0.41
1:C:191:ILE:O	1:C:195:GLN:HB2	2.21	0.41
1:B:92:GLU:OE1	1:C:63:PHE:CD2	2.74	0.41
1:D:124:GLU:O	1:D:125:GLN:C	2.56	0.41
1:B:78:LEU:HB2	1:B:184:ASP:HB3	2.03	0.41
1:D:193:ASN:N	1:D:193:ASN:OD1	2.54	0.41
1:C:83:SER:OG	1:C:165:LEU:HB3	2.21	0.41

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	133/165 (81%)	119 (90%)	13 (10%)	1 (1%)	21	47
1	B	132/165 (80%)	120 (91%)	11 (8%)	1 (1%)	21	47
1	C	135/165 (82%)	123 (91%)	11 (8%)	1 (1%)	24	50
1	D	133/165 (81%)	117 (88%)	14 (10%)	2 (2%)	11	29
All	All	533/660 (81%)	479 (90%)	49 (9%)	5 (1%)	19	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA
1	B	182	GLY
1	C	133	CYS
1	D	130	PRO
1	D	171	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	111/138 (80%)	101 (91%)	10 (9%)	10	24
1	B	110/138 (80%)	105 (96%)	5 (4%)	30	60
1	C	112/138 (81%)	109 (97%)	3 (3%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	111/138 (80%)	105 (95%)	6 (5%)	24	51
All	All	444/552 (80%)	420 (95%)	24 (5%)	24	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	65	SER
1	A	72	THR
1	A	125	GLN
1	A	133	CYS
1	A	163	ASP
1	A	169	SER
1	A	181	LYS
1	A	197	VAL
1	A	204	HIS
1	B	133	CYS
1	B	134	LEU
1	B	170	GLU
1	B	173	LEU
1	B	196	LYS
1	C	142	ARG
1	C	167	GLN
1	C	169	SER
1	D	78	LEU
1	D	133	CYS
1	D	163	ASP
1	D	170	GLU
1	D	184	ASP
1	D	193	ASN

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

Mol	Chain	Res	Type
1	B	195	GLN
1	C	190	ASN
1	D	74	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 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 [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	137/165 (83%)	-0.19	3 (2%) 62 62	41, 63, 104, 128	0
1	B	136/165 (82%)	-0.19	0 100 100	41, 64, 98, 110	0
1	C	139/165 (84%)	-0.19	1 (0%) 87 88	41, 63, 106, 140	0
1	D	137/165 (83%)	-0.16	0 100 100	42, 63, 100, 117	0
All	All	549/660 (83%)	-0.18	4 (0%) 87 88	41, 63, 100, 140	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	PRO	4.7
1	A	131	LYS	3.0
1	A	196	LYS	2.1
1	A	129	ASP	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.