Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 11:45 am BST

PDB ID	:	8CAF
Title	:	N8C_Fab3b in complex with NEDD8-CUL1(WHB)
Authors	:	Duda, D.M.; Yanishevski, D.; Henneberg, L.T.; Schulman, B.A.
Deposited on	:	2023-01-24
Resolution	:	2.66 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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
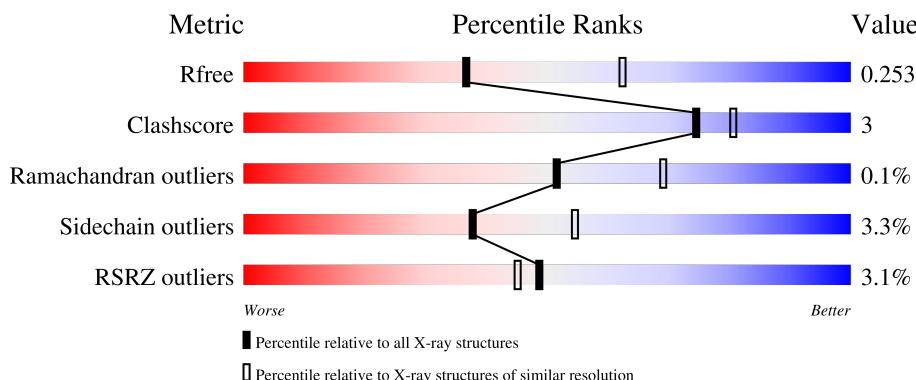
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
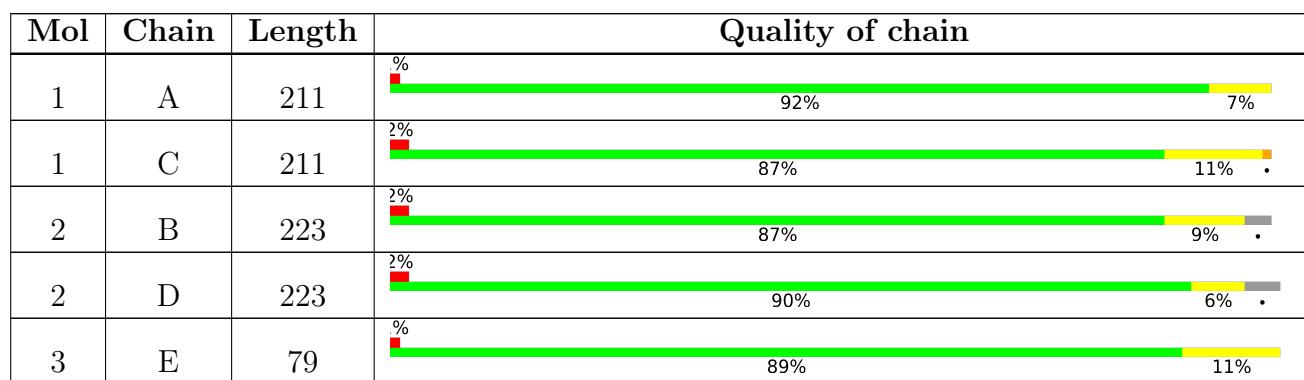
The reported resolution of this entry is 2.66 Å.

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	Percentile Ranks	Value
Rfree		0.253
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		3.3%
RSRZ outliers		3.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
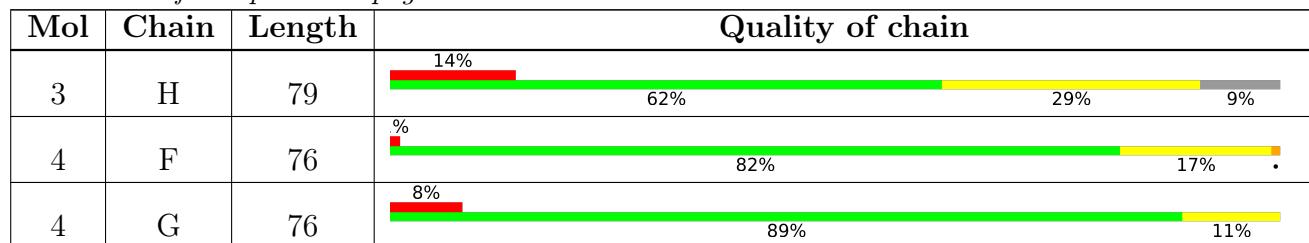
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	211	% 92% 7%
1	C	211	2% 87% 11% •
2	B	223	2% 87% 9% •
2	D	223	2% 90% 6% •
3	E	79	% 89% 11%

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Mol	Chain	Length	Quality of chain
3	H	79	14% ▬ 62% ▬ 29% ▬ 9%
4	F	76	% ▬ 82% ▬ 17% ▬ ·
4	G	76	8% ▬ 89% ▬ 11%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8808 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 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total 1606	C 1005	N 270	O 326	S 5	0	0	0
1	C	210	Total 1591	C 995	N 265	O 326	S 5	0	0	0

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total 1599	C 1014	N 267	O 313	S 5	0	0	0
2	D	215	Total 1599	C 1013	N 266	O 315	S 5	0	0	0

- Molecule 3 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	79	Total 625	C 401	N 112	O 109	S 3	0	0	0
3	H	72	Total 590	C 381	N 101	O 105	S 3	0	0	0

- Molecule 4 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	76	Total 599	C 378	N 104	O 115	S 2	0	0	0
4	G	76	Total 599	C 378	N 104	O 115	S 2	0	0	0
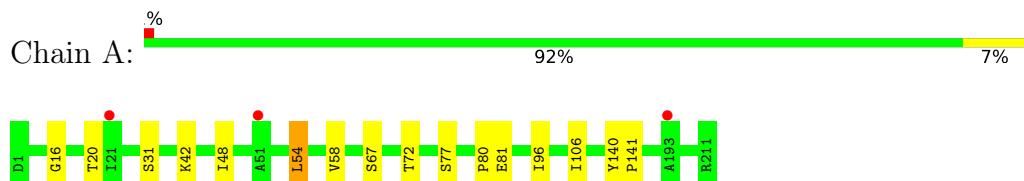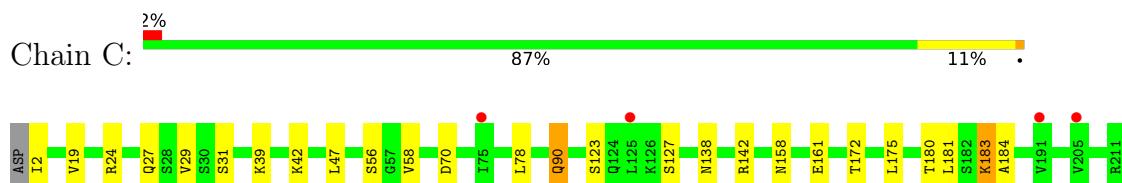
3 Residue-property plots ⓘ

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.
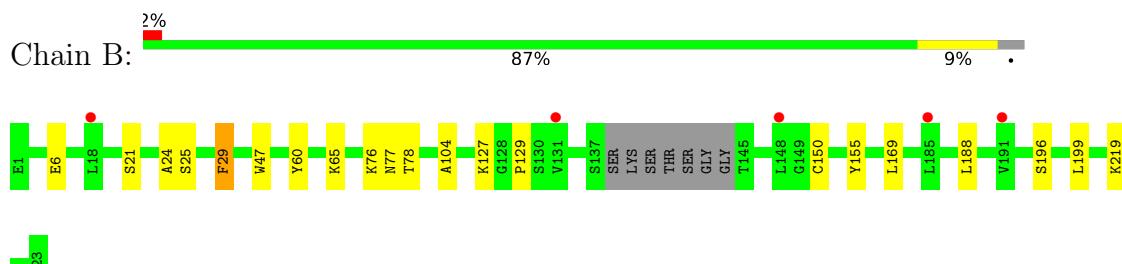
• Molecule 1: Fab Light Chain
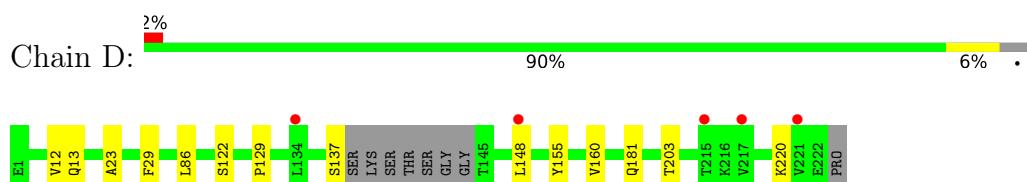
• Molecule 1: Fab Light Chain
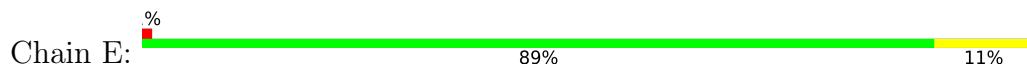
• Molecule 2: Fab Heavy Chain
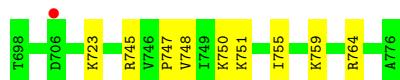
• Molecule 2: Fab Heavy Chain

• Molecule 3: Cullin-1

T698 D706 K723 R745 V746 P747 V748 I749 K750 K751 I755 K759 R764 A776

• Molecule 3: Cullin-1

Chain H:

14%

62% 29% 9%

THR THR HIS LYS N702 I703 E704 R707 K708 L709 L710 I711 Q712 R717 I718 K723 V724 L725 Q728 L731 G732 E733 Q737 F742 I753 D754 I755 L756 I757 E758 Y761 L762 E763 R764 V765 D766 GLU LYS D770 T771 Y772 L775 A776

• Molecule 4: NEDD8

Chain F:

%

82% 17% •

M1 L2 I3 K4 I13 E14 K22 R25 E34 R42 K48 K54 T55 I61 L67 V70 R74 G75 G76

• Molecule 4: NEDD8

Chain G:

8%

89% 11%

M1 L2 I3 L8 T9 I13 E14 K22 V23 E24 R42 S46 L62 S65 V70 L71 G76

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.37Å 106.87Å 180.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.33 – 2.66 102.37 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.3 (90.33-2.66) 98.3 (102.37-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.217 , 0.263 0.209 , 0.253	Depositor DCC
R_{free} test set	2876 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8808	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.44	0/1639	0.66	0/2225
1	C	0.49	0/1624	0.69	0/2208
2	B	0.50	0/1641	0.68	2/2241 (0.1%)
2	D	0.49	0/1640	0.67	0/2238
3	E	0.48	0/631	0.72	0/846
3	H	0.44	0/595	0.68	0/795
4	F	0.55	0/604	0.78	0/808
4	G	0.60	0/604	0.73	0/808
All	All	0.49	0/8978	0.69	2/12169 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	188	LEU	CA-CB-CG	5.99	129.07	115.30
2	B	169	LEU	CA-CB-CG	5.95	128.99	115.30

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	1606	0	1573	9	0
1	C	1591	0	1541	11	0
2	B	1599	0	1533	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1599	0	1546	6	0
3	E	625	0	657	6	0
3	H	590	0	634	12	0
4	F	599	0	638	7	0
4	G	599	0	638	3	0
All	All	8808	0	8760	56	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 (56) 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:C:161:GLU:HG2	1:C:175:LEU:HD21	1.74	0.68
4:F:74:ARG:HH11	3:H:761:TYR:HE1	1.42	0.68
1:A:80:PRO:HA	1:A:106:ILE:HG13	1.81	0.62
3:H:710:LEU:HD12	3:H:742:PHE:HE1	1.64	0.62
2:B:25:SER:HB2	2:D:23:ALA:HB1	1.85	0.59
3:H:754:ASP:HA	3:H:757:ILE:HG13	1.85	0.58
1:C:24:ARG:HG3	1:C:70:ASP:OD1	2.03	0.57
2:B:76:LYS:HB3	2:B:78:THR:HG23	1.88	0.54
1:C:39:LYS:HB2	1:C:42:LYS:HD3	1.90	0.53
1:C:47:LEU:HA	1:C:58:VAL:HG21	1.91	0.52
3:H:717:ARG:NH1	3:H:737:GLN:OE1	2.38	0.52
3:H:707:ARG:O	3:H:711:ILE:HG13	2.09	0.52
3:H:755:ILE:O	3:H:758:GLU:HG2	2.09	0.52
1:C:31:SER:HB2	3:E:723:LYS:HB2	1.93	0.51
1:C:29:VAL:HG11	1:C:90:GLN:NE2	2.29	0.48
4:G:42:ARG:HB2	4:G:70:VAL:HG22	1.94	0.48
3:H:762:LEU:HD22	3:H:772:TYR:HB3	1.95	0.48
2:B:129:PRO:HB3	2:B:155:TYR:HB3	1.96	0.48
1:C:19:VAL:HG21	1:C:78:LEU:HD22	1.95	0.48
3:H:763:GLU:HB3	3:H:775:LEU:HD11	1.96	0.47
1:C:158:ASN:OD1	1:C:158:ASN:N	2.42	0.47
3:E:745:ARG:HB2	3:E:747:PRO:HD2	1.96	0.47
3:E:755:ILE:HG22	3:E:759:LYS:HE2	1.96	0.47
1:A:81:GLU:H	1:A:81:GLU:HG3	1.43	0.47
3:E:750:LYS:NZ	3:E:764:ARG:HH21	2.14	0.46
1:C:138:ASN:HD22	1:C:172:THR:HG21	1.81	0.46
3:H:708:LYS:O	3:H:712:GLN:HG3	2.16	0.45
1:C:183:LYS:HD2	1:C:184:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:718:ILE:HD13	3:H:733:GLU:HB3	1.99	0.45
4:G:22:LYS:HB3	4:G:24:GLU:HG2	2.00	0.44
1:A:96:ILE:HB	2:B:47:TRP:CG	2.52	0.44
4:F:13:ILE:HD11	4:F:34:GLU:HG3	1.99	0.44
1:A:31:SER:HB2	3:H:723:LYS:HB2	1.99	0.44
2:D:203:THR:HG23	2:D:220:LYS:HD3	1.99	0.44
4:F:42:ARG:HB2	4:F:70:VAL:HG22	1.99	0.44
2:D:13:GLN:HE21	2:D:13:GLN:HB3	1.52	0.43
1:A:54:LEU:HD22	1:A:58:VAL:HB	2.00	0.43
1:C:2:ILE:N	1:C:27:GLN:HG3	2.34	0.43
4:F:48:LYS:HD2	4:F:48:LYS:HA	1.71	0.43
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.54	0.43
4:F:61:ILE:HD13	4:F:67:LEU:HD21	2.00	0.42
4:G:8:LEU:HD23	4:G:8:LEU:HA	1.83	0.42
2:B:60:TYR:HB2	2:B:65:LYS:HD2	2.01	0.42
2:D:181:GLN:HE21	2:D:181:GLN:HB2	1.69	0.42
2:D:129:PRO:HB3	2:D:155:TYR:HB3	2.01	0.42
1:A:16:GLY:HA2	1:A:77:SER:HB2	2.01	0.42
4:F:22:LYS:HA	4:F:55:THR:HA	2.00	0.42
3:E:751:LYS:O	3:E:755:ILE:HG13	2.20	0.42
3:E:745:ARG:HG3	3:E:748:VAL:HG23	2.01	0.41
1:A:48:ILE:HD13	1:A:54:LEU:HD23	2.03	0.41
2:B:24:ALA:HB3	2:B:29:PHE:HE1	1.86	0.41
2:D:12:VAL:HG11	2:D:86:LEU:HD13	2.04	0.41
2:B:104:ALA:HA	3:H:717:ARG:HD3	2.02	0.40
4:F:4:LYS:HE2	4:F:4:LYS:HB2	1.84	0.40
1:A:20:THR:HG23	1:A:72:THR:HG23	2.04	0.40
2:B:6:GLU:HA	2:B:21:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
1	C	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
2	B	212/223 (95%)	204 (96%)	7 (3%)	1 (0%)	29	43
2	D	211/223 (95%)	205 (97%)	6 (3%)	0	100	100
3	E	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
3	H	68/79 (86%)	67 (98%)	1 (2%)	0	100	100
4	F	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
4	G	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
All	All	1133/1178 (96%)	1096 (97%)	36 (3%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	LEU

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	185/187 (99%)	182 (98%)	3 (2%)	62	78
1	C	183/187 (98%)	175 (96%)	8 (4%)	28	43
2	B	173/182 (95%)	167 (96%)	6 (4%)	36	52
2	D	176/182 (97%)	171 (97%)	5 (3%)	43	61
3	E	66/74 (89%)	66 (100%)	0	100	100
3	H	66/74 (89%)	63 (96%)	3 (4%)	27	42
4	F	66/66 (100%)	62 (94%)	4 (6%)	18	29
4	G	66/66 (100%)	63 (96%)	3 (4%)	27	42
All	All	981/1018 (96%)	949 (97%)	32 (3%)	38	54

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	54	LEU
1	A	67	SER
2	B	29	PHE
2	B	77	ASN
2	B	127	LYS
2	B	150	CYS
2	B	196	SER
2	B	219	LYS
1	C	56	SER
1	C	90	GLN
1	C	123	SER
1	C	127	SER
1	C	142	ARG
1	C	180	THR
1	C	181	LEU
1	C	183	LYS
2	D	29	PHE
2	D	122	SER
2	D	137	SER
2	D	148	LEU
2	D	160	VAL
4	F	2	LEU
4	F	25	ARG
4	F	54	LYS
4	F	74	ARG
4	G	2	LEU
4	G	9	THR
4	G	65	SER
3	H	725	LEU
3	H	728	GLN
3	H	770	ASP

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

Mol	Chain	Res	Type
2	D	13	GLN
2	D	202	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	211/211 (100%)	0.60	3 (1%)	75	73	51, 73, 89, 109	0
1	C	210/211 (99%)	0.62	4 (1%)	66	63	45, 63, 102, 109	0
2	B	216/223 (96%)	0.65	5 (2%)	60	56	51, 62, 98, 113	0
2	D	215/223 (96%)	0.69	5 (2%)	60	56	45, 66, 96, 114	0
3	E	79/79 (100%)	0.58	1 (1%)	77	75	50, 68, 107, 111	0
3	H	72/79 (91%)	0.99	11 (15%)	2	1	59, 87, 101, 112	0
4	F	76/76 (100%)	0.82	1 (1%)	77	75	57, 69, 84, 96	0
4	G	76/76 (100%)	0.88	6 (7%)	12	10	56, 74, 91, 98	0
All	All	1155/1178 (98%)	0.69	36 (3%)	49	45	45, 68, 100, 114	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	758	GLU	3.5
3	H	704	GLU	2.9
1	C	191	VAL	2.9
1	A	193	ALA	2.8
3	H	765	VAL	2.8
4	F	14	GLU	2.8
3	H	762	LEU	2.7
4	G	13	ILE	2.7
1	C	125	LEU	2.7
4	G	46	SER	2.5
2	B	191	VAL	2.5
3	H	775	LEU	2.5
4	G	62	LEU	2.5
4	G	71	LEU	2.5
1	C	205	VAL	2.4
3	H	776	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	706	ASP	2.3
3	H	731	LEU	2.3
4	G	3	ILE	2.3
3	H	703	ILE	2.3
3	H	742	PHE	2.2
2	D	134	LEU	2.2
1	A	51	ALA	2.2
2	D	217	VAL	2.2
2	B	185	LEU	2.2
2	B	148	LEU	2.2
4	G	14	GLU	2.1
2	B	18	LEU	2.1
2	D	148	LEU	2.1
3	H	753	ILE	2.1
3	H	772	TYR	2.1
2	D	215	THR	2.1
1	C	75	ILE	2.1
2	D	221	VAL	2.0
1	A	21	ILE	2.0
2	B	131	VAL	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.