Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 02:38 AM EDT

PDB ID	:	5VL7
Title	:	PCSK9 complex with Fab33
Authors	:	Eigenbrot, C.; Shia, S.
Deposited on	:	2017-04-25
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

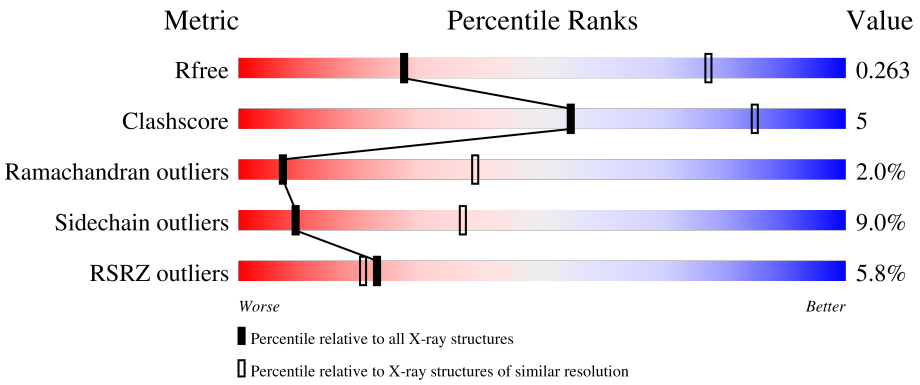
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	152	47% 12% • 39%
2	B	548	% 63% 16% • 20%
3	H	228	7% 77% 17% • •
4	L	214	15% 76% 21% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7194 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	92	740	474	133	131	2	0	0	0

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	437	3214	1982	586	615	31	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ILE	VAL	variant	UNP Q8NBP7
B	670	GLU	GLY	variant	UNP Q8NBP7
B	693	HIS	-	expression tag	UNP Q8NBP7
B	694	HIS	-	expression tag	UNP Q8NBP7
B	695	HIS	-	expression tag	UNP Q8NBP7
B	696	HIS	-	expression tag	UNP Q8NBP7
B	697	HIS	-	expression tag	UNP Q8NBP7
B	698	HIS	-	expression tag	UNP Q8NBP7
B	699	HIS	-	expression tag	UNP Q8NBP7
B	700	HIS	-	expression tag	UNP Q8NBP7

- Molecule 3 is a protein called Fab33 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	1630	1027	277	319	7	0	0	0

- Molecule 4 is a protein called Fab33 light chain.

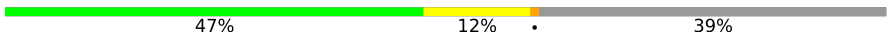
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	210	1610	1012	269	324	5	0	0	0

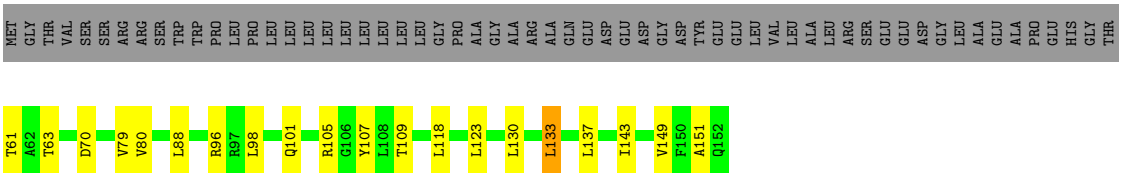
3 Residue-property plots (i)

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: Proprotein convertase subtilisin/kexin type 9

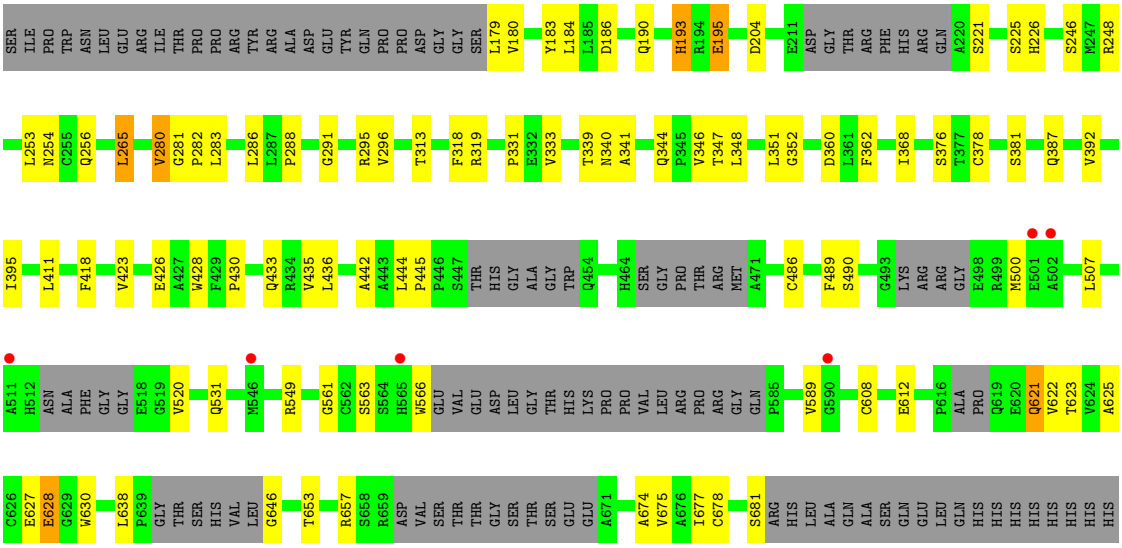
Chain A:





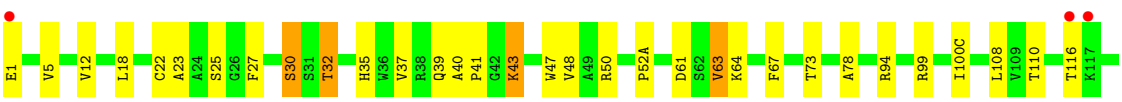
• Molecule 2: Proprotein convertase subtilisin/kexin type 9

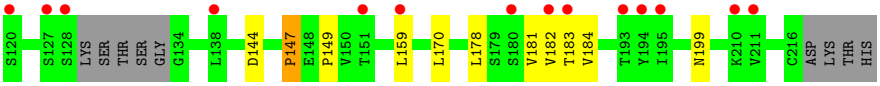
Chain B:



• Molecule 3: Fab33 heavy chain

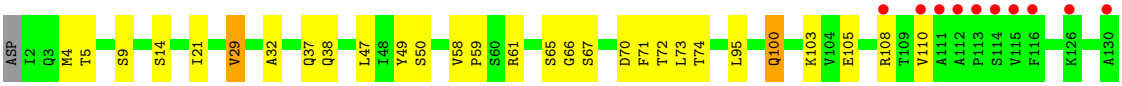
Chain H:

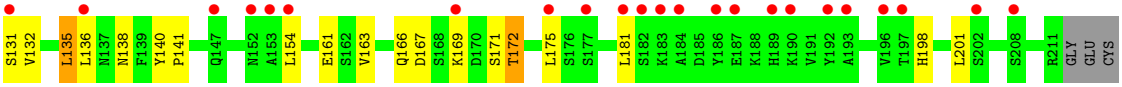




• Molecule 4: Fab33 light chain

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	92.28Å 142.52Å 253.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.75 – 3.50 37.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.75-3.50) 99.9 (37.75-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.199 , 0.245 0.213 , 0.263	Depositor DCC
R_{free} test set	903 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 86.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.42	0/757	0.68	0/1023
2	B	0.42	0/3264	0.67	0/4426
3	H	0.41	0/1668	0.69	0/2274
4	L	0.43	0/1646	0.69	0/2237
All	All	0.42	0/7335	0.68	0/9960

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	740	0	750	8	0
2	B	3214	0	3137	40	0
3	H	1630	0	1600	16	0
4	L	1610	0	1568	18	0
All	All	7194	0	7055	74	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 5.

All (74) 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)
4:L:108:ARG:HD3	4:L:171:SER:O	1.71	0.91
1:A:101:GLN:HB3	1:A:133:LEU:HD11	1.68	0.75
2:B:348:LEU:H	2:B:352:GLY:HA2	1.55	0.71
3:H:39:GLN:HE22	4:L:38:GLN:HE22	1.42	0.67
2:B:339:THR:HG23	2:B:362:PHE:HB3	1.76	0.66
2:B:418:PHE:CD1	2:B:445:PRO:HB3	2.32	0.64
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.79	0.64
2:B:340:ASN:HD21	2:B:344:GLN:HB2	1.63	0.64
2:B:368:ILE:HD12	2:B:387:GLN:HB3	1.80	0.62
3:H:5:VAL:HB	3:H:23:ALA:HB3	1.81	0.61
3:H:159:LEU:HD21	3:H:182:VAL:HG21	1.82	0.61
2:B:339:THR:CG2	2:B:362:PHE:HB3	2.32	0.59
2:B:392:VAL:HA	2:B:395:ILE:HD12	1.85	0.57
2:B:612:GLU:HG2	2:B:675:VAL:HG22	1.87	0.56
2:B:433:GLN:HA	2:B:436:LEU:HD12	1.89	0.55
4:L:105:GLU:OE2	4:L:140:TYR:HE1	1.90	0.55
4:L:198:HIS:HB3	4:L:201:LEU:HD13	1.88	0.54
2:B:621:GLN:HB3	2:B:657:ARG:HD2	1.89	0.54
4:L:21:ILE:HD12	4:L:73:LEU:HD23	1.89	0.54
2:B:341:ALA:HB1	3:H:73:THR:HG21	1.90	0.53
4:L:59:PRO:HB2	4:L:61:ARG:HG3	1.91	0.53
1:A:149:VAL:HG12	2:B:291:GLY:HA3	1.90	0.52
2:B:183:TYR:HE1	2:B:283:LEU:HD11	1.74	0.52
3:H:61:ASP:HA	3:H:64:LYS:HD3	1.92	0.52
4:L:161:GLU:HB3	4:L:175:LEU:HD11	1.91	0.52
3:H:116:THR:HG23	3:H:147:PRO:HD3	1.92	0.52
2:B:313:THR:HG22	2:B:333:VAL:HG12	1.92	0.52
2:B:561:GLY:HA2	2:B:677:ILE:HD12	1.91	0.51
2:B:630:TRP:HB3	2:B:678:CYS:HB3	1.91	0.51
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.92	0.51
4:L:140:TYR:CD1	4:L:141:PRO:HA	2.45	0.51
2:B:319:ARG:HG3	2:B:428:TRP:CH2	2.46	0.51
2:B:346:VAL:HG12	2:B:348:LEU:HG	1.93	0.50
2:B:490:SER:HB3	2:B:520:VAL:HG12	1.92	0.49
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.93	0.49
2:B:489:PHE:HA	2:B:646:GLY:HA3	1.95	0.48
3:H:100(C):ILE:HD13	4:L:49:TYR:HB2	1.94	0.48
2:B:180:VAL:HG22	2:B:282:PRO:HG2	1.95	0.48
4:L:100:GLN:H	4:L:100:GLN:HG3	1.50	0.48
3:H:27:PHE:HE2	3:H:32:THR:HG21	1.79	0.48
1:A:79:VAL:HG22	1:A:123:LEU:HD13	1.95	0.48
4:L:163:VAL:HG22	4:L:175:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HB2	1:A:137:LEU:HD11	1.96	0.47
2:B:368:ILE:O	2:B:381:SER:HA	2.14	0.47
3:H:30:SER:HA	3:H:52(A):PRO:HB2	1.96	0.47
2:B:313:THR:HG22	2:B:333:VAL:CG1	2.45	0.47
1:A:151:ALA:HB1	2:B:226:HIS:CE1	2.51	0.46
2:B:286:LEU:HG	2:B:288:PRO:HG3	1.97	0.46
4:L:29:VAL:HG13	4:L:32:ALA:HB3	1.97	0.46
4:L:108:ARG:HH11	4:L:172:THR:HA	1.81	0.46
3:H:35:HIS:HD2	3:H:47:TRP:NE1	2.15	0.45
2:B:638:LEU:HD13	2:B:675:VAL:HG21	1.98	0.45
3:H:63:VAL:HG13	3:H:67:PHE:HB2	1.99	0.45
2:B:183:TYR:CE1	2:B:283:LEU:HD11	2.53	0.43
2:B:486:CYS:HB3	2:B:500:MET:HG2	2.00	0.43
2:B:378:CYS:SG	3:H:99:ARG:HA	2.59	0.43
4:L:66:GLY:HA3	4:L:71:PHE:CD2	2.54	0.42
2:B:193:HIS:CD2	2:B:195:GLU:H	2.37	0.42
3:H:22:CYS:HB3	3:H:78:ALA:HB3	2.00	0.42
3:H:37:VAL:HG22	3:H:47:TRP:HA	2.01	0.42
2:B:625:ALA:HB2	2:B:653:THR:HG23	2.02	0.42
1:A:107:TYR:HB3	1:A:130:LEU:HD11	2.02	0.42
3:H:181:VAL:HG11	4:L:135:LEU:HD11	2.01	0.41
2:B:608:CYS:HA	2:B:678:CYS:O	2.20	0.41
4:L:47:LEU:HA	4:L:58:VAL:HG21	2.03	0.41
2:B:248:ARG:HH11	2:B:280:VAL:HG11	1.85	0.41
2:B:318:PHE:HA	2:B:351:LEU:HD13	2.02	0.41
4:L:167:ASP:O	4:L:171:SER:HA	2.20	0.41
2:B:184:LEU:HD11	2:B:186:ASP:HB2	2.03	0.41
1:A:80:VAL:HG22	1:A:143:ILE:HG12	2.02	0.41
2:B:430:PRO:HD2	2:B:433:GLN:HB2	2.02	0.41
1:A:151:ALA:HB2	2:B:253:LEU:HD13	2.03	0.40
2:B:265:LEU:HD11	2:B:296:VAL:CG2	2.51	0.40
2:B:622:VAL:HG13	2:B:674:ALA:HB2	2.03	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	90/152 (59%)	85 (94%)	5 (6%)	0	100	100
2	B	417/548 (76%)	386 (93%)	21 (5%)	10 (2%)	6	35
3	H	215/228 (94%)	196 (91%)	15 (7%)	4 (2%)	8	40
4	L	208/214 (97%)	181 (87%)	22 (11%)	5 (2%)	6	35
All	All	930/1142 (81%)	848 (91%)	63 (7%)	19 (2%)	7	39

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	147	PRO
4	L	67	SER
2	B	225	SER
2	B	254	ASN
2	B	281	GLY
3	H	144	ASP
4	L	138	ASN
4	L	166	GLN
4	L	169	LYS
2	B	204	ASP
2	B	628	GLU
2	B	426	GLU
2	B	442	ALA
3	H	41	PRO
2	B	531	GLN
2	B	193	HIS
4	L	110	VAL
2	B	331	PRO
3	H	149	PRO

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	79/127 (62%)	70 (89%)	9 (11%)	5 26
2	B	347/439 (79%)	323 (93%)	24 (7%)	15 47
3	H	181/189 (96%)	163 (90%)	18 (10%)	8 33
4	L	183/186 (98%)	163 (89%)	20 (11%)	6 29
All	All	790/941 (84%)	719 (91%)	71 (9%)	9 37

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	63	THR
1	A	70	ASP
1	A	88	LEU
1	A	96	ARG
1	A	105	ARG
1	A	109	THR
1	A	118	LEU
1	A	133	LEU
2	B	179	LEU
2	B	190	GLN
2	B	195	GLU
2	B	221	SER
2	B	246	SER
2	B	256	GLN
2	B	265	LEU
2	B	280	VAL
2	B	295	ARG
2	B	347	THR
2	B	360	ASP
2	B	376	SER
2	B	411	LEU
2	B	423	VAL
2	B	435	VAL
2	B	444	LEU
2	B	507	LEU
2	B	563	SER
2	B	566	TRP
2	B	621	GLN
2	B	623	THR
2	B	627	GLU
2	B	628	GLU
2	B	681	SER

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Mol	Chain	Res	Type
3	H	1	GLU
3	H	12	VAL
3	H	18	LEU
3	H	25	SER
3	H	30	SER
3	H	32	THR
3	H	43	LYS
3	H	48	VAL
3	H	50	ARG
3	H	63	VAL
3	H	94	ARG
3	H	108	LEU
3	H	110	THR
3	H	170	LEU
3	H	178	LEU
3	H	183	THR
3	H	184	VAL
3	H	199	ASN
4	L	4	MET
4	L	5	THR
4	L	9	SER
4	L	14	SER
4	L	29	VAL
4	L	50	SER
4	L	65	SER
4	L	70	ASP
4	L	72	THR
4	L	74	THR
4	L	95	LEU
4	L	100	GLN
4	L	103	LYS
4	L	131	SER
4	L	132	VAL
4	L	135	LEU
4	L	136	LEU
4	L	154	LEU
4	L	172	THR
4	L	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	193	HIS
2	B	417	HIS
2	B	591	HIS
3	H	35	HIS
3	H	39	GLN
3	H	76	ASN
3	H	200	HIS
4	L	100	GLN
4	L	124	GLN
4	L	166	GLN
4	L	198	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)

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	92/152 (60%)	-0.32	0 100 100	44, 80, 121, 149	0
2	B	437/548 (79%)	-0.14	6 (1%) 75 69	37, 78, 163, 197	0
3	H	219/228 (96%)	0.28	17 (7%) 13 13	55, 123, 240, 285	0
4	L	210/214 (98%)	0.45	33 (15%) 2 2	40, 111, 215, 269	0
All	All	958/1142 (83%)	0.07	56 (5%) 23 20	37, 91, 203, 285	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	182	SER	6.0
3	H	183	THR	5.8
3	H	194	TYR	5.5
3	H	182	VAL	5.3
4	L	181	LEU	4.6
4	L	111	ALA	3.7
4	L	202	SER	3.5
4	L	153	ALA	3.5
4	L	197	THR	3.4
4	L	193	ALA	3.3
3	H	120	SER	3.2
2	B	590	GLY	3.2
3	H	193	THR	3.1
4	L	192	TYR	2.9
4	L	187	GLU	2.9
4	L	130	ALA	2.9
2	B	546	MET	2.9
4	L	208	SER	2.8
3	H	127	SER	2.8
4	L	186	TYR	2.7
4	L	152	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	154	LEU	2.7
3	H	116	THR	2.7
3	H	211	VAL	2.7
3	H	210	LYS	2.7
4	L	175	LEU	2.7
3	H	151	THR	2.6
4	L	112	ALA	2.6
4	L	114	SER	2.5
3	H	1	GLU	2.5
4	L	116	PHE	2.4
4	L	126	LYS	2.4
4	L	184	ALA	2.4
4	L	131	SER	2.4
4	L	183	LYS	2.4
3	H	138	LEU	2.4
3	H	117	LYS	2.4
3	H	180	SER	2.4
4	L	177	SER	2.4
4	L	115	VAL	2.3
4	L	108	ARG	2.3
2	B	511	ALA	2.3
4	L	136	LEU	2.3
4	L	196	VAL	2.3
4	L	169	LYS	2.3
3	H	195	ILE	2.3
3	H	128	SER	2.2
4	L	189	HIS	2.2
2	B	502	ALA	2.1
4	L	110	VAL	2.1
2	B	501	GLU	2.1
3	H	159	LEU	2.1
2	B	565	HIS	2.1
4	L	190	LYS	2.1
4	L	113	PRO	2.1
4	L	147	GLN	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.