Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 09:03 AM EDT

PDB ID	:	4K8R
Title	:	An Antibody Against the C-terminal Domain of PCSK9 lowers LDL Cholesterol Levels in vivo
Authors	:	Schiele, F.; Nar, H.
Deposited on	:	2013-04-18
Resolution	:	3.22 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 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:

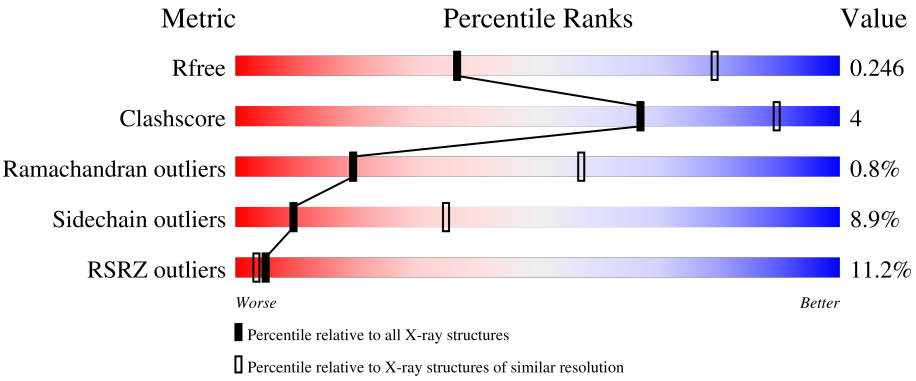
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 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	92	82% 17% •
2	B	548	2% 71% 17% • 10%
3	C	214	29% 87% 12%
4	D	234	39% 80% 17% • •
5	H	238	78% 13% • 7%

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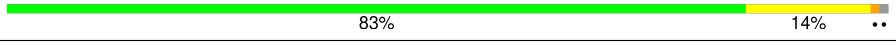
Mol	Chain	Length	Quality of chain
6	L	217	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11245 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
1	A	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	492	Total	C	N	O	S	0	0	0
			3659	2261	676	690	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ILE	VAL	ENGINEERED MUTATION	UNP Q8NBP7
B	670	GLU	GLY	ENGINEERED MUTATION	UNP Q8NBP7
B	693	LEU	-	EXPRESSION TAG	UNP Q8NBP7
B	694	GLU	-	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 Fab1, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1628	1019	273	332	4			

- Molecule 4 is a protein called Fab1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	229	Total	C	N	O	S	2	0	0
			1708	1070	286	345	7			

- Molecule 5 is a protein called Fab3H42, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	221	Total	C	N	O	S	0	0	0
			1660	1051	274	328	7			

- Molecule 6 is a protein called Fab3H42, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	214	Total	C	N	O	S	0	0	0
			1568	975	263	326	4			

- Molecule 7 is water.

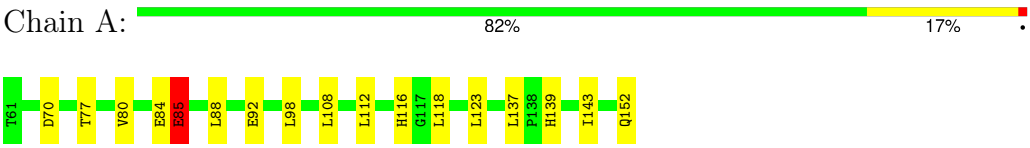
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total	O	0	0
			31	31		
7	B	94	Total	O	0	0
			94	94		
7	C	11	Total	O	0	0
			11	11		
7	D	8	Total	O	0	0
			8	8		
7	H	79	Total	O	0	0
			79	79		
7	L	59	Total	O	0	0
			59	59		

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.

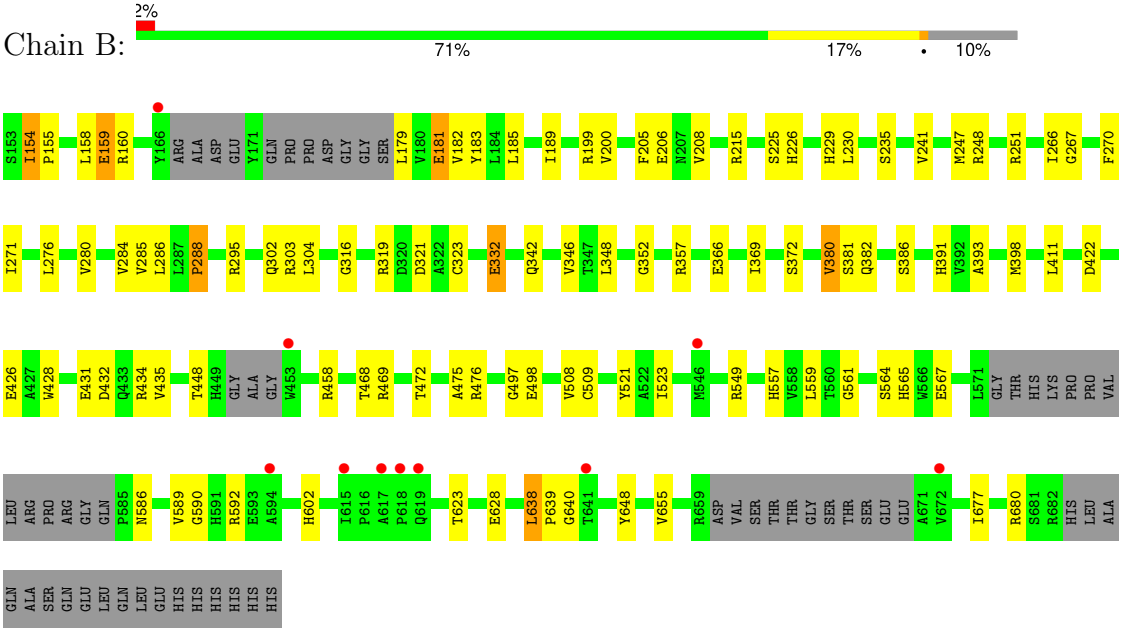
• Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain A:



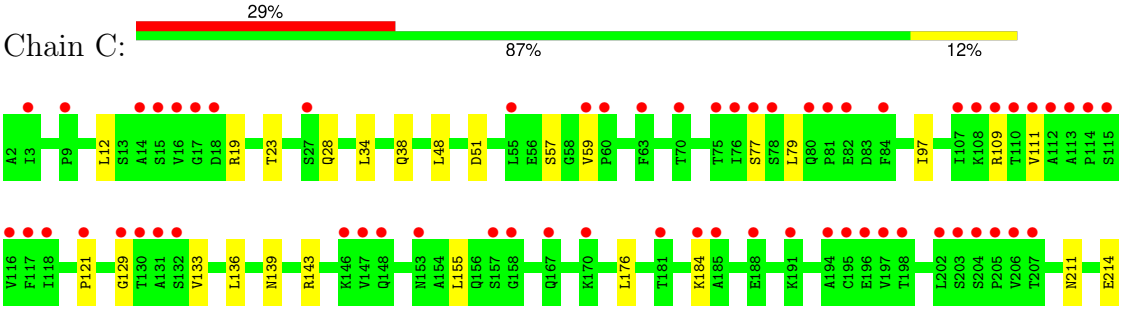
• Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain B:



• Molecule 3: Fab1, light chain

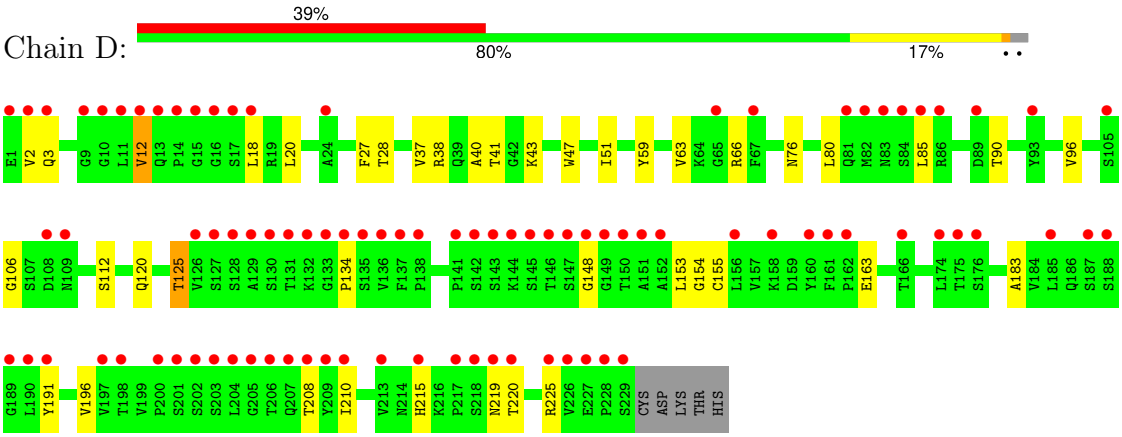
Chain C:



CYS

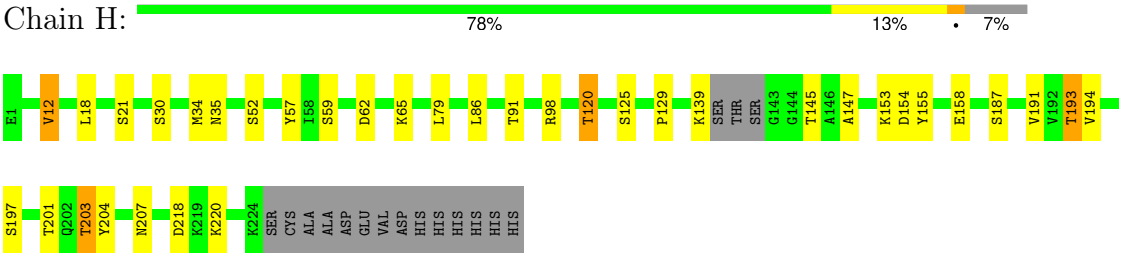
• Molecule 4: Fab1, heavy chain

Chain D:



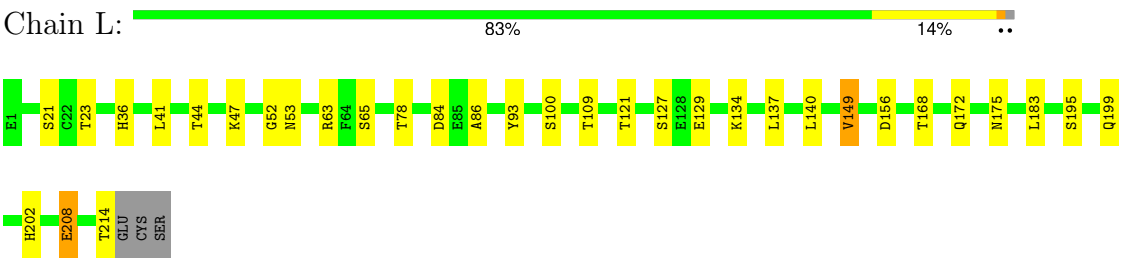
• Molecule 5: Fab3H42, heavy chain

Chain H:



• Molecule 6: Fab3H42, light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	262.19Å 138.65Å 69.54Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	40.00 – 3.22 36.60 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-3.22) 99.3 (36.60-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.167 , 0.226 0.179 , 0.246	Depositor DCC
R_{free} test set	1956 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 98.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11245	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

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	0.44	0/757	0.67	0/1023
2	B	0.40	0/3729	0.66	0/5064
3	C	0.41	0/1661	0.61	0/2254
4	D	0.39	0/1750	0.61	0/2385
5	H	0.42	0/1701	0.70	0/2313
6	L	0.41	0/1605	0.68	0/2192
All	All	0.41	0/11203	0.66	0/15231

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

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	7	0
2	B	3659	0	3567	44	0
3	C	1628	0	1588	9	0
4	D	1708	0	1640	12	0
5	H	1660	0	1610	11	0
6	L	1568	0	1518	8	0
7	A	31	0	0	0	0
7	B	94	0	0	3	0
7	C	11	0	0	0	0
7	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	79	0	0	0	0
7	L	59	0	0	0	0
All	All	11245	0	10673	85	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 4.

All (85) 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)
2:B:200:VAL:HG12	2:B:247:MET:HB2	1.71	0.72
1:A:88:LEU:HD13	1:A:116:HIS:HB3	1.76	0.67
3:C:48:LEU:HA	3:C:59:VAL:HG21	1.76	0.67
5:H:34:MET:HB3	5:H:79:LEU:HD22	1.77	0.65
3:C:129:GLY:HA2	3:C:184:LYS:HB2	1.77	0.65
6:L:199:GLN:HG2	6:L:208:GLU:HG3	1.80	0.64
2:B:230:LEU:HD21	2:B:386:SER:HB3	1.81	0.62
1:A:84:GLU:O	1:A:85:GLU:HB2	2.03	0.59
3:C:121:PRO:HD3	3:C:133:VAL:HG22	1.85	0.58
3:C:38:GLN:HB2	3:C:48:LEU:HD11	1.86	0.57
5:H:129:PRO:HB3	5:H:155:TYR:HB3	1.86	0.57
2:B:181:GLU:HG2	2:B:248:ARG:HD2	1.87	0.56
6:L:93:TYR:HA	6:L:100:SER:HA	1.88	0.55
3:C:19:ARG:HG2	3:C:77:SER:HA	1.89	0.55
2:B:523:ILE:HD13	2:B:648:TYR:HB3	1.88	0.54
2:B:208:VAL:HG11	2:B:251:ARG:HG2	1.91	0.53
6:L:36:HIS:CE1	6:L:52:GLY:H	2.26	0.53
2:B:561:GLY:HA2	2:B:677:ILE:HD13	1.93	0.51
6:L:41:LEU:HD23	6:L:86:ALA:HB2	1.92	0.51
6:L:63:ARG:NH1	6:L:84:ASP:OD1	2.44	0.51
2:B:286:LEU:HD13	2:B:393:ALA:HB2	1.94	0.50
2:B:321:ASP:OD1	2:B:323:CYS:HB2	2.11	0.50
2:B:521:TYR:HA	7:B:892:HOH:O	2.11	0.50
2:B:205:PHE:HE2	2:B:266:ILE:HG22	1.77	0.50
2:B:372:SER:HB2	2:B:380:VAL:HB	1.93	0.49
4:D:12:VAL:HG11	4:D:85:LEU:HD13	1.93	0.49
2:B:241:VAL:HG21	2:B:391:HIS:HA	1.95	0.49
2:B:638:LEU:HD23	2:B:639:PRO:HD2	1.96	0.48
2:B:155:PRO:HD2	2:B:158:LEU:HD12	1.95	0.48
4:D:37:VAL:HG22	4:D:47:TRP:HA	1.95	0.48
2:B:154:ILE:HG22	2:B:159:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.95	0.48
5:H:147:ALA:HB2	5:H:193:THR:HG23	1.96	0.48
5:H:203:THR:HB	5:H:220:LYS:HE2	1.95	0.48
2:B:199:ARG:HD3	2:B:235:SER:HB2	1.96	0.48
5:H:12:VAL:HG11	5:H:86:LEU:HD12	1.96	0.47
2:B:426:GLU:HB3	7:B:805:HOH:O	2.13	0.47
2:B:215:ARG:HG2	5:H:59:SER:HB3	1.95	0.47
4:D:90:THR:HG23	4:D:125:THR:HA	1.97	0.47
2:B:229:HIS:CE1	2:B:382:GLN:HB2	2.50	0.47
2:B:431:GLU:HA	2:B:434:ARG:HG3	1.95	0.46
2:B:346:VAL:HG22	2:B:366:GLU:HB2	1.98	0.46
5:H:12:VAL:HG21	5:H:18:LEU:HG	1.96	0.46
5:H:52:SER:HB2	5:H:57:TYR:HB2	1.98	0.46
2:B:183:TYR:HB2	2:B:285:VAL:HG22	1.98	0.45
2:B:426:GLU:HB2	2:B:434:ARG:HD3	1.98	0.45
1:A:118:LEU:HD11	2:B:304:LEU:HG	1.98	0.45
2:B:469:ARG:NH2	3:C:97:ILE:HD11	2.30	0.45
3:C:211:ASN:HB2	3:C:214:GLU:HB2	1.97	0.45
2:B:590:GLY:HA2	2:B:639:PRO:HG3	1.98	0.44
2:B:208:VAL:CG1	2:B:251:ARG:HG2	2.47	0.44
6:L:137:LEU:HB2	6:L:183:LEU:HB3	2.00	0.44
1:A:152:GLN:OE1	2:B:316:GLY:HA2	2.18	0.44
5:H:62:ASP:HA	5:H:65:LYS:HD2	2.00	0.44
4:D:154:GLY:HA3	4:D:196:VAL:HG12	1.99	0.43
4:D:208:THR:HG23	4:D:225:ARG:HE	1.82	0.43
1:A:98:LEU:HB2	1:A:137:LEU:HD11	2.01	0.43
2:B:623:THR:HG22	2:B:655:VAL:HA	1.99	0.43
2:B:348:LEU:HD12	2:B:352:GLY:HA2	2.00	0.43
3:C:136:LEU:HD13	4:D:196:VAL:HG21	2.01	0.43
4:D:40:ALA:HB3	4:D:43:LYS:HB2	2.01	0.43
4:D:134:PRO:HG3	4:D:215:HIS:HB2	2.00	0.42
2:B:226:HIS:CE1	2:B:230:LEU:HD11	2.55	0.42
2:B:205:PHE:CE2	2:B:266:ILE:HG22	2.55	0.42
2:B:557:HIS:CE1	2:B:602:HIS:HB2	2.55	0.42
2:B:332:GLU:H	2:B:332:GLU:CD	2.23	0.42
4:D:20:LEU:HD12	4:D:80:LEU:HD23	2.02	0.42
1:A:112:LEU:HB2	1:A:123:LEU:HD23	2.01	0.42
4:D:183:ALA:HB1	4:D:191:TYR:HB3	2.02	0.41
2:B:475:ALA:HB3	2:B:509:CYS:HB3	2.02	0.41
2:B:286:LEU:O	2:B:288:PRO:HD3	2.20	0.41
3:C:51:ASP:HB2	4:D:112:SER:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:VAL:HG13	4:D:27:PHE:CD2	2.55	0.41
2:B:497:GLY:HA3	2:B:565:HIS:HA	2.02	0.41
2:B:160:ARG:HD2	7:B:834:HOH:O	2.21	0.41
2:B:267:GLY:O	2:B:270:PHE:HB3	2.21	0.41
1:A:80:VAL:HG22	1:A:143:ILE:HG12	2.02	0.41
2:B:185:LEU:HD11	2:B:271:ILE:HD11	2.02	0.41
5:H:91:THR:HG23	5:H:120:THR:HA	2.03	0.41
6:L:129:GLU:HG2	6:L:134:LYS:HB2	2.02	0.41
2:B:476:ARG:HB3	2:B:508:VAL:HG12	2.02	0.41
6:L:149:VAL:HG12	6:L:202:HIS:HB2	2.03	0.40
2:B:182:VAL:HG22	2:B:284:VAL:HB	2.03	0.40
5:H:194:VAL:HG11	5:H:204:TYR:CE2	2.57	0.40
2:B:319:ARG:HG3	2:B:428:TRP:CH2	2.56	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	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	50
2	B	481/548 (88%)	451 (94%)	27 (6%)	3 (1%)	25	63
3	C	211/214 (99%)	191 (90%)	18 (8%)	2 (1%)	17	55
4	D	227/234 (97%)	208 (92%)	16 (7%)	3 (1%)	12	46
5	H	217/238 (91%)	205 (94%)	11 (5%)	1 (0%)	29	66
6	L	212/217 (98%)	204 (96%)	7 (3%)	1 (0%)	29	66
All	All	1438/1543 (93%)	1345 (94%)	82 (6%)	11 (1%)	19	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
2	B	357	ARG
3	C	111	VAL
3	C	139	ASN
4	D	41	THR
4	D	148	GLY
2	B	640	GLY
6	L	156	ASP
5	H	154	ASP
2	B	280	VAL
4	D	106	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	79/79 (100%)	73 (92%)	6 (8%)	13 44
2	B	392/439 (89%)	357 (91%)	35 (9%)	9 35
3	C	185/186 (100%)	175 (95%)	10 (5%)	22 57
4	D	190/195 (97%)	171 (90%)	19 (10%)	7 29
5	H	186/201 (92%)	167 (90%)	19 (10%)	7 29
6	L	177/180 (98%)	159 (90%)	18 (10%)	7 29
All	All	1209/1280 (94%)	1102 (91%)	107 (9%)	9 35

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	77	THR
1	A	85	GLU
1	A	92	GLU
1	A	108	LEU
1	A	139	HIS
2	B	154	ILE
2	B	159	GLU

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Mol	Chain	Res	Type
2	B	179	LEU
2	B	181	GLU
2	B	189	ILE
2	B	206	GLU
2	B	225	SER
2	B	276	LEU
2	B	288	PRO
2	B	295	ARG
2	B	302	GLN
2	B	303	ARG
2	B	332	GLU
2	B	342	GLN
2	B	369	ILE
2	B	380	VAL
2	B	381	SER
2	B	398	MET
2	B	411	LEU
2	B	422	ASP
2	B	432	ASP
2	B	435	VAL
2	B	448	THR
2	B	458	ARG
2	B	468	THR
2	B	472	THR
2	B	498	GLU
2	B	559	LEU
2	B	564	SER
2	B	567	GLU
2	B	586	ASN
2	B	592	ARG
2	B	628	GLU
2	B	638	LEU
2	B	680	ARG
3	C	12	LEU
3	C	23	THR
3	C	28	GLN
3	C	34	LEU
3	C	57	SER
3	C	79	LEU
3	C	109	ARG
3	C	143	ARG
3	C	155	LEU

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Mol	Chain	Res	Type
3	C	176	LEU
4	D	3	GLN
4	D	12	VAL
4	D	18	LEU
4	D	28	THR
4	D	38	ARG
4	D	51	ILE
4	D	59	TYR
4	D	63	VAL
4	D	66	ARG
4	D	76	ASN
4	D	96	VAL
4	D	120	GLN
4	D	125	THR
4	D	153	LEU
4	D	155	CYS
4	D	163	GLU
4	D	210	ILE
4	D	219	ASN
4	D	220	THR
5	H	12	VAL
5	H	21	SER
5	H	30	SER
5	H	35	ASN
5	H	98	ARG
5	H	120	THR
5	H	125	SER
5	H	139	LYS
5	H	145	THR
5	H	153	LYS
5	H	158	GLU
5	H	187	SER
5	H	191	VAL
5	H	193	THR
5	H	197	SER
5	H	201	THR
5	H	203	THR
5	H	207	ASN
5	H	218	ASP
6	L	21	SER
6	L	23	THR
6	L	44	THR

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Mol	Chain	Res	Type
6	L	47	LYS
6	L	53	ASN
6	L	65	SER
6	L	78	THR
6	L	109	THR
6	L	121	THR
6	L	127	SER
6	L	140	LEU
6	L	149	VAL
6	L	168	THR
6	L	172	GLN
6	L	175	ASN
6	L	195	SER
6	L	208	GLU
6	L	214	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	H	181	GLN

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

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, 95^{th} 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	92/92 (100%)	-0.52	0 100 100	23, 44, 71, 81	0
2	B	492/548 (89%)	-0.18	10 (2%) 65 52	21, 57, 115, 145	0
3	C	213/214 (99%)	1.41	62 (29%) 0 0	99, 154, 174, 199	0
4	D	229/234 (97%)	1.81	91 (39%) 0 0	85, 159, 197, 224	1 (0%)
5	H	221/238 (92%)	-0.48	0 100 100	22, 40, 58, 118	0
6	L	214/217 (98%)	-0.47	0 100 100	22, 40, 64, 95	0
All	All	1461/1543 (94%)	0.25	163 (11%) 5 3	21, 57, 172, 224	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	147	SER	8.1
4	D	143	SER	7.8
4	D	146	THR	7.7
4	D	201	SER	7.6
3	C	108	LYS	7.5
4	D	217	PRO	7.3
4	D	202	SER	7.0
4	D	145	SER	6.7
4	D	206	THR	6.5
4	D	148	GLY	6.4
3	C	116	VAL	6.2
4	D	205	GLY	6.0
4	D	162	PRO	5.9
4	D	229	SER	5.5
4	D	166	THR	5.3
4	D	14	PRO	5.2
4	D	200	PRO	5.1
3	C	184	LYS	5.1
3	C	115	SER	5.0

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Mol	Chain	Res	Type	RSRZ
4	D	150	THR	5.0
3	C	113	ALA	5.0
4	D	149	GLY	4.9
3	C	114	PRO	4.9
4	D	187	SER	4.7
4	D	142	SER	4.6
4	D	189	GLY	4.6
4	D	203	SER	4.5
4	D	144	LYS	4.5
4	D	10	GLY	4.5
4	D	225	ARG	4.5
4	D	198	THR	4.4
4	D	204	LEU	4.3
3	C	148	GLN	4.3
4	D	209	TYR	4.2
3	C	55	LEU	4.2
3	C	205	PRO	4.2
4	D	218	SER	4.2
4	D	83	ASN	4.2
3	C	109	ARG	4.1
4	D	128	SER	4.1
3	C	82	GLU	4.1
3	C	77	SER	4.1
4	D	11	LEU	4.1
4	D	161	PHE	4.1
3	C	15	SER	4.1
3	C	157	SER	4.0
4	D	127	SER	4.0
3	C	110	THR	4.0
4	D	17	SER	4.0
4	D	197	VAL	4.0
4	D	176	SER	4.0
4	D	219	ASN	4.0
4	D	207	GLN	3.9
4	D	152	ALA	3.9
4	D	131	THR	3.9
3	C	18	ASP	3.9
4	D	188	SER	3.8
3	C	81	PRO	3.8
4	D	9	GLY	3.8
4	D	141	PRO	3.8
3	C	111	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	107	ILE	3.7
4	D	129	ALA	3.7
4	D	158	LYS	3.6
3	C	130	THR	3.6
3	C	75	THR	3.5
4	D	108	ASP	3.5
4	D	226	VAL	3.4
3	C	206	VAL	3.4
3	C	188	GLU	3.4
3	C	204	SER	3.4
3	C	185	ALA	3.4
3	C	80	GLN	3.3
3	C	195	CYS	3.3
4	D	160	TYR	3.3
3	C	117	PHE	3.3
3	C	203	SER	3.2
4	D	109	ASN	3.2
3	C	112	ALA	3.2
2	B	453	TRP	3.2
3	C	118	ILE	3.1
3	C	78	SER	3.1
4	D	67	PHE	3.0
4	D	135	SER	3.0
2	B	166	TYR	3.0
4	D	89	ASP	3.0
3	C	84	PHE	3.0
3	C	158	GLY	2.9
3	C	198	THR	2.9
4	D	132	LYS	2.9
4	D	191	TYR	2.9
4	D	137	PHE	2.9
3	C	17	GLY	2.9
3	C	76	ILE	2.9
4	D	208	THR	2.9
3	C	202	LEU	2.9
4	D	151	ALA	2.8
3	C	3	ILE	2.8
3	C	194	ALA	2.8
4	D	134	PRO	2.8
4	D	85	LEU	2.7
4	D	105	SER	2.7
4	D	138	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	196	GLU	2.7
4	D	175	THR	2.7
3	C	191	LYS	2.7
4	D	18	LEU	2.7
4	D	228	PRO	2.7
4	D	16	GLY	2.6
4	D	65	GLY	2.6
4	D	81	GLN	2.6
3	C	63	PHE	2.6
4	D	215	HIS	2.6
4	D	133	GLY	2.6
4	D	210	ILE	2.6
2	B	672	VAL	2.6
4	D	220	THR	2.5
4	D	190	LEU	2.5
3	C	207	THR	2.5
3	C	197	VAL	2.4
3	C	27	SER	2.4
4	D	156	LEU	2.4
4	D	84	SER	2.4
3	C	167	GLN	2.4
3	C	132	SER	2.4
3	C	131	ALA	2.4
3	C	129	GLY	2.3
2	B	619	GLN	2.3
4	D	24	ALA	2.3
4	D	93	TYR	2.3
3	C	9	PRO	2.3
4	D	185	LEU	2.3
2	B	546	MET	2.3
4	D	15	GLY	2.3
3	C	153	ASN	2.3
4	D	174	LEU	2.3
4	D	1	GLU	2.3
4	D	13	GLN	2.3
2	B	615	ILE	2.3
4	D	130	SER	2.3
3	C	170	LYS	2.3
4	D	126	VAL	2.3
2	B	641	THR	2.2
2	B	594	ALA	2.2
3	C	14	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	12	VAL	2.2
3	C	121	PRO	2.1
4	D	2	VAL	2.1
3	C	16	VAL	2.1
4	D	213	VAL	2.1
3	C	59	VAL	2.1
2	B	618	PRO	2.1
4	D	82	MET	2.1
3	C	70	THR	2.1
4	D	86	ARG	2.1
4	D	3	GLN	2.1
2	B	617	ALA	2.1
4	D	136	VAL	2.0
3	C	147	VAL	2.0
3	C	60	PRO	2.0
4	D	227	GLU	2.0
3	C	146	LYS	2.0
3	C	181	THR	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 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.