Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:05 pm BST

PDB ID	:	3SQO
Title	:	PCSK9 J16 Fab complex
Authors	:	Strop, P.
Deposited on	:	2011-07-05
Resolution	:	2.70 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 ①) were used in the production of this report:

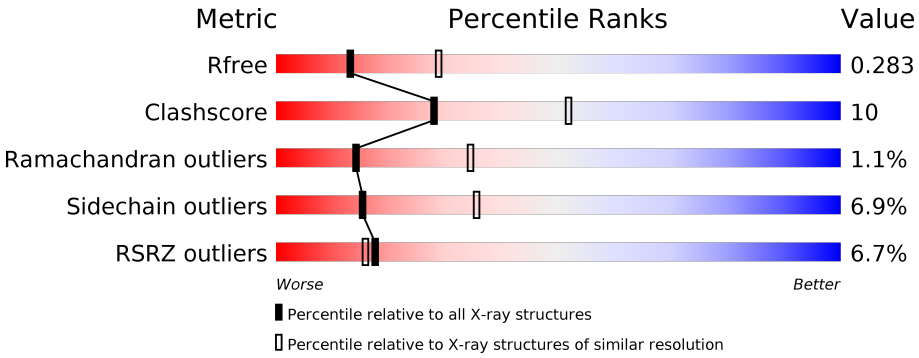
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	540	6% 69% 19% • 9%
2	H	219	11% 76% 18% • •
3	L	214	4% 79% 18% •
4	P	122	% 61% 12% • 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7658 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	491	Total	C	N	O	S	0	0	0
			3629	2238	668	691	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ILE	VAL	CONFLICT	UNP Q8NBP7
A	670	GLU	GLY	CONFLICT	UNP Q8NBP7

- Molecule 2 is a protein called J16 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1608	1012	270	318	8			

- Molecule 3 is a protein called J16 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1647	1032	280	330	5			

- Molecule 4 is a protein called PCSK9 prodomain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	92	Total	C	N	O	S	0	1	0
			742	475	134	131	2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		

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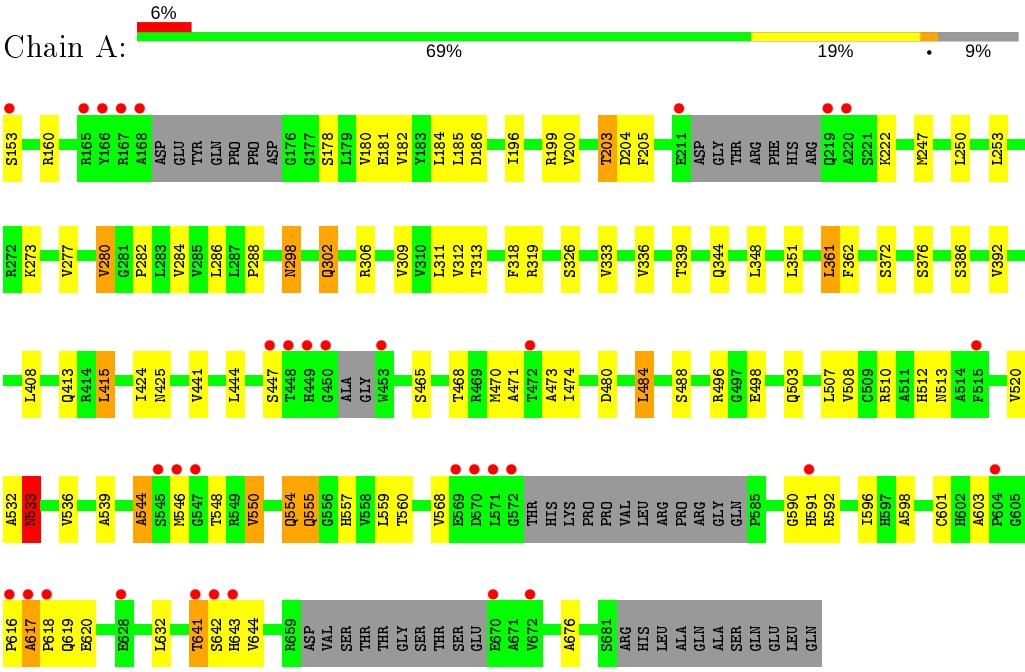
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total O 2 2	0	0
5	L	4	Total O 4 4	0	0
5	P	3	Total O 3 3	0	0

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.

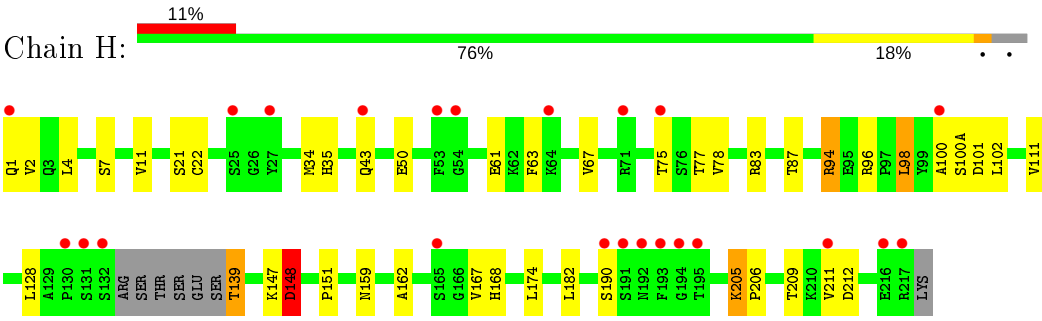
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain A:



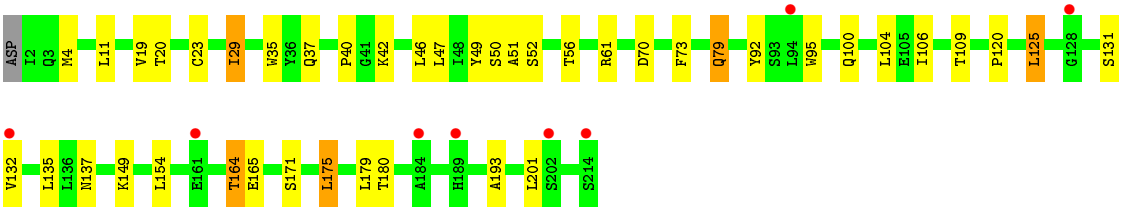
- Molecule 2: J16 Heavy chain

Chain H:

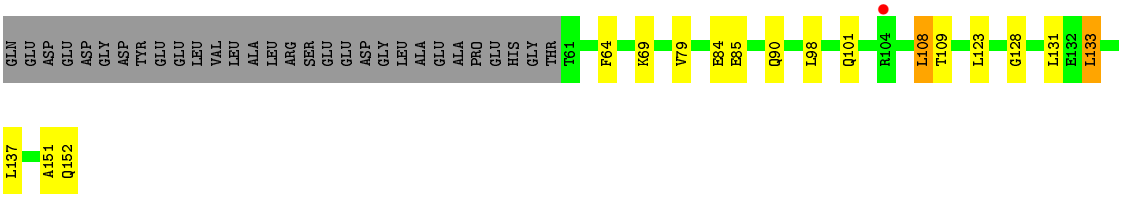


- Molecule 3: J16 Light chain

Chain L:



- Molecule 4: PCSK9 prodomain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.92Å 70.98Å 109.16Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.70) 96.5 (29.71-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.283 0.227 , 0.283	Depositor DCC
R_{free} test set	1721 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7658	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	0.43	0/3696	0.59	0/5019
2	H	0.36	0/1646	0.53	0/2240
3	L	0.43	0/1683	0.58	0/2282
4	P	0.51	0/766	0.58	0/1034
All	All	0.43	0/7791	0.57	0/10575

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	3629	0	3539	87	0
2	H	1608	0	1564	29	0
3	L	1647	0	1606	28	0
4	P	742	0	751	13	0
5	A	23	0	0	3	0
5	H	2	0	0	0	0
5	L	4	0	0	0	0
5	P	3	0	0	4	0
All	All	7658	0	7460	149	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 10.

All (149) 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:A:531:GLN:O	1:A:532:ALA:HB2	1.58	1.00
1:A:471:ALA:HB3	1:A:512:HIS:HA	1.50	0.93
3:L:120:PRO:HD3	3:L:132:VAL:HG12	1.51	0.89
4:P:64:PHE:CD1	4:P:131:LEU:HD21	2.07	0.89
1:A:531:GLN:OE1	1:A:531:GLN:CA	2.30	0.78
1:A:531:GLN:O	1:A:532:ALA:CB	2.29	0.75
1:A:531:GLN:OE1	1:A:531:GLN:HA	1.87	0.74
1:A:203:THR:OG1	1:A:250:LEU:HD23	1.88	0.74
1:A:555:GLN:HA	1:A:555:GLN:HE21	1.54	0.73
1:A:531:GLN:N	1:A:531:GLN:CD	2.36	0.71
1:A:471:ALA:HB2	1:A:513:ASN:HB2	1.73	0.71
4:P:64:PHE:CE1	4:P:131:LEU:HD21	2.26	0.70
4:P:69[A]:LYS:NZ	5:P:7:HOH:O	2.24	0.70
1:A:617:ALA:HB3	1:A:618:PRO:HD3	1.76	0.67
2:H:111:VAL:HG23	2:H:111:VAL:O	1.95	0.67
3:L:40:PRO:HG2	3:L:165:GLU:HG2	1.76	0.67
1:A:336:VAL:HG21	1:A:392:VAL:HG21	1.78	0.66
1:A:395:ILE:HG23	1:A:444:LEU:HD23	1.78	0.66
3:L:175:LEU:C	3:L:175:LEU:HD12	2.16	0.65
1:A:544:ALA:HB2	1:A:592:ARG:CZ	2.27	0.65
2:H:83:ARG:O	2:H:111:VAL:HG21	1.97	0.64
1:A:531:GLN:OE1	1:A:531:GLN:N	2.29	0.64
4:P:131:LEU:HD22	5:P:26:HOH:O	1.97	0.64
2:H:94:ARG:O	2:H:100(A):SER:HA	1.97	0.64
1:A:399:MET:HE1	1:A:415:LEU:CD1	2.30	0.62
1:A:503:GLN:HE21	1:A:508:VAL:HG21	1.65	0.62
1:A:550:VAL:HG22	1:A:596:ILE:HG23	1.82	0.62
1:A:344:GLN:NE2	1:A:425:ASN:HB3	2.16	0.60
1:A:503:GLN:NE2	1:A:508:VAL:HG21	2.17	0.60
2:H:139:THR:N	2:H:190:SER:HG	2.00	0.60
3:L:4:MET:HE3	3:L:23:CYS:SG	2.43	0.59
1:A:184:LEU:HD13	1:A:286:LEU:HD23	1.83	0.59
1:A:312:VAL:HG11	1:A:392:VAL:CG2	2.33	0.58
1:A:468:THR:HG22	5:A:32:HOH:O	2.02	0.58
3:L:29:ILE:HB	3:L:92:TYR:HB2	1.84	0.58
2:H:35:HIS:NE2	2:H:50:GLU:OE2	2.37	0.58
4:P:131:LEU:HB2	5:P:26:HOH:O	2.02	0.58
1:A:185:LEU:HD11	1:A:271:ILE:HD11	1.85	0.57
3:L:131:SER:HB3	3:L:180:THR:HG23	1.85	0.57
1:A:399:MET:HE1	1:A:415:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:GLU:HB2	3:L:95:TRP:CH2	2.40	0.57
4:P:98:LEU:HB2	4:P:137:LEU:HD11	1.87	0.56
2:H:209:THR:CG2	2:H:211:VAL:HG23	2.36	0.56
1:A:513:ASN:HD22	1:A:520:VAL:HG13	1.71	0.55
1:A:539:ALA:HB2	1:A:550:VAL:HG13	1.88	0.55
1:A:484:LEU:HD22	1:A:601:CYS:SG	2.47	0.55
1:A:548:THR:HG22	1:A:596:ILE:HG22	1.90	0.54
4:P:79:VAL:HG22	4:P:123:LEU:HD13	1.89	0.54
1:A:312:VAL:HG11	1:A:392:VAL:HG23	1.90	0.53
2:H:98:LEU:HD22	3:L:49:TYR:CD1	2.43	0.53
1:A:302:GLN:HE22	1:A:306:ARG:CZ	2.21	0.53
1:A:507:LEU:HD21	1:A:536:VAL:HG23	1.90	0.53
1:A:181:GLU:HG3	1:A:280:VAL:HG21	1.91	0.53
1:A:603:ALA:HB1	1:A:606:LEU:HG	1.91	0.53
1:A:273:LYS:O	1:A:277:VAL:HG23	2.08	0.52
1:A:488:SER:HA	1:A:523:ILE:HD12	1.90	0.52
2:H:159:ASN:HB2	2:H:162:ALA:HB3	1.90	0.52
2:H:2:VAL:HG22	2:H:102:LEU:HD22	1.92	0.52
3:L:164:THR:HG23	3:L:165:GLU:O	2.10	0.51
2:H:111:VAL:O	2:H:111:VAL:CG2	2.58	0.51
3:L:149:LYS:HB2	3:L:193:ALA:HB3	1.93	0.51
2:H:61:GLU:OE2	3:L:95:TRP:CZ2	2.64	0.51
1:A:632:LEU:HD13	1:A:676:ALA:HB1	1.93	0.50
2:H:11:VAL:CG2	2:H:151:PRO:HG3	2.42	0.50
1:A:253:LEU:HD13	4:P:151:ALA:HB2	1.92	0.50
1:A:474:ILE:HD11	1:A:510:ARG:HH11	1.76	0.50
1:A:530:PRO:O	1:A:531:GLN:O	2.30	0.50
3:L:29:ILE:HB	3:L:92:TYR:CB	2.40	0.50
1:A:318:PHE:HA	1:A:351:LEU:HD22	1.93	0.50
1:A:339:THR:HG21	1:A:424:ILE:CD1	2.41	0.50
1:A:200:VAL:HG22	1:A:247:MET:HB2	1.94	0.50
1:A:302:GLN:NE2	1:A:306:ARG:CZ	2.75	0.49
1:A:559:LEU:CD1	1:A:598:ALA:HB1	2.42	0.49
2:H:182:LEU:C	2:H:182:LEU:HD12	2.33	0.49
1:A:336:VAL:HG21	1:A:392:VAL:CG2	2.42	0.49
1:A:424:ILE:HD11	1:A:441:VAL:CG2	2.42	0.49
3:L:179:LEU:HD12	3:L:180:THR:N	2.27	0.49
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.48	0.49
4:P:108:LEU:HD13	4:P:109:THR:N	2.28	0.49
4:P:101:GLN:HE21	4:P:133:LEU:HD11	1.78	0.48
2:H:87:THR:OG1	2:H:111:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ALA:HB3	1:A:512:HIS:CA	2.34	0.48
1:A:180:VAL:HG22	1:A:282:PRO:HG2	1.95	0.48
1:A:568:VAL:O	1:A:568:VAL:HG23	2.13	0.48
1:A:554:GLN:HB2	1:A:557:HIS:CG	2.48	0.48
1:A:339:THR:HG23	1:A:362:PHE:HB3	1.94	0.47
2:H:167:VAL:CG1	2:H:168:HIS:N	2.78	0.47
2:H:4:LEU:HD21	2:H:34:MET:HE1	1.97	0.47
3:L:50:SER:O	3:L:51:ALA:HB3	2.14	0.47
2:H:4:LEU:CD2	2:H:34:MET:HE1	2.45	0.47
1:A:554:GLN:HE21	1:A:554:GLN:HA	1.80	0.47
1:A:313:THR:HB	1:A:333:VAL:HG11	1.96	0.46
3:L:154:LEU:O	3:L:154:LEU:HD12	2.15	0.46
2:H:2:VAL:HG22	2:H:102:LEU:CD2	2.45	0.46
1:A:253:LEU:HD22	1:A:257:GLY:O	2.16	0.46
2:H:167:VAL:HG12	2:H:168:HIS:N	2.31	0.45
4:P:64:PHE:CG	4:P:131:LEU:HD21	2.51	0.45
3:L:154:LEU:C	3:L:154:LEU:HD12	2.37	0.45
1:A:617:ALA:HB3	1:A:618:PRO:CD	2.45	0.45
2:H:101:ASP:HB3	3:L:46:LEU:HD23	1.99	0.45
2:H:61:GLU:OE2	3:L:95:TRP:HZ2	2.00	0.45
1:A:309:VAL:O	1:A:311:LEU:HD12	2.17	0.45
1:A:641:THR:HG21	1:A:644:VAL:CG1	2.47	0.45
1:A:471:ALA:HB2	1:A:513:ASN:N	2.31	0.45
3:L:11:LEU:CD2	3:L:19:VAL:HG13	2.47	0.45
2:H:11:VAL:HG22	2:H:151:PRO:HG3	1.99	0.44
1:A:205:PHE:CE1	1:A:266:ILE:HG22	2.52	0.44
2:H:205:LYS:N	2:H:206:PRO:CD	2.80	0.44
1:A:496:ARG:HD2	5:A:27:HOH:O	2.16	0.44
1:A:548:THR:HG22	1:A:596:ILE:CG2	2.48	0.44
3:L:29:ILE:O	3:L:29:ILE:CG1	2.65	0.44
1:A:182:VAL:HG22	1:A:284:VAL:HB	1.99	0.43
1:A:641:THR:HG22	1:A:642:SER:H	1.84	0.43
2:H:7:SER:HB3	2:H:21:SER:HB3	2.00	0.43
1:A:153:SER:N	3:L:56:THR:HG1	2.16	0.43
1:A:471:ALA:HA	5:A:32:HOH:O	2.18	0.43
1:A:468:THR:HG23	1:A:470:MET:H	1.84	0.42
1:A:250:LEU:HD11	1:A:271:ILE:CG1	2.50	0.42
1:A:532:ALA:O	1:A:533:ASN:C	2.57	0.42
2:H:63:PHE:O	2:H:67:VAL:HG12	2.19	0.42
3:L:120:PRO:HB2	3:L:125:LEU:HD11	2.01	0.42
1:A:344:GLN:HE22	1:A:425:ASN:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:104:LEU:HA	3:L:104:LEU:HD23	1.94	0.42
1:A:613:HIS:CE1	1:A:615:ILE:HD11	2.55	0.42
1:A:615:ILE:HG21	1:A:619:GLN:HG3	2.02	0.42
1:A:203:THR:O	1:A:204:ASP:HB2	2.20	0.42
1:A:361:LEU:HD12	1:A:361:LEU:N	2.35	0.42
3:L:106:ILE:HG21	3:L:171:SER:OG	2.20	0.42
1:A:196:ILE:HD12	1:A:200:VAL:HG21	2.02	0.41
3:L:11:LEU:HD21	3:L:19:VAL:HG13	2.02	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.03	0.41
3:L:61:ARG:CZ	3:L:79:GLN:HG3	2.49	0.41
1:A:530:PRO:HD2	1:A:531:GLN:NE2	2.34	0.41
1:A:531:GLN:H	1:A:531:GLN:CD	2.22	0.41
1:A:484:LEU:HD13	1:A:560:THR:HG21	2.02	0.41
2:H:147:LYS:HG2	2:H:148:ASP:CG	2.40	0.41
2:H:75:THR:OG1	2:H:77:THR:HG22	2.21	0.41
1:A:386:SER:OG	4:P:152:GLN:C	2.59	0.41
1:A:507:LEU:CD2	1:A:536:VAL:HG23	2.51	0.41
2:H:34:MET:HG3	2:H:78:VAL:HG21	2.03	0.41
1:A:186:ASP:OD2	1:A:288:PRO:HG2	2.20	0.41
1:A:533:ASN:N	1:A:533:ASN:OD1	2.54	0.41
1:A:632:LEU:CD1	1:A:676:ALA:HB1	2.50	0.41
1:A:298:ASN:ND2	1:A:326:SER:OG	2.53	0.41
1:A:465:SER:HB3	1:A:473:ALA:HB2	2.02	0.41
1:A:539:ALA:CB	1:A:550:VAL:HG13	2.50	0.40
4:P:128:GLY:HA2	5:P:26:HOH:O	2.20	0.40
1:A:590:GLY:HA3	1:A:596:ILE:HD12	2.04	0.40
1:A:641:THR:HG21	1:A:644:VAL:CG2	2.52	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	479/540 (89%)	447 (93%)	25 (5%)	7 (2%)	10 26
2	H	205/219 (94%)	186 (91%)	16 (8%)	3 (2%)	10 26
3	L	211/214 (99%)	201 (95%)	10 (5%)	0	100 100
4	P	91/122 (75%)	86 (94%)	4 (4%)	1 (1%)	14 34
All	All	986/1095 (90%)	920 (93%)	55 (6%)	11 (1%)	14 34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	SER
1	A	531	GLN
2	H	100	ALA
1	A	533	ASN
1	A	544	ALA
4	P	84	GLU
1	A	616	PRO
2	H	148	ASP
2	H	43	GLN
1	A	280	VAL
1	A	617	ALA

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	389/431 (90%)	360 (92%)	29 (8%)	13 31
2	H	182/190 (96%)	171 (94%)	11 (6%)	19 42
3	L	186/187 (100%)	172 (92%)	14 (8%)	13 31
4	P	80/103 (78%)	76 (95%)	4 (5%)	24 51
All	All	837/911 (92%)	779 (93%)	58 (7%)	15 35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ARG
1	A	178	SER
1	A	199	ARG
1	A	203	THR
1	A	222	LYS
1	A	298	ASN
1	A	302	GLN
1	A	319	ARG
1	A	348	LEU
1	A	361	LEU
1	A	372	SER
1	A	376	SER
1	A	401	SER
1	A	408	LEU
1	A	413	GLN
1	A	415	LEU
1	A	480	ASP
1	A	484	LEU
1	A	498	GLU
1	A	531	GLN
1	A	533	ASN
1	A	546	MET
1	A	550	VAL
1	A	554	GLN
1	A	555	GLN
1	A	591	HIS
1	A	620	GLU
1	A	641	THR
1	A	643	HIS
2	H	1	GLN
2	H	22	CYS
2	H	94	ARG
2	H	96	ARG
2	H	98	LEU
2	H	128	LEU
2	H	139	THR
2	H	148	ASP
2	H	174	LEU
2	H	205	LYS
2	H	212	ASP
3	L	20	THR
3	L	29	ILE
3	L	42	LYS

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Mol	Chain	Res	Type
3	L	52	SER
3	L	70	ASP
3	L	79	GLN
3	L	100	GLN
3	L	109	THR
3	L	125	LEU
3	L	135	LEU
3	L	137	ASN
3	L	164	THR
3	L	175	LEU
3	L	201	LEU
4	P	85	GLU
4	P	90	GLN
4	P	108	LEU
4	P	133	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	219	GLN
1	A	298	ASN
1	A	302	GLN
1	A	344	GLN
1	A	413	GLN
1	A	513	ASN
1	A	554	GLN
1	A	555	GLN
1	A	587	GLN
1	A	652	ASN
2	H	204	HIS
3	L	79	GLN
3	L	100	GLN
3	L	160	GLN
4	P	65	HIS
4	P	101	GLN

5.3.3 RNA

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 carbohydrates 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, 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	491/540 (90%)	0.31	35 (7%) 16 14	23, 46, 89, 132	0
2	H	211/219 (96%)	0.56	23 (10%) 5 4	40, 72, 104, 153	0
3	L	213/214 (99%)	0.11	8 (3%) 40 39	35, 57, 91, 118	0
4	P	92/122 (75%)	-0.17	1 (1%) 80 82	26, 39, 51, 61	0
All	All	1007/1095 (91%)	0.28	67 (6%) 17 16	23, 53, 95, 153	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	194	GLY	13.9
1	A	448	THR	9.5
2	H	195	THR	7.6
2	H	131	SER	6.9
1	A	571	LEU	5.9
1	A	168	ALA	5.9
1	A	545	SER	5.7
1	A	450	GLY	5.4
1	A	220	ALA	5.3
3	L	214	SER	5.2
1	A	546	MET	5.2
2	H	193	PHE	4.9
1	A	570	ASP	4.8
1	A	167	ARG	4.6
1	A	572	GLY	4.5
1	A	165	ARG	4.5
2	H	1	GLN	4.4
2	H	53	PHE	4.4
1	A	166	TYR	4.2
1	A	618	PRO	4.0
2	H	192	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	191	SER	3.8
2	H	54	GLY	3.4
2	H	132	SER	3.3
1	A	569	GLU	3.2
1	A	515	PHE	3.0
2	H	217	ARG	3.0
1	A	604	PRO	3.0
2	H	43	GLN	2.9
1	A	153	SER	2.9
1	A	447	SER	2.9
1	A	547	GLY	2.8
2	H	190	SER	2.8
1	A	453	TRP	2.8
1	A	643	HIS	2.8
2	H	27	TYR	2.8
1	A	219	GLN	2.7
3	L	94	LEU	2.7
1	A	641	THR	2.7
1	A	472	THR	2.5
1	A	211	GLU	2.4
1	A	628	GLU	2.4
1	A	642	SER	2.3
1	A	670	GLU	2.3
2	H	165	SER	2.2
3	L	161	GLU	2.2
1	A	531	GLN	2.2
2	H	75	THR	2.2
2	H	130	PRO	2.2
3	L	132	VAL	2.2
1	A	615	ILE	2.2
4	P	104	ARG	2.2
1	A	617	ALA	2.1
3	L	184	ALA	2.1
1	A	616	PRO	2.1
1	A	672	VAL	2.1
2	H	64	LYS	2.1
3	L	189	HIS	2.1
2	H	100	ALA	2.1
3	L	128	GLY	2.1
1	A	449	HIS	2.1
2	H	71	ARG	2.1
1	A	591	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	25	SER	2.0
2	H	211	VAL	2.0
2	H	216	GLU	2.0
3	L	202	SER	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.