



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 3H42 / pdb_00003h42
Title : Crystal structure of PCSK9 in complex with Fab from LDLR competitive antibody
Authors : Piper, D.E.; Walker, N.P.C.; Romanow, W.G.; Thibault, S.T.; Tsai, M.M.; Yang, E.
Deposited on : 2009-04-17
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

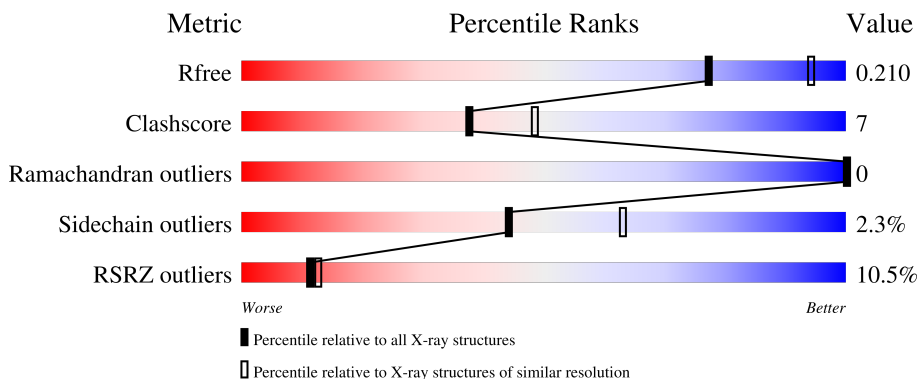
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

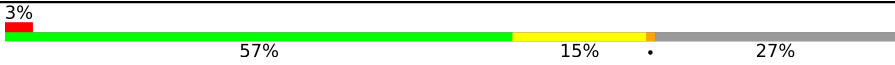
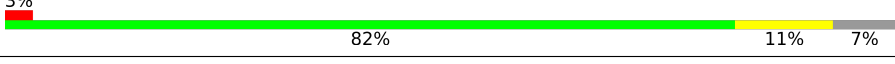
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	126	
2	B	540	
3	L	217	
4	H	238	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8196 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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q8NBP7
A	28	ALA	-	expression tag	UNP Q8NBP7
A	29	MET	-	expression tag	UNP Q8NBP7
A	30	GLY	-	expression tag	UNP Q8NBP7

- 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 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	533	ALA	ASN	engineered mutation	UNP Q8NBP7
B	620	GLY	GLU	SEE REMARK 999	UNP Q8NBP7

- Molecule 3 is a protein called Fab from LDLR competitive antibody: Light chain.

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

- Molecule 4 is a protein called Fab from LDLR competitive antibody: Heavy chain.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	233	HIS	-	expression tag	PDB 3H42
H	234	HIS	-	expression tag	PDB 3H42
H	235	HIS	-	expression tag	PDB 3H42
H	236	HIS	-	expression tag	PDB 3H42
H	237	HIS	-	expression tag	PDB 3H42
H	238	HIS	-	expression tag	PDB 3H42

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

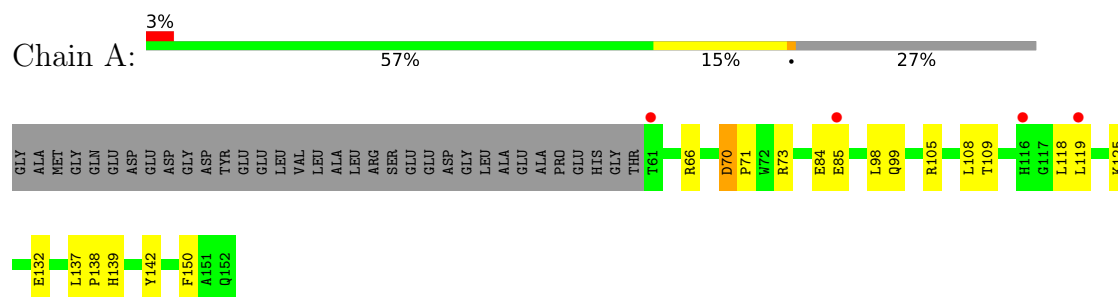
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	178	Total	O	0	0
			178	178		
6	L	159	Total	O	0	0
			159	159		
6	H	155	Total	O	0	0
			155	155		

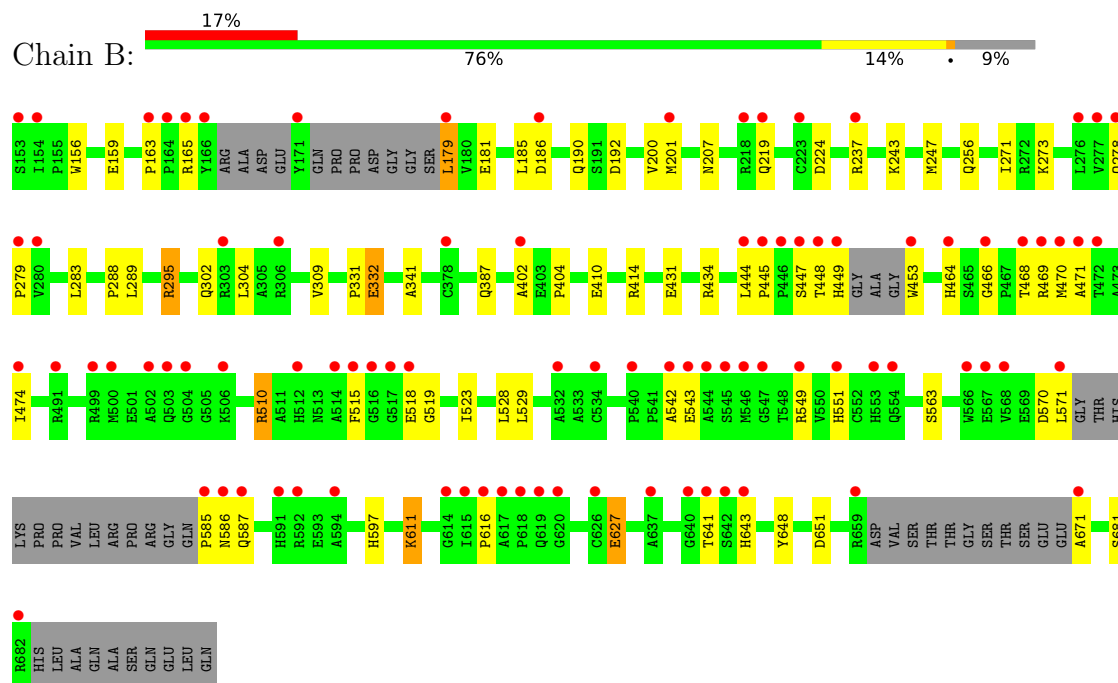
3 Residue-property plots

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.

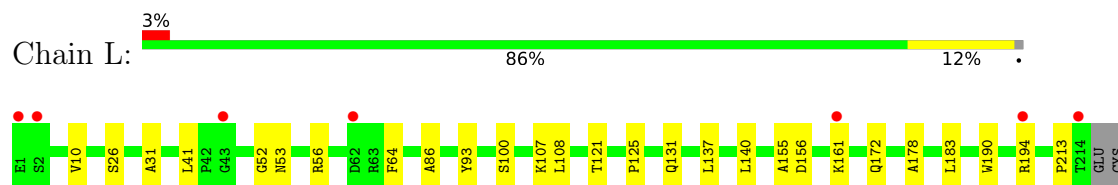
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



- Molecule 2: Proprotein convertase subtilisin/kexin type 9

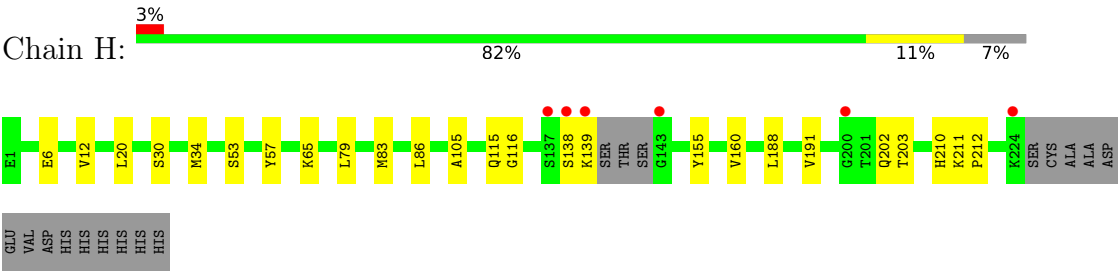


- Molecule 3: Fab from LDLR competitive antibody: Light chain



SER

● Molecule 4: Fab from LDLR competitive antibody: Heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.72Å 137.35Å 69.89Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.30) 99.8 (40.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.209 0.191 , 0.210	Depositor DCC
R_{free} test set	5376 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8196	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

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	0.33	0/757	0.65	0/1023
2	B	0.34	0/3729	0.72	3/5064 (0.1%)
3	L	0.35	0/1605	0.71	0/2192
4	H	0.35	0/1701	0.71	0/2313
All	All	0.35	0/7792	0.71	3/10592 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	466	GLY	CA-C-N	5.72	125.33	119.56
2	B	466	GLY	C-N-CA	5.72	125.33	119.56
2	B	651	ASP	CB-CA-C	-5.09	110.31	117.23

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	15	0
2	B	3659	0	3572	57	0
3	L	1568	0	1518	18	0
4	H	1660	0	1610	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	76	0	0	2	0
6	B	178	0	0	1	0
6	H	155	0	0	1	0
6	L	159	0	0	2	0
All	All	8196	0	7450	105	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 7.

All (105) 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:474:ILE:HD11	2:B:510:ARG:HH21	1.40	0.84
2:B:200:VAL:HG12	2:B:247:MET:HB2	1.60	0.82
1:A:66:ARG:HH21	1:A:73:ARG:HD2	1.43	0.81
2:B:474:ILE:HD11	2:B:510:ARG:NH2	1.97	0.80
2:B:402:ALA:HB1	2:B:448:THR:HG23	1.65	0.77
2:B:414:ARG:HH11	2:B:414:ARG:HG3	1.50	0.74
2:B:468:THR:HB	2:B:471:ALA:HB2	1.71	0.73
2:B:332:GLU:H	2:B:332:GLU:CD	2.00	0.69
2:B:469:ARG:HB2	2:B:515:PHE:HD2	1.58	0.68
2:B:278:GLN:HB3	2:B:279:PRO:HD2	1.76	0.68
2:B:302:GLN:HA	2:B:332:GLU:HG3	1.76	0.67
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.78	0.66
2:B:186:ASP:OD1	2:B:288:PRO:HG2	1.97	0.65
4:H:138:SER:C	4:H:139:LYS:HD2	2.21	0.65
2:B:570:ASP:C	2:B:571:LEU:HD12	2.23	0.64
2:B:523:ILE:HD13	2:B:648:TYR:HB3	1.80	0.63
3:L:125:PRO:HD3	3:L:137:LEU:CD2	2.28	0.63
1:A:84:GLU:O	1:A:85:GLU:HB2	2.01	0.60
1:A:66:ARG:NH2	1:A:73:ARG:HD2	2.17	0.58
3:L:108:LEU:C	3:L:108:LEU:HD23	2.28	0.58
2:B:304:LEU:HD22	2:B:309:VAL:HG21	1.86	0.58
2:B:641:THR:HG22	2:B:643:HIS:H	1.69	0.57
2:B:414:ARG:HG3	2:B:414:ARG:NH1	2.18	0.56
2:B:468:THR:HG22	2:B:470:MET:H	1.71	0.56
2:B:445:PRO:C	2:B:447:SER:H	2.13	0.55
2:B:448:THR:O	2:B:449:HIS:HB2	2.05	0.55
2:B:179:LEU:HD13	2:B:404:PRO:HG3	1.89	0.54
2:B:611:LYS:HB3	2:B:611:LYS:NZ	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:20:LEU:HG	4:H:83:MET:HE2	1.90	0.54
4:H:34:MET:HB3	4:H:79:LEU:HD22	1.91	0.53
4:H:160:VAL:CG2	4:H:188:LEU:HD21	2.38	0.53
2:B:256:GLN:HB3	4:H:57:TYR:CZ	2.44	0.53
4:H:6:GLU:CD	4:H:116:GLY:H	2.17	0.52
3:L:125:PRO:HD3	3:L:137:LEU:HD21	1.91	0.52
2:B:331:PRO:HD2	2:B:332:GLU:OE2	2.10	0.51
2:B:474:ILE:CD1	2:B:510:ARG:HH21	2.20	0.51
4:H:202:GLN:HE21	4:H:203:THR:N	2.08	0.51
1:A:118:LEU:O	1:A:119:LEU:HD23	2.12	0.50
3:L:140:LEU:CD1	4:H:191:VAL:HG21	2.42	0.50
4:H:188:LEU:C	4:H:188:LEU:HD12	2.37	0.50
1:A:142:TYR:CE1	2:B:295:ARG:HG2	2.47	0.49
4:H:160:VAL:HG22	4:H:188:LEU:HD21	1.95	0.49
1:A:132:GLU:HG2	6:A:177:HOH:O	2.13	0.48
2:B:283:LEU:HD21	2:B:309:VAL:HG22	1.95	0.48
2:B:464:HIS:NE2	2:B:519:GLY:HA3	2.28	0.48
2:B:563:SER:HB2	2:B:597:HIS:HB2	1.96	0.48
2:B:190:GLN:NE2	2:B:192:ASP:HB2	2.28	0.48
4:H:160:VAL:HG12	4:H:210:HIS:CD2	2.48	0.48
2:B:542:ALA:O	2:B:543:GLU:HB2	2.14	0.47
3:L:155:ALA:O	3:L:156:ASP:HB2	2.15	0.47
3:L:26:SER:O	3:L:31:ALA:HB2	2.15	0.47
2:B:283:LEU:HD23	2:B:283:LEU:H	1.79	0.47
3:L:56:ARG:HD3	3:L:64:PHE:O	2.14	0.47
3:L:156:ASP:OD1	3:L:194:ARG:HB2	2.16	0.46
2:B:289:LEU:HD12	2:B:289:LEU:C	2.40	0.46
3:L:137:LEU:HD12	3:L:183:LEU:HD23	1.98	0.46
2:B:224:ASP:HB2	6:B:759:HOH:O	2.16	0.46
2:B:156:TRP:CZ3	2:B:341:ALA:HA	2.50	0.45
3:L:41:LEU:HD23	3:L:86:ALA:HB2	1.98	0.45
4:H:115:GLN:NE2	6:H:461:HOH:O	2.49	0.45
2:B:190:GLN:HE21	2:B:192:ASP:H	1.64	0.45
2:B:387:GLN:NE2	2:B:387:GLN:H	2.15	0.45
3:L:125:PRO:HD3	3:L:137:LEU:HD23	1.98	0.44
2:B:611:LYS:HD3	2:B:627:GLU:OE2	2.18	0.44
4:H:202:GLN:HE21	4:H:203:THR:H	1.64	0.44
4:H:211:LYS:N	4:H:212:PRO:CD	2.81	0.44
1:A:105:ARG:HH21	1:A:105:ARG:HG3	1.82	0.44
1:A:84:GLU:O	1:A:85:GLU:CB	2.65	0.44
1:A:150:PHE:CG	4:H:105:ALA:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ARG:O	2:B:243:LYS:HD3	2.19	0.43
2:B:571:LEU:HD12	2:B:571:LEU:N	2.32	0.43
1:A:138:PRO:O	1:A:139:HIS:HB2	2.19	0.43
2:B:453:TRP:CZ3	2:B:681:SER:HB2	2.53	0.43
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.91	0.43
2:B:332:GLU:CD	2:B:332:GLU:N	2.74	0.43
3:L:190:TRP:CZ2	3:L:213:PRO:HA	2.54	0.43
1:A:70:ASP:N	1:A:71:PRO:HD2	2.33	0.43
4:H:12:VAL:HG11	4:H:86:LEU:HD13	2.00	0.43
4:H:65:LYS:HE2	4:H:65:LYS:HB2	1.77	0.42
2:B:431:GLU:HA	2:B:434:ARG:HD2	2.02	0.42
2:B:616:PRO:HA	2:B:671:ALA:HB2	2.01	0.42
3:L:10:VAL:HG12	6:L:456:HOH:O	2.20	0.42
3:L:93:TYR:HA	3:L:100:SER:HA	2.00	0.42
2:B:469:ARG:HB2	2:B:515:PHE:CD2	2.46	0.42
2:B:273:LYS:HE2	2:B:273:LYS:HB2	1.86	0.42
1:A:108:LEU:HD12	6:A:167:HOH:O	2.20	0.41
2:B:445:PRO:C	2:B:447:SER:N	2.78	0.41
3:L:161:LYS:HB2	6:L:484:HOH:O	2.19	0.41
2:B:185:LEU:O	2:B:288:PRO:HD2	2.21	0.41
3:L:172:GLN:OE1	3:L:178:ALA:HB2	2.21	0.41
2:B:549:ARG:HH11	2:B:587:GLN:HE22	1.67	0.41
1:A:98:LEU:HB2	1:A:137:LEU:HD11	2.02	0.41
2:B:414:ARG:NH1	2:B:414:ARG:CG	2.82	0.41
2:B:302:GLN:HA	2:B:332:GLU:CG	2.47	0.41
3:L:194:ARG:HA	3:L:194:ARG:HD3	1.92	0.41
4:H:30:SER:O	4:H:53:SER:HB2	2.21	0.41
2:B:185:LEU:HD12	2:B:185:LEU:N	2.36	0.41
2:B:585:PRO:O	2:B:586:ASN:HB2	2.20	0.41
2:B:163:PRO:HG3	2:B:444:LEU:O	2.22	0.40
1:A:99:GLN:HG2	1:A:109:THR:OG1	2.21	0.40
2:B:469:ARG:HG3	2:B:470:MET:HG2	2.04	0.40
3:L:52:GLY:O	3:L:53:ASN:HB2	2.22	0.40
2:B:410:GLU:HA	2:B:528:LEU:HD11	2.04	0.40
2:B:551:HIS:HB2	2:B:586:ASN:O	2.22	0.40
4:H:155:TYR:CE1	4:H:160:VAL:HG13	2.57	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	90/126 (71%)	87 (97%)	3 (3%)	0	100	100
2	B	481/540 (89%)	466 (97%)	15 (3%)	0	100	100
3	L	212/217 (98%)	207 (98%)	5 (2%)	0	100	100
4	H	217/238 (91%)	216 (100%)	1 (0%)	0	100	100
All	All	1000/1121 (89%)	976 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	79/104 (76%)	77 (98%)	2 (2%)	42	60
2	B	392/429 (91%)	378 (96%)	14 (4%)	31	47
3	L	177/180 (98%)	174 (98%)	3 (2%)	53	72
4	H	186/201 (92%)	186 (100%)	0	100	100
All	All	834/914 (91%)	815 (98%)	19 (2%)	44	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	125	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	159	GLU
2	B	165	ARG
2	B	179	LEU
2	B	181	GLU
2	B	201	MET
2	B	207	ASN
2	B	219	GLN
2	B	295	ARG
2	B	332	GLU
2	B	510	ARG
2	B	518	GLU
2	B	529	LEU
2	B	611	LYS
2	B	627	GLU
3	L	107	LYS
3	L	121	THR
3	L	131	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
2	B	190	GLN
2	B	382	GLN
2	B	387	GLN
2	B	553	HIS
2	B	557	HIS
2	B	587	GLN
2	B	643	HIS
3	L	40	GLN
4	H	3	GLN
4	H	39	GLN
4	H	82	GLN
4	H	84	ASN
4	H	115	GLN
4	H	202	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	92/126 (73%)	-0.02	4 (4%) 40 41	22, 39, 56, 69	0
2	B	492/540 (91%)	0.82	90 (18%) 3 4	23, 48, 93, 116	0
3	L	214/217 (98%)	-0.08	7 (3%) 49 51	23, 36, 61, 75	0
4	H	221/238 (92%)	-0.01	6 (2%) 56 58	23, 38, 57, 91	0
All	All	1019/1121 (90%)	0.37	107 (10%) 11 13	22, 41, 83, 116	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	546	MET	7.1
2	B	453	TRP	7.0
2	B	515	PHE	6.8
2	B	171	TYR	6.4
2	B	166	TYR	6.3
2	B	571	LEU	6.3
2	B	447	SER	6.0
2	B	179	LEU	5.5
2	B	280	VAL	5.2
2	B	449	HIS	5.1
2	B	544	ALA	5.1
2	B	469	ARG	5.1
2	B	643	HIS	5.0
4	H	139	LYS	5.0
2	B	545	SER	5.0
3	L	214	THR	4.8
2	B	617	ALA	4.7
2	B	470	MET	4.5
2	B	277	VAL	4.5
2	B	585	PRO	4.4
2	B	448	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	446	PRO	4.4
2	B	682	ARG	4.3
4	H	138	SER	4.3
2	B	468	THR	4.3
2	B	153	SER	4.3
4	H	143	GLY	4.3
1	A	61	THR	4.2
2	B	620	GLY	4.1
2	B	642	SER	4.0
2	B	516	GLY	4.0
2	B	671	ALA	3.9
4	H	137	SER	3.9
2	B	568	VAL	3.8
2	B	659	ARG	3.8
2	B	553	HIS	3.7
2	B	471	ALA	3.6
2	B	279	PRO	3.6
2	B	641	THR	3.6
2	B	549	ARG	3.5
4	H	200	GLY	3.5
2	B	378	CYS	3.5
1	A	85	GLU	3.4
2	B	619	GLN	3.4
2	B	445	PRO	3.4
2	B	504	GLY	3.4
2	B	547	GLY	3.3
2	B	640	GLY	3.3
2	B	616	PRO	3.3
2	B	466	GLY	3.3
2	B	586	ASN	3.3
2	B	165	ARG	3.2
4	H	224	LYS	3.1
2	B	615	ILE	3.1
3	L	161	LYS	3.1
2	B	514	ALA	3.1
2	B	499	ARG	3.0
2	B	503	GLN	2.9
2	B	164	PRO	2.9
2	B	223	CYS	2.9
3	L	1	GLU	2.8
3	L	194	ARG	2.8
2	B	303	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	554	GLN	2.7
2	B	543	GLU	2.7
2	B	276	LEU	2.7
2	B	186	ASP	2.6
3	L	43	GLY	2.6
2	B	542	ALA	2.6
2	B	218	ARG	2.6
2	B	444	LEU	2.5
2	B	278	GLN	2.5
2	B	518	GLU	2.5
2	B	491	ARG	2.4
2	B	626	CYS	2.4
2	B	474	ILE	2.4
2	B	506	LYS	2.4
2	B	201	MET	2.4
2	B	618	PRO	2.4
2	B	517	GLY	2.4
2	B	219	GLN	2.4
2	B	592	ARG	2.4
2	B	464	HIS	2.3
2	B	551	HIS	2.3
2	B	587	GLN	2.3
2	B	540	PRO	2.3
2	B	402	ALA	2.3
1	A	116	HIS	2.3
2	B	534	CYS	2.3
2	B	567	GLU	2.3
1	A	119	LEU	2.2
2	B	532	ALA	2.2
2	B	237	ARG	2.2
2	B	512	HIS	2.2
2	B	591	HIS	2.2
2	B	502	ALA	2.2
2	B	594	ALA	2.2
2	B	500	MET	2.2
2	B	163	PRO	2.2
3	L	62	ASP	2.1
2	B	306	ARG	2.1
2	B	637	ALA	2.1
2	B	472	THR	2.0
2	B	154	ILE	2.0
2	B	614	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	566	TRP	2.0
3	L	2	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	B	1	1/1	0.86	0.38	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.