



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:01 AM GMT

PDB ID : 3M0C
Title : The X-ray Crystal Structure of PCSK9 in Complex with the LDL receptor
Authors : Spraggon, G.; Hampton, E.N.
Deposited on : 2010-03-02
Resolution : 7.01 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

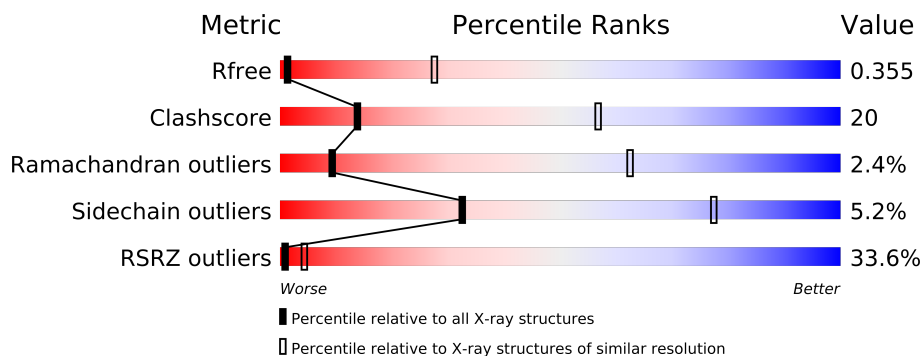
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 7.01 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}	66092	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	124	
2	B	546	
3	C	791	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7705 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1	0
			748	479	136	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total	C	N	O	S	0	1	0
			3618	2234	668	684	32			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	TYR	ASP	ENGINEERED	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

- Molecule 3 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	430	Total	C	N	O	S	0	0	0
			3336	2079	578	647	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	768	HIS	-	EXPRESSION TAG	UNP P01130
C	769	HIS	-	EXPRESSION TAG	UNP P01130
C	770	HIS	-	EXPRESSION TAG	UNP P01130

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	HIS	-	EXPRESSION TAG	UNP P01130
C	772	HIS	-	EXPRESSION TAG	UNP P01130
C	773	HIS	-	EXPRESSION TAG	UNP P01130

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

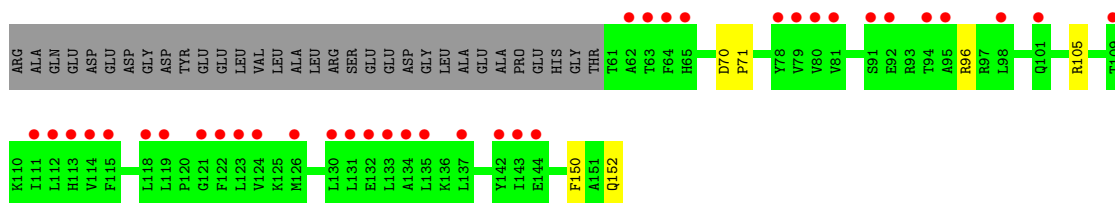
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Ca 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

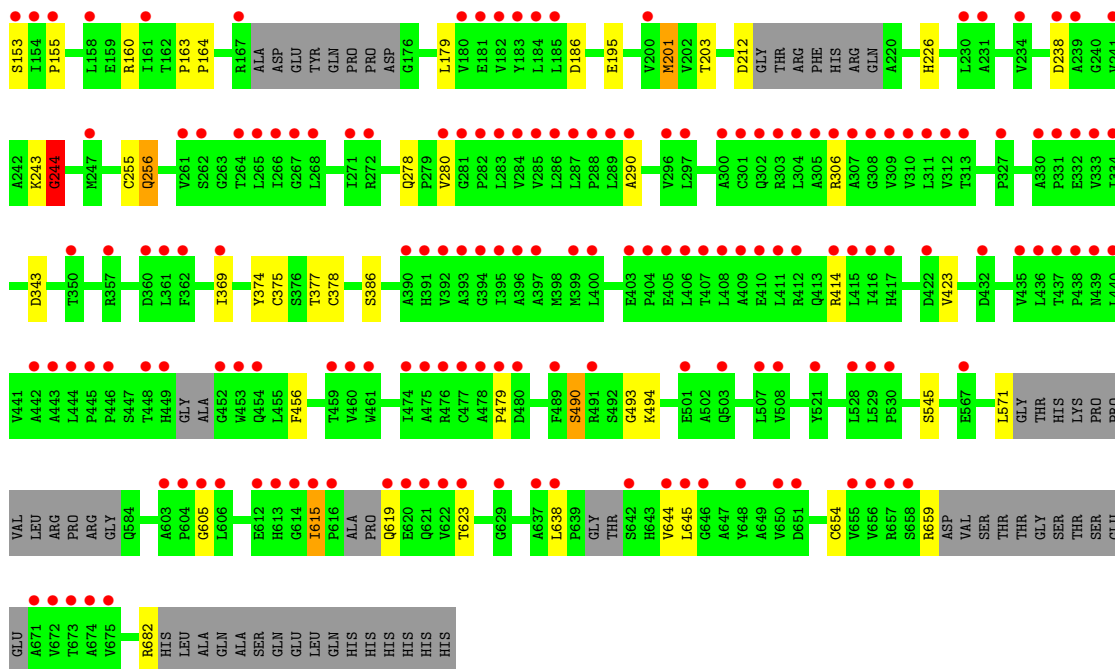
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain A:



- Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain B:



- Molecule 3: Low-density lipoprotein receptor

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	322.91Å 322.91Å 76.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	279.64 – 7.01 279.64 – 7.01	Depositor EDS
% Data completeness (in resolution range)	82.2 (279.64-7.01) 97.7 (279.64-7.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 6.74Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.341 , 0.362 0.339 , 0.355	Depositor DCC
R_{free} test set	337 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	247.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 182.2	EDS
Estimated twinning fraction	0.189 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	0 of 7313 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	7705	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	0.80	0/768	0.77	0/1037
2	B	0.73	3/3687 (0.1%)	0.75	1/5003 (0.0%)
3	C	0.65	3/3405 (0.1%)	1.09	21/4628 (0.5%)
All	All	0.70	6/7860 (0.1%)	0.91	22/10668 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	487	ARG	CD-NE	-17.20	1.17	1.46
3	C	444	TYR	N-CA	-17.05	1.12	1.46
3	C	343	CYS	CB-SG	-8.72	1.67	1.82
2	B	654	CYS	CB-SG	-6.39	1.71	1.82
2	B	255	CYS	C-N	-5.59	1.21	1.34
2	B	256	GLN	C-N	-5.31	1.23	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	428	ARG	NE-CZ-NH2	-9.01	115.80	120.30
3	C	518	PRO	N-CA-CB	8.64	113.67	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	517	THR	CA-C-O	-8.61	102.01	120.10
3	C	346	LEU	N-CA-C	7.29	130.68	111.00
3	C	444	TYR	N-CA-CB	6.68	122.63	110.60
3	C	367	HIS	N-CA-C	-6.67	93.00	111.00
3	C	518	PRO	CA-N-CD	-6.61	102.25	111.50
2	B	179	LEU	CA-CB-CG	6.42	130.07	115.30
3	C	499	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	C	281	CYS	N-CA-C	-6.22	94.21	111.00
3	C	272	ASP	N-CA-C	-6.01	94.77	111.00
3	C	366	PRO	N-CA-C	5.98	127.64	112.10
3	C	287	GLU	C-N-CD	5.77	140.52	128.40
3	C	286	ASP	N-CA-C	-5.76	95.45	111.00
3	C	612	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	C	518	PRO	N-CD-CG	5.64	111.66	103.20
3	C	263	CYS	N-CA-C	-5.61	95.86	111.00
3	C	262	LYS	N-CA-C	-5.56	95.98	111.00
3	C	274	VAL	N-CA-C	5.53	125.94	111.00
3	C	630	ASP	CB-CG-OD2	-5.33	113.50	118.30
3	C	263	CYS	CA-CB-SG	5.32	123.57	114.00
3	C	268	CYS	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	B	494	LYS	Peptide
3	C	517	THR	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	748	0	0	4	2
2	B	3618	0	0	22	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3336	0	0	136	8
4	C	3	0	0	0	0
All	All	7705	0	0	151	8

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:340:PRO:O	3:C:342:THR:N	1.58	1.35
3:C:323:PHE:CZ	3:C:351:GLU:OE2	1.94	1.21
3:C:463:ILE:CG2	3:C:644:ASN:CB	2.25	1.14
3:C:527:ASN:CA	3:C:661:LEU:CD1	2.27	1.13
2:B:377:THR:OG1	3:C:309:ASN:ND2	1.91	1.03
3:C:323:PHE:CE2	3:C:351:GLU:OE2	2.14	1.00
3:C:339:ASP:OD1	3:C:342:THR:CG2	2.11	0.99
2:B:153:SER:O	3:C:298:LEU:O	1.82	0.96
3:C:342:THR:CG2	3:C:343:CYS:N	2.28	0.93
3:C:374:VAL:CG2	3:C:375:GLY:N	2.30	0.92
3:C:375:GLY:O	3:C:635:HIS:NE2	2.04	0.91
2:B:369:ILE:CD1	3:C:301:ASN:OD1	2.19	0.90
3:C:486:LYS:CD	3:C:658:TYR:CE1	2.57	0.88
3:C:644:ASN:O	3:C:646:CYS:N	2.08	0.86
2:B:378:CYS:CB	3:C:307:VAL:CG1	2.52	0.86
3:C:463:ILE:CG2	3:C:644:ASN:CA	2.54	0.85
3:C:464:HIS:CD2	3:C:646:CYS:SG	2.70	0.85
3:C:280:ASP:N	3:C:286:ASP:OD2	2.13	0.81
3:C:337:CYS:C	3:C:342:THR:OG1	2.19	0.81
3:C:339:ASP:CA	3:C:340:PRO:O	2.30	0.80
3:C:487:ARG:N	3:C:658:TYR:OH	2.17	0.77
3:C:262:LYS:O	3:C:264:HIS:N	2.20	0.75
3:C:509:PHE:CZ	3:C:664:PRO:CB	2.69	0.74
3:C:488:LYS:CG	3:C:679:ASP:OD1	2.35	0.74
1:A:152:GLN:C	2:B:386:SER:OG	2.26	0.73
3:C:256:GLU:O	3:C:258:PRO:N	2.21	0.73
3:C:344:SER:O	3:C:345:GLN:OE1	2.07	0.73
3:C:340:PRO:O	3:C:342:THR:CA	2.38	0.71
3:C:263:CYS:SG	3:C:267:GLU:N	2.63	0.71
3:C:643:VAL:CG1	3:C:644:ASN:C	2.60	0.70
2:B:378:CYS:SG	3:C:307:VAL:CG1	2.80	0.70
3:C:340:PRO:C	3:C:342:THR:N	2.40	0.70
3:C:643:VAL:CA	3:C:644:ASN:CB	2.70	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:261:PHE:CD2	3:C:262:LYS:N	2.60	0.70
3:C:269:ILE:O	3:C:270:THR:OG1	2.10	0.69
3:C:337:CYS:SG	3:C:348:VAL:C	2.72	0.68
3:C:342:THR:CG2	3:C:347:CYS:CB	2.71	0.68
3:C:270:THR:CG2	3:C:271:LEU:N	2.56	0.68
3:C:337:CYS:SG	3:C:349:ASN:CB	2.83	0.67
3:C:270:THR:CG2	3:C:272:ASP:N	2.57	0.67
3:C:286:ASP:C	3:C:287:GLU:CG	2.63	0.67
3:C:527:ASN:ND2	3:C:674:THR:OG1	2.29	0.66
3:C:259:ASN:O	3:C:270:THR:CB	2.43	0.66
3:C:488:LYS:CD	3:C:677:CYS:O	2.45	0.65
3:C:261:PHE:O	3:C:263:CYS:N	2.28	0.65
3:C:340:PRO:O	3:C:341:ASP:C	2.30	0.65
3:C:275:CYS:CA	3:C:287:GLU:CG	2.75	0.65
3:C:486:LYS:CD	3:C:658:TYR:CD1	2.80	0.65
3:C:292:CYS:C	3:C:294:THR:N	2.51	0.64
3:C:256:GLU:O	3:C:258:PRO:CD	2.46	0.64
3:C:261:PHE:O	3:C:267:GLU:O	2.16	0.63
3:C:644:ASN:O	3:C:647:GLU:N	2.32	0.62
3:C:292:CYS:O	3:C:294:THR:N	2.33	0.62
3:C:260:LYS:CA	3:C:270:THR:OG1	2.48	0.61
3:C:463:ILE:CG2	3:C:644:ASN:CG	2.67	0.61
3:C:374:VAL:O	3:C:376:SER:N	2.33	0.61
3:C:367:HIS:O	3:C:368:THR:CG2	2.48	0.60
3:C:261:PHE:C	3:C:263:CYS:N	2.54	0.60
3:C:486:LYS:CB	3:C:658:TYR:CE1	2.84	0.60
3:C:644:ASN:C	3:C:646:CYS:N	2.51	0.60
3:C:281:CYS:O	3:C:283:ASP:N	2.35	0.59
2:B:186:ASP:OD1	2:B:226:HIS:ND1	2.36	0.59
3:C:338:GLN:N	3:C:342:THR:OG1	2.36	0.59
3:C:356:CYS:O	3:C:371:CYS:SG	2.60	0.59
3:C:278:ALA:O	3:C:286:ASP:OD2	2.21	0.59
3:C:333:ASP:CB	3:C:351:GLU:CG	2.81	0.58
3:C:283:ASP:C	3:C:285:SER:N	2.54	0.58
3:C:464:HIS:NE2	3:C:646:CYS:SG	2.76	0.58
3:C:269:ILE:CD1	3:C:280:ASP:O	2.52	0.58
3:C:486:LYS:CB	3:C:658:TYR:CZ	2.86	0.58
3:C:276:ASN:O	3:C:277:MET:C	2.42	0.58
3:C:289:ILE:O	3:C:289:ILE:CG1	2.52	0.57
2:B:155:PRO:CD	3:C:298:LEU:CD2	2.82	0.57
3:C:334:ILE:O	3:C:335:ASP:C	2.43	0.56
3:C:262:LYS:O	3:C:263:CYS:C	2.44	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:263:CYS:SG	3:C:266:GLY:CA	2.93	0.56
3:C:297:CYS:O	3:C:299:ASP:N	2.38	0.56
3:C:643:VAL:CG1	3:C:645:TRP:N	2.69	0.56
3:C:339:ASP:CA	3:C:340:PRO:C	2.72	0.55
3:C:486:LYS:CG	3:C:658:TYR:CE1	2.88	0.55
3:C:643:VAL:CB	3:C:645:TRP:N	2.70	0.55
3:C:370:ALA:O	3:C:372:LYS:N	2.39	0.55
2:B:153:SER:O	3:C:298:LEU:CB	2.55	0.55
3:C:281:CYS:C	3:C:283:ASP:N	2.61	0.53
3:C:362:PHE:O	3:C:363:GLN:CD	2.48	0.53
3:C:335:ASP:C	3:C:349:ASN:ND2	2.62	0.52
3:C:297:CYS:C	3:C:299:ASP:N	2.62	0.52
3:C:463:ILE:CG2	3:C:644:ASN:N	2.73	0.52
3:C:276:ASN:OD1	3:C:276:ASN:O	2.27	0.52
3:C:643:VAL:CG1	3:C:645:TRP:CA	2.88	0.51
3:C:337:CYS:SG	3:C:349:ASN:N	2.84	0.51
3:C:489:THR:N	3:C:679:ASP:OD2	2.44	0.51
3:C:486:LYS:CB	3:C:658:TYR:OH	2.59	0.50
3:C:526:LEU:O	3:C:661:LEU:CD1	2.59	0.50
2:B:343:ASP:CB	2:B:423:VAL:CG1	2.89	0.50
3:C:335:ASP:CA	3:C:349:ASN:ND2	2.75	0.50
3:C:339:ASP:N	3:C:342:THR:CB	2.75	0.50
3:C:370:ALA:C	3:C:372:LYS:N	2.66	0.49
3:C:322:GLY:O	3:C:333:ASP:CG	2.51	0.49
2:B:201:MET:CE	2:B:203:THR:CG2	2.91	0.48
3:C:464:HIS:CD2	3:C:646:CYS:CB	2.96	0.48
3:C:344:SER:C	3:C:345:GLN:OE1	2.52	0.48
3:C:286:ASP:OD1	3:C:287:GLU:CG	2.62	0.48
3:C:263:CYS:CB	3:C:267:GLU:N	2.77	0.48
3:C:489:THR:N	3:C:679:ASP:OD1	2.47	0.47
2:B:374:TYR:CZ	3:C:319:CYS:O	2.67	0.47
2:B:414:ARG:NH2	2:B:456:PHE:CE2	2.83	0.47
1:A:150:PHE:N	2:B:290:ALA:O	2.47	0.47
3:C:406:ARG:NH2	3:C:427:GLN:OE1	2.48	0.47
3:C:322:GLY:O	3:C:333:ASP:CB	2.63	0.46
3:C:333:ASP:OD1	3:C:334:ILE:N	2.48	0.46
3:C:276:ASN:N	3:C:287:GLU:OE2	2.48	0.46
3:C:508:GLY:CA	3:C:662:PRO:CB	2.93	0.46
1:A:150:PHE:O	2:B:290:ALA:N	2.50	0.45
3:C:289:ILE:C	3:C:291:GLU:N	2.70	0.45
3:C:643:VAL:CG1	3:C:644:ASN:O	2.63	0.45
3:C:346:LEU:O	3:C:346:LEU:CG	2.61	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:195:GLU:OE1	2:B:238:ASP:N	2.49	0.45
3:C:286:ASP:O	3:C:287:GLU:CG	2.64	0.45
3:C:338:GLN:O	3:C:341:ASP:C	2.55	0.45
3:C:290:LYS:O	3:C:291:GLU:CB	2.64	0.45
3:C:643:VAL:CG1	3:C:648:ARG:CB	2.95	0.45
3:C:273:LYS:CG	3:C:273:LYS:O	2.64	0.45
3:C:373:ALA:O	3:C:374:VAL:O	2.36	0.44
3:C:256:GLU:C	3:C:258:PRO:CD	2.85	0.44
3:C:527:ASN:CB	3:C:661:LEU:CD1	2.93	0.44
3:C:286:ASP:O	3:C:287:GLU:CB	2.65	0.44
3:C:526:LEU:CD1	3:C:662:PRO:CG	2.96	0.44
3:C:336:GLU:N	3:C:349:ASN:ND2	2.66	0.44
3:C:335:ASP:CB	3:C:349:ASN:ND2	2.82	0.43
2:B:490:SER:OG	2:B:493:GLY:N	2.51	0.43
3:C:337:CYS:CB	3:C:349:ASN:CB	2.97	0.43
3:C:340:PRO:O	3:C:342:THR:CB	2.67	0.42
3:C:336:GLU:N	3:C:349:ASN:OD1	2.53	0.42
3:C:394:ASP:OD1	3:C:396:SER:OG	2.38	0.41
3:C:273:LYS:CE	3:C:280:ASP:OD2	2.67	0.41
2:B:212:ASP:N	2:B:256:GLN:OE1	2.53	0.41
1:A:70:ASP:N	1:A:71:PRO:CD	2.83	0.41
3:C:289:ILE:O	3:C:291:GLU:N	2.54	0.41
2:B:605:GLY:O	2:B:682:ARG:N	2.54	0.41
3:C:348:VAL:CG2	3:C:355:LYS:O	2.68	0.41
3:C:299:ASP:O	3:C:302:GLY:N	2.53	0.41
3:C:287:GLU:O	3:C:288:PRO:C	2.52	0.41
2:B:615:ILE:CD1	2:B:619:GLN:NE2	2.84	0.41
2:B:306:ARG:NH1	2:B:479:PRO:CG	2.84	0.41
2:B:243:LYS:O	2:B:244:GLY:C	2.58	0.41
3:C:269:ILE:CG1	3:C:269:ILE:O	2.69	0.40
3:C:337:CYS:SG	3:C:348:VAL:N	2.94	0.40
3:C:644:ASN:O	3:C:645:TRP:C	2.54	0.40
3:C:463:ILE:O	3:C:644:ASN:ND2	2.55	0.40
3:C:263:CYS:CB	3:C:267:GLU:O	2.69	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:164:PRO:CA	3:C:284:TRP:CA[3_655]	1.95	0.25
2:B:164:PRO:CA	3:C:284:TRP:CB[3_655]	1.98	0.22
2:B:164:PRO:CB	3:C:286:ASP:O[3_655]	2.01	0.19

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105[A]:ARG:CZ	3:C:530:ASP:OD1[4.545]	2.07	0.13
2:B:164:PRO:C	3:C:284:TRP:CB[3.655]	2.08	0.12
2:B:163:PRO:O	3:C:284:TRP:CB[3.655]	2.10	0.10
1:A:105[A]:ARG:NE	3:C:530:ASP:OD1[4.545]	2.15	0.05
2:B:160:ARG:NE	3:C:282:ARG:CB[3.655]	2.17	0.03

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	33	85
3	C	426/791 (54%)	362 (85%)	43 (10%)	21 (5%)	3	43
All	All	988/1461 (68%)	911 (92%)	53 (5%)	24 (2%)	9	62

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	257	GLY
3	C	271	LEU
3	C	287	GLU
3	C	291	GLU
3	C	340	PRO
3	C	341	ASP
3	C	366	PRO
3	C	374	VAL
3	C	645	TRP
2	B	244	GLY
3	C	293	GLY
3	C	298	LEU
3	C	335	ASP
3	C	375	GLY
2	B	545	SER
3	C	263	CYS

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Mol	Chain	Res	Type
3	C	281	CYS
3	C	282	ARG
3	C	300	ASN
3	C	258	PRO
3	C	277	MET
3	C	320	PRO
3	C	266	GLY
2	B	280	VAL

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	80/104 (77%)	79 (99%)	1 (1%)	80	95
2	B	389/437 (89%)	378 (97%)	11 (3%)	56	88
3	C	374/691 (54%)	342 (91%)	32 (9%)	15	59
All	All	843/1232 (68%)	799 (95%)	44 (5%)	32	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
2	B	201	MET
2	B	278	GLN
2	B	375	CYS
2	B	490	SER
2	B	571	LEU
2	B	615	ILE
2	B	623	THR
2	B	638	LEU
2	B	644	VAL
2	B	645	LEU
2	B	659	ARG
3	C	256	GLU
3	C	261	PHE
3	C	263	CYS

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Mol	Chain	Res	Type
3	C	283	ASP
3	C	285	SER
3	C	289	ILE
3	C	290	LYS
3	C	317	CYS
3	C	318	LEU
3	C	335	ASP
3	C	336	GLU
3	C	337	CYS
3	C	339	ASP
3	C	341	ASP
3	C	342	THR
3	C	343	CYS
3	C	356	CYS
3	C	362	PHE
3	C	365	ASP
3	C	366	PRO
3	C	367	HIS
3	C	371	CYS
3	C	411	LEU
3	C	428	ARG
3	C	444	TYR
3	C	499	ARG
3	C	520	LYS
3	C	543	ASN
3	C	612	ARG
3	C	614	THR
3	C	623	GLU
3	C	643	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 3 ligands modelled in this entry, 3 are 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.

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	92/124 (74%)	2.09	37 (40%) 1 4	106, 181, 209, 231	0
2	B	486/546 (89%)	1.80	164 (33%) 1 4	81, 178, 253, 349	0
3	C	430/791 (54%)	1.86	139 (32%) 1 4	79, 170, 278, 322	1 (0%)
All	All	1008/1461 (68%)	1.85	340 (33%) 1 4	79, 176, 268, 349	1 (0%)

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	633	LEU	15.6
2	B	332	GLU	12.9
2	B	309	VAL	12.7
3	C	380	LEU	12.6
2	B	311	LEU	12.4
2	B	310	VAL	11.0
3	C	642	GLY	10.4
3	C	632	VAL	10.3
3	C	648	ARG	10.1
2	B	283	LEU	9.9
2	B	285	VAL	9.8
2	B	284	VAL	9.7
2	B	529	LEU	9.7
3	C	649	THR	9.4
2	B	304	LEU	9.3
3	C	591	ALA	9.0
3	C	546	THR	9.0
3	C	641	ARG	9.0
2	B	406	LEU	8.8
2	B	286	LEU	8.6
2	B	393	ALA	8.6
3	C	381	PHE	8.5
3	C	393	LEU	8.5

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Mol	Chain	Res	Type	RSRZ
3	C	510	MET	8.4
1	A	118	LEU	8.2
3	C	511	TYR	8.2
2	B	183	TYR	8.1
3	C	412	ASP	8.1
2	B	308	GLY	8.0
3	C	621	LEU	7.9
2	B	530	PRO	7.7
2	B	300	ALA	7.6
2	B	312	VAL	7.5
2	B	408	LEU	7.5
2	B	396	ALA	7.5
2	B	305	ALA	7.5
2	B	449	HIS	7.4
3	C	379	TYR	7.4
3	C	643	VAL	7.3
2	B	331	PRO	7.3
2	B	672	VAL	7.1
2	B	301	CYS	7.0
2	B	395	ILE	7.0
3	C	592	VAL	7.0
2	B	415	LEU	6.9
2	B	621	GLN	6.9
3	C	547	LEU	6.8
2	B	657	ARG	6.8
3	C	411	LEU	6.8
3	C	545	ILE	6.8
3	C	645	TRP	6.8
2	B	287	LEU	6.8
2	B	412	ARG	6.7
3	C	598	PHE	6.7
2	B	454	GLN	6.5
3	C	391	MET	6.3
2	B	671	ALA	6.3
3	C	512	TRP	6.3
2	B	615	ILE	6.3
2	B	185	LEU	6.2
2	B	282	PRO	6.2
3	C	413	THR	6.2
2	B	265	LEU	6.2
1	A	80	VAL	6.2
3	C	502	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	182	VAL	6.1
3	C	378	ALA	6.1
3	C	468	TYR	6.1
1	A	111	ILE	6.0
2	B	303	ARG	6.0
2	B	399	MET	6.0
2	B	268	LEU	6.0
3	C	458	LEU	6.0
2	B	307	ALA	6.0
2	B	403	GLU	5.9
2	B	306	ARG	5.9
3	C	634	PHE	5.8
3	C	578	LEU	5.8
1	A	122	PHE	5.7
1	A	133	LEU	5.7
1	A	131	LEU	5.7
3	C	390	LYS	5.6
3	C	555	TYR	5.6
2	B	184	LEU	5.5
2	B	281	GLY	5.4
2	B	264	THR	5.4
2	B	435	VAL	5.4
2	B	673	THR	5.4
2	B	461	TRP	5.3
2	B	453	TRP	5.3
3	C	453	GLN	5.3
1	A	135	LEU	5.3
3	C	651	LEU	5.3
1	A	134	ALA	5.3
3	C	401	LEU	5.3
1	A	143	ILE	5.3
2	B	616	PRO	5.2
3	C	506	VAL	5.2
1	A	130	LEU	5.2
3	C	597	VAL	5.2
3	C	503	VAL	5.1
3	C	590	LEU	5.1
2	B	334	ILE	5.1
2	B	444	LEU	5.0
2	B	648	TYR	5.0
2	B	619	GLN	5.0
3	C	382	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	638	LEU	5.0
3	C	607	ILE	5.0
2	B	333	VAL	4.9
2	B	411	LEU	4.9
2	B	622	VAL	4.9
3	C	479	VAL	4.9
3	C	556	TRP	4.9
3	C	640	PRO	4.9
2	B	620	GLU	4.9
1	A	64	PHE	4.9
2	B	436	LEU	4.8
3	C	459	ALA	4.8
2	B	442	ALA	4.8
2	B	476	ARG	4.7
2	B	404	PRO	4.7
2	B	297	LEU	4.7
2	B	491	ARG	4.7
3	C	487	ARG	4.7
3	C	484	GLY	4.7
3	C	425	LEU	4.7
3	C	593	PHE	4.7
2	B	272	ARG	4.6
2	B	407	THR	4.6
3	C	402	ILE	4.6
3	C	554	LEU	4.6
2	B	360	ASP	4.5
3	C	490	LEU	4.5
3	C	622	ALA	4.5
2	B	155	PRO	4.5
2	B	651	ASP	4.5
2	B	327	PRO	4.4
1	A	126	MET	4.4
2	B	391	HIS	4.4
3	C	528	GLY	4.4
2	B	452	GLY	4.4
3	C	501	ILE	4.4
2	B	410	GLU	4.3
3	C	473	VAL	4.3
2	B	405	GLU	4.3
3	C	534	LEU	4.3
3	C	599	TRP	4.3
1	A	98	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	445	PRO	4.3
2	B	239	ALA	4.3
3	C	631	MET	4.2
1	A	119	LEU	4.2
2	B	392	VAL	4.2
2	B	400	LEU	4.2
1	A	95	ALA	4.2
2	B	261	VAL	4.1
3	C	549	LEU	4.1
3	C	613	LEU	4.1
1	A	121	GLY	4.1
2	B	623	THR	4.1
3	C	629	GLU	4.1
3	C	521	ILE	4.0
3	C	467	ILE	4.0
3	C	456	ASP	4.0
2	B	296	VAL	4.0
3	C	672	LYS	4.0
3	C	277	MET	4.0
2	B	448	THR	3.9
2	B	567	GLU	3.9
2	B	361	LEU	3.9
2	B	658	SER	3.9
2	B	438	PRO	3.9
3	C	507	HIS	3.9
1	A	79	VAL	3.9
2	B	437	THR	3.9
3	C	505	PRO	3.9
3	C	448	ILE	3.9
2	B	414	ARG	3.9
2	B	302	GLN	3.9
2	B	637	ALA	3.8
3	C	388	VAL	3.8
3	C	430	ILE	3.8
2	B	613	HIS	3.8
2	B	612	GLU	3.8
3	C	421	TYR	3.8
3	C	522	LYS	3.8
3	C	550	LEU	3.8
1	A	142	TYR	3.8
3	C	486	LYS	3.7
3	C	594	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	417	HIS	3.7
3	C	609	SER	3.7
3	C	460	VAL	3.7
2	B	614	GLY	3.7
3	C	480	ALA	3.6
2	B	271	ILE	3.6
3	C	583	ARG	3.6
2	B	313	THR	3.6
2	B	181	GLU	3.5
3	C	596	LYS	3.5
3	C	491	PHE	3.5
2	B	650	VAL	3.5
2	B	503	GLN	3.5
2	B	480	ASP	3.5
3	C	420	ILE	3.5
1	A	123	LEU	3.5
3	C	416	ALA	3.4
2	B	606	LEU	3.4
2	B	394	GLY	3.4
2	B	280	VAL	3.4
3	C	608	PHE	3.4
2	B	231	ALA	3.3
3	C	603	ILE	3.3
2	B	247	MET	3.3
3	C	389	ARG	3.3
2	B	262	SER	3.3
2	B	289	LEU	3.3
3	C	618	VAL	3.3
2	B	674	ALA	3.3
3	C	567	ILE	3.3
2	B	443	ALA	3.3
3	C	523	LYS	3.2
3	C	564	ILE	3.2
3	C	410	ALA	3.2
3	C	477	VAL	3.2
3	C	639	GLN	3.2
2	B	656	VAL	3.1
1	A	113	HIS	3.1
3	C	298	LEU	3.1
3	C	428	ARG	3.1
2	B	479	PRO	3.1
1	A	137	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	602	ILE	3.1
3	C	612	ARG	3.1
2	B	153	SER	3.1
3	C	647	GLU	3.1
1	A	115	PHE	3.1
2	B	397	ALA	3.1
2	B	416	ILE	3.1
3	C	535	VAL	3.1
2	B	507	LEU	3.1
2	B	161	ILE	3.0
3	C	447	VAL	3.0
1	A	63	THR	3.0
2	B	154	ILE	3.0
3	C	526	LEU	3.0
1	A	132	GLU	3.0
2	B	266	ILE	3.0
2	B	440	LEU	3.0
3	C	638	THR	2.9
2	B	200	VAL	2.9
1	A	112	LEU	2.9
1	A	78	TYR	2.9
2	B	478	ALA	2.9
1	A	81	VAL	2.8
3	C	644	ASN	2.8
3	C	610	ALA	2.8
3	C	409	VAL	2.8
1	A	114	VAL	2.8
2	B	460	VAL	2.8
2	B	501	GLU	2.8
2	B	508	VAL	2.7
1	A	65	HIS	2.7
1	A	144	GLU	2.7
3	C	659	LEU	2.7
3	C	569	VAL	2.7
3	C	577	ILE	2.7
3	C	485	VAL	2.7
1	A	92	GLU	2.7
3	C	619	ASN	2.7
2	B	409	ALA	2.7
3	C	483	LYS	2.6
1	A	124	VAL	2.6
2	B	439	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	646	GLY	2.6
2	B	288	PRO	2.6
2	B	238	ASP	2.6
2	B	475	ALA	2.6
3	C	615	GLY	2.6
1	A	109	THR	2.6
2	B	350	THR	2.6
1	A	91	SER	2.6
1	A	94	THR	2.5
2	B	446	PRO	2.5
2	B	642	SER	2.5
2	B	362	PHE	2.5
3	C	469	TRP	2.5
3	C	650	THR	2.5
3	C	504	ASP	2.5
2	B	644	VAL	2.5
2	B	267	GLY	2.5
1	A	101	GLN	2.4
3	C	422	TRP	2.4
2	B	432	ASP	2.4
2	B	655	VAL	2.4
2	B	357	ARG	2.3
2	B	422	ASP	2.3
2	B	629	GLY	2.3
3	C	524	GLY	2.3
2	B	489	PHE	2.3
3	C	429	MET	2.3
2	B	241	VAL	2.3
3	C	655	GLY	2.3
3	C	454	ALA	2.3
3	C	530	ASP	2.3
2	B	234	VAL	2.3
2	B	477	CYS	2.3
2	B	521	TYR	2.3
3	C	455	PRO	2.3
2	B	180	VAL	2.3
2	B	230	LEU	2.3
3	C	423	SER	2.3
3	C	392	THR	2.2
3	C	654	GLY	2.2
3	C	620	LEU	2.2
2	B	158	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	435	LEU	2.2
1	A	62	ALA	2.2
2	B	605	GLY	2.2
2	B	390	ALA	2.2
2	B	528	LEU	2.2
2	B	459	THR	2.2
3	C	462	TRP	2.2
3	C	407	ASN	2.2
3	C	517	THR	2.1
3	C	405	LEU	2.1
2	B	369	ILE	2.1
2	B	603	ALA	2.1
2	B	604	PRO	2.1
2	B	167	ARG	2.1
3	C	482	THR	2.1
2	B	645	LEU	2.1
2	B	675	VAL	2.1
3	C	509	PHE	2.1
3	C	586	HIS	2.1
2	B	290	ALA	2.1
2	B	474	ILE	2.0
3	C	466	ASN	2.0
2	B	330	ALA	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	C	1002	1/1	0.41	0.82	153,153,153,153	0
4	CA	C	1003	1/1	0.26	-0.68	170,170,170,170	0
4	CA	C	1001	1/1	0.30	-0.68	136,136,136,136	0

6.5 Other polymers ⓘ

There are no such residues in this entry.