



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 01:52 PM EDT

PDB ID : 5OCA
Title : PCSK9:Fab Complex with Dextran Sulfate
Authors : Thirup, S.S.; Vilstrup, J.P.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

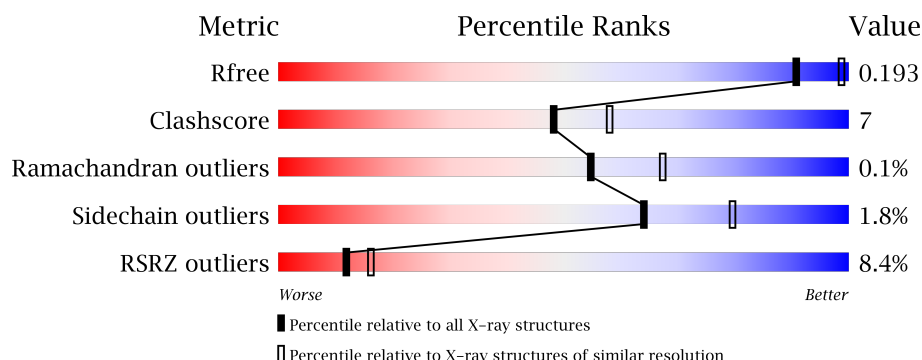
1 Overall quality at a glance

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>61%</div> <div>10%</div> <div>27%</div> </div>
2	B	540	<div> <div>13%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
3	H	238	<div> <div>3%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
4	L	217	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	9QZ	A	201[A]	-	-	-	X
5	9QZ	A	201[B]	-	-	-	X
6	NA	B	701	-	-	-	X
6	NA	B	702	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8500 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	495	Total	C	N	O	S	0	1	0
			3665	2261	679	693	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ILE	VAL	conflict	UNP Q8NBP7
B	533	ALA	ASN	conflict	UNP Q8NBP7
B	620	GLY	GLU	conflict	UNP Q8NBP7
B	670	GLU	GLY	conflict	UNP Q8NBP7

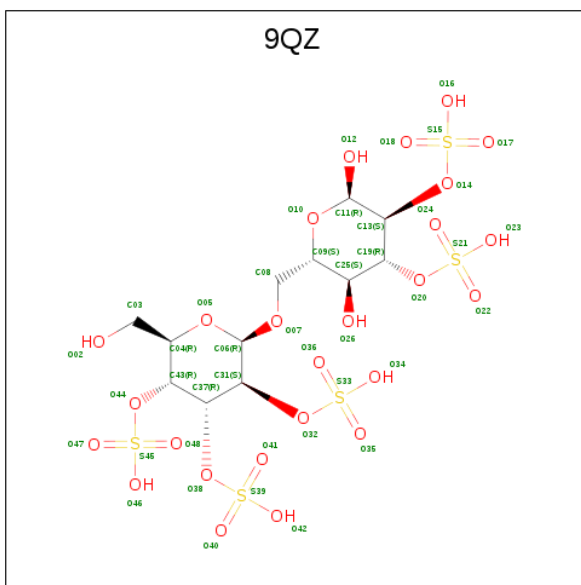
- Molecule 3 is a protein called Fab from LDLR competitive antibody: Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	1	0
			1648	1044	271	326	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	1	0
			1571	977	263	327	4			

- Molecule 5 is [(2 {R},3 {S},4 {R},5 {R},6 {R})-2-[(2 {S},3 {S},4 {R},5 {S},6 {R})-3,6-bis (oxidanyl)-4,5-disulfooxy-oxan-2-yl]methoxy]-6-(hydroxymethyl)-3,5-disulfooxy-oxan-4-yl] hydrogen sulfate (three-letter code: 9QZ) (formula: C₁₂H₂₂O₂₆S₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	1
			86	24	52	10		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Na 2 2	0	0

- Molecule 7 is water.

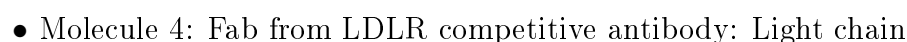
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	90	Total O 90 90	0	0
7	B	233	Total O 233 233	0	0
7	H	227	Total O 227 227	0	0

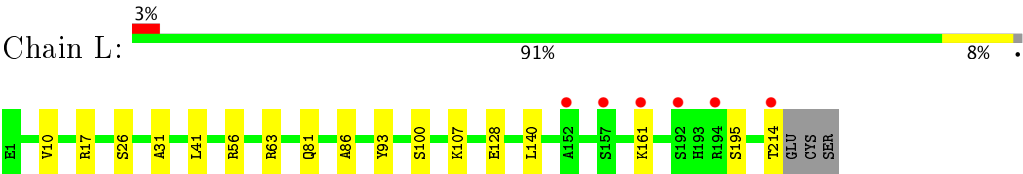
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	238	Total 238	O 238	0	0

- Molecule 1: Proprotein convertase subtilisin/kexin type 9





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)	38.29 – 2.30 38.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.29-2.30) 99.8 (38.29-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.167 , 0.195 0.164 , 0.193	Depositor DCC
R_{free} test set	5375 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	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	0.96	EDS
Total number of atoms	8500	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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, 9QZ

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	0.47	0/757	0.57	1/1023 (0.1%)
2	B	0.42	0/3736	0.60	0/5073
3	H	0.51	0/1692	0.63	0/2302
4	L	0.45	0/1611	0.60	1/2200 (0.0%)
All	All	0.45	0/7796	0.60	2/10598 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	L	63	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	119	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	469	ARG	Peptide

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	18	0
2	B	3665	0	3586	59	0
3	H	1648	0	1597	20	0
4	L	1571	0	1523	12	0
5	A	86	0	0	4	0
6	B	2	0	0	0	0
7	A	90	0	0	3	0
7	B	233	0	0	10	1
7	H	227	0	0	5	3
7	L	238	0	0	6	0
All	All	8500	0	7456	104	3

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 (104) 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)
3:H:203:THR:O	7:H:301:HOH:O	1.90	0.90
2:B:258[A]:LYS:NZ	7:B:802:HOH:O	2.05	0.87
3:H:134:LEU:HD22	3:H:150:CYS:CA	2.06	0.85
2:B:159:GLU:OE2	7:B:801:HOH:O	1.98	0.81
2:B:469:ARG:HE	2:B:516:GLY:H	1.27	0.78
1:A:87:HIS:H	1:A:90:GLN:HE21	1.32	0.77
4:L:161:LYS:O	7:L:302:HOH:O	2.07	0.72
4:L:17:ARG:NH1	7:L:304:HOH:O	2.23	0.72
1:A:69:LYS:NZ	7:A:301:HOH:O	2.21	0.72
1:A:139:HIS:NE2	5:A:201[B]:9QZ:O22	2.26	0.69
2:B:469:ARG:HB3	2:B:515:PHE:HA	1.74	0.68
2:B:414:ARG:HH11	2:B:414:ARG:HG3	1.58	0.67
1:A:87:HIS:H	1:A:90:GLN:NE2	1.94	0.66
1:A:66:ARG:NE	1:A:73:ARG:HH11	1.95	0.65
2:B:469:ARG:HB2	2:B:515:PHE:CD2	2.31	0.65
3:H:134:LEU:HD22	3:H:150:CYS:C	2.18	0.64
2:B:500:MET:HB3	2:B:507:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.79	0.64
2:B:469:ARG:HE	2:B:516:GLY:N	1.96	0.63
2:B:391:HIS:HB3	7:B:1005:HOH:O	1.99	0.62
2:B:555:GLN:NE2	7:B:806:HOH:O	2.33	0.62
4:L:81:GLN:NE2	7:L:305:HOH:O	2.24	0.62
2:B:611:LYS:HD2	2:B:627:GLU:OE2	1.99	0.62
3:H:6:GLU:CD	3:H:116:GLY:H	2.03	0.61
3:H:134:LEU:HD22	3:H:150:CYS:N	2.17	0.60
1:A:66:ARG:HD2	1:A:73:ARG:NH1	2.17	0.59
2:B:154:ILE:HD11	2:B:159:GLU:HB2	1.85	0.59
3:H:134:LEU:HD22	3:H:150:CYS:HA	1.83	0.59
4:L:107:LYS:C	4:L:107:LYS:HD3	2.25	0.57
1:A:116:HIS:HB2	7:A:371:HOH:O	2.05	0.56
2:B:414:ARG:NH1	2:B:414:ARG:HG3	2.20	0.56
2:B:566:TRP:NE1	2:B:569:GLU:OE1	2.35	0.56
1:A:150:PHE:CG	3:H:105:ALA:HB2	2.40	0.56
3:H:12:VAL:HG21	3:H:18:LEU:HG	1.86	0.56
3:H:134:LEU:CD2	3:H:150:CYS:C	2.75	0.55
2:B:304:LEU:HD22	2:B:309:VAL:HG21	1.89	0.54
2:B:256:GLN:HB3	3:H:57:TYR:CZ	2.43	0.54
2:B:495:ARG:HH11	2:B:644:VAL:HG12	1.73	0.53
2:B:283:LEU:HD21	2:B:309:VAL:HG22	1.90	0.52
2:B:196:ILE:HD12	2:B:200:VAL:HG11	1.92	0.52
1:A:132:GLU:HG2	7:A:333:HOH:O	2.10	0.51
2:B:186:ASP:OD1	2:B:288:PRO:HG2	2.11	0.51
2:B:302:GLN:HG3	2:B:332:GLU:OE2	2.12	0.50
2:B:302:GLN:NE2	2:B:332:GLU:OE2	2.40	0.50
2:B:469:ARG:NH2	2:B:513:ASN:HD21	2.09	0.50
2:B:218:ARG:NH1	7:B:815:HOH:O	2.45	0.50
2:B:483:LEU:HD23	2:B:507:LEU:HD22	1.93	0.50
2:B:492:SER:N	2:B:518:GLU:OE2	2.44	0.49
2:B:454:GLN:N	7:B:814:HOH:O	2.45	0.49
1:A:66:ARG:CD	1:A:73:ARG:HH11	2.25	0.49
1:A:104:ARG:NH2	5:A:201[A]:9QZ:O22	2.46	0.49
3:H:203:THR:HB	7:H:334:HOH:O	2.12	0.49
2:B:200:VAL:HG23	2:B:247:MET:HB2	1.94	0.49
2:B:469:ARG:CB	2:B:515:PHE:HA	2.43	0.48
4:L:56:ARG:NH2	7:L:301:HOH:O	2.03	0.48
4:L:214:THR:OG1	7:L:303:HOH:O	2.20	0.48
1:A:99:GLN:HG2	1:A:109:THR:OG1	2.14	0.48
3:H:165:ASN:ND2	7:H:301:HOH:O	2.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:HIS:CE1	2:B:519:GLY:HA3	2.49	0.47
1:A:117:GLY:O	2:B:303:ARG:NH2	2.47	0.47
2:B:496:ARG:HG3	2:B:514:ALA:HA	1.96	0.47
2:B:638:LEU:HA	2:B:638:LEU:HD23	1.77	0.46
3:H:2:VAL:HG12	3:H:112:VAL:HG11	1.97	0.46
2:B:418:PHE:CD2	2:B:445:PRO:HB3	2.50	0.46
2:B:469:ARG:HH21	2:B:513:ASN:HD21	1.64	0.46
2:B:523:ILE:HD13	2:B:648:TYR:HB3	1.97	0.46
2:B:588:CYS:HB3	2:B:596:ILE:HD11	1.96	0.46
2:B:469:ARG:HH22	2:B:519:GLY:N	2.13	0.46
4:L:41:LEU:HD23	4:L:86:ALA:HB2	1.97	0.45
2:B:468:THR:HB	2:B:471:ALA:HB2	1.97	0.45
2:B:194:ARG:NH2	7:B:811:HOH:O	2.40	0.45
2:B:295:ARG:HD2	7:B:958:HOH:O	2.16	0.45
2:B:423:VAL:HG22	7:B:856:HOH:O	2.16	0.45
2:B:477:CYS:H	2:B:506:LYS:HZ1	1.63	0.45
1:A:66:ARG:HD2	1:A:73:ARG:HH11	1.82	0.45
2:B:217:HIS:HE1	7:H:391:HOH:O	2.00	0.45
2:B:503:GLN:NE2	2:B:510:ARG:HH11	2.16	0.44
2:B:431:GLU:HA	2:B:434:ARG:HD2	2.00	0.44
2:B:302:GLN:HA	2:B:332:GLU:HG3	2.00	0.44
2:B:477:CYS:H	2:B:506:LYS:NZ	2.16	0.43
3:H:89:GLU:CD	3:H:89:GLU:H	2.21	0.43
4:L:10:VAL:HG12	7:L:417:HOH:O	2.18	0.43
2:B:345:PRO:HB2	2:B:428:TRP:CD2	2.53	0.43
1:A:66:ARG:HE	1:A:73:ARG:HH11	1.63	0.43
2:B:156:TRP:CZ3	2:B:341:ALA:HA	2.53	0.43
2:B:345:PRO:HD3	2:B:424:ILE:HG23	2.00	0.43
3:H:143:GLY:O	7:H:302:HOH:O	2.21	0.43
3:H:2:VAL:HG11	3:H:112:VAL:HG21	2.00	0.43
2:B:467:PRO:O	2:B:469:ARG:HD3	2.18	0.42
3:H:134:LEU:HD11	3:H:151:LEU:HB2	2.00	0.42
4:L:93:TYR:HA	4:L:100:SER:HA	2.00	0.42
2:B:194:ARG:NH1	2:B:237:ARG:NH1	2.66	0.42
2:B:638:LEU:HB2	2:B:673:THR:HB	2.00	0.42
1:A:66:ARG:HE	1:A:73:ARG:HD2	1.84	0.42
3:H:160:VAL:HG12	3:H:210:HIS:CD2	2.55	0.42
3:H:219:LYS:NZ	4:L:128:GLU:OE2	2.53	0.42
2:B:248:ARG:NH1	7:B:818:HOH:O	2.53	0.42
3:H:191:VAL:HG21	4:L:140:LEU:CD1	2.49	0.42
4:L:26:SER:O	4:L:31:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	5:A:201[B]:9QZ:O40	2.20	0.41
1:A:97:ARG:NH2	5:A:201[B]:9QZ:C06	2.84	0.41
2:B:302:GLN:CG	2:B:332:GLU:OE2	2.69	0.41
2:B:206:GLU:OE2	2:B:251:ARG:NH2	2.54	0.40
2:B:643:HIS:N	2:B:643:HIS:ND1	2.69	0.40

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
7:H:491:HOH:O	7:H:491:HOH:O 2_556	1.92	0.28
7:H:461:HOH:O	7:H:491:HOH:O 2_556	2.01	0.19
7:B:986:HOH:O	7:H:498:HOH:O 1_554	2.18	0.02

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%)	85 (94%)	5 (6%)	0	100	100
2	B	486/540 (90%)	464 (96%)	21 (4%)	1 (0%)	51	63
3	H	216/238 (91%)	213 (99%)	3 (1%)	0	100	100
4	L	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
All	All	1005/1121 (90%)	970 (96%)	34 (3%)	1 (0%)	55	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	514	ALA

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%)	53	70
2	B	392/429 (91%)	383 (98%)	9 (2%)	56	73
3	H	185/201 (92%)	182 (98%)	3 (2%)	68	82
4	L	178/180 (99%)	177 (99%)	1 (1%)	89	95
All	All	834/914 (91%)	819 (98%)	15 (2%)	64	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	119	LEU
2	B	165	ARG
2	B	274	SER
2	B	283	LEU
2	B	295	ARG
2	B	375	CYS
2	B	447	SER
2	B	546	MET
2	B	659	ARG
2	B	681	SER
3	H	21	SER
3	H	134	LEU
3	H	224	LYS
4	L	195	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
2	B	587	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	9QZ	A	201[A]	-	44,44,44	3.40	23 (52%)	51,70,70	1.56	7 (13%)
5	9QZ	A	201[B]	-	44,44,44	3.37	23 (52%)	51,70,70	1.42	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	9QZ	A	201[A]	-	-	0/32/72/72	0/2/2/2
5	9QZ	A	201[B]	-	-	1/32/72/72	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201[A]	9QZ	O07-C08	2.70	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201[B]	9QZ	O23-S21	2.84	1.66	1.50
5	A	201[B]	9QZ	O46-S45	2.87	1.66	1.50
5	A	201[B]	9QZ	O42-S39	2.92	1.66	1.50
5	A	201[A]	9QZ	O46-S45	2.95	1.66	1.50
5	A	201[A]	9QZ	O23-S21	2.99	1.66	1.50
5	A	201[B]	9QZ	O07-C08	2.99	1.49	1.43
5	A	201[A]	9QZ	O42-S39	2.99	1.66	1.50
5	A	201[A]	9QZ	O05-C04	3.23	1.52	1.44
5	A	201[A]	9QZ	O34-S33	3.36	1.68	1.50
5	A	201[B]	9QZ	O34-S33	3.36	1.68	1.50
5	A	201[A]	9QZ	O16-S15	3.42	1.69	1.50
5	A	201[B]	9QZ	O16-S15	3.54	1.69	1.50
5	A	201[B]	9QZ	O05-C04	3.60	1.53	1.44
5	A	201[A]	9QZ	O20-S21	3.68	1.67	1.56
5	A	201[B]	9QZ	O32-S33	3.71	1.67	1.56
5	A	201[B]	9QZ	O14-S15	3.73	1.67	1.56
5	A	201[B]	9QZ	O38-S39	3.74	1.67	1.56
5	A	201[A]	9QZ	O32-S33	3.89	1.68	1.56
5	A	201[A]	9QZ	O38-S39	3.91	1.68	1.56
5	A	201[B]	9QZ	O20-S21	3.96	1.68	1.56
5	A	201[A]	9QZ	O14-S15	4.11	1.68	1.56
5	A	201[A]	9QZ	O10-C11	5.06	1.52	1.43
5	A	201[B]	9QZ	O10-C11	5.12	1.52	1.43
5	A	201[B]	9QZ	O35-S33	5.24	1.65	1.45
5	A	201[A]	9QZ	O35-S33	5.25	1.65	1.45
5	A	201[A]	9QZ	O44-S45	5.31	1.72	1.56
5	A	201[B]	9QZ	O40-S39	5.34	1.65	1.45
5	A	201[B]	9QZ	O44-S45	5.36	1.72	1.56
5	A	201[B]	9QZ	O24-S21	5.39	1.65	1.45
5	A	201[B]	9QZ	O22-S21	5.39	1.65	1.45
5	A	201[B]	9QZ	O48-S45	5.41	1.66	1.45
5	A	201[B]	9QZ	O41-S39	5.42	1.66	1.45
5	A	201[A]	9QZ	O48-S45	5.42	1.66	1.45
5	A	201[A]	9QZ	O17-S15	5.48	1.66	1.45
5	A	201[A]	9QZ	O24-S21	5.53	1.66	1.45
5	A	201[A]	9QZ	O40-S39	5.54	1.66	1.45
5	A	201[A]	9QZ	O41-S39	5.55	1.66	1.45
5	A	201[B]	9QZ	O17-S15	5.55	1.66	1.45
5	A	201[B]	9QZ	O47-S45	5.56	1.66	1.45
5	A	201[A]	9QZ	O22-S21	5.58	1.66	1.45
5	A	201[A]	9QZ	O47-S45	5.62	1.66	1.45
5	A	201[B]	9QZ	O18-S15	5.62	1.66	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201[A]	9QZ	O18-S15	5.70	1.67	1.45
5	A	201[B]	9QZ	O36-S33	5.73	1.67	1.45
5	A	201[A]	9QZ	O36-S33	5.76	1.67	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	201[B]	9QZ	C03-C04-C43	-2.21	107.21	113.24
5	A	201[B]	9QZ	C19-C25-C09	2.03	114.03	109.67
5	A	201[A]	9QZ	C11-O10-C09	2.20	117.36	113.39
5	A	201[B]	9QZ	O05-C06-O07	2.36	115.63	110.02
5	A	201[A]	9QZ	O05-C04-C43	2.42	114.71	109.75
5	A	201[B]	9QZ	C31-C37-C43	2.43	115.84	110.46
5	A	201[B]	9QZ	O07-C06-C31	2.44	113.02	108.20
5	A	201[B]	9QZ	O10-C09-C08	2.69	112.00	106.64
5	A	201[B]	9QZ	O20-C19-C13	2.69	114.62	108.52
5	A	201[A]	9QZ	O44-C43-C37	2.92	115.14	108.52
5	A	201[A]	9QZ	C37-C43-C04	2.96	116.85	110.55
5	A	201[B]	9QZ	C19-O20-S21	3.01	124.76	118.97
5	A	201[B]	9QZ	C37-C43-C04	3.66	118.35	110.55
5	A	201[B]	9QZ	O05-C04-C43	4.23	118.40	109.75
5	A	201[A]	9QZ	O10-C09-C25	4.27	117.53	109.66
5	A	201[A]	9QZ	O07-C06-C31	4.31	116.72	108.20
5	A	201[A]	9QZ	C19-C25-C09	4.73	119.81	109.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	201[B]	9QZ	S21-O20-C19-C13

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	201[A]	9QZ	1	0
5	A	201[B]	9QZ	3	0

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, 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%)	0.01	4 (4%) 36 43	23, 40, 58, 76	0
2	B	495/540 (91%)	0.80	70 (14%) 3 4	24, 49, 103, 137	0
3	H	219/238 (92%)	0.06	6 (2%) 55 62	24, 38, 55, 73	0
4	L	214/217 (98%)	-0.09	6 (2%) 53 61	24, 38, 62, 81	0
All	All	1020/1121 (90%)	0.38	86 (8%) 12 16	23, 42, 88, 137	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	517	GLY	14.1
2	B	515	PHE	9.8
2	B	570	ASP	7.9
2	B	546	MET	7.9
2	B	166	TYR	6.7
2	B	643	HIS	6.1
2	B	165	ARG	5.8
2	B	448	THR	5.7
2	B	449	HIS	5.6
2	B	164	PRO	5.6
2	B	468	THR	5.5
2	B	619	GLN	5.4
2	B	153	SER	5.3
2	B	167	ARG	5.3
2	B	571	LEU	5.0
2	B	469	ARG	4.9
2	B	642	SER	4.8
2	B	616	PRO	4.8
2	B	553	HIS	4.7
2	B	615	ILE	4.7
2	B	467	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	168	ALA	4.7
2	B	279	PRO	4.7
2	B	545	SER	4.6
2	B	542	ALA	4.6
2	B	573	THR	4.4
2	B	617	ALA	4.3
2	B	516	GLY	4.3
2	B	618	PRO	4.2
2	B	547	GLY	4.1
2	B	278	GLN	4.0
2	B	659	ARG	4.0
2	B	447	SER	4.0
1	A	85	GLU	3.8
2	B	543	GLU	3.8
2	B	470	MET	3.8
2	B	505	GLY	3.7
2	B	471	ALA	3.7
2	B	544	ALA	3.6
2	B	277	VAL	3.6
2	B	506	LYS	3.6
2	B	641	THR	3.5
4	L	194	ARG	3.5
2	B	163	PRO	3.5
2	B	640	GLY	3.5
2	B	569	GLU	3.4
2	B	504	GLY	3.4
4	L	161	LYS	3.3
2	B	280	VAL	3.2
2	B	493	GLY	3.2
2	B	492	SER	3.1
2	B	554	GLN	3.1
2	B	514	ALA	3.1
2	B	671	ALA	2.9
2	B	592	ARG	2.8
3	H	103	TRP	2.8
3	H	1	GLU	2.8
2	B	244	GLY	2.6
4	L	157	SER	2.6
2	B	572	GLY	2.6
2	B	568	VAL	2.6
4	L	192	SER	2.6
1	A	151	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	494	LYS	2.6
2	B	567	GLU	2.5
2	B	258[A]	LYS	2.5
4	L	214	THR	2.4
1	A	149	VAL	2.4
4	L	152	ALA	2.4
2	B	518	GLU	2.4
2	B	672	VAL	2.4
2	B	502	ALA	2.3
2	B	289	LEU	2.3
1	A	61	THR	2.3
2	B	237	ARG	2.3
2	B	303	ARG	2.3
3	H	100	TYR	2.3
3	H	137	SER	2.2
2	B	314	ALA	2.2
2	B	287	LEU	2.2
3	H	201	THR	2.2
2	B	179	LEU	2.1
2	B	682	ARG	2.1
2	B	446	PRO	2.1
3	H	200	GLY	2.0
2	B	537	HIS	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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NA	B	702	1/1	0.94	0.58	17.38	55,55,55,55	0
5	9QZ	A	201[A]	43/43	0.65	0.46	6.71	72,89,94,100	43
5	9QZ	A	201[B]	43/43	0.65	0.46	6.56	60,89,94,98	43
6	NA	B	701	1/1	0.94	0.24	2.27	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.