Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 06:30 AM BST

PDB ID	:	5OCA
Title	:	PCSK9:Fab Complex with Dextran Sulfate
Authors	:	Thirup, S.S.; Vilstrup, J.P.
Deposited on	:	2017-06-30
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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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.
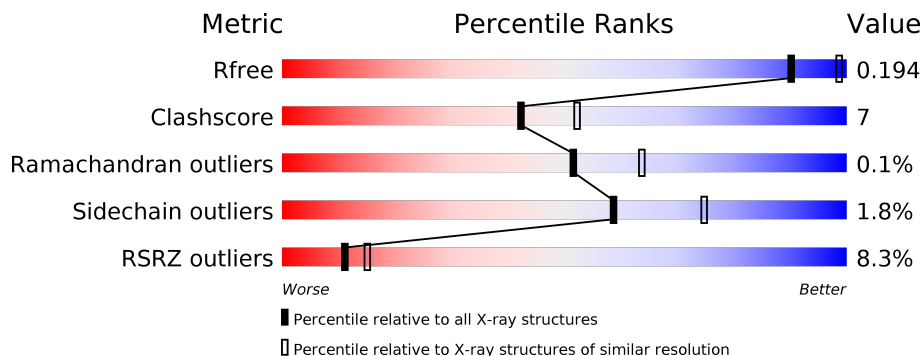
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	126	3% / 61% / 10% · / 27%
2	B	540	13% / 77% / 14% · 8%
3	H	238	3% / 83% / 8% 8%
4	L	217	3% / 91% / 8% ·
5	C	2	100%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TWD	C	1[A]	-	-	-	X
5	TWD	C	1[B]	-	-	-	X
5	TWA	C	2[A]	-	-	-	X
5	TWA	C	2[B]	-	-	-	X

2 Entry composition (i)

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 1571	C 977	N 263	O 327	S 4	0	1	0

- Molecule 5 is an oligosaccharide called 2,3,4-tri-O-sulfo-beta-D-altropyranose-(1-6)-2,3-di-O-sulfo-alpha-L-glucopyranose.
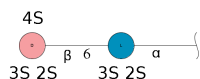
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total 86	C 24	O 52	S 10	0	2	0

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total 90	O 90	0	0
7	B	233	Total 233	O 233	0	0
7	H	227	Total 227	O 227	0	0
7	L	238	Total 238	O 238	0	0

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
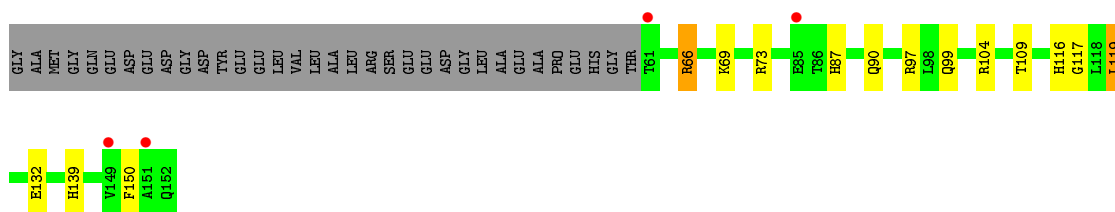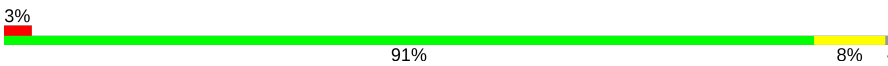
- Molecule 2: Proprotein convertase subtilisin/kexin type 9
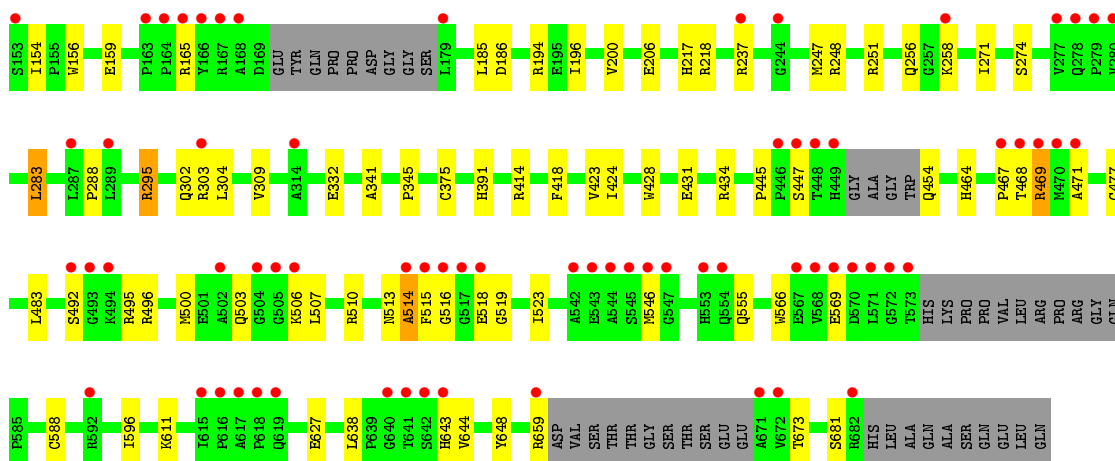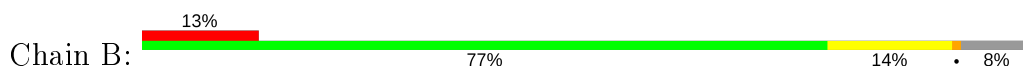
- Molecule 3: Fab from LDLR competitive antibody: Heavy chain
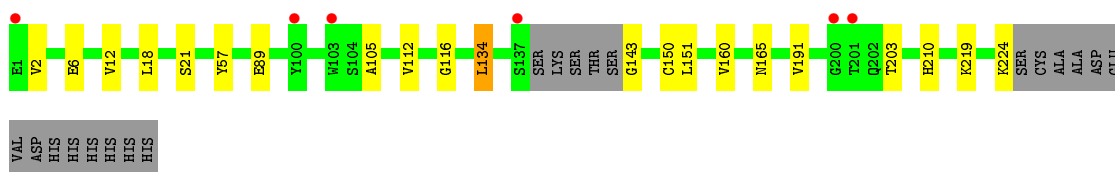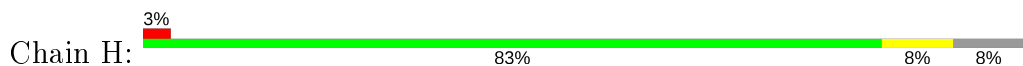
• Molecule 4: Fab from LDLR competitive antibody: Light chain

Chain L:

• Molecule 5: 2,3,4-tri-O-sulfo-beta-D-altropyranose-(1-6)-2,3-di-O-sulfo-alpha-L-glucopyranose

Chain C:

4   Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	2.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.167 , 0.195 0.167 , 0.194	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)	0.34 , 52.8	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h-2*l,-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.*

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[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 (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 (i)

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	C	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:C:1[B]:TWD: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:C:1[A]:TWD: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:C:2[B]:TWA:O40	2.20	0.41
1:A:97:ARG:NH2	5:C:2[B]:TWA:C1	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/126 (71%)	85 (94%)	5 (6%)	0	100	100
2	B	486/540 (90%)	464 (96%)	21 (4%)	1 (0%)	47	58
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%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	514	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	79/104 (76%)	77 (98%)	2 (2%)	47	65
2	B	392/429 (91%)	383 (98%)	9 (2%)	50	67
3	H	185/201 (92%)	182 (98%)	3 (2%)	62	78
4	L	178/180 (99%)	177 (99%)	1 (1%)	86	94
All	All	834/914 (91%)	819 (98%)	15 (2%)	59	75

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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

4 monosaccharides are modelled in this entry.

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	TWD	C	1[A]	5	20,20,20	2.90	9 (45%)	23,31,31	1.63	4 (17%)
5	TWD	C	1[B]	5	20,20,20	2.86	9 (45%)	23,31,31	1.34	5 (21%)
5	TWA	C	2[A]	5	23,23,24	3.31	13 (56%)	24,36,38	1.44	5 (20%)
5	TWA	C	2[B]	5	23,23,24	3.30	13 (56%)	24,36,38	1.63	5 (20%)

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	TWD	C	1[A]	5	-	7/12/32/32	0/1/1/1
5	TWD	C	1[B]	5	-	5/12/32/32	0/1/1/1
5	TWA	C	2[A]	5	-	9/17/34/37	0/1/1/1
5	TWA	C	2[B]	5	-	9/17/34/37	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2[A]	TWA	O36-S33	5.18	1.67	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2[B]	TWA	O36-S33	5.15	1.67	1.45
5	C	1[A]	TWD	O18-S15	5.12	1.67	1.45
5	C	2[B]	TWA	O4-S45	5.09	1.72	1.57
5	C	1[B]	TWD	O18-S15	5.05	1.66	1.45
5	C	2[A]	TWA	O47-S45	5.04	1.66	1.45
5	C	2[A]	TWA	O4-S45	5.04	1.72	1.57
5	C	1[A]	TWD	O22-S21	5.01	1.66	1.45
5	C	2[B]	TWA	O47-S45	4.99	1.66	1.45
5	C	1[B]	TWD	O17-S15	4.99	1.66	1.45
5	C	2[A]	TWA	O41-S39	4.98	1.66	1.45
5	C	2[A]	TWA	O40-S39	4.97	1.66	1.45
5	C	1[A]	TWD	O24-S21	4.96	1.66	1.45
5	C	1[A]	TWD	O17-S15	4.92	1.66	1.45
5	C	2[A]	TWA	O48-S45	4.87	1.66	1.45
5	C	2[B]	TWA	O41-S39	4.86	1.66	1.45
5	C	2[B]	TWA	O48-S45	4.86	1.66	1.45
5	C	1[B]	TWD	O22-S21	4.84	1.65	1.45
5	C	1[B]	TWD	O24-S21	4.83	1.65	1.45
5	C	2[B]	TWA	O40-S39	4.79	1.65	1.45
5	C	2[B]	TWA	O5-C5	4.77	1.53	1.43
5	C	2[A]	TWA	O35-S33	4.71	1.65	1.45
5	C	2[B]	TWA	O35-S33	4.70	1.65	1.45
5	C	2[A]	TWA	O5-C5	4.33	1.52	1.43
5	C	1[A]	TWD	O2-S15	3.86	1.68	1.57
5	C	1[B]	TWD	O5-C1	3.83	1.52	1.42
5	C	1[A]	TWD	O5-C1	3.79	1.52	1.42
5	C	1[B]	TWD	O3-S21	3.72	1.68	1.57
5	C	2[A]	TWA	O3-S39	3.67	1.68	1.57
5	C	2[A]	TWA	O2-S33	3.65	1.68	1.57
5	C	2[B]	TWA	O3-S39	3.51	1.67	1.57
5	C	1[B]	TWD	O2-S15	3.49	1.67	1.57
5	C	2[B]	TWA	O2-S33	3.48	1.67	1.57
5	C	1[A]	TWD	O3-S21	3.45	1.67	1.57
5	C	1[B]	TWD	O16-S15	3.19	1.69	1.50
5	C	1[A]	TWD	O16-S15	3.08	1.69	1.50
5	C	2[B]	TWA	O34-S33	3.02	1.68	1.50
5	C	2[A]	TWA	O34-S33	3.02	1.68	1.50
5	C	2[A]	TWA	O42-S39	2.68	1.66	1.50
5	C	1[A]	TWD	O23-S21	2.68	1.66	1.50
5	C	2[A]	TWA	O46-S45	2.64	1.66	1.50
5	C	2[B]	TWA	O42-S39	2.62	1.66	1.50
5	C	2[B]	TWA	O46-S45	2.57	1.66	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1[B]	TWD	O23-S21	2.54	1.66	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1[A]	TWD	C3-C4-C5	4.77	119.81	109.66
5	C	2[B]	TWA	O5-C5-C4	4.44	118.40	110.07
5	C	1[A]	TWD	O5-C5-C4	4.32	117.53	109.69
5	C	2[B]	TWA	C3-C4-C5	3.73	118.35	110.55
5	C	1[B]	TWD	C3-O3-S21	3.05	124.76	118.88
5	C	2[A]	TWA	O4-C4-C3	3.04	115.14	108.48
5	C	2[A]	TWA	C3-C4-C5	3.02	116.85	110.55
5	C	2[B]	TWA	O2-C2-C3	2.90	109.86	106.65
5	C	1[B]	TWD	O5-C1-C2	2.86	118.90	109.93
5	C	1[B]	TWD	O3-C3-C2	2.80	114.62	108.48
5	C	2[A]	TWA	O2-C2-C3	2.78	109.73	106.65
5	C	2[B]	TWA	C4-C3-C2	2.53	115.84	110.55
5	C	2[A]	TWA	O5-C5-C4	2.48	114.71	110.07
5	C	1[B]	TWD	O5-C5-C6	2.24	112.00	106.44
5	C	2[B]	TWA	C6-C5-C4	-2.10	107.21	113.33
5	C	1[A]	TWD	O2-C2-C3	2.06	113.00	108.48
5	C	1[B]	TWD	C3-C4-C5	2.05	114.03	109.66
5	C	1[A]	TWD	O5-C1-C2	2.05	116.36	109.93
5	C	2[A]	TWA	O3-C3-C4	2.02	112.92	108.48

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1[B]	TWD	C2-C3-O3-S21
5	C	2[B]	TWA	C1-C2-O2-S33
5	C	2[B]	TWA	C3-C2-O2-S33
5	C	2[B]	TWA	C4-O4-S45-O46
5	C	1[A]	TWD	C2-O2-S15-O16
5	C	2[A]	TWA	C1-C2-O2-S33
5	C	2[A]	TWA	C3-C4-O4-S45
5	C	2[A]	TWA	C2-O2-S33-O34
5	C	2[A]	TWA	C2-O2-S33-O35
5	C	2[A]	TWA	C4-O4-S45-O46
5	C	2[A]	TWA	C4-O4-S45-O48
5	C	2[B]	TWA	O5-C5-C6-O6
5	C	1[A]	TWD	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	2[B]	TWA	C4-C5-C6-O6
5	C	1[B]	TWD	O5-C5-C6-O6
5	C	1[A]	TWD	O5-C5-C6-O6
5	C	1[A]	TWD	C2-O2-S15-O17
5	C	2[A]	TWA	C2-O2-S33-O36
5	C	2[A]	TWA	C4-O4-S45-O47
5	C	2[A]	TWA	C3-C2-O2-S33
5	C	1[B]	TWD	C1-C2-O2-S15
5	C	1[A]	TWD	C1-C2-O2-S15
5	C	1[B]	TWD	C3-C2-O2-S15
5	C	1[A]	TWD	C3-C2-O2-S15
5	C	1[A]	TWD	C2-O2-S15-O18
5	C	2[B]	TWA	C2-O2-S33-O34
5	C	2[B]	TWA	C3-O3-S39-O42
5	C	2[B]	TWA	C4-O4-S45-O47
5	C	2[B]	TWA	C4-O4-S45-O48
5	C	1[B]	TWD	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1[B]	TWD	1	0
5	C	2[B]	TWA	2	0
5	C	1[A]	TWD	1	0

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	92/126 (73%)	0.01	4 (4%)	35	42	23, 40, 58, 76	0
2	B	495/540 (91%)	0.80	69 (13%)	2	4	24, 49, 103, 137	0
3	H	219/238 (92%)	0.06	6 (2%)	54	62	24, 38, 55, 73	0
4	L	214/217 (98%)	-0.09	6 (2%)	53	60	24, 38, 62, 81	0
All	All	1020/1121 (90%)	0.38	85 (8%)	11	15	23, 42, 88, 137	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	517	GLY	13.9
2	B	515	PHE	9.7
2	B	546	MET	8.0
2	B	570	ASP	7.9
2	B	166	TYR	6.7
2	B	643	HIS	6.1
2	B	448	THR	5.8
2	B	165	ARG	5.7
2	B	449	HIS	5.7
2	B	164	PRO	5.6
2	B	468	THR	5.6
2	B	619	GLN	5.5
2	B	153	SER	5.4
2	B	167	ARG	5.3
2	B	571	LEU	5.1
2	B	469	ARG	5.0
2	B	616	PRO	4.9
2	B	615	ILE	4.9
2	B	553	HIS	4.8
2	B	642	SER	4.7
2	B	467	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	545	SER	4.7
2	B	279	PRO	4.7
2	B	168	ALA	4.6
2	B	542	ALA	4.6
2	B	573	THR	4.5
2	B	617	ALA	4.4
2	B	618	PRO	4.3
2	B	516	GLY	4.2
2	B	547	GLY	4.2
2	B	659	ARG	4.1
2	B	278	GLN	4.0
2	B	447	SER	4.0
2	B	470	MET	3.9
1	A	85	GLU	3.8
2	B	543	GLU	3.8
2	B	471	ALA	3.8
2	B	505	GLY	3.7
2	B	544	ALA	3.7
2	B	277	VAL	3.6
2	B	506	LYS	3.5
4	L	194	ARG	3.5
2	B	640	GLY	3.5
2	B	163	PRO	3.5
2	B	504	GLY	3.5
2	B	641	THR	3.4
2	B	569	GLU	3.3
4	L	161	LYS	3.3
2	B	280	VAL	3.2
2	B	554	GLN	3.1
2	B	514	ALA	3.1
2	B	493	GLY	3.1
2	B	492	SER	3.1
2	B	671	ALA	2.9
2	B	592	ARG	2.9
3	H	1	GLU	2.8
3	H	103	TRP	2.8
4	L	157	SER	2.7
2	B	244	GLY	2.7
2	B	572	GLY	2.7
1	A	151	ALA	2.6
4	L	192	SER	2.6
2	B	568	VAL	2.5

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

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(Å²)	Q<0.9
5	TWD	C	1[B]	20/20	0.63	0.42	60,86,91,91	20
5	TWD	C	1[A]	20/20	0.63	0.42	74,91,95,100	20
5	TWA	C	2[B]	23/24	0.69	0.46	72,90,94,98	23
5	TWA	C	2[A]	23/24	0.69	0.46	72,87,92,93	23

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(Å^2)	Q<0.9
6	NA	B	701	1/1	0.94	0.24	51,51,51,51	0
6	NA	B	702	1/1	0.94	0.58	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.