

Full wwPDB X-ray Structure Validation Report (i)

May 26, 2022 – 04:15 pm BST

PDB ID	:	7ZFC
Title	:	SARS-CoV-2 Beta RBD in complex with nanobody C1, Omi-18 and Omi-31
		Fabs
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Deposited on	:	2022-04-01
Resolution	:	3.24 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.24 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	1619(3.28-3.20)		
Clashscore	141614	1755 (3.28-3.20)		
Ramachandran outliers	138981	1728 (3.28-3.20)		
Sidechain outliers	138945	1727 (3.28-3.20)		
RSRZ outliers	127900	1567 (3.28-3.20)		

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 <=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	
			24%	
1	Н	233	80%	18% •
			22%	
2	L	216	86%	12% •
			12%	
3	Μ	131	79%	15% 5%
			10%	
4	А	222	80%	17% •
			10%	
5	В	213	79%	17% •



Mol	Chain	Length	Quality of chain		
6	Е	202	4% 73%	23%	·
7	С	2	100%		



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8954 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 Omi-31 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Н	228	Total	C	N	0	S	0	0	0
		_	1704	1075	288	334	7	_	-	

• Molecule 2 is a protein called Omi-31 light chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	L	213	Total 1578	C 981	N 267	O 326	${S \over 4}$	0	1	0

• Molecule 3 is a protein called Nanobody C1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	М	124	Total 973	C 612	N 167	0 190	${S \atop 4}$	0	2	0

• Molecule 4 is a protein called Omi-18 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Δ	215	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	A	210	1586	1000	268	311	7		U	0

• Molecule 5 is a protein called Omi-18 light chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	В	207	Total 1557	C 968	N 267	0 318	${S \atop 4}$	0	0	0

• Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	Е	193	Total 1532	C 984	N 255	O 286	${ m S} 7$	0	0	0



Chain	Residue	Modelled	Actual	Comment	Reference
Е	327	HIS	-	expression tag	UNP P0DTC2
Е	328	HIS	-	expression tag	UNP P0DTC2
Е	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
Е	331	HIS	-	expression tag	UNP P0DTC2
Е	332	HIS	-	expression tag	UNP P0DTC2
Е	417	ASN	LYS	variant	UNP P0DTC2
Е	484	LYS	GLU	variant	UNP P0DTC2
Е	501	TYR	ASN	variant	UNP P0DTC2
Е	527	LYS	-	expression tag	UNP P0DTC2
Е	528	LYS	-	expression tag	UNP P0DTC2

There are 11 discrepancies between the modelled and reference sequences:

• Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
7	С	2	Total 24	C 14	N 1	O 9	0	0	0



3 Residue-property plots (i)

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: Omi-31 heavy chain

 \bullet Molecule 4: Omi-18 heavy chain





Chain C:

100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	105.00Å 105.00Å 234.48Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	84.78 - 3.24	Depositor
Resolution (A)	84.78 - 3.24	EDS
% Data completeness	99.6 (84.78-3.24)	Depositor
(in resolution range)	99.8 (84.78-3.24)	EDS
R _{merge}	0.27	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.99 (at 3.26 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D D.	0.244 , 0.299	Depositor
n, n_{free}	0.243 , 0.297	DCC
R_{free} test set	1205 reflections $(4.89%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	125.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8954	wwPDB-VP
Average B, all atoms $(Å^2)$	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: FUC, NAG

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).

Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Н	0.25	0/1746	0.49	0/2378
2	L	0.25	0/1618	0.48	0/2212
3	М	0.24	0/1004	0.50	0/1366
4	А	0.25	0/1620	0.51	0/2209
5	В	0.25	0/1596	0.48	0/2185
6	Е	0.26	0/1576	0.47	0/2146
All	All	0.25	0/9160	0.49	0/12496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	Н	1704	0	1671	26	0
2	L	1578	0	1529	18	0
3	М	973	0	922	13	0
4	А	1586	0	1563	21	0
5	В	1557	0	1494	30	0
6	Е	1532	0	1444	33	0
7	С	24	0	22	2	0
All	All	8954	0	8645	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:L:35:ASN:HD21	2:L:99:ARG:HH12	1.23	0.83	
1:H:109:ARG:NH1	2:L:94:GLU:OE2	2.15	0.78	
6:E:365:TYR:H	6:E:388:ASN:HD21	1.32	0.76	
4:A:199:ILE:HG12	4:A:214:ARG:HG2	1.72	0.71	
4:A:29:VAL:HG13	4:A:34:MET:HG3	1.72	0.71	
5:B:90:TRP:HA	5:B:90:TRP:CE3	2.25	0.71	
5:B:25:ASN:N	5:B:25:ASN:OD1	2.20	0.70	
6:E:475:ALA:HB3	6:E:487:ASN:HB3	1.74	0.69	
5:B:4:LEU:HD11	5:B:89:VAL:HG13	1.73	0.69	
2:L:35:ASN:HD21	2:L:99:ARG:NH1	1.92	0.67	
4:A:173:VAL:HG12	5:B:163:THR:HG23	1.77	0.66	
4:A:82:MET:HB3	4:A:85:LEU:HD21	1.80	0.64	
4:A:123:PRO:HB3	4:A:149:TYR:HB3	1.80	0.63	
4:A:92:VAL:HG22	4:A:112:THR:HG22	1.80	0.62	
2:L:11:SER:HB2	2:L:110:LEU:HD11	1.81	0.62	
2:L:84:GLU:HB2	2:L:109:VAL:HG23	1.82	0.61	
5:B:94:ARG:HH21	6:E:409:GLN:HG3	1.65	0.61	
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.83	0.61	
5:B:90:TRP:HA	5:B:90:TRP:HE3	1.65	0.60	
4:A:163:LEU:HD21	4:A:186:VAL:HG21	1.83	0.60	
1:H:2:VAL:HG23	1:H:117:VAL:HG11	1.84	0.59	
3:M:110:SER:HB3	6:E:378:LYS:NZ	2.17	0.59	
1:H:57:ALA:HB1	6:E:449:TYR:HB3	1.83	0.59	
5:B:139:ASP:OD1	5:B:168:GLN:NE2	2.37	0.58	
5:B:133:LEU:HD12	5:B:179:LEU:HD23	1.86	0.57	
5:B:11:SER:HB3	5:B:107:LEU:HD21	1.86	0.57	
5:B:94:ARG:NH2	6:E:409:GLN:HG3	2.18	0.57	
6:E:406:GLU:OE1	6:E:495:TYR:OH	2.19	0.57	
7:C:1:NAG:H4	7:C:2:FUC:H5	1.85	0.56	
4:A:48:VAL:HG13	4:A:63:VAL:HG21	1.86	0.56	
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.35	0.56	
3:M:105:ASP:HB2	6:E:378:LYS:HE3	1.87	0.56	
5:B:12:VAL:HG21	5:B:18:ALA:HB2	1.87	0.55	
6:E:365:TYR:H	6:E:388:ASN:ND2	2.02	0.55	
4:A:22:CYS:HB3	4:A:78:LEU:HB3	1.89	0.55	
6:E:485:GLY:H	6:E:488:CYS:HB2	1.72	0.55	
3:M:110:SER:HB3	6:E:378:LYS:HZ1	1.72	0.55	



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:B:54:PRO:HG2	5:B:57:ILE:HD12	1.89	0.54	
3:M:17[B]:SER:OG	3:M:82:GLN:NE2	2.40	0.54	
6:E:339:GLY:HA2	7:C:1:NAG:O7	2.06	0.54	
2:L:40:LEU:HD23	2:L:85:ALA:HB2	1.90	0.53	
4:A:6:GLU:H	4:A:109:GLN:HE22	1.57	0.53	
6:E:350:VAL:HG22	6:E:422:ASN:HB3	1.90	0.52	
5:B:16:GLN:HG2	5:B:17:THR:H	1.75	0.52	
2:L:86:ASP:OD1	2:L:106:LYS:HG2	2.10	0.51	
4:A:35:THR:HG22	4:A:50:LEU:HB3	1.93	0.51	
6:E:336:CYS:HB2	6:E:363:ALA:HB2	1.93	0.51	
5:B:53:ARG:HD3	5:B:61:PHE:O	2.10	0.51	
1:H:174:LEU:HD21	1:H:197:VAL:HG21	1.91	0.51	
6:E:357:ARG:NH2	6:E:394:ASN:OD1	2.44	0.50	
4:A:34:MET:HB3	4:A:78:LEU:HD22	1.92	0.50	
5:B:105:THR:HG21	5:B:142:PRO:HB3	1.93	0.50	
1:H:31:SER:H	1:H:54:ILE:HG21	1.76	0.50	
1:H:28:THR:O	1:H:32:TYR:HB2	2.11	0.50	
4:A:32:ASN:HD21	6:E:475:ALA:HB1	1.77	0.50	
1:H:102:HIS:HB2	1:H:113:ASP:HB2	1.92	0.49	
3:M:91:THR:HG23	3:M:121:THR:HA	1.95	0.49	
1:H:47:TRP:HE3	1:H:61:ALA:HB2	1.78	0.48	
1:H:53:PRO:HB3	1:H:74:LYS:HE2	1.95	0.48	
2:L:47:LEU:HD21	2:L:50:TYR:HB3	1.95	0.48	
5:B:114:PRO:HB3	5:B:140:PHE:HB3	1.95	0.48	
4:A:100:GLN:HB3	5:B:90:TRP:CZ2	2.50	0.47	
3:M:5:VAL:HB	3:M:23:ALA:HB3	1.96	0.47	
5:B:12:VAL:HG12	5:B:16:GLN:HB3	1.96	0.47	
2:L:117:PRO:HB3	2:L:143:PHE:HB3	1.97	0.47	
2:L:136:LEU:HD12	2:L:182:LEU:HD23	1.97	0.47	
1:H:47:TRP:CE3	1:H:61:ALA:HB2	2.51	0.46	
1:H:114:GLY:H	2:L:99:ARG:HH22	1.63	0.46	
3:M:73:HIS:HB3	3:M:76:ASN:OD1	2.15	0.46	
4:A:204:HIS:HB3	4:A:209:THR:HB	1.97	0.46	
6:E:403:ARG:HG2	6:E:505:TYR:HA	1.96	0.46	
1:H:89:GLU:OE1	1:H:89:GLU:N	2.48	0.46	
4:A:42:GLY:HA3	5:B:164:THR:HG21	1.96	0.46	
4:A:146:VAL:HG11	4:A:154:VAL:HG21	1.97	0.46	
6:E:365:TYR:N	6:E:388:ASN:HD21	2.08	0.46	
6:E:439:ASN:O	6:E:443:SER:OG	2.34	0.46	
4:A:120:THR:HG22	4:A:207:SER:HB3	1.98	0.46	
5:B:29:ALA:HB2	6:E:501:TYR:CE2	2.50	0.46	



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:B:133:LEU:HB2	5:B:179:LEU:HB3	1.98	0.45	
5:B:32:VAL:HG21	5:B:70:ALA:HB2	1.98	0.45	
5:B:18:ALA:HB2	5:B:77:ILE:HD11	1.97	0.45	
2:L:92:TRP:CZ3	2:L:98:GLY:HA2	2.52	0.45	
6:E:359:SER:O	6:E:361:CYS:N	2.42	0.45	
6:E:376:THR:HB	6:E:435:ALA:HB3	1.98	0.45	
1:H:14:PRO:HD2	1:H:128:SER:HA	1.97	0.45	
1:H:51:VAL:HG23	1:H:58:LYS:HB3	1.99	0.45	
4:A:11:LEU:HA	4:A:114:THR:O	2.17	0.45	
2:L:22:CYS:HB3	2:L:72:ALA:HB3	1.98	0.45	
3:M:52:SER:O	3:M:56:ASN:N	2.49	0.45	
5:B:46:VAL:HA	5:B:57:ILE:HD13	1.99	0.45	
5:B:27:ASP:OD1	5:B:65:ASN:ND2	2.46	0.45	
6:E:518:LEU:HD21	6:E:521:PRO:HB3	1.97	0.45	
4:A:33:TYR:OH	6:E:455:LEU:O	2.27	0.45	
6:E:352:ALA:HB1	6:E:466:ARG:HH21	1.82	0.45	
6:E:398:ASP:HB2	6:E:512:VAL:HB	1.98	0.44	
6:E:392:PHE:CE1	6:E:395:VAL:HG23	2.53	0.44	
2:L:187:GLU:OE1	2:L:187:GLU:N	2.51	0.43	
3:M:107:TRP:CH2	6:E:503:VAL:HG12	2.54	0.43	
1:H:116:ASP:N	1:H:116:ASP:OD1	2.51	0.43	
3:M:76:ASN:ND2	3:M:80:TYR:OH	2.52	0.43	
5:B:151:ALA:O	5:B:153:SER:N	2.52	0.43	
1:H:52:ILE:HG22	1:H:55:LEU:H	1.83	0.43	
4:A:14:PRO:HD3	4:A:116:SER:O	2.19	0.42	
2:L:35:ASN:HB2	2:L:49:ILE:O	2.19	0.42	
2:L:39:GLN:O	2:L:85:ALA:HB1	2.19	0.42	
1:H:98:ARG:HG2	1:H:117:VAL:HB	2.01	0.42	
6:E:401:VAL:HG22	6:E:509:ARG:HG2	2.00	0.42	
1:H:161:PHE:HA	1:H:162:PRO:HA	1.85	0.42	
3:M:99:GLY:HA3	3:M:101:PHE:CE2	2.54	0.42	
1:H:40:ALA:HB3	1:H:43:LEU:HD12	2.02	0.41	
5:B:46:VAL:HA	5:B:57:ILE:CD1	2.50	0.41	
1:H:67:ARG:O	1:H:83:LEU:HD12	2.21	0.41	
6:E:414:GLN:O	6:E:424:LYS:NZ	2.53	0.41	
5:B:150:LYS:HB2	5:B:193:SER:HB2	2.02	0.41	
5:B:121:PRO:HD3	5:B:133:LEU:HD23	2.02	0.41	
2:L:84:GLU:HG3	2:L:107:LEU:O	2.21	0.41	
1:H:31:SER:HA	1:H:54:ILE:HD13	2.03	0.41	
1:H:57:ALA:HA	6:E:449:TYR:CD2	2.56	0.41	
3:M:32:TYR:CE2	3:M:53:VAL:HG21	2.56	0.41	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:HIS:HB2	1:H:113:ASP:CB	2.51	0.41
5:B:94:ARG:HH22	6:E:408:ARG:CG	2.33	0.40
1:H:199:VAL:HG11	1:H:209:TYR:CE1	2.57	0.40
6:E:335:LEU:HD23	6:E:335:LEU:HA	1.90	0.40
2:L:7:PRO:HA	2:L:8:PRO:HD3	1.97	0.40
3:M:40:ALA:HB3	3:M:43:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	Н	226/233~(97%)	217 (96%)	9 (4%)	0	100	100
2	L	212/216~(98%)	199 (94%)	13 (6%)	0	100	100
3	М	124/131~(95%)	121 (98%)	3 (2%)	0	100	100
4	А	211/222~(95%)	201 (95%)	7(3%)	3(1%)	11	43
5	В	205/213~(96%)	190 (93%)	14 (7%)	1 (0%)	29	64
6	Ε	191/202~(95%)	172 (90%)	18 (9%)	1 (0%)	29	64
All	All	1169/1217~(96%)	1100 (94%)	64 (6%)	5 (0%)	34	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	В	152	ASP
4	А	100	GLN
4	А	2	VAL
4	А	41	PRO
6	Е	362	VAL



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	Н	190/195~(97%)	186~(98%)	4 (2%)	53	77
2	L	179/182~(98%)	178 (99%)	1 (1%)	86	93
3	М	105/110~(96%)	105 (100%)	0	100	100
4	А	177/185~(96%)	176~(99%)	1 (1%)	86	93
5	В	175/181~(97%)	174 (99%)	1 (1%)	86	93
6	Е	165/175~(94%)	163~(99%)	2 (1%)	71	86
All	All	991/1028~(96%)	982~(99%)	9 (1%)	78	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	59	HIS
1	Н	65	GLN
1	Н	107	TRP
1	Н	110	PHE
2	L	39	GLN
4	А	168	HIS
5	В	25	ASN
6	Е	489	TYR
6	Е	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	Н	103	HIS
2	L	35	ASN
6	Е	388	ASN

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)

2 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).

Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	\mathbf{ths}	В	ond ang	les
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
7	NAG	С	1	6,7	14,14,15	0.42	0	$17,\!19,\!21$	1.09	1 (5%)
7	FUC	С	2	7	10,10,11	0.87	0	14,14,16	1.10	1 (7%)

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
7	NAG	С	1	6,7	-	2/6/23/26	0/1/1/1
7	FUC	С	2	7	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	С	1	NAG	C1-O5-C5	4.14	117.80	112.19
7	С	2	FUC	O5-C5-C4	2.55	114.09	109.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	С	1	NAG	C4-C5-C6-O6
7	С	1	NAG	O5-C5-C6-O6



There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	С	1	NAG	2	0
7	С	2	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	Н	228/233~(97%)	1.36	55 (24%) 0 1	88, 148, 285, 377	0
2	L	213/216~(98%)	1.35	48 (22%) 0 1	89, 147, 266, 321	0
3	М	124/131~(94%)	0.91	16 (12%) 3 3	102, 134, 176, 201	0
4	А	215/222~(96%)	0.87	23 (10%) 6 4	96, 130, 180, 292	0
5	В	207/213~(97%)	0.77	21 (10%) 7 5	98, 137, 187, 262	0
6	Е	193/202~(95%)	0.68	9 (4%) 31 21	90, 117, 179, 221	0
All	All	1180/1217~(96%)	1.01	172 (14%) 2 2	88, 135, 250, 377	0

All (172) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	L	124	PRO	14.8
4	А	219	SER	13.2
2	L	150	VAL	10.5
1	Н	140	ALA	9.4
1	Н	141	PRO	9.3
2	L	135	THR	8.7
2	L	121	LEU	8.5
2	L	159	VAL	8.4
2	L	125	SER	7.2
1	Н	148	GLY	7.2
1	Н	138	PRO	7.1
1	Н	145	SER	7.0
2	L	137	VAL	6.8
1	Н	153	LEU	6.6
1	Н	204	LEU	6.5
1	Н	139	LEU	6.4
1	Н	147	SER	6.4
2	L	160	LYS	6.2
1	Н	199	VAL	6.1



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Mol	Chain	Res	Type	RSRZ				
2	L	197	CYS	6.0				
2	L	115	ALA	5.9				
1	Н	142	SER	5.8				
3	М	10	GLY	5.7				
2	L	199	VAL	5.5				
1	Н	137	PHE	5.4				
1	Н	200	PRO	5.4				
2	L	123	PRO	5.0				
2	L	120	THR	5.0				
1	Н	209	TYR	4.9				
2	L	122	PHE	4.8				
5	В	28	GLY	4.7				
1	Н	136	VAL	4.7				
2	L	136	LEU	4.6				
2	L	152	TRP	4.6				
2	L	139	LEU	4.4				
2	L	181	TYR	4.2				
3	М	11[A]	LEU	4.0				
1	Н	208	THR	4.0				
1	Н	151	ALA	4.0				
2	L	164	GLU	3.9				
1	Н	1	GLU	3.9				
2	L	146	GLY	3.9				
2	L	204	SER	3.8				
5	В	193	SER	3.8				
5	В	199	GLU	3.7				
4	А	119	SER	3.7				
1	Н	187	SER	3.7				
5	В	144	ALA	3.7				
1	Н	228	PRO	3.7				
2	L	134	ALA	3.7				
2	L	195	TYR	3.6				
1	Н	197	VAL	3.6				
2	L	210	VAL	3.6				
5	В	96	HIS	3.5				
1	Н	156	LEU	3.5				
5	В	4	LEU	3.4				
1	Н	179	HIS	3.4				
2	L	209	THR	3.4				
1	Н	227	GLU	3.4				
1	Н	155	CYS	3.4				
1	Н	222	VAL	3.3				

222VAL3.3Continued on next page...



Mol	Chain	Res	Type	RSRZ
2	L	114	LYS	3.3
1	Н	198	THR	3.3
1	Н	174	LEU	3.3
4	А	116	SER	3.2
4	А	215	VAL	3.2
1	Н	207	GLN	3.2
5	В	29	ALA	3.2
4	А	67	PHE	3.2
5	В	192	TYR	3.2
5	В	21	THR	3.1
2	L	116	ASN	3.1
4	А	193	LEU	3.1
2	L	151	ALA	3.1
5	В	27	ASP	3.1
4	А	85	LEU	3.1
1	Н	135	SER	3.0
2	L	138	CYS	3.0
1	Н	178	VAL	3.0
4	А	131	SER	3.0
4	А	184	SER	3.0
6	Е	497	PHE	3.0
2	L	148	VAL	2.9
2	L	184	LEU	2.9
2	L	206	VAL	2.9
1	Н	167	VAL	2.8
1	Н	225	ARG	2.8
2	L	163	VAL	2.8
2	L	158	PRO	2.8
6	Е	423	TYR	2.8
1	Н	169	TRP	2.8
5	В	143	GLY	2.7
6	Е	375	SER	2.7
5	В	70	ALA	2.7
4	А	48	VAL	2.7
1	Н	149	GLY	2.7
1	Н	213	VAL	2.7
2	L	182	LEU	2.7
4	А	198	TYR	2.7
6	Е	505	TYR	2.7
4	А	120	THR	2.6
5	В	152	ASP	2.6
1	Н	48	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	Н	154	GLY	2.6
3	М	70	ILE	2.6
3	М	40	ALA	2.5
4	А	154	VAL	2.5
3	М	27	PHE	2.5
1	Н	175	THR	2.5
5	В	88	GLN	2.5
3	М	65	LYS	2.5
4	А	133	LYS	2.5
5	В	20	ILE	2.5
1	Н	146	THR	2.5
3	М	30	ASP	2.5
1	Н	81	MET	2.4
6	Е	429	PHE	2.4
6	Е	424	LYS	2.4
2	L	90	ALA	2.4
2	L	189	TRP	2.4
5	В	145	VAL	2.4
2	L	117	PRO	2.4
1	Н	190	LEU	2.4
3	М	93	ILE	2.3
4	А	129	ALA	2.3
1	Н	226	VAL	2.3
4	А	115	VAL	2.3
6	Е	338	PHE	2.3
1	Н	150	THR	2.3
3	М	122	VAL	2.3
1	Н	184	VAL	2.3
2	L	31	SER	2.3
2	L	192	HIS	2.3
2	L	37	TYR	2.3
1	Н	101	LEU	2.3
2	L	140	ILE	2.3
1	Н	69	THR	2.2
2	L	179	SER	2.2
3	М	100	ARG	2.2
5	В	190	ARG	2.2
4	А	79	TYR	2.2
1	Н	110	PHE	2.2
2	L	76	ILE	2.2
6	Е	378	LYS	2.2
2	L	112	GLN	2.2

112GLN2.2Continued on next page...



Mol	Chain	Res	Type	RSRZ
2	L	198	GLN	2.2
1	Н	36	TRP	2.1
1	Н	214	ASN	2.1
1	Н	64	PHE	2.1
1	Н	206	THR	2.1
3	М	68	PHE	2.1
4	А	183	SER	2.1
1	Н	152	ALA	2.1
3	М	31	PHE	2.1
4	А	82	MET	2.1
5	В	45	LEU	2.1
3	М	83	MET	2.1
4	А	182	LEU	2.1
5	В	22	CYS	2.1
6	Е	515	PHE	2.1
1	Н	131	THR	2.1
4	А	188	VAL	2.0
3	М	59	THR	2.0
2	L	127	GLU	2.0
5	В	156	VAL	2.0
4	А	163	LEU	2.0
2	L	202	GLU	2.0
1	Н	20	VAL	2.0
3	М	62	ASP	2.0
3	М	95	TYR	2.0
4	А	210	LYS	2.0
5	В	191	SER	2.0

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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, 95^{th} 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	$B-factors(A^2)$	Q<0.9
7	NAG	С	1	14/15	0.75	0.27	156,191,221,229	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
7	FUC	С	2	10/11	0.78	0.37	215,248,267,293	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

