

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8SDH
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with
		neutralizing antibody CC25.56
Authors	:	Yuan, M.; Wilson, I.A.
Deposited on	:	2023-04-06
Resolution	:	2.84 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

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 2.84 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.



Motric	Whole archive	Similar resolution
WIEthte	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	$1031 \ (2.86-2.82)$
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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		
1	А	205	9%	21%	• 5%
	 	200	13%	21/0	
	В	205	71%	23%	• 5%
2	С	223	74%	24%	•
2	Н	223	83%	13%	••
		214	2%		
3	D	214	77%	18%	••



Mol	Chain	Length	Quality of chain	Quality of chain					
3	L	214	2%	20%	•••				
4	Е	2	100%						



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9606 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	105	Total	С	Ν	0	\mathbf{S}	0	0	0
1	А	195	1541	988	257	288	8	0	0	U
1	D	105	Total	С	Ν	0	S	0	0	0
1	D	195	1535	984	256	287	8	0	0	U

• Molecule 1 is a protein called Spike protein S1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	531	GLY	-	expression tag	UNP P0DTC2
А	532	HIS	-	expression tag	UNP P0DTC2
А	533	HIS	-	expression tag	UNP P0DTC2
А	534	HIS	-	expression tag	UNP P0DTC2
А	535	HIS	-	expression tag	UNP P0DTC2
А	536	HIS	-	expression tag	UNP P0DTC2
А	537	HIS	-	expression tag	UNP P0DTC2
В	531	GLY	-	expression tag	UNP P0DTC2
В	532	HIS	-	expression tag	UNP P0DTC2
В	533	HIS	-	expression tag	UNP P0DTC2
В	534	HIS	-	expression tag	UNP P0DTC2
В	535	HIS	-	expression tag	UNP P0DTC2
В	536	HIS	-	expression tag	UNP P0DTC2
В	537	HIS	-	expression tag	UNP P0DTC2

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Neutralizing antibody CC25.56 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	тт	916	Total	С	Ν	0	S	0	0	0
	11	210	1626	1037	271	310	8			
0	C	222	Total	С	Ν	0	S	0	0	0
			1664	1058	278	320	8	0	0	

• Molecule 3 is a protein called Neutralizing antibody CC25.56 Light Chain.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	т	210	Total	С	Ν	0	S	0	0	0
0		210	1573	986	265	318	4	0		
2	П	210	Total	С	Ν	0	S	0	1	0
0		210	1584	995	266	319	4	0	1	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Е	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	В	1	Total C 14 8	N 1	O 5	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	7	Total O 7 7	0	0
6	В	3	Total O 3 3	0	0
6	Н	6	Total O 6 6	0	0
6	L	7	Total O 7 7	0	0
6	С	10	Total O 10 10	0	0
6	D	8	Total O 8 8	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: Spike protein S1





• Molecule 3: Neutralizing antibody CC25.56 Light Chain



• Molecule 3: Neutralizing antibody CC25.56 Light Chain



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	171.05Å 105.59Å 98.99Å	Depositor
a, b, c, α , β , γ	90.00° 117.31° 90.00°	Depositor
Bosolution(A)	47.69 - 2.84	Depositor
Resolution (A)	47.69 - 2.84	EDS
% Data completeness	98.8 (47.69-2.84)	Depositor
(in resolution range)	98.8 (47.69-2.84)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.48 (at 2.86 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
D D.	0.246 , 0.283	Depositor
Λ, Λ_{free}	0.249 , 0.287	DCC
R_{free} test set	1914 reflections (5.23%)	wwPDB-VP
Wilson B-factor $(Å^2)$	54.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 38.1	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9606	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% 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: 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		
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/1585	0.62	3/2158~(0.1%)	
1	В	0.27	0/1579	0.51	0/2150	
2	С	0.32	0/1708	0.65	2/2325~(0.1%)	
2	Н	0.29	0/1669	0.57	1/2272~(0.0%)	
3	D	0.27	0/1627	0.56	2/2227~(0.1%)	
3	L	0.26	0/1615	0.50	0/2211	
All	All	0.29	0/9783	0.57	8/13343~(0.1%)	

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
3	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	497	PHE	C-N-CA	10.59	148.17	121.70
3	D	50	TYR	C-N-CD	-9.90	98.82	120.60
1	А	497	PHE	O-C-N	-9.78	107.06	122.70
2	Н	227	LYS	CD-CE-NZ	-8.66	91.78	111.70
2	С	206	ILE	CG1-CB-CG2	-8.63	92.42	111.40
2	С	206	ILE	CA-CB-CG1	8.24	126.66	111.00
1	А	497	PHE	CA-C-N	6.57	131.64	117.20
3	D	129	LYS	CA-CB-CG	5.11	124.65	113.40

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	50	TYR	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	А	1541	0	1454	30	0
1	В	1535	0	1441	37	0
2	С	1664	0	1642	39	0
2	Н	1626	0	1603	16	0
3	D	1584	0	1521	29	0
3	L	1573	0	1513	31	0
4	Е	28	0	25	0	0
5	В	14	0	13	0	0
6	А	7	0	0	0	0
6	В	3	0	0	0	0
6	С	10	0	0	0	0
6	D	8	0	0	0	0
6	Н	6	0	0	0	0
6	L	7	0	0	0	0
All	All	9606	0	9212	171	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 9.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:L:29:GLY:HA2	3:L:66:ASN:HD21	1.36	0.90
1:A:521:PRO:HG3	1:B:409:GLN:HG3	1.61	0.80
3:L:66:ASN:HD22	3:L:67:SER:N	1.83	0.75
2:C:210:ASN:HB2	2:C:217:LYS:HD2	1.69	0.74
3:D:181:LEU:HD12	3:D:185:GLN:HG3	1.71	0.72
1:B:340:GLU:OE1	1:B:356:LYS:NZ	2.22	0.72
3:D:130:ALA:HB3	3:D:181:LEU:O	1.89	0.71



	ti c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:51:ILE:HD12	2:C:57:THR:HG22	1.71	0.70	
2:C:139:LEU:HD11	2:C:197:LEU:HD11	1.75	0.69	
2:H:227:LYS:HZ1	3:L:122:SER:CB	2.06	0.67	
3:L:29:GLY:HA2	3:L:66:ASN:ND2	2.09	0.66	
1:A:341:VAL:HG23	1:A:342:PHE:HD1	1.61	0.66	
2:H:152:THR:HG22	2:H:210:ASN:HB3	1.78	0.66	
2:C:125:PRO:HB3	2:C:139:LEU:HD13	1.78	0.66	
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.30	0.65	
1:B:458:LYS:NZ	1:B:474:GLN:O	2.29	0.65	
2:C:18:LEU:HD12	2:C:82(C):LEU:HD11	1.79	0.63	
2:C:209:VAL:O	2:C:217:LYS:HG3	1.98	0.63	
1:A:360:ASN:H	1:A:523:THR:HB	1.63	0.62	
1:B:434:ILE:HB	1:B:511:VAL:HG12	1.80	0.62	
3:L:105:THR:HG21	3:L:141:PRO:HB3	1.81	0.62	
3:D:189:HIS:HD1	3:D:192:TYR:HH	1.47	0.61	
1:B:365:TYR:HA	1:B:368:LEU:HD12	1.83	0.61	
3:L:136:ILE:HG21	3:L:196:VAL:HG11	1.84	0.60	
1:A:369:TYR:O	1:A:369:TYR:HD1	1.85	0.59	
3:L:66:ASN:HD22	3:L:67:SER:H	1.49	0.58	
2:C:112:PHE:HB2	2:C:147:PHE:CZ	2.38	0.58	
3:L:83:GLU:HG3	3:L:106:VAL:HG23	1.84	0.58	
2:H:212:LYS:HG2	2:H:213:PRO:HD3	1.84	0.58	
2:C:23:LYS:NZ	2:C:75:ILE:O	2.36	0.58	
3:D:128:ASN:O	3:D:128:ASN:ND2	2.37	0.57	
3:D:195:GLN:NE2	3:D:206:GLU:OE2	2.19	0.57	
3:D:127:ALA:HB1	3:D:129:LYS:NZ	2.19	0.57	
3:L:90:LEU:HD12	3:L:91:TRP:H	1.69	0.57	
2:C:194:SER:HA	2:C:197:LEU:HD23	1.85	0.57	
2:C:176:VAL:HB	3:D:162:THR:HG22	1.86	0.57	
3:L:90:LEU:HD12	3:L:91:TRP:N	2.20	0.57	
1:B:355:ARG:HD3	1:B:398:ASP:OD1	2.05	0.57	
1:B:342:PHE:CZ	1:B:511:VAL:HG11	2.40	0.56	
2:H:114:GLN:HG2	2:H:116:LYS:HB2	1.86	0.56	
2:C:101:ASP:HA	3:D:46:VAL:HG21	1.87	0.56	
2:H:125:PRO:HD3	2:H:139:LEU:HD13	1.86	0.56	
3:L:4:LEU:HD22	3:L:23:CYS:SG	2.45	0.56	
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.40	0.56	
3:L:48:ILE:HG22	3:L:49:TYR:O	2.06	0.55	
2:C:118:PRO:HB3	2:C:146:TYR:HB3	1.86	0.55	
2:H:227:LYS:NZ	3:L:122:SER:HB3	2.21	0.55	
1:B:388:ASN:HB2	1:B:527:PRO:HD2	1.89	0.54	



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:D:119:PRO:HA	3:D:132:LEU:HD13	1.88	0.54	
1:B:365:TYR:CD2	1:B:387:LEU:HD22	2.42	0.54	
1:B:393:THR:N	1:B:516:GLU:O	2.40	0.54	
2:H:227:LYS:NZ	3:L:122:SER:CB	2.69	0.54	
3:L:18:THR:HG23	3:L:76:SER:HA	1.90	0.54	
2:C:210:ASN:HB2	2:C:217:LYS:NZ	2.22	0.54	
1:B:369:TYR:HA	1:B:377:PHE:CE2	2.43	0.54	
2:C:40:MET:HB2	2:C:43:LYS:HG3	1.90	0.53	
1:A:455:LEU:HD12	1:A:456:PHE:CZ	2.44	0.53	
2:C:166:THR:O	2:C:170:VAL:HG22	2.10	0.52	
2:H:118:PRO:HB3	2:H:146:TYR:HB3	1.91	0.51	
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.35	0.51	
3:L:28:ILE:N	3:L:28:ILE:HD12	2.26	0.51	
3:L:29:GLY:CA	3:L:66:ASN:HD21	2.17	0.51	
2:C:152:THR:OG1	2:C:210:ASN:HB3	2.11	0.51	
3:D:185:GLN:O	3:D:189:HIS:ND1	2.44	0.51	
2:C:4:LEU:HD12	2:C:92:CYS:SG	2.51	0.50	
3:D:127:ALA:HB1	3:D:129:LYS:HZ2	1.76	0.50	
3:D:149:LYS:HZ1	3:D:154:PRO:HB3	1.77	0.50	
3:D:151:ASP:OD1	3:D:190:ARG:HG2	2.11	0.50	
1:A:398:ASP:O	1:A:511:VAL:HA	2.12	0.50	
1:B:417:LYS:O	1:B:421:TYR:HB2	2.12	0.49	
3:D:135:LEU:HD23	3:D:176:SER:HB3	1.94	0.49	
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.47	0.49	
3:D:128:ASN:C	3:D:129:LYS:HD3	2.31	0.49	
2:H:176:VAL:HB	3:L:162:THR:HG22	1.95	0.49	
2:C:210:ASN:N	2:C:217:LYS:HZ2	2.11	0.49	
3:D:68:GLU:HG2	3:D:69:ASN:OD1	2.13	0.49	
3:L:50:TYR:HB3	3:L:51:PRO:HD3	1.95	0.48	
1:A:471:GLU:OE2	3:D:31:LYS:NZ	2.46	0.48	
2:C:147:PHE:HD1	2:C:148:PRO:CA	2.27	0.48	
3:D:28:ILE:HG22	3:D:33:VAL:HG21	1.96	0.48	
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.49	0.48	
2:H:94:ARG:NH2	2:H:101:ASP:OD2	2.39	0.48	
2:C:209:VAL:C	2:C:217:LYS:HG3	2.34	0.48	
3:L:68:GLU:H	3:L:68:GLU:CD	2.16	0.48	
2:C:4:LEU:HD12	2:C:22:CYS:SG	2.53	0.48	
1:A:417:LYS:O	1:A:421:TYR:HB2	2.14	0.47	
3:D:189:HIS:CE1	3:D:192:TYR:HH	2.31	0.47	
1:B:353:TRP:O	1:B:466:ARG:NH1	2.47	0.47	
1:B:398:ASP:O	1:B:511:VAL:HA	2.14	0.47	



	A L	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:506:GLN:HB2	1:A:508:TYR:HE1	1.79	0.47	
1:B:394:ASN:HB2	1:B:516:GLU:OE2	2.14	0.47	
2:C:36:TRP:CZ3	2:C:92:CYS:HB3	2.49	0.47	
1:B:365:TYR:CE2	1:B:387:LEU:HD22	2.49	0.47	
1:B:409:GLN:NE2	1:B:418:ILE:HB	2.30	0.47	
1:B:517:LEU:HD13	1:B:519:HIS:H	1.80	0.46	
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.51	0.46	
2:C:116:LYS:HB2	2:C:116:LYS:HE2	1.65	0.46	
3:L:49:TYR:HB2	3:L:53:ASP:HB3	1.97	0.46	
2:C:101:ASP:OD1	2:C:101:ASP:N	2.48	0.46	
3:D:35:TRP:HB2	3:D:48:ILE:HG22	1.97	0.46	
2:C:210:ASN:CB	2:C:217:LYS:HD2	2.40	0.45	
1:A:506:GLN:HB2	1:A:508:TYR:CE1	2.51	0.45	
1:B:377:PHE:CE1	1:B:434:ILE:HG12	2.51	0.45	
3:L:135:LEU:HD23	3:L:176:SER:HB3	1.98	0.45	
3:L:13:VAL:HG23	3:L:78:VAL:HG21	1.99	0.45	
3:L:28:ILE:HG23	3:L:33:VAL:HG21	1.99	0.45	
2:C:211:HIS:HB3	2:C:216:THR:HB	1.98	0.45	
1:A:376:THR:HB	1:A:435:ALA:HB3	1.98	0.45	
1:B:409:GLN:HE22	1:B:418:ILE:H	1.65	0.45	
1:A:342:PHE:CZ	1:A:511:VAL:HG21	2.51	0.45	
3:L:141:PRO:HD2	3:L:199:GLU:OE1	2.17	0.45	
2:C:165:LEU:HD23	2:C:190:VAL:HG21	1.99	0.45	
1:B:376:THR:HB	1:B:435:ALA:HB3	1.97	0.44	
2:H:87:THR:HG23	2:H:110:THR:HA	1.99	0.44	
1:B:409:GLN:NE2	1:B:418:ILE:H	2.15	0.44	
3:D:186:TRP:CZ2	3:D:211:PRO:HA	2.53	0.44	
1:A:502:GLY:O	1:A:506:GLN:HG2	2.18	0.44	
3:L:129:LYS:HA	3:L:129:LYS:HD2	1.67	0.44	
2:C:101:ASP:O	2:C:102:ILE:HD13	2.17	0.44	
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.99	0.44	
2:H:29:PHE:CD2	2:H:76:SER:HA	2.52	0.43	
3:L:4:LEU:HD23	3:L:4:LEU:HA	1.77	0.43	
2:C:36:TRP:CE2	2:C:80:LEU:HB2	2.53	0.43	
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.53	0.43	
1:B:350:VAL:O	1:B:353:TRP:HD1	2.01	0.43	
1:B:403:ARG:HG3	1:B:495:TYR:CE1	2.53	0.43	
2:C:147:PHE:HD1	2:C:148:PRO:N	2.16	0.43	
3:L:186:TRP:CZ2	3:L:211:PRO:HA	2.53	0.43	
1:B:369:TYR:HA	1:B:377:PHE:HE2	1.82	0.43	
2:C:220:LYS:HA	2:C:220:LYS:HD3	1.82	0.43	



	AL O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:342:PHE:HZ	1:B:434:ILE:HD12	1.83	0.43	
2:H:194:SER:O	2:H:197:LEU:HB2	2.19	0.43	
2:C:123:LEU:HD12	2:C:141:CYS:N	2.33	0.43	
1:A:389:ASP:N	1:A:389:ASP:OD1	2.52	0.43	
2:C:123:LEU:HB3	3:D:118:PHE:CD1	2.54	0.43	
2:C:122:PRO:HD3	2:C:220:LYS:HE3	2.01	0.42	
2:C:174:PRO:HG2	3:D:165:SER:OG	2.18	0.42	
1:A:498:GLN:HA	1:A:499:PRO:HD3	1.90	0.42	
1:B:378:LYS:HD3	1:B:379:CYS:N	2.33	0.42	
3:D:17:LYS:HD3	3:D:17:LYS:HA	1.61	0.42	
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.55	0.42	
3:L:13:VAL:HG21	3:L:78:VAL:HG11	2.02	0.42	
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.54	0.42	
2:C:93:ALA:HB1	2:C:100(D):PHE:HB3	2.01	0.42	
1:A:468:ILE:HD11	3:D:51:PRO:HD3	2.02	0.42	
1:B:415:THR:OG1	1:B:416:GLY:N	2.53	0.42	
2:H:38:ARG:HB2	2:H:48:MET:SD	2.60	0.42	
1:B:403:ARG:HD2	1:B:505:TYR:HD1	1.84	0.42	
3:D:162:THR:HG23	3:D:176:SER:O	2.19	0.42	
1:A:341:VAL:HG23	1:A:342:PHE:CD1	2.49	0.42	
1:A:350:VAL:O	1:A:353:TRP:HD1	2.02	0.42	
1:A:405:ASP:OD1	1:A:405:ASP:N	2.51	0.41	
3:D:36:TYR:CE2	3:D:46:VAL:HG22	2.55	0.41	
1:A:393:THR:CG2	1:A:520:ALA:HB3	2.50	0.41	
1:A:396:TYR:HB2	1:A:514:SER:HB2	2.02	0.41	
1:A:424:LYS:HE2	1:A:424:LYS:HB2	1.84	0.41	
2:C:12:LYS:O	2:C:111:VAL:HA	2.20	0.41	
1:A:427:ASP:N	1:A:427:ASP:OD1	2.53	0.41	
3:D:13:VAL:HG11	3:D:19:ALA:HB2	2.02	0.41	
1:A:393:THR:HG21	1:A:520:ALA:HB3	2.03	0.41	
1:A:335:LEU:HD22	1:A:362:VAL:O	2.21	0.41	
1:A:393:THR:N	1:A:516:GLU:O	2.54	0.41	
1:B:386:LYS:HA	1:B:389:ASP:OD2	2.20	0.41	
1:B:442:ASP:HB3	1:B:451:TYR:HE2	1.86	0.41	
3:L:25:GLY:CA	3:L:28:ILE:HD11	2.51	0.41	
2:C:105:GLN:H	2:C:105:GLN:CD	2.24	0.41	
1:A:440:ASN:OD1	1:A:440:ASN:N	2.47	0.40	
2:H:211:HIS:CD2	2:H:213:PRO:HD2	2.56	0.40	
2:H:51:ILE:HD12	2:H:57:THR:HG22	2.03	0.40	
2:C:147:PHE:HA	2:C:148:PRO:HA	1.89	0.40	
3:D:140:TYR:CD1	3:D:141:PRO:HA	2.56	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	А	193/205~(94%)	190~(98%)	3~(2%)	0	100	100
1	В	193/205~(94%)	189~(98%)	4 (2%)	0	100	100
2	С	220/223~(99%)	215~(98%)	4 (2%)	1 (0%)	29	51
2	Н	212/223~(95%)	207~(98%)	5(2%)	0	100	100
3	D	209/214~(98%)	202~(97%)	6 (3%)	1 (0%)	29	51
3	L	208/214~(97%)	199~(96%)	8 (4%)	1 (0%)	29	51
All	All	1235/1284~(96%)	1202 (97%)	30 (2%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	132	THR
3	D	51	PRO
3	L	51	PRO

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 Outlier		Percentiles	
1	А	167/177~(94%)	159~(95%)	8 (5%)	25 49	
1	В	165/177~(93%)	161 (98%)	4(2%)	49 72	



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	С	186/187~(100%)	174 (94%)	12 (6%)	17	33
2	Н	181/187~(97%)	171 (94%)	10 (6%)	21	41
3	D	176/179~(98%)	167~(95%)	9~(5%)	24	45
3	L	175/179~(98%)	163~(93%)	12 (7%)	15	31
All	All	1050/1086~(97%)	995~(95%)	55~(5%)	23	44

Continued from previous page...

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	340	GLU
1	А	367	VAL
1	А	369	TYR
1	А	387	LEU
1	А	389	ASP
1	А	408	ARG
1	А	427	ASP
1	А	501	ASN
1	В	368	LEU
1	В	373	SER
1	В	377	PHE
1	В	514	SER
2	Н	25	SER
2	Н	48	MET
2	Н	85	SER
2	Н	113	ASN
2	Н	142	LEU
2	Н	187	SER
2	Н	194	SER
2	Н	197	LEU
2	Н	207	CYS
2	Н	208	ASN
3	L	9	SER
3	L	30	SER
3	L	46	VAL
3	L	53	ASP
3	L	63	SER
3	L	65	SER
3	L	66	ASN
3	L	156	LYS
3	L	164	PRO
3	L	171	ASN



7.6.1			m
Mol	Chain	Res	Туре
3	L	191	SER
3	L	197	THR
2	С	22	CYS
2	С	62	SER
2	С	67	VAL
2	С	73	LYS
2	С	89	MET
2	С	112	PHE
2	С	147	PHE
2	С	167	SER
2	С	188	SER
2	С	207	CYS
2	С	212	LYS
2	С	225	GLU
3	D	2	SER
3	D	70	THR
3	D	108	GLN
3	D	151	ASP
3	D	152	SER
3	D	153	SER
3	D	162	THR
3	D	176	SER
3	D	212	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	409	GLN
2	Н	3	GLN
3	L	34	HIS
3	L	42	GLN
3	L	66	ASN
3	L	126	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)

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).

Mol Tw	Turne	Chain	Dec	Tinle	Bond lengths			Bond angles		
	туре	be Chain Res Lin	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	Е	1	4,1	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	Е	2	4	14,14,15	0.25	0	17,19,21	0.43	0

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
4	NAG	Е	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	1	NAG	C4-C5-C6-O6
4	Е	2	NAG	O5-C5-C6-O6
4	Е	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.





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)

1 ligand is 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 Cha	Chain	Dec	Tink	Bond lengths			Bond angles			
	Type	Chain	n res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	1001	1	14,14,15	0.29	0	17,19,21	0.44	0



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	NAG	В	1001	1	-	0/6/23/26	0/1/1/1

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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	195/205~(95%)	0.67	18 (9%) 9 5	30, 67, 109, 124	0
1	В	195/205~(95%)	0.74	26 (13%) 3 2	39, 74, 119, 131	0
2	С	222/223~(99%)	0.41	6 (2%) 54 49	28, 52, 87, 106	0
2	Н	216/223~(96%)	0.30	7 (3%) 47 41	31, 48, 80, 125	0
3	D	210/214~(98%)	0.30	5 (2%) 59 54	34, 52, 84, 96	0
3	L	210/214~(98%)	0.18	4 (1%) 66 62	29, 49, 70, 97	0
All	All	1248/1284~(97%)	0.43	66 (5%) 26 20	28, 54, 102, 131	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	2	SER	6.8
1	В	372	ALA	4.7
1	А	528	LYS	4.6
2	Н	228	SER	4.3
1	А	338	PHE	4.2
1	А	370	ASN	4.0
1	В	389	ASP	4.0
1	В	440	ASN	3.9
1	В	334	ASN	3.7
1	А	527	PRO	3.7
1	В	523	THR	3.7
1	А	334	ASN	3.6
1	В	365	TYR	3.6
1	В	515	PHE	3.6
1	А	387	LEU	3.6
3	D	2	SER	3.5
1	В	364	ASP	3.5
1	А	432	CYS	3.5
1	А	372	ALA	3.4



Mol	Chain	Res	Type	RSRZ	
1	В	369 TYR		3.4	
3	D	125	LEU	3.3	
3	L	210	ALA	3.3	
1	В	390	LEU	3.1	
1	В	521	PRO	3.0	
1	В	524	VAL	3.0	
1	А	434	ILE	2.9	
1	А	503	VAL	2.8	
1	В	387	LEU	2.8	
1	В	341	VAL	2.8	
1	В	394	ASN	2.8	
2	С	206	ILE	2.8	
2	Н	227	LYS	2.8	
2	Н	136	THR	2.7	
1	A	441	LEU	2.7	
2	С	228	SER	2.7	
1	В	400	PHE	2.7	
1	В	388	ASN	2.7	
1	В	384	PRO	2.6	
3	D	156	LYS	2.6	
1	В	391	CYS	2.6	
1	А	342	PHE	2.5	
3	D	25	GLY	2.5	
1	А	363	ALA	2.4	
1	А	337	PRO	2.4	
1	В	342	PHE	2.4	
1	А	365	TYR	2.4	
2	С	142	LEU	2.4	
1	В	362	VAL	2.4	
1	В	518	LEU	2.3	
2	С	164	ALA	2.3	
1	В	374	PHE	2.3	
1	А	368	LEU	2.2	
2	Н	139	LEU	2.2	
1	В	370	ASN	2.2	
2	Н	197	LEU	2.2	
3	L	190	ARG	2.2	
2	С	217	LYS	2.2	
2	Н	137	ALA	2.1	
1	A	526	GLY	2.1	
3	L	192	TYR	2.1	
1	А	442	ASP	2.1	



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Mol	Chain	Res	Type	RSRZ
1	В	392	PHE	2.1
3	D	193	SER	2.1
1	В	363	ALA	2.1
2	Н	205	TYR	2.0
2	С	224	VAL	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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAG	Е	1	14/15	0.65	0.29	90,108,115,117	0
4	NAG	Е	2	14/15	0.73	0.31	92,112,117,122	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)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	NAG	В	1001	14/15	0.78	0.35	99,110,111,115	0

6.5 Other polymers (i)

There are no such residues in this entry.

