



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 PM UTC

PDB ID : 9PSP / pdb_00009psp
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies BoWLB-1173 and CC12.3
Authors : Feng, Z.; Wilson, I.A.
Deposited on : 2025-07-25
Resolution : 2.81 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

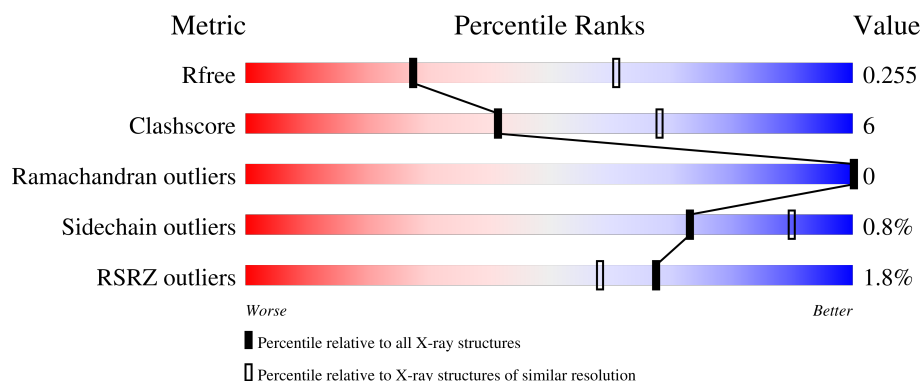
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.






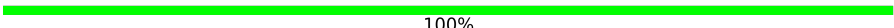
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	T	209	 3% 81% 12% 7%
1	U	209	 2% 77% 16% 7%
2	K	220	 2% 88% 12%
2	M	220	 83% 17%
3	N	215	 86% 13%

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Mol	Chain	Length	Quality of chain
3	W	215	 85% 15%
4	A	221	 3% 83% 14% •
4	H	221	 3% 81% 15% •
5	B	221	 2% 78% 20% •
5	L	221	 2% 81% 17% •
6	V	2	 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16598 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 Spike protein S1 receptor binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	8			
1	U	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	534	SER	-	expression tag	UNP P0DTC2
T	535	GLY	-	expression tag	UNP P0DTC2
T	536	HIS	-	expression tag	UNP P0DTC2
T	537	HIS	-	expression tag	UNP P0DTC2
T	538	HIS	-	expression tag	UNP P0DTC2
T	539	HIS	-	expression tag	UNP P0DTC2
T	540	HIS	-	expression tag	UNP P0DTC2
T	541	HIS	-	expression tag	UNP P0DTC2
U	534	SER	-	expression tag	UNP P0DTC2
U	535	GLY	-	expression tag	UNP P0DTC2
U	536	HIS	-	expression tag	UNP P0DTC2
U	537	HIS	-	expression tag	UNP P0DTC2
U	538	HIS	-	expression tag	UNP P0DTC2
U	539	HIS	-	expression tag	UNP P0DTC2
U	540	HIS	-	expression tag	UNP P0DTC2
U	541	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC12.3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	220	Total	C	N	O	S	0	0	0
			1644	1040	272	325	7			
2	M	220	Total	C	N	O	S	0	0	0
			1644	1040	272	325	7			

- Molecule 3 is a protein called CC12.3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	214	Total	C	N	O	S	0	0	0
			1641	1024	280	332	5			
3	N	214	Total	C	N	O	S	0	0	0
			1641	1024	280	332	5			

- Molecule 4 is a protein called BoWLB-1173 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	213	Total	C	N	O	S	0	0	0
			1588	1010	256	315	7			
4	A	214	Total	C	N	O	S	0	0	0
			1592	1012	257	316	7			

- Molecule 5 is a protein called BoWLB-1173 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	217	Total	C	N	O	S	0	0	0
			1691	1064	279	342	6			
5	B	217	Total	C	N	O	S	0	0	0
			1691	1064	279	342	6			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



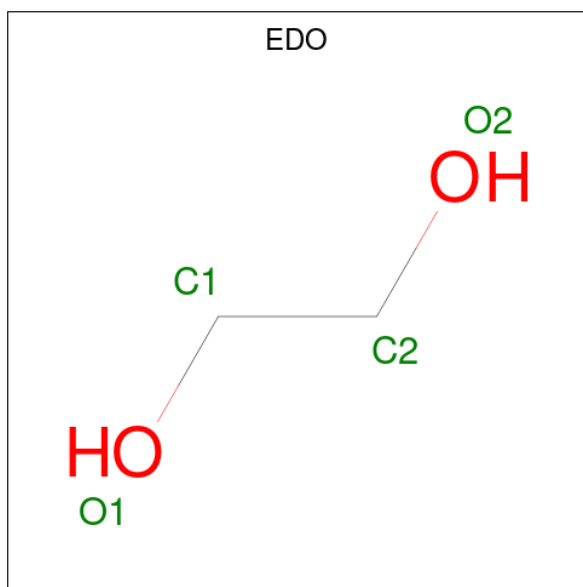
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	U	1	Total	C	O	0	0
			7	4	3		
8	K	1	Total	C	O	0	0
			7	4	3		
8	K	1	Total	C	O	0	0
			7	4	3		

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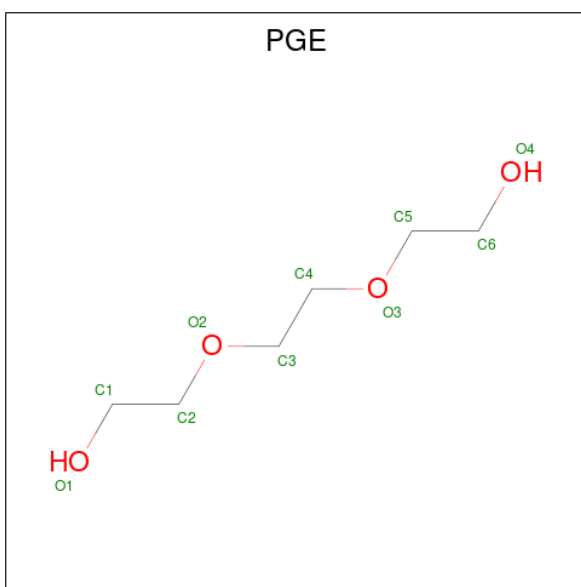
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	K	1	Total	C	O	0	0
			7	4	3		
8	W	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



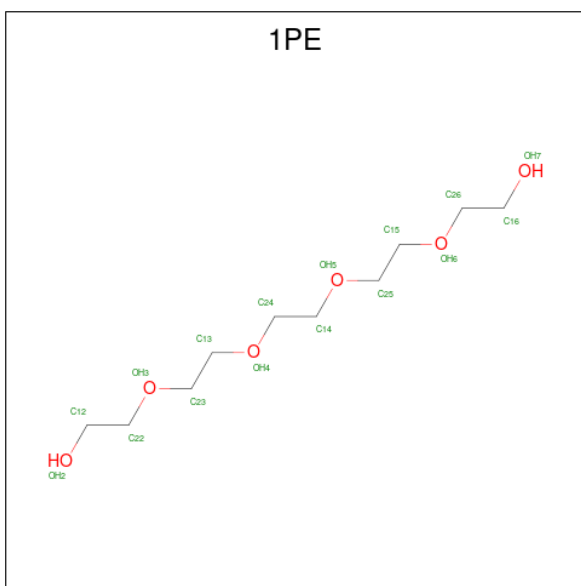
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	N	1	Total	C	O	0	0
			10	6	4		
10	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			16	10	6		

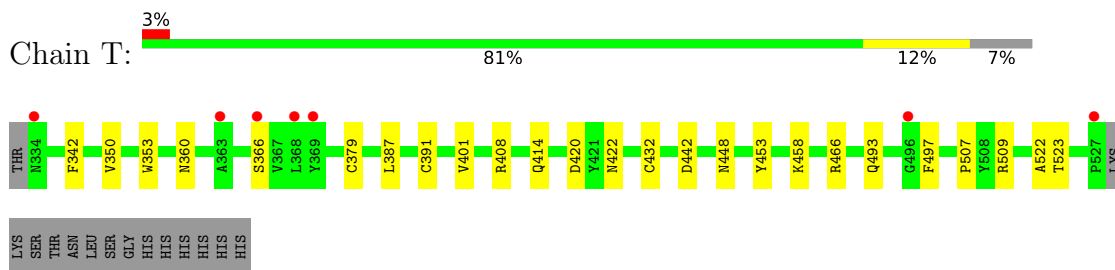
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	T	24	Total 24	O 24	0	0
12	U	25	Total 25	O 25	0	0
12	K	40	Total 40	O 40	0	0
12	W	38	Total 38	O 38	0	0
12	M	30	Total 30	O 30	0	0
12	N	37	Total 37	O 37	0	0
12	H	24	Total 24	O 24	0	0
12	L	12	Total 12	O 12	0	0
12	A	29	Total 29	O 29	0	0
12	B	18	Total 18	O 18	0	0

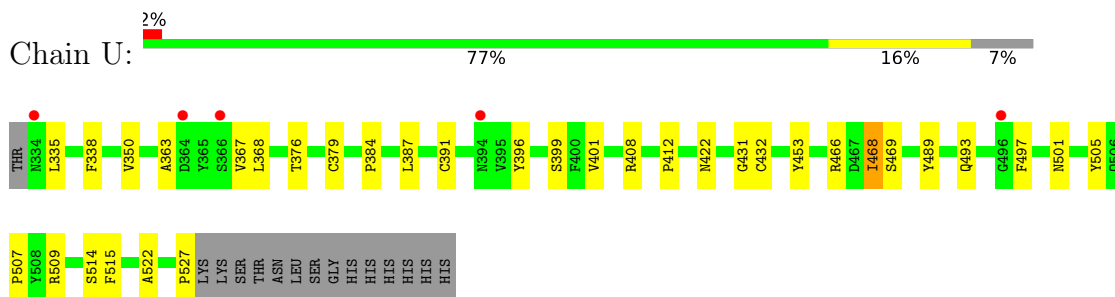
3 Residue-property plots [i](#)

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.

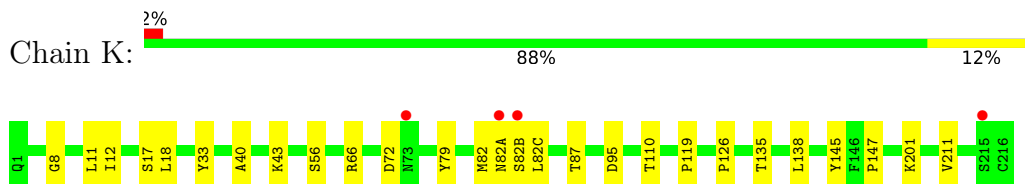
- Molecule 1: Spike protein S1 receptor binding domain



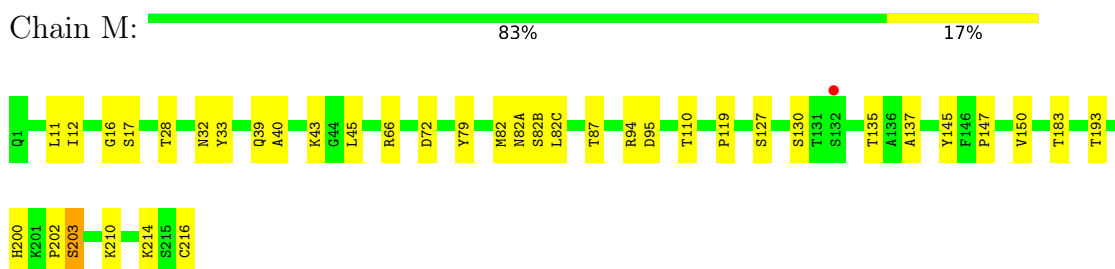
- Molecule 1: Spike protein S1 receptor binding domain




- Molecule 2: CC12.3 Fab heavy chain



- Molecule 2: CC12.3 Fab heavy chain




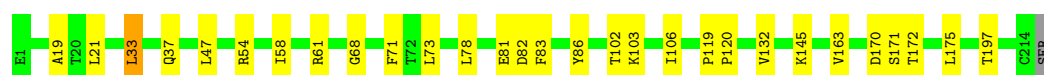
- Molecule 3: CC12.3 Fab light chain

Chain W:  85% 15%




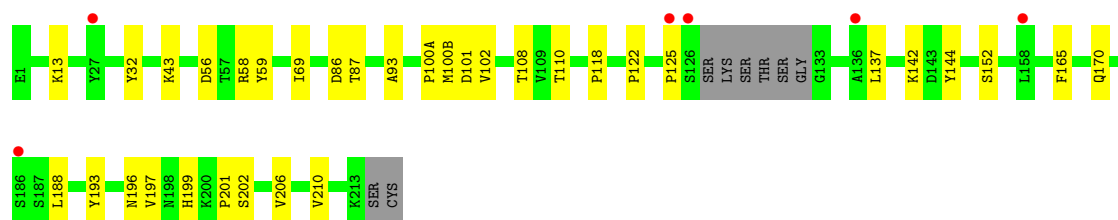
- Molecule 3: CC12.3 Fab light chain

Chain N:  86% 13%




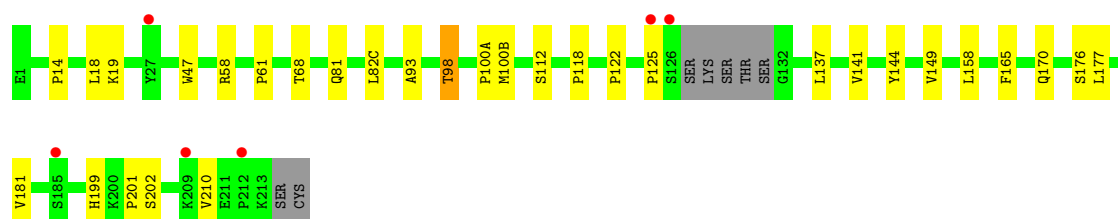
- Molecule 4: BoWLB-1173 Fab heavy chain

Chain H:  3% 81% 15%




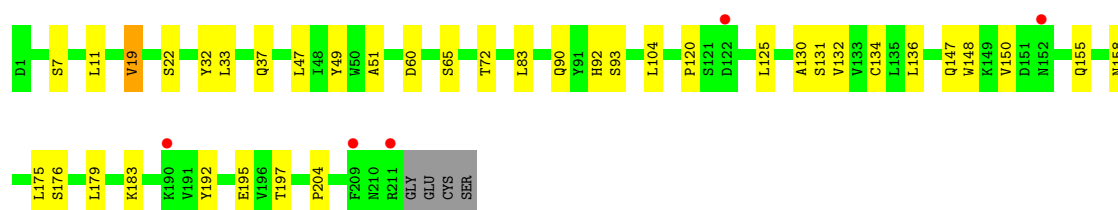
- Molecule 4: BoWLB-1173 Fab heavy chain

Chain A:  3% 83% 14%

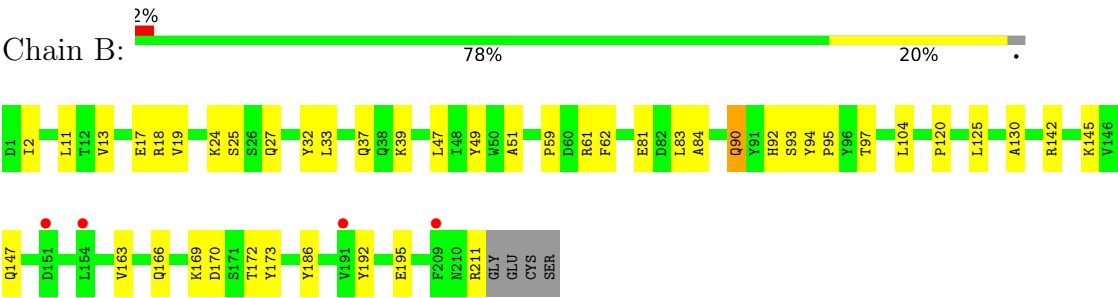


- Molecule 5: BoWLB-1173 Fab light chain

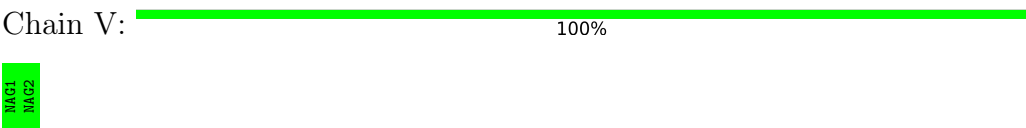
Chain L:  2% 81% 17%



• Molecule 5: BoWLB-1173 Fab light chain



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.20Å 101.05Å 127.83Å 92.25° 100.66° 90.09°	Depositor
Resolution (Å)	47.96 – 2.81 47.96 – 2.81	Depositor EDS
% Data completeness (in resolution range)	92.7 (47.96-2.81) 95.5 (47.96-2.81)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.195 , 0.247 0.200 , 0.255	Depositor DCC
R_{free} test set	3215 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l 0.064 for -h,k,-l 0.012 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16598	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: PEG, 1PE, EDO, NAG, PGE

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	T	0.10	0/1580	0.26	0/2151
1	U	0.08	0/1580	0.23	0/2151
2	K	0.10	0/1684	0.28	0/2292
2	M	0.10	0/1684	0.27	0/2292
3	N	0.10	0/1676	0.29	0/2274
3	W	0.09	0/1676	0.28	0/2274
4	A	0.10	0/1633	0.27	0/2229
4	H	0.11	0/1629	0.28	0/2224
5	B	0.10	0/1729	0.28	0/2346
5	L	0.09	0/1729	0.28	0/2346
All	All	0.10	0/16600	0.27	0/22579

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

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	T	1536	0	1452	15	0
1	U	1536	0	1452	20	0
2	K	1644	0	1604	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1644	0	1604	22	0
3	N	1641	0	1597	20	0
3	W	1641	0	1597	24	0
4	A	1592	0	1562	20	0
4	H	1588	0	1559	22	0
5	B	1691	0	1646	33	0
5	L	1691	0	1646	26	0
6	V	28	0	25	0	0
7	T	14	0	13	1	0
8	K	21	0	30	2	0
8	U	7	0	10	0	0
8	W	7	0	10	0	0
9	W	4	0	6	0	0
10	A	10	0	14	4	0
10	N	10	0	14	1	0
11	H	16	0	22	2	0
12	A	29	0	0	1	0
12	B	18	0	0	6	0
12	H	24	0	0	3	0
12	K	40	0	0	0	0
12	L	12	0	0	0	0
12	M	30	0	0	1	0
12	N	37	0	0	1	0
12	T	24	0	0	2	0
12	U	25	0	0	1	0
12	W	38	0	0	2	0
All	All	16598	0	15863	207	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 6.

All (207) 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)
4:A:58:ARG:HB2	10:A:301:PGE:H1	1.64	0.79
1:U:489:TYR:OH	2:M:94:ARG:NH2	2.16	0.78
1:U:412:PRO:HB2	10:A:301:PGE:H6	1.68	0.75
3:N:83:PHE:CG	3:N:106:ILE:HG22	2.21	0.75
3:W:106:ILE:HD11	3:W:171:SER:HB3	1.70	0.74
4:A:93:ALA:HB3	4:A:100(B):MET:HE2	1.71	0.72
2:M:66:ARG:NH1	2:M:82(B):SER:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:90:GLN:OE1	5:B:97:THR:OG1	2.11	0.69
4:H:58:ARG:HD3	11:H:301:1PE:H252	1.75	0.69
4:A:125:PRO:HG3	4:A:137:LEU:HB3	1.74	0.68
5:B:93:SER:N	12:B:301:HOH:O	2.16	0.68
4:H:122:PRO:HB3	4:H:210:VAL:HG23	1.77	0.66
5:B:33:LEU:HB3	5:B:51:ALA:HB2	1.78	0.66
1:U:468:ILE:HD11	3:W:158:ASN:HB3	1.78	0.65
2:K:66:ARG:NH1	2:K:82(B):SER:O	2.27	0.65
3:N:81:GLU:OE2	4:H:13:LYS:NZ	2.29	0.65
2:K:12:ILE:HG21	2:K:82(C):LEU:HD13	1.79	0.64
2:M:12:ILE:HG21	2:M:82(C):LEU:HD13	1.80	0.64
1:T:353:TRP:O	1:T:466:ARG:NH1	2.31	0.64
4:H:125:PRO:HG3	4:H:137:LEU:HB3	1.80	0.63
5:B:18:ARG:NH2	12:B:303:HOH:O	2.31	0.63
3:N:68:GLY:N	12:N:402:HOH:O	2.32	0.63
2:K:126:PRO:HG3	2:K:138:LEU:HB3	1.80	0.63
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.82	0.62
1:T:360:ASN:H	1:T:523:THR:HB	1.64	0.62
3:W:68:GLY:N	12:W:402:HOH:O	2.31	0.62
8:K:303:PEG:H32	3:W:94:SER:HB3	1.81	0.62
1:T:408:ARG:NH1	1:T:414:GLN:OE1	2.33	0.62
5:L:90:GLN:HE21	5:L:93:SER:H	1.48	0.62
3:N:106:ILE:HD11	3:N:171:SER:OG	2.00	0.61
5:B:92:HIS:N	12:B:301:HOH:O	2.31	0.61
5:B:2:ILE:HG23	5:B:27:GLN:HB3	1.81	0.61
3:W:183:LYS:NZ	3:W:187:GLU:OE2	2.34	0.60
1:T:458:LYS:NZ	12:T:705:HOH:O	2.33	0.60
1:T:342:PHE:HB2	7:T:601:NAG:H82	1.84	0.60
4:A:118:PRO:HB3	4:A:144:TYR:HB3	1.84	0.60
3:N:83:PHE:CD1	3:N:106:ILE:HG22	2.37	0.59
3:W:120:PRO:HD3	3:W:132:VAL:HG22	1.83	0.59
5:B:93:SER:O	12:B:301:HOH:O	2.17	0.59
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.85	0.58
4:H:32:TYR:OH	4:H:101:ASP:OD1	2.21	0.58
2:K:11:LEU:HB2	2:K:147:PRO:HG3	1.86	0.58
1:U:367:VAL:HG13	1:U:368:LEU:HD13	1.87	0.57
2:K:87:THR:HG23	2:K:110:THR:HA	1.85	0.57
5:L:33:LEU:HB3	5:L:51:ALA:HB2	1.86	0.57
2:M:130:SER:OG	2:M:137:ALA:O	2.21	0.57
5:B:11:LEU:HD22	5:B:104:LEU:HD12	1.85	0.57
4:H:152:SER:HB2	4:H:196:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:120:PRO:HG3	5:L:130:ALA:HB1	1.87	0.56
2:M:39:GLN:HB2	2:M:45:LEU:HD23	1.89	0.54
4:A:170:GLN:OE1	4:A:176:SER:OG	2.22	0.54
4:A:165:PHE:O	4:A:177:LEU:HD11	2.07	0.54
2:M:72:ASP:HB2	2:M:79:TYR:HE2	1.72	0.54
5:B:25:SER:OG	5:B:27:GLN:O	2.26	0.54
3:W:37:GLN:HB2	3:W:47:LEU:HD11	1.89	0.54
3:W:106:ILE:HD11	3:W:171:SER:CB	2.37	0.53
5:L:32:TYR:HB2	5:L:92:HIS:HB2	1.90	0.53
2:M:127:SER:H	2:M:130:SER:HB3	1.74	0.53
2:K:56:SER:HA	8:K:302:PEG:H32	1.91	0.52
3:W:2:ILE:HG13	3:W:26:SER:HB3	1.90	0.52
5:B:211:ARG:HH11	5:B:211:ARG:HG2	1.73	0.52
5:L:155:GLN:HB3	5:L:158:ASN:HD21	1.74	0.52
1:U:338:PHE:HE2	1:U:363:ALA:HB1	1.73	0.52
2:M:28:THR:O	2:M:32:ASN:ND2	2.40	0.52
4:A:141:VAL:O	4:A:177:LEU:N	2.43	0.52
1:U:350:VAL:HG22	1:U:422:ASN:HB3	1.91	0.51
5:L:158:ASN:OD1	5:L:158:ASN:N	2.44	0.51
3:W:60:ASP:OD1	3:W:60:ASP:N	2.43	0.51
4:H:118:PRO:HB3	4:H:144:TYR:HB3	1.93	0.51
3:N:103:LYS:HD3	10:N:301:PGE:H62	1.93	0.51
5:B:13:VAL:HG11	5:B:19:VAL:HG22	1.93	0.51
3:N:61:ARG:NE	3:N:82:ASP:OD2	2.43	0.51
1:U:408:ARG:NH2	12:U:705:HOH:O	2.44	0.50
3:N:82:ASP:O	3:N:86:TYR:OH	2.18	0.50
5:B:24:LYS:NZ	12:B:302:HOH:O	2.27	0.50
3:W:106:ILE:HG13	3:W:166:GLN:HE22	1.75	0.50
5:B:186:TYR:O	5:B:192:TYR:OH	2.29	0.50
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.47	0.50
4:H:100(A):PRO:HG3	5:L:49:TYR:HB2	1.94	0.50
2:K:82:MET:SD	2:K:82(C):LEU:HD21	2.52	0.49
2:K:119:PRO:HB3	2:K:145:TYR:HB3	1.94	0.49
2:M:135:THR:HG23	2:M:183:THR:HG23	1.94	0.49
5:B:61:ARG:NH2	5:B:81:GLU:OE1	2.42	0.49
5:B:166:GLN:HG3	5:B:173:TYR:CZ	2.48	0.49
5:B:37:GLN:HB2	5:B:47:LEU:HD11	1.93	0.49
3:N:83:PHE:CD2	3:N:106:ILE:HG22	2.47	0.49
5:B:90:GLN:NE2	12:B:301:HOH:O	2.22	0.49
2:M:200:HIS:CD2	2:M:202:PRO:HD2	2.48	0.49
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:350:VAL:HG22	1:T:422:ASN:HB3	1.94	0.48
3:N:21:LEU:HD22	3:N:102:THR:HG21	1.95	0.48
5:B:170:ASP:OD2	5:B:172:THR:OG1	2.28	0.48
5:B:17:GLU:HG2	5:B:18:ARG:H	1.78	0.48
5:L:147:GLN:NE2	5:L:195:GLU:OE1	2.47	0.48
2:M:216:CYS:O	12:M:301:HOH:O	2.20	0.48
4:A:98:THR:HG21	10:A:301:PGE:H3	1.96	0.48
4:A:158:LEU:HD21	4:A:181:VAL:HG21	1.96	0.48
3:W:82:ASP:O	3:W:86:TYR:OH	2.21	0.47
5:L:136:LEU:HB2	5:L:175:LEU:HB3	1.96	0.47
2:M:193:THR:HB	2:M:210:LYS:HE2	1.96	0.47
4:A:141:VAL:HB	4:A:177:LEU:HB3	1.95	0.47
1:T:391:CYS:HB3	1:T:522:ALA:HB1	1.96	0.47
2:K:72:ASP:HB2	2:K:79:TYR:HE2	1.79	0.47
3:W:155:GLN:OE1	3:W:158:ASN:ND2	2.39	0.47
5:L:134:CYS:HB2	5:L:148:TRP:CH2	2.49	0.47
5:B:32:TYR:HB2	5:B:92:HIS:HB2	1.95	0.47
2:K:8:GLY:O	2:K:18:LEU:HD21	2.14	0.47
3:W:33:LEU:HD22	3:W:71:PHE:CG	2.49	0.47
5:B:39:LYS:HG2	5:B:84:ALA:HB2	1.97	0.47
5:L:132:VAL:HB	5:L:179:LEU:HB3	1.96	0.47
4:A:122:PRO:HB3	4:A:210:VAL:HG12	1.97	0.47
1:U:469:SER:HB2	3:W:157:GLY:HA3	1.95	0.46
4:H:86:ASP:OD2	12:H:401:HOH:O	2.21	0.46
1:T:366:SER:N	12:T:703:HOH:O	2.48	0.46
4:A:19:LYS:HG3	4:A:81:GLN:HB2	1.97	0.46
2:K:17:SER:OG	2:K:82(A):ASN:HA	2.15	0.46
4:H:199:HIS:CD2	4:H:201:PRO:HD2	2.51	0.46
5:B:147:GLN:HB3	5:B:195:GLU:HB3	1.98	0.46
3:N:21:LEU:HD12	3:N:73:LEU:HD23	1.98	0.46
2:M:11:LEU:HB2	2:M:147:PRO:HG3	1.97	0.46
5:B:11:LEU:HD21	5:B:13:VAL:HG13	1.97	0.46
1:U:401:VAL:HG22	1:U:509:ARG:HG2	1.98	0.46
4:H:125:PRO:HG2	4:H:188:LEU:HD21	1.98	0.46
1:U:384:PRO:HA	1:U:387:LEU:HG	1.98	0.46
4:H:197:VAL:HB	4:H:206:VAL:HG22	1.98	0.46
5:L:92:HIS:ND1	5:L:93:SER:OG	2.48	0.46
3:N:170:ASP:OD2	3:N:172:THR:OG1	2.32	0.46
1:T:442:ASP:O	1:T:448:ASN:ND2	2.42	0.45
1:U:501:ASN:HB3	1:U:505:TYR:HB2	1.98	0.45
5:B:120:PRO:HG3	5:B:130:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:165:PHE:CZ	5:L:176:SER:HB3	2.51	0.45
1:T:401:VAL:HG22	1:T:509:ARG:HG2	1.99	0.45
1:U:335:LEU:HD23	1:U:335:LEU:H	1.81	0.45
1:T:497:PHE:CE2	1:T:507:PRO:HB3	2.52	0.45
1:U:431:GLY:HA2	1:U:515:PHE:HD2	1.82	0.45
4:H:137:LEU:HD21	4:H:193:TYR:CD2	2.52	0.45
4:H:142:LYS:HE2	4:H:170:GLN:HE22	1.81	0.44
4:A:47:TRP:NE1	12:A:404:HOH:O	2.33	0.44
4:A:137:LEU:HD13	4:A:210:VAL:HG21	1.98	0.44
5:L:11:LEU:HD21	5:L:19:VAL:HG11	2.00	0.44
3:W:83:PHE:CD1	3:W:106:ILE:HG22	2.53	0.44
2:M:82:MET:SD	2:M:82(C):LEU:HD21	2.58	0.44
5:L:60:ASP:N	5:L:60:ASP:OD1	2.46	0.44
1:U:497:PHE:CE2	1:U:507:PRO:HB3	2.53	0.43
3:W:61:ARG:NE	3:W:82:ASP:OD2	2.47	0.43
4:A:18:LEU:HB2	4:A:82(C):LEU:HD11	2.00	0.43
4:A:100(A):PRO:HG3	5:B:49:TYR:HB2	2.00	0.43
5:B:142:ARG:HD3	5:B:163:VAL:HG11	2.00	0.43
1:U:466:ARG:HH11	3:W:155:GLN:NE2	2.16	0.43
2:M:200:HIS:ND1	2:M:203:SER:HB3	2.34	0.43
4:H:56:ASP:OD1	11:H:301:1PE:H151	2.19	0.43
4:H:59:TYR:HH	4:H:69:ILE:H	1.65	0.43
4:A:14:PRO:HD3	4:A:112:SER:O	2.18	0.43
2:K:33:TYR:HB2	2:K:95:ASP:O	2.17	0.43
2:M:214:LYS:NZ	3:N:119:PRO:HG2	2.34	0.43
2:K:201:LYS:HA	2:K:201:LYS:HD2	1.69	0.43
1:U:453:TYR:CZ	1:U:493:GLN:HB3	2.53	0.43
4:H:93:ALA:HB1	4:H:100(B):MET:HB3	2.01	0.43
5:L:37:GLN:HB2	5:L:47:LEU:HD11	2.01	0.43
5:L:125:LEU:O	5:L:183:LYS:HE2	2.19	0.43
1:T:387:LEU:HD12	1:T:387:LEU:HA	1.89	0.42
2:M:87:THR:HG23	2:M:110:THR:HA	2.00	0.42
4:A:199:HIS:CD2	4:A:201:PRO:HD2	2.53	0.42
1:T:453:TYR:CZ	1:T:493:GLN:HB3	2.54	0.42
2:M:40:ALA:HB3	2:M:43:LYS:HB2	2.01	0.42
5:B:145:LYS:HA	5:B:145:LYS:HD2	1.73	0.42
3:W:145:LYS:HB3	3:W:197:THR:HB	2.01	0.42
4:H:101:ASP:OD1	4:H:102:VAL:HG23	2.19	0.42
5:L:90:GLN:NE2	5:L:93:SER:O	2.53	0.42
4:H:87:THR:HG23	4:H:110:THR:HA	2.01	0.42
3:W:35:TRP:HB2	3:W:48:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:ILE:HD11	2:M:16:GLY:HA3	2.00	0.42
3:N:145:LYS:HB3	3:N:197:THR:HB	2.02	0.42
3:N:163:VAL:HG22	3:N:175:LEU:HD12	2.02	0.42
4:H:101:ASP:OD2	12:H:402:HOH:O	2.22	0.42
5:L:197:THR:HG22	5:L:204:PRO:HB3	2.02	0.42
10:A:301:PGE:H4	5:B:94:TYR:CZ	2.55	0.42
1:T:420:ASP:OD2	2:K:56:SER:OG	2.25	0.41
3:W:163:VAL:HG22	3:W:175:LEU:HD12	2.02	0.41
1:U:391:CYS:HB3	1:U:522:ALA:HB1	2.02	0.41
4:H:43:LYS:NZ	12:H:404:HOH:O	2.36	0.41
5:L:120:PRO:HB3	5:L:131:SER:H	1.85	0.41
2:K:12:ILE:HB	2:K:18:LEU:HD12	2.03	0.41
5:L:7:SER:HG	5:L:22:SER:HG	1.64	0.41
5:L:65:SER:HB3	5:L:72:THR:HB	2.02	0.41
5:L:150:VAL:HG22	5:L:192:TYR:CD1	2.55	0.41
5:B:59:PRO:HG2	5:B:62:PHE:CE1	2.54	0.41
3:W:120:PRO:HG3	3:W:130:ALA:HB1	2.02	0.41
5:L:125:LEU:HD23	5:L:125:LEU:HA	1.94	0.41
3:N:19:ALA:HB2	3:N:78:LEU:HD11	2.02	0.41
5:L:83:LEU:HD12	5:L:104:LEU:O	2.21	0.41
1:U:396:TYR:HB2	1:U:514:SER:HB3	2.03	0.41
3:W:24:ARG:NH2	12:W:411:HOH:O	2.54	0.41
2:M:17:SER:OG	2:M:82(A):ASN:HA	2.20	0.41
5:B:169:LYS:HE3	5:B:169:LYS:HB2	1.96	0.41
1:T:379:CYS:HA	1:T:432:CYS:HA	2.02	0.40
2:M:33:TYR:HB2	2:M:95:ASP:O	2.21	0.40
4:A:61:PRO:HD2	5:B:95:PRO:HG3	2.04	0.40
1:U:363:ALA:O	1:U:527:PRO:HD3	2.22	0.40
1:U:379:CYS:HA	1:U:432:CYS:HA	2.03	0.40
3:N:54:ARG:HG2	3:N:58:ILE:HB	2.03	0.40
5:L:150:VAL:HG22	5:L:192:TYR:HD1	1.86	0.40
3:W:126:LYS:HB2	3:W:126:LYS:HE2	1.84	0.40
2:K:40:ALA:HB3	2:K:43:LYS:HB2	2.04	0.40
4:A:199:HIS:ND1	4:A:202:SER:OG	2.52	0.40
5:B:83:LEU:HD12	5:B:104:LEU:O	2.21	0.40
5:B:125:LEU:HD12	5:B:125:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

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	T	192/209 (92%)	187 (97%)	5 (3%)	0	100	100
1	U	192/209 (92%)	187 (97%)	5 (3%)	0	100	100
2	K	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
2	M	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
3	N	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
3	W	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
4	A	210/221 (95%)	207 (99%)	3 (1%)	0	100	100
4	H	209/221 (95%)	205 (98%)	4 (2%)	0	100	100
5	B	215/221 (97%)	208 (97%)	7 (3%)	0	100	100
5	L	215/221 (97%)	209 (97%)	6 (3%)	0	100	100
All	All	2093/2172 (96%)	2045 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	T	167/181 (92%)	167 (100%)	0	100	100
1	U	167/181 (92%)	164 (98%)	3 (2%)	51	80
2	K	186/186 (100%)	184 (99%)	2 (1%)	65	86
2	M	186/186 (100%)	184 (99%)	2 (1%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	185/186 (100%)	184 (100%)	1 (0%)	81	93
3	W	185/186 (100%)	185 (100%)	0	100	100
4	A	180/187 (96%)	177 (98%)	3 (2%)	53	81
4	H	180/187 (96%)	178 (99%)	2 (1%)	65	86
5	B	195/198 (98%)	194 (100%)	1 (0%)	81	93
5	L	195/198 (98%)	194 (100%)	1 (0%)	81	93
All	All	1826/1876 (97%)	1811 (99%)	15 (1%)	73	90

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

Mol	Chain	Res	Type
1	U	376	THR
1	U	399	SER
1	U	468	ILE
2	K	135	THR
2	K	211	VAL
2	M	150	VAL
2	M	203	SER
3	N	33	LEU
4	H	108	THR
4	H	202	SER
5	L	19	VAL
4	A	68	THR
4	A	98	THR
4	A	149	VAL
5	B	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	370	ASN
1	T	493	GLN
1	U	493	GLN
2	K	3	GLN
2	K	39	GLN
2	K	199	ASN
3	W	38	GLN
3	N	138	ASN
4	H	76	ASN

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Mol	Chain	Res	Type
4	H	170	GLN
5	B	42	GLN
5	B	155	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 ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	V	1	1,6	14,14,15	0.74	0	17,19,21	0.98	0
6	NAG	V	2	6	14,14,15	0.71	0	17,19,21	0.82	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
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	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.

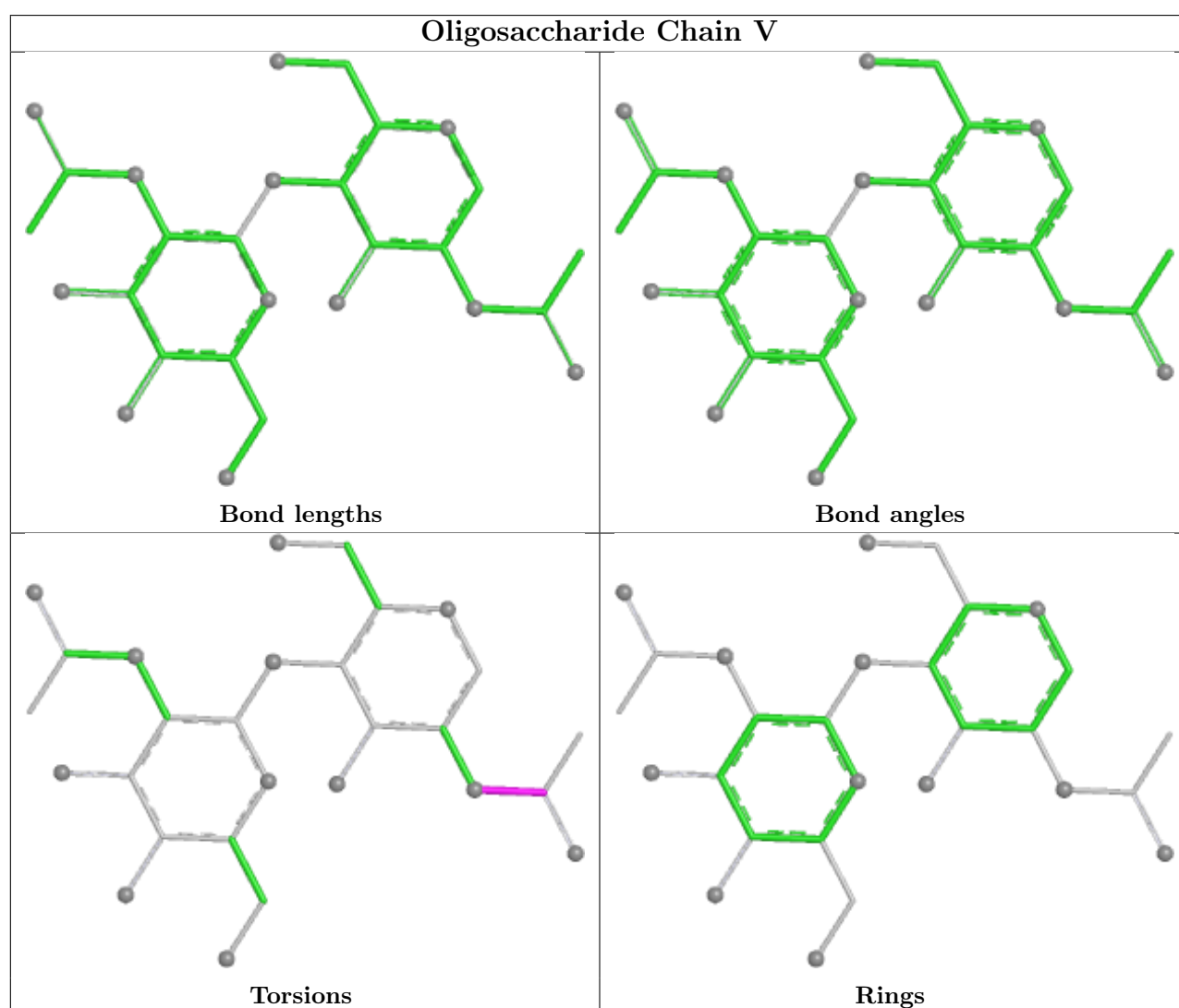
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2

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 ⓘ

10 ligands 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	$\# Z > 2$
9	EDO	W	302	-	3,3,3	0.25	0	2,2,2	0.33	0
10	PGE	N	301	-	9,9,9	0.32	0	8,8,8	0.50	0
8	PEG	U	601	-	6,6,6	0.25	0	5,5,5	0.23	0
11	1PE	H	301	-	15,15,15	0.29	0	14,14,14	0.19	0
10	PGE	A	301	-	9,9,9	0.32	0	8,8,8	0.54	0
8	PEG	W	301	-	6,6,6	0.25	0	5,5,5	0.42	0
7	NAG	T	601	1	14,14,15	0.70	0	17,19,21	0.88	0
8	PEG	K	302	-	6,6,6	0.26	0	5,5,5	0.23	0
8	PEG	K	303	-	6,6,6	0.25	0	5,5,5	0.23	0
8	PEG	K	301	-	6,6,6	0.26	0	5,5,5	0.23	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
9	EDO	W	302	-	-	0/1/1/1	-
10	PGE	N	301	-	-	2/7/7/7	-
8	PEG	U	601	-	-	2/4/4/4	-
11	1PE	H	301	-	-	2/13/13/13	-
10	PGE	A	301	-	-	1/7/7/7	-
8	PEG	W	301	-	-	0/4/4/4	-
7	NAG	T	601	1	-	0/6/23/26	0/1/1/1
8	PEG	K	302	-	-	0/4/4/4	-
8	PEG	K	303	-	-	0/4/4/4	-
8	PEG	K	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	301	1PE	OH5-C14-C24-OH4
11	H	301	1PE	OH7-C16-C26-OH6
8	U	601	PEG	O1-C1-C2-O2
8	K	301	PEG	C4-C3-O2-C2
8	K	301	PEG	O1-C1-C2-O2
10	A	301	PGE	O1-C1-C2-O2
10	N	301	PGE	C3-C4-O3-C5
10	N	301	PGE	C1-C2-O2-C3
8	U	601	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	301	PGE	1	0
11	H	301	1PE	2	0
10	A	301	PGE	4	0
7	T	601	NAG	1	0
8	K	302	PEG	1	0
8	K	303	PEG	1	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	T	194/209 (92%)	-0.00	7 (3%) 46 37	24, 39, 73, 89	0
1	U	194/209 (92%)	0.03	5 (2%) 57 47	26, 41, 75, 92	0
2	K	220/220 (100%)	-0.26	4 (1%) 67 58	23, 36, 62, 84	0
2	M	220/220 (100%)	-0.17	1 (0%) 87 82	24, 38, 65, 82	0
3	N	214/215 (99%)	-0.26	0 100 100	27, 39, 54, 84	0
3	W	214/215 (99%)	-0.31	1 (0%) 87 82	26, 38, 55, 85	0
4	A	214/221 (96%)	0.03	6 (2%) 55 44	31, 45, 84, 94	0
4	H	213/221 (96%)	0.14	6 (2%) 55 44	27, 46, 89, 99	0
5	B	217/221 (98%)	0.41	4 (1%) 67 58	38, 63, 81, 96	0
5	L	217/221 (98%)	0.45	5 (2%) 61 51	31, 64, 95, 107	0
All	All	2117/2172 (97%)	0.00	39 (1%) 67 58	23, 43, 82, 107	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	496	GLY	3.4
5	B	154	LEU	3.3
4	H	27	TYR	3.2
2	K	82(B)	SER	3.0
1	T	527	PRO	3.0
1	U	334	ASN	3.0
5	L	190	LYS	3.0
1	T	366	SER	3.0
4	A	126	SER	2.9
5	B	209	PHE	2.9
5	B	191	VAL	2.8
4	H	125	PRO	2.6
3	W	30	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	158	LEU	2.5
5	L	209	PHE	2.5
4	H	126	SER	2.5
4	A	185	SER	2.5
2	K	73	ASN	2.5
2	K	82(A)	ASN	2.5
5	L	211	ARG	2.5
1	T	496	GLY	2.4
1	U	364	ASP	2.3
4	A	27	TYR	2.3
1	U	394	ASN	2.3
1	T	363	ALA	2.2
1	T	334	ASN	2.2
1	T	368	LEU	2.2
1	U	366	SER	2.2
4	H	136	ALA	2.2
4	A	209	LYS	2.1
2	M	132	SER	2.1
4	H	186	SER	2.1
5	L	152	ASN	2.1
2	K	215	SER	2.1
4	A	125	PRO	2.1
5	B	151	ASP	2.1
1	T	369	TYR	2.1
4	A	212	PRO	2.0
5	L	122	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

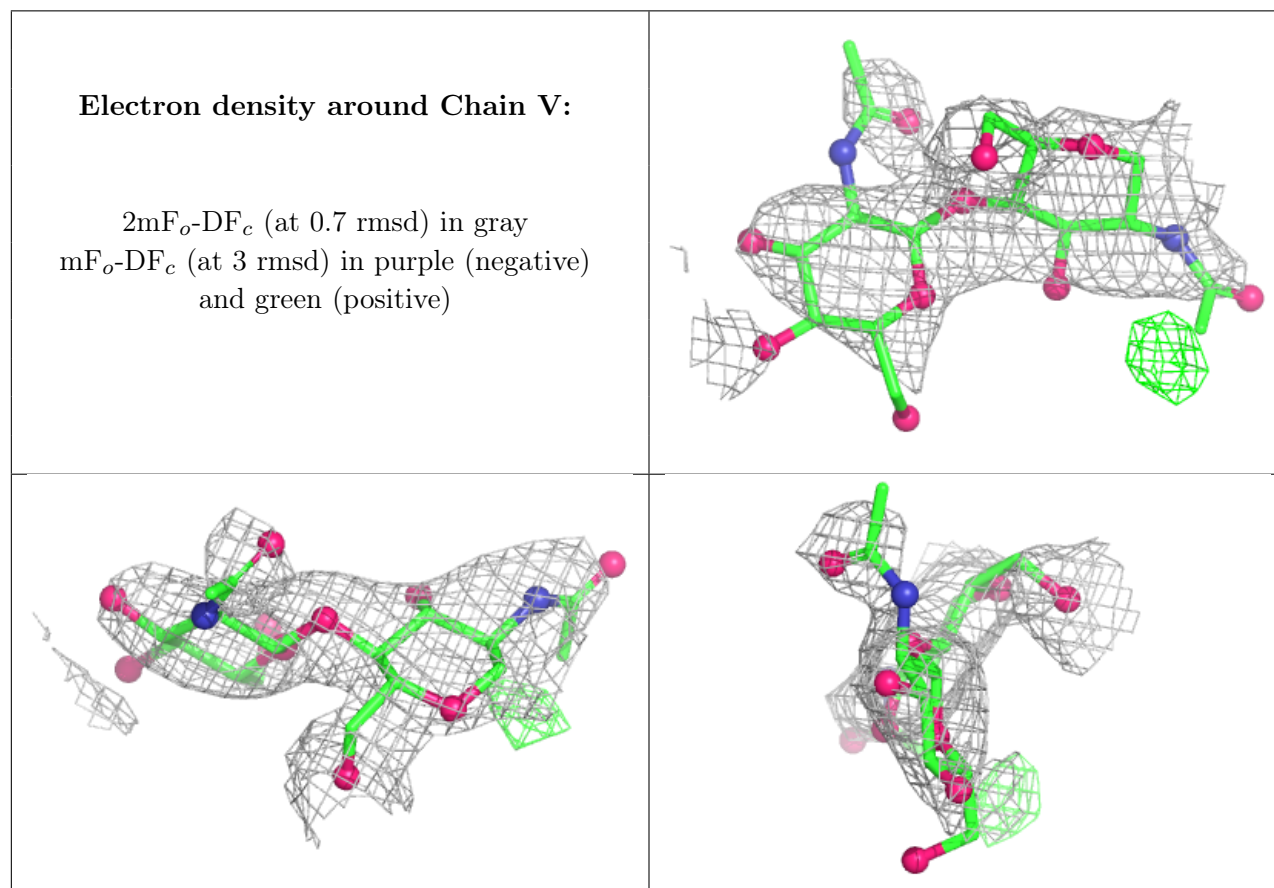
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
6	NAG	V	1	14/15	-	-	75,88,97,104	0
6	NAG	V	2	14/15	-	-	83,107,113,116	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, 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
7	NAG	T	601	14/15	0.64	0.16	60,82,89,96	0
8	PEG	U	601	7/7	0.74	0.22	50,58,66,74	0
8	PEG	K	301	7/7	0.81	0.18	37,48,56,64	0
10	PGE	N	301	10/10	0.87	0.14	28,47,61,68	0
8	PEG	K	303	7/7	0.88	0.11	43,48,53,64	0
8	PEG	K	302	7/7	0.88	0.13	36,49,57,69	0
9	EDO	W	302	4/4	0.92	0.11	35,43,44,44	0
11	1PE	H	301	16/16	0.92	0.12	26,44,72,79	0
10	PGE	A	301	10/10	0.93	0.11	27,36,50,52	0
8	PEG	W	301	7/7	0.95	0.08	33,37,41,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.