



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:14 AM UTC

PDB ID : 9PSN / pdb_00009psn
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies BoWLB-105 and CC12.3
Authors : Feng, Z.; Wilson, I.A.
Deposited on : 2025-07-25
Resolution : 2.54 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

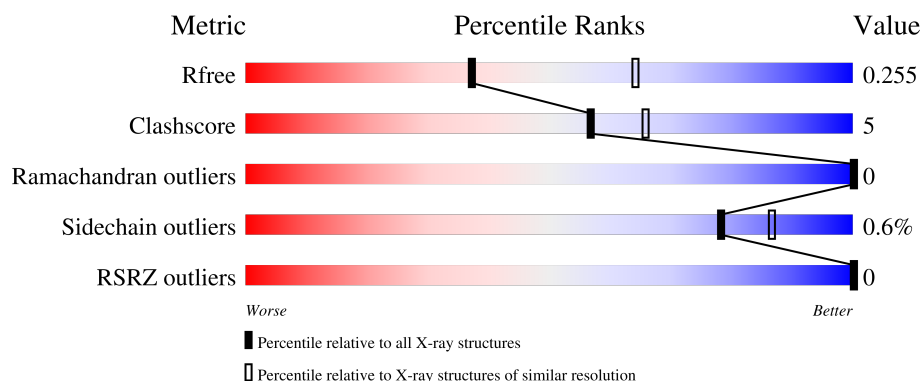
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	E	209	 83% 10% 7%
1	T	209	 86% 7% 7%
2	J	220	 90% 10%
2	M	220	 88% 12%
3	K	215	 84% 16%

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Mol	Chain	Length	Quality of chain
3	N	215	 88% 12%
4	O	221	 87% 10% •
4	Q	221	 88% 8% •
5	P	221	 82% 15% ••
5	R	221	 90% 8% •
6	A	2	 50% 50%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17097 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	E	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	8			
1	T	194	Total	C	N	O	S	0	1	0
			1540	988	256	288	8			

There are 16 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	220	Total	C	N	O	S	0	2	0
			1654	1046	274	327	7			
2	M	220	Total	C	N	O	S	0	1	0
			1648	1042	273	326	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	214	Total	C	N	O	S	0	0	0
			1641	1024	280	332	5			
3	N	214	Total	C	N	O	S	0	1	0
			1645	1027	280	333	5			

- Molecule 4 is a protein called BoWLB-105 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	215	Total	C	N	O	S	0	0	0
			1597	1014	258	318	7			
4	Q	212	Total	C	N	O	S	0	0	0
			1581	1006	255	313	7			

- Molecule 5 is a protein called BoWLB-105 Fab light chain.

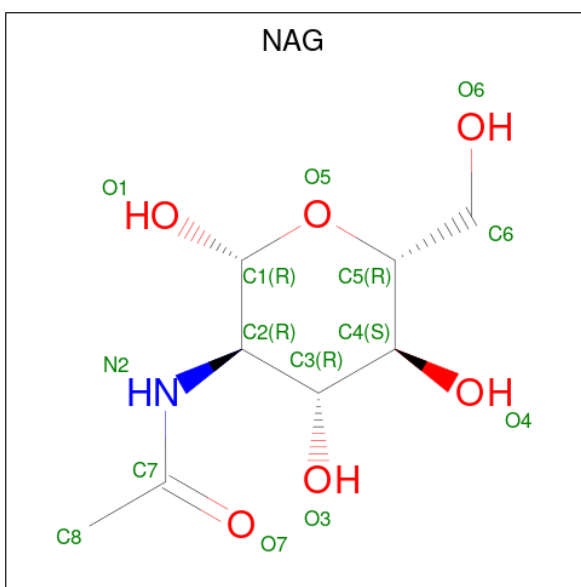
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	217	Total	C	N	O	S	0	0	0
			1691	1064	279	342	6			
5	R	217	Total	C	N	O	S	0	0	0
			1691	1064	279	342	6			

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



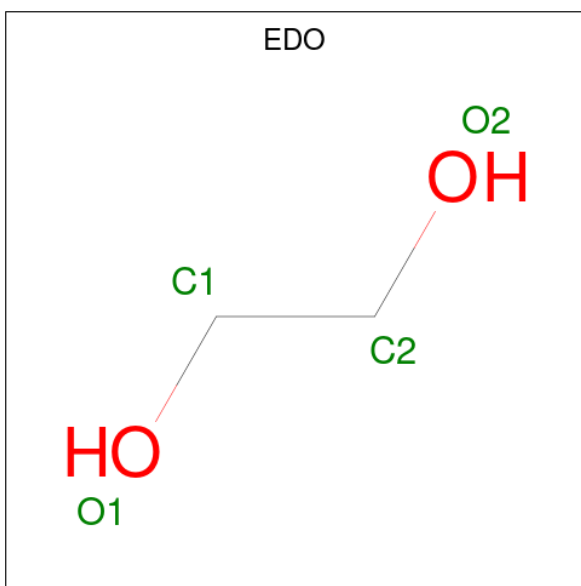
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



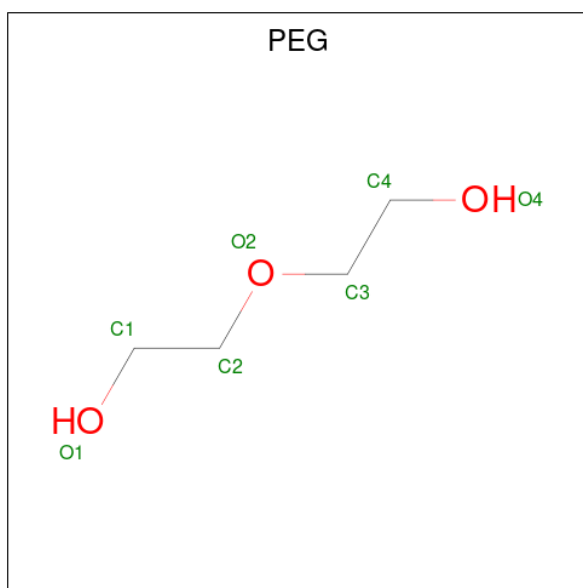
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



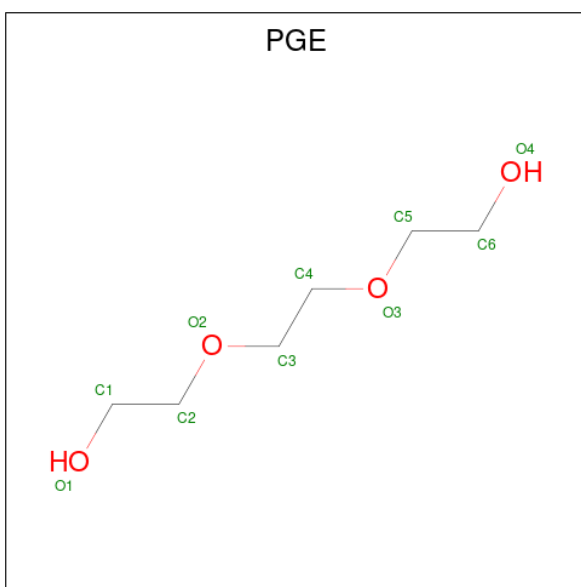
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



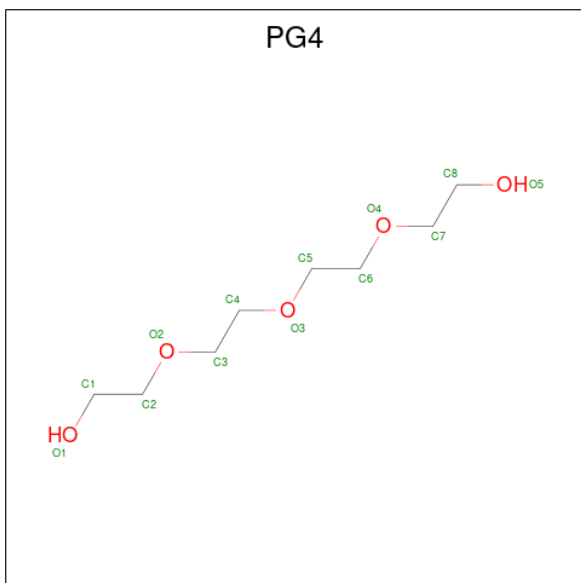
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total	C	O	0	0
			7	4	3		
9	J	1	Total	C	O	0	0
			7	4	3		
9	J	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	N	1	Total	C	O	0	0
			7	4	3		
9	N	1	Total	C	O	0	0
			7	4	3		

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



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

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $\text{C}_8\text{H}_{18}\text{O}_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	O	1	Total	C	O	0	0
			13	8	5		
11	Q	1	Total	C	O	0	0
			13	8	5		

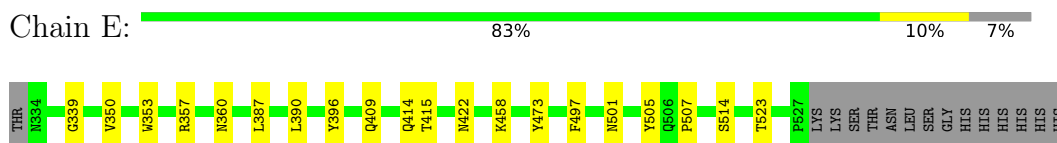
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	63	Total	O	0	0
			63	63		
12	T	67	Total	O	0	0
			67	67		
12	J	87	Total	O	0	0
			87	87		
12	K	84	Total	O	0	0
			84	84		
12	M	91	Total	O	0	0
			91	91		
12	N	99	Total	O	0	0
			99	99		
12	O	66	Total	O	0	0
			66	66		
12	P	50	Total	O	0	0
			50	50		
12	Q	63	Total	O	0	0
			63	63		
12	R	27	Total	O	0	0
			27	27		

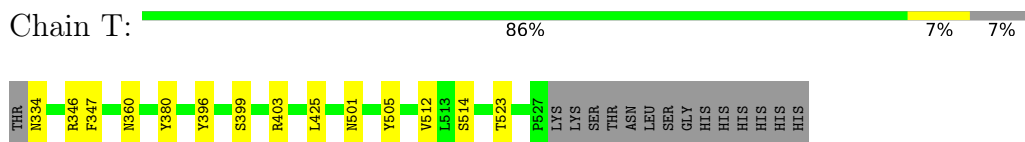
3 Residue-property plots

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.

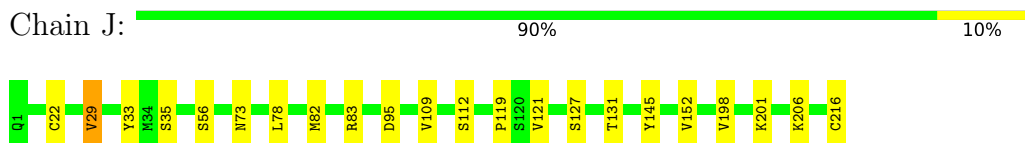
- Molecule 1: Spike protein S1 receptor binding domain



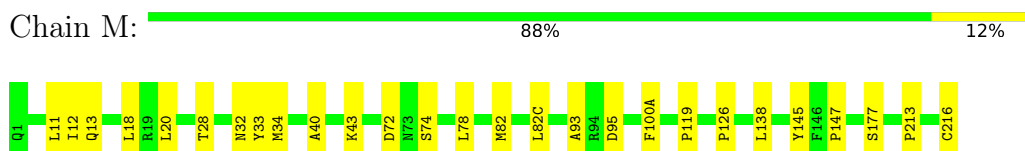
- Molecule 1: Spike protein S1 receptor binding domain



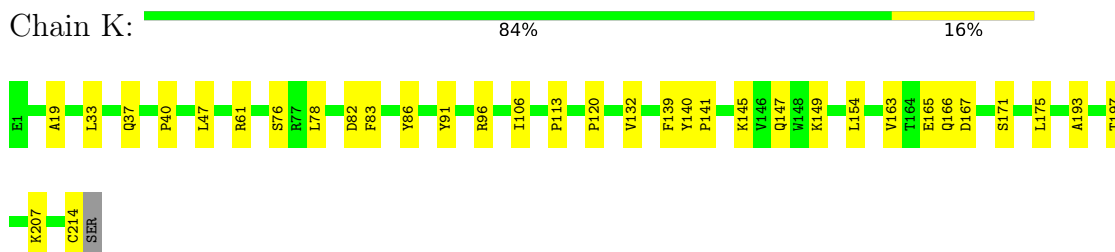
- Molecule 2: CC12.3 Fab heavy chain



- Molecule 2: CC12.3 Fab heavy chain



- Molecule 3: CC12.3 Fab light chain



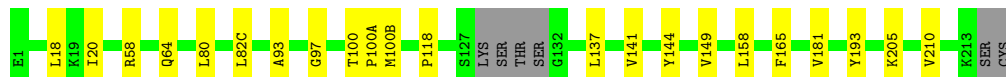
- Molecule 3: CC12.3 Fab light chain

Chain N:  88% 12%




- Molecule 4: BoWLB-105 Fab heavy chain

Chain O:  87% 10% .




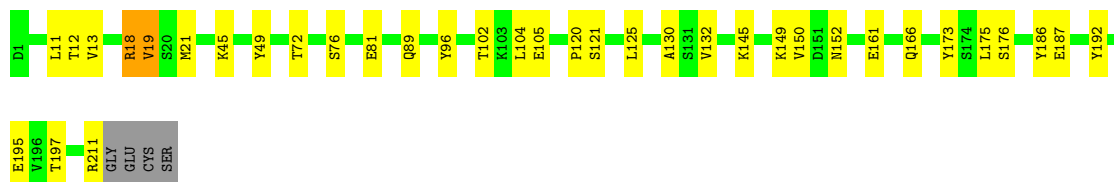
- Molecule 4: BoWLB-105 Fab heavy chain

Chain Q:  88% 8% .



- Molecule 5: BoWLB-105 Fab light chain

Chain P:  82% 15% ..



- Molecule 5: BoWLB-105 Fab light chain

Chain R:  90% 8% .



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

Chain A:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.13Å 100.86Å 127.54Å 87.92° 79.18° 89.89°	Depositor
Resolution (Å)	42.02 – 2.54 42.02 – 2.54	Depositor EDS
% Data completeness (in resolution range)	90.5 (42.02-2.54) 92.7 (42.02-2.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.203 , 0.255	Depositor DCC
R_{free} test set	1965 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,h-l 0.099 for -h,k,-l 0.017 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17097	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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, EDO, NAG, PG4, 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	E	0.11	0/1580	0.26	0/2151
1	T	0.11	0/1587	0.29	0/2161
2	J	0.12	0/1697	0.29	0/2310
2	M	0.12	0/1688	0.29	0/2297
3	K	0.12	0/1676	0.31	0/2274
3	N	0.11	0/1683	0.29	0/2284
4	O	0.11	0/1638	0.27	0/2235
4	Q	0.12	0/1622	0.31	0/2214
5	P	0.11	0/1729	0.28	0/2346
5	R	0.11	0/1729	0.29	0/2346
All	All	0.11	0/16629	0.29	0/22618

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	E	1536	0	1452	14	0
1	T	1540	0	1459	9	0
2	J	1654	0	1614	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1648	0	1605	17	0
3	K	1641	0	1597	23	0
3	N	1645	0	1603	13	0
4	O	1597	0	1565	13	0
4	Q	1581	0	1552	13	0
5	P	1691	0	1646	23	0
5	R	1691	0	1646	14	0
6	A	28	0	25	0	0
7	E	14	0	13	1	0
8	E	8	0	12	1	0
8	J	4	0	6	0	0
9	J	21	0	30	3	0
9	K	14	0	20	0	0
9	N	21	0	30	2	0
10	K	20	0	26	1	0
10	M	10	0	14	0	0
10	N	10	0	14	0	0
11	O	13	0	18	2	0
11	Q	13	0	18	5	0
12	E	63	0	0	2	0
12	J	87	0	0	3	0
12	K	84	0	0	1	0
12	M	91	0	0	1	0
12	N	99	0	0	1	0
12	O	66	0	0	0	0
12	P	50	0	0	3	0
12	Q	63	0	0	0	0
12	R	27	0	0	1	0
12	T	67	0	0	2	0
All	All	17097	0	15965	150	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 5.

All (150) 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)
5:R:11:LEU:HD23	5:R:104:LEU:HD13	1.69	0.75
2:J:29:VAL:HG22	2:J:73:ASN:HD22	1.53	0.74
4:Q:158:LEU:HD21	4:Q:181:VAL:HG11	1.68	0.73
3:K:83:PHE:CG	3:K:106:ILE:HG22	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:GLN:HA	1:E:414:GLN:HG2	1.70	0.72
2:M:126:PRO:HG3	2:M:138:LEU:HB3	1.76	0.67
2:J:83:ARG:NH2	12:J:402:HOH:O	2.29	0.66
5:R:33:LEU:HB3	5:R:51:ALA:HB2	1.76	0.66
2:J:121:VAL:O	12:J:401:HOH:O	2.13	0.66
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.78	0.65
2:M:34:MET:HE3	2:M:78:LEU:HB2	1.80	0.64
5:R:37:GLN:HB2	5:R:47:LEU:HD11	1.78	0.64
2:M:12:ILE:HD13	2:M:18:LEU:HD13	1.80	0.63
4:Q:150:THR:HG22	4:Q:198:ASN:HB3	1.81	0.63
1:E:387:LEU:HA	1:E:390:LEU:HD12	1.81	0.61
4:O:58:ARG:HB2	11:O:301:PG4:H42	1.82	0.61
3:K:149:LYS:HB2	3:K:193:ALA:HB3	1.83	0.61
2:M:216:CYS:SG	12:M:448:HOH:O	2.56	0.60
4:Q:162:VAL:HG22	4:Q:181:VAL:HG22	1.83	0.59
3:K:207:LYS:NZ	12:K:401:HOH:O	2.26	0.59
5:P:81:GLU:OE2	12:P:301:HOH:O	2.16	0.59
4:Q:118:PRO:HB3	4:Q:144:TYR:HB3	1.86	0.58
3:K:83:PHE:CD1	3:K:106:ILE:HG22	2.39	0.57
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.84	0.57
5:P:18:ARG:HG2	5:P:76:SER:HA	1.85	0.57
5:P:45:LYS:NZ	12:P:307:HOH:O	2.36	0.57
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.85	0.57
5:R:11:LEU:HD21	5:R:19:VAL:HG21	1.87	0.56
3:N:145:LYS:HB3	3:N:197:THR:HB	1.88	0.56
11:Q:300:PG4:H41	5:R:94:TYR:HE2	1.70	0.55
1:T:346:ARG:NH2	12:T:603:HOH:O	2.33	0.55
5:P:166:GLN:HG2	5:P:173:TYR:CE1	2.42	0.55
2:J:56:SER:HA	9:J:303:PEG:H31	1.87	0.55
3:N:170:ASP:HB3	4:O:205:LYS:HD2	1.89	0.55
1:E:415:THR:HG21	9:J:303:PEG:H32	1.89	0.55
3:K:37:GLN:HB2	3:K:47:LEU:HD11	1.89	0.55
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.88	0.55
4:Q:39:GLN:HE22	5:R:38:GLN:HE22	1.55	0.55
3:K:147:GLN:HG2	3:K:154:LEU:HD11	1.90	0.53
4:Q:100(A):PRO:HG3	5:R:49:TYR:HB2	1.89	0.53
2:J:35:SER:OG	2:J:95:ASP:OD2	2.24	0.53
5:P:152:ASN:ND2	12:P:308:HOH:O	2.42	0.53
4:O:118:PRO:HB3	4:O:144:TYR:HB3	1.91	0.52
5:P:13:VAL:HG21	5:P:19:VAL:HG21	1.92	0.52
3:K:167:ASP:HA	10:K:303:PGE:H4	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:97:GLY:O	4:Q:100:THR:OG1	2.26	0.52
4:Q:58:ARG:HH12	11:Q:300:PG4:H71	1.73	0.52
2:M:126:PRO:HD2	2:M:213:PRO:HA	1.90	0.52
4:O:97:GLY:O	4:O:100:THR:OG1	2.28	0.52
3:N:18:ARG:HH11	3:N:74:THR:HG21	1.75	0.51
5:P:120:PRO:HD3	5:P:132:VAL:HG22	1.93	0.51
5:P:150:VAL:HG22	5:P:192:TYR:HD1	1.74	0.51
3:K:82:ASP:O	3:K:86:TYR:OH	2.19	0.51
5:R:30:LYS:NZ	12:R:301:HOH:O	2.42	0.51
4:O:93:ALA:HB1	4:O:100(B):MET:HB3	1.92	0.51
3:N:48:ILE:HD13	3:N:54:ARG:HA	1.91	0.50
2:J:127:SER:O	2:J:131:THR:OG1	2.24	0.49
1:E:360:ASN:H	1:E:523:THR:HB	1.76	0.49
2:J:112:SER:HB2	9:J:302:PEG:H12	1.94	0.49
3:N:124:GLN:O	3:N:127:SER:OG	2.27	0.49
3:K:145:LYS:HB3	3:K:197:THR:HB	1.93	0.49
5:P:105:GLU:OE1	5:P:173:TYR:OH	2.31	0.49
1:E:458:LYS:HE3	1:E:473:TYR:CE1	2.47	0.49
3:K:106:ILE:HD11	3:K:171:SER:OG	2.13	0.48
1:T:501:ASN:HB3	1:T:505:TYR:HB2	1.94	0.48
2:M:33:TYR:HB2	2:M:95:ASP:O	2.12	0.48
4:O:137:LEU:HD21	4:O:193:TYR:CD2	2.48	0.48
3:N:106:ILE:HD11	3:N:171:SER:HB3	1.94	0.48
5:P:186:TYR:O	5:P:192:TYR:OH	2.31	0.48
2:J:152:VAL:HG22	2:J:198:VAL:HG22	1.95	0.47
3:K:166:GLN:NE2	3:K:171:SER:O	2.46	0.47
5:P:89:GLN:HE21	5:P:96:TYR:HB3	1.80	0.47
1:E:501:ASN:HB3	1:E:505:TYR:HB2	1.97	0.47
4:Q:93:ALA:HB1	4:Q:100(B):MET:HB3	1.97	0.47
2:J:82:MET:HE1	2:J:109:VAL:HG21	1.97	0.47
1:T:396:TYR:HB2	1:T:514:SER:HB2	1.97	0.46
2:M:34:MET:HB3	2:M:78:LEU:HD22	1.97	0.46
5:P:11:LEU:HD23	5:P:104:LEU:HD13	1.97	0.46
1:T:360:ASN:H	1:T:523:THR:HB	1.81	0.46
11:Q:300:PG4:H51	11:Q:300:PG4:H32	1.82	0.45
3:K:120:PRO:HD3	3:K:132:VAL:HG22	1.98	0.45
2:M:93:ALA:HB1	2:M:100(A):PHE:HB3	1.97	0.45
4:O:100(A):PRO:HG3	5:P:49:TYR:HB2	1.98	0.45
4:O:20:ILE:HD11	4:O:80:LEU:HD23	1.98	0.45
5:P:149:LYS:HE2	5:P:195:GLU:HB2	1.98	0.45
5:R:120:PRO:HG3	5:R:130:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:18:LEU:HB2	4:O:82(C):LEU:HD11	1.98	0.45
2:M:12:ILE:HG21	2:M:82(C):LEU:HD13	1.99	0.45
1:E:357:ARG:NE	12:E:705:HOH:O	2.42	0.45
3:K:19:ALA:HB2	3:K:78:LEU:HD11	1.99	0.44
4:O:141:VAL:HG11	4:O:149:VAL:HG11	1.99	0.44
11:Q:300:PG4:H41	5:R:94:TYR:CE2	2.51	0.44
3:N:35:TRP:HB2	3:N:48:ILE:HB	1.99	0.44
3:N:61:ARG:HB2	3:N:76:SER:O	2.17	0.44
1:E:458:LYS:NZ	12:E:710:HOH:O	2.48	0.44
4:Q:47:TRP:HD1	4:Q:100(B):MET:HE1	1.82	0.44
5:R:13:VAL:HG22	5:R:104:LEU:HD11	2.00	0.44
9:N:303:PEG:H11	9:N:303:PEG:H31	1.77	0.44
1:E:339:GLY:HA2	7:E:601:NAG:H83	2.00	0.44
3:K:163:VAL:HG22	3:K:175:LEU:HD12	1.99	0.44
5:P:161:GLU:HG2	5:P:175:LEU:HD21	2.00	0.44
2:M:13:GLN:H	2:M:13:GLN:CD	2.26	0.44
5:R:83:LEU:HD11	5:R:166:GLN:HB3	1.99	0.43
2:J:22:CYS:HB3	2:J:78:LEU:HB3	2.00	0.43
3:K:61:ARG:HB2	3:K:76:SER:O	2.18	0.43
1:E:396:TYR:HB2	1:E:514:SER:HB3	2.01	0.43
5:P:121:SER:O	5:P:125:LEU:HG	2.17	0.43
4:O:137:LEU:HD21	4:O:193:TYR:HD2	1.82	0.43
2:J:33:TYR:HB2	2:J:95:ASP:O	2.18	0.43
1:E:409:GLN:HG2	8:E:603:EDO:H12	2.00	0.43
1:E:350:VAL:HG22	1:E:422:ASN:HB3	2.00	0.42
3:K:106:ILE:HD11	3:K:171:SER:CB	2.49	0.42
3:N:60:ASP:OD1	3:N:60:ASP:N	2.52	0.42
5:P:21:MET:HG2	5:P:102:THR:HG21	2.02	0.42
5:P:187:GLU:O	5:P:211:ARG:NH2	2.52	0.42
4:O:158:LEU:HD21	4:O:181:VAL:HG21	2.02	0.42
3:K:40:PRO:HG2	3:K:165:GLU:HG2	2.00	0.42
3:K:140:TYR:CG	3:K:141:PRO:HA	2.55	0.42
5:R:119:PRO:HB3	5:R:209:PHE:CE2	2.55	0.42
2:J:206:LYS:HE3	2:J:206:LYS:HB2	1.90	0.42
3:N:143:GLU:H	3:N:143:GLU:CD	2.27	0.42
5:P:120:PRO:HG3	5:P:130:ALA:HB1	2.01	0.42
5:P:12:THR:HG22	5:P:105:GLU:HB2	2.01	0.42
2:M:72:ASP:OD1	2:M:74:SER:OG	2.30	0.42
2:M:177:SER:C	9:N:303:PEG:H12	2.45	0.41
2:M:20:LEU:HG	2:M:82:MET:HE3	2.02	0.41
1:E:350:VAL:O	1:E:353:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:425:LEU:HD21	1:T:512:VAL:HG11	2.02	0.41
2:J:201:LYS:NZ	12:J:415:HOH:O	2.51	0.41
5:P:145:LYS:HB3	5:P:197:THR:HB	2.02	0.41
3:K:91:TYR:HA	3:K:96:ARG:HG2	2.03	0.41
3:K:106:ILE:HD11	3:K:171:SER:HB3	2.02	0.41
2:M:28:THR:O	2:M:32:ASN:ND2	2.44	0.41
2:M:11:LEU:HB2	2:M:147:PRO:HG3	2.03	0.41
11:O:301:PG4:H61	11:O:301:PG4:H41	1.76	0.41
1:T:380:TYR:HE2	11:Q:300:PG4:H31	1.85	0.41
1:T:403:ARG:HD2	12:N:459:HOH:O	2.20	0.41
2:J:216:CYS:HB2	3:K:214:CYS:SG	2.61	0.41
4:Q:39:GLN:HE22	5:R:38:GLN:NE2	2.19	0.41
4:Q:47:TRP:CD1	4:Q:100(B):MET:HE1	2.56	0.41
1:T:334:ASN:N	12:T:614:HOH:O	2.55	0.40
1:E:497:PHE:CD2	1:E:507:PRO:HB3	2.57	0.40
4:O:165:PHE:CE2	5:P:176:SER:HB3	2.57	0.40
2:M:40:ALA:HB3	2:M:43:LYS:HB2	2.02	0.40
4:Q:12:LYS:HE3	4:Q:18:LEU:HD13	2.03	0.40
1:T:347:PHE:CE2	1:T:399:SER:HB2	2.56	0.40
3:K:113:PRO:HB3	3:K:139:PHE:HB3	2.03	0.40
3:K:154:LEU:HD12	3:K:154:LEU:HA	1.72	0.40
3:N:106:ILE:HG13	3:N:166:GLN:HE22	1.86	0.40
5:P:13:VAL:HG22	5:P:104:LEU:HD11	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	Percentiles	
1	E	192/209 (92%)	186 (97%)	6 (3%)	0	100	100
1	T	193/209 (92%)	190 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	220/220 (100%)	218 (99%)	2 (1%)	0	100	100
2	M	219/220 (100%)	215 (98%)	4 (2%)	0	100	100
3	K	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
3	N	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
4	O	211/221 (96%)	209 (99%)	2 (1%)	0	100	100
4	Q	208/221 (94%)	206 (99%)	2 (1%)	0	100	100
5	P	215/221 (97%)	211 (98%)	4 (2%)	0	100	100
5	R	215/221 (97%)	211 (98%)	4 (2%)	0	100	100
All	All	2098/2172 (97%)	2056 (98%)	42 (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	E	167/181 (92%)	167 (100%)	0	100	100
1	T	168/181 (93%)	168 (100%)	0	100	100
2	J	187/186 (100%)	186 (100%)	1 (0%)	81	88
2	M	186/186 (100%)	186 (100%)	0	100	100
3	K	185/186 (100%)	184 (100%)	1 (0%)	81	88
3	N	186/186 (100%)	182 (98%)	4 (2%)	45	64
4	O	181/187 (97%)	179 (99%)	2 (1%)	65	79
4	Q	179/187 (96%)	179 (100%)	0	100	100
5	P	195/198 (98%)	192 (98%)	3 (2%)	57	74
5	R	195/198 (98%)	195 (100%)	0	100	100
All	All	1829/1876 (98%)	1818 (99%)	11 (1%)	78	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	29	VAL
3	K	33	LEU
3	N	11	LEU
3	N	72	THR
3	N	105	GLU
3	N	213	GLU
4	O	64	GLN
4	O	210	VAL
5	P	18	ARG
5	P	19	VAL
5	P	72	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	414	GLN
1	E	493	GLN
1	T	360	ASN
1	T	370	ASN
1	T	450	ASN
1	T	481	ASN
1	T	519	HIS
2	J	73	ASN
2	J	105	GLN
2	J	204	ASN
3	K	199	GLN
2	M	1	GLN
3	N	89	GLN
3	N	155	GLN
4	O	203	ASN
5	P	42	GLN
5	P	124	GLN
4	Q	198	ASN
5	R	29	GLN
5	R	38	GLN
5	R	42	GLN
5	R	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	A	1	6,1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
6	NAG	A	2	6	14,14,15	0.72	0	17,19,21	0.87	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	A	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	A	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1	NAG	C2-N2-C7	2.02	125.60	122.90

There are no chirality outliers.

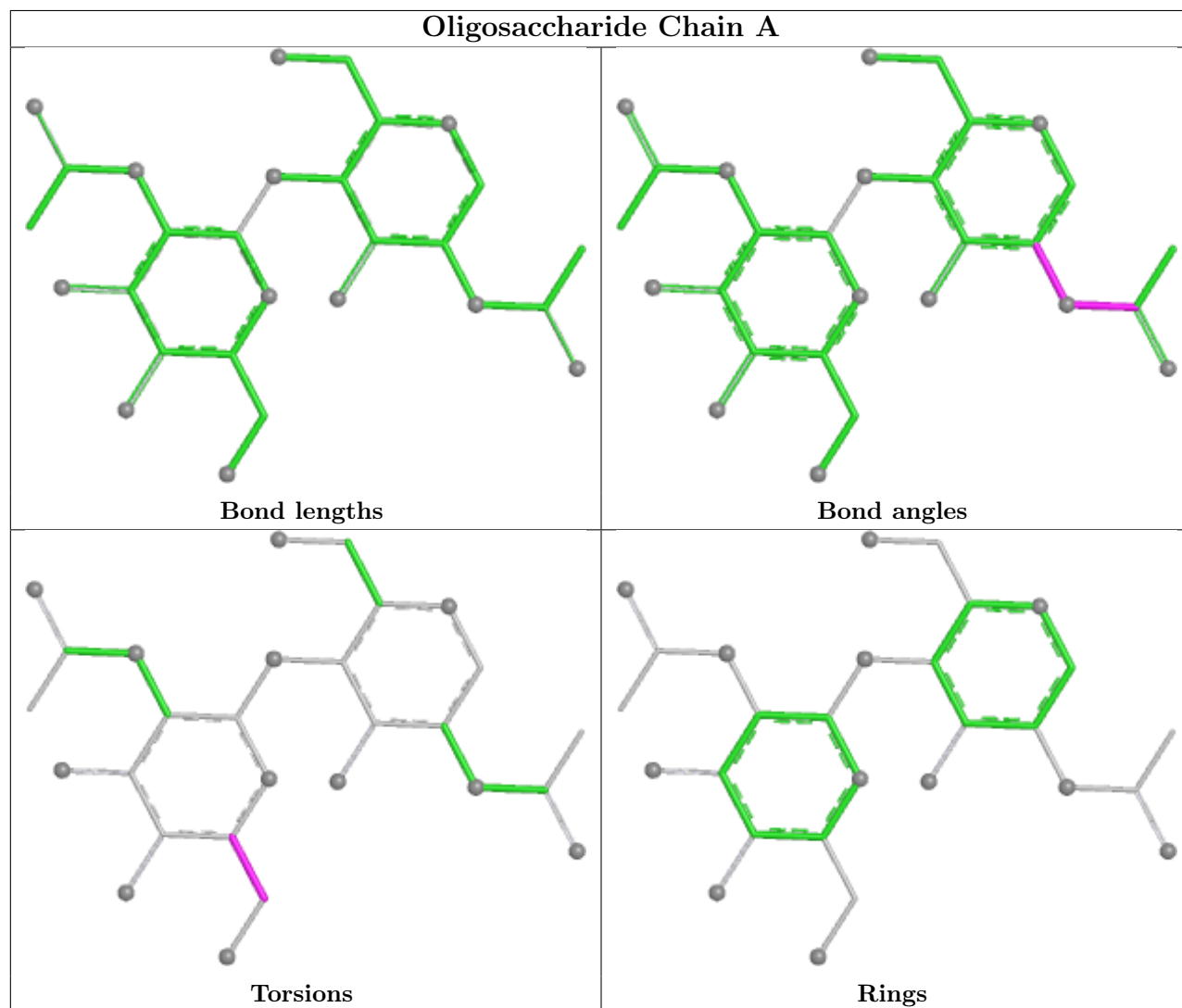
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2	NAG	C4-C5-C6-O6
6	A	2	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](#)

18 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	PEG	N	304	-	6,6,6	0.25	0	5,5,5	0.23	0
10	PGE	N	302	-	9,9,9	0.33	0	8,8,8	0.52	0
11	PG4	Q	300	-	12,12,12	0.29	0	11,11,11	0.26	0
9	PEG	K	302	-	6,6,6	0.26	0	5,5,5	0.18	0
10	PGE	M	301	-	9,9,9	0.32	0	8,8,8	0.53	0
7	NAG	E	601	1	14,14,15	0.71	0	17,19,21	1.21	1 (5%)
8	EDO	E	602	-	3,3,3	0.25	0	2,2,2	0.37	0
9	PEG	J	302	-	6,6,6	0.26	0	5,5,5	0.25	0
11	PG4	O	301	-	12,12,12	0.28	0	11,11,11	0.15	0
9	PEG	J	301	-	6,6,6	0.25	0	5,5,5	0.26	0
10	PGE	K	301	-	9,9,9	0.32	0	8,8,8	0.46	0
9	PEG	N	301	-	6,6,6	0.25	0	5,5,5	0.22	0
9	PEG	J	303	-	6,6,6	0.25	0	5,5,5	0.24	0
9	PEG	N	303	-	6,6,6	0.24	0	5,5,5	0.19	0
9	PEG	K	304	-	6,6,6	0.25	0	5,5,5	0.25	0
8	EDO	J	304	-	3,3,3	0.27	0	2,2,2	0.09	0
8	EDO	E	603	-	3,3,3	0.25	0	2,2,2	0.29	0
10	PGE	K	303	-	9,9,9	0.33	0	8,8,8	0.39	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	PEG	N	304	-	-	1/4/4/4	-
10	PGE	N	302	-	-	3/7/7/7	-
11	PG4	Q	300	-	-	5/10/10/10	-
9	PEG	K	302	-	-	0/4/4/4	-
10	PGE	M	301	-	-	3/7/7/7	-
7	NAG	E	601	1	-	2/6/23/26	0/1/1/1
8	EDO	E	602	-	-	0/1/1/1	-
9	PEG	J	302	-	-	1/4/4/4	-
11	PG4	O	301	-	-	4/10/10/10	-
9	PEG	J	301	-	-	0/4/4/4	-
10	PGE	K	301	-	-	2/7/7/7	-
9	PEG	N	301	-	-	2/4/4/4	-
9	PEG	J	303	-	-	1/4/4/4	-
9	PEG	N	303	-	-	3/4/4/4	-
9	PEG	K	304	-	-	1/4/4/4	-
8	EDO	J	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	E	603	-	-	0/1/1/1	-
10	PGE	K	303	-	-	0/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	601	NAG	C2-N2-C7	3.15	127.12	122.90

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	M	301	PGE	O2-C3-C4-O3
11	Q	300	PG4	O2-C3-C4-O3
9	N	301	PEG	O1-C1-C2-O2
11	Q	300	PG4	C3-C4-O3-C5
10	N	302	PGE	O3-C5-C6-O4
11	Q	300	PG4	O3-C5-C6-O4
10	N	302	PGE	O2-C3-C4-O3
9	N	303	PEG	O1-C1-C2-O2
9	N	301	PEG	C4-C3-O2-C2
9	N	304	PEG	C4-C3-O2-C2
10	N	302	PGE	C6-C5-O3-C4
11	O	301	PG4	C6-C5-O3-C4
9	J	303	PEG	O2-C3-C4-O4
9	J	302	PEG	C1-C2-O2-C3
7	E	601	NAG	C3-C2-N2-C7
10	K	301	PGE	C6-C5-O3-C4
10	K	301	PGE	C1-C2-O2-C3
9	N	303	PEG	C1-C2-O2-C3
11	O	301	PG4	C8-C7-O4-C6
11	O	301	PG4	O2-C3-C4-O3
10	M	301	PGE	C4-C3-O2-C2
7	E	601	NAG	C1-C2-N2-C7
10	M	301	PGE	C6-C5-O3-C4
11	Q	300	PG4	O1-C1-C2-O2
9	N	303	PEG	C4-C3-O2-C2
11	Q	300	PG4	C1-C2-O2-C3
11	O	301	PG4	O3-C5-C6-O4
9	K	304	PEG	O2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	300	PG4	5	0
7	E	601	NAG	1	0
9	J	302	PEG	1	0
11	O	301	PG4	2	0
9	J	303	PEG	2	0
9	N	303	PEG	2	0
8	E	603	EDO	1	0
10	K	303	PGE	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 [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(Å ²)	Q<0.9
1	E	194/209 (92%)	-1.55	0 100 100	18, 33, 68, 86	0
1	T	194/209 (92%)	-1.55	0 100 100	15, 34, 71, 89	1 (0%)
2	J	220/220 (100%)	-1.63	0 100 100	14, 30, 57, 97	2 (0%)
2	M	220/220 (100%)	-1.60	0 100 100	17, 31, 59, 78	1 (0%)
3	K	214/215 (99%)	-1.63	0 100 100	16, 31, 49, 71	0
3	N	214/215 (99%)	-1.61	0 100 100	19, 32, 49, 84	1 (0%)
4	O	215/221 (97%)	-1.47	0 100 100	24, 41, 86, 104	0
4	Q	212/221 (95%)	-1.47	0 100 100	24, 41, 85, 100	0
5	P	217/221 (98%)	-1.36	0 100 100	27, 60, 89, 98	0
5	R	217/221 (98%)	-1.34	0 100 100	34, 59, 81, 89	0
All	All	2117/2172 (97%)	-1.52	0 100 100	14, 37, 78, 104	5 (0%)

There are no RSRZ outliers to report.

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.

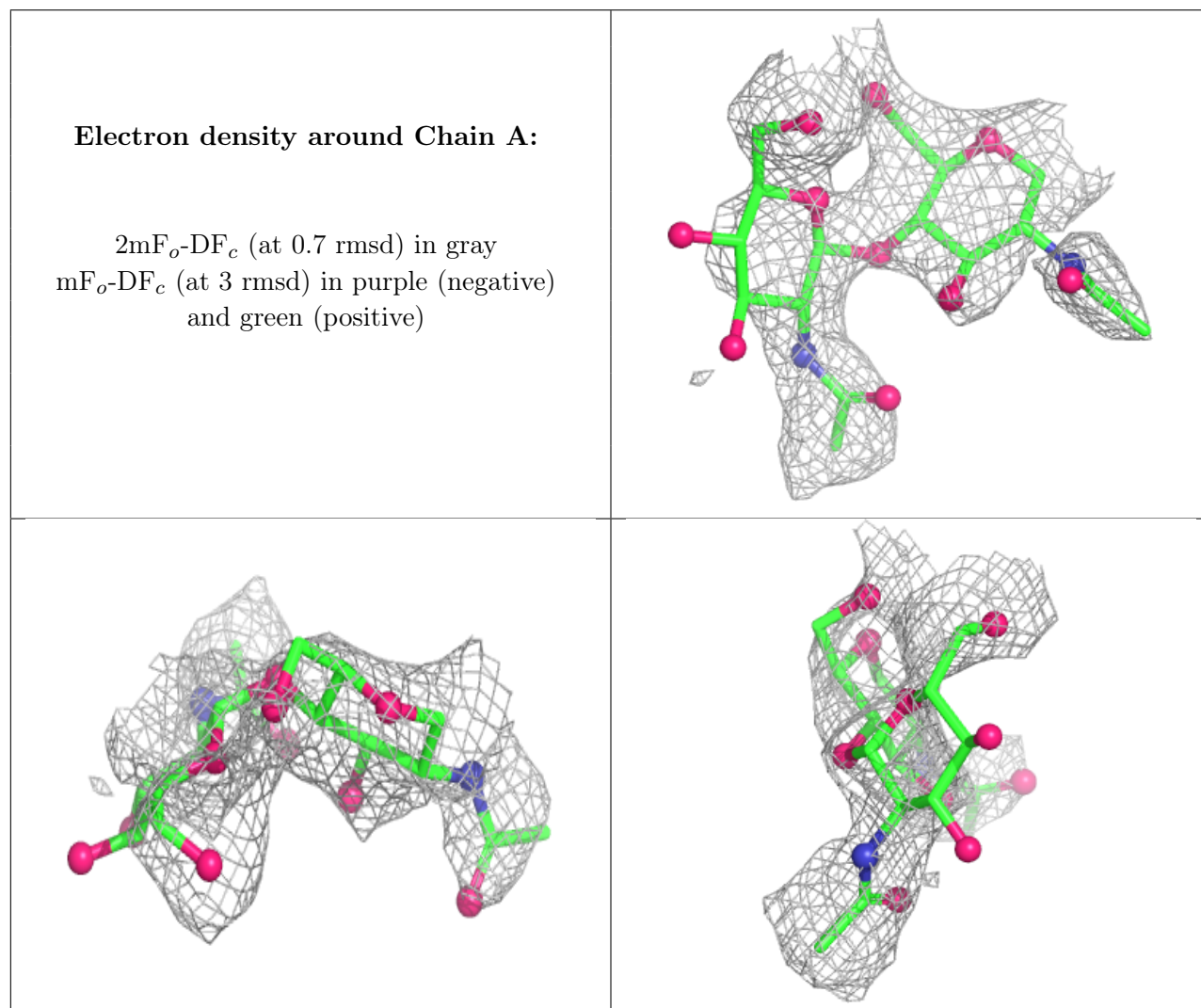
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	1	14/15	-	-	65,90,93,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	2	14/15	-	-	65,106,114,115	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 ⓘ

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(\AA^2)	Q<0.9
9	PEG	N	304	7/7	0.96	0.08	54,59,71,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	PEG	J	301	7/7	0.98	0.05	43,61,63,69	0
9	PEG	J	302	7/7	0.98	0.06	42,43,62,66	0
9	PEG	K	302	7/7	0.98	0.04	49,50,54,55	0
7	NAG	E	601	14/15	0.98	0.05	71,84,97,99	0
8	EDO	E	603	4/4	0.99	0.05	40,45,50,50	0
9	PEG	J	303	7/7	0.99	0.03	29,38,55,58	0
8	EDO	J	304	4/4	0.99	0.04	28,31,49,51	0
9	PEG	K	304	7/7	0.99	0.04	29,37,57,60	0
9	PEG	N	301	7/7	0.99	0.04	44,44,52,55	0
9	PEG	N	303	7/7	0.99	0.07	19,35,64,65	0
8	EDO	E	602	4/4	0.99	0.06	30,42,43,55	0
10	PGE	K	301	10/10	0.99	0.04	29,43,57,57	0
10	PGE	K	303	10/10	0.99	0.04	44,59,65,73	0
10	PGE	M	301	10/10	0.99	0.04	42,59,69,79	0
10	PGE	N	302	10/10	0.99	0.04	24,43,54,55	0
11	PG4	O	301	13/13	0.99	0.03	24,38,49,58	0
11	PG4	Q	300	13/13	0.99	0.04	33,47,53,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.