



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:06 AM BST

PDB ID : 3U2S
Title : Crystal Structure of PG9 Fab in Complex with V1V2 Region from HIV-1 strain ZM109
Authors : McLellan, J.S.; Pancera, M.; Kwong, P.D.
Deposited on : 2011-10-04
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

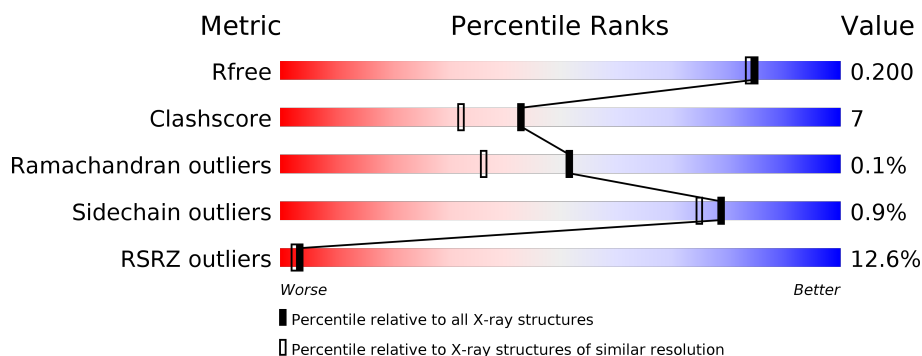
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	248	<div> <div>19%</div> <div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	H	248	<div> <div>2%</div> <div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
2	B	216	<div> <div>4%</div> <div> <div>87%</div> <div>11%</div> </div> </div>
2	L	216	<div> <div>3%</div> <div> <div>88%</div> <div>9%</div> </div> </div>
3	C	124	<div> <div>28%</div> <div> <div>56%</div> <div>16%</div> <div>27%</div> </div> </div>
3	G	124	<div> <div>26%</div> <div> <div>56%</div> <div>15%</div> <div>27%</div> </div> </div>

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Mol	Chain	Length	Quality of chain	
4	D	7		
4	E	7		

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16931 atoms, of which 7771 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 PG9 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	230	Total	C	H	N	O	S	0	0	0
			3447	1122	1667	298	351	9			
1	A	227	Total	C	H	N	O	S	0	0	0
			3415	1113	1652	295	346	9			

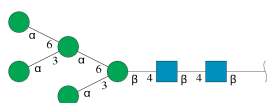
- Molecule 2 is a protein called PG9 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	211	Total	C	H	N	O	S	0	0	0
			3103	974	1537	267	321	4			
2	B	211	Total	C	H	N	O	S	0	0	0
			3103	974	1537	267	321	4			

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	90	Total	C	H	N	O	S	0	0	0
			1379	440	677	117	141	4			
3	C	90	Total	C	H	N	O	S	0	0	0
			1386	442	681	117	142	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



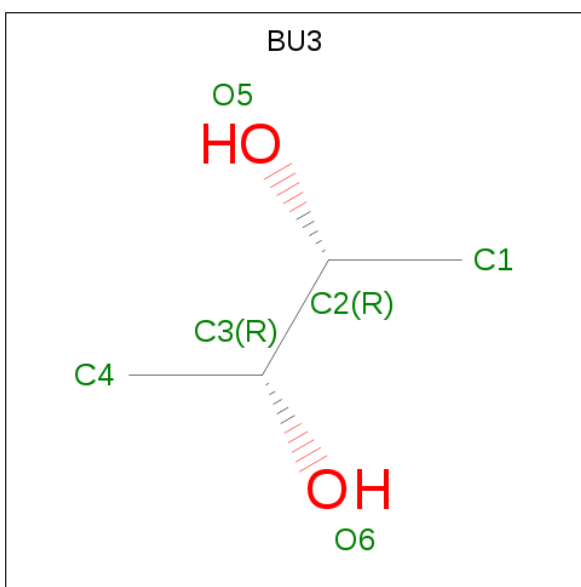
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



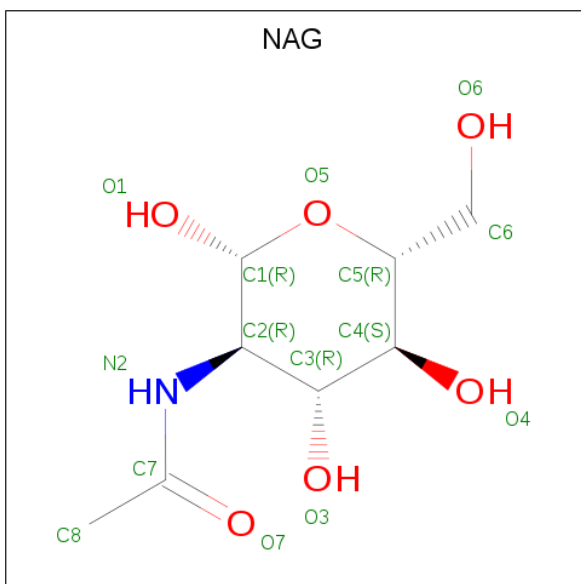
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	H	O	0	0
			16	4	10	2		
6	B	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

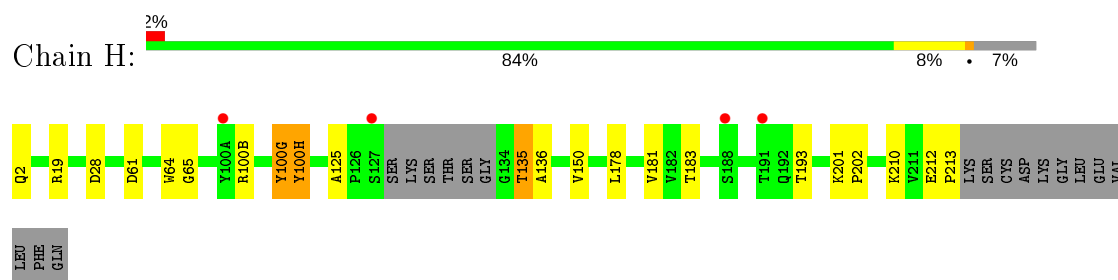
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	232	Total	O	0	0
			232	232		
8	L	186	Total	O	0	0
			186	186		
8	G	38	Total	O	0	0
			38	38		
8	A	203	Total	O	0	0
			203	203		
8	B	154	Total	O	0	0
			154	154		
8	C	34	Total	O	0	0
			34	34		

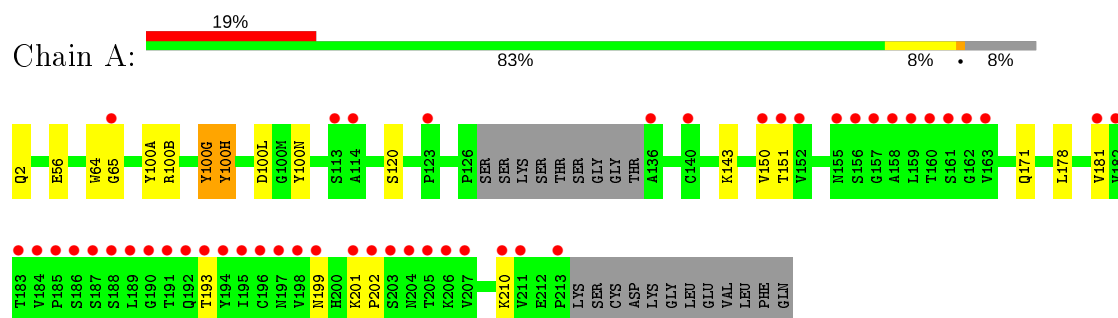
3 Residue-property plots

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.

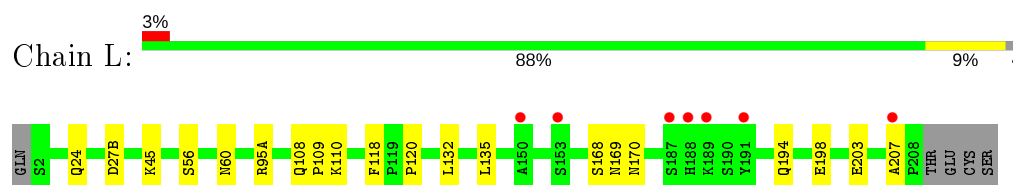
- Molecule 1: PG9 heavy chain



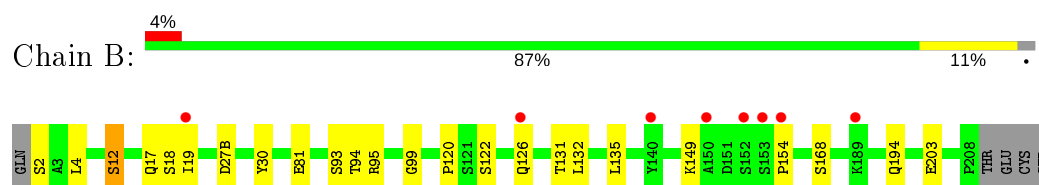
- Molecule 1: PG9 heavy chain



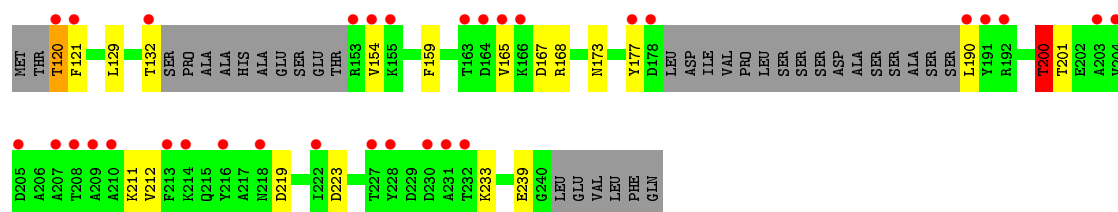
- Molecule 2: PG9 light chain



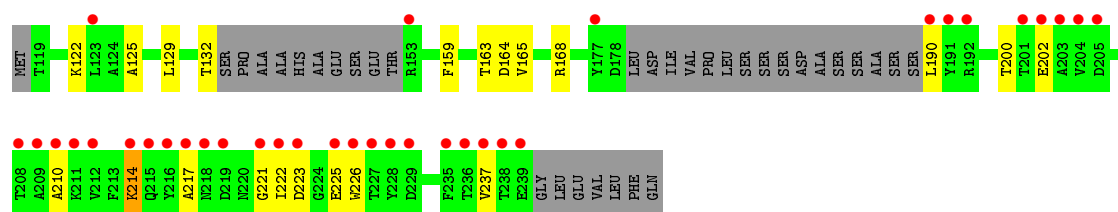
- Molecule 2: PG9 light chain



- Molecule 3: Envelope glycoprotein gp120



- Molecule 3: Envelope glycoprotein gp120



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.47Å 86.56Å 94.88Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	41.58 – 1.80 41.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (41.58-1.80) 90.9 (41.58-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_755)	Depositor
R, R_{free}	0.178 , 0.205 0.174 , 0.200	Depositor DCC
R_{free} test set	6169 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l 0.007 for -k,-h,-l 0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16931	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, BU3, TYS, SO4, PCA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/1770	0.53	0/2409
1	H	0.39	0/1787	0.54	0/2432
2	B	0.35	0/1601	0.52	0/2180
2	L	0.37	0/1601	0.53	0/2180
3	C	0.27	0/714	0.44	0/967
3	G	0.28	0/711	0.52	0/962
All	All	0.36	0/8184	0.52	0/11130

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	200	THR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	1652	1662	21	0
1	H	1780	1667	1677	21	0
2	B	1566	1537	1533	18	0
2	L	1566	1537	1533	22	0
3	C	705	681	680	20	0
3	G	702	677	676	17	0
4	D	83	0	70	0	0
4	E	83	0	70	0	0
5	B	15	0	0	0	0
5	H	5	0	0	0	0
5	L	5	0	0	1	0
6	B	6	10	10	0	0
6	L	6	10	10	0	0
7	C	14	0	13	0	0
7	G	14	0	13	0	0
8	A	203	0	0	7	0
8	B	154	0	0	5	0
8	C	34	0	0	2	0
8	G	38	0	0	6	0
8	H	232	0	0	5	1
8	L	186	0	0	10	1
All	All	9160	7771	7947	110	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (110) 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)
1:H:181:VAL:HG11	2:L:135:LEU:HD13	1.42	1.02
3:G:173:ASN:OD1	8:G:456:HOH:O	1.82	0.96
2:L:56:SER:HG	1:A:100(A):TYR:HH	1.20	0.89
1:A:171:GLN:NE2	8:A:377:HOH:O	2.10	0.84
2:L:207:ALA:O	8:L:668:HOH:O	1.97	0.82
1:A:100(H):TYS:S	8:A:748:HOH:O	2.41	0.79
3:C:221:GLY:O	8:C:416:HOH:O	2.01	0.78
3:G:233:LYS:NZ	8:G:591:HOH:O	2.16	0.78
2:L:24:GLN:OE1	8:L:261:HOH:O	2.01	0.78
3:G:120:THR:HA	8:G:769:HOH:O	1.82	0.77
1:H:181:VAL:HG11	2:L:135:LEU:CD1	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:200:THR:O	3:G:201:THR:HG23	1.85	0.77
1:H:64:TRP:O	8:H:690:HOH:O	2.03	0.75
5:L:214:SO4:O4	8:L:697:HOH:O	2.04	0.74
3:G:120:THR:N	8:G:769:HOH:O	2.27	0.68
2:L:110:LYS:NZ	8:L:239:HOH:O	2.10	0.67
2:L:118:PHE:HE2	2:L:135:LEU:HD12	1.60	0.67
3:G:120:THR:CA	8:G:769:HOH:O	2.40	0.67
3:G:219:ASP:OD1	8:G:692:HOH:O	2.14	0.66
2:B:17:GLN:HG2	2:B:18:SER:N	2.12	0.65
2:L:110:LYS:CE	8:L:239:HOH:O	2.45	0.63
1:A:100(N):TYR:OH	8:A:549:HOH:O	2.14	0.62
1:H:135:THR:CG2	1:H:183:THR:HG23	2.30	0.61
3:C:225:GLU:O	8:C:800:HOH:O	2.16	0.61
1:H:135:THR:HG23	1:H:183:THR:HG23	1.84	0.60
2:B:2:SER:CA	8:B:689:HOH:O	2.49	0.60
1:H:193:THR:HG23	1:H:210:LYS:HE3	1.83	0.60
1:H:100(H):TYS:S	3:G:168:ARG:NH1	2.74	0.59
1:H:61:ASP:OD1	2:L:95(A):ARG:NH2	2.34	0.59
1:A:100(A):TYR:OH	8:A:761:HOH:O	2.16	0.59
2:B:2:SER:HA	8:B:689:HOH:O	2.03	0.59
2:L:108:GLN:HB2	2:L:109:PRO:HD2	1.85	0.58
3:C:132:THR:CG2	3:C:190:LEU:HD23	2.34	0.58
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.86	0.58
3:C:122:LYS:HG2	3:C:200:THR:HG22	1.85	0.58
2:B:12:SER:HB3	8:B:278:HOH:O	2.03	0.58
3:G:129:LEU:HD23	3:G:159:PHE:HB3	1.86	0.58
1:A:201:LYS:HB2	1:A:202:PRO:HD3	1.86	0.57
2:B:2:SER:N	8:B:689:HOH:O	2.38	0.57
3:C:132:THR:HG23	3:C:190:LEU:HD23	1.88	0.56
3:C:226:TRP:CD2	3:C:237:VAL:HG12	2.42	0.55
2:L:60:ASN:HB3	8:L:807:HOH:O	2.06	0.55
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.38	0.54
2:L:169:ASN:O	2:L:170:ASN:HB2	2.09	0.53
3:G:121:PHE:CE1	3:G:233:LYS:HD2	2.45	0.52
1:H:150:VAL:CG2	1:H:178:LEU:HD21	2.40	0.52
1:A:120:SER:OG	8:A:721:HOH:O	2.18	0.52
1:A:100(L):ASP:OD1	3:C:168:ARG:NH2	2.42	0.52
3:G:132:THR:HG22	3:G:190:LEU:HD23	1.91	0.51
1:H:100(H):TYS:O1	3:G:168:ARG:NH1	2.43	0.51
2:L:120:PRO:HD3	2:L:132:LEU:HD23	1.93	0.51
2:L:45:LYS:NZ	8:L:401:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:GLN:HG2	2:B:18:SER:H	1.74	0.51
2:B:18:SER:O	2:B:19:ILE:HD13	2.11	0.51
3:G:223:ASP:O	3:G:239:GLU:HG2	2.11	0.51
3:C:132:THR:HG23	3:C:190:LEU:CD2	2.41	0.50
1:A:65:GLY:HA2	8:A:260:HOH:O	2.11	0.50
1:A:151:THR:CG2	1:A:199:ASN:HB3	2.42	0.50
1:A:100(H):TYS:O3	8:A:748:HOH:O	2.19	0.49
2:B:149:LYS:HD3	2:B:154:PRO:HA	1.94	0.49
3:C:217:ALA:HB1	3:C:222:ILE:HB	1.93	0.49
1:A:181:VAL:HG11	2:B:135:LEU:CD1	2.43	0.49
3:C:129:LEU:HD23	3:C:159:PHE:HB3	1.95	0.49
2:B:122:SER:O	2:B:126:GLN:HG3	2.13	0.48
3:C:132:THR:CG2	3:C:190:LEU:CD2	2.92	0.48
3:C:125:ALA:HA	3:C:237:VAL:HG22	1.95	0.48
1:A:150:VAL:CG2	1:A:178:LEU:HD21	2.43	0.47
2:B:168:SER:OG	8:B:750:HOH:O	2.20	0.47
2:B:120:PRO:HD3	2:B:132:LEU:CD2	2.45	0.47
3:C:202:GLU:N	3:C:202:GLU:OE1	2.48	0.47
1:H:135:THR:CG2	1:H:136:ALA:N	2.78	0.47
3:G:165:VAL:HG12	3:G:167:ASP:OD2	2.14	0.47
1:H:19:ARG:NE	8:H:297:HOH:O	2.35	0.47
3:G:223:ASP:N	3:G:239:GLU:OE1	2.37	0.46
1:H:125:ALA:O	8:H:323:HOH:O	2.20	0.46
1:A:150:VAL:HG23	1:A:178:LEU:HD21	1.97	0.46
3:C:210:ALA:O	3:C:214:LYS:HD3	2.16	0.46
1:H:150:VAL:HG23	1:H:178:LEU:HD21	1.97	0.46
1:H:65:GLY:HA2	8:H:321:HOH:O	2.15	0.46
2:L:45:LYS:HD2	8:L:229:HOH:O	2.15	0.46
3:C:226:TRP:CE3	3:C:237:VAL:HG12	2.51	0.46
2:L:45:LYS:CD	8:L:229:HOH:O	2.64	0.45
1:A:178:LEU:HD12	1:A:178:LEU:C	2.37	0.45
3:G:154:VAL:HG22	3:G:177:TYR:HD1	1.83	0.44
1:A:143:LYS:NZ	2:B:131:THR:OG1	2.41	0.44
3:G:211:LYS:HD3	3:G:212:VAL:N	2.32	0.44
2:L:118:PHE:CE2	2:L:135:LEU:HD12	2.46	0.44
1:H:178:LEU:HD12	1:H:178:LEU:C	2.38	0.43
1:H:212:GLU:HB2	1:H:213:PRO:HD2	1.99	0.43
2:B:194:GLN:HG2	2:B:203:GLU:HG3	2.00	0.43
1:A:64:TRP:HA	1:A:65:GLY:HA2	1.78	0.43
3:C:223:ASP:N	3:C:223:ASP:OD2	2.51	0.43
3:C:226:TRP:CE3	3:C:237:VAL:CG1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:THR:O	2:B:95:ARG:HB2	2.19	0.43
2:L:168:SER:HB2	2:B:81:GLU:OE1	2.19	0.43
1:H:100(B):ARG:NH1	1:H:100(G):TYS:O2	2.52	0.42
1:H:135:THR:HG21	1:H:183:THR:HG23	1.99	0.42
2:B:4:LEU:HB2	2:B:99:GLY:HA2	2.02	0.42
2:L:194:GLN:HG2	2:L:203:GLU:HG3	2.02	0.42
1:H:201:LYS:N	1:H:202:PRO:CD	2.83	0.42
2:L:110:LYS:HE3	2:L:198:GLU:HB2	2.02	0.41
2:B:30:TYR:OH	2:B:93:SER:HA	2.19	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.83	0.41
3:C:132:THR:HG22	3:C:190:LEU:HD23	2.03	0.41
3:C:164:ASP:N	3:C:164:ASP:OD1	2.49	0.41
1:H:28:ASP:OD2	8:H:678:HOH:O	2.22	0.41
3:C:165:VAL:HB	3:C:168:ARG:HG2	2.03	0.40
2:L:45:LYS:NZ	8:L:229:HOH:O	2.55	0.40
1:A:100(B):ARG:NH1	1:A:100(G):TYS:O2	2.50	0.40
1:A:151:THR:HG22	1:A:199:ASN:HB3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:338:HOH:O	8:L:277:HOH:O[2_645]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/248 (89%)	217 (98%)	4 (2%)	0	100	100
1	H	224/248 (90%)	221 (99%)	3 (1%)	0	100	100
2	B	209/216 (97%)	204 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	209/216 (97%)	203 (97%)	6 (3%)	0	100	100
3	C	84/124 (68%)	82 (98%)	1 (1%)	1 (1%)	13	3
3	G	84/124 (68%)	82 (98%)	2 (2%)	0	100	100
All	All	1031/1176 (88%)	1009 (98%)	21 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	163	THR

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	A	189/207 (91%)	188 (100%)	1 (0%)	88	87
1	H	191/207 (92%)	190 (100%)	1 (0%)	88	87
2	B	178/183 (97%)	176 (99%)	2 (1%)	73	68
2	L	178/183 (97%)	177 (99%)	1 (1%)	86	84
3	C	77/105 (73%)	76 (99%)	1 (1%)	69	62
3	G	76/105 (72%)	74 (97%)	2 (3%)	46	32
All	All	889/990 (90%)	881 (99%)	8 (1%)	78	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	135	THR
2	L	27(B)	ASP
3	G	120	THR
3	G	200	THR
1	A	56	GLU
2	B	12	SER
2	B	27(B)	ASP

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Mol	Chain	Res	Type
3	C	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	188	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TYS	A	100(H)	1	15,16,17	1.17	1 (6%)	18,22,24	0.73	0
1	TYS	H	100(G)	-	15,16,17	1.12	1 (6%)	18,22,24	0.97	1 (5%)
1	PCA	H	2	1	7,8,9	2.04	2 (28%)	9,10,12	2.10	5 (55%)
1	TYS	H	100(H)	1	15,16,17	1.19	1 (6%)	18,22,24	0.65	1 (5%)
1	TYS	A	100(G)	-	15,16,17	1.17	2 (13%)	18,22,24	0.86	1 (5%)
1	PCA	A	2	1	7,8,9	2.08	2 (28%)	9,10,12	1.74	4 (44%)

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
1	TYS	A	100(H)	1	-	1/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYS	H	100(G)	-	-	2/10/11/13	0/1/1/1
1	PCA	H	2	1	-	0/0/11/13	0/1/1/1
1	TYS	H	100(H)	1	-	3/10/11/13	0/1/1/1
1	TYS	A	100(G)	-	-	1/10/11/13	0/1/1/1
1	PCA	A	2	1	-	0/0/11/13	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	PCA	CD-N	4.60	1.46	1.34
1	H	2	PCA	CD-N	4.31	1.45	1.34
1	A	100(H)	TYS	OH-S	3.06	1.62	1.58
1	H	2	PCA	CA-N	2.98	1.50	1.46
1	H	100(H)	TYS	OH-S	2.85	1.62	1.58
1	A	2	PCA	CA-N	2.79	1.49	1.46
1	H	100(G)	TYS	OH-S	2.38	1.61	1.58
1	A	100(G)	TYS	OH-S	2.30	1.61	1.58
1	A	100(G)	TYS	OH-CZ	-2.10	1.39	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2	PCA	CA-N-CD	-3.01	103.27	113.58
1	H	2	PCA	OE-CD-CG	-2.97	121.58	126.76
1	H	2	PCA	CG-CD-N	2.73	115.46	108.39
1	H	100(G)	TYS	OH-CZ-CE2	2.70	123.96	118.64
1	A	2	PCA	CA-N-CD	-2.64	104.55	113.58
1	H	2	PCA	CB-CA-N	2.57	110.69	103.30
1	A	100(G)	TYS	OH-CZ-CE2	2.47	123.50	118.64
1	A	2	PCA	CB-CA-N	2.43	110.27	103.30
1	H	2	PCA	CB-CA-C	-2.17	109.71	112.70
1	A	2	PCA	CG-CD-N	2.17	114.00	108.39
1	A	2	PCA	OE-CD-CG	-2.06	123.17	126.76
1	H	100(H)	TYS	O3-S-OH	2.02	110.69	105.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	100(H)	TYS	CZ-OH-S-O3
1	H	100(G)	TYS	CE1-CZ-OH-S

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Mol	Chain	Res	Type	Atoms
1	H	100(G)	TYS	CE2-CZ-OH-S
1	H	100(H)	TYS	CZ-OH-S-O1
1	H	100(H)	TYS	CZ-OH-S-O3
1	A	100(G)	TYS	CZ-OH-S-O3
1	H	100(H)	TYS	CZ-OH-S-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	100(H)	TYS	2	0
1	H	100(G)	TYS	1	0
1	H	100(H)	TYS	2	0
1	A	100(G)	TYS	1	0

5.5 Carbohydrates [i](#)

14 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	$\# Z > 2$
4	NAG	D	1	3,4	14,14,15	0.60	0	17,19,21	1.14	2 (11%)
4	NAG	D	2	4	14,14,15	0.65	0	17,19,21	0.93	0
4	BMA	D	3	4	11,11,12	0.78	0	15,15,17	1.03	1 (6%)
4	MAN	D	4	4	11,11,12	0.65	0	15,15,17	1.07	0
4	MAN	D	5	4	11,11,12	0.71	0	15,15,17	0.55	0
4	MAN	D	6	4	11,11,12	0.66	0	15,15,17	1.04	0
4	MAN	D	7	4	11,11,12	0.65	0	15,15,17	0.88	0
4	NAG	E	1	3,4	14,14,15	0.52	0	17,19,21	0.71	0
4	NAG	E	2	4	14,14,15	0.76	1 (7%)	17,19,21	0.79	0
4	BMA	E	3	4	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
4	MAN	E	4	4	11,11,12	0.78	0	15,15,17	0.98	0
4	MAN	E	5	4	11,11,12	0.71	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	E	6	4	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
4	MAN	E	7	4	11,11,12	0.65	0	15,15,17	0.78	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	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	MAN	E	7	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	-2.09	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	O5-C5-C6	3.21	112.23	107.20
4	D	3	BMA	C1-C2-C3	2.45	112.68	109.67
4	E	3	BMA	C1-C2-C3	2.38	112.60	109.67
4	D	1	NAG	C2-N2-C7	-2.11	119.90	122.90
4	E	6	MAN	C2-C3-C4	-2.01	107.42	110.89
4	E	6	MAN	C1-C2-C3	-2.00	107.20	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	7	MAN	C4-C5-C6-O6
4	D	7	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
5	SO4	B	216	-	4,4,4	0.14	0	6,6,6	0.14	0
5	SO4	L	214	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	215	-	4,4,4	0.13	0	6,6,6	0.12	0
6	BU3	L	213	-	4,5,5	1.23	1 (25%)	6,6,6	0.71	0
7	NAG	G	573	3	14,14,15	0.55	0	17,19,21	0.74	0
5	SO4	H	226	-	4,4,4	0.16	0	6,6,6	0.10	0
7	NAG	C	573	3	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
6	BU3	B	213	-	4,5,5	1.23	1 (25%)	6,6,6	0.71	0
5	SO4	B	214	-	4,4,4	0.14	0	6,6,6	0.09	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
7	NAG	G	573	3	-	0/6/23/26	0/1/1/1
7	NAG	C	573	3	-	0/6/23/26	0/1/1/1
6	BU3	B	213	-	-	0/4/4/4	-
6	BU3	L	213	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	213	BU3	O6-C3	-2.08	1.37	1.43
6	B	213	BU3	O6-C3	-2.07	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	573	NAG	O5-C1-C2	-2.38	107.53	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	214	SO4	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	A	224/248 (90%)	1.05	47 (20%) 1 0	16, 36, 95, 131	0
1	H	227/248 (91%)	0.35	4 (1%) 68 64	16, 30, 63, 85	0
2	B	211/216 (97%)	0.45	8 (3%) 40 35	19, 40, 68, 83	0
2	L	211/216 (97%)	0.33	7 (3%) 46 40	16, 34, 69, 85	0
3	C	90/124 (72%)	1.93	35 (38%) 0 0	30, 68, 109, 126	0
3	G	90/124 (72%)	1.81	32 (35%) 0 0	38, 66, 100, 133	0
All	All	1053/1176 (89%)	0.78	133 (12%) 3 2	16, 39, 90, 133	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	190	LEU	8.5
1	A	191	THR	8.2
3	C	221	GLY	8.2
3	C	190	LEU	7.6
1	A	158	ALA	7.5
3	G	222	ILE	7.2
1	A	192	GLN	7.0
3	C	153	ARG	6.7
3	C	218	ASN	6.7
3	C	215	GLN	6.5
3	G	210	ALA	6.5
1	A	159	LEU	6.4
3	G	191	TYR	6.4
3	C	219	ASP	6.0
3	C	216	TYR	5.9
1	A	195	ILE	5.9
3	C	222	ILE	5.9
3	G	153	ARG	5.8
1	A	190	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
3	C	217	ALA	5.3
1	A	156	SER	5.2
3	C	191	TYR	5.2
3	G	121	PHE	5.2
3	G	209	ALA	5.2
1	A	181	VAL	5.1
3	G	205	ASP	5.1
1	A	194	TYR	4.9
1	A	204	ASN	4.8
1	A	188	SER	4.8
1	A	193	THR	4.6
3	C	227	THR	4.6
3	G	192	ARG	4.5
3	G	164	ASP	4.4
3	G	165	VAL	4.3
3	G	204	VAL	4.3
3	C	204	VAL	4.3
3	G	203	ALA	4.1
3	G	232	THR	4.1
3	C	228	TYR	4.1
1	A	189	LEU	4.0
2	L	189	LYS	4.1
2	B	152	SER	4.0
3	C	237	VAL	3.9
3	C	225	GLU	3.9
1	A	201	LYS	3.9
1	A	150	VAL	3.9
2	L	150	ALA	3.8
1	A	205	THR	3.8
3	C	238	THR	3.8
3	C	192	ARG	3.8
1	A	185	PRO	3.8
3	G	166	LYS	3.7
3	G	177	TYR	3.7
3	C	211	LYS	3.6
1	A	151	THR	3.6
1	A	196	CYS	3.6
1	A	184	VAL	3.6
1	A	210	LYS	3.6
1	A	157	GLY	3.6
1	A	152	VAL	3.5
3	C	229	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	THR	3.4
3	C	210	ALA	3.4
1	A	162	GLY	3.3
3	C	226	TRP	3.4
1	A	211	VAL	3.3
3	G	120	THR	3.3
3	C	212	VAL	3.3
1	A	202	PRO	3.2
1	A	182	VAL	3.2
3	G	216	TYR	3.2
2	B	189	LYS	3.1
2	B	153	SER	3.1
3	G	178	ASP	3.1
1	H	100(A)	TYR	3.1
3	C	236	THR	3.0
1	A	123	PRO	3.0
1	A	207	VAL	3.0
3	C	123	LEU	3.0
2	B	150	ALA	2.9
1	H	127	SER	2.9
3	C	235	PHE	2.9
3	G	218	ASN	2.9
2	B	126	GLN	2.9
1	A	183	THR	2.9
1	A	199	ASN	2.8
3	C	239	GLU	2.8
1	H	191	THR	2.8
3	G	214	LYS	2.8
3	G	132	THR	2.8
3	G	163	THR	2.8
1	A	206	LYS	2.8
3	C	208	THR	2.8
1	A	65	GLY	2.7
3	G	227	THR	2.7
1	A	155	ASN	2.7
3	G	207	ALA	2.7
3	C	201	THR	2.6
3	G	155	LYS	2.6
3	C	209	ALA	2.6
3	G	228	TYR	2.6
3	C	214	LYS	2.6
1	A	203	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	202	GLU	2.5
3	G	231	ALA	2.4
1	A	186	SER	2.4
1	A	198	VAL	2.4
1	A	136	ALA	2.3
1	A	161	SER	2.3
2	L	187	SER	2.3
2	L	188	HIS	2.3
2	L	191	TYR	2.3
2	B	19	ILE	2.3
1	A	140	CYS	2.3
3	C	205	ASP	2.3
1	A	187	SER	2.2
3	C	177	TYR	2.2
1	H	188	SER	2.2
2	L	207	ALA	2.2
3	C	223	ASP	2.2
1	A	163	VAL	2.2
2	B	154	PRO	2.1
3	C	203	ALA	2.1
1	A	213	PRO	2.1
3	G	154	VAL	2.1
3	G	208	THR	2.1
1	A	197	ASN	2.1
3	G	213	PHE	2.1
1	A	114	ALA	2.1
2	B	140	TYR	2.0
3	G	230	ASP	2.0
1	A	113	SER	2.0
2	L	153	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	TYS	H	100(H)	16/17	0.89	0.11	30,36,91,100	0
1	TYS	H	100(G)	16/17	0.93	0.12	30,38,88,90	0
1	TYS	A	100(H)	16/17	0.93	0.11	24,34,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TYS	A	100(G)	16/17	0.93	0.11	27,32,75,76	0
1	PCA	H	2	8/9	0.96	0.09	30,39,48,54	0
1	PCA	A	2	8/9	0.97	0.11	19,24,33,33	0

6.3 Carbohydrates

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
4	MAN	E	7	11/12	0.81	0.23	74,80,87,88	0
4	MAN	D	7	11/12	0.86	0.16	52,68,75,80	0
4	NAG	E	2	14/15	0.91	0.10	28,36,45,53	0
4	BMA	D	3	11/12	0.93	0.08	25,34,42,52	0
4	NAG	D	2	14/15	0.93	0.09	24,31,43,44	0
4	BMA	E	3	11/12	0.94	0.08	31,43,53,60	0
4	NAG	E	1	14/15	0.95	0.09	28,34,43,50	0
4	MAN	E	6	11/12	0.95	0.10	23,27,40,43	0
4	MAN	D	5	11/12	0.96	0.09	20,23,26,27	0
4	MAN	E	4	11/12	0.97	0.13	25,28,33,37	0
4	MAN	E	5	11/12	0.97	0.12	22,26,32,36	0
4	MAN	D	6	11/12	0.97	0.12	21,25,38,54	0
4	NAG	D	1	14/15	0.98	0.09	26,32,41,43	0
4	MAN	D	4	11/12	0.98	0.09	21,25,28,28	0

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
6	BU3	L	213	6/6	0.81	0.14	34,44,58,60	0
7	NAG	G	573	14/15	0.87	0.15	39,46,53,59	0
5	SO4	B	214	5/5	0.88	0.10	67,79,95,103	0
7	NAG	C	573	14/15	0.92	0.08	31,38,47,51	0
5	SO4	B	216	5/5	0.92	0.20	59,62,77,88	0
5	SO4	B	215	5/5	0.93	0.22	40,57,71,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	L	214	5/5	0.94	0.22	78,83,90,96	0
5	SO4	H	226	5/5	0.94	0.15	76,80,89,94	0
6	BU3	B	213	6/6	0.95	0.11	34,44,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.