



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID : 3SDY
Title : Crystal Structure of Broadly Neutralizing Antibody CR8020 Bound to the Influenza A H3 Hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2011-06-09
Resolution : 2.85 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

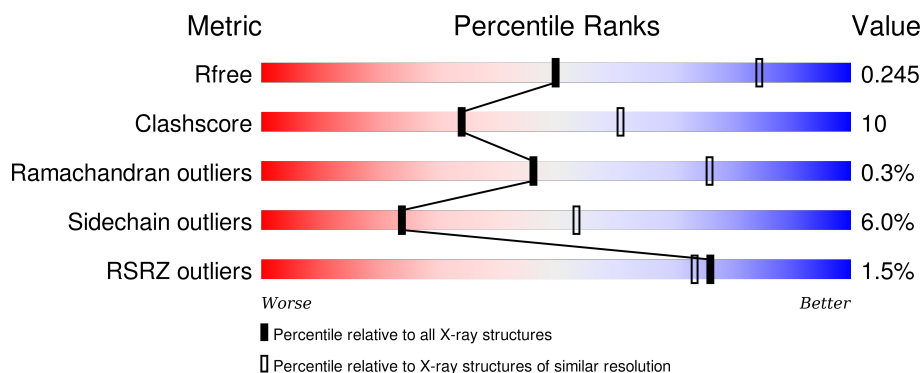
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	323	<div> <div>2%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
2	B	176	<div> <div>78%</div> <div>18%</div> <div>..</div> </div>
3	H	227	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>
4	L	216	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	FUC	A	606	X	-	-	-
8	FUC	B	206	X	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14620 atoms, of which 7155 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	319	4868	1542	2407	433	473	13	2407	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
A	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
A	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
A	10	GLY	-	EXPRESSION TAG	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	172	2696	863	1305	243	279	6	1305	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Antibody CR8020, Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	221	3286	1056	1617	276	330	7	1617	0	0

- Molecule 4 is a protein called Antibody CR8020, Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	215	Total	C	H	N	O	S	1609	0	0
			3255	1026	1609	285	328	7			

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	4	Total	C	H	N	O		43	0
			93	28	43	2	20			
5	A	4	Total	C	H	N	O		43	0
			93	28	43	2	20			

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	6	Total	C	H	N	O		62	0
			133	40	62	2	29			

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	2	Total	C	H	N	O		25	0
			53	16	25	2	10			

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	4	Total	C	H	N	O		44	0
			93	28	44	2	19			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

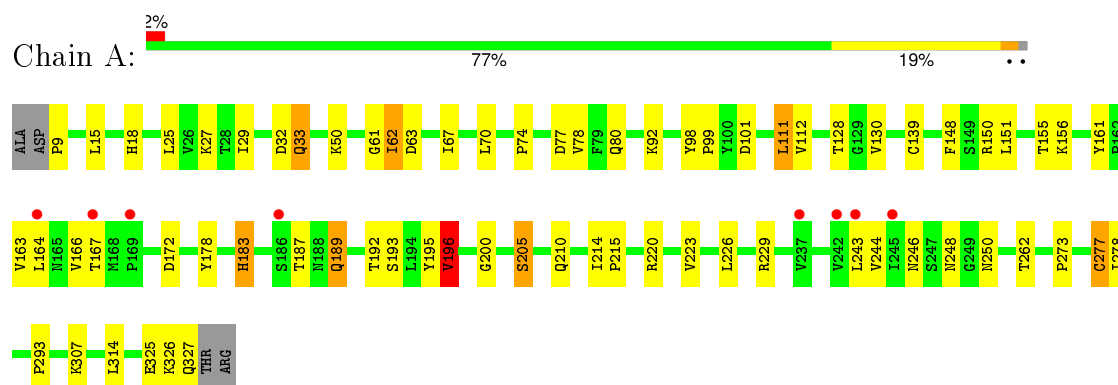


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total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

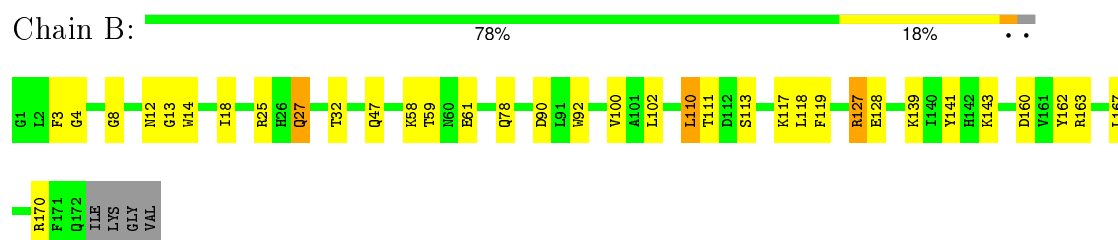
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

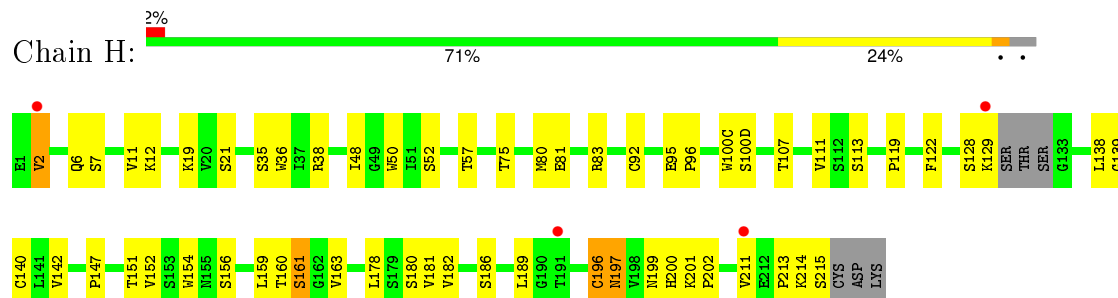
- Molecule 1: Hemagglutinin HA1 chain



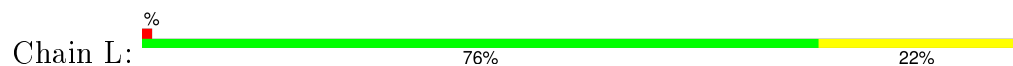
- Molecule 2: Hemagglutinin HA2 chain

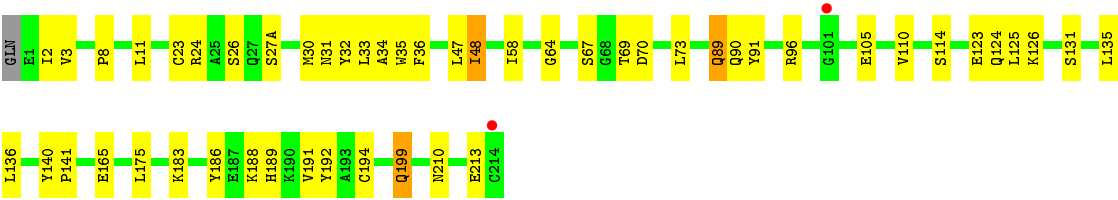


- Molecule 3: Antibody CR8020, Heavy Chain



- Molecule 4: Antibody CR8020, Light Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	197.75Å 197.75Å 197.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 2.85 46.61 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.1 (46.61-2.85) 99.3 (46.61-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.202 , 0.235 0.211 , 0.245	Depositor DCC
R_{free} test set	3035 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.3	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 59904 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14620	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, FUC, 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	0.28	0/2518	0.50	0/3430
2	B	0.32	0/1415	0.49	0/1902
3	H	0.28	0/1705	0.50	0/2329
4	L	0.30	0/1680	0.52	0/2278
All	All	0.29	0/7318	0.50	0/9939

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
6	A	1	0
8	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	606	FUC	C1
8	B	206	FUC	C1

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	A	2461	2407	2411	56	0
2	B	1391	1305	1306	27	0
3	H	1669	1617	1618	38	0
4	L	1646	1609	1612	37	0
5	A	100	86	86	4	0
6	A	71	62	61	3	0
7	A	28	25	25	0	0
8	B	49	44	43	0	0
9	A	5	0	0	0	0
9	B	15	0	0	1	0
9	L	30	0	0	0	0
All	All	7465	7155	7162	148	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 10.

All (148) 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:L:210:ASN:HB2	4:L:213:GLU:HG3	1.59	0.85
3:H:138:LEU:HD13	3:H:211:VAL:HG21	1.63	0.81
1:A:195:TYR:O	1:A:196:VAL:HG23	1.84	0.78
1:A:220:ARG:HD2	1:A:229:ARG:HG3	1.69	0.74
3:H:35:SER:HB2	3:H:95:GLU:HG3	1.75	0.69
1:A:111:LEU:HD12	1:A:112:VAL:N	2.10	0.66
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.76	0.66
4:L:47:LEU:HA	4:L:58:ILE:CD1	2.27	0.64
1:A:130:VAL:HG23	1:A:155:THR:O	1.99	0.62
1:A:325:GLU:HG2	2:B:13:GLY:O	2.00	0.62
3:H:163:VAL:HG22	3:H:182:VAL:HG22	1.82	0.62
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.83	0.61
1:A:25:LEU:HB3	1:A:33:GLN:HG3	1.82	0.60
3:H:181:VAL:HG11	4:L:135:LEU:CD2	2.32	0.60
4:L:32:TYR:HB3	4:L:91:TYR:CE1	2.36	0.60
6:A:601:NAG:H61	6:A:602:NAG:C7	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:246:ASN:HA	2.03	0.58
4:L:24:ARG:NH1	4:L:70:ASP:HB2	2.18	0.58
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.85	0.58
1:A:25:LEU:HD13	1:A:33:GLN:HG2	1.86	0.57
3:H:201:LYS:N	3:H:202:PRO:HD2	2.21	0.56
4:L:8:PRO:HG2	4:L:11:LEU:CD2	2.36	0.55
4:L:125:LEU:O	4:L:183:LYS:CE	2.54	0.55
1:A:25:LEU:HD13	1:A:33:GLN:CG	2.37	0.55
4:L:188:LYS:HE3	4:L:189:HIS:CE1	2.42	0.55
3:H:6:GLN:HB3	3:H:107:THR:HG23	1.89	0.55
1:A:155:THR:HG22	1:A:156:LYS:H	1.72	0.54
3:H:178:LEU:HD12	3:H:178:LEU:C	2.28	0.54
2:B:58:LYS:HG3	9:B:177:SO4:O3	2.06	0.54
1:A:223:VAL:HG22	1:A:229:ARG:NH1	2.23	0.54
3:H:200:HIS:CE1	3:H:202:PRO:HG2	2.43	0.53
1:A:326:LYS:O	1:A:327:GLN:CB	2.55	0.53
3:H:7:SER:O	3:H:107:THR:CG2	2.57	0.53
1:A:98:TYR:CE2	1:A:226:LEU:HD13	2.44	0.53
1:A:277:CYS:SG	1:A:278:ILE:N	2.82	0.53
1:A:214:ILE:N	1:A:214:ILE:HD12	2.24	0.52
1:A:111:LEU:HD12	1:A:111:LEU:C	2.30	0.52
5:A:701:NAG:H61	5:A:702:NAG:HN2	1.74	0.52
3:H:38:ARG:HB3	3:H:48:ILE:HD11	1.91	0.52
3:H:156:SER:H	3:H:197:ASN:HD21	1.58	0.52
1:A:50:LYS:HB3	1:A:273:PRO:HG2	1.92	0.52
3:H:35:SER:CB	3:H:95:GLU:HG3	2.39	0.51
3:H:36:TRP:CE2	3:H:80:MET:HB2	2.45	0.51
1:A:205:SER:HB3	1:A:210:GLN:HG3	1.92	0.51
1:A:307:LYS:HD3	2:B:61:GLU:HB2	1.91	0.51
4:L:32:TYR:HB3	4:L:91:TYR:CD1	2.46	0.51
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.45	0.50
2:B:3:PHE:CE1	2:B:113:SER:HB2	2.46	0.50
1:A:314:LEU:HB3	2:B:100:VAL:HG21	1.94	0.50
4:L:191:VAL:HG22	4:L:210:ASN:ND2	2.26	0.50
3:H:6:GLN:HB3	3:H:107:THR:CG2	2.41	0.50
4:L:188:LYS:HE3	4:L:189:HIS:NE2	2.27	0.49
1:A:9:PRO:HB3	2:B:143:LYS:NZ	2.27	0.49
1:A:192:THR:HA	1:A:196:VAL:O	2.12	0.49
1:A:195:TYR:CE2	1:A:250:ASN:HA	2.46	0.49
2:B:14:TRP:CH2	2:B:25:ARG:HG3	2.48	0.49
1:A:148:PHE:HB2	1:A:151:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:90:GLN:CD	4:L:90:GLN:O	2.51	0.49
4:L:191:VAL:HG22	4:L:210:ASN:HD22	1.78	0.49
2:B:47:GLN:CD	2:B:110:LEU:HD11	2.34	0.49
1:A:161:TYR:H	1:A:196:VAL:HG21	1.78	0.48
3:H:181:VAL:HG11	4:L:135:LEU:HD21	1.94	0.48
3:H:50:TRP:CH2	3:H:52:SER:HB2	2.48	0.48
1:A:220:ARG:HH11	1:A:229:ARG:HG3	1.78	0.48
3:H:181:VAL:HG11	4:L:135:LEU:HD22	1.94	0.48
1:A:326:LYS:O	1:A:327:GLN:HG3	2.14	0.47
3:H:159:LEU:HD21	3:H:182:VAL:HG11	1.95	0.47
4:L:31:ASN:HD21	4:L:67:SER:HB2	1.79	0.47
1:A:326:LYS:O	1:A:327:GLN:HB2	2.13	0.47
4:L:125:LEU:O	4:L:183:LYS:HE2	2.15	0.47
3:H:151:THR:HB	3:H:199:ASN:HB3	1.96	0.47
3:H:11:VAL:HG21	3:H:147:PRO:HG3	1.97	0.47
1:A:15:LEU:HD21	2:B:118:LEU:HG	1.97	0.47
1:A:15:LEU:CD2	2:B:119:PHE:HA	2.45	0.46
1:A:187:THR:HB	1:A:189:GLN:HE21	1.80	0.46
3:H:186:SER:O	3:H:189:LEU:CB	2.63	0.46
3:H:7:SER:O	3:H:107:THR:HG22	2.15	0.46
2:B:163:ARG:HG2	2:B:167:LEU:HD12	1.97	0.46
3:H:186:SER:O	3:H:189:LEU:HB3	2.16	0.46
4:L:110:VAL:HG21	4:L:199:GLN:HE22	1.81	0.46
1:A:130:VAL:CG2	1:A:155:THR:O	2.64	0.46
1:A:293:PRO:HA	2:B:59:THR:HG21	1.98	0.46
3:H:83:ARG:O	3:H:111:VAL:HG11	2.16	0.46
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.15	0.45
4:L:123:GLU:O	4:L:126:LYS:HB2	2.16	0.45
1:A:99:PRO:HB3	1:A:223:VAL:CG2	2.46	0.45
2:B:18:ILE:HD11	3:H:100(C):TRP:CE3	2.52	0.45
3:H:213:PRO:O	3:H:214:LYS:HB3	2.17	0.45
1:A:61:GLY:C	1:A:62:ILE:HG12	2.36	0.45
4:L:8:PRO:HG2	4:L:11:LEU:HD23	1.99	0.44
1:A:9:PRO:HB3	2:B:143:LYS:HZ3	1.81	0.44
5:A:702:NAG:H61	5:A:703:BMA:H2	1.98	0.44
4:L:135:LEU:HD12	4:L:136:LEU:N	2.33	0.44
5:A:702:NAG:H62	5:A:703:BMA:O2	2.18	0.44
1:A:220:ARG:NH1	1:A:229:ARG:HB2	2.33	0.44
3:H:12:LYS:O	3:H:111:VAL:HA	2.18	0.44
3:H:122:PHE:CE2	4:L:124:GLN:HG3	2.53	0.44
1:A:326:LYS:O	1:A:327:GLN:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:502:NAG:O3	5:A:505:MAN:H5	2.18	0.44
1:A:74:PRO:HD3	1:A:139:CYS:SG	2.57	0.44
2:B:162:TYR:CD2	2:B:162:TYR:N	2.86	0.44
3:H:100(D):SER:OG	4:L:89:GLN:NE2	2.51	0.43
1:A:77:ASP:O	1:A:80:GLN:HG3	2.18	0.43
4:L:175:LEU:C	4:L:175:LEU:HD23	2.38	0.43
1:A:27:LYS:HG2	1:A:32:ASP:O	2.18	0.43
1:A:187:THR:HB	1:A:189:GLN:HG2	2.00	0.43
1:A:189:GLN:O	1:A:193:SER:CB	2.67	0.43
4:L:47:LEU:HA	4:L:58:ILE:HD13	2.00	0.43
3:H:119:PRO:HB2	3:H:142:VAL:HG13	2.01	0.43
3:H:160:THR:HG22	3:H:161:SER:N	2.33	0.43
3:H:19:LYS:HG3	3:H:81:GLU:HB2	2.01	0.43
3:H:95:GLU:HB3	3:H:96:PRO:HD2	2.00	0.43
4:L:48:ILE:HD12	4:L:64:GLY:N	2.33	0.43
2:B:127:ARG:HB3	2:B:128:GLU:H	1.60	0.42
4:L:3:VAL:HB	4:L:26:SER:HB3	2.01	0.42
3:H:138:LEU:HD12	3:H:139:GLY:N	2.34	0.42
2:B:4:GLY:O	2:B:8:GLY:HA3	2.19	0.42
1:A:74:PRO:CD	1:A:139:CYS:SG	3.07	0.42
4:L:140:TYR:CG	4:L:141:PRO:HA	2.54	0.42
4:L:140:TYR:C	4:L:140:TYR:CD1	2.92	0.42
1:A:195:TYR:O	1:A:196:VAL:CG2	2.62	0.42
1:A:163:VAL:CG2	1:A:248:ASN:HD22	2.31	0.42
4:L:8:PRO:HG2	4:L:11:LEU:HD21	2.01	0.42
2:B:113:SER:O	2:B:117:LYS:HG3	2.20	0.42
4:L:36:PHE:HE2	4:L:89:GLN:HG2	1.85	0.42
3:H:152:VAL:HG11	3:H:180:SER:CB	2.50	0.42
2:B:141:TYR:CD1	2:B:170:ARG:HG2	2.55	0.42
4:L:186:TYR:O	4:L:192:TYR:OH	2.38	0.42
4:L:34:ALA:HA	4:L:48:ILE:O	2.20	0.41
3:H:2:VAL:O	3:H:2:VAL:HG12	2.20	0.41
4:L:140:TYR:CD1	4:L:141:PRO:N	2.88	0.41
1:A:67:ILE:O	1:A:70:LEU:HB3	2.19	0.41
1:A:183:HIS:CD2	1:A:195:TYR:OH	2.72	0.41
1:A:307:LYS:HE2	2:B:92:TRP:CZ2	2.54	0.41
4:L:23:CYS:HB2	4:L:35:TRP:CH2	2.56	0.41
3:H:128:SER:O	3:H:129:LYS:C	2.59	0.41
2:B:27:GLN:HB2	2:B:32:THR:HG22	2.02	0.41
6:A:601:NAG:H61	6:A:602:NAG:H82	2.03	0.41
2:B:58:LYS:O	2:B:58:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:HA	2:B:32:THR:HG22	2.03	0.41
1:A:200:GLY:O	1:A:215:PRO:HD2	2.20	0.41
2:B:110:LEU:HD23	2:B:111:THR:N	2.35	0.41
1:A:80:GLN:HB3	1:A:150:ARG:NH2	2.36	0.41
1:A:178:TYR:CD1	1:A:243:LEU:HD22	2.56	0.41
6:A:601:NAG:C6	6:A:602:NAG:H82	2.52	0.40
3:H:154:TRP:CZ3	3:H:196:CYS:HB3	2.56	0.40
4:L:30:MET:HG2	4:L:32:TYR:CZ	2.56	0.40
2:B:139:LYS:HD3	2:B:141:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/323 (98%)	310 (98%)	5 (2%)	2 (1%)	30	63
2	B	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
3	H	217/227 (96%)	206 (95%)	10 (5%)	1 (0%)	34	67
4	L	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
All	All	917/942 (97%)	888 (97%)	26 (3%)	3 (0%)	46	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	62	ILE
3	H	2	VAL

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	280/283 (99%)	262 (94%)	18 (6%)	22	50
2	B	146/149 (98%)	139 (95%)	7 (5%)	31	65
3	H	186/192 (97%)	176 (95%)	10 (5%)	27	59
4	L	184/185 (100%)	171 (93%)	13 (7%)	18	44
All	All	796/809 (98%)	748 (94%)	48 (6%)	24	53

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	33	GLN
1	A	63	ASP
1	A	78	VAL
1	A	92	LYS
1	A	101	ASP
1	A	111	LEU
1	A	128	THR
1	A	166	VAL
1	A	167	THR
1	A	172	ASP
1	A	183	HIS
1	A	189	GLN
1	A	196	VAL
1	A	205	SER
1	A	244	VAL
1	A	262	THR
1	A	277	CYS
2	B	12	ASN
2	B	27	GLN
2	B	78	GLN
2	B	90	ASP
2	B	110	LEU
2	B	127	ARG

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Mol	Chain	Res	Type
2	B	160	ASP
3	H	21	SER
3	H	57	THR
3	H	75	THR
3	H	92	CYS
3	H	113	SER
3	H	140	CYS
3	H	161	SER
3	H	196	CYS
3	H	197	ASN
3	H	215	SER
4	L	2	ILE
4	L	27(A)	SER
4	L	33	LEU
4	L	48	ILE
4	L	69	THR
4	L	89	GLN
4	L	96	ARG
4	L	105	GLU
4	L	114	SER
4	L	131	SER
4	L	165	GLU
4	L	194	CYS
4	L	199	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	54	ASN
1	A	137	ASN
1	A	183	HIS
1	A	189	GLN
1	A	210	GLN
2	B	26	HIS
2	B	78	GLN
2	B	125	GLN
2	B	168	ASN
2	B	172	GLN
3	H	164	HIS
3	H	197	ASN
4	L	89	GLN

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Mol	Chain	Res	Type
4	L	138	ASN
4	L	155	GLN
4	L	199	GLN
4	L	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	H	1	3	7,8,9	1.95	2 (28%)	9,10,12	1.96	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
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	PCA	CA-N	3.26	1.50	1.46
3	H	1	PCA	CD-N	3.87	1.46	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	PCA	CA-N-CD	-3.09	103.45	113.81
3	H	1	PCA	OE-CD-CG	-2.42	121.41	126.81
3	H	1	PCA	CB-CA-C	-2.33	109.57	112.76
3	H	1	PCA	CB-CA-N	2.34	110.03	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

20 carbohydrates 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	NAG	A	501	1,5	14,14,15	0.52	0	15,19,21	1.70	1 (6%)
5	NAG	A	502	5	14,14,15	0.39	0	15,19,21	0.81	0
5	BMA	A	503	5	11,11,12	0.60	0	14,15,17	0.98	2 (14%)
5	MAN	A	505	5	11,11,12	0.59	0	14,15,17	0.96	1 (7%)
6	NAG	A	601	1,6	14,14,15	0.48	0	15,19,21	0.76	0
6	NAG	A	602	6	14,14,15	0.51	0	15,19,21	0.71	0
6	BMA	A	603	6	11,11,12	0.58	0	14,15,17	0.86	0
6	MAN	A	604	6	11,11,12	0.56	0	14,15,17	1.07	2 (14%)
6	MAN	A	605	6	11,11,12	0.57	0	14,15,17	0.95	1 (7%)
6	FUC	A	606	6	10,10,11	0.56	0	14,14,16	1.42	3 (21%)
5	NAG	A	701	1,5	14,14,15	0.52	0	15,19,21	1.16	1 (6%)
5	NAG	A	702	5	14,14,15	0.59	0	15,19,21	0.92	0
5	BMA	A	703	5	11,11,12	0.57	0	14,15,17	1.79	3 (21%)
5	MAN	A	704	5	11,11,12	0.60	0	14,15,17	0.86	0
7	NAG	A	801	1,7	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
7	NAG	A	802	7	14,14,15	0.43	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	201	8,2	14,14,15	0.32	0	15,19,21	2.23	4 (26%)
8	NAG	B	202	8	14,14,15	0.56	0	15,19,21	0.71	0
8	BMA	B	203	8	11,11,12	0.66	0	14,15,17	1.20	2 (14%)
8	FUC	B	206	8	10,10,11	0.88	1 (10%)	14,14,16	2.24	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	502	5	-	0/6/23/26	0/1/1/1
5	BMA	A	503	5	-	0/2/19/22	0/1/1/1
5	MAN	A	505	5	-	0/2/19/22	0/1/1/1
6	NAG	A	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	602	6	-	0/6/23/26	0/1/1/1
6	BMA	A	603	6	-	0/2/19/22	0/1/1/1
6	MAN	A	604	6	-	0/2/19/22	0/1/1/1
6	MAN	A	605	6	-	0/2/19/22	0/1/1/1
6	FUC	A	606	6	1/1/5/5	0/0/17/20	0/1/1/1
5	NAG	A	701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	702	5	-	0/6/23/26	0/1/1/1
5	BMA	A	703	5	-	0/2/19/22	0/1/1/1
5	MAN	A	704	5	-	0/2/19/22	0/1/1/1
7	NAG	A	801	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	802	7	-	0/6/23/26	0/1/1/1
8	NAG	B	201	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	202	8	-	0/6/23/26	0/1/1/1
8	BMA	B	203	8	-	0/2/19/22	0/1/1/1
8	FUC	B	206	8	1/1/5/5	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	206	FUC	O5-C1	-2.01	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	206	FUC	C1-C2-C3	-5.15	103.45	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	206	FUC	C1-O5-C5	-3.68	106.69	112.38
8	B	201	NAG	C4-C3-C2	-3.24	106.19	111.23
5	A	703	BMA	O3-C3-C2	-2.93	104.70	110.00
6	A	606	FUC	C1-C2-C3	-2.20	106.94	109.54
8	B	201	NAG	C6-C5-C4	-2.20	107.59	113.02
8	B	206	FUC	C2-C3-C4	-2.05	107.55	111.04
8	B	201	NAG	C3-C4-C5	2.01	113.70	110.20
5	A	505	MAN	O5-C5-C6	2.04	111.76	107.35
6	A	604	MAN	C1-O5-C5	2.10	114.91	112.25
5	A	503	BMA	O5-C5-C6	2.10	111.90	107.35
7	A	801	NAG	C1-O5-C5	2.10	114.92	112.25
8	B	206	FUC	O5-C5-C4	2.11	113.18	109.53
6	A	604	MAN	C1-C2-C3	2.19	112.13	109.54
6	A	606	FUC	O5-C5-C6	2.20	109.77	106.13
5	A	703	BMA	O5-C5-C6	2.22	112.16	107.35
8	B	203	BMA	O5-C5-C6	2.39	112.53	107.35
8	B	206	FUC	O2-C2-C1	2.40	114.01	109.21
6	A	605	MAN	O5-C5-C6	2.41	112.56	107.35
7	A	802	NAG	C1-O5-C5	2.56	115.49	112.25
5	A	503	BMA	C1-C2-C3	2.69	112.73	109.54
6	A	606	FUC	O5-C1-C2	2.74	115.30	110.86
8	B	206	FUC	C3-C4-C5	3.03	114.83	109.72
5	A	701	NAG	C1-O5-C5	3.18	116.28	112.25
8	B	203	BMA	C1-C2-C3	3.49	113.67	109.54
5	A	703	BMA	C1-C2-C3	5.15	115.63	109.54
5	A	501	NAG	C1-O5-C5	5.99	119.86	112.25
8	B	201	NAG	C1-O5-C5	6.58	120.60	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	206	FUC	C1
6	A	606	FUC	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	NAG	1	0
5	A	505	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	3	0
6	A	602	NAG	3	0
5	A	701	NAG	1	0
5	A	702	NAG	3	0
5	A	703	BMA	2	0

5.6 Ligand geometry [i](#)

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	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.20	0
9	SO4	B	177	-	4,4,4	0.24	0	6,6,6	0.11	0
9	SO4	B	178	-	4,4,4	0.25	0	6,6,6	0.22	0
9	SO4	B	179	-	4,4,4	0.22	0	6,6,6	0.08	0
9	SO4	L	215	-	4,4,4	0.22	0	6,6,6	0.18	0
9	SO4	L	216	-	4,4,4	0.23	0	6,6,6	0.10	0
9	SO4	L	217	-	4,4,4	0.21	0	6,6,6	0.08	0
9	SO4	L	218	-	4,4,4	0.22	0	6,6,6	0.11	0
9	SO4	L	219	-	4,4,4	0.20	0	6,6,6	0.14	0
9	SO4	L	220	-	4,4,4	0.22	0	6,6,6	0.10	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
9	SO4	B	177	-	-	0/0/0/0	0/0/0/0
9	SO4	B	178	-	-	0/0/0/0	0/0/0/0
9	SO4	B	179	-	-	0/0/0/0	0/0/0/0
9	SO4	L	215	-	-	0/0/0/0	0/0/0/0
9	SO4	L	216	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	L	217	-	-	0/0/0/0	0/0/0/0
9	SO4	L	218	-	-	0/0/0/0	0/0/0/0
9	SO4	L	219	-	-	0/0/0/0	0/0/0/0
9	SO4	L	220	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	177	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 [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	A	319/323 (98%)	-0.03	8 (2%) 61 56	55, 108, 165, 189	0
2	B	172/176 (97%)	-0.10	0 100 100	49, 77, 126, 160	0
3	H	220/227 (96%)	0.01	4 (1%) 71 68	63, 97, 150, 184	0
4	L	215/216 (99%)	-0.11	2 (0%) 85 84	64, 88, 121, 171	0
All	All	926/942 (98%)	-0.05	14 (1%) 76 73	49, 92, 153, 189	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	214	CYS	3.9
3	H	129	LYS	3.8
1	A	245	ILE	3.7
1	A	186	SER	2.6
1	A	167	THR	2.4
3	H	211	VAL	2.4
1	A	243	LEU	2.4
1	A	164	LEU	2.3
1	A	169	PRO	2.2
1	A	242	VAL	2.2
3	H	191	THR	2.1
3	H	2	VAL	2.1
4	L	101	GLY	2.0
1	A	237	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PCA	H	1	8/9	0.77	0.34	-	140,152,171,171	5

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
8	FUC	B	206	10/11	0.92	0.27	5.04	9,9,133,160	11
5	NAG	A	702	14/15	0.88	0.38	1.37	164,171,177,185	12
5	NAG	A	501	14/15	0.80	0.20	0.38	121,155,178,194	12
8	NAG	B	201	14/15	0.94	0.13	-0.58	89,121,136,148	11
6	NAG	A	601	14/15	0.86	0.16	-0.64	110,122,138,143	11
6	BMA	A	603	11/12	0.90	0.18	-0.97	110,122,137,142	8
6	MAN	A	604	11/12	0.95	0.17	-0.97	93,114,127,142	10
7	NAG	A	801	14/15	0.95	0.13	-1.03	90,107,119,137	12
5	NAG	A	701	14/15	0.90	0.14	-2.19	153,169,175,176	12
6	NAG	A	602	14/15	0.93	0.14	-	111,122,135,137	12
8	BMA	B	203	11/12	0.57	0.42	-	181,194,205,213	10
5	MAN	A	505	11/12	0.60	0.30	-	177,196,206,209	10
8	NAG	B	202	14/15	0.86	0.23	-	118,156,178,194	12
6	FUC	A	606	10/11	0.94	0.12	-	9,9,131,135	11
5	MAN	A	704	11/12	0.74	0.34	-	215,230,238,239	10
5	NAG	A	502	14/15	0.75	0.41	-	130,161,175,185	12
5	BMA	A	703	11/12	0.82	0.32	-	186,191,204,216	9
5	BMA	A	503	11/12	0.20	0.37	-	184,202,216,217	9
6	MAN	A	605	11/12	0.89	0.28	-	130,145,154,156	10
7	NAG	A	802	14/15	0.84	0.14	-	115,144,159,167	13

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
9	SO4	L	216	5/5	0.93	0.23	-0.20	150,151,161,164	0
9	SO4	B	178	5/5	0.98	0.12	-2.13	96,113,118,118	0
9	SO4	L	215	5/5	0.92	0.18	-	118,132,139,139	0
9	SO4	L	220	5/5	0.90	0.19	-	162,163,166,168	0
9	SO4	B	177	5/5	0.90	0.15	-	153,163,171,174	0
9	SO4	A	1	5/5	0.95	0.14	-	111,117,124,124	0
9	SO4	B	179	5/5	0.75	0.24	-	210,213,214,214	0
9	SO4	L	217	5/5	0.93	0.20	-	145,153,158,164	0
9	SO4	L	219	5/5	0.77	0.18	-	142,162,169,174	0
9	SO4	L	218	5/5	0.91	0.19	-	147,159,164,175	0

6.5 Other polymers [i](#)

There are no such residues in this entry.