



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:59 PM GMT

PDB ID : 4IRZ
Title : Crystal structure of A4b7 headpiece complexed with Fab Natalizumab
Authors : Yu, Y.; Schurpf, T.; Springer, T.A.
Deposited on : 2013-01-15
Resolution : 2.84 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

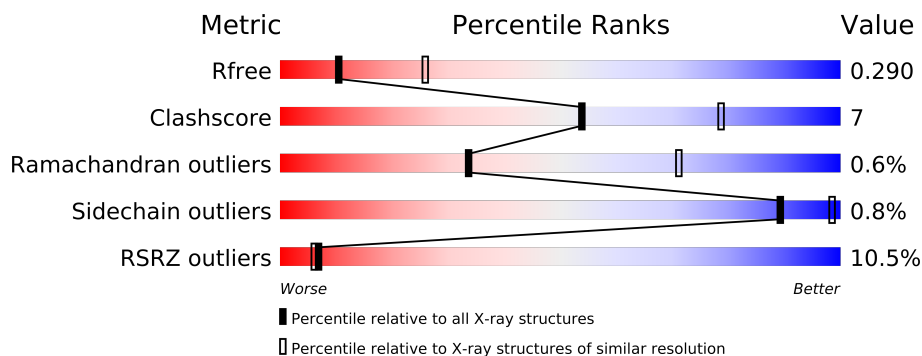
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2270 (2.88-2.80)
Clashscore	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)
RSRZ outliers	66119	2274 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	597	
2	L	210	
3	H	222	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	3105	-	X
7	PEG	A	611	-	X
8	NDS	A	612	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15763 atoms, of which 7752 are hydrogens and 0 are deuterium.

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 (with D amino acids) called Integrin alpha4 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	592	Total	C	H	N	O	S	38	3	0
			9051	2896	4454	794	884	23			

- Molecule 2 is a protein (with D amino acids) called Fab Natalizumab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	208	Total	C	H	N	O	S	0	0	0
			3192	1017	1571	273	325	6			

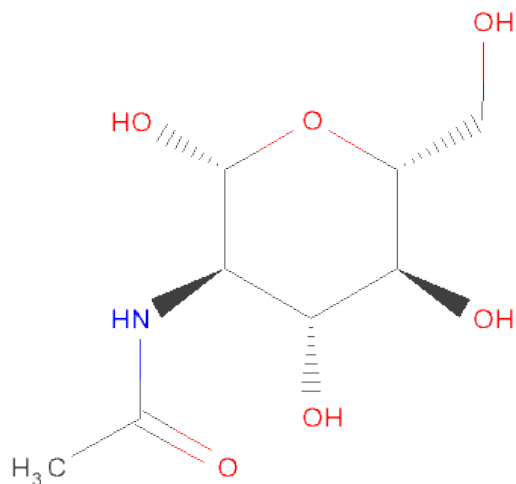
- Molecule 3 is a protein (with D amino acids) called Fab Natalizumab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	217	Total	C	H	N	O	S	0	2	0
			3274	1048	1612	278	327	9			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

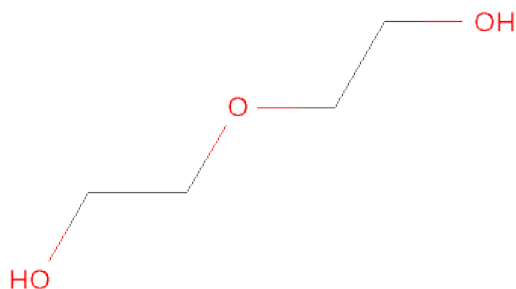


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

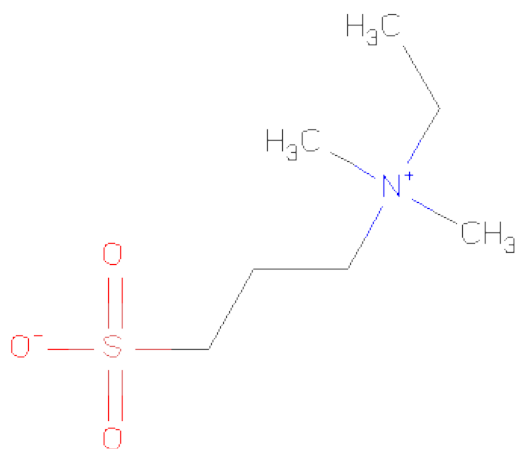
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is ETHYL DIMETHYL AMMONIO PROPANE SULFONATE (three-letter code: NDS) (formula: $C_7H_{17}NO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	S	0	0
			29	7	17	1	3	1		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total 1	Na 1	0	0

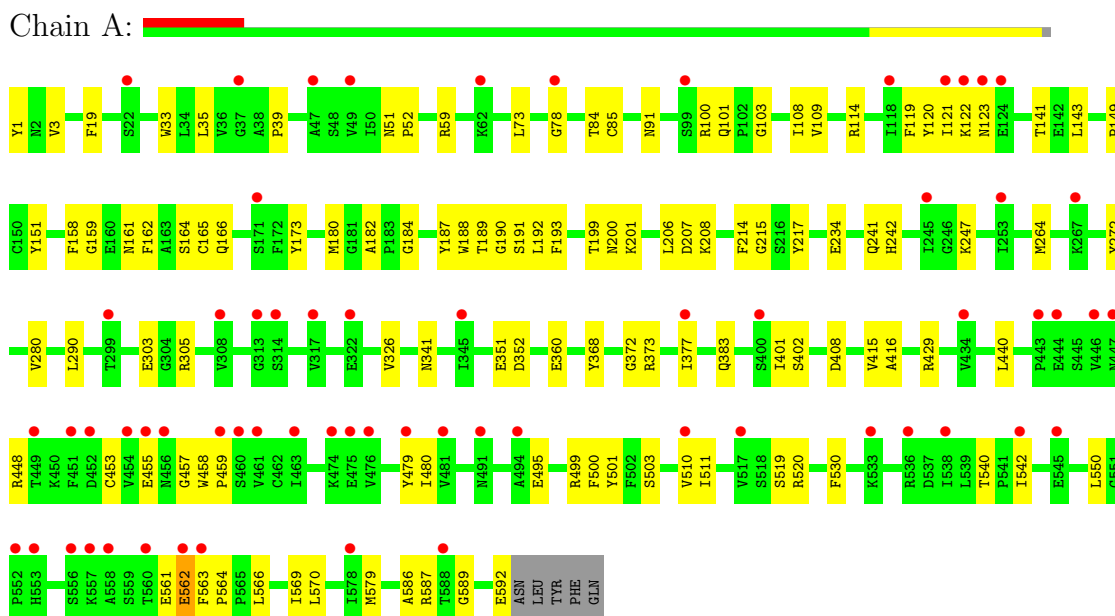
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	9	Total 9	O 9	0	0
10	L	4	Total 4	O 4	0	0

3 Residue-property plots

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: Integrin alpha4 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.61Å 77.89Å 217.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 2.84 44.62 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.62-2.84) 99.7 (44.62-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.237 , 0.287 0.239 , 0.290	Depositor DCC
R_{free} test set	1535 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 30297 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15763	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, NA, CA, NDS, PEG

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	0.23	0/4698	0.40	0/6361
2	L	0.23	0/1658	0.40	0/2253
3	H	0.23	0/1702	0.39	0/2317
All	All	0.23	0/8058	0.40	0/10931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4597	4454	0	68	1
2	L	1621	1571	0	25	0
3	H	1662	1612	0	20	0
4	A	3	0	0	0	0
5	A	56	54	0	0	0
6	A	39	34	0	0	0
7	A	7	10	0	0	0
8	A	12	17	0	0	0
9	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	9	0	0	2	0
10	L	4	0	0	0	0
All	All	8011	7752	0	108	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:169:ASP:OD2	2:L:171:THR:OG1	2.05	0.74
3:H:210:HIS:ND1	3:H:213:SER:OG	2.24	0.70
2:L:122:GLU:OE1	2:L:122:GLU:N	2.25	0.69
1:A:455:GLU:OE2	1:A:501:TYR:OH	2.14	0.66
1:A:499:ARG:NH2	1:A:540:THR:O	2.30	0.65
1:A:234:GLU:N	1:A:234:GLU:OE1	2.31	0.64
1:A:100:ARG:NH2	1:A:103:GLY:O	2.32	0.63
3:H:89:GLU:N	3:H:89:GLU:OE1	2.34	0.61
1:A:1:TYR:HA	1:A:383:GLN:HB2	1.88	0.56
1:A:114:ARG:NH1	1:A:166:GLN:OE1	2.40	0.55
2:L:83:ILE:CD1	2:L:165:GLN:HB2	2.36	0.55
1:A:440:LEU:HB2	1:A:579[A]:MET:SD	2.48	0.53
2:L:29:ILE:HD11	2:L:71:TYR:CE2	2.43	0.52
1:A:158:PHE:O	1:A:164:SER:OG	2.27	0.52
2:L:117:PHE:CE1	3:H:148:LEU:HA	2.45	0.52
1:A:448[B]:ARG:NH2	1:A:589:GLY:O	2.42	0.52
1:A:429:ARG:CZ	1:A:566:LEU:HD21	2.41	0.51
2:L:33:MET:HE3	2:L:88:CYS:HB2	1.92	0.51
1:A:373:ARG:NH2	10:A:705:HOH:O	2.45	0.50
1:A:201:LYS:NZ	3:H:30:LYS:O	2.45	0.50
3:H:211:LYS:N	3:H:212:PRO:CD	2.75	0.50
1:A:189:THR:HG22	1:A:214:PHE:HA	1.94	0.49
1:A:280:VAL:HG23	1:A:351:GLU:OE2	2.13	0.49
1:A:35:LEU:CD1	1:A:108:ILE:HD13	2.42	0.49
1:A:208:LYS:HE2	2:L:30:ASN:HB3	1.95	0.49
1:A:33:TRP:CZ3	1:A:59:ARG:HB2	2.48	0.48
1:A:550:LEU:HG	1:A:570:LEU:HG	1.95	0.48
2:L:39:THR:HG23	2:L:40:PRO:HD2	1.94	0.48
1:A:448[B]:ARG:HB2	1:A:448[B]:ARG:NH1	2.28	0.48
2:L:123:GLN:OE1	3:H:153:LYS:NZ	2.47	0.48
3:H:11:VAL:HB	3:H:157:PRO:HG3	1.94	0.48
1:A:264:MET:HE1	1:A:290:LEU:HD13	1.95	0.48
1:A:569:ILE:HG12	1:A:570:LEU:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:563:PHE:N	1:A:564:PRO:HD3	2.29	0.47
1:A:303:GLU:N	1:A:303:GLU:OE2	2.47	0.47
1:A:408:ASP:CG	10:A:703:HOH:O	2.52	0.47
2:L:80:PRO:HA	2:L:105:ILE:HD13	1.96	0.47
1:A:519:SER:O	1:A:520:ARG:HB2	2.13	0.47
3:H:33:TYR:HB2	3:H:99:GLU:HB3	1.97	0.47
2:L:83:ILE:O	2:L:84:ALA:HB2	2.15	0.47
1:A:561:GLU:HG2	1:A:562:GLU:N	2.30	0.47
3:H:48:MET:HE1	3:H:81:MET:CE	2.44	0.47
1:A:372:GLY:HA2	1:A:377:ILE:HG22	1.96	0.46
2:L:174:LEU:HD23	2:L:175:SER:N	2.30	0.46
1:A:184:GLY:HA2	1:A:188:TRP:CE3	2.51	0.46
1:A:119:PHE:O	1:A:120:TYR:HB2	2.15	0.46
1:A:143:LEU:HG	1:A:143:LEU:O	2.15	0.46
1:A:3:VAL:HG12	1:A:383:GLN:OE1	2.15	0.46
1:A:586:ALA:O	1:A:587:ARG:CB	2.64	0.45
2:L:141:ARG:NH2	2:L:162:VAL:HG21	2.31	0.45
1:A:161:ASN:HB3	3:H:104:ASN:O	2.16	0.45
1:A:199:THR:O	1:A:200:ASN:HB2	2.17	0.45
2:L:33:MET:CE	2:L:88:CYS:HB2	2.47	0.45
1:A:401:ILE:HG22	1:A:402:SER:N	2.32	0.45
2:L:130:SER:HA	2:L:178:LEU:O	2.17	0.45
1:A:85:CYS:HB2	1:A:151:TYR:OH	2.17	0.44
1:A:305:ARG:HD3	1:A:326:VAL:HG12	2.00	0.44
1:A:121:ILE:O	1:A:123:ASN:N	2.49	0.44
1:A:165:CYS:HB2	1:A:182:ALA:HB1	1.99	0.44
1:A:448[B]:ARG:CZ	1:A:448[B]:ARG:HB2	2.47	0.44
1:A:500:PHE:CE1	1:A:542:ILE:HG21	2.53	0.44
1:A:510:VAL:HG22	1:A:511:ILE:N	2.32	0.44
1:A:360:GLU:OE2	1:A:368:TYR:OH	2.36	0.44
1:A:429:ARG:NH2	1:A:566:LEU:HD21	2.32	0.44
3:H:81:MET:C	3:H:81:MET:SD	2.96	0.44
1:A:341:ASN:O	1:A:352:ASP:O	2.35	0.44
1:A:100:ARG:HG2	1:A:101:GLN:N	2.34	0.43
3:H:211:LYS:HB2	3:H:212:PRO:HD3	1.99	0.43
2:L:65:SER:OG	2:L:72:THR:OG1	2.36	0.43
1:A:503:SER:OG	1:A:530:PHE:CE2	2.71	0.43
3:H:64:PHE:O	3:H:65:GLN:C	2.57	0.43
1:A:182:ALA:O	1:A:190:GLY:HA2	2.18	0.43
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.00	0.43
1:A:51:ASN:N	1:A:52:PRO:CD	2.82	0.43
3:H:149:GLY:HA2	3:H:164:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:35:TRP:CE2	2:L:73:PHE:HB2	2.54	0.43
3:H:36:TRP:CE2	3:H:81:MET:HB2	2.53	0.43
1:A:415:VAL:HG12	1:A:416:ALA:N	2.34	0.43
1:A:519:SER:O	1:A:520:ARG:CB	2.67	0.43
1:A:215:GLY:O	1:A:241:GLN:HB2	2.19	0.42
2:L:148:LYS:NZ	2:L:194:GLU:OE2	2.50	0.42
1:A:480:ILE:CG1	1:A:550:LEU:HD22	2.49	0.42
3:H:158:GLU:CB	3:H:159:PRO:HA	2.49	0.42
1:A:108:ILE:HG22	1:A:109:VAL:N	2.35	0.42
2:L:80:PRO:HA	2:L:105:ILE:CD1	2.49	0.42
3:H:149:GLY:HA2	3:H:164:TRP:CH2	2.54	0.41
1:A:187:TYR:O	1:A:188:TRP:HB2	2.20	0.41
2:L:11:LEU:C	2:L:11:LEU:HD12	2.40	0.41
2:L:141:ARG:NH1	2:L:172:TYR:CE1	2.88	0.41
1:A:73:LEU:HD23	1:A:141:THR:HB	2.03	0.41
1:A:84:THR:O	1:A:84:THR:HG22	2.19	0.41
1:A:108:ILE:CG2	1:A:109:VAL:N	2.82	0.41
1:A:162:PHE:CD2	1:A:193:PHE:HZ	2.38	0.41
3:H:201:THR:OG1	3:H:202:LYS:N	2.54	0.41
1:A:191:SER:OG	1:A:192:LEU:N	2.54	0.41
1:A:242:HIS:CD2	1:A:247:LYS:HD2	2.56	0.41
1:A:206:LEU:O	1:A:208:LYS:N	2.54	0.41
2:L:39:THR:CG2	2:L:40:PRO:HD2	2.51	0.41
2:L:149:VAL:HG13	2:L:191:TYR:CZ	2.56	0.41
2:L:192:ALA:HA	2:L:206:LYS:O	2.21	0.41
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.56	0.40
1:A:242:HIS:CD2	1:A:247:LYS:HE3	2.56	0.40
1:A:51:ASN:O	1:A:91:ASN:HA	2.22	0.40
1:A:149:PRO:HG3	1:A:180:MET:HE1	2.04	0.40
3:H:99:GLU:HG2	3:H:108:TYR:HB3	2.03	0.40
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.56	0.40
1:A:457:GLY:O	1:A:459:PRO:HD3	2.21	0.40
1:A:495[B]:GLU:N	1:A:495[B]:GLU:OE1	2.53	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	Distance(Å)	Clash(Å)
1:A:217:TYR:OH	1:A:592:GLU:OE1[3_545]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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	$\# Z > 2$
6	NAG	A	3196	1,6	12,14,15	0.65	0	15,19,21	1.12	2 (13%)
6	NAG	A	3197	6	12,14,15	0.69	1 (8%)	15,19,21	0.86	1 (6%)
6	BMA	A	3198	6	10,11,12	0.81	1 (10%)	11,15,17	1.11	1 (9%)

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	3196	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	3197	6	-	0/6/23/26	0/1/1/1
6	BMA	A	3198	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3197	NAG	O5-C5	-2.09	1.41	1.45
6	A	3198	BMA	O5-C5	-2.02	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3198	BMA	O5-C5-C6	3.32	110.47	106.98
6	A	3197	NAG	O5-C5-C6	2.25	109.34	106.98
6	A	3196	NAG	O5-C5-C6	2.12	109.21	106.98
6	A	3196	NAG	C3-C4-C5	2.02	113.80	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	3046	1	12,14,15	0.69	1 (8%)	15,19,21	0.83	1 (6%)
5	NAG	A	3105	1	12,14,15	0.68	1 (8%)	15,19,21	0.79	1 (6%)
5	NAG	A	3485	1	12,14,15	0.68	1 (8%)	15,19,21	0.88	1 (6%)
5	NAG	A	3505	1	12,14,15	0.69	1 (8%)	15,19,21	0.81	1 (6%)
7	PEG	A	611	-	6,6,6	0.52	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NDS	A	612	-	11,11,11	0.99	0	16,16,16	1.85	2 (12%)

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	3046	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3105	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3485	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3505	1	-	0/6/23/26	0/1/1/1
7	PEG	A	611	-	-	0/4/4/4	0/0/0/0
8	NDS	A	612	-	-	0/11/11/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3505	NAG	O5-C5	-2.10	1.41	1.45
5	A	3105	NAG	O5-C5	-2.09	1.41	1.45
5	A	3046	NAG	O5-C5	-2.04	1.41	1.45
5	A	3485	NAG	O5-C5	-2.01	1.41	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	612	NDS	O2-S1-O1	-5.82	101.21	112.44
8	A	612	NDS	C3-C4-S1	-2.91	109.38	113.20
5	A	3485	NAG	O5-C5-C6	2.58	109.69	106.98
5	A	3046	NAG	O5-C5-C6	2.44	109.54	106.98
5	A	3105	NAG	O5-C5-C6	2.29	109.39	106.98
5	A	3505	NAG	O5-C5-C6	2.17	109.25	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	592/597 (99%)	0.67	64 (10%)	6 6	22, 56, 119, 207	8 (1%)
2	L	208/210 (99%)	0.82	32 (15%)	3 2	29, 67, 118, 176	0
3	H	217/222 (97%)	0.46	11 (5%)	27 28	31, 60, 116, 164	0
All	All	1017/1029 (98%)	0.66	107 (10%)	7 6	22, 58, 118, 207	8 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	195	VAL	6.7
1	A	449	THR	6.2
1	A	451	PHE	5.3
2	L	109	VAL	5.1
2	L	145	VAL	4.9
1	A	553	HIS	4.8
2	L	143	ALA	4.6
1	A	557	LYS	4.5
2	L	114	VAL	4.5
1	A	447	ASN	4.4
2	L	193	CYS	4.3
1	A	558	ALA	4.2
2	L	124	LEU	4.1
1	A	552	PRO	3.9
1	A	510	VAL	3.9
1	A	322	GLU	3.8
3	H	138	SER	3.8
2	L	200	LEU	3.8
1	A	533	LYS	3.7
1	A	118	ILE	3.6
3	H	136	PRO	3.6
1	A	560	THR	3.6
2	L	132	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	H	192	VAL	3.6
1	A	517	VAL	3.5
1	A	578	ILE	3.5
1	A	455	GLU	3.4
2	L	201	SER	3.3
2	L	196	THR	3.3
1	A	556	SER	3.3
2	L	180	LEU	3.2
1	A	443	PRO	3.2
1	A	124	GLU	3.2
1	A	171	SER	3.0
2	L	204	VAL	3.0
1	A	99	SER	3.0
1	A	78	GLY	3.0
1	A	536	ARG	3.0
1	A	22	SER	3.0
2	L	131	VAL	3.0
1	A	476	VAL	3.0
1	A	314	SER	2.9
1	A	123	ASN	2.9
1	A	538	ILE	2.8
1	A	452	ASP	2.8
1	A	463	ILE	2.7
2	L	19	VAL	2.7
1	A	479	TYR	2.7
2	L	198	GLN	2.7
3	H	221	VAL	2.7
1	A	456	ASN	2.7
2	L	197	HIS	2.6
2	L	190	VAL	2.6
1	A	345	ILE	2.6
2	L	147	TRP	2.6
2	L	108	THR	2.6
2	L	209	ASN	2.6
1	A	494	ALA	2.5
1	A	122	LYS	2.5
1	A	62	LYS	2.5
1	A	459	PRO	2.5
1	A	253	ILE	2.5
3	H	194	VAL	2.5
1	A	49	VAL	2.5
1	A	444	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	222	GLU	2.4
1	A	313	GLY	2.4
1	A	121	ILE	2.4
1	A	377	ILE	2.4
1	A	563	PHE	2.4
3	H	29	ILE	2.4
2	L	105	ILE	2.4
1	A	491	ASN	2.4
2	L	183	ALA	2.4
3	H	196	SER	2.4
1	A	454	VAL	2.3
2	L	134	LEU	2.3
1	A	308	VAL	2.3
1	A	461	VAL	2.3
1	A	542	ILE	2.2
1	A	317	VAL	2.2
1	A	434	VAL	2.2
1	A	545	GLU	2.2
2	L	206	LYS	2.2
2	L	103	VAL	2.2
1	A	562	GLU	2.2
1	A	400	SER	2.2
3	H	146	ALA	2.2
2	L	208	PHE	2.1
3	H	153	LYS	2.1
2	L	162	VAL	2.1
1	A	245	ILE	2.1
1	A	588	THR	2.1
2	L	205	THR	2.1
1	A	267	LYS	2.1
1	A	299	THR	2.0
1	A	474	LYS	2.0
1	A	475	GLU	2.0
1	A	481	VAL	2.0
2	L	144	LYS	2.0
1	A	37	GLY	2.0
1	A	460	SER	2.0
1	A	446	VAL	2.0
2	L	4	MET	2.0
2	L	159	GLN	2.0
1	A	47	ALA	2.0
3	H	193	THR	2.0

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

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	3197	14/15	0.27	2.22	98,116,135,140	0
6	NAG	A	3196	14/15	0.19	-0.54	48,59,78,79	0
6	BMA	A	3198	11/12	0.22	-	146,151,181,181	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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	NDS	A	612	12/12	0.54	4.22	59,76,94,94	0
7	PEG	A	611	7/7	0.39	2.41	55,66,71,73	17
5	NAG	A	3105	14/15	0.31	2.24	75,93,111,112	0
5	NAG	A	3485	14/15	0.34	1.16	55,67,77,80	28
5	NAG	A	3505	14/15	0.29	0.35	42,52,63,67	28
5	NAG	A	3046	14/15	0.18	-0.45	79,91,110,110	0
9	NA	H	301	1/1	0.16	-1.30	57,57,57,57	0
4	CA	A	2006	1/1	0.10	-1.38	57,57,57,57	0
4	CA	A	2005	1/1	0.08	-1.59	55,55,55,55	0
4	CA	A	2007	1/1	0.10	-2.26	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.