



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:00 PM GMT

PDB ID : 4WK2
Title : Metal Ion and Ligand Binding of Integrin
Authors : Xia, W.; Springer, T.A.
Deposited on : 2014-10-01
Resolution : 2.50 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

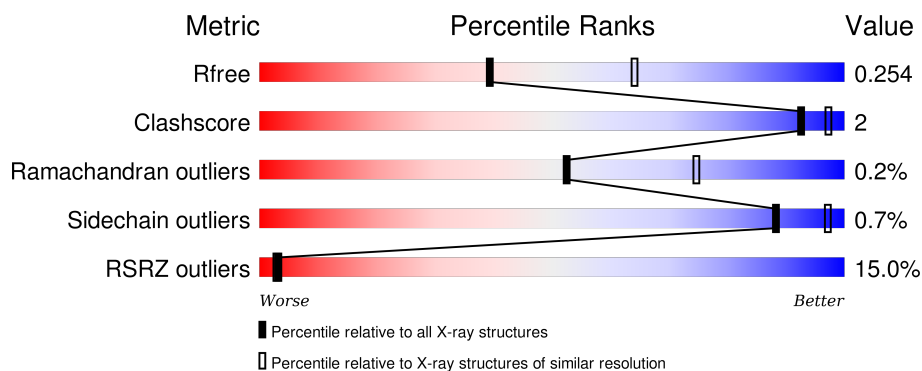
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	452	<div> <div>11%</div> <div>96%</div> </div>
2	B	445	<div> <div>18%</div> <div>92%</div> </div>
3	C	6	<div> <div>17%</div> <div>100%</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
8	NAG	B	509	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13981 atoms, of which 6767 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	0	1	0
			6558	2149	3180	553	668	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	VAL	ILE	engineered mutation	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6593	2082	3270	563	654	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	THR	SER	conflict	UNP P05556

- Molecule 3 is a protein called GLY-ARG-GLY-ASP-SER-PRO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	6	Total	C	H	N	O		0	0	0
			75	22	34	9	10				

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	A	4	Total	Ca	0	0
			4	4		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	7	Total	C	H	N	O	0	0
			157	46	74	2	35		

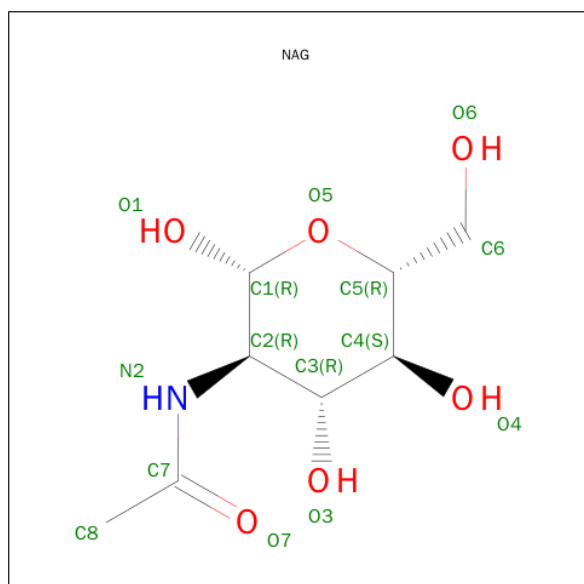
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	A	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
6	B	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	B	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	4	Total	C	H	N	O	0	0
			96	28	46	2	20		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

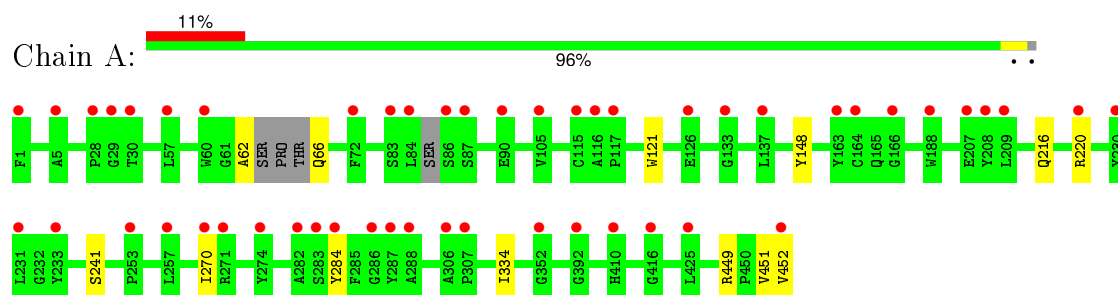
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	84	Total	O	0	0
			84	84		
10	B	80	Total	O	0	0
			80	80		

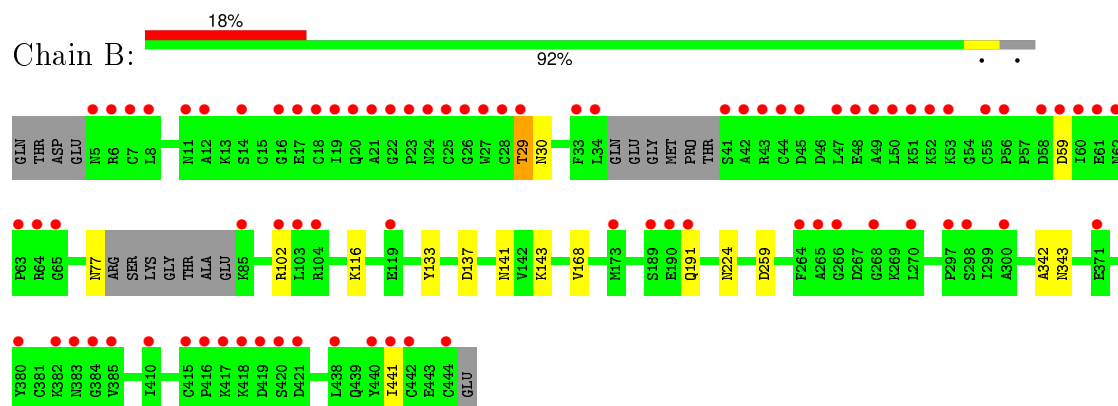
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

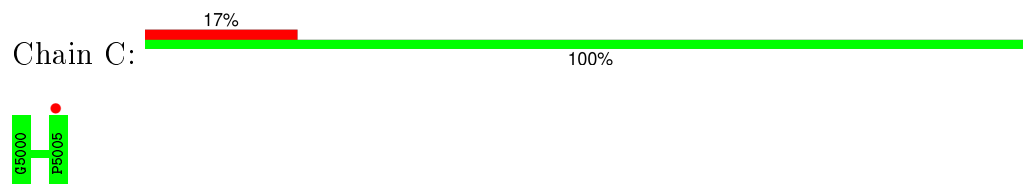
• Molecule 1: Integrin alpha-5



• Molecule 2: Integrin beta-1



• Molecule 3: GLY-ARG-GLY-ASP-SER-PRO



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.98Å 118.39Å 170.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 2.50 42.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (42.57-2.50) 98.2 (42.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.210 , 0.254 0.211 , 0.254	Depositor DCC
R_{free} test set	1998 reflections (4.68%)	DCC
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42741 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13981	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, BMA, CA, NAG, 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	0.23	0/3473	0.39	0/4733
2	B	0.22	0/3379	0.39	0/4560
3	C	0.19	0/41	0.32	0/52
All	All	0.23	0/6893	0.39	0/9345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3378	3180	3177	8	0
2	B	3323	3270	3274	13	0
3	C	41	34	34	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
5	A	83	74	71	6	0
6	A	56	53	50	3	0
6	B	56	54	50	0	0
7	A	50	46	43	0	0
8	A	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	42	42	39	3	0
9	B	1	0	0	0	0
10	A	84	0	0	1	0
10	B	80	0	0	3	0
All	All	7214	6767	6751	26	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 2.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:507:BMA:C6	5:A:509:MAN:C1	2.42	0.97
2:B:137:ASP:HB2	8:B:509:NAG:O7	1.75	0.86
1:A:241:SER:HB2	6:A:518:NAG:H82	1.60	0.83
2:B:137:ASP:CB	8:B:509:NAG:O7	2.33	0.76
2:B:259:ASP:OD2	10:B:614:HOH:O	2.08	0.72
5:A:507:BMA:O6	5:A:509:MAN:C2	2.37	0.72
1:A:449:ARG:NH2	10:A:668:HOH:O	2.30	0.63
2:B:30:ASN:N	2:B:59:ASP:OD1	2.33	0.62
5:A:507:BMA:H61	5:A:509:MAN:C1	2.31	0.58
2:B:29:THR:OG1	2:B:59:ASP:O	2.26	0.53
2:B:133:TYR:OH	2:B:191:GLN:NE2	2.42	0.53
1:A:148:TYR:OH	1:A:216:GLN:NE2	2.42	0.53
2:B:141:ASN:ND2	2:B:343:ASN:OD1	2.42	0.53
1:A:62:ALA:O	1:A:66:GLN:NE2	2.41	0.52
1:A:220:ARG:NH2	5:A:509:MAN:C1	2.73	0.52
1:A:241:SER:HB2	6:A:518:NAG:C8	2.38	0.48
1:A:451:VAL:HG22	1:A:452:VAL:H	1.79	0.47
2:B:29:THR:N	2:B:59:ASP:OD1	2.43	0.46
2:B:102:ARG:NH1	2:B:441:ILE:HD11	2.31	0.46
2:B:137:ASP:HB3	8:B:509:NAG:O7	2.16	0.45
2:B:77:ASN:HB3	2:B:116:LYS:NZ	2.33	0.44
2:B:143:LYS:NZ	10:B:633:HOH:O	2.51	0.43
2:B:342:ALA:O	10:B:680:HOH:O	2.21	0.43
1:A:220:ARG:NH2	5:A:511:MAN:O5	2.52	0.42
5:A:509:MAN:O5	5:A:511:MAN:C1	2.68	0.42
6:A:518:NAG:H61	6:A:519:NAG:N2	2.34	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/452 (98%)	427 (96%)	15 (3%)	1 (0%)	52	75
2	B	421/445 (95%)	398 (94%)	22 (5%)	1 (0%)	52	75
3	C	4/6 (67%)	4 (100%)	0	0	100	100
All	All	868/903 (96%)	829 (96%)	37 (4%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
2	B	168	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	355/358 (99%)	352 (99%)	3 (1%)	86	96
2	B	380/395 (96%)	378 (100%)	2 (0%)	92	98
3	C	4/4 (100%)	4 (100%)	0	100	100
All	All	739/757 (98%)	734 (99%)	5 (1%)	88	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	TRP

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Mol	Chain	Res	Type
1	A	284	TYR
1	A	334	ILE
2	B	29	THR
2	B	224	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	221	GLN
2	B	141	ASN
2	B	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 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	505	1,5	14,14,15	0.35	0	15,19,21	0.28	0
5	NAG	A	506	5	14,14,15	0.24	0	15,19,21	0.41	0
5	BMA	A	507	5	11,11,12	0.66	0	14,15,17	0.76	0
5	MAN	A	508	5	11,11,12	0.73	0	14,15,17	1.02	2 (14%)
5	MAN	A	509	5	11,11,12	0.25	0	14,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	510	5	11,11,12	0.24	0	14,15,17	0.56	0
5	MAN	A	511	5	11,11,12	0.26	0	14,15,17	0.61	0
6	NAG	A	512	1,6	14,14,15	0.23	0	15,19,21	0.31	0
6	NAG	A	513	6	14,14,15	0.24	0	15,19,21	0.85	1 (6%)
7	NAG	A	514	1,7	14,14,15	0.35	0	15,19,21	0.27	0
7	NAG	A	515	7	14,14,15	0.26	0	15,19,21	0.30	0
7	BMA	A	516	7	11,11,12	0.57	0	14,15,17	0.87	0
7	MAN	A	517	7	11,11,12	0.60	0	14,15,17	1.34	3 (21%)
6	NAG	A	518	1,6	14,14,15	0.28	0	15,19,21	0.53	0
6	NAG	A	519	6	14,14,15	0.29	0	15,19,21	0.53	0
6	NAG	B	504	2,6	14,14,15	0.29	0	15,19,21	0.60	0
6	NAG	B	505	6	14,14,15	0.26	0	15,19,21	0.59	0
6	NAG	B	506	2,6	14,14,15	0.26	0	15,19,21	0.23	0
6	NAG	B	507	6	14,14,15	0.19	0	15,19,21	0.33	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
5	NAG	A	505	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	506	5	-	0/6/23/26	0/1/1/1
5	BMA	A	507	5	-	0/2/19/22	0/1/1/1
5	MAN	A	508	5	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	5	-	0/2/19/22	0/1/1/1
5	MAN	A	511	5	-	0/2/19/22	0/1/1/1
6	NAG	A	512	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	513	6	-	0/6/23/26	0/1/1/1
7	NAG	A	514	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	515	7	-	0/6/23/26	0/1/1/1
7	BMA	A	516	7	-	0/2/19/22	0/1/1/1
7	MAN	A	517	7	-	0/2/19/22	0/1/1/1
6	NAG	A	518	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	519	6	-	0/6/23/26	0/1/1/1
6	NAG	B	504	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	505	6	-	0/6/23/26	0/1/1/1
6	NAG	B	506	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	507	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	517	MAN	O2-C2-C3	-2.17	105.75	110.12
5	A	508	MAN	O2-C2-C3	-2.16	105.78	110.12
7	A	517	MAN	O5-C1-C2	2.06	114.20	110.86
6	A	513	NAG	C1-O5-C5	2.07	114.87	112.25
5	A	508	MAN	C1-O5-C5	2.11	114.92	112.25
7	A	517	MAN	C1-O5-C5	3.34	116.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	BMA	3	0
5	A	509	MAN	5	0
5	A	511	MAN	2	0
6	A	518	NAG	3	0
6	A	519	NAG	1	0

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	$\# Z > 2$
8	NAG	A	520	1	14,14,15	0.27	0	15,19,21	0.53	0
8	NAG	B	508	2	14,14,15	0.23	0	15,19,21	0.31	0
8	NAG	B	509	2	14,14,15	0.33	0	15,19,21	0.35	0
8	NAG	B	510	2	14,14,15	0.29	0	15,19,21	0.57	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
8	NAG	A	520	1	-	0/6/23/26	0/1/1/1
8	NAG	B	508	2	-	0/6/23/26	0/1/1/1
8	NAG	B	509	2	-	0/6/23/26	0/1/1/1
8	NAG	B	510	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	509	NAG	3	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	448/452 (99%)	0.67	50 (11%) 7 7	49, 79, 130, 216	0
2	B	427/445 (95%)	1.06	81 (18%) 2 1	46, 83, 173, 286	0
3	C	6/6 (100%)	0.65	1 (16%) 2 2	92, 101, 127, 138	0
All	All	881/903 (97%)	0.86	132 (14%) 3 3	46, 81, 163, 286	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	ILE	9.6
1	A	84	LEU	9.4
2	B	416	PRO	6.3
1	A	86	SER	6.2
2	B	7	CYS	6.0
2	B	21	ALA	5.9
2	B	42	ALA	5.6
2	B	19	ILE	5.6
2	B	417	LYS	5.6
2	B	6	ARG	5.5
2	B	44	CYS	5.5
2	B	418	LYS	5.3
2	B	50	LEU	5.2
2	B	12	ALA	5.1
2	B	24	ASN	5.1
2	B	56	PRO	5.1
2	B	8	LEU	5.0
2	B	22	GLY	4.9
2	B	119	GLU	4.8
2	B	419	ASP	4.8
2	B	20	GLN	4.7
1	A	29	GLY	4.6
2	B	421	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	25	CYS	4.5
1	A	87	SER	4.3
2	B	53	LYS	4.2
2	B	62	ASN	4.1
2	B	33	PHE	4.0
2	B	59	ASP	3.9
1	A	30	THR	3.9
2	B	410	ILE	3.8
2	B	45	ASP	3.8
1	A	90	GLU	3.8
2	B	34	LEU	3.8
2	B	55	CYS	3.7
2	B	415	CYS	3.7
2	B	48	GLU	3.7
2	B	441	ILE	3.7
2	B	442	CYS	3.6
2	B	270	LEU	3.6
2	B	298	SER	3.6
2	B	52	LYS	3.6
1	A	126	GLU	3.5
2	B	103	LEU	3.5
1	A	137	LEU	3.4
1	A	283	SER	3.4
2	B	104	ARG	3.4
2	B	23	PRO	3.3
2	B	64	ARG	3.3
2	B	26	GLY	3.3
2	B	85	LYS	3.3
1	A	28	PRO	3.3
2	B	63	PRO	3.2
1	A	271	ARG	3.2
2	B	27	TRP	3.2
2	B	384	GLY	3.1
2	B	43	ARG	3.1
2	B	14	SER	3.1
2	B	190	GLU	3.1
1	A	287	TYR	2.9
1	A	286	GLY	2.9
1	A	282	ALA	2.9
2	B	300	ALA	2.8
2	B	47	LEU	2.8
2	B	58	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	29	THR	2.8
2	B	264	PHE	2.8
2	B	265	ALA	2.8
1	A	230	TYR	2.8
1	A	83	SER	2.7
2	B	5	ASN	2.7
1	A	164	CYS	2.7
1	A	284	TYR	2.7
2	B	18	CYS	2.7
2	B	28	CYS	2.7
2	B	61	GLU	2.6
1	A	352	GLY	2.6
1	A	392	GLY	2.6
2	B	65	GLY	2.6
1	A	1	PHE	2.6
2	B	385	VAL	2.6
1	A	253	PRO	2.6
1	A	270	ILE	2.5
3	C	5005	PRO	2.5
1	A	188	TRP	2.5
1	A	425	LEU	2.5
2	B	444	CYS	2.5
2	B	297	PRO	2.4
2	B	173	MET	2.4
2	B	49	ALA	2.4
2	B	102	ARG	2.4
2	B	420	SER	2.4
2	B	380	TYR	2.3
2	B	11	ASN	2.3
1	A	207	GLU	2.3
1	A	208	TYR	2.3
2	B	440	TYR	2.3
1	A	416	GLY	2.3
1	A	105	VAL	2.2
2	B	16	GLY	2.2
1	A	233	TYR	2.2
2	B	51	LYS	2.2
1	A	452	VAL	2.2
1	A	166	GLY	2.2
1	A	231	LEU	2.2
1	A	306	ALA	2.2
2	B	17	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	257	LEU	2.2
1	A	115	CYS	2.1
1	A	410	HIS	2.1
2	B	41	SER	2.1
1	A	116	ALA	2.1
1	A	57	LEU	2.1
1	A	72	PHE	2.1
1	A	117	PRO	2.1
2	B	191	GLN	2.1
1	A	274	TYR	2.1
2	B	438	LEU	2.1
1	A	5	ALA	2.1
1	A	288	ALA	2.1
1	A	209	LEU	2.1
2	B	371	GLU	2.1
2	B	383	ASN	2.1
1	A	133	GLY	2.1
1	A	163	TYR	2.1
2	B	266	GLY	2.1
1	A	307	PRO	2.1
2	B	189	SER	2.1
1	A	220	ARG	2.0
1	A	60	TRP	2.0
2	B	382	LYS	2.0
2	B	268	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
7	NAG	A	514	14/15	0.94	0.20	1.27	85,103,116,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	505	14/15	0.91	0.19	-0.15	66,79,93,95	0
5	NAG	A	506	14/15	0.96	0.13	-0.96	87,95,110,114	0
6	NAG	A	518	14/15	0.86	0.13	-1.32	148,169,200,203	0
6	NAG	A	512	14/15	0.88	0.11	-4.03	97,107,125,128	0
5	MAN	A	510	11/12	0.82	0.28	-	77,105,127,140	0
7	BMA	A	516	11/12	0.70	0.37	-	139,146,174,175	0
5	MAN	A	511	11/12	0.74	0.53	-	145,151,181,182	0
6	NAG	A	519	14/15	0.73	0.37	-	69,110,135,143	0
6	NAG	B	505	14/15	0.82	0.23	-	105,130,157,165	0
7	NAG	A	515	14/15	0.83	0.20	-	115,126,147,151	0
6	NAG	B	504	14/15	0.82	0.15	-	58,102,129,134	0
7	MAN	A	517	11/12	0.74	0.41	-	149,151,181,181	0
5	MAN	A	509	11/12	0.67	0.21	-	134,141,169,169	0
5	BMA	A	507	11/12	0.81	0.11	-	112,125,150,150	0
6	NAG	B	506	14/15	0.90	0.21	-	99,115,135,138	0
6	NAG	B	507	14/15	0.71	0.40	-	124,132,156,156	0
5	MAN	A	508	11/12	0.85	0.14	-	119,124,149,150	0
6	NAG	A	513	14/15	0.68	0.28	-	119,129,154,154	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	B	509	14/15	0.68	0.40	3.32	156,159,190,191	0
9	MG	B	501	1/1	0.95	0.20	0.55	59,59,59,59	0
8	NAG	A	520	14/15	0.88	0.22	-0.18	110,120,142,144	0
4	CA	B	503	1/1	0.97	0.22	-0.47	66,66,66,66	0
4	CA	A	502	1/1	0.98	0.10	-0.78	73,73,73,73	0
4	CA	B	502	1/1	0.63	0.13	-0.92	156,156,156,156	0
4	CA	A	503	1/1	0.96	0.09	-1.38	66,66,66,66	0
4	CA	A	504	1/1	0.96	0.06	-1.43	81,81,81,81	0
4	CA	A	501	1/1	0.96	0.06	-2.23	87,87,87,87	0
8	NAG	B	508	14/15	0.83	0.36	-	121,135,161,162	0
8	NAG	B	510	14/15	0.81	0.33	-	129,138,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.