



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4BTY
Title : Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
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Deposited on : 2013-06-19
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

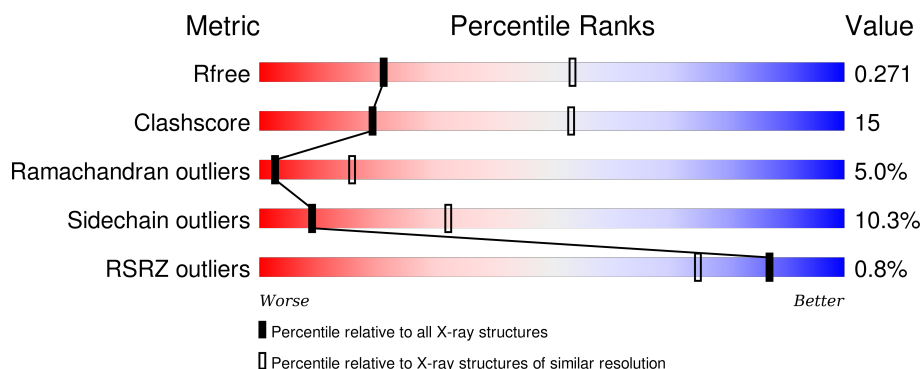
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	737	 63% 28% 6% .
1	B	737	 62% 28% 5% . .

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
4	NAG	B	1771	X	-	-	-
5	NAG	A	1768	X	-	-	-
5	NAG	A	1770	X	-	-	-
7	NAG	B	1765	X	-	-	-
7	BMA	B	1767	-	-	X	-
7	MAN	B	1768	X	-	-	-
7	MAN	B	1769	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11484 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5604	3595	968	1021	20			
1	B	707	Total	C	N	O	S	0	0	0
			5567	3574	957	1016	20			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

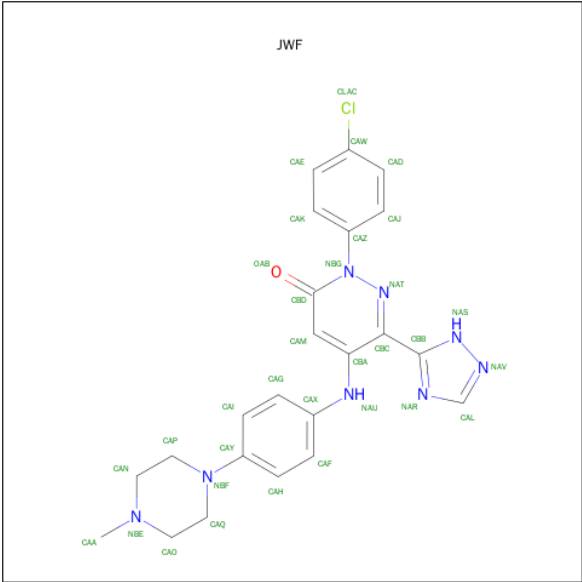
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 5-[4-(4-METHYLPYPERAZIN-1-YL)PHENYLAMINO]-2-(4-CHLOROPHENYL)-6-(1H-1,2,4-TRIAZOL-5-YL)-3(2H)-PYRIDAZINONE (three-letter code: JWF) (formula: C₂₃H₂₃ClN₈O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			33	23	1	8	1		
6	B	1	Total	C	Cl	N	O	0	0
			33	23	1	8	1		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	5	Total	C	N	O	0	0
			61	34	2	25		

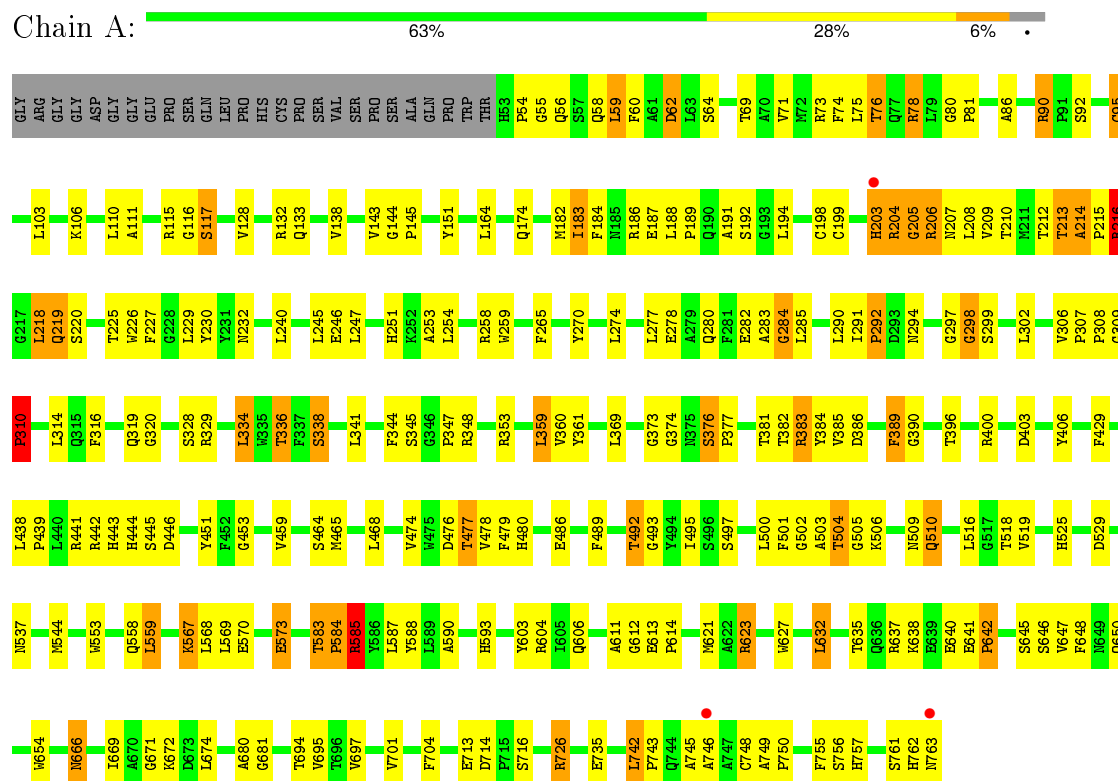
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	26	Total	O	0	0
			26	26		
8	B	14	Total	O	0	0
			14	14		

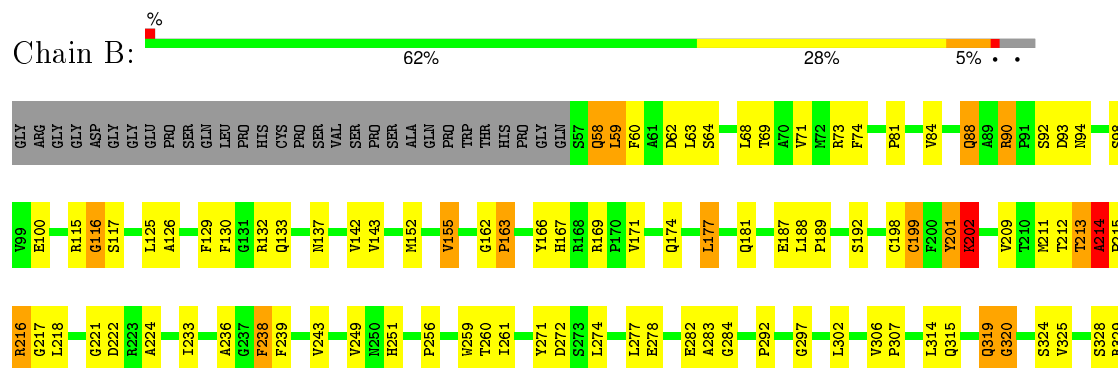
3 Residue-property plots

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: MEMBRANE PRIMARY AMINE OXIDASE



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.74Å 226.74Å 218.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.20 – 3.10 49.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	76.2 (49.20-3.10) 76.2 (49.15-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.246 0.217 , 0.271	Depositor DCC
R_{free} test set	2314 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 45763 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, CA, JWF, TPQ, CU, 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	0.67	1/5769 (0.0%)	0.89	5/7867 (0.1%)
1	B	0.66	1/5730 (0.0%)	0.88	1/7815 (0.0%)
All	All	0.66	2/11499 (0.0%)	0.88	6/15682 (0.0%)

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
1	A	0	2
1	B	0	7
4	B	1	0
7	B	3	0
All	All	4	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	ASN	CG-ND2	6.88	1.50	1.32
1	B	592	ASN	CG-ND2	5.50	1.46	1.32

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	A	529	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	529	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	258	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	585	ARG	NE-CZ-NH2	-5.69	117.46	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1765	NAG	C1
7	B	1768	MAN	C1
7	B	1769	MAN	C1
4	B	1771	NAG	C1

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	PRO	Peptide
1	A	438	LEU	Peptide
1	B	162	GLY	Peptide
1	B	202	LYS	Peptide
1	B	213	THR	Peptide

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	5604	0	5335	169	0
1	B	5567	0	5299	182	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	28	0	25	1	0
4	B	28	0	25	1	0
5	A	56	0	52	1	0
5	B	28	0	26	4	0
6	A	33	0	23	5	0
6	B	33	0	23	3	0
7	B	61	0	52	9	0
8	A	26	0	0	2	0
8	B	14	0	0	4	0
All	All	11484	0	10860	337	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 15.

The worst 5 of 337 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:B:592:ASN:ND2	5:B:1772:NAG:C1	1.90	1.35
1:B:592:ASN:ND2	5:B:1772:NAG:O5	1.62	1.32
7:B:1767:BMA:O4	7:B:1769:MAN:H2	1.33	1.25
7:B:1767:BMA:C4	7:B:1769:MAN:H2	1.79	1.13
1:B:592:ASN:HD22	5:B:1772:NAG:C1	1.59	1.00

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	708/737 (96%)	596 (84%)	73 (10%)	39 (6%)	2	13
1	B	704/737 (96%)	593 (84%)	79 (11%)	32 (4%)	3	17
All	All	1412/1474 (96%)	1189 (84%)	152 (11%)	71 (5%)	3	16

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	116	GLY
1	A	203	HIS
1	A	204	ARG
1	A	206	ARG

5.3.2 Protein sidechains [i](#)

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	588/610 (96%)	527 (90%)	61 (10%)	9	32
1	B	584/610 (96%)	524 (90%)	60 (10%)	9	32
All	All	1172/1220 (96%)	1051 (90%)	121 (10%)	9	32

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	THR
1	B	98	SER
1	B	634	VAL
1	A	713	GLU
1	B	58	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	592	ASN
1	B	593	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	TPQ	A	471	1	13,14,15	1.30	3 (23%)	15,19,21	1.67	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPQ	B	471	1	13,14,15	1.30	1 (7%)	15,19,21	1.72	2 (13%)

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	TPQ	A	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1	-	0/4/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C6-C5	-2.24	1.38	1.44
1	A	471	TPQ	C6-C1	2.01	1.39	1.34
1	A	471	TPQ	C3-C4	2.42	1.39	1.35
1	B	471	TPQ	C3-C4	2.70	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	TPQ	C1-C6-C5	-2.83	121.25	122.97
1	B	471	TPQ	O5-C5-C4	2.38	122.97	119.16
1	A	471	TPQ	O5-C5-C4	2.77	123.60	119.16
1	A	471	TPQ	C6-C1-C2	4.08	121.32	118.44
1	B	471	TPQ	C6-C1-C2	4.72	121.78	118.44

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

9 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	$\# Z > 2$
4	NAG	A	1765	1,4	14,14,15	0.56	0	15,19,21	1.54	3 (20%)
4	NAG	A	1766	4	14,14,15	0.67	0	15,19,21	1.34	2 (13%)
7	NAG	B	1765	1,7	14,14,15	0.68	0	15,19,21	2.15	6 (40%)
7	NAG	B	1766	7	14,14,15	0.49	0	15,19,21	1.85	1 (6%)
7	BMA	B	1767	7	11,11,12	1.28	2 (18%)	14,15,17	2.53	7 (50%)
7	MAN	B	1768	7	11,11,12	1.68	3 (27%)	14,15,17	1.85	5 (35%)
7	MAN	B	1769	7	11,11,12	0.26	0	14,15,17	0.61	0
4	NAG	B	1770	1,4	14,14,15	0.79	0	15,19,21	2.03	5 (33%)
4	NAG	B	1771	4	14,14,15	0.68	0	15,19,21	2.44	4 (26%)

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	A	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1766	4	-	0/6/23/26	0/1/1/1
7	NAG	B	1765	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	B	1766	7	-	0/6/23/26	0/1/1/1
7	BMA	B	1767	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1768	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	B	1769	7	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	B	1770	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1771	4	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1767	BMA	O6-C6	2.08	1.51	1.42
7	B	1768	MAN	C4-C3	2.31	1.58	1.52
7	B	1767	BMA	O3-C3	2.76	1.49	1.43
7	B	1768	MAN	C1-C2	3.30	1.60	1.52
7	B	1768	MAN	C2-C3	3.51	1.57	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1765	NAG	O4-C4-C3	-4.68	99.80	110.34
4	B	1771	NAG	O7-C7-C8	-3.37	115.87	122.06
7	B	1765	NAG	C3-C4-C5	-3.31	104.43	110.20
7	B	1768	MAN	C1-O5-C5	-3.25	108.12	112.25
4	B	1770	NAG	C4-C3-C2	-2.54	107.28	111.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1771	NAG	C1
7	B	1765	NAG	C1
7	B	1769	MAN	C1
7	B	1768	MAN	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1765	NAG	1	0
7	B	1765	NAG	1	0
7	B	1767	BMA	8	0
7	B	1769	MAN	8	0
4	B	1770	NAG	1	0
4	B	1771	NAG	1	0

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	1767	1	14,14,15	0.81	0	15,19,21	2.35	7 (46%)
5	NAG	A	1768	1	14,14,15	0.97	1 (7%)	15,19,21	3.19	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1769	1	14,14,15	0.75	0	15,19,21	2.29	5 (33%)
5	NAG	A	1770	1	14,14,15	2.73	3 (21%)	15,19,21	3.54	6 (40%)
6	JWF	A	2000	-	32,37,37	2.57	9 (28%)	36,52,52	2.32	7 (19%)
5	NAG	B	1772	-	14,14,15	0.27	0	15,19,21	0.53	0
5	NAG	B	1773	1	14,14,15	1.64	2 (14%)	15,19,21	2.77	3 (20%)
6	JWF	B	2000	-	32,37,37	2.45	6 (18%)	36,52,52	2.47	11 (30%)

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	1767	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1768	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	1769	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1770	1	1/1/5/7	0/6/23/26	0/1/1/1
6	JWF	A	2000	-	-	0/13/26/26	0/5/5/5
5	NAG	B	1772	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1773	1	-	0/6/23/26	0/1/1/1
6	JWF	B	2000	-	-	0/13/26/26	0/5/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2000	JWF	NAV-NAS	-8.90	1.18	1.37
6	B	2000	JWF	CBC-CBB	-8.50	1.33	1.49
6	B	2000	JWF	NAV-NAS	-7.46	1.21	1.37
6	A	2000	JWF	CBC-CBB	-7.34	1.36	1.49
6	A	2000	JWF	CAZ-NBG	-4.30	1.35	1.44

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2000	JWF	NAR-CBB-NAS	-9.58	107.20	114.88
6	B	2000	JWF	NAR-CBB-NAS	-8.46	108.09	114.88
5	A	1770	NAG	O7-C7-C8	-4.56	113.70	122.06
6	A	2000	JWF	CBA-CBC-NAT	-4.36	115.86	121.12
5	A	1767	NAG	C3-C4-C5	-3.97	103.28	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1768	NAG	C1
5	A	1770	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1768	NAG	1	0
6	A	2000	JWF	5	0
5	B	1772	NAG	4	0
6	B	2000	JWF	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 [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	710/737 (96%)	-0.24	3 (0%) 93 85	58, 83, 112, 163	0
1	B	706/737 (95%)	-0.14	9 (1%) 79 62	63, 84, 115, 180	0
All	All	1416/1474 (96%)	-0.19	12 (0%) 87 75	58, 83, 115, 180	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ALA	4.1
1	B	744	GLN	4.0
1	B	745	ALA	4.0
1	A	203	HIS	3.5
1	A	763	ASN	3.3

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(Å ²)	Q<0.9
1	TPQ	A	471	14/15	0.94	0.24	-	68,74,80,80	0
1	TPQ	B	471	14/15	0.97	0.31	-	68,76,90,94	0

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
4	NAG	A	1765	14/15	0.96	0.17	0.12	78,83,93,101	0
7	NAG	B	1765	14/15	0.90	0.16	-1.02	74,82,91,94	0
4	NAG	B	1770	14/15	0.94	0.14	-1.38	97,105,126,137	0
7	NAG	B	1766	14/15	0.94	0.17	-	100,110,119,123	0
7	MAN	B	1769	11/12	0.56	0.36	-	89,129,154,162	0
7	BMA	B	1767	11/12	0.80	0.30	-	113,133,158,163	0
4	NAG	B	1771	14/15	0.90	0.23	-	106,130,141,143	0
4	NAG	A	1766	14/15	0.85	0.24	-	101,123,145,157	0
7	MAN	B	1768	11/12	0.81	0.49	-	87,119,138,139	0

6.4 Ligands [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
6	JWF	B	2000	33/33	0.91	0.21	-0.11	71,78,101,108	0
5	NAG	A	1767	14/15	0.87	0.20	-0.31	93,104,130,130	0
6	JWF	A	2000	33/33	0.96	0.18	-0.31	71,90,120,127	0
3	CA	B	1763	1/1	0.95	0.05	-2.14	72,72,72,72	0
3	CA	A	1764	1/1	0.77	0.13	-2.48	94,94,94,94	0
3	CA	B	1764	1/1	0.93	0.11	-2.55	81,81,81,81	0
3	CA	A	1763	1/1	0.96	0.05	-2.73	71,71,71,71	0
5	NAG	B	1773	14/15	0.76	0.46	-	118,149,156,156	0
5	NAG	A	1769	14/15	0.63	0.56	-	127,148,167,183	0
5	NAG	A	1768	14/15	0.67	0.28	-	121,169,177,179	0
5	NAG	A	1770	14/15	0.54	0.61	-	114,149,166,170	0
5	NAG	B	1772	14/15	0.64	0.21	-	98,134,157,157	0
2	CU	A	1762	1/1	0.89	0.20	-	85,85,85,85	0
2	CU	B	1762	1/1	0.90	0.24	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.