



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 AM UTC

PDB ID : 5AF9 / pdb_00005af9
Title : Thrombin in complex with 4-Methoxy-N-(2-pyridinyl)benzamide
Authors : Ruehmann, E.; Heine, A.; Klebe, G.
Deposited on : 2015-01-20
Resolution : 1.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

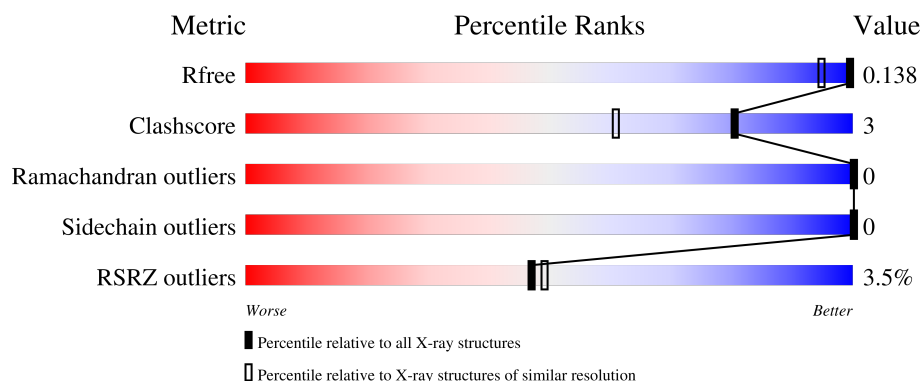
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.18 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}	180053	1789 (1.20-1.16)
Clashscore	190562	1845 (1.20-1.16)
Ramachandran outliers	187476	1789 (1.20-1.16)
Sidechain outliers	187428	1789 (1.20-1.16)
RSRZ outliers	180081	1787 (1.20-1.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	258	2% 93% ••
2	I	12	33% 67% 17% 8% 8%
3	L	29	7% 97% •

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5051 atoms, of which 2276 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 THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	H	250	4141	1339	2050	370	368	14	0	12	0

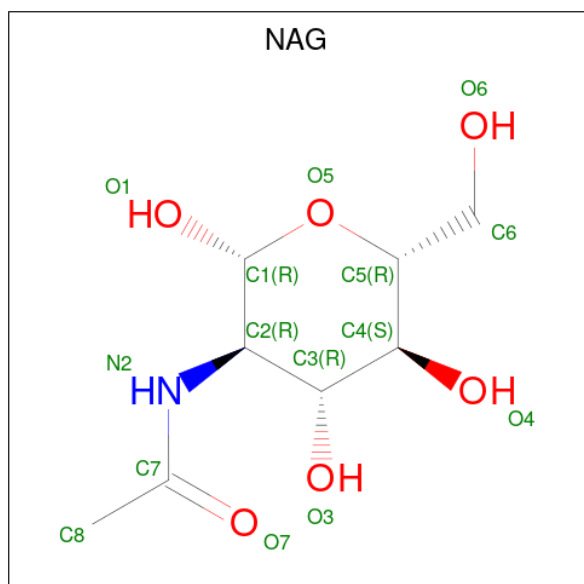
- Molecule 2 is a protein called HIRUDIN VARIANT-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	11	89	58	11	19	1	0	0	0

- Molecule 3 is a protein called THROMBIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	28	463	150	226	37	49	1	0	2	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

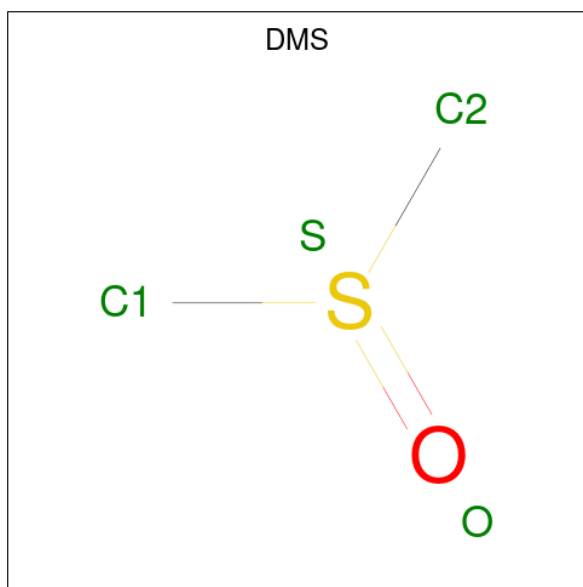


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

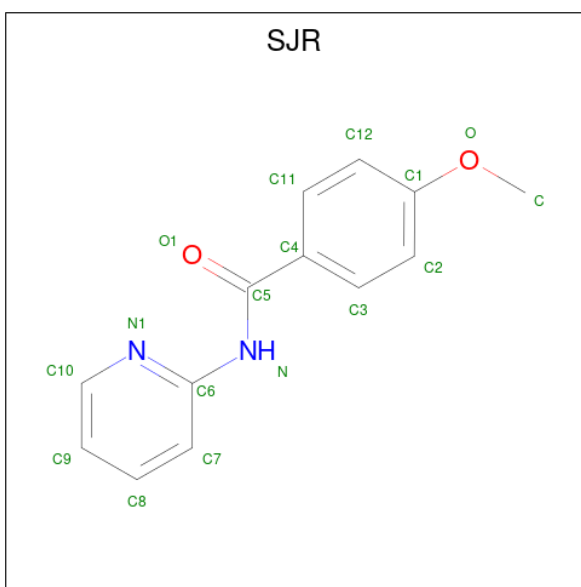
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Na	0	0
			2	2		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



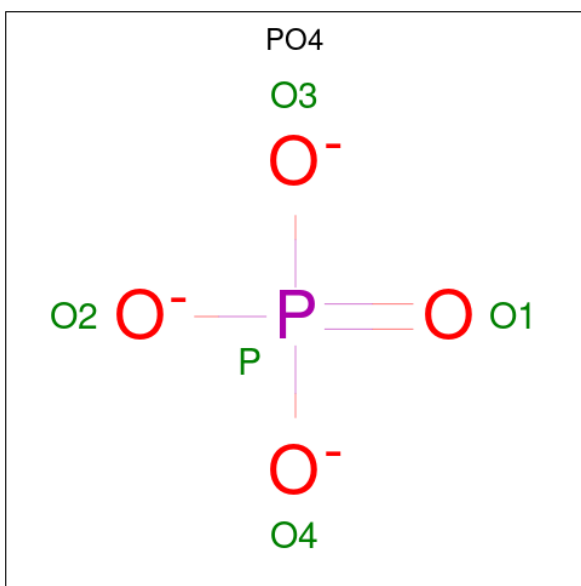
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	O	S	0	0
			4	2	1	1		
6	H	1	Total	C	O	S	0	1
			8	4	2	2		

- Molecule 7 is 4-methoxy-N-(pyridin-2-yl)benzamide (CCD ID: SJR) (formula: C₁₃H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	N	O	0	0
			17	13	2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



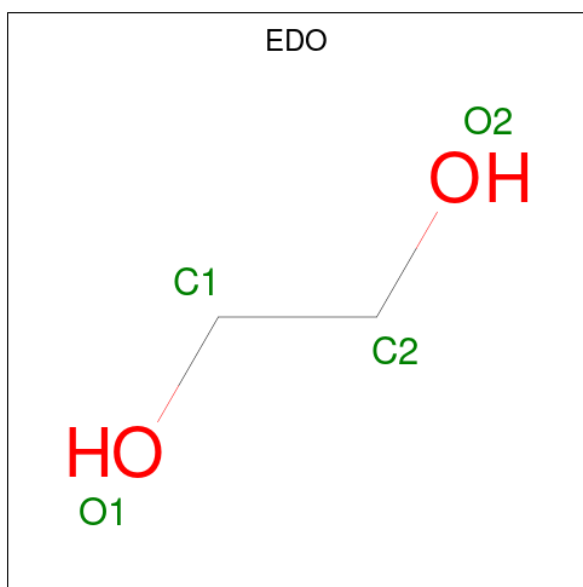
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			6	3	3		
9	H	1	Total	C	O	0	0
			6	3	3		
9	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	246	Total 252	O 252	0	6
11	H	1	Total 1	O 1	0	0
11	I	6	Total 6	O 6	0	0
11	L	27	Total 27	O 27	0	0

i

• Molecule 1: THROMBIN HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.03Å 71.25Å 72.14Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	70.96 – 1.18 70.96 – 1.18	Depositor EDS
% Data completeness (in resolution range)	95.1 (70.96-1.18) 95.1 (70.96-1.18)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.121 , 0.137 0.124 , 0.138	Depositor DCC
R_{free} test set	5435 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5051	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GOL, DMS, TYS, SJR, PO4, NA, NAG

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	H	0.62	1/2161 (0.0%)	0.72	0/2922
2	I	0.36	0/73	0.48	0/97
3	L	0.59	0/242	0.73	0/323
All	All	0.61	1/2476 (0.0%)	0.71	0/3342

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	60(G)	ASN	CG-ND2	5.75	1.45	1.33

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	H	2091	2050	2065	6	0
2	I	89	0	68	4	0
3	L	237	226	229	0	0
4	H	14	0	13	0	0
5	H	2	0	0	0	0
6	H	12	0	18	3	0
7	H	17	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	5	0	0	0	0
9	H	18	0	24	6	0
10	H	4	0	6	0	0
11	H	253	0	0	0	0
11	I	6	0	0	0	0
11	L	27	0	0	0	0
All	All	2775	2276	2435	13	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 3.

All (13) 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)
6:H:1249[B]:DMS:H23	9:H:1252:GOL:O3	1.84	0.78
1:H:101:ARG:HE	9:H:1253:GOL:H32	1.66	0.61
2:I:522:ILE:HD11	2:I:527:LEU:HD11	1.82	0.61
6:H:1249[A]:DMS:H12	9:H:1252:GOL:O3	2.09	0.52
1:H:101:ARG:HE	9:H:1253:GOL:C3	2.24	0.50
2:I:526:TYS:C	2:I:527:LEU:HD12	2.44	0.47
1:H:211:GLY:HA2	1:H:229:THR:O	2.15	0.46
6:H:1249[B]:DMS:H23	9:H:1252:GOL:HO3	1.81	0.46
2:I:522:ILE:CD1	2:I:527:LEU:HD11	2.44	0.45
1:H:179:ASN:HD21	9:H:1253:GOL:H32	1.82	0.45
2:I:522:ILE:CG1	2:I:527:LEU:HD11	2.48	0.43
1:H:201:MET:SD	1:H:210:MET:HG3	2.59	0.43
1:H:84:MET:HE3	1:H:109:LYS:HD2	2.01	0.42

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	H	258/258 (100%)	251 (97%)	7 (3%)	0	100	100
2	I	8/12 (67%)	8 (100%)	0	0	100	100
3	L	28/29 (97%)	27 (96%)	1 (4%)	0	100	100
All	All	294/299 (98%)	286 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	223/224 (100%)	223 (100%)	0	100	100
2	I	6/10 (60%)	6 (100%)	0	100	100
3	L	25/27 (93%)	25 (100%)	0	100	100
All	All	254/261 (97%)	254 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	H	151	GLN
1	H	179	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$
2	TYS	I	526	2	15,16,17	1.46	3 (20%)	15,22,24	1.12	1 (6%)

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
2	TYS	I	526	2	-	0/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	526	TYS	CE1-CD1	2.92	1.43	1.38
2	I	526	TYS	OH-S	-2.92	1.52	1.58
2	I	526	TYS	CD2-CG	2.08	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	526	TYS	OH-S-O1	-2.70	99.34	107.56

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
2	I	526	TYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
6	DMS	H	1249[B]	-	3,3,3	0.62	0	3,3,3	0.46	0
6	DMS	H	1248	-	3,3,3	0.65	0	3,3,3	0.36	0
9	GOL	H	1253	-	5,5,5	0.39	0	5,5,5	0.62	0
7	SJR	H	1250	-	18,18,18	0.19	0	23,23,23	0.44	0
9	GOL	H	1254	-	5,5,5	0.40	0	5,5,5	0.28	0
9	GOL	H	1252	-	5,5,5	0.37	0	5,5,5	0.88	0
6	DMS	H	1249[A]	-	3,3,3	0.58	0	3,3,3	0.28	0
8	PO4	H	1251	-	4,4,4	1.26	0	6,6,6	1.46	2 (33%)
10	EDO	H	1255	-	3,3,3	0.46	0	2,2,2	0.29	0
4	NAG	H	1060	1	14,14,15	1.98	5 (35%)	17,19,21	0.96	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	GOL	H	1253	-	-	0/4/4/4	-
7	SJR	H	1250	-	-	0/10/10/10	0/2/2/2
9	GOL	H	1254	-	-	2/4/4/4	-
9	GOL	H	1252	-	-	2/4/4/4	-
10	EDO	H	1255	-	-	0/1/1/1	-
4	NAG	H	1060	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1060	NAG	C7-N2	4.33	1.48	1.34
4	H	1060	NAG	O5-C5	3.17	1.49	1.43
4	H	1060	NAG	C4-C3	-3.11	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1060	NAG	C3-C2	-2.31	1.47	1.52
4	H	1060	NAG	C6-C5	-2.05	1.45	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1251	PO4	O4-P-O1	-2.58	101.81	110.95
8	H	1251	PO4	O3-P-O2	2.29	115.03	107.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	1254	GOL	O2-C2-C3-O3
4	H	1060	NAG	O5-C5-C6-O6
9	H	1252	GOL	O1-C1-C2-C3
9	H	1254	GOL	C1-C2-C3-O3
4	H	1060	NAG	C4-C5-C6-O6
9	H	1252	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1249[B]	DMS	2	0
9	H	1253	GOL	3	0
9	H	1252	GOL	3	0
6	H	1249[A]	DMS	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	H	250/258 (96%)	-0.25	4 (1%) 70 74	6, 18, 35, 43	12 (4%)
2	I	10/12 (83%)	1.90	4 (40%) 1 1	27, 36, 44, 45	0
3	L	28/29 (96%)	-0.14	2 (7%) 22 25	10, 16, 32, 37	2 (7%)
All	All	288/299 (96%)	-0.16	10 (3%) 47 49	6, 17, 37, 45	14 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	147	THR	5.0
2	I	527	LEU	4.9
3	L	14(K)	ILE	3.9
1	H	186(C)	GLY	3.6
1	H	245	PHE	3.3
1	H	186(A)	ASP	3.1
2	I	528	GLN	3.1
2	I	518	ASP	2.9
3	L	1(C)	GLU	2.7
2	I	522	ILE	2.2

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TYS	I	526	16/17	0.98	0.07	25,28,36,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	1060	14/15	0.79	0.14	40,43,49,49	0
9	GOL	H	1253	6/6	0.80	0.20	34,36,37,38	6
9	GOL	H	1252	6/6	0.90	0.16	22,36,38,39	6
9	GOL	H	1254	6/6	0.91	0.13	24,31,33,35	6
10	EDO	H	1255	4/4	0.92	0.13	21,25,26,27	0
7	SJR	H	1250	17/17	0.94	0.10	18,20,30,30	0
8	PO4	H	1251	5/5	0.96	0.08	17,19,20,20	5
6	DMS	H	1248	4/4	0.98	0.08	14,15,17,18	4
6	DMS	H	1249[A]	4/4	0.98	0.08	22,24,25,25	4
6	DMS	H	1249[B]	4/4	0.98	0.08	28,28,28,29	4
5	NA	H	1247	1/1	1.00	0.01	15,15,15,15	0
5	NA	H	1246	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.