



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YO8
Title : Structure of the C-terminal domain of human thrombospondin-2
Authors : Carlson, C.B.; Bernstein, D.A.; Annis, D.S.; Misenheimer, T.M.; Hannah, B.A.; Mosher, D.F.; Keck, J.L.
Deposited on : 2005-01-26
Resolution : 2.60 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

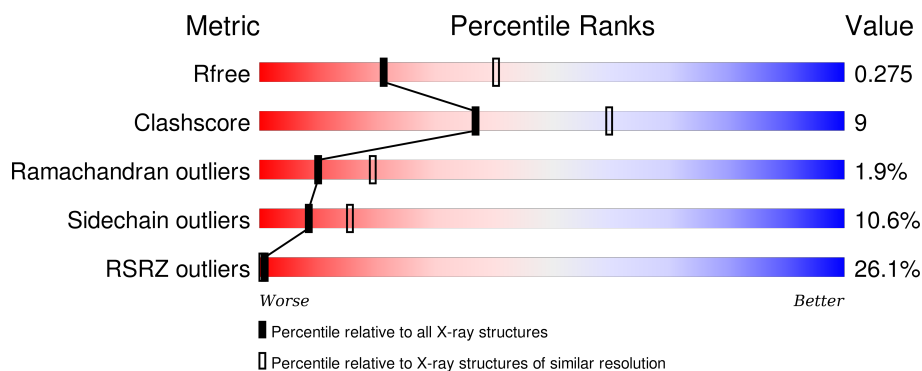
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	634	

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
2	MAN	A	3	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5085 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 thrombospondin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	Se	0	0	0
			4844	2949	837	1017	36	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	CLONING ARTIFACT	UNP P35442
A	549	ASP	-	CLONING ARTIFACT	UNP P35442
A	550	PRO	-	CLONING ARTIFACT	UNP P35442
A	675	MSE	MET	MODIFIED RESIDUE	UNP P35442
A	964	MSE	MET	MODIFIED RESIDUE	UNP P35442
A	1041	MSE	MET	MODIFIED RESIDUE	UNP P35442
A	1134	MSE	MET	MODIFIED RESIDUE	UNP P35442
A	1159	MSE	MET	MODIFIED RESIDUE	UNP P35442
A	1173	ALA	-	EXPRESSION TAG	UNP P35442
A	1174	ALA	-	EXPRESSION TAG	UNP P35442
A	1175	GLY	-	EXPRESSION TAG	UNP P35442
A	1176	HIS	-	EXPRESSION TAG	UNP P35442
A	1177	HIS	-	EXPRESSION TAG	UNP P35442
A	1178	HIS	-	EXPRESSION TAG	UNP P35442
A	1179	HIS	-	EXPRESSION TAG	UNP P35442
A	1180	HIS	-	EXPRESSION TAG	UNP P35442
A	1181	HIS	-	EXPRESSION TAG	UNP P35442

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	Ca	0	0
			30	30		

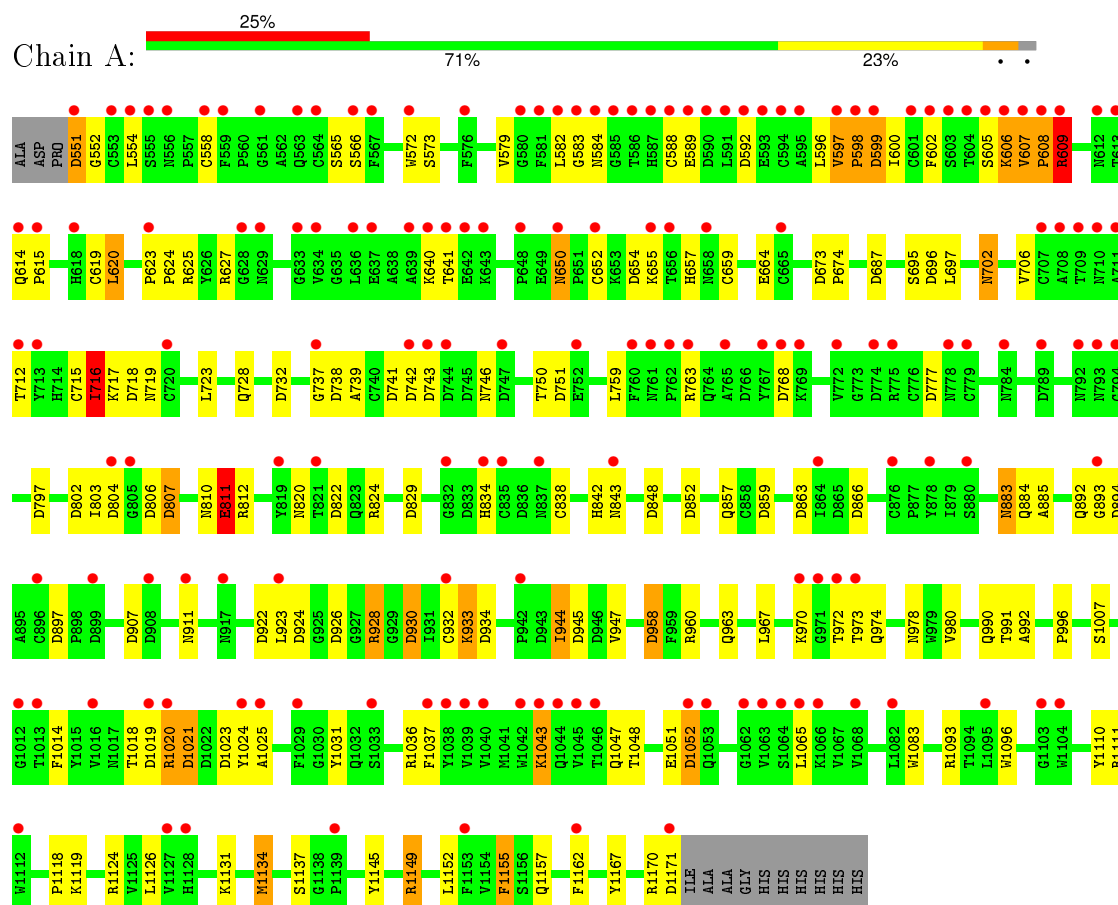
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	116	Total	O	0	0
			116	116		

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: thrombospondin-2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.44Å 121.59Å 155.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 26.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.60) 94.9 (26.86-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.284 0.215 , 0.275	Depositor DCC
R_{free} test set	2575 reflections (10.94%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26140 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: 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	0.57	0/4962	0.87	27/6755 (0.4%)

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
2	A	1	0

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	866	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	738	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	797	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	718	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	958	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	924	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	945	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	930	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	592	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	848	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	926	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	654	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	852	ASP	CB-CG-OD2	5.30	123.08	118.30
1	A	1171	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	863	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	802	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	804	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	934	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	768	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	687	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	551	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	599	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	859	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	732	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	907	ASP	CB-CG-OD2	5.06	122.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	3	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4248	87	0
2	A	39	0	34	0	0
3	A	28	0	25	0	0
4	A	28	0	26	5	0
5	A	30	0	0	0	0
6	A	116	0	0	1	0
All	All	5085	0	4333	87	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 9.

All (87) 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:A:597:VAL:HB	1:A:598:PRO:CD	1.90	1.02
1:A:597:VAL:HB	1:A:598:PRO:HD3	1.03	0.99
1:A:597:VAL:CB	1:A:598:PRO:HD3	1.93	0.97
1:A:719:ASN:H	1:A:728:GLN:HE22	1.25	0.83
1:A:608:PRO:O	1:A:609:ARG:HB2	1.79	0.81
1:A:810:ASN:O	1:A:811:GLU:HB3	1.83	0.78
1:A:751:ASP:HB3	6:A:1320:HOH:O	1.85	0.75
1:A:978:ASN:H	1:A:990:GLN:HE21	1.35	0.74
1:A:1110:TYR:CE2	1:A:1134:MSE:HE3	2.23	0.73
1:A:606:LYS:HB3	1:A:608:PRO:HD2	1.71	0.71
1:A:572:TRP:NE1	4:A:6:NAG:H82	2.10	0.66
1:A:572:TRP:CD1	4:A:6:NAG:C8	2.78	0.66
1:A:972:THR:C	1:A:974:GLN:H	1.99	0.66
1:A:883:ASN:HD22	1:A:884:GLN:N	1.95	0.64
1:A:572:TRP:HE1	4:A:6:NAG:H82	1.63	0.64
1:A:607:VAL:H	1:A:608:PRO:CD	2.11	0.64
1:A:978:ASN:H	1:A:990:GLN:NE2	1.95	0.63
1:A:1024:TYR:HB2	1:A:1155:PHE:HB3	1.80	0.63
1:A:883:ASN:ND2	1:A:885:ALA:H	1.97	0.63
1:A:958:ASP:OD1	1:A:960:ARG:HB2	2.00	0.61
1:A:607:VAL:H	1:A:608:PRO:HD3	1.65	0.61
1:A:883:ASN:HD22	1:A:883:ASN:C	2.04	0.61
1:A:607:VAL:N	1:A:608:PRO:CD	2.65	0.60
1:A:1124:ARG:CZ	1:A:1126:LEU:HD21	2.32	0.60
1:A:695:SER:HB3	1:A:702:ASN:HD21	1.66	0.60
1:A:715:CYS:O	1:A:716:ILE:HB	2.03	0.59
1:A:978:ASN:N	1:A:990:GLN:HE21	2.01	0.59
1:A:614:GLN:HB2	1:A:615:PRO:HD3	1.84	0.58
1:A:810:ASN:O	1:A:811:GLU:CB	2.52	0.57
1:A:990:GLN:NE2	1:A:992:ALA:H	2.03	0.57
1:A:552:GLY:O	4:A:6:NAG:H83	2.05	0.56
1:A:602:PHE:O	1:A:609:ARG:HG3	2.06	0.55
1:A:572:TRP:CD1	4:A:6:NAG:H82	2.41	0.55
1:A:719:ASN:N	1:A:728:GLN:HE22	2.01	0.55
1:A:1152:LEU:HD13	1:A:1162:PHE:CG	2.42	0.53
1:A:928:ARG:NH1	1:A:932:CYS:O	2.38	0.53
1:A:990:GLN:HE22	1:A:992:ALA:H	1.55	0.53
1:A:609:ARG:NH2	1:A:623:PRO:HB3	2.25	0.52
1:A:582:LEU:N	1:A:589:GLU:O	2.42	0.51
1:A:883:ASN:HD22	1:A:885:ALA:H	1.57	0.51
1:A:650:ASN:HD21	1:A:652:CYS:HB2	1.75	0.51
1:A:657:HIS:HD2	1:A:659:CYS:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ARG:HB3	1:A:1145:TYR:CE2	2.47	0.50
1:A:1043:LYS:HZ1	1:A:1047:GLN:HB3	1.76	0.50
1:A:763:ARG:HH11	1:A:763:ARG:HG3	1.77	0.50
1:A:582:LEU:HG	1:A:583:GLY:H	1.76	0.49
1:A:1043:LYS:NZ	1:A:1047:GLN:HB3	2.28	0.49
1:A:609:ARG:HH11	1:A:620:LEU:HB3	1.78	0.48
1:A:972:THR:C	1:A:974:GLN:N	2.62	0.48
1:A:719:ASN:H	1:A:728:GLN:NE2	2.04	0.48
1:A:829:ASP:HB3	1:A:842:HIS:CD2	2.48	0.48
1:A:820:ASN:HB3	1:A:834:HIS:HD2	1.79	0.48
1:A:598:PRO:HG2	1:A:600:ILE:HG13	1.96	0.47
1:A:715:CYS:O	1:A:716:ILE:CB	2.63	0.47
1:A:1152:LEU:HD13	1:A:1162:PHE:CB	2.44	0.47
1:A:723:LEU:HD23	1:A:739:ALA:HB1	1.96	0.47
1:A:650:ASN:C	1:A:650:ASN:HD22	2.17	0.47
1:A:843:ASN:HB3	1:A:857:GLN:HG3	1.96	0.47
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.43	0.47
1:A:1124:ARG:NH2	1:A:1126:LEU:HD21	2.30	0.46
1:A:1023:ASP:HA	1:A:1043:LYS:HE2	1.96	0.46
1:A:1018:THR:OG1	1:A:1020:ARG:HG2	2.16	0.46
1:A:737:GLY:O	1:A:741:ASP:HB2	2.16	0.46
1:A:624:PRO:O	1:A:625:ARG:HB2	2.16	0.45
1:A:674:PRO:HD2	1:A:944:ILE:HG23	1.99	0.45
1:A:1021:ASP:HB3	1:A:1157:GLN:OE1	2.16	0.45
1:A:1031:TYR:HA	1:A:1037:PHE:HB3	1.98	0.45
1:A:1096:TRP:CE2	1:A:1137:SER:HA	2.51	0.45
1:A:697:LEU:HD13	1:A:1111:ARG:HB2	1.99	0.45
1:A:803:ILE:HG23	1:A:810:ASN:HD21	1.82	0.44
1:A:947:VAL:HB	1:A:1167:TYR:O	2.18	0.44
1:A:963:GLN:OE1	1:A:1149:ARG:NH2	2.37	0.43
1:A:743:ASP:OD2	1:A:746:ASN:HA	2.19	0.43
1:A:609:ARG:HD3	1:A:609:ARG:HA	1.85	0.42
1:A:922:ASP:HA	1:A:930:ASP:OD1	2.19	0.42
1:A:673:ASP:OD2	1:A:933:LYS:O	2.38	0.41
1:A:657:HIS:CD2	1:A:659:CYS:HB2	2.56	0.41
1:A:1110:TYR:CE2	1:A:1134:MSE:CE	3.00	0.41
1:A:806:ASP:O	1:A:807:ASP:HB2	2.19	0.41
1:A:892:GLN:HB3	1:A:897:ASP:HB2	2.03	0.41
1:A:1043:LYS:HE3	1:A:1083:TRP:CZ2	2.56	0.41
1:A:893:GLY:O	1:A:894:ASP:C	2.59	0.41
1:A:1007:SER:HA	1:A:1118:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:PHE:CE2	1:A:1025:ALA:HB3	2.55	0.41
1:A:673:ASP:HA	1:A:674:PRO:HA	1.86	0.40
1:A:944:ILE:H	1:A:944:ILE:HG13	1.50	0.40
1:A:996:PRO:HD3	1:A:1155:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/634 (98%)	550 (89%)	57 (9%)	12 (2%)	10	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	VAL
1	A	598	PRO
1	A	609	ARG
1	A	716	ILE
1	A	584	ASN
1	A	608	PRO
1	A	706	VAL
1	A	811	GLU
1	A	973	THR
1	A	558	CYS
1	A	970	LYS
1	A	607	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	540/544 (99%)	483 (89%)	57 (11%)	8 15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	551	ASP
1	A	554	LEU
1	A	565	SER
1	A	566	SER
1	A	573	SER
1	A	579	VAL
1	A	588	CYS
1	A	596	LEU
1	A	599	ASP
1	A	605	SER
1	A	606	LYS
1	A	609	ARG
1	A	619	CYS
1	A	620	LEU
1	A	627	ARG
1	A	640	LYS
1	A	641	THR
1	A	650	ASN
1	A	655	LYS
1	A	664	GLU
1	A	702	ASN
1	A	712	THR
1	A	716	ILE
1	A	717	LYS
1	A	742	ASP
1	A	750	THR
1	A	759	LEU
1	A	807	ASP
1	A	811	GLU
1	A	812	ARG

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Mol	Chain	Res	Type
1	A	822	ASP
1	A	824	ARG
1	A	838	CYS
1	A	883	ASN
1	A	911	ASN
1	A	923	LEU
1	A	928	ARG
1	A	933	LYS
1	A	944	ILE
1	A	967	LEU
1	A	980	VAL
1	A	991	THR
1	A	1019	ASP
1	A	1020	ARG
1	A	1021	ASP
1	A	1043	LYS
1	A	1048	THR
1	A	1051	GLU
1	A	1052	ASP
1	A	1065	LEU
1	A	1093	ARG
1	A	1119	LYS
1	A	1131	LYS
1	A	1134	MSE
1	A	1149	ARG
1	A	1155	PHE
1	A	1170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	ASN
1	A	657	HIS
1	A	728	GLN
1	A	834	HIS
1	A	842	HIS
1	A	883	ASN
1	A	911	ASN
1	A	990	GLN
1	A	1091	GLN
1	A	1113	HIS

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 ⓘ

5 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	$\# Z > 2$
2	NAG	A	1	1,2	14,14,15	0.71	1 (7%)	15,19,21	1.27	1 (6%)
2	NAG	A	2	2	14,14,15	0.62	0	15,19,21	0.70	0
2	MAN	A	3	2	11,11,12	0.64	0	14,15,17	2.19	3 (21%)
3	NAG	A	4	1,3	14,14,15	0.67	0	15,19,21	1.02	1 (6%)
3	NAG	A	5	3	14,14,15	0.48	0	15,19,21	0.68	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	A	3	2	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	A	4	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	C1-C2	2.12	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	NAG	C4-C3-C2	2.76	115.53	111.23
2	A	3	MAN	O5-C1-C2	2.95	115.65	110.86
2	A	1	NAG	C1-O5-C5	4.27	117.67	112.25
2	A	3	MAN	C1-C2-C3	5.07	115.54	109.54
2	A	3	MAN	C1-O5-C5	5.40	119.10	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	3	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 30 are monoatomic - leaving 2 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	$\# Z > 2$
4	NAG	A	6	1	14,14,15	0.65	0	15,19,21	0.96	0
4	NAG	A	7	1	14,14,15	0.58	0	15,19,21	1.19	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
4	NAG	A	6	1	-	0/6/23/26	0/1/1/1
4	NAG	A	7	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	7	NAG	C1-O5-C5	3.89	117.18	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6	NAG	5	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	616/634 (97%)	1.55	161 (26%) 1 0	40, 61, 122, 158	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	15.0
1	A	582	LEU	9.4
1	A	576	PHE	9.2
1	A	566	SER	8.1
1	A	607	VAL	7.8
1	A	634	VAL	7.8
1	A	973	THR	7.7
1	A	972	THR	7.5
1	A	641	THR	6.9
1	A	595	ALA	6.7
1	A	709	THR	6.2
1	A	712	THR	6.2
1	A	603	SER	5.8
1	A	710	ASN	5.4
1	A	588	CYS	5.2
1	A	594	CYS	5.2
1	A	1171	ASP	5.2
1	A	581	PHE	5.1
1	A	587	HIS	5.0
1	A	1039	VAL	4.7
1	A	551	ASP	4.7
1	A	556	ASN	4.6
1	A	580	GLY	4.5
1	A	584	ASN	4.5
1	A	629	ASN	4.4
1	A	615	PRO	4.4
1	A	1040	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	804	ASP	4.3
1	A	606	LYS	4.3
1	A	642	GLU	4.0
1	A	899	ASP	4.0
1	A	1042	TRP	4.0
1	A	762	PRO	4.0
1	A	597	VAL	4.0
1	A	761	ASN	3.9
1	A	589	GLU	3.9
1	A	737	GLY	3.9
1	A	614	GLN	3.9
1	A	779	CYS	3.8
1	A	835	CYS	3.7
1	A	742	ASP	3.7
1	A	628	GLY	3.7
1	A	1025	ALA	3.7
1	A	711	ALA	3.7
1	A	1052	ASP	3.6
1	A	1065	LEU	3.6
1	A	1153	PHE	3.4
1	A	708	ALA	3.4
1	A	942	PRO	3.3
1	A	558	CYS	3.3
1	A	602	PHE	3.3
1	A	767	TYR	3.3
1	A	639	ALA	3.3
1	A	752	GLU	3.2
1	A	1053	GLN	3.2
1	A	585	GLY	3.2
1	A	1045	VAL	3.2
1	A	559	PHE	3.2
1	A	599	ASP	3.2
1	A	971	GLY	3.2
1	A	1082	LEU	3.2
1	A	713	TYR	3.1
1	A	864	ILE	3.1
1	A	608	PRO	3.1
1	A	605	SER	3.1
1	A	1063	VAL	3.1
1	A	586	THR	3.1
1	A	1020	ARG	3.0
1	A	652	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	843	ASN	3.0
1	A	1013	THR	3.0
1	A	707	CYS	3.0
1	A	778	ASN	3.0
1	A	893	GLY	3.0
1	A	604	THR	2.9
1	A	834	HIS	2.8
1	A	637	GLU	2.8
1	A	1044	GLN	2.8
1	A	1139	PRO	2.8
1	A	794	GLY	2.8
1	A	792	ASN	2.8
1	A	970	LYS	2.8
1	A	821	THR	2.7
1	A	837	ASN	2.7
1	A	591	LEU	2.7
1	A	1037	PHE	2.7
1	A	555	SER	2.7
1	A	760	PHE	2.7
1	A	1103	GLY	2.6
1	A	1024	TYR	2.6
1	A	609	ARG	2.6
1	A	618	HIS	2.6
1	A	593	GLU	2.6
1	A	648	PRO	2.6
1	A	636	LEU	2.5
1	A	1062	GLY	2.5
1	A	896	CYS	2.5
1	A	1064	SER	2.5
1	A	789	ASP	2.5
1	A	878	TYR	2.5
1	A	1046	THR	2.4
1	A	564	CYS	2.4
1	A	768	ASP	2.4
1	A	554	LEU	2.4
1	A	650	ASN	2.4
1	A	601	CYS	2.4
1	A	613	THR	2.3
1	A	747	ASP	2.3
1	A	1095	LEU	2.3
1	A	658	ASN	2.3
1	A	572	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1038	TYR	2.3
1	A	1043	LYS	2.3
1	A	1128	HIS	2.3
1	A	612	ASN	2.3
1	A	784	ASN	2.3
1	A	832	GLY	2.3
1	A	1112	TRP	2.3
1	A	655	LYS	2.3
1	A	774	ASP	2.2
1	A	1066	LYS	2.2
1	A	592	ASP	2.2
1	A	765	ALA	2.2
1	A	563	GLN	2.2
1	A	1012	GLY	2.2
1	A	1068	VAL	2.2
1	A	793	ASN	2.2
1	A	656	THR	2.2
1	A	932	CYS	2.2
1	A	1029	PHE	2.2
1	A	553	CYS	2.2
1	A	805	GLY	2.2
1	A	561	GLY	2.2
1	A	917	ASN	2.2
1	A	876	CYS	2.2
1	A	769	LYS	2.2
1	A	775	ARG	2.2
1	A	744	ASP	2.2
1	A	1104	TRP	2.1
1	A	640	LYS	2.1
1	A	908	ASP	2.1
1	A	720	CYS	2.1
1	A	598	PRO	2.1
1	A	911	ASN	2.1
1	A	643	LYS	2.1
1	A	880	SER	2.1
1	A	1019	ASP	2.1
1	A	772	VAL	2.1
1	A	567	PHE	2.1
1	A	1162	PHE	2.1
1	A	623	PRO	2.1
1	A	763	ARG	2.1
1	A	1016	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	743	ASP	2.0
1	A	665	CYS	2.0
1	A	923	LEU	2.0
1	A	1033	SER	2.0
1	A	590	ASP	2.0
1	A	633	GLY	2.0
1	A	819	TYR	2.0
1	A	1127	VAL	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
3	NAG	A	4	14/15	0.76	0.22	-0.50	80,89,98,107	0
2	MAN	A	3	11/12	0.57	0.29	-	133,136,137,138	0
3	NAG	A	5	14/15	0.62	0.45	-	115,123,126,127	0
2	NAG	A	1	14/15	0.53	0.37	-	114,119,121,122	0
2	NAG	A	2	14/15	0.40	0.80	-	123,127,131,132	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
4	NAG	A	6	14/15	0.74	0.33	0.26	103,117,128,133	0
5	CA	A	1190	1/1	0.99	0.17	-1.42	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	A	1208	1/1	0.95	0.10	-1.94	58,58,58,58	0
5	CA	A	1188	1/1	0.84	0.10	-1.95	55,55,55,55	0
5	CA	A	1195	1/1	0.98	0.12	-2.10	53,53,53,53	0
5	CA	A	1204	1/1	0.96	0.14	-2.11	70,70,70,70	0
5	CA	A	1206	1/1	0.93	0.11	-2.21	62,62,62,62	0
5	CA	A	1198	1/1	0.98	0.11	-2.25	50,50,50,50	0
5	CA	A	1200	1/1	0.97	0.07	-2.36	62,62,62,62	0
5	CA	A	1196	1/1	0.97	0.12	-2.36	52,52,52,52	0
5	CA	A	1201	1/1	0.90	0.08	-2.42	70,70,70,70	0
5	CA	A	1191	1/1	0.99	0.08	-2.45	53,53,53,53	0
5	CA	A	1189	1/1	0.97	0.07	-2.47	61,61,61,61	0
5	CA	A	1192	1/1	0.96	0.10	-2.48	55,55,55,55	0
5	CA	A	1194	1/1	0.94	0.11	-2.49	55,55,55,55	0
5	CA	A	1185	1/1	0.99	0.11	-2.56	57,57,57,57	0
5	CA	A	1187	1/1	0.87	0.09	-2.56	70,70,70,70	0
5	CA	A	1186	1/1	0.96	0.13	-2.65	58,58,58,58	0
5	CA	A	1197	1/1	0.92	0.13	-2.68	63,63,63,63	0
5	CA	A	1199	1/1	0.89	0.11	-2.80	59,59,59,59	0
5	CA	A	1202	1/1	0.76	0.14	-2.81	71,71,71,71	0
5	CA	A	1209	1/1	0.96	0.13	-2.87	45,45,45,45	0
5	CA	A	1205	1/1	0.94	0.14	-3.07	72,72,72,72	0
5	CA	A	1193	1/1	0.98	0.07	-3.10	57,57,57,57	0
5	CA	A	1184	1/1	0.81	0.12	-3.25	74,74,74,74	0
5	CA	A	1210	1/1	0.93	0.14	-3.39	51,51,51,51	0
5	CA	A	1211	1/1	0.94	0.08	-3.60	116,116,116,116	0
5	CA	A	1183	1/1	0.97	0.08	-4.23	50,50,50,50	0
5	CA	A	1203	1/1	0.93	0.08	-4.36	81,81,81,81	0
5	CA	A	1207	1/1	0.93	0.07	-5.54	65,65,65,65	0
5	CA	A	1182	1/1	0.96	0.08	-6.75	46,46,46,46	0
4	NAG	A	7	14/15	0.67	0.32	-	140,146,149,149	0

6.5 Other polymers ⓘ

There are no such residues in this entry.