



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1E03
Title : PLASMA ALPHA ANTITHROMBIN-III AND PENTASACCHARIDE
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Deposited on : 2000-03-09
Resolution : 2.90 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

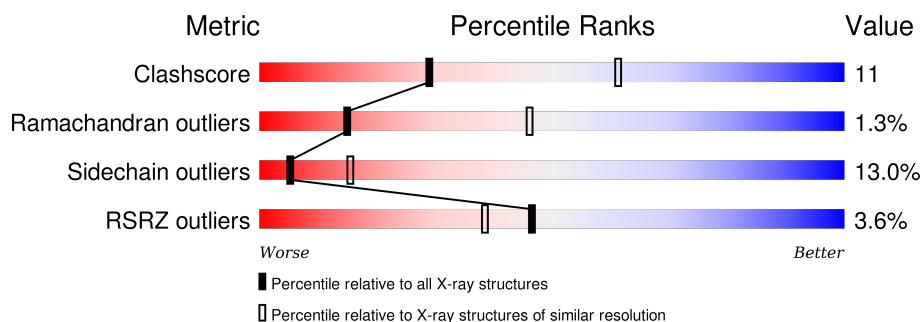
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	I	432	
1	L	432	

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	NAG	I	802	X	-	-	-
4	NAG	L	841	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	L	842	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7001 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.

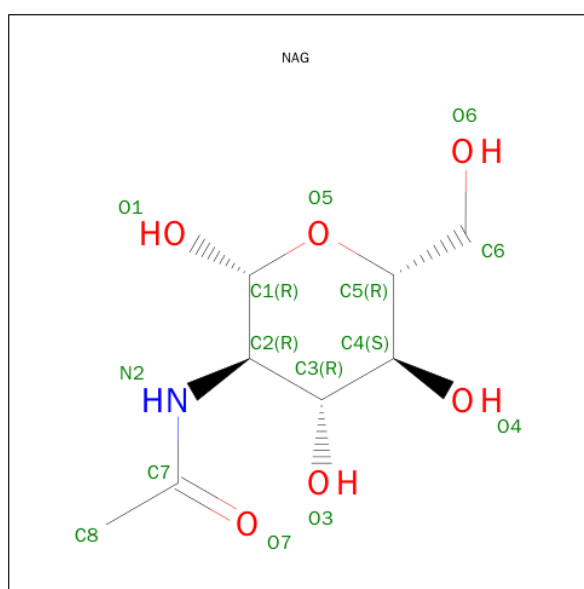
- Molecule 1 is a protein called ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	418	Total	C	N	O	S	0	0	0
			3279	2090	546	626	17			
1	L	423	Total	C	N	O	S	0	0	0
			3335	2122	560	635	18			

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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

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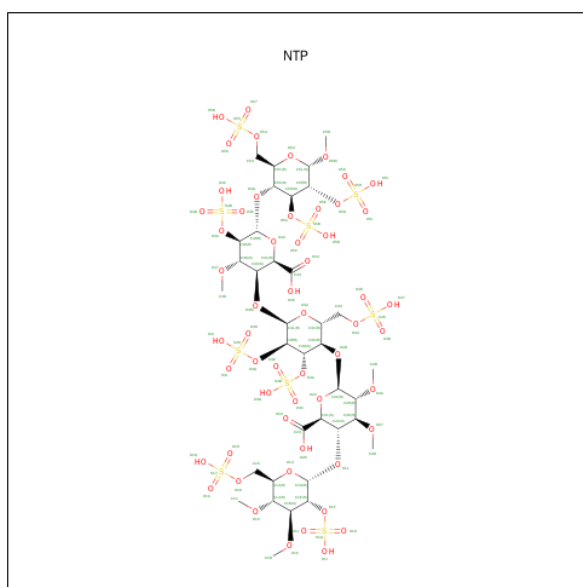
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is HEPARIN PENTASACCHARIDE (three-letter code: NTP) (formula: $C_{36}H_{60}O_{55}S_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	O	S	0	0
			100	36	55	9		
5	L	1	Total	C	O	S	0	0
			100	36	55	9		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	8	Total	O	0	0
			8	8		

- Molecule 1: ANTITHROMBIN-III



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.51Å 87.07Å 97.35Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.90) 94.6 (19.94-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.252 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.8	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23386 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NTP, BMA, 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	I	0.46	0/3345	1.00	2/4531 (0.0%)
1	L	0.47	0/3401	1.04	6/4601 (0.1%)
All	All	0.47	0/6746	1.02	8/9132 (0.1%)

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	L	0	1
2	I	1	0
All	All	1	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	47	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	L	47	ARG	CD-NE-CZ	7.05	133.47	123.60
1	I	200	ASP	CB-CG-OD1	6.14	123.83	118.30
1	L	200	ASP	CB-CG-OD1	6.14	123.82	118.30
1	L	222	LYS	N-CA-CB	5.57	120.63	110.60
1	L	17	MET	CA-CB-CG	5.49	122.64	113.30
1	I	322	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	L	40	ILE	CB-CA-C	-5.01	101.57	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	802	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	6	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	I	3279	0	3200	76	0
1	L	3335	0	3278	58	0
2	I	28	0	25	0	0
3	I	14	0	13	1	0
3	L	14	0	13	0	0
4	I	39	0	34	1	0
4	L	78	0	68	3	0
5	I	100	0	49	10	0
5	L	100	0	49	16	0
6	I	6	0	0	0	0
6	L	8	0	0	1	0
All	All	7001	0	6729	156	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 11.

All (156) 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:L:901:NTP:O1H	5:L:901:NTP:H1D2	1.33	1.25
5:L:901:NTP:O1H	5:L:901:NTP:C1D	1.90	1.17
5:L:901:NTP:C1K	5:L:901:NTP:H282	1.85	1.07
5:L:901:NTP:H1K	5:L:901:NTP:H282	1.08	1.04
5:L:901:NTP:S1G	5:L:901:NTP:H1D3	2.09	0.91
5:L:901:NTP:S1G	5:L:901:NTP:C1D	2.64	0.85
1:L:20:MET:HE2	4:L:841:NAG:H4	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:901:NTP:C28	5:I:901:NTP:O2A	2.31	0.79
1:L:129:ARG:HD3	1:L:417:LEU:HD21	1.65	0.79
5:L:901:NTP:H113	5:L:901:NTP:O1C	1.83	0.78
5:L:901:NTP:C11	5:L:901:NTP:O1C	2.34	0.75
1:I:144:ASN:HB3	1:I:217:ASN:HA	1.70	0.74
5:L:901:NTP:H3L	5:L:901:NTP:H483	1.70	0.74
5:I:901:NTP:H283	5:I:901:NTP:O2A	1.89	0.73
1:I:141:VAL:HG23	1:I:220:TYR:HB3	1.71	0.73
5:I:901:NTP:H4F	5:I:901:NTP:H531	1.71	0.71
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.71	0.70
5:L:901:NTP:H1D3	5:L:901:NTP:O1F	1.91	0.70
5:I:901:NTP:H151	5:I:901:NTP:H112	1.75	0.68
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.77	0.65
1:I:183:ARG:NH2	1:I:204:SER:HA	2.12	0.64
1:I:218:THR:HG22	1:I:370:LYS:HB3	1.80	0.64
1:L:7:ILE:HD12	1:L:15:ILE:HD13	1.79	0.63
1:L:211:THR:HA	1:L:391:ALA:O	1.99	0.62
1:L:270:LEU:HD23	1:L:283:LEU:HD12	1.80	0.62
1:L:428:ASN:HD21	1:L:430:CYS:HB2	1.63	0.62
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.82	0.61
1:I:274:PHE:HD2	1:I:279:ILE:HG22	1.65	0.61
1:I:264:ALA:O	1:I:265:GLU:HB2	2.00	0.61
1:I:48:VAL:HG13	1:I:126:LEU:HB2	1.84	0.60
1:L:20:MET:HB2	4:L:841:NAG:H61	1.85	0.58
1:L:198:ILE:HG23	1:L:370:LYS:HG2	1.86	0.58
5:I:901:NTP:H282	5:I:901:NTP:H2B2	1.86	0.58
1:L:49:TRP:CZ2	1:L:53:LYS:HD2	2.39	0.58
1:L:365:SER:HB3	1:L:392:GLY:H	1.69	0.57
1:I:202:ILE:HD13	1:I:207:ILE:HD11	1.86	0.56
5:I:901:NTP:H282	5:I:901:NTP:C2B	2.36	0.56
1:L:222:LYS:HD2	1:L:381:GLU:HG3	1.89	0.55
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.89	0.55
1:L:43:ALA:HA	5:L:901:NTP:H1D2	1.89	0.55
1:I:139:LYS:NZ	1:I:197:ARG:HH22	2.05	0.55
4:L:861:NAG:H62	4:L:862:NAG:N2	2.22	0.54
1:I:25:SER:HB2	1:I:26:PRO:CD	2.38	0.54
1:I:134:ALA:HA	1:I:279:ILE:HD13	1.90	0.54
1:I:22:ILE:HD12	1:I:24:ARG:HE	1.72	0.53
1:I:124:ALA:HB2	1:I:165:VAL:HG22	1.90	0.53
1:I:190:VAL:HG11	1:I:201:VAL:HG21	1.91	0.53
1:I:130:LEU:HD13	1:I:421:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:LYS:HD2	1:I:119:ILE:HG21	1.90	0.52
1:L:57:ARG:HB2	1:L:107:LYS:HG3	1.90	0.52
1:L:284:ILE:HB	1:L:409:LEU:HB2	1.91	0.52
5:L:901:NTP:H1K	5:L:901:NTP:C28	2.05	0.52
1:I:163:GLU:HB2	1:I:169:LYS:HG2	1.92	0.52
1:I:204:SER:O	1:I:205:GLU:HB2	2.09	0.51
1:I:390:ILE:HA	1:L:319:HIS:HB2	1.92	0.51
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.46	0.51
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.91	0.50
1:L:295:VAL:HG13	1:L:307:TRP:HH2	1.76	0.50
1:I:44:THR:HG21	1:I:417:LEU:HD13	1.93	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.12	0.50
1:I:273:PRO:HA	1:I:280:THR:HG22	1.94	0.50
1:I:7:ILE:HG23	1:I:164:LEU:HG	1.94	0.49
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.47	0.49
1:L:63:TYR:HE2	1:L:296:GLU:HG2	1.77	0.49
4:I:841:NAG:H62	4:I:842:NAG:N2	2.28	0.49
1:I:391:ALA:O	1:L:321:PRO:HD3	2.12	0.49
5:L:901:NTP:S1G	5:L:901:NTP:H1D2	2.36	0.49
1:I:139:LYS:HZ3	1:I:197:ARG:HH22	1.61	0.49
1:I:25:SER:CB	1:I:26:PRO:CD	2.90	0.49
1:I:300:THR:HB	1:I:301:PRO:HD2	1.94	0.49
1:L:55:ASN:HB2	6:L:2001:HOH:O	2.12	0.49
1:L:364:VAL:HG22	1:L:390:ILE:HD13	1.95	0.48
1:I:198:ILE:HD11	1:I:220:TYR:HB2	1.96	0.48
1:I:70:LYS:HD3	1:I:76:ILE:HD13	1.96	0.48
1:I:186:ILE:HG21	1:I:202:ILE:HD12	1.95	0.47
1:I:108:PHE:O	1:I:111:ILE:HG12	2.14	0.47
1:I:75:ASN:HB3	1:I:325:ILE:HG12	1.96	0.47
1:L:149:ASP:HB3	1:L:152:LEU:HD12	1.94	0.47
5:I:901:NTP:C28	5:I:901:NTP:C2B	2.91	0.47
1:L:355:VAL:HG21	1:L:359:ARG:HB3	1.96	0.47
1:I:316:LEU:HB3	1:I:400:VAL:HG12	1.96	0.47
1:L:40:ILE:H	1:L:40:ILE:HG13	1.51	0.47
1:I:392:GLY:HA3	1:L:321:PRO:HG3	1.96	0.47
1:L:282:VAL:HG21	1:L:308:LEU:HD21	1.97	0.47
1:I:56:SER:HA	1:I:420:ILE:HD12	1.96	0.47
1:I:131:TYR:HD1	1:I:140:LEU:HD23	1.79	0.47
5:I:901:NTP:O2A	5:I:901:NTP:H282	2.14	0.46
1:I:198:ILE:HG23	1:I:370:LYS:HG2	1.97	0.46
1:L:39:LYS:NZ	1:L:46:ARG:HH22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:901:NTP:O1F	5:L:901:NTP:C1D	2.49	0.46
5:I:901:NTP:C4F	5:I:901:NTP:H531	2.40	0.46
1:I:201:VAL:HG11	1:I:216:VAL:HG13	1.98	0.46
1:L:152:LEU:HD13	1:L:212:VAL:HG13	1.97	0.46
1:L:17:MET:O	1:L:18:ASN:C	2.54	0.46
1:L:395:LEU:O	1:L:397:PRO:HD3	2.15	0.46
1:L:299:LEU:HD11	1:L:304:LEU:HD12	1.98	0.46
1:I:47:ARG:O	1:I:50:GLU:HG2	2.16	0.46
1:I:51:LEU:HD21	1:I:123:PHE:CD2	2.51	0.45
1:L:57:ARG:CB	1:L:107:LYS:HG3	2.46	0.45
1:L:71:ASN:O	1:L:74:ASP:HB2	2.16	0.45
1:I:131:TYR:HE2	3:I:821:NAG:H82	1.81	0.45
1:I:135:ASN:O	1:I:136:LYS:C	2.55	0.45
1:L:359:ARG:HG2	1:L:361:ASP:OD1	2.17	0.45
1:I:105:VAL:HG21	1:I:340:LEU:HB2	1.97	0.45
1:I:224:LEU:HD12	1:I:378:GLU:O	2.17	0.45
1:I:92:LEU:HD21	1:I:161:ILE:HG21	1.99	0.45
1:L:190:VAL:HG11	1:L:201:VAL:CG2	2.46	0.45
1:I:263:VAL:HB	1:I:264:ALA:H	1.60	0.45
1:I:120:HIS:H	1:I:120:HIS:CD2	2.34	0.45
1:L:47:ARG:NH1	1:L:114:LYS:HB3	2.32	0.44
1:L:286:PRO:HG3	1:L:292:LEU:HD13	1.97	0.44
1:L:204:SER:O	1:L:205:GLU:HB2	2.17	0.44
1:L:40:ILE:HD11	1:L:46:ARG:NE	2.32	0.44
1:I:145:ARG:HB2	1:I:189:TRP:CH2	2.53	0.44
1:L:40:ILE:HD11	1:L:46:ARG:HE	1.83	0.44
1:I:261:ARG:HG3	1:I:263:VAL:HG13	1.98	0.44
1:L:71:ASN:OD1	1:L:73:ASN:HB2	2.18	0.43
1:I:324:ARG:CG	1:I:374:GLU:HG3	2.49	0.43
1:I:343:LEU:HD11	1:I:351:LEU:HD21	1.99	0.43
5:L:901:NTP:H3L	5:L:901:NTP:O3K	2.18	0.43
1:I:274:PHE:CD2	1:I:279:ILE:HG22	2.49	0.43
1:I:149:ASP:HA	1:I:173:LEU:O	2.18	0.43
1:I:236:LYS:HA	1:I:236:LYS:HD2	1.91	0.43
1:I:139:LYS:O	1:I:221:PHE:HA	2.19	0.43
1:I:40:ILE:HA	1:I:41:PRO:HD3	1.89	0.43
1:L:147:PHE:HB3	1:L:173:LEU:HD12	2.01	0.43
1:I:198:ILE:HG21	1:I:218:THR:HG21	2.01	0.42
1:L:38:GLN:O	1:L:39:LYS:C	2.57	0.42
1:I:63:TYR:OH	1:I:425:ARG:HB2	2.18	0.42
1:I:130:LEU:HD11	1:I:419:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:MET:HG2	1:L:17:MET:O	2.20	0.42
1:I:175:PHE:O	1:I:209:GLU:HA	2.19	0.42
1:I:152:LEU:HD22	1:I:360:ASP:OD2	2.20	0.42
1:I:217:ASN:O	1:I:369:HIS:HA	2.20	0.42
1:I:7:ILE:HD13	1:I:7:ILE:H	1.83	0.42
1:L:428:ASN:HD22	1:L:428:ASN:C	2.23	0.42
1:L:405:ASN:OD1	1:L:406:ARG:N	2.53	0.42
1:L:40:ILE:HG23	1:L:49:TRP:CG	2.56	0.41
1:I:197:ARG:NH2	1:I:381:GLU:OE2	2.53	0.41
1:L:229:PHE:CD2	1:L:254:GLN:HB2	2.56	0.41
1:I:332:LYS:O	1:I:336:GLN:HG3	2.20	0.41
5:I:901:NTP:H483	5:I:901:NTP:H3L	2.02	0.41
1:L:39:LYS:HZ3	1:L:46:ARG:HH22	1.68	0.41
1:I:391:ALA:HB2	1:L:285:LEU:HD21	2.02	0.41
1:I:299:LEU:HA	1:I:299:LEU:HD12	1.92	0.41
1:I:76:ILE:HG22	1:I:77:PHE:H	1.85	0.41
1:L:287:LYS:O	1:L:288:PRO:C	2.59	0.41
1:L:13:ARG:HG3	5:L:901:NTP:S3H	2.61	0.41
1:I:292:LEU:HD21	1:I:425:ARG:HG3	2.02	0.41
1:I:119:ILE:O	1:I:123:PHE:HD2	2.04	0.41
1:L:324:ARG:HA	1:L:373:LEU:O	2.20	0.41
1:L:229:PHE:HB2	1:L:377:GLU:HA	2.02	0.41
1:L:45:ASN:O	1:L:46:ARG:C	2.58	0.40
1:I:96:ASN:HB3	1:I:97:ASP:H	1.66	0.40
1:I:255:GLU:HG2	1:I:317:VAL:HG22	2.03	0.40
1:L:5:VAL:HB	1:L:6:ASP:H	1.59	0.40

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	I	414/432 (96%)	371 (90%)	36 (9%)	7 (2%)	11	38
1	L	419/432 (97%)	376 (90%)	39 (9%)	4 (1%)	19	54
All	All	833/864 (96%)	747 (90%)	75 (9%)	11 (1%)	15	46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	136	LYS
1	I	179	ALA
1	I	356	ALA
1	L	357	GLU
1	L	358	GLY
1	I	77	PHE
1	I	332	LYS
1	L	18	ASN
1	L	288	PRO
1	I	407	PRO
1	I	429	PRO

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	I	356/383 (93%)	309 (87%)	47 (13%)	5	14
1	L	365/383 (95%)	318 (87%)	47 (13%)	5	16
All	All	721/766 (94%)	627 (87%)	94 (13%)	5	15

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	ILE
1	I	9	THR
1	I	15	ILE
1	I	61	THR
1	I	76	ILE

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Mol	Chain	Res	Type
1	I	81	LEU
1	I	82	SER
1	I	96	ASN
1	I	114	LYS
1	I	129	ARG
1	I	137	SER
1	I	139	LYS
1	I	141	VAL
1	I	142	SER
1	I	144	ASN
1	I	151	SER
1	I	162	SER
1	I	165	VAL
1	I	169	LYS
1	I	171	GLN
1	I	180	GLU
1	I	182	SER
1	I	197	ARG
1	I	200	ASP
1	I	228	LYS
1	I	246	SER
1	I	272	LEU
1	I	284	ILE
1	I	304	LEU
1	I	310	GLU
1	I	316	LEU
1	I	322	ARG
1	I	327	ASP
1	I	330	SER
1	I	334	GLN
1	I	338	MET
1	I	341	VAL
1	I	345	SER
1	I	351	LEU
1	I	355	VAL
1	I	381	GLU
1	I	390	ILE
1	I	400	VAL
1	I	428	ASN
1	I	429	PRO
1	I	430	CYS
1	I	431	VAL

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Mol	Chain	Res	Type
1	L	6	ASP
1	L	14	ASP
1	L	15	ILE
1	L	17	MET
1	L	18	ASN
1	L	23	TYR
1	L	40	ILE
1	L	46	ARG
1	L	47	ARG
1	L	74	ASP
1	L	78	LEU
1	L	113	GLU
1	L	116	SER
1	L	123	PHE
1	L	136	LYS
1	L	138	SER
1	L	145	ARG
1	L	204	SER
1	L	205	GLU
1	L	209	GLU
1	L	213	LEU
1	L	227	SER
1	L	230	SER
1	L	235	ARG
1	L	236	LYS
1	L	237	GLU
1	L	248	SER
1	L	254	GLN
1	L	262	ARG
1	L	263	VAL
1	L	298	GLU
1	L	304	LEU
1	L	312	GLU
1	L	315	MET
1	L	330	SER
1	L	331	LEU
1	L	334	GLN
1	L	340	LEU
1	L	348	LYS
1	L	360	ASP
1	L	389	VAL
1	L	394	SER

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Mol	Chain	Res	Type
1	L	402	PHE
1	L	414	GLU
1	L	418	ASN
1	L	419	THR
1	L	428	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	120	HIS
1	I	428	ASN
1	L	118	GLN
1	L	120	HIS
1	L	428	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

11 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	I	801	1,2	14,14,15	1.60	2 (14%)	15,19,21	3.94	3 (20%)
2	NAG	I	802	2	14,14,15	1.62	3 (21%)	15,19,21	1.22	2 (13%)
4	NAG	I	841	1,4	14,14,15	1.23	1 (7%)	15,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	842	4	14,14,15	1.31	1 (7%)	15,19,21	1.66	3 (20%)
4	BMA	I	843	4	11,11,12	1.00	1 (9%)	14,15,17	0.90	0
4	NAG	L	841	1,4	14,14,15	1.25	1 (7%)	15,19,21	0.86	1 (6%)
4	NAG	L	842	4	14,14,15	1.52	4 (28%)	15,19,21	3.03	6 (40%)
4	BMA	L	843	4	11,11,12	0.94	1 (9%)	14,15,17	1.12	2 (14%)
4	NAG	L	861	1,4	14,14,15	1.27	1 (7%)	15,19,21	1.43	3 (20%)
4	NAG	L	862	4	14,14,15	1.25	1 (7%)	15,19,21	2.00	3 (20%)
4	BMA	L	863	4	11,11,12	1.04	2 (18%)	14,15,17	1.45	1 (7%)

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	I	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	802	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	I	841	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	842	4	-	0/6/23/26	0/1/1/1
4	BMA	I	843	4	-	0/2/19/22	0/1/1/1
4	NAG	L	841	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	842	4	-	0/6/23/26	0/1/1/1
4	BMA	L	843	4	-	0/2/19/22	0/1/1/1
4	NAG	L	861	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	862	4	-	0/6/23/26	0/1/1/1
4	BMA	L	863	4	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	801	NAG	O5-C5	-3.81	1.35	1.43
4	L	842	NAG	O7-C7	-3.79	1.14	1.23
4	I	842	NAG	O7-C7	-3.69	1.14	1.23
4	L	862	NAG	O7-C7	-3.65	1.14	1.23
4	I	841	NAG	O7-C7	-3.57	1.14	1.23
4	L	841	NAG	O7-C7	-3.56	1.14	1.23
2	I	802	NAG	O7-C7	-3.54	1.15	1.23
2	I	801	NAG	O7-C7	-3.52	1.15	1.23
4	L	861	NAG	O7-C7	-3.47	1.15	1.23
2	I	802	NAG	O5-C1	-3.15	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	802	NAG	C1-C2	-2.90	1.48	1.52
4	L	842	NAG	C2-N2	-2.23	1.42	1.46
4	L	842	NAG	C3-C2	-2.11	1.47	1.52
4	L	863	BMA	O5-C1	-2.07	1.40	1.43
4	I	843	BMA	C1-C2	2.22	1.57	1.52
4	L	863	BMA	C1-C2	2.23	1.57	1.52
4	L	843	BMA	C1-C2	2.28	1.57	1.52
4	L	842	NAG	C4-C3	2.52	1.59	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	801	NAG	C4-C3-C2	-5.56	102.58	111.23
4	L	842	NAG	C4-C3-C2	-4.54	104.17	111.23
4	L	863	BMA	C1-C2-C3	-4.45	104.27	109.54
4	L	862	NAG	C4-C3-C2	-4.33	104.50	111.23
2	I	802	NAG	C4-C3-C2	-3.45	105.87	111.23
4	L	842	NAG	O4-C4-C3	-2.90	103.81	110.34
4	L	861	NAG	C4-C3-C2	-2.68	107.06	111.23
4	L	861	NAG	O5-C5-C6	-2.28	102.42	107.35
4	I	842	NAG	C4-C3-C2	-2.28	107.69	111.23
4	I	842	NAG	O4-C4-C3	-2.27	105.24	110.34
4	L	843	BMA	C1-C2-C3	-2.23	106.91	109.54
4	L	843	BMA	C3-C4-C5	-2.06	106.61	110.20
2	I	802	NAG	C3-C4-C5	2.11	113.88	110.20
4	L	841	NAG	O4-C4-C5	2.20	115.07	109.24
2	I	801	NAG	O5-C5-C6	2.22	112.15	107.35
4	L	862	NAG	O4-C4-C5	2.60	116.12	109.24
4	L	842	NAG	O4-C4-C5	2.96	117.08	109.24
4	L	861	NAG	C3-C4-C5	3.08	115.57	110.20
4	I	842	NAG	C1-O5-C5	4.39	117.83	112.25
4	L	842	NAG	C3-C2-N2	5.12	122.82	110.56
4	L	842	NAG	C1-O5-C5	5.17	118.81	112.25
4	L	862	NAG	C1-O5-C5	5.35	119.04	112.25
4	L	842	NAG	C2-N2-C7	5.84	130.54	123.04
2	I	801	NAG	C1-O5-C5	13.72	129.66	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	802	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	841	NAG	1	0
4	I	842	NAG	1	0
4	L	841	NAG	2	0
4	L	861	NAG	1	0
4	L	862	NAG	1	0

5.6 Ligand geometry

4 ligands 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	$\# Z > 2$
3	NAG	I	821	1	14,14,15	1.23	1 (7%)	15,19,21	0.81	0
5	NTP	I	901	-	98,104,104	1.03	3 (3%)	140,162,162	1.29	8 (5%)
3	NAG	L	801	1	14,14,15	1.30	1 (7%)	15,19,21	1.97	2 (13%)
5	NTP	L	901	-	98,104,104	1.02	2 (2%)	140,162,162	0.94	6 (4%)

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
3	NAG	I	821	1	-	0/6/23/26	0/1/1/1
5	NTP	I	901	-	-	0/76/184/184	0/5/5/5
3	NAG	L	801	1	-	0/6/23/26	0/1/1/1
5	NTP	L	901	-	-	0/76/184/184	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	801	NAG	O7-C7	-3.61	1.14	1.23
3	I	821	NAG	O7-C7	-3.57	1.14	1.23
5	I	901	NTP	O3G-C3F	-2.71	1.40	1.46
5	I	901	NTP	O3A-C39	-2.29	1.41	1.46
5	L	901	NTP	O3A-C39	-2.21	1.41	1.46
5	L	901	NTP	C20-C21	2.17	1.56	1.52
5	I	901	NTP	C20-C21	2.21	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	901	NTP	C39-O3A-S3B	-3.21	112.66	118.77
5	L	901	NTP	C1E-O1F-S1G	-2.66	113.71	118.77
5	L	901	NTP	C29-C26-C20	-2.30	105.36	110.43
5	L	901	NTP	C5F-C59-C50	-2.12	105.75	110.43
5	L	901	NTP	O1L-C1K-C1E	-2.10	104.73	109.05
5	I	901	NTP	O1L-C1K-C1E	-2.01	104.90	109.05
3	L	801	NAG	C4-C3-C2	-2.01	108.10	111.23
5	L	901	NTP	C4F-O42-C41	2.10	115.42	112.17
5	I	901	NTP	O52-C51-C50	2.14	114.27	109.75
5	L	901	NTP	O42-C4F-C49	2.22	113.95	109.47
5	I	901	NTP	O3G-C3F-C39	2.61	114.26	108.48
5	I	901	NTP	O5M-C5L-C5F	3.30	113.46	107.82
5	I	901	NTP	C2C-O22-C21	3.42	117.47	112.17
5	I	901	NTP	O5G-C5F-C5L	4.06	113.17	107.65
3	L	801	NAG	C1-O5-C5	6.94	121.05	112.25
5	I	901	NTP	O3G-C3F-C3L	7.64	118.05	107.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	821	NAG	1	0
5	I	901	NTP	10	0
5	L	901	NTP	16	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	I	418/432 (96%)	-0.36	15 (3%) 46 38	13, 43, 90, 126	0
1	L	423/432 (97%)	-0.46	15 (3%) 48 40	11, 33, 86, 133	0
All	All	841/864 (97%)	-0.41	30 (3%) 46 38	11, 38, 90, 133	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	38	GLN	5.3
1	I	28	LYS	4.4
1	I	384	ALA	4.4
1	L	34	GLU	4.3
1	I	385	SER	4.0
1	I	382	ALA	4.0
1	I	383	ALA	3.8
1	I	38	GLN	3.8
1	L	26	PRO	3.8
1	L	25	SER	3.7
1	I	37	GLU	3.7
1	I	27	GLU	3.3
1	I	359	ARG	3.3
1	I	15	ILE	3.0
1	I	357	GLU	3.0
1	L	399	ARG	2.9
1	L	33	ASP	2.9
1	L	27	GLU	2.9
1	L	134	ALA	2.9
1	L	397	PRO	2.8
1	I	360	ASP	2.7
1	L	135	ASN	2.7
1	L	358	GLY	2.5
1	I	26	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	32	GLU	2.4
1	L	398	ASN	2.4
1	I	14	ASP	2.4
1	L	402	PHE	2.2
1	L	36	SER	2.2
1	I	380	SER	2.1

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
4	NAG	L	842	14/15	0.69	0.34	4.46	94,100,105,107	0
4	NAG	L	841	14/15	0.86	0.24	3.37	74,81,91,94	0
4	NAG	I	841	14/15	0.91	0.19	0.10	63,68,81,94	0
4	NAG	L	862	14/15	0.77	0.41	-	113,119,122,123	0
4	NAG	I	842	14/15	0.76	0.36	-	106,112,123,132	0
4	BMA	I	843	11/12	0.40	0.51	-	141,145,146,147	0
2	NAG	I	802	14/15	0.74	0.60	-	127,128,131,132	0
4	BMA	L	843	11/12	0.74	0.41	-	109,109,110,111	0
2	NAG	I	801	14/15	0.83	0.46	-	116,122,125,125	0
4	BMA	L	863	11/12	0.70	0.42	-	116,117,118,118	0
4	NAG	L	861	14/15	0.70	0.35	-	85,95,98,106	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(\AA^2)	Q<0.9
5	NTP	L	901	100/100	0.96	0.12	-0.65	27,39,53,56	0
5	NTP	I	901	100/100	0.94	0.14	-0.85	42,61,76,77	0
3	NAG	I	821	14/15	0.70	0.55	-	125,127,130,131	0
3	NAG	L	801	14/15	0.75	0.49	-	103,110,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.