



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1E04
Title : PLASMA BETA ANTITHROMBIN-III
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Deposited on : 2000-03-09
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

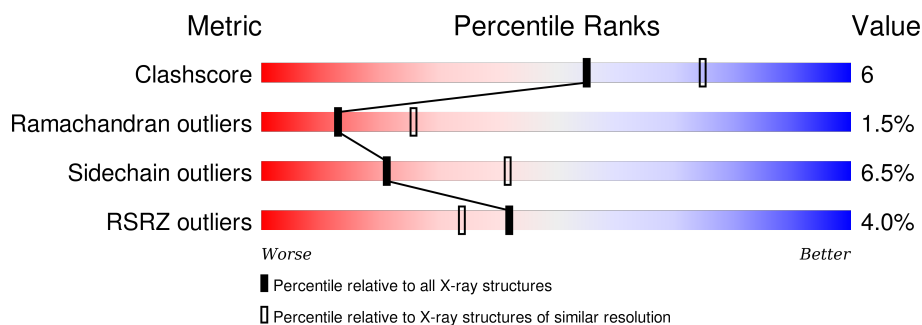
1 Overall quality at a glance

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))
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	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	L	801	-	-	-	X
2	NAG	L	841	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	I	863	-	-	-	X
5	GOL	L	901	-	-	-	X
6	MAN	L	864	-	-	-	X
7	PO4	L	501	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6728 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	403	Total	C	N	O	S	0	0	0
			3179	2032	529	602	16			
1	L	412	Total	C	N	O	S	0	0	0
			3225	2057	536	614	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		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).

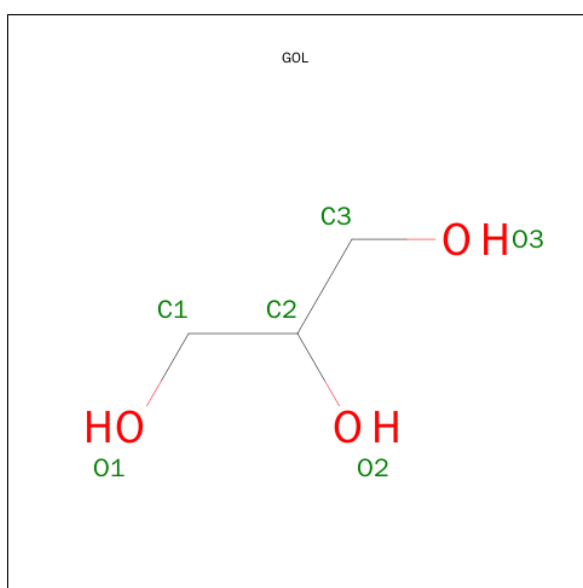


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			11	6	5		

- 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		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

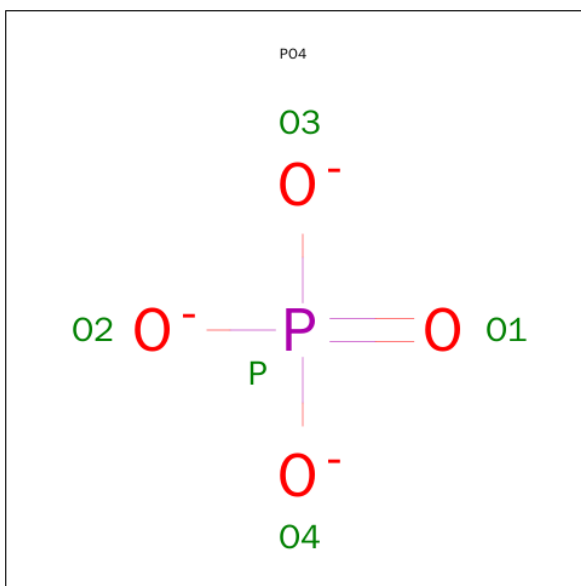


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	O	P	0	0
			5	4	1		

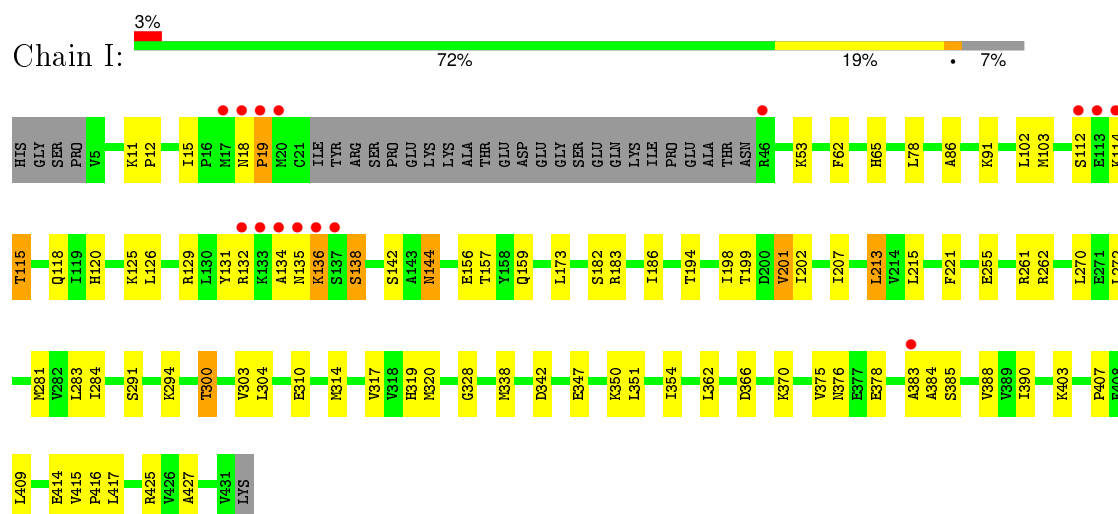
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	51	Total	O	0	0
			51	51		
8	L	33	Total	O	0	0
			33	33		

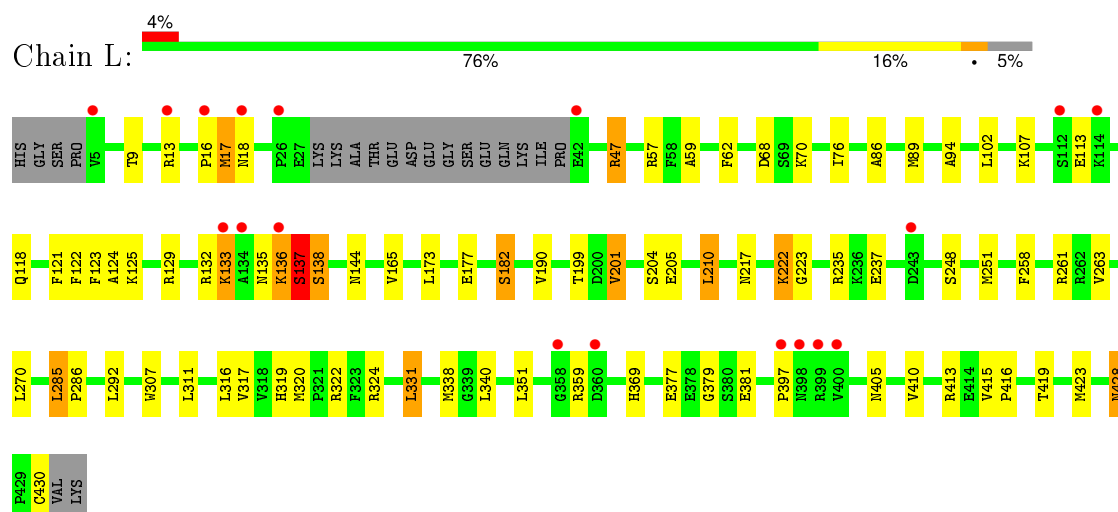
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ANTITHROMBIN-III



• 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	62.05Å 99.34Å 88.59Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 94.6 (19.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.243 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	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 30594 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6728	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: GOL, PO4, BMA, 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	I	0.41	0/3242	0.87	1/4384 (0.0%)
1	L	0.39	0/3289	0.84	1/4452 (0.0%)
All	All	0.40	0/6531	0.86	2/8836 (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	I	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	I	262	ARG	CD-NE-CZ	7.24	133.73	123.60
1	L	285	LEU	CA-CB-CG	5.71	128.43	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	134	ALA	Mainchain

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	I	3179	0	3139	42	0
1	L	3225	0	3155	41	0
2	I	56	0	50	2	0
2	L	56	0	50	2	0
3	I	11	0	10	0	0
4	I	39	0	34	0	0
5	I	6	0	8	0	0
5	L	6	0	8	1	0
6	L	61	0	52	0	0
7	L	5	0	0	0	0
8	I	51	0	0	2	0
8	L	33	0	0	0	0
All	All	6728	0	6506	83	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 6.

All (83) 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:L:86:ALA:HA	1:L:89:MET:HE3	1.66	0.75
1:I:388:VAL:HG22	1:L:317:VAL:HB	1.70	0.74
1:I:86:ALA:HA	1:I:144:ASN:HD21	1.52	0.73
1:L:47:ARG:HD3	1:L:113:GLU:HG3	1.71	0.72
1:I:194:THR:HG21	1:I:198:ILE:HD12	1.73	0.70
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.76	0.68
1:L:331:LEU:HD21	1:L:369:HIS:HB2	1.76	0.66
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.80	0.64
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.80	0.63
1:I:156:GLU:HA	1:I:159:GLN:HE21	1.64	0.62
1:L:428:ASN:ND2	1:L:430:CYS:H	2.01	0.59
1:L:428:ASN:HD22	1:L:430:CYS:H	1.52	0.58
1:I:11:LYS:HB3	1:I:12:PRO:HD2	1.86	0.57
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.71	0.56
1:I:198:ILE:HG23	1:I:370:LYS:HD3	1.88	0.56
1:I:354:ILE:HG22	1:I:362:LEU:HD13	1.88	0.56
1:L:173:LEU:HD13	1:L:182:SER:HB3	1.90	0.54
1:L:270:LEU:HD13	1:L:316:LEU:HD11	1.90	0.54
1:L:144:ASN:HD22	1:L:217:ASN:HA	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:300:THR:HG23	1:I:303:VAL:HB	1.90	0.53
1:I:376:ASN:HD21	1:I:383:ALA:HA	1.73	0.53
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.92	0.52
1:I:173:LEU:HD13	1:I:182:SER:HB3	1.92	0.52
1:L:210:LEU:HA	1:L:359:ARG:HH22	1.75	0.52
1:I:270:LEU:HD21	1:I:272:LEU:HD21	1.93	0.51
1:L:204:SER:O	1:L:205:GLU:HB2	2.11	0.51
1:I:320:MET:HE1	1:I:375:VAL:HG11	1.92	0.50
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.93	0.50
1:L:222:LYS:HD3	1:L:381:GLU:HB2	1.93	0.49
1:I:213:LEU:HD11	1:I:354:ILE:HD13	1.95	0.48
1:I:18:ASN:HB3	1:I:19:PRO:HD2	1.94	0.48
1:I:291:SER:HB3	1:I:294:LYS:HG3	1.96	0.48
1:I:261:ARG:HG2	1:I:310:GLU:HB3	1.97	0.47
1:I:425:ARG:HD3	1:I:427:ALA:HB2	1.96	0.47
1:I:15:ILE:HG21	1:I:120:HIS:HB2	1.97	0.47
1:I:135:ASN:O	1:I:136:LYS:C	2.53	0.47
1:L:102:LEU:HG	1:L:340:LEU:HD11	1.97	0.47
1:L:222:LYS:HG2	1:L:381:GLU:HG3	1.97	0.47
1:I:126:LEU:HD12	1:I:417:LEU:HD13	1.95	0.47
1:L:59:ALA:O	1:L:423:MET:HE1	2.15	0.47
1:I:114:LYS:O	1:I:115:THR:C	2.54	0.46
1:L:261:ARG:HB3	1:L:311:LEU:HD23	1.98	0.46
1:L:132:ARG:O	1:L:133:LYS:HB2	2.14	0.46
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.97	0.45
1:I:328:GLY:HA2	1:I:370:LYS:HG3	1.98	0.45
1:L:237:GLU:OE1	1:L:251:MET:HG3	2.17	0.45
1:I:390:ILE:HA	1:L:319:HIS:HB2	1.99	0.45
1:L:125:LYS:O	1:L:129:ARG:HG2	2.17	0.45
1:L:263:VAL:HG11	1:L:307:TRP:CD1	2.51	0.44
1:I:62:PHE:HA	1:I:338:MET:HE1	1.99	0.44
1:I:125:LYS:O	1:I:129:ARG:HG2	2.18	0.43
1:I:378:GLU:HG3	1:I:384:ALA:HB3	2.00	0.43
1:L:16:PRO:O	1:L:17:MET:C	2.55	0.43
1:I:65:HIS:HB2	8:I:2002:HOH:O	2.18	0.43
1:I:284:ILE:HB	1:I:409:LEU:HB2	2.00	0.43
1:L:47:ARG:HG2	1:L:122:PHE:CE2	2.54	0.43
1:L:18:ASN:HB2	2:L:842:NAG:H83	2.00	0.43
1:I:138:SER:HB3	1:I:221:PHE:CE1	2.54	0.42
2:I:801:NAG:H62	2:I:802:NAG:N2	2.34	0.42
1:I:86:ALA:HB1	1:I:215:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:PRO:HD3	1:L:292:LEU:HD13	2.01	0.42
1:I:131:TYR:CE1	1:I:142:SER:HB2	2.54	0.42
1:I:415:VAL:HB	1:I:416:PRO:CD	2.48	0.42
1:I:202:ILE:HG21	1:I:207:ILE:HD12	2.02	0.42
1:L:413:ARG:HD2	5:L:901:GOL:H12	2.02	0.42
1:L:18:ASN:HB2	2:L:842:NAG:C8	2.50	0.42
1:L:89:MET:CE	1:L:217:ASN:HB2	2.49	0.41
1:I:11:LYS:HB3	1:I:12:PRO:CD	2.49	0.41
1:L:121:PHE:CZ	1:L:125:LYS:HE3	2.56	0.41
1:L:190:VAL:HG21	1:L:201:VAL:HG21	2.01	0.41
1:L:124:ALA:HB2	1:L:165:VAL:HG13	2.02	0.41
1:L:70:LYS:HD2	1:L:76:ILE:HG12	2.01	0.41
1:I:281:MET:CE	1:I:283:LEU:HD21	2.51	0.41
2:I:841:NAG:H62	2:I:842:NAG:N2	2.35	0.41
1:L:136:LYS:O	1:L:137:SER:C	2.58	0.41
1:I:62:PHE:HA	1:I:338:MET:CE	2.51	0.41
1:I:91:LYS:HE2	1:I:103:MET:SD	2.61	0.41
1:L:322:ARG:HD2	1:L:377:GLU:OE1	2.20	0.41
1:L:223:GLY:O	1:L:379:GLY:HA3	2.21	0.41
1:L:57:ARG:HB3	1:L:107:LYS:HG3	2.03	0.41
1:I:201:VAL:HG22	8:I:2015:HOH:O	2.21	0.40
1:L:113:GLU:HB3	1:L:118:GLN:OE1	2.21	0.40
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.03	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	I	399/432 (92%)	373 (94%)	21 (5%)	5 (1%)	15	30
1	L	408/432 (94%)	380 (93%)	21 (5%)	7 (2%)	11	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	807/864 (93%)	753 (93%)	42 (5%)	12 (2%)	13	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	13	ARG
1	I	112	SER
1	I	19	PRO
1	I	115	THR
1	L	138	SER
1	I	136	LYS
1	L	17	MET
1	L	133	LYS
1	L	136	LYS
1	L	137	SER
1	L	397	PRO
1	I	407	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	347/383 (91%)	325 (94%)	22 (6%)	22	44
1	L	349/383 (91%)	326 (93%)	23 (7%)	21	40
All	All	696/766 (91%)	651 (94%)	45 (6%)	21	42

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	53	LYS
1	I	78	LEU
1	I	102	LEU
1	I	118	GLN
1	I	132	ARG
1	I	138	SER

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Mol	Chain	Res	Type
1	I	144	ASN
1	I	157	THR
1	I	183	ARG
1	I	199	THR
1	I	201	VAL
1	I	213	LEU
1	I	300	THR
1	I	304	LEU
1	I	314	MET
1	I	342	ASP
1	I	347	GLU
1	I	350	LYS
1	I	351	LEU
1	I	366	ASP
1	I	385	SER
1	I	414	GLU
1	L	9	THR
1	L	47	ARG
1	L	68	ASP
1	L	123	PHE
1	L	135	ASN
1	L	137	SER
1	L	138	SER
1	L	177	GLU
1	L	182	SER
1	L	199	THR
1	L	201	VAL
1	L	210	LEU
1	L	222	LYS
1	L	235	ARG
1	L	248	SER
1	L	285	LEU
1	L	320	MET
1	L	324	ARG
1	L	331	LEU
1	L	405	ASN
1	L	410	VAL
1	L	419	THR
1	L	428	ASN

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

Mol	Chain	Res	Type
1	I	118	GLN
1	I	144	ASN
1	I	159	GLN
1	I	334	GLN
1	L	55	ASN
1	L	144	ASN
1	L	217	ASN
1	L	336	GLN
1	L	405	ASN
1	L	428	ASN

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 ⓘ

16 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	1.24	1 (7%)	15,19,21	0.84	1 (6%)
2	NAG	I	802	2	14,14,15	1.23	1 (7%)	15,19,21	1.74	1 (6%)
2	NAG	I	841	1,2	14,14,15	1.25	1 (7%)	15,19,21	0.74	1 (6%)
2	NAG	I	842	2	14,14,15	1.22	1 (7%)	15,19,21	1.42	2 (13%)
4	NAG	I	861	1,4	14,14,15	1.34	1 (7%)	15,19,21	0.95	1 (6%)
4	NAG	I	862	4	14,14,15	1.25	1 (7%)	15,19,21	0.85	0
4	BMA	I	863	4	11,11,12	1.01	1 (9%)	14,15,17	1.27	2 (14%)
2	NAG	L	801	1,2	14,14,15	1.21	1 (7%)	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	802	2	14,14,15	1.24	1 (7%)	15,19,21	0.89	1 (6%)
2	NAG	L	841	1,2	14,14,15	1.40	2 (14%)	15,19,21	1.35	1 (6%)
2	NAG	L	842	2	14,14,15	1.25	1 (7%)	15,19,21	0.95	1 (6%)
6	NAG	L	861	1,6	14,14,15	1.28	2 (14%)	15,19,21	2.23	2 (13%)
6	NAG	L	862	6	14,14,15	1.26	1 (7%)	15,19,21	1.83	4 (26%)
6	BMA	L	863	6	11,11,12	1.68	4 (36%)	14,15,17	3.80	6 (42%)
6	MAN	L	864	6	11,11,12	0.95	0	14,15,17	1.52	2 (14%)
6	MAN	L	868	6	11,11,12	0.97	1 (9%)	14,15,17	1.29	2 (14%)

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	-	0/6/23/26	0/1/1/1
2	NAG	I	841	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	842	2	-	0/6/23/26	0/1/1/1
4	NAG	I	861	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	862	4	-	0/6/23/26	0/1/1/1
4	BMA	I	863	4	-	0/2/19/22	0/1/1/1
2	NAG	L	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	802	2	-	0/6/23/26	0/1/1/1
2	NAG	L	841	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	842	2	-	0/6/23/26	0/1/1/1
6	NAG	L	861	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	862	6	-	0/6/23/26	0/1/1/1
6	BMA	L	863	6	-	0/2/19/22	0/1/1/1
6	MAN	L	864	6	-	0/2/19/22	1/1/1/1
6	MAN	L	868	6	-	0/2/19/22	1/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	802	NAG	O7-C7	-3.74	1.14	1.23
2	I	802	NAG	O7-C7	-3.73	1.14	1.23
2	I	801	NAG	O7-C7	-3.72	1.14	1.23
4	I	862	NAG	O7-C7	-3.71	1.14	1.23
2	L	841	NAG	O7-C7	-3.70	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	862	NAG	O7-C7	-3.68	1.14	1.23
2	L	801	NAG	O7-C7	-3.67	1.14	1.23
2	I	842	NAG	O7-C7	-3.67	1.14	1.23
4	I	861	NAG	O7-C7	-3.66	1.14	1.23
2	I	841	NAG	O7-C7	-3.64	1.14	1.23
6	L	861	NAG	O7-C7	-3.64	1.14	1.23
2	L	842	NAG	O7-C7	-3.57	1.14	1.23
6	L	863	BMA	O2-C2	-2.18	1.38	1.43
6	L	861	NAG	O5-C1	2.33	1.47	1.43
6	L	863	BMA	C2-C3	2.35	1.55	1.52
6	L	868	MAN	C1-C2	2.42	1.58	1.52
4	I	863	BMA	C1-C2	2.51	1.58	1.52
6	L	863	BMA	C4-C5	2.70	1.58	1.53
6	L	863	BMA	C1-C2	2.73	1.58	1.52
2	L	841	NAG	O5-C1	2.87	1.48	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	863	BMA	C1-C2-C3	-9.41	98.41	109.54
6	L	861	NAG	C1-O5-C5	-7.66	102.52	112.25
6	L	863	BMA	O5-C1-C2	-4.71	103.21	110.86
6	L	863	BMA	C3-C4-C5	-4.67	102.05	110.20
2	L	841	NAG	C1-O5-C5	-4.34	106.74	112.25
2	I	842	NAG	C6-C5-C4	-3.32	104.82	113.02
4	I	863	BMA	O5-C1-C2	-2.64	106.57	110.86
4	I	863	BMA	C1-C2-C3	-2.52	106.56	109.54
6	L	862	NAG	O4-C4-C3	-2.48	104.75	110.34
6	L	868	MAN	O5-C1-C2	-2.37	107.01	110.86
2	L	801	NAG	C1-O5-C5	-2.32	109.30	112.25
4	I	861	NAG	C4-C3-C2	-2.23	107.77	111.23
2	I	841	NAG	C4-C3-C2	-2.13	107.92	111.23
6	L	868	MAN	C1-C2-C3	-2.02	107.15	109.54
6	L	863	BMA	O5-C5-C6	2.02	111.72	107.35
2	I	801	NAG	C2-N2-C7	2.15	125.80	123.04
6	L	864	MAN	O5-C5-C6	2.17	112.04	107.35
2	L	842	NAG	C1-O5-C5	2.17	115.00	112.25
2	L	802	NAG	C2-N2-C7	2.24	125.92	123.04
6	L	862	NAG	C4-C3-C2	2.45	115.04	111.23
6	L	861	NAG	C3-C4-C5	2.72	114.93	110.20
6	L	863	BMA	O4-C4-C3	2.76	116.55	110.34
2	I	842	NAG	C1-O5-C5	3.20	116.31	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	862	NAG	C3-C4-C5	3.27	115.91	110.20
6	L	864	MAN	C1-O5-C5	3.71	116.95	112.25
6	L	862	NAG	C2-N2-C7	4.55	128.88	123.04
2	I	802	NAG	C2-N2-C7	5.72	130.39	123.04
6	L	863	BMA	O3-C3-C4	6.69	125.39	110.34

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	864	MAN	C1-C2-C3-C4-C5-O5
6	L	868	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	801	NAG	1	0
2	I	802	NAG	1	0
2	I	841	NAG	1	0
2	I	842	NAG	1	0
2	L	842	NAG	2	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	MAN	I	803	-	11,11,12	0.82	0	14,15,17	0.99	1 (7%)
5	GOL	I	901	-	5,5,5	0.70	0	5,5,5	0.41	0
7	PO4	L	501	-	4,4,4	0.65	0	6,6,6	0.27	0
5	GOL	L	901	-	5,5,5	0.72	0	5,5,5	0.44	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
3	MAN	I	803	-	-	0/2/19/22	1/1/1/1
5	GOL	I	901	-	-	0/4/4/4	0/0/0/0
7	PO4	L	501	-	-	0/0/0/0	0/0/0/0
5	GOL	L	901	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	803	MAN	C1-C2-C3	-2.05	107.11	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	803	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	901	GOL	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

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	403/432 (93%)	-0.24	15 (3%) 45 37	26, 45, 82, 127	0
1	L	412/432 (95%)	-0.18	18 (4%) 38 30	26, 47, 98, 120	0
All	All	815/864 (94%)	-0.21	33 (4%) 42 34	26, 45, 95, 127	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	135	ASN	7.1
1	L	134	ALA	5.6
1	I	134	ALA	5.6
1	I	19	PRO	5.0
1	L	398	ASN	4.9
1	I	17	MET	4.8
1	I	20	MET	4.5
1	I	112	SER	4.1
1	L	400	VAL	3.9
1	I	18	ASN	3.7
1	L	5	VAL	3.6
1	I	136	LYS	3.5
1	L	26	PRO	3.5
1	L	112	SER	3.3
1	I	113	GLU	3.1
1	L	42	GLU	3.0
1	I	133	LYS	3.0
1	L	136	LYS	2.8
1	L	13	ARG	2.8
1	I	46	ARG	2.7
1	I	114	LYS	2.7
1	L	243	ASP	2.6
1	L	399	ARG	2.5
1	L	114	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	358	GLY	2.4
1	L	397	PRO	2.4
1	I	132	ARG	2.2
1	L	18	ASN	2.2
1	L	360	ASP	2.2
1	L	16	PRO	2.1
1	L	133	LYS	2.1
1	I	383	ALA	2.1
1	I	137	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	BMA	I	863	11/12	0.15	0.70	19.35	155,156,156,156	0
6	MAN	L	864	11/12	0.72	0.44	13.76	138,140,140,141	0
2	NAG	L	801	14/15	0.65	0.39	6.33	104,107,114,121	0
2	NAG	L	841	14/15	0.75	0.31	2.19	99,106,113,121	0
2	NAG	I	841	14/15	0.86	0.19	0.05	67,73,83,91	0
2	NAG	I	802	14/15	0.74	0.70	-	129,133,136,136	0
6	NAG	L	861	14/15	0.82	0.33	-	87,92,100,109	0
4	NAG	I	861	14/15	0.66	0.47	-	120,129,134,141	0
6	MAN	L	868	11/12	0.50	0.55	-	149,150,151,152	0
2	NAG	L	842	14/15	0.78	0.52	-	126,129,130,131	0
6	NAG	L	862	14/15	0.78	0.37	-	117,120,126,131	0
2	NAG	I	801	14/15	0.72	0.42	-	105,110,118,124	0
6	BMA	L	863	11/12	0.62	0.57	-	136,140,143,146	0
2	NAG	I	842	14/15	0.74	0.56	-	96,102,103,103	0
4	NAG	I	862	14/15	0.56	0.74	-	146,150,151,153	0
2	NAG	L	802	14/15	0.72	0.61	-	127,129,130,130	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
7	PO4	L	501	5/5	0.86	0.32	5.79	83,83,84,85	0
5	GOL	L	901	6/6	0.95	0.17	2.91	47,49,49,49	0
5	GOL	I	901	6/6	0.90	0.19	1.33	55,59,60,60	0
3	MAN	I	803	11/12	0.75	0.45	-	139,139,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.