



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:49 pm GMT

PDB ID : 3KCG
Title : Crystal structure of the antithrombin-factor IXa-pentasaccharide complex
Authors : Huntington, J.A.; Johnson, D.J.D.
Deposited on : 2009-10-21
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

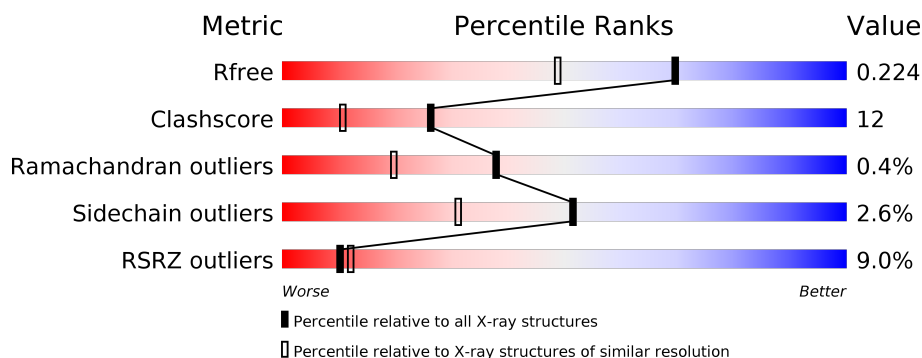
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	L	59	<div> <div>39%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>8%</div> <div>8%</div> </div> </div>
2	H	235	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
3	I	432	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>

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
6	NAG	I	841	-	-	-	X
8	MPD	I	5276	-	-	-	X
8	MPD	I	5277	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6669 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 Coagulation factor IXa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	54	Total	C	N	O	S	0	0	0
			377	231	69	70	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	84	MET	-	INITIATING METHIONINE	UNP P00740

- Molecule 2 is a protein called Coagulation factor IXa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	235	Total	C	N	O	S	0	12	0
			1938	1227	341	360	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	ENGINEERED	UNP P00740

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	419	Total	C	N	O	S	0	24	0
			3483	2213	597	653	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Ca 1 1	0	0

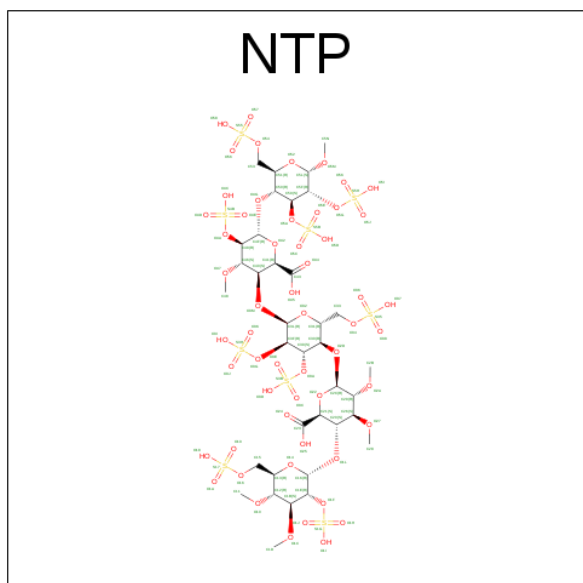
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	2	Total C N O 24 14 1 9	0	0
5	I	2	Total C N O 24 14 1 9	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 is HEPARIN PENTASACCHARIDE (three-letter code: NTP) (formula: $C_{36}H_{60}O_{55}S_9$).



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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	I	1	Total	C	O	0	0
			8	6	2		
8	I	1	Total	C	O	0	0
			8	6	2		

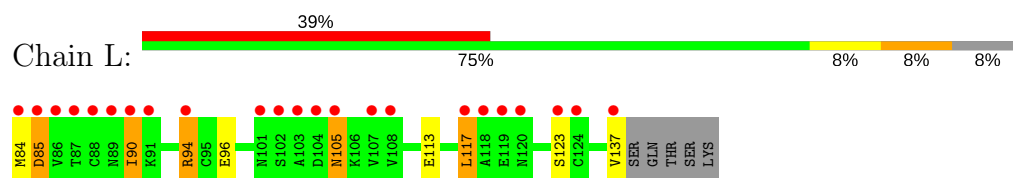
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	28	Total	O	0	0
			28	28		
9	H	292	Total	O	0	0
			292	292		
9	I	347	Total	O	0	0
			347	347		

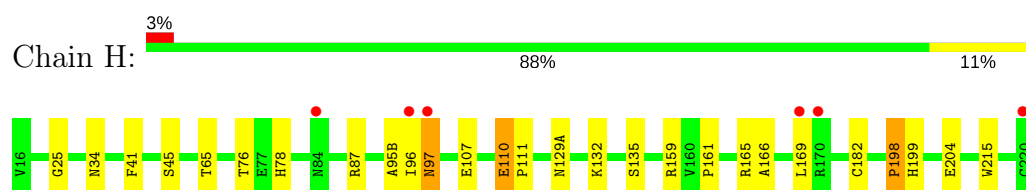
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

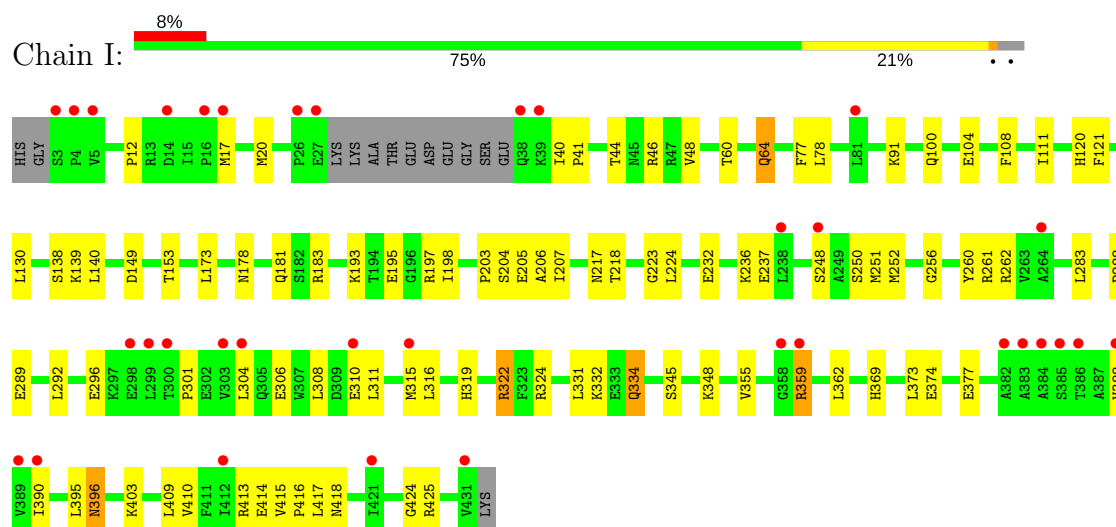
- Molecule 1: Coagulation factor IXa light chain



- Molecule 2: Coagulation factor IXa heavy chain



- Molecule 3: Antithrombin-III



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.78Å 88.44Å 147.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.05 – 1.70 38.05 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.05-1.70) 99.1 (38.05-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.70Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.230 0.226 , 0.224	Depositor DCC
R_{free} test set	5638 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, NAG, NTP, CA, FUC, 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	L	0.31	0/382	0.57	0/518
2	H	0.34	0/1983	0.67	1/2687 (0.0%)
3	I	0.31	0/3551	0.60	0/4799
All	All	0.32	0/5916	0.62	1/8004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	199	HIS	N-CA-C	-5.94	94.95	111.00

There are no chirality outliers.

There are no planarity outliers.

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	L	377	0	335	15	0
2	H	1938	0	1869	29	0
3	I	3483	0	3401	88	0
4	H	1	0	0	0	0
5	I	48	0	44	1	0
6	I	39	0	34	2	0
7	I	100	0	58	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	16	0	28	1	0
9	H	292	0	0	4	0
9	I	347	0	0	4	0
9	L	28	0	0	1	0
All	All	6669	0	5769	138	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 12.

All (138) 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)
3:I:359:ARG:H	3:I:359:ARG:HD3	1.13	1.07
3:I:359:ARG:HH21	3:I:359:ARG:HG2	1.15	1.07
3:I:60[A]:THR:HG21	3:I:301:PRO:HG3	1.41	1.02
3:I:359:ARG:N	3:I:359:ARG:HD3	1.84	0.92
3:I:424:GLY:C	3:I:425[A]:ARG:CA	2.44	0.86
3:I:64[A]:GLN:HA	3:I:64[A]:GLN:HE21	1.40	0.85
3:I:359:ARG:H	3:I:359:ARG:CD	1.86	0.83
7:I:433:NTP:H152	7:I:433:NTP:H112	1.60	0.81
3:I:20:MET:CE	6:I:841:NAG:H2	2.19	0.73
3:I:292:LEU:HD11	3:I:409:LEU:HG	1.70	0.72
2:H:34:ASN:HB2	2:H:65[B]:THR:HG23	1.73	0.71
3:I:261:ARG:NH1	3:I:310:GLU:HB3	2.06	0.69
3:I:193:LYS:HG3	5:I:902:FUC:O3	1.92	0.69
3:I:183[A]:ARG:HB2	3:I:207:ILE:HD11	1.74	0.69
3:I:359:ARG:CG	3:I:359:ARG:HH21	2.01	0.68
2:H:87[B]:ARG:HB3	2:H:107:GLU:HB3	1.76	0.68
3:I:359:ARG:NH2	3:I:359:ARG:HG2	1.94	0.67
3:I:183[B]:ARG:HB2	3:I:207:ILE:HD11	1.76	0.66
2:H:159[B]:ARG:HH22	2:H:161:PRO:HB3	1.61	0.66
3:I:198:ILE:HD13	3:I:218:THR:HB	1.78	0.64
3:I:324:ARG:HG2	3:I:374:GLU:HG3	1.79	0.63
2:H:34:ASN:HB2	2:H:65[B]:THR:CG2	2.29	0.63
7:I:433:NTP:O2A	7:I:433:NTP:H282	1.99	0.63
3:I:319:HIS:HB2	3:I:403[A]:LYS:HA	1.80	0.63
3:I:319:HIS:HB2	3:I:403[B]:LYS:HA	1.80	0.62
2:H:76:THR:HG22	2:H:78[A]:HIS:HD2	1.65	0.61
2:H:41:PHE:HA	3:I:395:LEU:HB2	1.83	0.60
3:I:308:LEU:HD13	3:I:413:ARG:NH1	2.17	0.60
3:I:203:PRO:HG2	3:I:206:ALA:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:433:NTP:H1D2	7:I:433:NTP:O1F	2.03	0.59
1:L:94:ARG:HH11	1:L:94:ARG:CG	2.15	0.59
2:H:45:SER:OG	2:H:198:PRO:HB3	2.03	0.58
1:L:113:GLU:HG3	9:H:587:HOH:O	2.03	0.58
1:L:85:ASP:HB3	1:L:105:ASN:OD1	2.04	0.58
7:I:433:NTP:H2B3	7:I:433:NTP:O2D	2.04	0.57
3:I:252:MET:SD	3:I:377:GLU:HG3	2.44	0.57
1:L:84:MET:O	1:L:85:ASP:HB2	2.03	0.57
3:I:359:ARG:NH2	9:I:571:HOH:O	2.37	0.57
3:I:415:VAL:HB	3:I:416:PRO:HD3	1.87	0.57
2:H:165[A]:ARG:O	2:H:169:LEU:HD13	2.06	0.56
3:I:60[A]:THR:CG2	3:I:301:PRO:HG3	2.26	0.56
3:I:108:PHE:O	3:I:111:ILE:HG12	2.06	0.56
3:I:261:ARG:HD3	3:I:262:ARG:N	2.21	0.55
7:I:433:NTP:H112	7:I:433:NTP:C15	2.32	0.55
3:I:60[A]:THR:HG21	3:I:301:PRO:CG	2.28	0.55
3:I:20:MET:HE2	6:I:841:NAG:H2	1.88	0.54
3:I:283:LEU:CD2	3:I:410:VAL:HG12	2.37	0.54
1:L:94:ARG:HG2	1:L:94:ARG:NH1	2.22	0.54
7:I:433:NTP:H1K	7:I:433:NTP:O27	2.07	0.54
3:I:417:LEU:O	3:I:418:ASN:HB2	2.08	0.54
2:H:97[B]:ASN:O	2:H:97[B]:ASN:OD1	2.26	0.53
2:H:110[A]:GLU:OE1	2:H:111:PRO:HD2	2.09	0.53
3:I:236:LYS:HD2	3:I:248:SER:OG	2.09	0.53
3:I:332[A]:LYS:HE2	9:I:616:HOH:O	2.09	0.52
3:I:183[B]:ARG:CB	3:I:207:ILE:HD11	2.39	0.52
7:I:433:NTP:H482	7:I:433:NTP:O4A	2.10	0.52
3:I:44:THR:HG21	3:I:417:LEU:HD11	1.91	0.52
3:I:120:HIS:H	3:I:120:HIS:CD2	2.27	0.52
3:I:60[B]:THR:HG21	3:I:301:PRO:HD3	1.91	0.51
2:H:96:ILE:O	2:H:97[A]:ASN:CB	2.57	0.51
3:I:288:PRO:O	3:I:289:GLU:CB	2.58	0.51
3:I:304:LEU:C	3:I:304:LEU:HD23	2.31	0.51
2:H:96:ILE:O	2:H:97[A]:ASN:HB2	2.11	0.51
2:H:215:TRP:CE3	3:I:390:ILE:HG23	2.46	0.50
2:H:182[B]:CYS:SG	2:H:225:TYR:HB2	2.52	0.50
2:H:129(A):ASN:O	2:H:132[A]:LYS:HG2	2.12	0.50
2:H:95(B):ALA:C	2:H:96:ILE:HD13	2.32	0.49
1:L:137:VAL:HG21	2:H:25:GLY:HA3	1.93	0.49
2:H:135:SER:OG	2:H:159[B]:ARG:NE	2.43	0.49
1:L:94:ARG:NH1	1:L:94:ARG:CG	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:60[A]:THR:O	3:I:64[A]:GLN:HG2	2.13	0.49
7:I:433:NTP:S1G	7:I:433:NTP:H1D2	2.53	0.49
1:L:90:ILE:HG13	1:L:90:ILE:O	2.12	0.49
1:L:94:ARG:HH11	1:L:94:ARG:CB	2.26	0.49
3:I:139:LYS:HE3	3:I:197:ARG:NH2	2.27	0.48
7:I:433:NTP:H152	7:I:433:NTP:C11	2.38	0.48
3:I:359:ARG:CG	3:I:359:ARG:NH2	2.67	0.48
3:I:355:VAL:HB	3:I:362:LEU:HD22	1.94	0.48
2:H:165[B]:ARG:HH11	2:H:165[B]:ARG:CG	2.26	0.48
9:H:659:HOH:O	3:I:388:VAL:HA	2.13	0.47
3:I:237:GLU:OE1	3:I:251[A]:MET:HG2	2.14	0.47
2:H:165[B]:ARG:NH1	2:H:165[B]:ARG:HG2	2.28	0.47
2:H:96:ILE:O	2:H:97[B]:ASN:ND2	2.48	0.47
3:I:130:LEU:HB2	8:I:5276:MPD:HM2	1.96	0.47
1:L:113:GLU:HG2	9:L:584:HOH:O	2.14	0.47
3:I:261:ARG:HH12	3:I:310:GLU:HB3	1.77	0.47
3:I:44:THR:HG21	3:I:417:LEU:CD1	2.45	0.47
1:L:94:ARG:HH11	1:L:94:ARG:HG2	1.79	0.47
2:H:165[B]:ARG:HG3	9:H:664:HOH:O	2.15	0.46
3:I:261:ARG:HD3	3:I:262:ARG:H	1.79	0.46
3:I:256:GLY:HA2	3:I:315:MET:HE1	1.97	0.46
3:I:138:SER:CB	3:I:223:GLY:HA2	2.46	0.46
3:I:232[A]:GLU:H	3:I:232[A]:GLU:CD	2.19	0.46
3:I:91:LYS:C	3:I:91:LYS:HD3	2.37	0.46
1:L:117:LEU:HD23	1:L:123:SER:O	2.15	0.46
2:H:76:THR:HG22	2:H:78[A]:HIS:CD2	2.49	0.46
3:I:181:GLN:HG3	9:I:756:HOH:O	2.16	0.46
3:I:64[A]:GLN:CA	3:I:64[A]:GLN:HE21	2.14	0.46
3:I:331[B]:LEU:HD11	3:I:369:HIS:HB2	1.98	0.45
3:I:100:GLN:O	3:I:104:GLU:HG3	2.17	0.45
3:I:261:ARG:HB3	3:I:311:LEU:HD23	1.98	0.45
1:L:90:ILE:O	1:L:90:ILE:CG1	2.64	0.45
3:I:334:GLN:N	3:I:334:GLN:HE21	2.02	0.45
1:L:96:GLU:HG3	2:H:204:GLU:HG2	1.98	0.45
2:H:96:ILE:O	2:H:97[B]:ASN:CB	2.63	0.45
3:I:40:ILE:HD12	3:I:46[B]:ARG:NH1	2.31	0.45
3:I:306:GLU:O	3:I:310:GLU:HG3	2.17	0.45
3:I:283:LEU:HD22	3:I:410:VAL:HG12	1.99	0.44
3:I:292:LEU:O	3:I:296:GLU:HG3	2.17	0.44
3:I:17:MET:HG3	3:I:120:HIS:HE1	1.82	0.44
2:H:132[B]:LYS:HB2	2:H:132[B]:LYS:HE2	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:153[B]:THR:HG23	9:I:450:HOH:O	2.18	0.43
3:I:395:LEU:O	3:I:396:ASN:HB3	2.18	0.43
3:I:195:GLU:HB2	3:I:197:ARG:NH1	2.34	0.43
3:I:260:TYR:CG	3:I:261:ARG:N	2.87	0.42
3:I:140:LEU:C	3:I:140:LEU:HD23	2.40	0.42
1:L:105:ASN:HA	1:L:105:ASN:HD22	1.57	0.42
2:H:165[B]:ARG:NH1	2:H:165[B]:ARG:CG	2.83	0.42
3:I:40:ILE:HA	3:I:41:PRO:HD3	1.92	0.42
3:I:149:ASP:HA	3:I:173:LEU:O	2.20	0.42
2:H:132[A]:LYS:HD2	9:H:624:HOH:O	2.19	0.41
3:I:183[A]:ARG:NE	3:I:204:SER:HA	2.36	0.41
3:I:40:ILE:HD12	3:I:46[B]:ARG:CZ	2.51	0.41
3:I:183[A]:ARG:CA	3:I:207:ILE:HD11	2.51	0.41
3:I:204:SER:O	3:I:205:GLU:HB2	2.21	0.41
3:I:395:LEU:HA	3:I:395:LEU:HD23	1.97	0.41
2:H:165[B]:ARG:O	2:H:166:ALA:C	2.59	0.41
3:I:12:PRO:HG3	3:I:121:PHE:CE2	2.56	0.40
3:I:345:SER:HB3	3:I:348:LYS:HB2	2.04	0.40
3:I:178:ASN:OD1	3:I:181:GLN:NE2	2.54	0.40
3:I:250:SER:HB2	3:I:322[A]:ARG:CG	2.51	0.40
3:I:77:PHE:CE2	3:I:373:LEU:HB2	2.57	0.40
7:I:433:NTP:H482	7:I:433:NTP:S4B	2.62	0.40
3:I:48:VAL:HG21	7:I:433:NTP:O1A	2.21	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	L	52/59 (88%)	46 (88%)	5 (10%)	1 (2%)	9 1
2	H	245/235 (104%)	237 (97%)	6 (2%)	2 (1%)	22 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	I	439/432 (102%)	426 (97%)	12 (3%)	1 (0%)	51 31
All	All	736/726 (101%)	709 (96%)	23 (3%)	4 (0%)	38 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97[A]	ASN
2	H	97[B]	ASN
1	L	85	ASP
3	I	396	ASN

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	L	38/53 (72%)	34 (90%)	4 (10%)	8 1
2	H	206/197 (105%)	203 (98%)	3 (2%)	70 55
3	I	374/382 (98%)	363 (97%)	11 (3%)	48 26
All	All	618/632 (98%)	600 (97%)	18 (3%)	51 26

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	90	ILE
1	L	94	ARG
1	L	105	ASN
1	L	117	LEU
2	H	110[A]	GLU
2	H	110[B]	GLU
2	H	198	PRO
3	I	64[A]	GLN
3	I	64[B]	GLN
3	I	78	LEU
3	I	217	ASN

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Mol	Chain	Res	Type
3	I	224	LEU
3	I	316	LEU
3	I	322[A]	ARG
3	I	322[B]	ARG
3	I	334	GLN
3	I	359	ARG
3	I	414	GLU

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

Mol	Chain	Res	Type
1	L	89	ASN
2	H	84	ASN
3	I	120	HIS
3	I	181	GLN
3	I	334	GLN

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 ⓘ

7 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	$\# Z > 2$
5	NAG	I	801	3,5	14,14,15	0.48	0	15,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	I	802	5	9,10,11	0.46	0	13,14,16	0.44	0
6	NAG	I	841	3,6	14,14,15	0.53	0	15,19,21	0.73	1 (6%)
6	NAG	I	842	6	14,14,15	0.65	0	15,19,21	1.05	1 (6%)
6	MAN	I	843	6	11,11,12	1.14	1 (9%)	13,15,17	1.44	2 (15%)
5	NAG	I	901	3,5	14,14,15	0.51	0	15,19,21	0.73	0
5	FUC	I	902	5	9,10,11	0.52	0	13,14,16	0.54	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
5	NAG	I	801	3,5	-	0/6/23/26	0/1/1/1
5	FUC	I	802	5	-	0/0/17/20	0/1/1/1
6	NAG	I	841	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	842	6	-	1/6/23/26	0/1/1/1
6	MAN	I	843	6	-	0/2/19/22	0/1/1/1
5	NAG	I	901	3,5	-	0/6/23/26	0/1/1/1
5	FUC	I	902	5	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	843	MAN	C1-C2	2.96	1.59	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	843	MAN	C3-C4-C5	-2.34	106.09	110.22
6	I	842	NAG	C4-C3-C2	-2.08	107.98	111.02
6	I	841	NAG	C2-N2-C7	-2.05	119.96	122.94
6	I	843	MAN	C1-C2-C3	3.98	114.70	109.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	842	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	841	NAG	2	0
5	I	902	FUC	1	0

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
7	NTP	I	433	-	98,104,104	1.61	10 (10%)	126,162,162	1.19	12 (9%)
8	MPD	I	5276	-	7,7,7	0.43	0	9,10,10	0.41	0
8	MPD	I	5277	-	7,7,7	0.41	0	9,10,10	0.34	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
7	NTP	I	433	-	-	0/76/184/184	0/5/5/5
8	MPD	I	5276	-	-	0/5/5/5	0/0/0/0
8	MPD	I	5277	-	-	0/5/5/5	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	433	NTP	O16-S17	-4.65	1.43	1.56
7	I	433	NTP	O54-S55	-4.62	1.43	1.56
7	I	433	NTP	O3G-S3H	-4.60	1.43	1.56
7	I	433	NTP	O34-S35	-4.59	1.43	1.56
7	I	433	NTP	O1F-S1G	-4.56	1.43	1.56
7	I	433	NTP	O4A-S4B	-4.56	1.43	1.56
7	I	433	NTP	O5A-S5B	-4.54	1.43	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	433	NTP	O3A-S3B	-4.52	1.43	1.56
7	I	433	NTP	O5G-S5H	-4.51	1.43	1.56
7	I	433	NTP	O5M-C5L	2.27	1.44	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	433	NTP	C1E-O1F-S1G	-4.31	110.67	118.97
7	I	433	NTP	C5F-O5G-S5H	-3.93	111.41	118.97
7	I	433	NTP	C3F-O3G-S3H	-3.89	111.48	118.97
7	I	433	NTP	C59-O5A-S5B	-3.00	113.20	118.97
7	I	433	NTP	C39-O3A-S3B	-2.87	113.44	118.97
7	I	433	NTP	C4F-O4G-C50	-2.74	111.33	118.00
7	I	433	NTP	C15-C13-C12	-2.53	107.03	113.30
7	I	433	NTP	C49-O4A-S4B	-2.51	114.15	118.97
7	I	433	NTP	C1K-O1L-C20	-2.29	112.41	118.00
7	I	433	NTP	C5N-O5M-C5L	-2.28	109.72	113.29
7	I	433	NTP	O32-C31-C30	2.10	114.04	109.75
7	I	433	NTP	O16-C15-C13	2.65	112.73	107.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	433	NTP	11	0
8	I	5276	MPD	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	L	54/59 (91%)	1.66	23 (42%) 0 0	25, 45, 60, 62	0
2	H	235/235 (100%)	0.11	7 (2%) 51 56	13, 23, 39, 52	2 (0%)
3	I	419/432 (96%)	0.41	34 (8%) 13 15	18, 31, 58, 75	0
All	All	708/726 (97%)	0.41	64 (9%) 10 12	13, 29, 57, 75	2 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	220	CYS	8.7
3	I	3	SER	8.7
3	I	4	PRO	8.6
3	I	386	THR	7.7
1	L	118	ALA	6.4
1	L	84	MET	6.1
3	I	388	VAL	6.0
3	I	38	GLN	5.5
3	I	26	PRO	5.5
2	H	84	ASN	5.2
1	L	89	ASN	4.6
2	H	245	THR	4.5
1	L	102	SER	4.4
1	L	103	ALA	4.3
3	I	384	ALA	4.2
3	I	299	LEU	4.2
1	L	90	ILE	3.9
3	I	431	VAL	3.9
3	I	264	ALA	3.5
1	L	104	ASP	3.4
1	L	88	CYS	3.4
3	I	27	GLU	3.4
1	L	123	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	108	VAL	3.3
3	I	359	ARG	3.2
1	L	119	GLU	3.0
1	L	86	VAL	3.0
3	I	412[A]	ILE	2.9
2	H	96	ILE	2.9
1	L	117	LEU	2.9
1	L	94	ARG	2.8
1	L	120	ASN	2.8
3	I	304	LEU	2.8
3	I	390	ILE	2.8
1	L	105	ASN	2.8
3	I	383	ALA	2.7
1	L	85	ASP	2.7
3	I	298	GLU	2.6
3	I	382	ALA	2.6
3	I	303	VAL	2.5
3	I	14	ASP	2.5
1	L	87	THR	2.5
1	L	91	LYS	2.5
3	I	389	VAL	2.5
3	I	385	SER	2.4
3	I	81	LEU	2.3
3	I	17	MET	2.3
2	H	97[A]	ASN	2.3
1	L	107	VAL	2.3
3	I	310	GLU	2.3
3	I	315	MET	2.2
2	H	170	ARG	2.1
3	I	421	ILE	2.1
1	L	124	CYS	2.1
3	I	5	VAL	2.1
3	I	16	PRO	2.1
1	L	101	ASN	2.1
3	I	39	LYS	2.0
3	I	300	THR	2.0
1	L	137	VAL	2.0
2	H	169	LEU	2.0
3	I	238	LEU	2.0
3	I	248	SER	2.0
3	I	358	GLY	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
6	NAG	I	841	14/15	0.83	0.17	2.34	49,54,55,60	0
5	NAG	I	901	14/15	0.63	0.49	-	64,68,71,73	0
5	FUC	I	802	10/11	0.49	0.49	-	75,75,76,77	0
5	NAG	I	801	14/15	0.64	0.39	-	62,68,70,73	0
5	FUC	I	902	10/11	0.69	0.59	-	75,76,76,77	0
6	NAG	I	842	14/15	0.87	0.19	-	62,66,67,70	0
6	MAN	I	843	11/12	0.52	0.42	-	74,76,77,78	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
8	MPD	I	5276	8/8	0.83	0.45	9.05	61,62,63,63	0
8	MPD	I	5277	8/8	0.92	0.21	4.46	61,62,62,63	0
7	NTP	I	433	100/100	0.95	0.09	-0.55	26,32,40,42	0
4	CA	H	500	1/1	0.98	0.06	-1.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.