



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:46 AM GMT

PDB ID : 1TB6  
Title : 2.5A Crystal Structure of the Antithrombin-Thrombin-Heparin Ternary Complex  
Authors : Li, W.; Johnson, D.J.; Esmon, C.T.; Huntington, J.A.  
Deposited on : 2004-05-19  
Resolution : 2.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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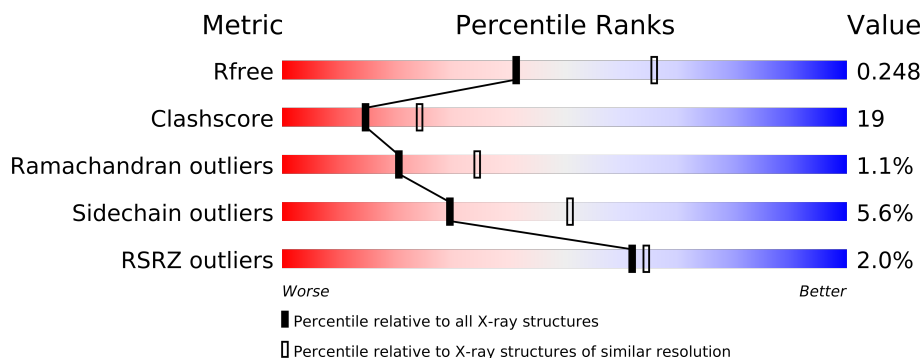
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	49	
2	H	259	
3	I	432	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6324 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	43	Total	C	N	O	S	0	0	0
			343	219	52	71	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	259	Total	C	N	O	S	0	0	0
			2070	1324	362	370	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	ENGINEERED	UNP P00734

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	412	Total	C	N	O	S	0	0	0
			3271	2091	553	607	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	317	CYS	VAL	ENGINEERED	UNP P01008
I	401	CYS	THR	ENGINEERED	UNP P01008

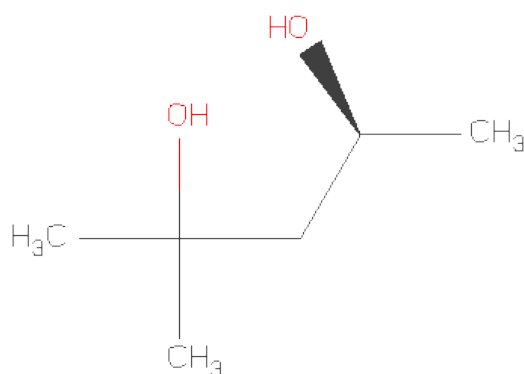
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	3	Total	C	N	O	0	0
			38	22	2	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	ENGINEERED	UNP P00734

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

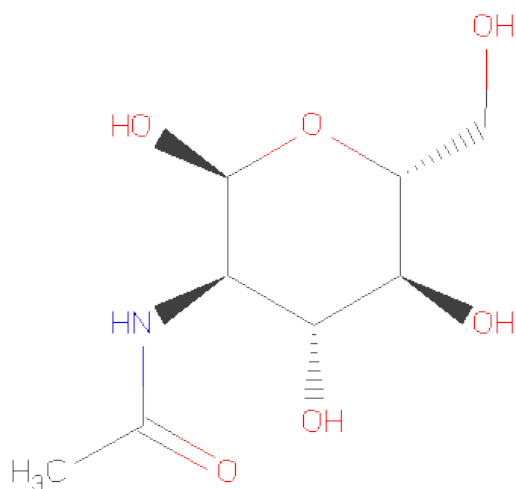
- Molecule 6 is a polymer of unknown type called SUGAR (16-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	16	Total	C	O	S	0	0
			278	127	134	17		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	317	CYS	VAL	ENGINEERED	UNP P01008
I	401	CYS	THR	ENGINEERED	UNP P01008

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

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

There are 3 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	317	CYS	VAL	ENGINEERED	UNP P01008
I	401	CYS	THR	ENGINEERED	UNP P01008

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	317	CYS	VAL	ENGINEERED	UNP P01008
I	401	CYS	THR	ENGINEERED	UNP P01008

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	3	Total	O	0	0
			3	3		
10	H	47	Total	O	0	0
			47	47		
10	I	96	Total	O	0	0
			96	96		

### 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.

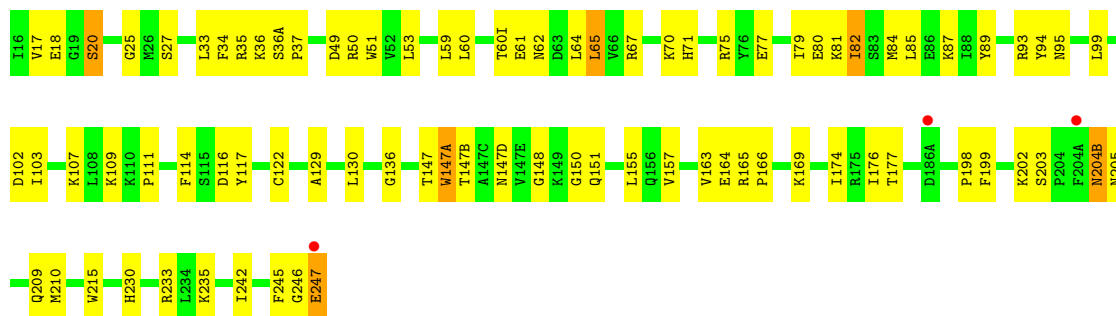
- Molecule 1: thrombin

Chain L: 



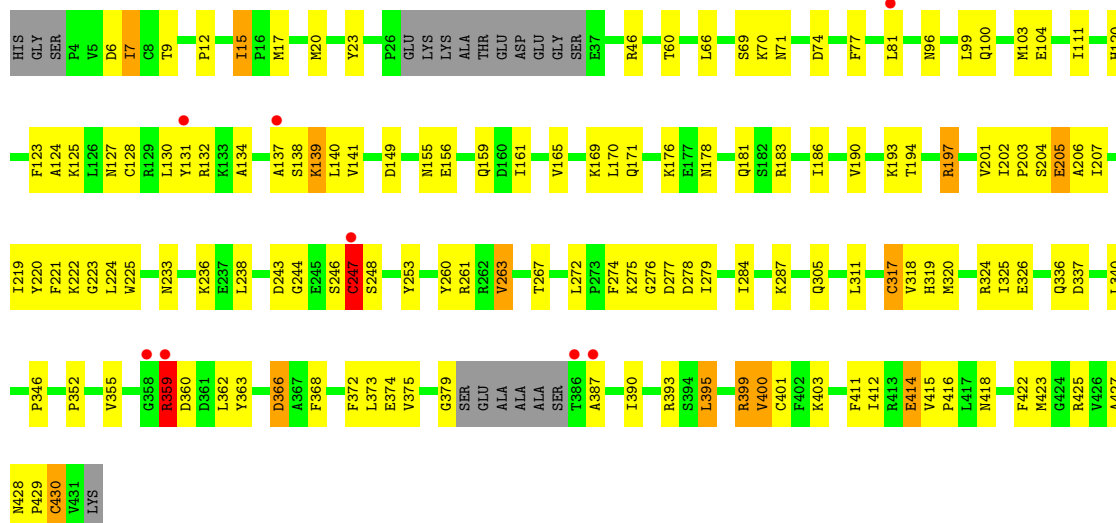
- Molecule 2: thrombin

Chain H: 



- Molecule 3: Antithrombin-III

Chain I: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.41Å 88.40Å 117.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.46 – 2.50 37.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.46-2.50) 99.4 (37.46-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.245 0.211 , 0.248	Depositor DCC
$R_{free}$ test set	1301 reflections (4.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.6	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32246 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, NDG, GU3, GU2, GU1, GU0, GU6, GU5, GU4, GU9, GU8, 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	0.34	0/350	0.60	0/470
2	H	0.36	0/2125	0.67	1/2876 (0.0%)
3	I	0.40	0/3337	0.67	1/4508 (0.0%)
All	All	0.38	0/5812	0.67	2/7854 (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
6	I	7	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	317	CYS	CA-CB-SG	6.18	125.12	114.00
2	H	247	GLU	N-CA-C	5.56	126.00	111.00

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	434	GU6	C4,C3,C5,C2
6	I	446	GU6	C5,C3,C4

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	343	0	315	26	0
2	H	2070	0	2022	77	0
3	I	3271	0	3248	116	1
4	H	38	0	34	4	0
5	H	32	0	56	9	0
5	I	32	0	56	5	0
6	I	278	0	185	32	0
7	I	14	0	13	1	0
8	I	61	0	52	2	0
9	I	39	0	34	0	0
10	H	47	0	0	3	0
10	I	96	0	0	5	0
10	L	3	0	0	0	0
All	All	6324	0	6015	234	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (234) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:324:ARG:HH12	3:I:374:GLU:HG3	1.21	1.02
3:I:7:ILE:HD13	3:I:7:ILE:H	1.25	0.98
1:L:1(I):ARG:HG2	1:L:1(I):ARG:HH11	1.39	0.85
2:H:71:HIS:HB2	5:H:782:MPD:H11	1.59	0.84
3:I:355:VAL:HG21	3:I:360:ASP:HB3	1.59	0.83
6:I:436:GU5:H5	6:I:437:GU8:H62	1.64	0.78
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.64	0.77
1:L:1(I):ARG:HG2	1:L:1(I):ARG:NH1	1.98	0.77
3:I:324:ARG:NH1	3:I:374:GLU:HG3	1.99	0.76
3:I:324:ARG:HG3	3:I:324:ARG:HH11	1.51	0.76
2:H:93:ARG:NH1	6:I:434:GU6:H61	2.00	0.76
3:I:414:GLU:OE1	3:I:416:PRO:HD2	1.85	0.76
6:I:445:GU1:H83	6:I:445:GU1:H72	1.66	0.75
3:I:326:GLU:HG3	3:I:326:GLU:O	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:61:GLU:CG	2:H:87:LYS:HA	2.16	0.74
3:I:96:ASN:OD1	7:I:801:NDG:H5	1.88	0.73
3:I:139:LYS:O	3:I:221:PHE:HA	1.88	0.73
3:I:7:ILE:CD1	3:I:7:ILE:H	2.02	0.72
3:I:81:LEU:HD11	3:I:127:ASN:HD21	1.55	0.69
3:I:246:SER:O	3:I:247:CYS:HB2	1.93	0.69
1:L:1(I):ARG:HH21	2:H:247:GLU:C	1.95	0.68
6:I:438:GU9:H1	6:I:439:GU8:O3	1.92	0.68
2:H:67:ARG:HG2	2:H:82:ILE:HG12	1.76	0.67
1:L:1(K):ASN:HD21	1:L:1(I):ARG:CB	2.09	0.65
1:L:1(H):THR:HG22	2:H:247:GLU:HA	1.78	0.65
6:I:443:GU8:H73	6:I:444:GU5:H61	1.76	0.65
1:L:1(K):ASN:HD21	1:L:1(I):ARG:HB3	1.61	0.64
3:I:415:VAL:HB	3:I:416:PRO:HD3	1.79	0.64
2:H:59:LEU:HD22	2:H:64:LEU:HD11	1.79	0.64
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.33	0.64
3:I:15:ILE:HD13	3:I:15:ILE:N	2.13	0.63
3:I:159:GLN:HB3	3:I:169:LYS:HD2	1.80	0.63
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.81	0.63
3:I:127:ASN:HB3	5:I:864:MPD:H11	1.80	0.62
3:I:60:THR:HA	5:I:865:MPD:H31	1.81	0.62
1:L:1(K):ASN:OD1	1:L:1(I):ARG:HB2	1.99	0.62
3:I:120:HIS:H	3:I:120:HIS:CD2	2.18	0.62
3:I:186:ILE:HG21	3:I:202:ILE:HD12	1.81	0.62
1:L:1(I):ARG:CG	1:L:1(I):ARG:HH11	2.13	0.61
3:I:7:ILE:HD13	3:I:7:ILE:N	2.08	0.60
2:H:67:ARG:NH2	2:H:82:ILE:HD11	2.15	0.60
1:L:5:PRO:HB2	2:H:116:ASP:HA	1.82	0.60
3:I:128:CYS:HB3	3:I:132:ARG:HH21	1.67	0.60
3:I:425:ARG:HD3	3:I:427:ALA:HB2	1.82	0.59
3:I:190:VAL:HG11	3:I:201:VAL:HG21	1.84	0.59
2:H:34:PHE:HB2	2:H:65:LEU:HD22	1.85	0.59
1:L:5:PRO:CB	2:H:116:ASP:HA	2.33	0.58
2:H:81:LYS:HE3	10:H:801:HOH:O	2.03	0.58
6:I:437:GU8:H1	6:I:438:GU9:H62	1.84	0.58
3:I:170:LEU:C	3:I:170:LEU:HD23	2.24	0.58
2:H:174:ILE:HD13	3:I:390:ILE:HB	1.85	0.58
3:I:399:ARG:HH11	3:I:399:ARG:CG	2.16	0.58
6:I:444:GU5:H1	6:I:445:GU1:H82	1.86	0.58
2:H:60:LEU:HD11	4:H:778:NDG:H8C3	1.87	0.57
2:H:27:SER:H	5:H:782:MPD:H53	1.69	0.57
3:I:100:GLN:O	3:I:104:GLU:HG3	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:319:HIS:HB2	3:I:403:LYS:HA	1.85	0.57
3:I:276:GLY:O	3:I:277:ASP:HB2	2.05	0.56
3:I:125:LYS:HE3	10:I:912:HOH:O	2.05	0.56
2:H:35:ARG:HD2	2:H:37:PRO:O	2.05	0.56
2:H:80:GLU:O	2:H:81:LYS:HD2	2.06	0.56
6:I:438:GU9:H72	6:I:438:GU9:O1	2.06	0.56
3:I:272:LEU:N	3:I:272:LEU:HD12	2.21	0.55
3:I:238:LEU:HD22	3:I:246:SER:OG	2.07	0.55
3:I:134:ALA:O	3:I:138:SER:HB2	2.07	0.55
2:H:164:GLU:HB3	2:H:166:PRO:HD2	1.89	0.55
3:I:355:VAL:HG13	3:I:362:LEU:HD22	1.89	0.55
3:I:206:ALA:HB1	3:I:368:PHE:HZ	1.72	0.55
6:I:441:GU8:C7	6:I:442:GU9:H61	2.37	0.55
3:I:99:LEU:O	3:I:103:MET:HG2	2.06	0.54
2:H:25:GLY:H	5:H:782:MPD:H31	1.71	0.54
2:H:176:ILE:HG22	2:H:177:THR:N	2.23	0.54
3:I:305:GLN:OE1	3:I:418:ASN:ND2	2.41	0.54
3:I:66:LEU:O	3:I:70:LYS:HG3	2.08	0.54
3:I:400:VAL:CG1	3:I:401:CYS:N	2.70	0.54
3:I:12:PRO:HB2	6:I:446:GU6:O15	2.08	0.53
1:L:1(G):PHE:CD1	2:H:242:ILE:HD13	2.44	0.53
4:H:778:NDG:H6C1	4:H:780:FUC:O2	2.09	0.53
2:H:129:ALA:O	2:H:130:LEU:HB2	2.09	0.53
3:I:149:ASP:OD2	3:I:176:LYS:HG3	2.08	0.53
3:I:81:LEU:HD11	3:I:127:ASN:ND2	2.22	0.53
6:I:442:GU9:O1	6:I:442:GU9:H72	2.08	0.53
2:H:67:ARG:CZ	2:H:82:ILE:HD11	2.39	0.53
3:I:77:PHE:CE2	3:I:373:LEU:HB2	2.44	0.53
3:I:141:VAL:HG22	3:I:220:TYR:HB3	1.90	0.53
3:I:278:ASP:C	3:I:279:ILE:HD12	2.30	0.52
3:I:204:SER:O	3:I:205:GLU:CB	2.57	0.52
6:I:443:GU8:C7	6:I:444:GU5:H61	2.40	0.52
2:H:80:GLU:OE2	5:H:783:MPD:H51	2.10	0.52
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.45	0.52
3:I:204:SER:O	3:I:205:GLU:HB3	2.10	0.51
2:H:147:THR:HG21	2:H:147(D):ASN:HB3	1.92	0.51
2:H:155:LEU:CD2	5:H:782:MPD:H51	2.41	0.51
2:H:65:LEU:HD23	2:H:65:LEU:C	2.32	0.51
2:H:233:ARG:HH21	2:H:233:ARG:HG2	1.76	0.51
3:I:236:LYS:HE3	3:I:248:SER:OG	2.11	0.50
6:I:445:GU1:C8	6:I:445:GU1:H72	2.38	0.50
3:I:197:ARG:HG3	10:I:953:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:441:GU8:H73	6:I:442:GU9:H61	1.92	0.50
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.12	0.50
2:H:64:LEU:HB2	2:H:85:LEU:HD12	1.93	0.50
3:I:399:ARG:HH11	3:I:399:ARG:HG2	1.76	0.50
6:I:440:GU9:H1	6:I:441:GU8:C8	2.42	0.50
3:I:400:VAL:HG13	3:I:401:CYS:N	2.27	0.50
3:I:359:ARG:HG3	10:I:931:HOH:O	2.11	0.50
2:H:136:GLY:HA3	2:H:199:PHE:CE1	2.46	0.50
3:I:355:VAL:HG21	3:I:360:ASP:CB	2.36	0.49
2:H:169:LYS:HA	2:H:176:ILE:HD12	1.94	0.49
3:I:77:PHE:HB2	3:I:325:ILE:HG21	1.95	0.49
3:I:260:TYR:CZ	3:I:400:VAL:HG11	2.48	0.49
3:I:399:ARG:NH1	3:I:399:ARG:CG	2.75	0.49
2:H:165:ARG:N	2:H:166:PRO:CD	2.76	0.49
2:H:50:ARG:HH11	2:H:111:PRO:HG2	1.77	0.49
1:L:1:CYS:C	2:H:122:CYS:SG	2.92	0.49
2:H:36:LYS:HE3	2:H:64:LEU:O	2.12	0.48
1:L:1:CYS:O	2:H:122:CYS:SG	2.70	0.48
5:H:781:MPD:H13	10:I:955:HOH:O	2.12	0.48
3:I:324:ARG:HD3	3:I:372:PHE:HZ	1.78	0.48
3:I:20:MET:SD	3:I:352:PRO:HB2	2.53	0.48
6:I:437:GU8:H73	6:I:437:GU8:O1	2.13	0.48
2:H:169:LYS:HE3	10:H:805:HOH:O	2.12	0.48
6:I:444:GU5:H82	6:I:444:GU5:O2	2.14	0.48
3:I:225:TRP:CD1	3:I:379:GLY:HA2	2.48	0.48
6:I:437:GU8:H1	6:I:438:GU9:C6	2.44	0.48
1:L:1(H):THR:HG22	2:H:247:GLU:N	2.29	0.47
6:I:436:GU5:C7	10:I:944:HOH:O	2.62	0.47
6:I:439:GU8:O2	6:I:439:GU8:H83	2.14	0.47
3:I:77:PHE:CZ	3:I:373:LEU:HB2	2.50	0.47
3:I:139:LYS:HB2	3:I:222:LYS:O	2.14	0.47
5:H:781:MPD:H12	3:I:233:ASN:O	2.14	0.47
2:H:84:MET:HB2	2:H:109:LYS:HG3	1.97	0.47
2:H:99:LEU:O	2:H:102:ASP:HB2	2.14	0.47
3:I:324:ARG:HH11	3:I:324:ARG:CG	2.22	0.47
3:I:190:VAL:HG11	3:I:201:VAL:CG2	2.44	0.47
1:L:1(K):ASN:ND2	1:L:1(I):ARG:CB	2.78	0.47
3:I:161:ILE:O	3:I:165:VAL:HG12	2.14	0.47
3:I:128:CYS:HB3	3:I:132:ARG:NH2	2.30	0.46
6:I:439:GU8:O1	6:I:439:GU8:H73	2.15	0.46
3:I:183:ARG:NH2	3:I:204:SER:HB2	2.30	0.46
3:I:20:MET:HE3	8:I:841:NAG:H2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:441:GU8:H73	6:I:441:GU8:O1	2.15	0.46
1:L:14(C):GLU:OE1	2:H:202:LYS:NZ	2.38	0.46
2:H:36:LYS:HD2	2:H:62:ASN:O	2.16	0.45
3:I:261:ARG:CB	3:I:311:LEU:HD23	2.47	0.45
2:H:148:GLY:HA2	2:H:151:GLN:NE2	2.31	0.45
3:I:131:TYR:HB2	5:I:864:MPD:H13	1.97	0.45
3:I:138:SER:HB3	3:I:223:GLY:HA2	1.98	0.45
2:H:20:SER:O	2:H:157:VAL:HG12	2.16	0.45
3:I:346:PRO:HG3	3:I:363:TYR:CZ	2.52	0.45
3:I:130:LEU:CD2	3:I:414:GLU:HG3	2.46	0.45
3:I:287:LYS:HE3	3:I:287:LYS:HB2	1.81	0.45
1:L:1(G):PHE:HD1	2:H:242:ILE:HD13	1.82	0.45
1:L:1(M):PHE:CD2	2:H:235:LYS:HE2	2.52	0.45
2:H:163:VAL:HG12	2:H:164:GLU:N	2.33	0.45
2:H:129:ALA:HA	2:H:210:MET:HE1	1.98	0.45
3:I:46:ARG:NH2	6:I:447:GU2:O48	2.50	0.45
2:H:25:GLY:H	5:H:782:MPD:C3	2.29	0.44
3:I:243:ASP:OD1	3:I:244:GLY:N	2.49	0.44
2:H:61:GLU:CD	2:H:61:GLU:H	2.20	0.44
3:I:186:ILE:HG21	3:I:202:ILE:CD1	2.48	0.44
3:I:261:ARG:HB3	3:I:311:LEU:HD23	2.00	0.44
3:I:253:TYR:HA	3:I:318:VAL:O	2.18	0.44
2:H:36(A):SER:HA	2:H:37:PRO:C	2.37	0.44
1:L:13:GLU:HA	1:L:14(C):GLU:OE2	2.17	0.44
3:I:124:ALA:HB2	3:I:165:VAL:CG2	2.48	0.44
4:H:778:NDG:C6	4:H:780:FUC:O2	2.65	0.44
2:H:164:GLU:CB	2:H:166:PRO:HD2	2.48	0.44
3:I:203:PRO:HG3	5:I:867:MPD:O2	2.18	0.44
6:I:447:GU2:O1	6:I:448:GU3:H7B	2.18	0.44
1:L:1(H):THR:HG22	2:H:247:GLU:CA	2.46	0.43
3:I:17:MET:O	3:I:120:HIS:HE1	2.01	0.43
3:I:260:TYR:CG	3:I:261:ARG:N	2.86	0.43
1:L:7:PHE:O	1:L:8:GLU:C	2.56	0.43
1:L:1(K):ASN:HD21	1:L:1(I):ARG:HB2	1.80	0.43
6:I:444:GU5:H1	6:I:445:GU1:C8	2.48	0.43
2:H:49:ASP:O	2:H:111:PRO:HA	2.18	0.43
3:I:137:ALA:CB	3:I:275:LYS:HE2	2.48	0.43
1:L:1(K):ASN:ND2	1:L:1(I):ARG:HB2	2.33	0.43
3:I:324:ARG:HD3	3:I:372:PHE:CZ	2.54	0.43
6:I:445:GU1:H83	6:I:445:GU1:C7	2.41	0.43
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.33	0.43
2:H:215:TRP:CE3	3:I:390:ILE:HG12	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:284:ILE:HD13	3:I:411:PHE:HE2	1.84	0.43
3:I:125:LYS:NZ	6:I:445:GU1:O37	2.50	0.43
3:I:206:ALA:HB1	3:I:368:PHE:CZ	2.52	0.43
3:I:12:PRO:HG2	6:I:446:GU6:O17	2.18	0.43
2:H:215:TRP:HA	3:I:393:ARG:HG3	2.00	0.43
3:I:284:ILE:HD13	3:I:411:PHE:CE2	2.54	0.43
1:L:4:ARG:HA	1:L:5:PRO:HD3	1.91	0.43
3:I:346:PRO:HG3	3:I:363:TYR:CE2	2.54	0.43
3:I:320:MET:CE	3:I:375:VAL:HG11	2.49	0.43
6:I:439:GU8:C7	6:I:440:GU9:H61	2.49	0.42
2:H:117:TYR:CD1	5:H:782:MPD:HM3	2.54	0.42
2:H:80:GLU:C	2:H:81:LYS:HD2	2.40	0.42
6:I:439:GU8:H73	6:I:440:GU9:H61	2.01	0.42
2:H:147:THR:CG2	2:H:147(D):ASN:HD22	2.32	0.42
3:I:355:VAL:CG1	3:I:362:LEU:HD22	2.50	0.42
3:I:132:ARG:HD3	3:I:132:ARG:N	2.33	0.42
2:H:147:THR:CG2	2:H:147(A):TRP:N	2.82	0.42
3:I:178:ASN:HB3	3:I:181:GLN:HB2	2.01	0.42
3:I:366:ASP:HB3	3:I:368:PHE:CE2	2.55	0.42
3:I:412:ILE:HB	3:I:422:PHE:HB2	2.01	0.42
2:H:147:THR:CG2	2:H:147(B):THR:H	2.32	0.42
1:L:6:LEU:HA	1:L:10:LYS:HE2	2.02	0.42
2:H:60:LEU:HD11	4:H:778:NDG:C8	2.50	0.42
3:I:155:ASN:ND2	8:I:841:NAG:C7	2.82	0.42
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.94	0.42
2:H:50:ARG:HG3	2:H:51:TRP:CD1	2.55	0.42
3:I:6:ASP:OD1	3:I:9:THR:HG23	2.20	0.42
3:I:263:VAL:HG22	3:I:267:THR:O	2.20	0.42
2:H:89:TYR:OH	2:H:245:PHE:HB3	2.20	0.41
3:I:138:SER:CB	3:I:223:GLY:HA2	2.51	0.41
1:L:8:GLU:H	1:L:8:GLU:CD	2.24	0.41
2:H:17:VAL:O	2:H:18:GLU:HB2	2.20	0.41
3:I:423:MET:HE1	5:I:865:MPD:HM1	2.02	0.41
2:H:203:SER:O	2:H:205:ASN:HA	2.21	0.41
2:H:75:ARG:O	2:H:77:GLU:HG3	2.21	0.41
3:I:140:LEU:HD11	3:I:219:ILE:HD11	2.03	0.41
3:I:324:ARG:NH1	3:I:324:ARG:CG	2.81	0.41
2:H:79:ILE:HG23	2:H:117:TYR:CD2	2.56	0.41
3:I:15:ILE:HG12	3:I:15:ILE:O	2.20	0.41
6:I:444:GU5:H5	6:I:445:GU1:O38	2.21	0.41
2:H:198:PRO:HB3	2:H:209:GLN:NE2	2.36	0.41
2:H:130:LEU:HD21	2:H:230:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:324:ARG:HH12	3:I:374:GLU:CG	2.10	0.41
6:I:440:GU9:H1	6:I:441:GU8:O3	2.19	0.41
3:I:274:PHE:CD2	3:I:279:ILE:HG22	2.56	0.41
3:I:320:MET:HE1	3:I:375:VAL:HG11	2.02	0.41
3:I:336:GLN:HA	3:I:340:LEU:O	2.21	0.41
3:I:194:THR:O	3:I:197:ARG:HB2	2.20	0.41
3:I:395:LEU:HA	3:I:395:LEU:HD23	1.82	0.40
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.37	0.40
2:H:150:GLY:HA3	10:H:792:HOH:O	2.20	0.40
3:I:181:GLN:N	3:I:181:GLN:OE1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:207:ILE:O	3:I:399:ARG:NH2[4_455]	2.19	0.01

## 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	L	41/49 (84%)	35 (85%)	6 (15%)	0	100	100
2	H	257/259 (99%)	237 (92%)	20 (8%)	0	100	100
3	I	406/432 (94%)	378 (93%)	20 (5%)	8 (2%)	11	17
All	All	704/740 (95%)	650 (92%)	46 (6%)	8 (1%)	21	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	247	CYS
3	I	359	ARG
3	I	387	ALA
3	I	205	GLU
3	I	111	ILE

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Mol	Chain	Res	Type
3	I	430	CYS
3	I	429	PRO
3	I	263	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	L	36/43 (84%)	32 (89%)	4 (11%)	9	16
2	H	218/224 (97%)	209 (96%)	9 (4%)	41	67
3	I	358/382 (94%)	337 (94%)	21 (6%)	28	48
All	All	612/649 (94%)	578 (94%)	34 (6%)	30	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(K)	ASN
1	L	1(I)	ARG
1	L	1(E)	SER
1	L	14(K)	ILE
2	H	20	SER
2	H	33	LEU
2	H	60(I)	THR
2	H	65	LEU
2	H	82	ILE
2	H	94	TYR
2	H	95	ASN
2	H	147(A)	TRP
2	H	204(B)	ASN
3	I	7	ILE
3	I	15	ILE
3	I	69	SER
3	I	123	PHE
3	I	139	LYS
3	I	156	GLU
3	I	171	GLN

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Mol	Chain	Res	Type
3	I	193	LYS
3	I	197	ARG
3	I	224	LEU
3	I	247	CYS
3	I	317	CYS
3	I	337	ASP
3	I	359	ARG
3	I	366	ASP
3	I	395	LEU
3	I	399	ARG
3	I	400	VAL
3	I	414	GLU
3	I	428	ASN
3	I	430	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	H	151	GLN
2	H	204(B)	ASN
2	H	239	GLN
3	I	55	ASN
3	I	65	HIS
3	I	120	HIS
3	I	127	ASN
3	I	171	GLN
3	I	305	GLN
3	I	319	HIS
3	I	418	ASN
3	I	428	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

27 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$
4	NDG	H	778	2,4	12,14,15	0.57	0	15,19,21	0.94	1 (6%)
4	NAG	H	779	4	12,14,15	0.44	0	15,19,21	0.66	0
4	FUC	H	780	4	9,10,11	0.59	0	10,14,16	0.57	0
6	GU4	I	433	6	28,28,28	3.45	4 (14%)	45,45,45	1.37	7 (15%)
6	GU6	I	434	6	23,23,24	3.93	7 (30%)	32,36,38	2.84	9 (28%)
6	GU0	I	435	6	23,23,24	3.15	3 (13%)	32,36,38	1.22	3 (9%)
6	GU5	I	436	6	17,17,18	1.02	1 (5%)	20,24,26	0.87	0
6	GU8	I	437	6	14,14,15	0.58	0	14,18,20	0.78	1 (7%)
6	GU9	I	438	6	14,14,15	0.60	0	14,18,20	0.84	0
6	GU8	I	439	6	14,14,15	0.58	0	14,18,20	0.87	0
6	GU9	I	440	6	14,14,15	0.59	0	14,18,20	0.70	0
6	GU8	I	441	6	14,14,15	0.58	0	14,18,20	0.68	0
6	GU9	I	442	6	14,14,15	0.60	0	14,18,20	0.65	0
6	GU8	I	443	6	14,14,15	0.57	0	14,18,20	0.78	0
6	GU5	I	444	6	17,17,18	1.02	1 (5%)	20,24,26	0.82	0
6	GU1	I	445	6	14,14,15	0.73	0	15,19,21	1.54	1 (6%)
6	GU6	I	446	6	23,23,24	3.16	3 (13%)	32,36,38	1.38	7 (21%)
6	GU2	I	447	6	14,14,15	0.77	1 (7%)	15,19,21	1.53	1 (6%)
6	GU3	I	448	6	21,21,22	2.68	3 (14%)	27,31,33	1.38	3 (11%)
8	NAG	I	841	8,3	12,14,15	0.62	0	15,19,21	0.73	0
8	NAG	I	842	8	12,14,15	0.42	0	15,19,21	0.83	0
8	BMA	I	843	8	10,11,12	0.68	0	11,15,17	1.33	2 (18%)
8	MAN	I	844	8	10,11,12	0.49	0	11,15,17	0.23	0
8	MAN	I	845	8	10,11,12	0.43	0	11,15,17	0.37	0
9	NAG	I	861	9,3	12,14,15	0.51	0	15,19,21	0.70	0
9	NAG	I	862	9	12,14,15	0.68	0	15,19,21	0.67	0
9	BMA	I	863	9	10,11,12	0.44	0	11,15,17	0.35	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
4	NDG	H	778	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	779	4	-	0/6/23/26	0/1/1/1
4	FUC	H	780	4	-	0/0/17/20	0/1/1/1
6	GU4	I	433	6	-	0/21/41/41	0/1/1/1
6	GU6	I	434	6	4/4/7/8	0/16/32/36	0/1/1/1
6	GU0	I	435	6	-	0/16/32/36	0/1/1/1
6	GU5	I	436	6	-	0/10/26/30	0/1/1/1
6	GU8	I	437	6	-	0/7/23/27	0/1/1/1
6	GU9	I	438	6	-	0/7/23/27	0/1/1/1
6	GU8	I	439	6	-	0/7/23/27	0/1/1/1
6	GU9	I	440	6	-	0/7/23/27	0/1/1/1
6	GU8	I	441	6	-	0/7/23/27	0/1/1/1
6	GU9	I	442	6	-	0/7/23/27	0/1/1/1
6	GU8	I	443	6	-	0/7/23/27	0/1/1/1
6	GU5	I	444	6	-	0/10/26/30	0/1/1/1
6	GU1	I	445	6	-	0/8/24/28	0/1/1/1
6	GU6	I	446	6	3/3/7/8	0/16/32/36	0/1/1/1
6	GU2	I	447	6	-	0/8/24/28	0/1/1/1
6	GU3	I	448	6	-	0/15/31/35	0/1/1/1
8	NAG	I	841	8,3	-	0/6/23/26	0/1/1/1
8	NAG	I	842	8	-	0/6/23/26	0/1/1/1
8	BMA	I	843	8	-	0/2/19/22	0/1/1/1
8	MAN	I	844	8	-	0/2/19/22	0/1/1/1
8	MAN	I	845	8	-	0/2/19/22	0/1/1/1
9	NAG	I	861	9,3	-	0/6/23/26	0/1/1/1
9	NAG	I	862	9	-	0/6/23/26	0/1/1/1
9	BMA	I	863	9	-	0/2/19/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	448	GU3	O2-S2	-10.63	1.43	1.60
6	I	433	GU4	O2-S2	-10.00	1.43	1.59
6	I	435	GU0	O2-S2	-9.99	1.43	1.59
6	I	446	GU6	O2-S2	-9.96	1.43	1.59
6	I	446	GU6	O3-S3	-9.94	1.43	1.59
6	I	433	GU4	O4-S4	-9.88	1.43	1.59
6	I	434	GU6	O2-S2	-9.82	1.43	1.59
6	I	433	GU4	O3-S3	-9.82	1.43	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	435	GU0	O3-S3	-9.78	1.43	1.59
6	I	434	GU6	O3-S3	-9.72	1.44	1.59
6	I	434	GU6	C2-C3	-8.26	1.39	1.52
6	I	434	GU6	O2-C2	-6.18	1.36	1.46
6	I	434	GU6	O3-C3	-5.26	1.36	1.46
6	I	448	GU3	O6-S6	-4.03	1.43	1.57
6	I	434	GU6	O6-S6	-2.74	1.43	1.60
6	I	436	GU5	O6-S6	-2.71	1.43	1.60
6	I	444	GU5	O6-S6	-2.69	1.43	1.60
6	I	435	GU0	O6-S6	-2.69	1.43	1.60
6	I	433	GU4	O6-S6	-2.68	1.43	1.60
6	I	446	GU6	O6-S6	-2.67	1.43	1.60
6	I	448	GU3	O1-C1	2.24	1.44	1.40
6	I	434	GU6	O5-C5	-2.09	1.36	1.44
6	I	447	GU2	O48-C6	-2.03	1.23	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	434	GU6	O2-C2-C1	9.06	120.15	107.58
6	I	434	GU6	O5-C5-C6	6.47	117.75	107.86
6	I	434	GU6	O2-C2-C3	6.37	122.31	108.58
6	I	434	GU6	O3-C3-C2	5.64	123.35	107.99
6	I	447	GU2	O48-C6-C5	5.03	120.19	113.04
6	I	445	GU1	O38-C6-C5	4.90	119.99	113.04
6	I	448	GU3	C2-O2-S2	-4.40	111.20	118.37
6	I	433	GU4	C2-O2-S2	-3.67	112.27	118.20
8	I	843	BMA	O5-C5-C6	-3.52	103.28	106.98
6	I	434	GU6	C2-O2-S2	-3.42	112.67	118.20
6	I	448	GU3	C6-O6-S6	3.38	121.10	116.76
6	I	446	GU6	C3-O3-S3	-2.97	112.64	120.00
6	I	433	GU4	C4-O4-S4	-2.81	113.66	118.20
6	I	435	GU0	C2-O2-S2	-2.74	113.77	118.20
6	I	433	GU4	C3-O3-S3	-2.73	113.79	118.20
6	I	446	GU6	C2-O2-S2	-2.63	113.96	118.20
6	I	434	GU6	C1-C2-C3	2.59	117.20	110.79
6	I	435	GU0	O3-S3-O27	2.39	111.28	104.58
6	I	434	GU6	O17-S3-O3	2.37	111.22	105.80
8	I	843	BMA	C4-C3-C2	-2.27	107.46	110.50
6	I	435	GU0	O2-S2-O23	2.26	110.91	104.58
6	I	434	GU6	C1-O5-C5	2.26	117.25	112.41
6	I	446	GU6	O2-C2-C1	2.24	110.69	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	446	GU6	O2-S2-O13	2.17	110.64	104.58
6	I	448	GU3	C8-O1-C1	-2.16	110.05	113.33
6	I	433	GU4	O2-C2-C1	2.15	110.56	107.58
4	H	778	NDG	C2-N2-C7	-2.13	119.51	123.09
6	I	433	GU4	O3-S3-O27	2.11	110.48	104.58
6	I	437	GU8	C1-C2-C3	-2.11	105.58	110.79
6	I	446	GU6	O3-S3-O16	2.10	110.44	104.58
6	I	434	GU6	O2-S2-O14	2.07	110.38	104.58
6	I	446	GU6	O6-C6-C5	2.06	111.72	107.81
6	I	433	GU4	O2-S2-O11	2.05	110.30	104.58
6	I	433	GU4	O24-S4-O4	2.02	110.43	105.80
6	I	446	GU6	O17-S3-O3	2.01	110.39	105.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	434	GU6	C4
6	I	434	GU6	C3
6	I	434	GU6	C5
6	I	434	GU6	C2
6	I	446	GU6	C5
6	I	446	GU6	C3
6	I	446	GU6	C4

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

9 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	$\# Z  > 2$
5	MPD	H	781	-	7,7,7	0.60	0	10,10,10	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MPD	H	782	-	7,7,7	0.58	0	10,10,10	0.59	0
5	MPD	H	783	-	7,7,7	0.40	0	10,10,10	0.37	0
5	MPD	H	784	-	7,7,7	0.46	0	10,10,10	0.41	0
7	NDG	I	801	3	12,14,15	0.44	0	15,19,21	0.70	0
5	MPD	I	864	-	7,7,7	0.45	0	10,10,10	0.43	0
5	MPD	I	865	-	7,7,7	0.59	0	10,10,10	0.50	0
5	MPD	I	866	-	7,7,7	0.44	0	10,10,10	0.37	0
5	MPD	I	867	-	7,7,7	0.42	0	10,10,10	0.50	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	MPD	H	781	-	-	0/5/5/5	0/0/0/0
5	MPD	H	782	-	-	0/5/5/5	0/0/0/0
5	MPD	H	783	-	-	0/5/5/5	0/0/0/0
5	MPD	H	784	-	-	0/5/5/5	0/0/0/0
7	NDG	I	801	3	-	0/6/23/26	0/1/1/1
5	MPD	I	864	-	-	0/5/5/5	0/0/0/0
5	MPD	I	865	-	-	0/5/5/5	0/0/0/0
5	MPD	I	866	-	-	0/5/5/5	0/0/0/0
5	MPD	I	867	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	43/49 (87%)	0.17	2 (4%) 30 31	47, 64, 77, 90	0
2	H	259/259 (100%)	-0.07	3 (1%) 75 77	22, 42, 60, 83	0
3	I	412/432 (95%)	0.02	8 (1%) 64 66	22, 40, 70, 82	0
All	All	714/740 (96%)	-0.00	13 (1%) 62 68	22, 42, 70, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1(R)	SER	5.4
3	I	358	GLY	2.9
3	I	131	TYR	2.6
3	I	359	ARG	2.4
3	I	387	ALA	2.3
2	H	247	GLU	2.3
2	H	186(A)	ASP	2.3
1	L	14(K)	ILE	2.3
3	I	247	CYS	2.2
2	H	204(A)	PHE	2.2
3	I	137	ALA	2.2
3	I	81	LEU	2.1
3	I	386	THR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



### 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	I	842	14/15	0.14	-	46,58,66,78	0
8	MAN	I	845	11/12	0.52	-	118,123,125,125	0
6	GU9	I	440	14/15	0.34	-	73,75,77,77	0
4	NDG	H	778	14/15	0.28	-	67,74,84,86	0
6	GU8	I	441	14/15	0.28	-	74,75,76,77	0
8	BMA	I	843	11/12	0.22	-	91,103,110,115	0
4	NAG	H	779	14/15	0.44	-	89,92,94,94	0
9	NAG	I	861	14/15	0.33	-	87,92,94,98	0
6	GU2	I	447	14/15	0.18	-	65,66,70,70	0
8	NAG	I	841	14/15	0.16	-	42,48,50,51	0
9	BMA	I	863	11/12	0.40	-	106,108,108,109	0
4	FUC	H	780	10/11	0.31	-	86,89,91,92	0
6	GU6	I	434	23/24	0.17	-	41,52,64,67	0
8	MAN	I	844	11/12	0.50	-	119,122,123,124	0
6	GU1	I	445	14/15	0.16	-	58,59,62,63	0
6	GU4	I	433	28/28	0.12	-	43,54,60,61	0
6	GU0	I	435	23/24	0.12	-	28,43,47,51	0
6	GU3	I	448	21/22	0.13	-	58,63,74,75	0
6	GU9	I	442	14/15	0.15	-	71,74,76,76	0
6	GU9	I	438	14/15	0.24	-	70,75,76,76	0
6	GU5	I	444	17/18	0.10	-	47,54,57,57	0
6	GU5	I	436	17/18	0.10	-	43,46,51,53	0
9	NAG	I	862	14/15	0.55	-	102,104,106,107	0
6	GU6	I	446	23/24	0.15	-	53,65,70,71	0
6	GU8	I	443	14/15	0.23	-	63,69,71,72	0
6	GU8	I	439	14/15	0.23	-	76,77,79,79	0
6	GU8	I	437	14/15	0.15	-	49,55,59,62	0

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	I	865	8/8	0.26	-	72,73,74,75	0
5	MPD	H	784	8/8	0.27	-	77,77,78,78	0
5	MPD	I	864	8/8	0.31	-	83,84,86,87	0
5	MPD	H	781	8/8	0.29	-	76,76,77,78	0
5	MPD	I	866	8/8	0.23	-	89,90,91,91	0
5	MPD	I	867	8/8	0.27	-	98,98,99,99	0
5	MPD	H	782	8/8	0.49	-	97,99,100,100	0
7	NDG	I	801	14/15	0.40	-	78,82,84,85	0
5	MPD	H	783	8/8	0.25	-	68,69,73,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.