



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 1UMA / pdb_00001uma
Title : ALPHA-THROMBIN (HIRUGEN) COMPLEXED WITH NA-(N,N-DIMETHYLCARBAMOYL)-ALPHA-AZALYSINE
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Deposited on : 1996-03-26
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

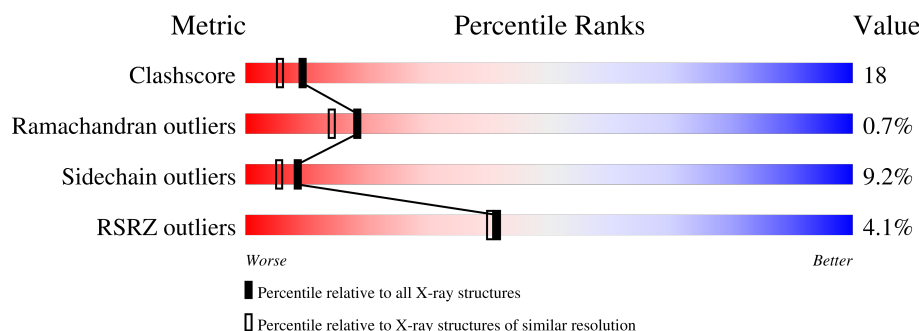
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	36	14% 56% 36% 8%
2	H	259	% 57% 32% 8% ...
3	I	10	40% 40% 40% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2658 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 ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	57	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	33	0	0
			2053	1310	362	367	14			

- Molecule 3 is a protein called HIRUDIN I.

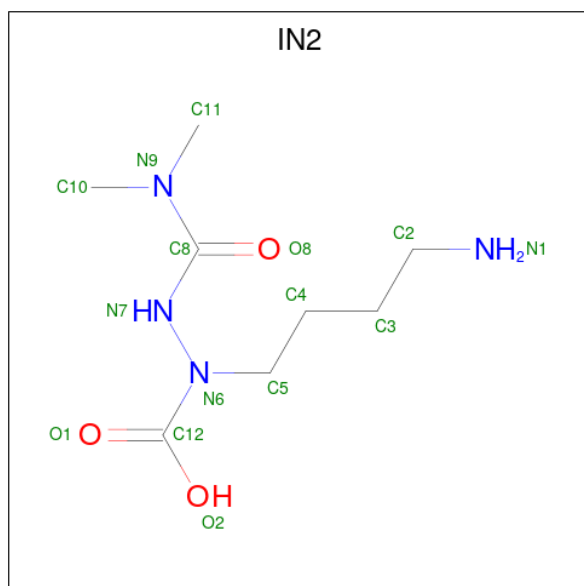
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	4	0	0
			95	59	10	25	1			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is N,N-DIMETHYLCARBAMOYL-ALPHA-AZALYSINE (CCD ID: IN2) (formula: $C_8H_{18}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			15	8	4	3		
5	H	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	21	Total	O	1	0
			21	21		
6	H	157	Total	O	5	0
			157	157		
6	I	2	Total	O	0	0
			2	2		

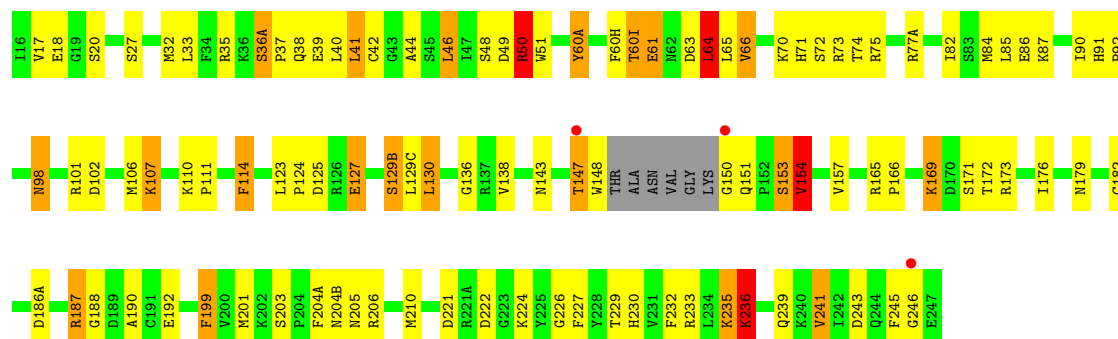
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ALPHA-THROMBIN



- Molecule 2: ALPHA-THROMBIN



- Molecule 3: HIRUDIN I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.15Å 71.90Å 72.30Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 93.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.85 (at 2.01Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 102.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2658	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, IN2, TYS

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	5.99	2/290 (0.7%)	1.83	6/384 (1.6%)
2	H	1.16	6/2107 (0.3%)	1.85	53/2846 (1.9%)
3	I	8.55	1/79 (1.3%)	1.46	0/103
All	All	2.77	9/2476 (0.4%)	1.83	59/3333 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	15	ARG	C-OXT	100.53	3.24	1.23
3	I	64	LEU	C-OXT	75.61	2.74	1.23
2	H	36(A)	SER	CB-OG	-23.26	0.95	1.42
2	H	153	SER	CB-OG	14.23	1.70	1.42
2	H	236	LYS	CE-NZ	-13.52	1.08	1.49
2	H	147	THR	C-O	9.27	1.34	1.23
2	H	27	SER	CB-OG	8.72	1.59	1.42
1	L	14(K)	ILE	CG1-CD1	8.56	1.85	1.51
2	H	236	LYS	CD-CE	6.77	1.72	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	PHE	CA-CB-CG	-9.39	104.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	147	THR	O-C-N	-9.18	112.16	123.36
1	L	14(J)	TYR	N-CA-C	-9.04	103.39	112.97
2	H	187	ARG	CD-NE-CZ	-8.99	111.81	124.40
1	L	1(A)	ASP	CA-CB-CG	-8.75	103.85	112.60
2	H	148	TRP	CB-CA-C	-8.63	93.70	110.10
2	H	205	ASN	CA-CB-CG	-8.48	104.12	112.60
2	H	148	TRP	N-CA-CB	-8.48	96.09	110.50
2	H	27	SER	N-CA-CB	7.86	121.00	110.79
2	H	243	ASP	N-CA-CB	7.52	121.41	110.20
2	H	60(I)	THR	N-CA-CB	-7.50	99.04	111.20
2	H	154	VAL	N-CA-CB	-7.34	100.11	112.44
2	H	148	TRP	N-CA-C	7.30	131.45	111.00
2	H	204(A)	PHE	CA-CB-CG	-7.20	106.60	113.80
2	H	27	SER	CB-CA-C	-6.98	101.01	111.27
2	H	147	THR	CA-C-O	-6.80	111.91	120.28
2	H	114	PHE	CA-CB-CG	-6.63	107.17	113.80
2	H	236	LYS	N-CA-CB	6.59	119.80	110.12
2	H	232	PHE	CA-CB-CG	-6.48	107.32	113.80
2	H	199	PHE	N-CA-C	-6.43	98.04	108.52
2	H	60(H)	PHE	CA-CB-CG	-6.34	107.46	113.80
2	H	157	VAL	CA-CB-CG2	6.27	121.05	110.40
2	H	190	ALA	N-CA-C	-6.25	102.11	110.55
1	L	1(A)	ASP	N-CA-C	-6.24	105.31	113.17
2	H	129(B)	SER	N-CA-C	6.21	119.02	111.82
1	L	14(A)	LYS	N-CA-C	6.13	119.86	112.38
2	H	187	ARG	NE-CZ-NH1	-6.11	115.39	121.50
2	H	171	SER	CA-C-N	-6.10	112.42	122.11
2	H	171	SER	C-N-CA	-6.10	112.42	122.11
2	H	236	LYS	CD-CE-NZ	6.04	131.23	111.90
2	H	235	LYS	N-CA-C	5.91	117.72	111.28
2	H	151	GLN	O-C-N	-5.88	115.86	121.57
2	H	205	ASN	OD1-CG-ND2	5.85	128.45	122.60
2	H	102	ASP	N-CA-CB	-5.83	102.18	110.58
1	L	15	ARG	NE-CZ-NH1	5.82	127.32	121.50
2	H	60(A)	TYR	CA-CB-CG	-5.73	103.58	113.90
2	H	241	VAL	N-CA-CB	5.71	118.31	110.54
2	H	186(A)	ASP	CB-CA-C	-5.62	101.30	110.85
2	H	138	VAL	CA-C-N	-5.58	113.82	122.59
2	H	138	VAL	C-N-CA	-5.58	113.82	122.59
1	L	14(K)	ILE	CB-CA-C	5.49	120.30	111.29
2	H	229	THR	CA-CB-OG1	-5.48	101.38	109.60
2	H	82	ILE	CA-CB-CG1	-5.45	101.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ARG	NE-CZ-NH2	-5.45	114.30	119.20
2	H	98	ASN	CA-CB-CG	-5.42	107.18	112.60
2	H	222	ASP	CA-CB-CG	-5.37	107.23	112.60
2	H	179	ASN	CA-CB-CG	-5.36	107.24	112.60
2	H	42	CYS	N-CA-CB	-5.34	101.47	110.49
2	H	44	ALA	CA-C-O	-5.29	115.48	121.25
2	H	147	THR	CB-CA-C	5.28	118.88	109.65
2	H	236	LYS	CB-CA-C	5.26	119.52	110.79
2	H	150	GLY	O-C-N	-5.24	114.62	123.00
2	H	50	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	H	64	LEU	N-CA-C	5.19	118.05	109.85
2	H	66	VAL	N-CA-CB	-5.19	104.19	111.25
2	H	84	MET	O-C-N	5.15	129.74	123.10
2	H	125	ASP	CA-CB-CG	-5.12	107.48	112.60
2	H	245	PHE	CA-CB-CG	5.09	118.89	113.80
2	H	42	CYS	CB-CA-C	-5.04	100.40	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	147	THR	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	L	287	0	278	17	3
2	H	2053	0	2018	71	3
3	I	95	0	73	5	0
4	H	14	0	13	0	0
5	H	29	0	34	1	0
6	H	157	0	0	7	0
6	I	2	0	0	1	0
6	L	21	0	0	0	0
All	All	2658	0	2416	85	3

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 18.

All (85) 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:14(K):ILE:CD1	1:L:14(K):ILE:CG1	1.85	1.52
2:H:153:SER:CB	2:H:153:SER:OG	1.70	1.37
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	1.87	0.97
1:L:1(F):GLY:HA2	2:H:235:LYS:NZ	1.87	0.90
2:H:51:TRP:CZ2	2:H:107:LYS:HE3	2.12	0.84
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.79	0.83
2:H:50:ARG:HH12	2:H:107:LYS:CD	1.97	0.76
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ3	1.51	0.75
3:I:58:GLU:H	3:I:58:GLU:CD	1.94	0.74
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.92	0.73
2:H:50:ARG:NH1	2:H:107:LYS:HE2	2.03	0.73
2:H:86:GLU:HB3	2:H:107:LYS:HG2	1.70	0.72
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.98	0.70
2:H:107:LYS:NZ	2:H:246:GLY:HA3	2.06	0.70
1:L:1(F):GLY:HA2	2:H:235:LYS:CE	2.23	0.69
2:H:35:ARG:O	2:H:38:GLN:HA	1.93	0.69
1:L:14(K):ILE:CD1	1:L:14(K):ILE:CB	2.71	0.67
2:H:50:ARG:HH12	2:H:107:LYS:CE	2.06	0.67
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.76	0.66
2:H:17:VAL:O	2:H:188:GLY:HA2	1.98	0.62
2:H:50:ARG:HH12	2:H:107:LYS:HE2	1.63	0.62
2:H:50:ARG:HH12	2:H:107:LYS:HD3	1.62	0.62
2:H:224:LYS:HE2	6:H:659:HOH:O	1.99	0.62
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.25	0.61
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.80	0.61
2:H:75:ARG:NH1	6:H:713:HOH:O	2.30	0.61
2:H:36(A):SER:HA	2:H:37:PRO:C	2.26	0.60
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.38	0.58
2:H:153:SER:OG	2:H:153:SER:CA	2.50	0.57
2:H:60(A):TYR:CE2	5:H:500:IN2:H21	2.40	0.57
2:H:236:LYS:HG2	6:H:689:HOH:O	2.04	0.56
2:H:73:ARG:HD2	6:H:698:HOH:O	2.06	0.56
2:H:50:ARG:NH2	2:H:86:GLU:OE1	2.39	0.55
2:H:107:LYS:HZ2	2:H:246:GLY:HA3	1.71	0.55
3:I:56:PHE:HB2	6:I:535:HOH:O	2.06	0.55
2:H:182:CYS:HA	2:H:226:GLY:O	2.06	0.55
1:L:1(E):SER:H	2:H:235:LYS:HZ1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.72	0.54
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.23	0.54
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.44	0.53
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.64	0.53
2:H:187:ARG:NH2	2:H:221:ASP:O	2.40	0.52
2:H:124:PRO:O	2:H:235:LYS:NZ	2.42	0.51
2:H:46:LEU:HD22	2:H:48:SER:O	2.11	0.51
2:H:35:ARG:HB3	2:H:39:GLU:HG3	1.92	0.51
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.93	0.50
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.13	0.48
2:H:169:LYS:NZ	6:H:634:HOH:O	2.46	0.48
2:H:70:LYS:HE3	2:H:72:SER:O	2.14	0.48
1:L:1(E):SER:H	2:H:235:LYS:NZ	2.11	0.47
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.43	0.47
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.45	0.47
2:H:51:TRP:CE2	2:H:107:LYS:HE3	2.47	0.47
2:H:98:ASN:OD1	2:H:98:ASN:N	2.41	0.47
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.80	0.46
1:L:1(E):SER:HA	2:H:123:LEU:O	2.16	0.46
2:H:114:PHE:HB3	6:H:624:HOH:O	2.15	0.45
2:H:114:PHE:CD1	2:H:114:PHE:N	2.79	0.45
2:H:61:GLU:H	2:H:61:GLU:HG2	1.42	0.45
2:H:127:GLU:H	2:H:127:GLU:CD	2.25	0.45
2:H:41:LEU:HD12	2:H:41:LEU:HA	1.84	0.44
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.16	0.44
2:H:77(A):ARG:HD2	6:H:684:HOH:O	2.17	0.44
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.33	0.44
1:L:14(C):GLU:O	1:L:14(G):LEU:CD2	2.66	0.44
1:L:1(F):GLY:HA2	2:H:235:LYS:HE2	1.99	0.43
2:H:60(I):THR:HB	2:H:63:ASP:OD2	2.18	0.43
2:H:127:GLU:CD	2:H:127:GLU:N	2.77	0.43
2:H:201:MET:SD	2:H:210:MET:HG3	2.58	0.43
2:H:153:SER:CB	2:H:153:SER:HG	2.13	0.42
1:L:14(D):ARG:HG2	1:L:14(E):GLU:N	2.24	0.42
2:H:35:ARG:CB	2:H:39:GLU:HG3	2.50	0.42
2:H:165:ARG:N	2:H:166:PRO:CD	2.82	0.42
2:H:74:THR:HA	3:I:56:PHE:CD1	2.56	0.41
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.35	0.41
2:H:176:ILE:HG23	2:H:176:ILE:HD12	1.82	0.41
2:H:18:GLU:HG3	2:H:187:ARG:HB2	2.01	0.41
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:HD3	2:H:111:PRO:N	2.36	0.41
2:H:41:LEU:HD23	2:H:64:LEU:CD2	2.51	0.41
2:H:51:TRP:CZ2	2:H:107:LYS:CE	2.96	0.41
2:H:110:LYS:HB3	2:H:111:PRO:HD2	2.02	0.40
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.57	0.40
2:H:230:HIS:CG	2:H:233:ARG:HG3	2.56	0.40
2:H:107:LYS:HE3	2:H:107:LYS:HB2	1.93	0.40

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:ARG:OXT	2:H:173:ARG:O[4_556]	1.48	0.72
1:L:15:ARG:NH2	2:H:172:THR:O[4_556]	2.07	0.13
1:L:15:ARG:NH2	2:H:169:LYS:O[4_556]	2.18	0.02

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	34/36 (94%)	25 (74%)	7 (21%)	2 (6%)	1	0
2	H	249/259 (96%)	239 (96%)	10 (4%)	0	100	100
3	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	290/305 (95%)	271 (93%)	17 (6%)	2 (1%)	18	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(L)	ASP
1	L	1(G)	PHE

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	31/31 (100%)	29 (94%)	2 (6%)	15	12
2	H	221/225 (98%)	200 (90%)	21 (10%)	8	5
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	3
All	All	261/265 (98%)	237 (91%)	24 (9%)	8	5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	9	LYS
2	H	20	SER
2	H	33	LEU
2	H	41	LEU
2	H	46	LEU
2	H	50	ARG
2	H	61	GLU
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	87	LYS
2	H	90	ILE
2	H	107	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	154	VAL
2	H	169	LYS
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
3	I	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	143	ASN
2	H	156	GLN
2	H	204(B)	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TYS	I	63	3	15,16,17	1.68	2 (13%)	15,22,24	1.91	3 (20%)

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	TYS	I	63	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-S	-5.31	1.48	1.58
3	I	63	TYS	OH-CZ	-3.01	1.37	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-CZ-CE1	4.76	128.03	118.70
3	I	63	TYS	OH-CZ-CE2	-3.97	110.92	118.70
3	I	63	TYS	OH-S-O2	2.39	114.83	107.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	IN2	H	600	2	13,13,14	1.09	2 (15%)	11,15,17	0.84	0
4	NAG	H	400	2	14,14,15	0.82	0	17,19,21	2.20	3 (17%)
5	IN2	H	500	-	11,14,14	1.36	2 (18%)	13,17,17	2.06	3 (23%)

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	IN2	H	600	2	-	1/10/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	400	2	-	2/6/23/26	0/1/1/1
5	IN2	H	500	-	-	4/14/17/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	500	IN2	C8-N7	-3.23	1.31	1.37
5	H	600	IN2	C8-N9	-2.45	1.32	1.35
5	H	600	IN2	C8-N7	-2.35	1.33	1.37
5	H	500	IN2	C8-N9	-2.23	1.32	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	C2-N2-C7	-5.46	115.59	122.90
4	H	400	NAG	O3-C3-C4	-5.44	97.56	110.38
5	H	500	IN2	O1-C12-N6	-5.27	115.18	123.19
5	H	500	IN2	C4-C5-N6	2.96	119.81	113.35
5	H	500	IN2	C5-N6-C12	2.67	129.80	121.62
4	H	400	NAG	O7-C7-C8	2.22	126.02	122.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAG	C8-C7-N2-C2
5	H	500	IN2	C4-C5-N6-N7
5	H	500	IN2	C4-C5-N6-C12
5	H	500	IN2	O8-C8-N7-N6
4	H	400	NAG	O7-C7-N2-C2
5	H	600	IN2	C2-C3-C4-C5
5	H	500	IN2	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	500	IN2	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	30/36 (83%)	0.45	5 (16%) 4 4	7, 33, 53, 66	3 (10%)
2	H	251/259 (96%)	-0.33	3 (1%) 76 76	19, 32, 57, 70	3 (1%)
3	I	9/10 (90%)	1.53	4 (44%) 0 1	33, 50, 72, 73	1 (11%)
All	All	290/305 (95%)	-0.19	12 (4%) 41 40	7, 32, 60, 73	7 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1(G)	PHE	7.0
1	L	1(E)	SER	6.0
1	L	14(K)	ILE	4.9
3	I	55	ASP	3.1
2	H	147	THR	3.1
1	L	14(D)	ARG	3.0
2	H	150	GLY	2.9
1	L	1(F)	GLY	2.7
3	I	61	GLU	2.4
3	I	62	GLU	2.4
2	H	246	GLY	2.4
3	I	64	LEU	2.3

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

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. 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	B-factors(Å ²)	Q<0.9
3	TYS	I	63	16/17	0.93	0.10	38,54,79,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	400	14/15	0.62	0.15	48,72,80,80	0
5	IN2	H	500	15/15	0.82	0.13	33,52,80,80	0
5	IN2	H	600	14/15	0.92	0.10	20,36,61,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.