Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:28 pm BST

PDB ID	:	1A61
Title	:	THROMBIN COMPLEXED WITH A BETA-MIMETIC THIAZOLE-CONTAINING INHIBITOR
Authors	:	St Charles, R.; Matthews, J.H.; Zhang, E.; Tulinsky, A.; Kahn, M.
Deposited on	:	1998-03-05
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

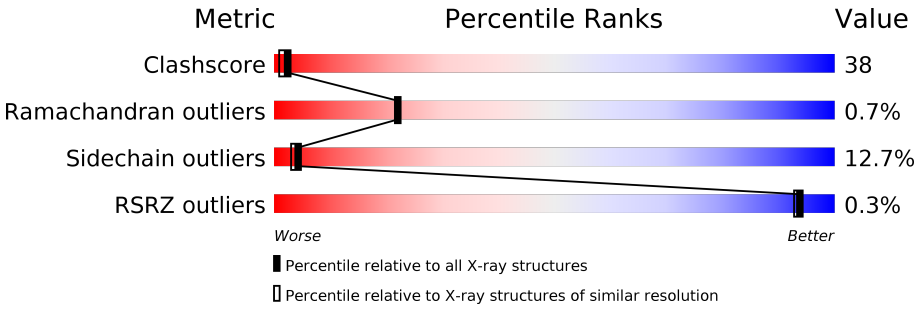
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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 <=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	31% 25% 17% · 25%
2	H	259	39% 37% 17% · ·
3	I	12	8% 17% 25% 33% 8% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2512 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 (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			2022	1290	358	360	14			

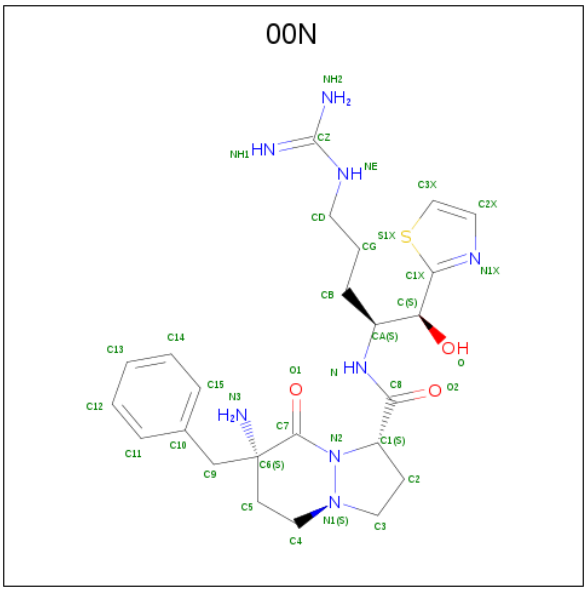
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			89	56	10	22	1			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	Na	0	0
			2	2		

- Molecule 5 is (1S,7S)-7-amino-7-benzyl-N-{(1S)-4-carbamimidamido-1-[(S)-hydroxy(1,3-thiazol-2-yl)methyl]butyl}-8-oxohexahydro-1H-pyrazolo[1,2-a]pyridazine-1-carboxamide (three-letter code: 00N) (formula: $C_{24}H_{34}N_8O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C N O S 36 24 8 3 1	0	0

- Molecule 6 is water.

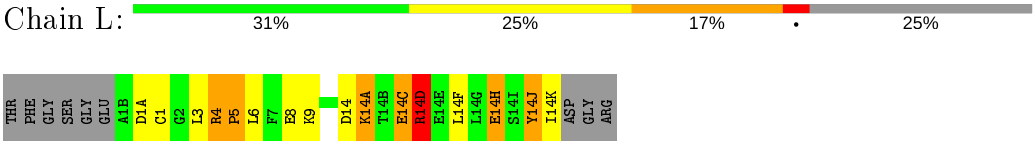
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	9	Total O 9 9	0	0
6	H	124	Total O 124 124	0	0
6	I	8	Total O 8 8	0	0

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.

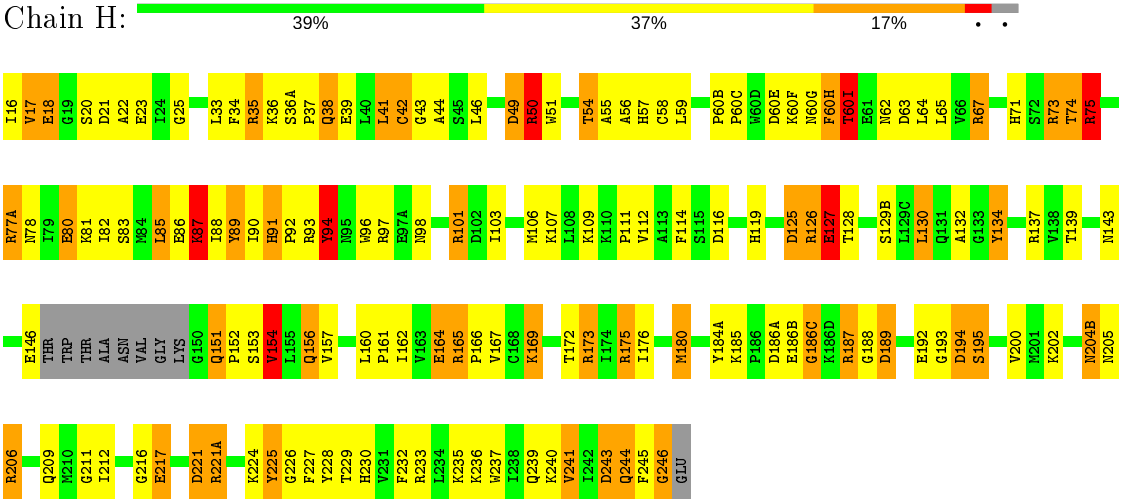
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L:



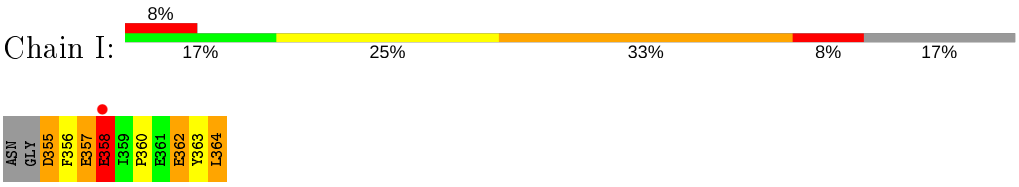
- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H:



- Molecule 3: HIRUGEN

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.85Å 72.41Å 72.97Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 50.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	76.0 (7.00-2.20) 76.9 (50.16-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.148 , (Not available) 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2512	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, 00N, 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	1.01	0/224	2.22	10/298 (3.4%)
2	H	0.95	1/2074 (0.0%)	2.26	73/2801 (2.6%)
3	I	0.97	0/73	2.18	5/96 (5.2%)
All	All	0.95	1/2371 (0.0%)	2.26	88/3195 (2.8%)

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
1	L	0	2
2	H	0	17
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	GLU	CD-OE1	-5.08	1.20	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	165	ARG	CD-NE-CZ	19.68	151.16	123.60
2	H	77(A)	ARG	NE-CZ-NH1	-15.53	112.53	120.30
2	H	126	ARG	NE-CZ-NH2	-14.86	112.87	120.30
2	H	75	ARG	NE-CZ-NH2	14.59	127.59	120.30
2	H	67	ARG	NE-CZ-NH2	14.07	127.33	120.30
2	H	243	ASP	CB-CG-OD2	-13.83	105.86	118.30
2	H	187	ARG	NE-CZ-NH1	-13.13	113.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	4	ARG	NE-CZ-NH2	11.78	126.19	120.30
2	H	233	ARG	NE-CZ-NH2	-11.47	114.57	120.30
2	H	194	ASP	CB-CG-OD1	-11.40	108.04	118.30
2	H	97	ARG	NE-CZ-NH2	-10.73	114.93	120.30
2	H	97	ARG	NE-CZ-NH1	10.65	125.62	120.30
2	H	137	ARG	NE-CZ-NH1	10.35	125.47	120.30
2	H	206	ARG	NE-CZ-NH1	-10.30	115.15	120.30
2	H	243	ASP	CA-CB-CG	10.18	135.80	113.40
2	H	35	ARG	CD-NE-CZ	-9.87	109.79	123.60
2	H	75	ARG	NE-CZ-NH1	-9.85	115.37	120.30
2	H	50	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	L	14	ASP	CB-CG-OD1	-9.13	110.08	118.30
2	H	101	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	H	189	ASP	CB-CG-OD2	8.82	126.23	118.30
2	H	233	ARG	CD-NE-CZ	-8.81	111.27	123.60
2	H	125	ASP	CB-CG-OD1	8.54	125.98	118.30
2	H	49	ASP	CB-CG-OD1	-8.00	111.10	118.30
2	H	67	ARG	NH1-CZ-NH2	-7.99	110.61	119.40
2	H	246	GLY	CA-C-O	-7.98	106.24	120.60
1	L	14	ASP	CB-CG-OD2	7.94	125.45	118.30
2	H	184(A)	TYR	CB-CG-CD1	-7.69	116.39	121.00
2	H	164	GLU	CG-CD-OE2	7.50	133.30	118.30
2	H	186(B)	GLU	OE1-CD-OE2	-7.44	114.37	123.30
2	H	243	ASP	CB-CA-C	7.42	125.24	110.40
2	H	38	GLN	CB-CG-CD	7.28	130.54	111.60
2	H	21	ASP	CB-CG-OD2	-7.27	111.75	118.30
2	H	164	GLU	OE1-CD-OE2	-7.23	114.63	123.30
2	H	192	GLU	CG-CD-OE2	7.12	132.53	118.30
3	I	357	GLU	OE1-CD-OE2	7.12	131.84	123.30
2	H	77(A)	ARG	NE-CZ-NH2	7.04	123.82	120.30
2	H	175	ARG	CD-NE-CZ	-6.97	113.84	123.60
2	H	243	ASP	CB-CG-OD1	6.92	124.53	118.30
2	H	94	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	H	126	ARG	CD-NE-CZ	-6.84	114.02	123.60
2	H	225	TYR	CB-CG-CD2	-6.80	116.92	121.00
2	H	187	ARG	CD-NE-CZ	-6.77	114.12	123.60
2	H	206	ARG	NH1-CZ-NH2	6.71	126.78	119.40
2	H	165	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	H	50	ARG	NE-CZ-NH1	-6.48	117.06	120.30
2	H	21	ASP	CB-CG-OD1	6.40	124.06	118.30
2	H	173	ARG	CD-NE-CZ	-6.37	114.68	123.60
2	H	154	VAL	N-CA-CB	-6.35	97.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	193	GLY	CA-C-O	-6.11	109.60	120.60
2	H	217	GLU	OE1-CD-OE2	-6.11	115.97	123.30
2	H	151	GLN	CA-CB-CG	-6.06	100.08	113.40
1	L	5	PRO	O-C-N	-5.99	113.12	122.70
2	H	93	ARG	NE-CZ-NH1	-5.99	117.31	120.30
2	H	22	ALA	N-CA-CB	-5.89	101.85	110.10
2	H	42	CYS	CA-CB-SG	5.89	124.60	114.00
3	I	362	GLU	N-CA-CB	5.88	121.19	110.60
1	L	14(D)	ARG	CD-NE-CZ	5.85	131.79	123.60
2	H	75	ARG	CD-NE-CZ	-5.85	115.42	123.60
2	H	127	GLU	CG-CD-OE1	5.83	129.96	118.30
2	H	87	LYS	N-CA-CB	-5.81	100.14	110.60
3	I	358	GLU	CB-CG-CD	5.74	129.69	114.20
1	L	14(C)	GLU	CG-CD-OE2	-5.70	106.89	118.30
1	L	14(J)	TYR	CB-CG-CD2	5.68	124.41	121.00
2	H	126	ARG	NH1-CZ-NH2	5.59	125.55	119.40
2	H	189	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	H	25	GLY	CA-C-O	-5.53	110.66	120.60
1	L	14(H)	GLU	OE1-CD-OE2	5.52	129.92	123.30
2	H	228	TYR	CB-CG-CD2	-5.51	117.69	121.00
2	H	192	GLU	OE1-CD-OE2	-5.50	116.70	123.30
2	H	18	GLU	CG-CD-OE1	5.49	129.29	118.30
2	H	54	THR	CA-CB-CG2	5.48	120.08	112.40
2	H	186(C)	GLY	C-N-CA	5.46	135.34	121.70
3	I	364	LEU	CB-CG-CD1	5.44	120.25	111.00
2	H	187	ARG	NH1-CZ-NH2	5.38	125.32	119.40
2	H	60(I)	THR	CA-CB-OG1	-5.33	97.82	109.00
2	H	73	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	L	14(C)	GLU	CG-CD-OE1	5.31	128.91	118.30
2	H	172	THR	N-CA-CB	-5.23	100.36	110.30
2	H	60(H)	PHE	CB-CG-CD1	-5.19	117.17	120.80
2	H	17	VAL	CG1-CB-CG2	-5.18	102.61	110.90
3	I	357	GLU	CG-CD-OE2	-5.18	107.94	118.30
2	H	221	ASP	CB-CA-C	5.17	120.75	110.40
2	H	137	ARG	O-C-N	5.07	130.81	122.70
2	H	206	ARG	CG-CD-NE	-5.05	101.19	111.80
1	L	4	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
2	H	74	THR	CA-CB-OG1	-5.04	98.42	109.00
2	H	226	GLY	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	119	HIS	Mainchain
2	H	134	TYR	Mainchain
2	H	156	GLN	Sidechain
2	H	160	LEU	Mainchain
2	H	161	PRO	Mainchain
2	H	180	MET	Mainchain
2	H	20	SER	Mainchain
2	H	212	ILE	Mainchain
2	H	232	PHE	Sidechain
2	H	60(H)	PHE	Mainchain
2	H	62	ASN	Mainchain
2	H	80	GLU	Mainchain
2	H	87	LYS	Mainchain
2	H	89	TYR	Sidechain
2	H	91	HIS	Mainchain
2	H	98	ASN	Sidechain,Mainchain
1	L	3	LEU	Mainchain
1	L	5	PRO	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	222	0	225	20	0
2	H	2022	0	1997	152	1
3	I	89	0	67	10	1
4	H	2	0	0	0	0
5	H	36	0	32	9	0
6	H	124	0	0	21	0
6	I	8	0	0	2	0
6	L	9	0	0	6	0
All	All	2512	0	2321	176	1

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 38.

All (176) 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)
2:H:75:ARG:HG3	2:H:75:ARG:NH1	1.30	1.15
2:H:75:ARG:CG	2:H:75:ARG:NH1	2.09	1.13
2:H:139:THR:HG22	2:H:157:VAL:HG22	1.15	1.08
2:H:244:GLN:HG2	2:H:245:PHE:CD2	1.88	1.08
2:H:51:TRP:CE3	6:H:548:HOH:O	2.13	0.99
2:H:107:LYS:NZ	2:H:246:GLY:HA3	1.78	0.98
2:H:75:ARG:CG	2:H:75:ARG:HH11	1.62	0.97
2:H:75:ARG:HG3	2:H:75:ARG:HH11	0.78	0.94
2:H:245:PHE:HE2	6:H:448:HOH:O	1.53	0.91
2:H:126:ARG:HB3	2:H:127:GLU:OE1	1.72	0.90
2:H:106:MET:C	6:H:548:HOH:O	2.10	0.89
2:H:164:GLU:OE1	2:H:167:VAL:HG21	1.73	0.89
2:H:50:ARG:HE	2:H:107:LYS:HE2	1.38	0.88
2:H:139:THR:CG2	2:H:157:VAL:HG22	2.04	0.86
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.58	0.83
2:H:195:SER:OG	5:H:372:00N:C1X	2.28	0.82
3:I:364:LEU:C	6:I:538:HOH:O	2.20	0.80
1:L:14(D):ARG:NH1	1:L:14(H):GLU:OE2	2.16	0.79
2:H:153:SER:HB3	6:H:442:HOH:O	1.81	0.79
2:H:169:LYS:NZ	2:H:169:LYS:HB3	1.91	0.78
2:H:85:LEU:HD11	2:H:106:MET:HE1	1.64	0.78
2:H:236:LYS:HE2	6:H:465:HOH:O	1.84	0.78
2:H:85:LEU:CD1	2:H:106:MET:CE	2.61	0.77
3:I:358:GLU:HG3	6:I:488:HOH:O	1.84	0.77
2:H:107:LYS:HZ2	2:H:246:GLY:HA3	1.46	0.77
2:H:50:ARG:HH21	2:H:107:LYS:HD3	1.54	0.73
2:H:169:LYS:CB	2:H:169:LYS:NZ	2.48	0.73
2:H:244:GLN:HG2	2:H:245:PHE:CE2	2.23	0.73
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.89	0.72
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.20	0.72
2:H:51:TRP:HE3	6:H:548:HOH:O	1.58	0.72
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.21	0.71
2:H:126:ARG:HB2	6:H:503:HOH:O	1.91	0.70
2:H:175:ARG:HD2	6:H:453:HOH:O	1.89	0.70
2:H:126:ARG:CB	6:H:503:HOH:O	2.37	0.70
2:H:17:VAL:O	2:H:18:GLU:HB2	1.92	0.70
2:H:116:ASP:OD1	6:H:421:HOH:O	2.09	0.69
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.75	0.69
2:H:85:LEU:HD13	2:H:106:MET:CE	2.23	0.69
2:H:189:ASP:OD2	5:H:372:00N:NH2	2.24	0.68
2:H:107:LYS:HZ1	2:H:246:GLY:HA3	1.54	0.68
2:H:86:GLU:OE2	2:H:107:LYS:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.93	0.68
2:H:74:THR:O	6:H:482:HOH:O	2.10	0.68
1:L:1(A):ASP:CA	6:L:478:HOH:O	2.41	0.67
1:L:1(A):ASP:C	6:L:478:HOH:O	2.34	0.67
2:H:50:ARG:HH21	2:H:107:LYS:CD	2.07	0.66
2:H:85:LEU:HD11	2:H:106:MET:CE	2.26	0.66
2:H:165:ARG:NH1	2:H:180:MET:O	2.29	0.65
1:L:14(D):ARG:NH2	1:L:14(H):GLU:OE1	2.29	0.65
3:I:358:GLU:CD	3:I:358:GLU:H	2.00	0.65
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.31	0.65
2:H:106:MET:O	6:H:548:HOH:O	2.13	0.63
2:H:60(I):THR:O	2:H:63:ASP:HB2	1.97	0.63
2:H:169:LYS:HB3	2:H:169:LYS:HZ1	1.64	0.63
2:H:59:LEU:HD13	2:H:88:ILE:HG21	1.80	0.63
2:H:18:GLU:HA	6:H:489:HOH:O	1.98	0.63
1:L:14(A):LYS:NZ	1:L:14(A):LYS:HB2	2.12	0.63
2:H:41:LEU:CD2	2:H:64:LEU:CD2	2.78	0.62
1:L:1(A):ASP:N	6:L:478:HOH:O	2.31	0.62
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE2	2.47	0.62
2:H:143:ASN:ND2	6:H:520:HOH:O	2.12	0.61
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.35	0.61
2:H:195:SER:CB	5:H:372:00N:C	2.78	0.61
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.36	0.61
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.00	0.60
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE1	2.50	0.60
2:H:50:ARG:NE	2:H:107:LYS:HE2	2.13	0.60
2:H:41:LEU:CD2	2:H:64:LEU:HD21	2.32	0.60
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.16	0.59
1:L:1(A):ASP:HB3	6:L:478:HOH:O	2.00	0.59
1:L:14(D):ARG:CZ	1:L:14(H):GLU:CD	2.72	0.58
1:L:1(A):ASP:CB	6:L:478:HOH:O	2.52	0.58
2:H:73:ARG:NH2	6:H:443:HOH:O	2.37	0.57
3:I:357:GLU:HG2	3:I:358:GLU:N	2.19	0.57
2:H:42:CYS:HB3	2:H:195:SER:O	2.03	0.57
3:I:360:PRO:HB2	3:I:362:GLU:OE2	2.04	0.56
2:H:217:GLU:OE1	2:H:224:LYS:NZ	2.37	0.56
2:H:130:LEU:HD22	2:H:162:ILE:HD13	1.88	0.56
2:H:245:PHE:CE2	6:H:448:HOH:O	2.40	0.56
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.38	0.55
2:H:35:ARG:O	2:H:38:GLN:HA	2.07	0.54
2:H:244:GLN:CG	2:H:245:PHE:CE2	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(A):ASP:OD2	1:L:9:LYS:HE2	2.07	0.54
2:H:134:TYR:HD1	2:H:134:TYR:N	2.04	0.54
2:H:60(I):THR:HG22	2:H:63:ASP:CG	2.28	0.53
2:H:41:LEU:HD23	2:H:64:LEU:HD21	1.89	0.53
2:H:216:GLY:O	5:H:372:00N:N3	2.34	0.53
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.72	0.53
2:H:134:TYR:CD1	2:H:134:TYR:N	2.77	0.52
2:H:41:LEU:HD23	2:H:64:LEU:CD2	2.39	0.52
2:H:49:ASP:OD2	2:H:111:PRO:CB	2.57	0.52
2:H:74:THR:HB	3:I:356:PHE:HA	1.91	0.52
2:H:85:LEU:HD23	2:H:85:LEU:N	2.25	0.52
2:H:16:ILE:HD13	2:H:194:ASP:OD2	2.10	0.52
2:H:187:ARG:NH2	2:H:221:ASP:O	2.38	0.52
2:H:38:GLN:O	2:H:39:GLU:HB3	2.09	0.51
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.45	0.51
2:H:165:ARG:O	2:H:169:LYS:HG3	2.10	0.51
2:H:107:LYS:N	6:H:548:HOH:O	2.40	0.51
1:L:4:ARG:HB2	1:L:8:GLU:OE1	2.09	0.51
2:H:89:TYR:OH	2:H:245:PHE:HB3	2.11	0.51
2:H:156:GLN:C	2:H:157:VAL:HG23	2.31	0.50
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.46	0.50
2:H:195:SER:CB	5:H:372:00N:O	2.60	0.50
2:H:126:ARG:CB	2:H:127:GLU:OE1	2.53	0.50
2:H:17:VAL:O	2:H:188:GLY:HA2	2.12	0.50
2:H:185:LYS:HD3	2:H:225:TYR:OH	2.11	0.50
1:L:14(A):LYS:NZ	6:L:514:HOH:O	2.44	0.50
2:H:49:ASP:N	2:H:49:ASP:OD1	2.42	0.49
2:H:125:ASP:OD1	2:H:128:THR:CB	2.61	0.49
2:H:194:ASP:O	2:H:195:SER:C	2.51	0.48
1:L:1(A):ASP:OD2	1:L:9:LYS:CE	2.61	0.48
2:H:211:GLY:HA2	2:H:229:THR:O	2.12	0.48
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.17	0.48
2:H:59:LEU:HD13	2:H:88:ILE:CG2	2.44	0.48
1:L:14(D):ARG:O	1:L:14(D):ARG:HG2	2.13	0.48
2:H:106:MET:N	6:H:548:HOH:O	2.46	0.47
2:H:56:ALA:HB2	2:H:103:ILE:O	2.13	0.47
2:H:49:ASP:O	2:H:111:PRO:HA	2.14	0.47
2:H:146:GLU:OE1	2:H:221(A):ARG:NE	2.47	0.47
2:H:167:VAL:HG11	2:H:185:LYS:HE2	1.97	0.46
2:H:54:THR:HG23	2:H:55:ALA:O	2.14	0.46
1:L:1:CYS:O	2:H:206:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.97	0.46
2:H:165:ARG:N	2:H:166:PRO:CD	2.78	0.46
2:H:239:GLN:O	2:H:240:LYS:C	2.54	0.46
2:H:75:ARG:N	2:H:75:ARG:HD3	2.31	0.46
2:H:195:SER:OG	5:H:372:00N:O	2.25	0.46
2:H:235:LYS:O	2:H:239:GLN:HB2	2.16	0.45
2:H:41:LEU:HA	2:H:41:LEU:HD12	1.72	0.45
2:H:132:ALA:HB1	2:H:164:GLU:HG3	1.99	0.45
2:H:37:PRO:O	2:H:39:GLU:HG2	2.16	0.45
2:H:60(E):ASP:OD2	6:H:425:HOH:O	2.21	0.45
2:H:74:THR:HG21	3:I:355:ASP:HB3	1.99	0.44
2:H:58:CYS:O	2:H:60(F):LYS:HE2	2.17	0.44
2:H:127:GLU:H	2:H:127:GLU:CD	2.20	0.44
2:H:67:ARG:HG2	2:H:82:ILE:HG12	2.00	0.44
2:H:18:GLU:HG3	2:H:187:ARG:CB	2.40	0.44
2:H:57:HIS:NE2	5:H:372:00N:N1X	2.65	0.44
2:H:60(F):LYS:HZ1	5:H:372:00N:H2X	1.83	0.44
2:H:175:ARG:HD2	2:H:175:ARG:HH11	1.54	0.44
2:H:73:ARG:NH1	6:H:439:HOH:O	2.45	0.44
2:H:156:GLN:O	2:H:157:VAL:HG23	2.17	0.44
2:H:60(G):ASN:ND2	6:H:441:HOH:O	2.42	0.44
2:H:94:TYR:HA	2:H:101:ARG:HB2	2.00	0.44
2:H:204(B):ASN:N	2:H:204(B):ASN:HD22	2.16	0.44
2:H:244:GLN:CD	2:H:245:PHE:CE2	2.91	0.44
3:I:357:GLU:CG	3:I:358:GLU:N	2.81	0.43
2:H:127:GLU:CD	2:H:127:GLU:N	2.71	0.43
2:H:204(B):ASN:H	2:H:204(B):ASN:HD22	1.65	0.43
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.63	0.43
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	2.18	0.43
2:H:60(F):LYS:NZ	5:H:372:00N:H2X	2.34	0.43
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.88	0.43
2:H:43:GLY:O	2:H:44:ALA:HB2	2.19	0.43
2:H:49:ASP:HB2	2:H:112:VAL:O	2.18	0.42
1:L:14(J):TYR:HE2	2:H:202:LYS:O	2.02	0.42
2:H:200:VAL:HG12	2:H:209:GLN:HA	2.01	0.42
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.54	0.42
2:H:38:GLN:O	2:H:39:GLU:CB	2.67	0.42
3:I:360:PRO:HG2	3:I:363:TYS:HE2	2.01	0.42
2:H:236:LYS:HA	2:H:236:LYS:HD3	1.81	0.41
2:H:156:GLN:O	2:H:157:VAL:CG2	2.69	0.41
2:H:125:ASP:OD1	2:H:128:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:LYS:HG2	3:I:364:LEU:HD12	2.02	0.41
2:H:130:LEU:CD2	2:H:162:ILE:CD1	2.99	0.41
2:H:77(A):ARG:HD2	2:H:77(A):ARG:HH11	1.65	0.41
2:H:59:LEU:HD13	2:H:88:ILE:HD13	2.01	0.41
2:H:164:GLU:H	2:H:164:GLU:CD	2.20	0.41
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.84	0.41
2:H:173:ARG:HH11	2:H:173:ARG:HD2	1.46	0.40
2:H:169:LYS:CB	2:H:169:LYS:HZ1	2.29	0.40
2:H:237:TRP:O	2:H:241:VAL:CG1	2.68	0.40
2:H:130:LEU:HD12	2:H:230:HIS:NE2	2.36	0.40
2:H:125:ASP:OD1	2:H:128:THR:OG1	2.28	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	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:NH1	3:I:357:GLU:OE1[2_555]	2.12	0.08

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	25/36 (69%)	23 (92%)	2 (8%)	0	100 100
2	H	246/259 (95%)	224 (91%)	20 (8%)	2 (1%)	19 19
3	I	7/12 (58%)	7 (100%)	0	0	100 100
All	All	278/307 (91%)	254 (91%)	22 (8%)	2 (1%)	22 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	186(C)	GLY

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Mol	Chain	Res	Type
2	H	195	SER

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	25/31 (81%)	21 (84%)	4 (16%)	2	2
2	H	218/225 (97%)	192 (88%)	26 (12%)	5	4
3	I	8/10 (80%)	6 (75%)	2 (25%)	0	0
All	All	251/266 (94%)	219 (87%)	32 (13%)	4	3

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(K)	ILE
2	H	33	LEU
2	H	36(A)	SER
2	H	41	LEU
2	H	46	LEU
2	H	50	ARG
2	H	60(I)	THR
2	H	65	LEU
2	H	75	ARG
2	H	81	LYS
2	H	83	SER
2	H	85	LEU
2	H	87	LYS
2	H	94	TYR
2	H	109	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	130	LEU

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Mol	Chain	Res	Type
2	H	154	VAL
2	H	169	LYS
2	H	186(A)	ASP
2	H	204(B)	ASN
2	H	205	ASN
2	H	221(A)	ARG
2	H	241	VAL
2	H	243	ASP
2	H	244	GLN
3	I	355	ASP
3	I	358	GLU

Some 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	156	GLN
2	H	204(B)	ASN
2	H	205	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	363	3	15,16,17	1.84	2 (13%)	18,22,24	1.58	5 (27%)

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	363	3	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	363	TYS	OH-S	5.35	1.66	1.58
3	I	363	TYS	OH-CZ	-3.75	1.36	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	363	TYS	OH-S-O2	-2.76	99.66	107.71
3	I	363	TYS	CG-CB-CA	-2.68	108.66	114.10
3	I	363	TYS	CB-CA-C	2.43	116.02	111.47
3	I	363	TYS	OH-S-O1	2.15	113.97	107.71
3	I	363	TYS	OH-CZ-CE1	2.15	122.86	118.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	363	TYS	CA-CB-CG-CD1
3	I	363	TYS	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	363	TYS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
5	00N	H	372	2	35,39,39	2.82	11 (31%)	32,55,55	5.74	19 (59%)

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	00N	H	372	2	-	5/23/57/57	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	372	00N	O-C	-8.84	1.25	1.42
5	H	372	00N	C9-C6	6.36	1.62	1.55
5	H	372	00N	C8-N	5.30	1.45	1.34
5	H	372	00N	C2-C3	4.72	1.61	1.52
5	H	372	00N	O2-C8	4.53	1.32	1.23
5	H	372	00N	C1-C8	-4.34	1.42	1.52
5	H	372	00N	O1-C7	3.93	1.28	1.22
5	H	372	00N	C5-C6	-3.24	1.50	1.54
5	H	372	00N	C9-C10	3.03	1.56	1.51
5	H	372	00N	C1X-S1X	2.25	1.80	1.73
5	H	372	00N	C12-C11	2.18	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	372	00N	CA-N-C8	18.99	156.63	123.07
5	H	372	00N	O2-C8-N	-11.15	102.27	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	372	00N	C1X-C-CA	9.61	122.08	111.31
5	H	372	00N	C9-C10-C15	-8.57	109.62	121.07
5	H	372	00N	C1-C8-N	7.47	133.23	116.58
5	H	372	00N	C9-C10-C11	7.09	130.54	121.07
5	H	372	00N	C4-C5-C6	6.66	119.07	112.97
5	H	372	00N	O-C-CA	6.43	125.19	107.99
5	H	372	00N	CB-CA-N	5.94	118.15	110.33
5	H	372	00N	NE-CZ-NH1	-5.43	111.15	120.70
5	H	372	00N	C7-N2-N1	4.74	127.97	120.23
5	H	372	00N	C2-C1-C8	-4.38	101.87	111.22
5	H	372	00N	O1-C7-N2	4.03	124.14	120.65
5	H	372	00N	C5-C4-N1	3.99	114.68	109.30
5	H	372	00N	C6-C9-C10	3.55	122.69	115.61
5	H	372	00N	C2-C3-N1	-3.47	94.99	103.68
5	H	372	00N	C-CA-N	3.18	116.08	110.05
5	H	372	00N	CG-CB-CA	-2.94	107.93	113.93
5	H	372	00N	O1-C7-C6	-2.63	114.96	122.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	372	00N	C-CA-N-C8
5	H	372	00N	NH2-CZ-NE-CD
5	H	372	00N	O2-C8-N-CA
5	H	372	00N	C1-C8-N-CA
5	H	372	00N	CB-CA-N-C8

There are no ring outliers.

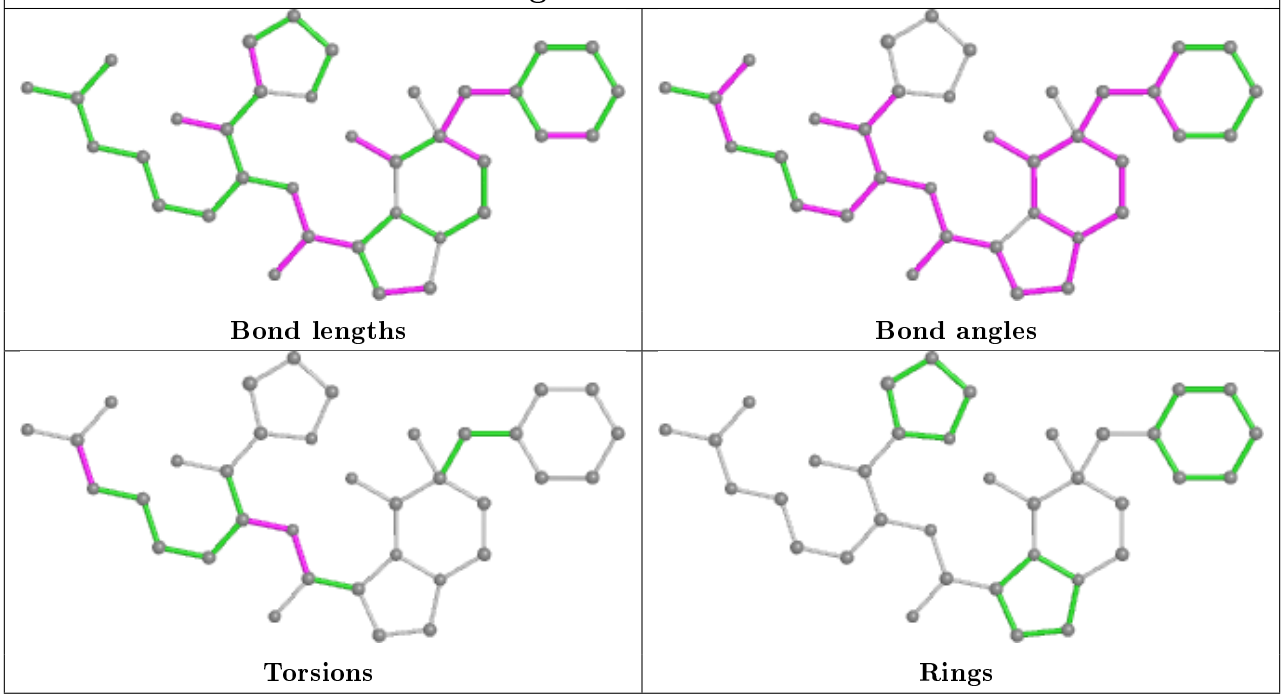
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	372	00N	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 00N H 372



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^{th} 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	27/36 (75%)	-0.51	0 100 100	16, 24, 42, 45	0
2	H	250/259 (96%)	-0.57	0 100 100	14, 25, 43, 50	0
3	I	9/12 (75%)	0.35	1 (11%) 5 4	42, 46, 49, 49	0
All	All	286/307 (93%)	-0.53	1 (0%) 94 93	14, 26, 44, 50	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	358	GLU	2.4

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, 95^{th} 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	363	16/17	0.96	0.12	33,41,49,50	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

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. The B-factors column lists the minimum,

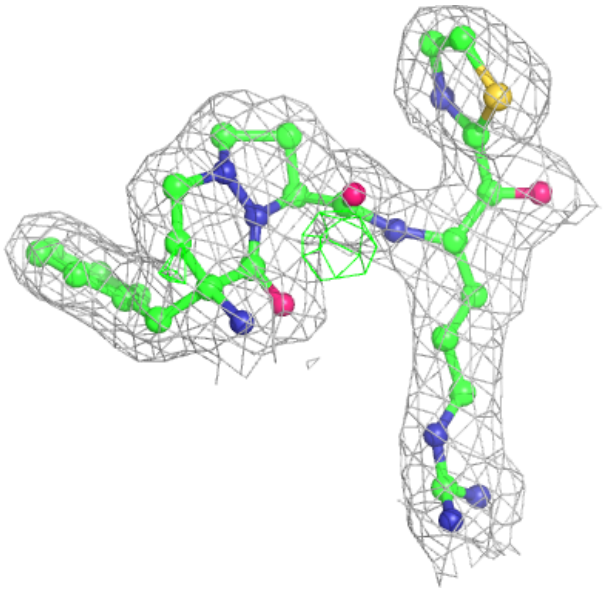
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

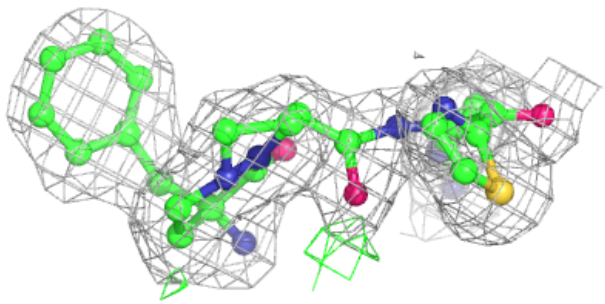
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	00N	H	372	36/36	0.96	0.11	12,24,31,33	0
4	NA	H	650	1/1	0.96	0.13	28,28,28,28	1
4	NA	H	651	1/1	0.98	0.06	26,26,26,26	0

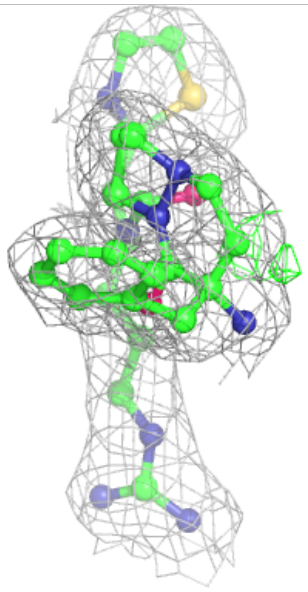
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 00N H 372:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.