



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:55 PM GMT

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 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>

---

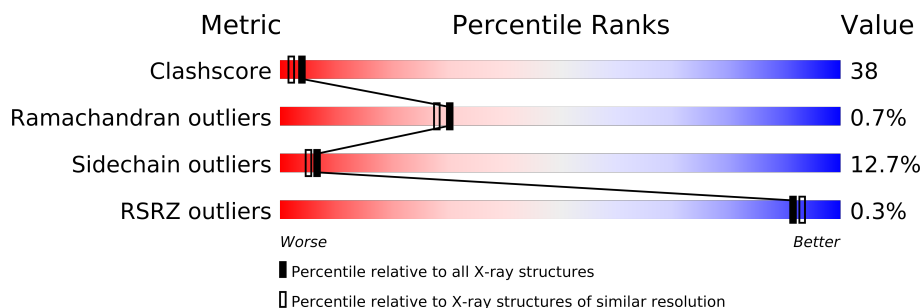
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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  $\geq 3$ , 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	36	
2	H	259	
3	I	12	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2512 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 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			

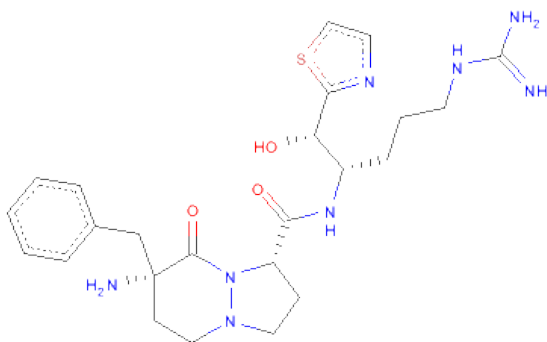
- Molecule 3 is a protein called HIRUGEN.

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<sub>24</sub>H<sub>34</sub>N<sub>8</sub>O<sub>3</sub>S).



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

- Molecule 6 is water.

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 77.0 (50.16-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.148 , (Not available) 0.147 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 14209 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 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	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

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 38.

All (176) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:85:LEU:HD11	2:H:106:MET:HE1	1.64	0.78
2:H:169:LYS:NZ	2:H:169:LYS:HB3	1.91	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:51:TRP:HE3	6:H:548:HOH:O	1.58	0.72
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.20	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
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.93	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:I:357:GLU:HG2	3:I:358:GLU:N	2.19	0.57
2:H:73:ARG:NH2	6:H:443:HOH:O	2.37	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:245:PHE:CE2	6:H:448:HOH:O	2.40	0.56
2:H:130:LEU:HD22	2:H:162:ILE:HD13	1.88	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:41:LEU:HD23	2:H:64:LEU:CD2	2.39	0.52
2:H:134:TYR:CD1	2:H:134:TYR:N	2.77	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:195:SER:CB	5:H:372:00N:O	2.60	0.50
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.46	0.50
2:H:126:ARG:CB	2:H:127:GLU:OE1	2.53	0.50
2:H:185:LYS:HD3	2:H:225:TYR:OH	2.11	0.50
2:H:17:VAL:O	2:H:188:GLY:HA2	2.12	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:HG2	1:L:14(D):ARG:O	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:75:ARG:HD3	2:H:75:ARG:N	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:CD	2:H:127:GLU:H	2.20	0.44
2:H:67:ARG:HG2	2:H:82:ILE:HG12	2.00	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:18:GLU:HG3	2:H:187:ARG:CB	2.40	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:244:GLN:CD	2:H:245:PHE:CE2	2.91	0.44
2:H:204(B):ASN:N	2:H:204(B):ASN:HD22	2.16	0.44
2:H:94:TYR:HA	2:H:101:ARG:HB2	2.00	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:94:TYR:CZ	2:H:96:TRP:HB3	2.54	0.42
2:H:200:VAL:HG12	2:H:209:GLN:HA	2.01	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:HD3	2:H:236:LYS:HA	1.81	0.41
2:H:156:GLN:O	2:H:157:VAL:CG2	2.69	0.41
2:H:36:LYS:HG2	3:I:364:LEU:HD12	2.02	0.41
2:H:125:ASP:OD1	2:H:128:THR:HB	2.21	0.41
2:H:164:GLU:CD	2:H:164:GLU:H	2.20	0.41
2:H:59:LEU:HD13	2:H:88:ILE:HD13	2.01	0.41
2:H:77(A):ARG:HD2	2:H:77(A):ARG:HH11	1.65	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:130:LEU:CD2	2:H:162:ILE:CD1	2.99	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	Distance(Å)	Clash(Å)
2:H:75:ARG:NH1	3:I:357:GLU:OE1[2.555]	2.12	0.08

## 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	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
2	H	246/259 (95%)	224 (91%)	20 (8%)	2 (1%)	27	24
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	278/307 (91%)	254 (91%)	22 (8%)	2 (1%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	186(C)	GLY
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%)	3	3
2	H	218/225 (97%)	192 (88%)	26 (12%)	8	6
3	I	8/10 (80%)	6 (75%)	2 (25%)	1	0
All	All	251/266 (94%)	219 (87%)	32 (13%)	6	5

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
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 chains 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	16,16,17	5.63	2 (12%)	20,22,24	1.44	5 (25%)

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	-	0/9/11/13	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	O-C	21.72	1.26	1.11
3	I	363	TYS	OH-CZ	-5.07	1.36	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	363	TYS	OH-S-O2	-2.76	99.66	107.64
3	I	363	TYS	OH-CZ-CE1	2.51	122.86	118.70
3	I	363	TYS	CG-CB-CA	-2.44	108.66	114.42
3	I	363	TYS	OH-S-O1	2.19	113.97	107.64
3	I	363	TYS	OH-CZ-CE2	-2.11	115.19	118.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	39,39,39	2.81	10 (25%)	52,55,55	4.85	28 (53%)

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	-	0/24/57/57	0/2/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	372	00N	O-C	-8.70	1.25	1.42
5	H	372	00N	C9-C6	7.27	1.62	1.55
5	H	372	00N	C1X-S1X	5.42	1.80	1.73
5	H	372	00N	C8-N	4.96	1.45	1.34
5	H	372	00N	C1-C8	-4.70	1.42	1.52
5	H	372	00N	O2-C8	4.54	1.32	1.23
5	H	372	00N	C2-C3	4.21	1.61	1.52
5	H	372	00N	C1X-C	4.13	1.56	1.51
5	H	372	00N	O1-C7	3.31	1.28	1.22
5	H	372	00N	C9-C10	2.71	1.56	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	372	00N	CA-N-C8	17.74	156.63	123.24
5	H	372	00N	C2X-N1X-C1X	13.96	126.64	104.90
5	H	372	00N	O2-C8-N	-10.73	102.27	122.93
5	H	372	00N	C9-C10-C15	-7.84	109.62	121.06
5	H	372	00N	C1-C8-N	7.49	133.23	116.70
5	H	372	00N	C1X-C-CA	7.16	122.08	109.17
5	H	372	00N	C9-C10-C11	6.50	130.54	121.06
5	H	372	00N	CB-CA-N	6.23	118.15	109.92
5	H	372	00N	O-C-CA	5.72	125.19	107.86
5	H	372	00N	C8-C1-N2	-5.48	100.06	112.08
5	H	372	00N	C5-C6-C9	-5.33	98.37	110.80
5	H	372	00N	C2-C1-C8	-5.16	101.87	111.15
5	H	372	00N	C5-C6-N3	5.10	116.52	108.72
5	H	372	00N	NE-CZ-NH1	-4.81	111.15	120.35
5	H	372	00N	C7-N2-N1	4.74	127.97	122.82
5	H	372	00N	C9-C6-C7	3.79	117.05	108.02
5	H	372	00N	C4-C5-C6	3.56	119.07	112.82
5	H	372	00N	C3-C2-C1	-3.55	98.15	104.38
5	H	372	00N	O1-C7-N2	3.46	124.14	120.82
5	H	372	00N	O-C-C1X	-3.39	102.40	110.53
5	H	372	00N	C6-C9-C10	3.34	122.69	115.73
5	H	372	00N	CG-CB-CA	-3.31	107.93	113.69
5	H	372	00N	C5-C4-N1	3.22	114.68	109.76
5	H	372	00N	C2-C3-N1	-3.17	94.99	103.77
5	H	372	00N	CB-CA-C	3.12	116.89	111.45
5	H	372	00N	C-CA-N	3.01	116.08	110.35
5	H	372	00N	O1-C7-C6	-2.27	114.96	121.42
5	H	372	00N	C3X-C2X-N1X	-2.23	103.42	109.66

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	27/36 (75%)	-0.39	0 100 100	16, 24, 42, 45	0
2	H	250/259 (96%)	-0.54	1 (0%) 90 92	14, 25, 43, 50	0
3	I	10/12 (83%)	-0.00	0 100 100	41, 46, 49, 49	0
All	All	287/307 (93%)	-0.50	1 (0%) 91 93	14, 26, 44, 50	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	245	PHE	2.0

### 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. 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
3	TYS	I	363	16/17	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. 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	00N	H	372	36/36	0.10	-	12,24,31,33	0
4	NA	H	651	1/1	0.05	-	26,26,26,26	0
4	NA	H	650	1/1	0.10	-	28,28,28,28	1

## 6.5 Other polymers

There are no such residues in this entry.