



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:06 PM GMT

PDB ID : 8KME  
Title : CRYSTAL STRUCTURE OF HUMAN ALPHA-THROMBIN INHIBITED  
WITH SEL2770.  
Authors : Mochalkin, I.; Tulinsky, A.  
Deposited on : 1999-03-21  
Resolution : 2.10 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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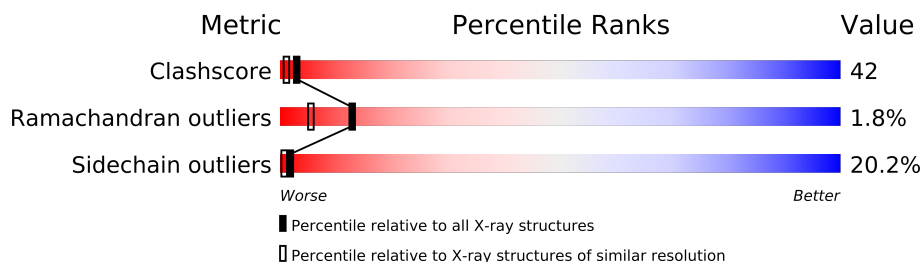
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.10 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	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	36	
2	2	259	
3	3	10	
4	4	7	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2457 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	1	26	Total	C	N	O	S	0	0	0
			214	134	35	44	1			

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	250	Total	C	N	O	S	0	0	0
			2005	1282	351	358	14			

- Molecule 3 is a protein called N-ACETYLMIRUDIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	S	0	0	0
			79	50	10	18	1			

- Molecule 4 is a protein called SEL2770.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	7	Total	C	N	O	0	0	1
			54	39	9	6			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	2	80	Total 80	O 80	0	0
6	3	8	Total 8	O 8	0	0
6	4	2	Total 2	O 2	0	0

### 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.

Note EDS was not executed.

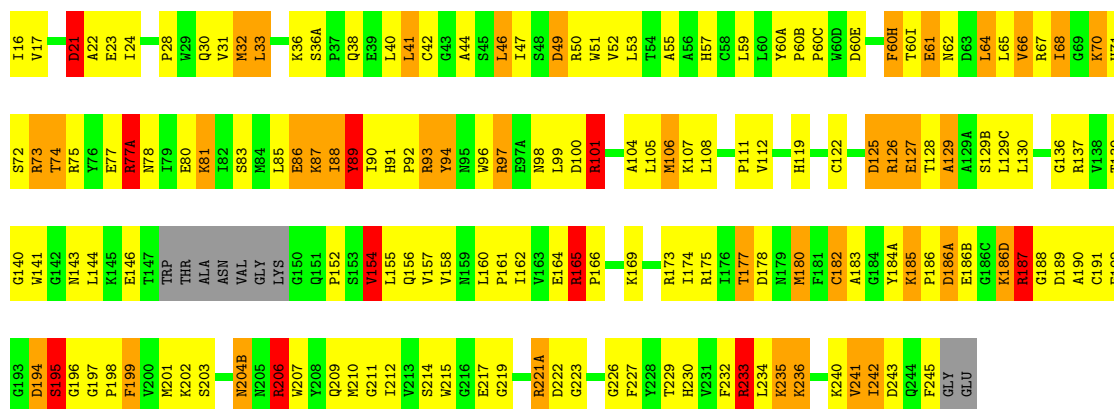
#### • Molecule 1: THROMBIN

Chain 1: 



#### • Molecule 2: THROMBIN

Chain 2: 



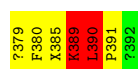
#### • Molecule 3: N-ACETYLHIRUDIN

Chain 3: 



#### • Molecule 4: SEL2770

Chain 4: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.66Å 72.00Å 73.45Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	9.00 – 2.10	Depositor
% Data completeness (in resolution range)	60.0 (9.00-2.10)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 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: OBN, ACE, CHG, NA, NH2, MLY, 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	1	1.07	0/216	1.63	2/287 (0.7%)
2	2	0.95	0/2057	1.76	36/2781 (1.3%)
3	3	1.53	0/63	1.62	0/82
4	4	1.03	0/16	2.21	1/23 (4.3%)
All	All	0.98	0/2352	1.75	39/3173 (1.2%)

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	1	0	1
2	2	0	12
4	4	0	2
All	All	0	15

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	126	ARG	NE-CZ-NH1	17.25	128.93	120.30
2	2	187	ARG	NE-CZ-NH1	-17.13	111.73	120.30
2	2	221(A)	ARG	NE-CZ-NH1	14.76	127.68	120.30
2	2	187	ARG	NE-CZ-NH2	14.00	127.30	120.30
2	2	73	ARG	NE-CZ-NH1	13.68	127.14	120.30
2	2	126	ARG	NE-CZ-NH2	-11.49	114.55	120.30
2	2	233	ARG	NE-CZ-NH2	10.96	125.78	120.30
2	2	233	ARG	NE-CZ-NH1	-10.37	115.12	120.30
2	2	206	ARG	NE-CZ-NH1	10.12	125.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	126	ARG	CD-NE-CZ	8.72	135.81	123.60
2	2	194	ASP	CB-CG-OD2	7.85	125.37	118.30
2	2	187	ARG	CD-NE-CZ	7.44	134.02	123.60
2	2	101	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	2	125	ASP	CB-CG-OD1	7.37	124.94	118.30
2	2	175	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	1	4	ARG	NE-CZ-NH2	6.91	123.75	120.30
2	2	221(A)	ARG	CD-NE-CZ	6.67	132.93	123.60
2	2	187	ARG	CG-CD-NE	-6.66	97.82	111.80
2	2	180	MET	O-C-N	6.40	132.94	122.70
2	2	77(A)	ARG	NE-CZ-NH2	6.39	123.50	120.30
2	2	73	ARG	CD-NE-CZ	6.37	132.52	123.60
2	2	194	ASP	CB-CG-OD1	-6.26	112.66	118.30
2	2	73	ARG	NE-CZ-NH2	-6.17	117.21	120.30
4	4	389	MLY	C-N-CA	6.00	136.70	121.70
2	2	77	GLU	O-C-N	5.94	132.21	122.70
2	2	42	CYS	CB-CA-C	-5.85	98.70	110.40
1	1	14(D)	ARG	NE-CZ-NH2	5.67	123.14	120.30
2	2	178	ASP	CB-CG-OD2	-5.57	113.29	118.30
2	2	154	VAL	N-CA-CB	-5.50	99.39	111.50
2	2	173	ARG	NE-CZ-NH2	5.41	123.01	120.30
2	2	60(H)	PHE	CB-CG-CD1	-5.31	117.08	120.80
2	2	21	ASP	CB-CG-OD2	-5.26	113.56	118.30
2	2	97	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	2	207	TRP	O-C-N	5.18	130.99	122.70
2	2	146	GLU	C-N-CA	5.16	134.60	121.70
2	2	89	TYR	N-CA-CB	5.14	119.85	110.60
2	2	137	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	2	210	MET	CA-CB-CG	-5.04	104.73	113.30
2	2	49	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	3	LEU	Mainchain
2	2	100	ASP	Mainchain
2	2	106	MET	Mainchain
2	2	129	ALA	Mainchain
2	2	158	VAL	Mainchain
2	2	160	LEU	Mainchain
2	2	165	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	2	187	ARG	Sidechain
2	2	199	PHE	Mainchain
2	2	206	ARG	Sidechain
2	2	66	VAL	Mainchain
2	2	88	ILE	Mainchain
2	2	93	ARG	Sidechain
4	4	389	MLY	Peptide
4	4	390	LEU	Peptide

## 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	1	214	0	214	17	0
2	2	2005	0	1970	178	1
3	3	79	0	59	7	0
4	4	54	0	58	12	0
5	2	2	0	0	0	0
6	1	13	0	0	1	0
6	2	80	0	0	5	1
6	3	8	0	0	1	0
6	4	2	0	0	0	0
All	All	2457	0	2301	196	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 42.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:236:LYS:HE2	2:2:236:LYS:H	1.13	1.14
2:2:21:ASP:HB3	2:2:154:VAL:HG12	1.50	0.92
2:2:174:ILE:HD11	4:4:391:PRO:HD3	1.49	0.92
2:2:91:HIS:CG	2:2:92:PRO:HD2	2.10	0.87
2:2:140:GLY:HA3	2:2:194:ASP:OD1	1.75	0.86
2:2:59:LEU:HD13	2:2:88:ILE:CG2	2.05	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:236:LYS:HE2	2:2:236:LYS:N	1.89	0.86
2:2:91:HIS:ND1	2:2:92:PRO:HD2	1.91	0.86
2:2:139:THR:HG22	2:2:157:VAL:HG22	1.58	0.83
2:2:165:ARG:HD3	2:2:169:LYS:HZ1	1.43	0.82
2:2:36:LYS:HD2	3:3:364:LEU:HD23	1.60	0.82
2:2:232:PHE:O	2:2:235:LYS:HB2	1.81	0.81
2:2:52:VAL:HG23	2:2:108:LEU:HD21	1.61	0.79
2:2:86:GLU:O	2:2:87:LYS:HG2	1.82	0.79
2:2:236:LYS:H	2:2:236:LYS:CE	1.94	0.78
1:1:3:LEU:HD11	2:2:206:ARG:HH11	1.47	0.78
2:2:235:LYS:C	2:2:235:LYS:HD3	2.03	0.77
2:2:60(I):THR:HG23	2:2:61:GLU:HG2	1.68	0.76
2:2:59:LEU:HD22	2:2:88:ILE:HD13	1.67	0.75
2:2:59:LEU:HD13	2:2:88:ILE:HG21	1.66	0.75
2:2:24:ILE:H	2:2:24:ILE:HD12	1.50	0.75
2:2:17:VAL:O	2:2:188:GLY:HA2	1.87	0.74
2:2:32:MET:HE3	2:2:70:LYS:HD3	1.68	0.73
2:2:21:ASP:HB3	2:2:154:VAL:CG1	2.19	0.73
2:2:143:ASN:HD21	2:2:192:GLU:HB3	1.54	0.73
2:2:60(B):PRO:HG2	2:2:96:TRP:CE2	2.22	0.73
2:2:80:GLU:C	2:2:81:LYS:HE2	2.08	0.72
1:1:3:LEU:HD11	2:2:206:ARG:NH1	2.03	0.72
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.20	0.72
2:2:53:LEU:HD23	2:2:209:GLN:OE1	1.91	0.71
2:2:143:ASN:ND2	2:2:192:GLU:HB3	2.06	0.71
2:2:36:LYS:CD	3:3:364:LEU:HD23	2.21	0.70
2:2:24:ILE:N	2:2:24:ILE:HD12	2.06	0.70
1:1:3:LEU:CD1	2:2:206:ARG:HH11	2.04	0.70
2:2:165:ARG:HD3	2:2:169:LYS:NZ	2.07	0.70
2:2:52:VAL:CG2	2:2:108:LEU:HD21	2.21	0.70
2:2:186:PRO:HD3	6:2:440:HOH:O	1.91	0.70
2:2:94:TYR:HE1	2:2:99:LEU:CD2	2.04	0.69
2:2:235:LYS:O	2:2:235:LYS:HD3	1.92	0.69
2:2:49:ASP:O	2:2:111:PRO:HA	1.92	0.69
2:2:186:PRO:HG3	2:2:223:GLY:N	2.06	0.69
1:1:14(G):LEU:HD21	2:2:202:LYS:HG2	1.75	0.68
2:2:60(H):PHE:HB3	2:2:64:LEU:HD21	1.74	0.68
2:2:98:ASN:HD21	2:2:177:THR:CG2	2.07	0.68
2:2:185:LYS:HG2	2:2:186(B):GLU:OE1	1.95	0.67
1:1:4:ARG:HG2	2:2:28:PRO:HG2	1.77	0.66
3:3:360:PRO:HA	6:3:467:HOH:O	1.95	0.66
1:1:1:CYS:O	2:2:206:ARG:HD3	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:4:389:MLY:N	4:4:389:MLY:HD3	2.12	0.65
2:2:217:GLU:HA	4:4:389:MLY:O	1.96	0.64
2:2:203:SER:HB3	2:2:204(B):ASN:ND2	2.13	0.64
6:2:709:HOH:O	4:4:385:CHG:H4	1.97	0.64
2:2:81:LYS:HE2	2:2:81:LYS:N	2.13	0.63
2:2:186(B):GLU:O	2:2:186(D):LYS:HE2	2.00	0.62
4:4:385:CHG:H6	4:4:385:CHG:O	1.99	0.61
2:2:94:TYR:CE1	2:2:99:LEU:CD2	2.83	0.61
4:4:379:ACE:O	4:4:389:MLY:HH13	2.01	0.60
2:2:51:TRP:CZ2	2:2:107:LYS:HD2	2.37	0.60
2:2:122:CYS:SG	2:2:206:ARG:HD2	2.41	0.60
2:2:129(C):LEU:HB3	2:2:201:MET:SD	2.42	0.60
2:2:108:LEU:CD1	2:2:112:VAL:CG1	2.79	0.60
1:1:7:PHE:HB3	1:1:12:LEU:O	2.00	0.60
2:2:204(B):ASN:C	2:2:204(B):ASN:HD22	2.05	0.59
2:2:36:LYS:HE3	6:2:715:HOH:O	2.03	0.59
2:2:94:TYR:HE1	2:2:99:LEU:HD22	1.66	0.59
2:2:165:ARG:HD3	2:2:169:LYS:CE	2.33	0.59
2:2:101:ARG:HG2	2:2:234:LEU:HD21	1.84	0.59
1:1:14:ASP:OD1	1:1:14(C):GLU:HB3	2.02	0.59
2:2:85:LEU:HD22	2:2:106:MET:HB3	1.84	0.58
2:2:59:LEU:CD2	2:2:88:ILE:HD13	2.31	0.58
2:2:22:ALA:CB	2:2:155:LEU:HD23	2.33	0.58
2:2:174:ILE:HD11	4:4:391:PRO:CD	2.29	0.58
2:2:60(B):PRO:HG2	2:2:96:TRP:CD2	2.39	0.58
1:1:3:LEU:CD1	2:2:206:ARG:NH1	2.64	0.58
2:2:203:SER:HB3	2:2:204(B):ASN:HD21	1.68	0.58
1:1:14(E):GLU:HG3	6:1:702:HOH:O	2.04	0.57
2:2:30:GLN:HE22	2:2:198:PRO:CD	2.17	0.57
4:4:389:MLY:HA	4:4:389:MLY:HH22	1.86	0.57
2:2:28:PRO:HB2	2:2:119:HIS:HB3	1.87	0.56
2:2:36:LYS:HD2	3:3:364:LEU:CD2	2.34	0.56
2:2:89:TYR:O	2:2:104:ALA:HA	2.05	0.56
2:2:204(B):ASN:HD22	2:2:206:ARG:H	1.52	0.56
2:2:98:ASN:HD22	2:2:180:MET:HE1	1.71	0.56
2:2:57:HIS:CD2	2:2:57:HIS:O	2.59	0.56
4:4:380:0BN:C8	4:4:380:0BN:C	2.83	0.56
2:2:91:HIS:CE1	2:2:92:PRO:HD2	2.40	0.56
2:2:31:VAL:HB	2:2:44:ALA:HB3	1.86	0.56
1:1:14:ASP:HB2	2:2:23:GLU:OE2	2.06	0.56
2:2:60(H):PHE:CB	2:2:64:LEU:HD21	2.36	0.55
2:2:32:MET:HG2	2:2:67:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:126:ARG:O	2:2:126:ARG:HG2	2.04	0.55
2:2:108:LEU:HD12	2:2:112:VAL:CG1	2.36	0.55
2:2:50:ARG:HH21	2:2:107:LYS:HE3	1.72	0.55
2:2:60(I):THR:CG2	2:2:61:GLU:N	2.70	0.55
2:2:86:GLU:O	2:2:87:LYS:CG	2.53	0.55
2:2:81:LYS:HE2	2:2:81:LYS:CA	2.37	0.54
2:2:165:ARG:HG2	2:2:166:PRO:HD3	1.89	0.54
2:2:217:GLU:O	2:2:221(A):ARG:HD2	2.08	0.54
2:2:32:MET:HE1	2:2:70:LYS:HE2	1.90	0.53
2:2:60(I):THR:HG23	2:2:61:GLU:H	1.73	0.53
2:2:60(B):PRO:N	2:2:60(C):PRO:HD2	2.23	0.53
2:2:215:TRP:HA	4:4:380:0BN:C4	2.38	0.53
2:2:32:MET:HG2	2:2:67:ARG:HD3	1.90	0.53
2:2:98:ASN:O	2:2:99:LEU:HB2	2.08	0.53
2:2:235:LYS:CD	2:2:235:LYS:C	2.77	0.53
2:2:64:LEU:CD1	2:2:88:ILE:HD11	2.39	0.53
2:2:22:ALA:HB2	2:2:157:VAL:HG23	1.90	0.52
2:2:188:GLY:O	2:2:189:ASP:HB2	2.10	0.52
2:2:98:ASN:ND2	2:2:177:THR:CG2	2.72	0.52
2:2:94:TYR:CE1	2:2:99:LEU:HD23	2.45	0.52
2:2:36:LYS:O	2:2:38:GLN:HG2	2.09	0.52
2:2:164:GLU:H	2:2:164:GLU:CD	2.12	0.52
2:2:32:MET:CE	2:2:70:LYS:HE2	2.40	0.51
2:2:91:HIS:ND1	2:2:92:PRO:CD	2.70	0.51
2:2:55:ALA:H	2:2:196:GLY:HA2	1.76	0.51
2:2:41:LEU:HD21	2:2:60(H):PHE:CD2	2.45	0.51
2:2:86:GLU:O	2:2:87:LYS:CB	2.59	0.51
2:2:105:LEU:HD13	2:2:242:ILE:CD1	2.40	0.51
2:2:177:THR:HG23	2:2:180:MET:HE3	1.93	0.51
2:2:33:LEU:O	2:2:40:LEU:HD12	2.11	0.50
2:2:91:HIS:CG	2:2:92:PRO:CD	2.89	0.50
2:2:87:LYS:HB3	2:2:89:TYR:CE1	2.46	0.50
2:2:98:ASN:ND2	2:2:177:THR:HG23	2.25	0.50
2:2:32:MET:HE3	2:2:70:LYS:CD	2.39	0.50
2:2:204(B):ASN:ND2	2:2:206:ARG:H	2.10	0.50
2:2:41:LEU:HD22	2:2:64:LEU:HD22	1.93	0.50
2:2:94:TYR:CE2	2:2:96:TRP:HB3	2.46	0.50
2:2:60(I):THR:CG2	2:2:61:GLU:H	2.25	0.49
2:2:59:LEU:HD22	2:2:88:ILE:CD1	2.41	0.49
2:2:80:GLU:O	2:2:81:LYS:HE2	2.11	0.49
2:2:71:HIS:CE1	2:2:154:VAL:HG13	2.48	0.48
2:2:31:VAL:HG12	2:2:32:MET:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:81:LYS:CE	2:2:81:LYS:CA	2.87	0.48
2:2:144:LEU:HD21	2:2:156:GLN:NE2	2.28	0.48
2:2:74:THR:HG22	2:2:75:ARG:N	2.28	0.48
2:2:161:PRO:O	2:2:183:ALA:HB1	2.15	0.47
2:2:127:GLU:CD	2:2:127:GLU:H	2.17	0.47
2:2:189:ASP:HB2	6:2:444:HOH:O	2.14	0.47
2:2:16:ILE:HD13	2:2:190:ALA:HA	1.97	0.47
2:2:64:LEU:HD12	2:2:88:ILE:HD11	1.96	0.46
2:2:165:ARG:CG	2:2:166:PRO:HD3	2.45	0.46
2:2:214:SER:HB3	2:2:227:PHE:O	2.15	0.46
2:2:98:ASN:HD21	2:2:177:THR:HG21	1.81	0.46
2:2:98:ASN:HD22	2:2:180:MET:CE	2.29	0.46
2:2:60(B):PRO:N	2:2:60(C):PRO:CD	2.78	0.45
2:2:186:PRO:HB3	2:2:222:ASP:HB3	1.98	0.45
2:2:219:GLY:O	4:4:380:0BN:H8	2.15	0.45
2:2:184(A):TYR:O	6:2:570:HOH:O	2.21	0.45
1:1:14(D):ARG:HD3	1:1:14(H):GLU:OE2	2.15	0.45
2:2:24:ILE:H	2:2:24:ILE:CD1	2.25	0.45
2:2:161:PRO:HG3	2:2:184(A):TYR:CE1	2.51	0.45
2:2:73:ARG:CG	2:2:141:TRP:HB3	2.46	0.45
2:2:215:TRP:HB2	4:4:389:MLY:HD2	1.98	0.45
1:1:7:PHE:CB	1:1:12:LEU:O	2.63	0.45
2:2:182:CYS:HA	2:2:226:GLY:O	2.17	0.45
2:2:211:GLY:HA2	2:2:229:THR:O	2.16	0.44
2:2:31:VAL:CG1	2:2:32:MET:N	2.80	0.44
2:2:93:ARG:HG2	2:2:93:ARG:HH11	1.83	0.44
2:2:240:LYS:O	2:2:240:LYS:HG3	2.17	0.44
2:2:61:GLU:OE1	2:2:87:LYS:HA	2.18	0.43
2:2:165:ARG:N	2:2:166:PRO:HD2	2.33	0.43
2:2:68:ILE:CD1	2:2:112:VAL:HG11	2.48	0.43
2:2:165:ARG:HD3	2:2:169:LYS:HE2	2.01	0.43
2:2:204(B):ASN:ND2	2:2:206:ARG:HB2	2.33	0.43
2:2:136:GLY:HA3	2:2:199:PHE:CZ	2.53	0.43
2:2:185:LYS:O	2:2:186(A):ASP:N	2.51	0.43
2:2:105:LEU:HD12	2:2:241:VAL:HG11	2.01	0.43
3:3:361:GLU:C	3:3:363:TYS:N	2.70	0.43
2:2:32:MET:HE3	2:2:70:LYS:CE	2.49	0.42
2:2:70:LYS:HE3	2:2:70:LYS:HB3	1.45	0.42
2:2:53:LEU:HD11	2:2:212:ILE:HD11	2.00	0.42
2:2:30:GLN:HE22	2:2:198:PRO:HD2	1.84	0.42
2:2:60(A):TYR:CE1	2:2:60(C):PRO:HG2	2.54	0.42
2:2:61:GLU:HG2	2:2:61:GLU:H	1.45	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:1(A):ASP:O	1:1:1(A):ASP:OD1	2.37	0.42
1:1:7:PHE:CA	1:1:12:LEU:O	2.68	0.42
2:2:243:ASP:C	2:2:245:PHE:N	2.73	0.42
2:2:52:VAL:HG23	2:2:108:LEU:CD2	2.41	0.42
2:2:60(B):PRO:HG2	2:2:96:TRP:CZ2	2.55	0.41
2:2:125:ASP:OD1	2:2:128:THR:HB	2.20	0.41
2:2:164:GLU:C	2:2:166:PRO:HD2	2.40	0.41
3:3:363:TYS:HD1	3:3:363:TYS:HA	1.69	0.41
2:2:230:HIS:CG	2:2:233:ARG:HG3	2.55	0.41
2:2:46:LEU:HD23	2:2:46:LEU:HA	1.92	0.41
1:1:14(A):LYS:HG2	1:1:14(A):LYS:H	1.69	0.41
2:2:59:LEU:HD13	2:2:88:ILE:HG23	1.99	0.41
2:2:94:TYR:CZ	2:2:96:TRP:HB3	2.56	0.41
2:2:105:LEU:HD12	2:2:241:VAL:CG1	2.51	0.41
2:2:195:SER:C	2:2:197:GLY:H	2.25	0.41
2:2:129:ALA:O	2:2:130:LEU:HB2	2.21	0.41
2:2:203:SER:CB	2:2:204(B):ASN:ND2	2.83	0.40
3:3:359:ILE:HD12	3:3:363:TYS:HB3	2.03	0.40
2:2:165:ARG:N	2:2:166:PRO:CD	2.85	0.40
2:2:191:CYS:O	2:2:194:ASP:HB2	2.20	0.40
2:2:32:MET:CE	2:2:70:LYS:CE	2.99	0.40
2:2:81:LYS:CE	2:2:81:LYS:N	2.82	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)
2:2:59:LEU:O	6:2:423:HOH:O[2.655]	2.11	0.09

## 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	1	24/36 (67%)	21 (88%)	3 (12%)	0	100	100
2	2	246/259 (95%)	219 (89%)	23 (9%)	4 (2%)	14	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	7/10 (70%)	7 (100%)	0	0	100	100
4	4	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	279/312 (89%)	248 (89%)	26 (9%)	5 (2%)	13	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	87	LYS
2	2	77(A)	ARG
4	4	390	LEU
2	2	101	ARG
2	2	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	1	24/31 (77%)	21 (88%)	3 (12%)	7	3
2	2	215/225 (96%)	170 (79%)	45 (21%)	1	0
3	3	6/9 (67%)	5 (83%)	1 (17%)	3	1
4	4	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	247/267 (92%)	197 (80%)	50 (20%)	2	1

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	14(D)	ARG
1	1	14(E)	GLU
2	2	21	ASP
2	2	32	MET
2	2	33	LEU
2	2	36(A)	SER
2	2	41	LEU
2	2	46	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	47	ILE
2	2	60(E)	ASP
2	2	61	GLU
2	2	62	ASN
2	2	64	LEU
2	2	65	LEU
2	2	66	VAL
2	2	68	ILE
2	2	70	LYS
2	2	72	SER
2	2	74	THR
2	2	77(A)	ARG
2	2	78	ASN
2	2	81	LYS
2	2	83	SER
2	2	86	GLU
2	2	89	TYR
2	2	90	ILE
2	2	94	TYR
2	2	97	ARG
2	2	127	GLU
2	2	129(B)	SER
2	2	152	PRO
2	2	154	VAL
2	2	162	ILE
2	2	165	ARG
2	2	177	THR
2	2	182	CYS
2	2	185	LYS
2	2	186(A)	ASP
2	2	186(D)	LYS
2	2	187	ARG
2	2	195	SER
2	2	204(B)	ASN
2	2	233	ARG
2	2	235	LYS
2	2	236	LYS
2	2	241	VAL
2	2	242	ILE
3	3	355	ASP
4	4	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such



sidechains are listed below:

Mol	Chain	Res	Type
2	2	30	GLN
2	2	71	HIS
2	2	78	ASN
2	2	98	ASN
2	2	143	ASN
2	2	156	GLN
2	2	204(B)	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
3	TYS	3	363	3	16,16,17	6.17	2 (12%)	20,22,24	2.10	6 (30%)
4	0BN	4	380	4	14,14,15	8.06	9 (64%)	16,18,20	2.43	6 (37%)
4	CHG	4	385	4	10,10,11	7.72	6 (60%)	10,12,14	1.41	2 (20%)
4	MLY	4	389	4	10,10,11	8.23	5 (50%)	9,11,13	2.83	2 (22%)

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	3	363	3	-	0/9/11/13	0/1/1/1
4	0BN	4	380	4	-	0/8/10/12	0/1/1/1
4	CHG	4	385	4	-	0/4/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLY	4	389	4	-	0/7/9/11	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	380	0BN	O-C	27.25	1.30	1.11
3	3	363	TYS	O-C	24.01	1.28	1.11
4	4	385	CHG	O-C	22.87	1.27	1.11
4	4	389	MLY	O-C	18.80	1.24	1.11
4	4	389	MLY	CB-CA	16.85	1.66	1.53
4	4	380	0BN	C6-C10	-8.49	1.40	1.49
4	4	380	0BN	C9-C3	-5.42	1.37	1.51
4	4	385	CHG	C1-CA	-4.99	1.41	1.53
3	3	363	TYS	OH-CZ	-4.63	1.37	1.42
4	4	380	0BN	C10-N2	-4.21	1.26	1.34
4	4	380	0BN	C8-C3	4.18	1.48	1.38
4	4	385	CHG	C6-C1	-3.64	1.44	1.53
4	4	385	CHG	CA-C	3.55	1.55	1.48
4	4	385	CHG	C5-C6	-3.49	1.43	1.53
4	4	389	MLY	CH2-NZ	-3.31	1.34	1.46
4	4	389	MLY	CA-C	3.24	1.54	1.48
4	4	389	MLY	CH1-NZ	-3.17	1.35	1.46
4	4	380	0BN	C9-CA	2.47	1.60	1.53
4	4	385	CHG	C3-C2	-2.47	1.46	1.53
4	4	380	0BN	C5-C4	-2.46	1.34	1.38
4	4	380	0BN	C5-C6	2.46	1.43	1.39
4	4	380	0BN	C8-C7	-2.45	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	389	MLY	C-CA-N	-7.68	106.16	113.83
4	4	380	0BN	C-CA-N	-7.49	106.35	113.83
3	3	363	TYS	C-CA-N	5.23	119.05	113.83
3	3	363	TYS	CG-CB-CA	-4.93	102.78	114.42
3	3	363	TYS	OH-S-O2	-2.74	99.72	107.64
3	3	363	TYS	OH-S-O1	2.73	115.54	107.64
4	4	380	0BN	C9-C3-C8	-2.73	115.55	120.90
4	4	380	0BN	C7-C8-C3	-2.49	117.37	121.05
4	4	380	0BN	C8-C3-C4	2.46	122.31	118.16
3	3	363	TYS	CB-CG-CD1	-2.45	116.09	120.90
4	4	389	MLY	CH2-NZ-CH1	2.40	116.28	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	380	0BN	C5-C4-C3	-2.35	117.58	121.05
4	4	380	0BN	C7-C6-C5	2.33	121.97	118.63
4	4	385	CHG	C6-C1-CA	-2.17	108.85	112.10
3	3	363	TYS	CZ-OH-S	2.10	122.12	118.98
4	4	385	CHG	C2-C1-C6	2.04	112.93	109.45

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.