



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:06 am BST

PDB ID : 1CA8
Title : Thrombin inhibitors with rigid tripeptidyl aldehydes
Authors : Krishnan, R.; Zhang, E.; Hakansson, K.; Arni, R.K.; Tulinsky, A.; Lim-Wilby, M.S.L.; Levy, O.E.; Semple, J.E.; Brunck, T.K.
Deposited on : 1998-04-27
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

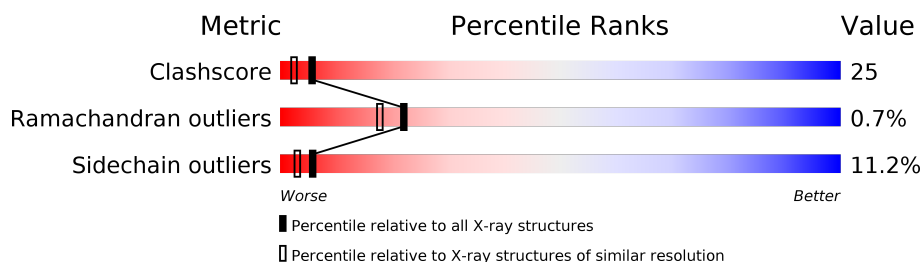
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	36	
2	B	259	
3	C	13	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2411 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	S	0	0	0
			208	131	32	44	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1969	1261	348	347	13			

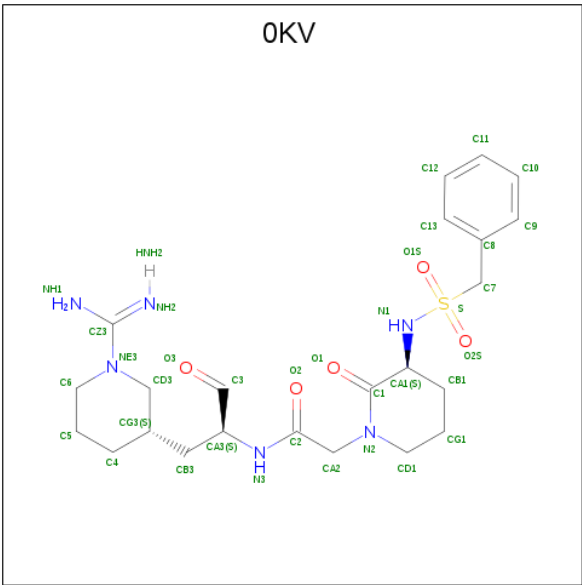
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	S	0	0	0
			63	40	8	14	1			

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

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

- Molecule 5 is 2-{(3S)-3-[(benzylsulfonyl)amino]-2-oxopiperidin-1-yl}-N-{(2S)-1-[(3S)-1-carbamimidoylpiperidin-3-yl]-3-oxopropan-2-yl}acetamide (three-letter code: 0KV) (formula: C₂₃H₃₄N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			35	23	6	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	121	Total	O	0	0
			121	121		
6	C	5	Total	O	0	0
			5	5		

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. 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. 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.

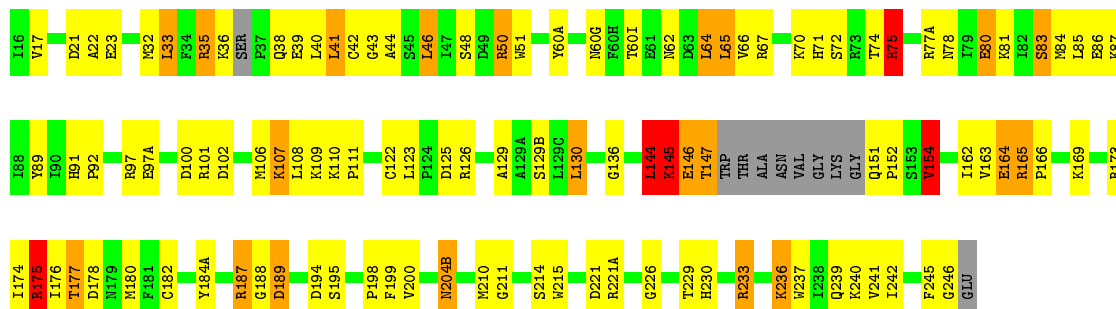
• Molecule 1: Thrombin light chain

Chain A: 




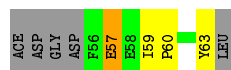
• Molecule 2: Thrombin heavy chain

Chain B: 



• Molecule 3: HIRUGEN

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.13 Å 72.12 Å 73.14 Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2411	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 0KV, 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	A	0.81	0/210	1.78	5/280 (1.8%)
2	B	1.04	9/2018 (0.4%)	1.73	43/2726 (1.6%)
3	C	0.76	0/48	1.53	1/63 (1.6%)
All	All	1.02	9/2276 (0.4%)	1.73	49/3069 (1.6%)

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	A	0	1
2	B	0	3
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	144	LEU	C-N	-28.40	0.68	1.34
2	B	174	ILE	C-N	9.27	1.55	1.34
2	B	146	GLU	CG-CD	6.59	1.61	1.51
2	B	146	GLU	CA-C	5.51	1.67	1.52
2	B	147	THR	N-CA	5.51	1.57	1.46
2	B	146	GLU	CD-OE2	5.38	1.31	1.25
2	B	146	GLU	CB-CG	5.37	1.62	1.52
2	B	146	GLU	CD-OE1	5.30	1.31	1.25
2	B	146	GLU	C-N	5.06	1.45	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	ARG	NE-CZ-NH1	15.20	127.90	120.30
2	B	97	ARG	NE-CZ-NH2	-13.46	113.57	120.30
2	B	144	LEU	O-C-N	-11.18	104.82	122.70
2	B	174	ILE	C-N-CA	-10.26	96.05	121.70
2	B	144	LEU	C-N-CA	10.05	146.83	121.70
2	B	101	ARG	NE-CZ-NH1	9.53	125.06	120.30
2	B	146	GLU	CB-CA-C	9.10	128.60	110.40
2	B	35	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	4	ARG	NE-CZ-NH2	7.85	124.23	120.30
2	B	67	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	B	233	ARG	CD-NE-CZ	7.34	133.88	123.60
2	B	175	ARG	NE-CZ-NH2	7.25	123.92	120.30
2	B	165	ARG	CD-NE-CZ	7.01	133.42	123.60
2	B	189	ASP	CB-CG-OD2	6.80	124.42	118.30
2	B	125	ASP	CB-CG-OD1	6.69	124.32	118.30
2	B	75	ARG	CD-NE-CZ	6.51	132.71	123.60
2	B	60(A)	TYR	CB-CG-CD1	-6.35	117.19	121.00
2	B	184(A)	TYR	CB-CG-CD1	-6.35	117.19	121.00
2	B	221(A)	ARG	NE-CZ-NH1	-6.32	117.14	120.30
2	B	221(A)	ARG	NE-CZ-NH2	6.21	123.40	120.30
2	B	146	GLU	OE1-CD-OE2	-6.08	116.01	123.30
2	B	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	B	42	CYS	CA-CB-SG	6.02	124.84	114.00
1	A	14	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	B	154	VAL	N-CA-CB	-5.84	98.64	111.50
2	B	80	GLU	CG-CD-OE2	-5.76	106.79	118.30
1	A	14(C)	GLU	CG-CD-OE1	-5.74	106.82	118.30
3	C	57	GLU	OE1-CD-OE2	5.68	130.12	123.30
2	B	164	GLU	OE1-CD-OE2	-5.60	116.58	123.30
2	B	83	SER	N-CA-CB	5.58	118.87	110.50
2	B	187	ARG	NE-CZ-NH1	-5.56	117.52	120.30
2	B	145	LYS	CB-CA-C	-5.56	99.29	110.40
2	B	97	ARG	NH1-CZ-NH2	5.54	125.50	119.40
2	B	100	ASP	CB-CG-OD2	-5.54	113.31	118.30
2	B	174	ILE	O-C-N	5.53	131.55	122.70
1	A	1(A)	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	4	ARG	NH1-CZ-NH2	-5.45	113.41	119.40
2	B	233	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	B	44	ALA	CB-CA-C	5.34	118.11	110.10
2	B	35	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	B	194	ASP	CB-CG-OD1	-5.30	113.53	118.30
2	B	173	ARG	N-CA-CB	5.21	119.98	110.60
2	B	164	GLU	CG-CD-OE2	5.20	128.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ASP	CB-CG-OD1	5.13	122.92	118.30
2	B	226	GLY	O-C-N	5.11	130.87	122.70
2	B	146	GLU	N-CA-C	-5.09	97.26	111.00
2	B	23	GLU	OE1-CD-OE2	5.08	129.40	123.30
2	B	180	MET	O-C-N	5.04	130.77	122.70
2	B	144	LEU	CA-C-N	5.01	128.21	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	PRO	Mainchain
2	B	122	CYS	Mainchain
2	B	144	LEU	Mainchain
2	B	177	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	A	208	0	203	1	0
2	B	1969	0	1916	108	0
3	C	63	0	43	8	0
4	B	2	0	0	0	0
5	B	35	0	33	6	0
6	A	8	0	0	0	0
6	B	121	0	0	9	0
6	C	5	0	0	2	0
All	All	2411	0	2195	114	0

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 25.

All (114) 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:B:195:SER:OG	5:B:248:0KV:C3	1.76	1.33
2:B:236:LYS:HE3	2:B:236:LYS:H	1.07	1.15
2:B:75:ARG:NH1	2:B:75:ARG:HA	1.67	1.07
2:B:236:LYS:N	2:B:236:LYS:HE3	1.80	0.96
2:B:236:LYS:CE	2:B:236:LYS:H	1.81	0.94
2:B:195:SER:HG	5:B:248:0KV:C3	1.75	0.91
3:C:60:PRO:HG2	3:C:63:TYS:HE2	1.53	0.89
2:B:239:GLN:C	2:B:240:LYS:CA	2.43	0.87
2:B:43:GLY:HA3	6:B:564:HOH:O	1.74	0.86
2:B:72:SER:OG	2:B:75:ARG:HG2	1.77	0.84
2:B:151:GLN:NE2	6:B:557:HOH:O	2.12	0.82
2:B:195:SER:OG	5:B:248:0KV:H3	1.75	0.82
2:B:77(A):ARG:O	6:B:499:HOH:O	1.97	0.81
2:B:75:ARG:CA	2:B:75:ARG:NH1	2.45	0.79
2:B:74:THR:O	6:B:450:HOH:O	2.01	0.77
2:B:71:HIS:CD2	2:B:154:VAL:HG22	2.22	0.75
2:B:178:ASP:HB3	2:B:233:ARG:HH11	1.52	0.73
2:B:75:ARG:HH12	3:C:57:GLU:CB	2.05	0.69
2:B:80:GLU:O	2:B:81:LYS:HD3	1.91	0.69
2:B:86:GLU:HB3	2:B:107:LYS:HG3	1.72	0.69
3:C:59:ILE:HG23	6:C:537:HOH:O	1.92	0.69
2:B:242:ILE:O	2:B:246:GLY:N	2.26	0.68
2:B:109:LYS:HB3	6:B:572:HOH:O	1.95	0.67
2:B:178:ASP:CB	2:B:233:ARG:HH11	2.06	0.67
2:B:195:SER:OG	5:B:248:0KV:CA3	2.44	0.65
2:B:35:ARG:HB2	2:B:41:LEU:HD13	1.78	0.65
2:B:75:ARG:NH1	3:C:57:GLU:OE1	2.31	0.64
2:B:164:GLU:H	2:B:164:GLU:CD	2.00	0.63
2:B:165:ARG:NH2	2:B:177:THR:O	2.32	0.62
2:B:75:ARG:HB3	2:B:75:ARG:HH11	1.63	0.61
2:B:85:LEU:HD13	2:B:106:MET:HE2	1.81	0.61
2:B:77(A):ARG:O	2:B:78:ASN:HB2	2.02	0.60
2:B:175:ARG:HG2	2:B:175:ARG:O	2.01	0.60
2:B:36:LYS:HG2	2:B:65:LEU:HD22	1.84	0.60
2:B:46:LEU:HD22	2:B:48:SER:O	2.02	0.60
2:B:75:ARG:HH12	3:C:57:GLU:HB2	1.65	0.60
2:B:130:LEU:CD2	2:B:162:ILE:CD1	2.80	0.59
2:B:50:ARG:NH1	2:B:108:LEU:O	2.35	0.59
2:B:71:HIS:CD2	2:B:154:VAL:CG2	2.86	0.58
2:B:75:ARG:HH11	2:B:75:ARG:CB	2.17	0.58
3:C:59:ILE:CG2	6:C:537:HOH:O	2.51	0.58
2:B:72:SER:OG	2:B:75:ARG:CG	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:PRO:HG2	3:C:63:TYS:CE2	2.28	0.58
2:B:50:ARG:HE	2:B:111:PRO:HD3	1.69	0.57
2:B:107:LYS:HG3	2:B:107:LYS:O	2.04	0.57
2:B:236:LYS:HG2	2:B:237:TRP:H	1.69	0.57
2:B:130:LEU:CD2	2:B:162:ILE:HD13	2.35	0.56
2:B:85:LEU:HD11	2:B:106:MET:HE1	1.86	0.56
2:B:165:ARG:O	2:B:169:LYS:HD3	2.06	0.56
2:B:50:ARG:HH11	2:B:107:LYS:HE2	1.69	0.55
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.08	0.55
2:B:86:GLU:CD	2:B:107:LYS:HD3	2.27	0.55
2:B:215:TRP:CE3	5:B:248:OKV:H9	2.41	0.55
2:B:187:ARG:NE	2:B:221:ASP:OD2	2.34	0.55
2:B:91:HIS:ND1	2:B:92:PRO:HD2	2.23	0.54
2:B:35:ARG:O	2:B:38:GLN:CA	2.56	0.54
2:B:145:LYS:HB2	2:B:147:THR:N	2.22	0.54
2:B:187:ARG:NH2	2:B:221:ASP:O	2.32	0.54
2:B:123:LEU:HD12	6:B:503:HOH:O	2.07	0.54
2:B:97(A):GLU:OE2	2:B:175:ARG:HD3	2.09	0.53
2:B:236:LYS:CE	2:B:236:LYS:N	2.56	0.53
2:B:75:ARG:HH12	3:C:57:GLU:HB3	1.74	0.52
2:B:35:ARG:HD3	2:B:39:GLU:OE2	2.10	0.52
5:B:248:OKV:HB1A	5:B:248:OKV:O2S	2.11	0.51
2:B:165:ARG:N	2:B:166:PRO:HD2	2.27	0.50
2:B:32:MET:HG3	2:B:40:LEU:HD13	1.92	0.50
2:B:35:ARG:NH1	2:B:39:GLU:OE2	2.36	0.50
2:B:75:ARG:HA	2:B:75:ARG:HH11	1.68	0.50
2:B:144:LEU:H	2:B:147:THR:C	2.15	0.49
2:B:126:ARG:O	2:B:126:ARG:CG	2.61	0.49
2:B:32:MET:HG3	2:B:40:LEU:CD1	2.43	0.49
2:B:102:ASP:OD2	2:B:214:SER:OG	2.25	0.49
2:B:130:LEU:HD22	2:B:162:ILE:HD13	1.94	0.49
2:B:35:ARG:CD	2:B:39:GLU:OE2	2.61	0.48
2:B:51:TRP:HZ2	2:B:246:GLY:HA3	1.79	0.48
2:B:87:LYS:HB3	2:B:89:TYR:CE1	2.49	0.48
2:B:75:ARG:NH1	2:B:75:ARG:CB	2.75	0.47
2:B:60(G):ASN:ND2	6:B:453:HOH:O	2.29	0.47
1:A:14(G):LEU:N	1:A:14(G):LEU:HD22	2.30	0.47
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.50	0.47
2:B:85:LEU:CD1	2:B:106:MET:CE	2.93	0.47
2:B:17:VAL:O	2:B:188:GLY:HA2	2.15	0.46
2:B:165:ARG:O	2:B:169:LYS:CD	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:HA	2:B:130:LEU:HD23	1.75	0.46
2:B:22:ALA:O	2:B:71:HIS:HE1	1.98	0.46
2:B:36:LYS:HE3	2:B:62:ASN:O	2.16	0.45
2:B:70:LYS:HE3	2:B:72:SER:O	2.16	0.45
2:B:129:ALA:HA	2:B:210:MET:HE1	1.97	0.45
2:B:130:LEU:HD23	2:B:162:ILE:CD1	2.47	0.45
2:B:230:HIS:ND1	2:B:233:ARG:HG3	2.32	0.45
2:B:43:GLY:CA	6:B:564:HOH:O	2.50	0.45
2:B:46:LEU:CD2	2:B:48:SER:O	2.64	0.44
2:B:33:LEU:CD2	2:B:64:LEU:HD22	2.47	0.44
2:B:204(B):ASN:C	2:B:204(B):ASN:ND2	2.70	0.44
2:B:145:LYS:CB	2:B:147:THR:N	2.79	0.43
2:B:233:ARG:O	2:B:236:LYS:HD2	2.18	0.43
2:B:91:HIS:CG	2:B:92:PRO:HD2	2.53	0.43
2:B:107:LYS:HE3	2:B:107:LYS:HB2	1.42	0.43
2:B:84:MET:O	2:B:109:LYS:HB2	2.18	0.43
2:B:86:GLU:HB3	2:B:107:LYS:CG	2.45	0.43
2:B:35:ARG:HB2	2:B:41:LEU:CD1	2.46	0.42
2:B:188:GLY:O	2:B:189:ASP:HB2	2.19	0.42
2:B:211:GLY:HA2	2:B:229:THR:O	2.18	0.42
2:B:145:LYS:HB2	2:B:147:THR:CA	2.49	0.42
2:B:178:ASP:HB2	2:B:233:ARG:HH11	1.84	0.42
2:B:178:ASP:CB	2:B:233:ARG:NH1	2.80	0.41
2:B:198:PRO:HB2	2:B:200:VAL:HG13	2.01	0.41
2:B:75:ARG:HG2	2:B:75:ARG:H	1.64	0.41
2:B:65:LEU:HD12	2:B:65:LEU:HA	1.97	0.41
2:B:236:LYS:HE2	2:B:236:LYS:HB3	1.84	0.40
2:B:89:TYR:CD1	2:B:89:TYR:N	2.89	0.40
2:B:187:ARG:NH1	2:B:187:ARG:HG2	2.36	0.40
2:B:110:LYS:N	6:B:572:HOH:O	2.53	0.40
2:B:151:GLN:HA	2:B:152:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

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	A	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
2	B	241/259 (93%)	230 (95%)	9 (4%)	2 (1%)	19	15
3	C	6/13 (46%)	6 (100%)	0	0	100	100
All	All	271/308 (88%)	259 (96%)	10 (4%)	2 (1%)	22	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	146	GLU
2	B	245	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	A	23/31 (74%)	19 (83%)	4 (17%)	2	1
2	B	205/225 (91%)	183 (89%)	22 (11%)	6	3
3	C	4/10 (40%)	4 (100%)	0	100	100
All	All	232/266 (87%)	206 (89%)	26 (11%)	6	3

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	10	LYS
1	A	14(A)	LYS
1	A	14(F)	LEU
2	B	33	LEU
2	B	41	LEU
2	B	46	LEU
2	B	50	ARG

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Mol	Chain	Res	Type
2	B	60(I)	THR
2	B	64	LEU
2	B	65	LEU
2	B	66	VAL
2	B	75	ARG
2	B	83	SER
2	B	107	LYS
2	B	129(B)	SER
2	B	130	LEU
2	B	145	LYS
2	B	154	VAL
2	B	163	VAL
2	B	175	ARG
2	B	176	ILE
2	B	182	CYS
2	B	204(B)	ASN
2	B	236	LYS
2	B	241	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	ASN
2	B	156	GLN
2	B	204(B)	ASN
2	B	205	ASN
2	B	239	GLN

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	C	63	3	15,16,17	0.92	1 (6%)	18,22,24	1.46	4 (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	C	63	3	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	63	TYS	OH-S	2.65	1.62	1.58

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	63	TYS	CG-CB-CA	-2.75	108.52	114.10
3	C	63	TYS	O2-S-O1	2.25	121.23	112.22
3	C	63	TYS	OH-S-O2	-2.17	101.36	107.71
3	C	63	TYS	CD1-CE1-CZ	-2.16	117.09	119.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	63	TYS	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	63	TYS	2	0

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	0KV	B	248	-	35,37,37	1.92	10 (28%)	45,51,51	3.50	18 (40%)

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	0KV	B	248	-	-	6/27/52/52	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	248	0KV	CZ3-NE3	4.63	1.45	1.35
5	B	248	0KV	C2-N3	4.10	1.42	1.34
5	B	248	0KV	CD3-NE3	3.59	1.51	1.46
5	B	248	0KV	S-N1	3.16	1.66	1.61
5	B	248	0KV	CA2-C2	3.03	1.57	1.52
5	B	248	0KV	C6-NE3	2.87	1.52	1.47
5	B	248	0KV	CA3-N3	2.80	1.50	1.46
5	B	248	0KV	CA1-N1	-2.76	1.41	1.46
5	B	248	0KV	CA1-C1	2.34	1.55	1.52
5	B	248	0KV	O2-C2	2.06	1.27	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	248	0KV	CA2-N2-C1	-10.92	109.89	119.70
5	B	248	0KV	CA2-C2-N3	-8.00	97.26	115.31
5	B	248	0KV	CG3-CB3-CA3	-7.57	104.34	114.52
5	B	248	0KV	C4-CG3-CD3	7.37	117.02	108.68
5	B	248	0KV	C3-CA3-N3	6.04	120.63	109.73
5	B	248	0KV	C2-CA2-N2	-5.94	99.40	113.60
5	B	248	0KV	O1-C1-N2	5.65	129.16	122.49
5	B	248	0KV	O2S-S-N1	-4.94	100.02	107.12
5	B	248	0KV	O2-C2-N3	4.30	130.22	122.95
5	B	248	0KV	CB1-CG1-CD1	3.94	116.38	110.85
5	B	248	0KV	O2S-S-O1S	3.65	124.64	119.35
5	B	248	0KV	O1-C1-CA1	-3.59	112.82	120.58
5	B	248	0KV	O2-C2-CA2	-3.03	115.78	121.08
5	B	248	0KV	CA3-N3-C2	-2.88	117.84	123.15
5	B	248	0KV	O1S-S-C7	-2.77	104.08	108.30
5	B	248	0KV	C7-C8-C9	-2.62	117.27	120.54
5	B	248	0KV	O2S-S-C7	2.60	112.26	108.30
5	B	248	0KV	C6-NE3-CZ3	2.10	124.89	118.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	248	0KV	O3-C3-CA3-CB3
5	B	248	0KV	O2-C2-N3-CA3
5	B	248	0KV	CA3-CB3-CG3-CD3
5	B	248	0KV	C1-CA1-N1-S
5	B	248	0KV	CB1-CA1-N1-S
5	B	248	0KV	O2-C2-CA2-N2

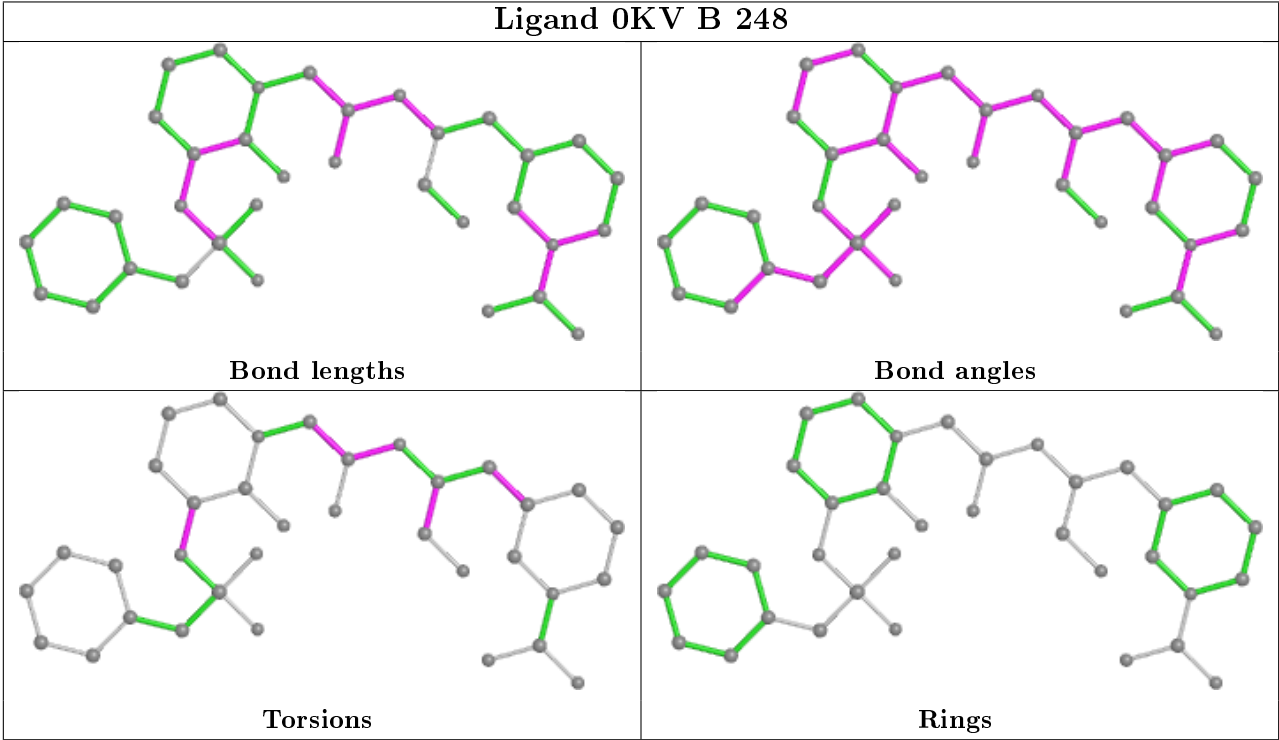
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	248	0KV	6	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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	144:LEU	C	145:LYS	N	0.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.