



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 AM UTC

PDB ID : 1BB0 / pdb_00001bb0
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 : 1998-04-28
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

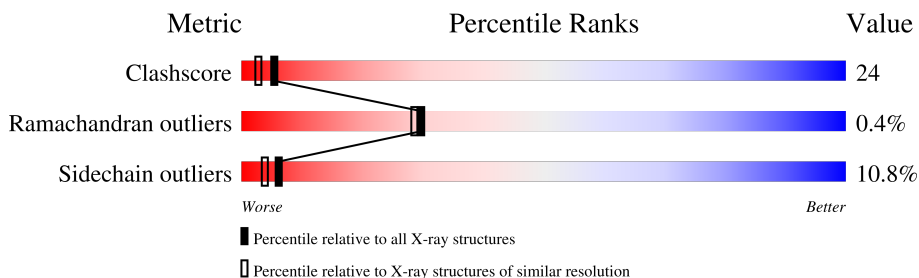
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

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 2412 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.

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

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	1970	1261	349	347	13	0	0	0

- Molecule 3 is a protein called HIRUGEN.

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

- Molecule 4 is SODIUM ION (CCD ID: 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-[(3R)-1-carbamimidoylpiperidin-3-yl]-3-oxopropan-2-yl}acetamide (CCD ID: 0IV) (formula: C₂₃H₃₄N₆O₅S).

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

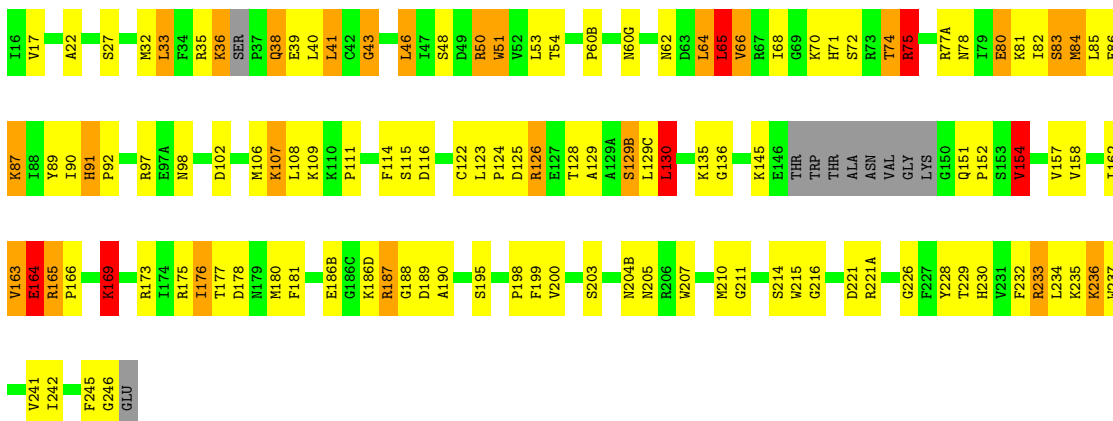
• Molecule 1: THROMBIN

Chain A:  47% 25% 28%




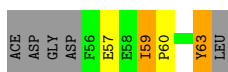
• Molecule 2: THROMBIN

Chain B:  49% 35% 10% • •



• Molecule 3: HIRUGEN

Chain C:  31% 15% 15% 38%



4 Data and refinement statistics

Xtrriage (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	71.14Å 72.26Å 72.73Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.10)	Depositor
R_{merge}	0.06	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.	Xtrriage
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: NA, TYS, OIV

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	0.87	0/210	1.96	5/280 (1.8%)
2	B	0.94	0/2020	2.04	76/2731 (2.8%)
3	C	0.74	0/48	1.85	1/63 (1.6%)
All	All	0.93	0/2278	2.03	82/3074 (2.7%)

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	1
All	All	0	2

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	ARG	CA-C-N	11.16	137.07	121.66
2	B	175	ARG	C-N-CA	11.16	137.07	121.66
2	B	154	VAL	N-CA-CB	-9.84	98.75	112.52
2	B	38	GLN	CA-C-O	-9.42	110.67	120.84
2	B	180	MET	CA-C-O	-9.06	111.17	121.40
2	B	164	GLU	CB-CG-CD	7.96	126.12	112.60
2	B	163	VAL	CA-C-N	7.40	131.34	120.90
2	B	163	VAL	C-N-CA	7.40	131.34	120.90
2	B	27	SER	CA-C-O	7.27	128.18	121.34
2	B	74	THR	N-CA-C	6.98	122.90	113.97
2	B	176	ILE	CA-CB-CG2	6.96	122.33	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	ALA	N-CA-C	-6.81	101.74	110.53
2	B	228	TYR	CA-C-O	-6.67	113.31	121.11
2	B	27	SER	CB-CA-C	6.66	119.41	111.15
2	B	97	ARG	NE-CZ-NH2	-6.66	113.21	119.20
2	B	205	ASN	CA-CB-CG	-6.61	105.99	112.60
2	B	116	ASP	CA-CB-CG	6.59	119.19	112.60
2	B	165	ARG	CD-NE-CZ	6.48	133.47	124.40
2	B	180	MET	O-C-N	6.46	130.99	123.17
2	B	221(A)	ARG	CA-C-O	-6.42	113.73	121.05
2	B	91	HIS	CA-CB-CG	-6.39	107.41	113.80
2	B	27	SER	N-CA-CB	-6.36	103.53	110.71
2	B	233	ARG	NE-CZ-NH1	6.36	127.86	121.50
2	B	82	ILE	CA-C-O	-6.33	113.75	120.53
2	B	98	ASN	CA-C-O	-6.25	112.53	119.34
2	B	176	ILE	N-CA-CB	-6.24	103.72	110.53
2	B	158	VAL	CA-C-N	6.18	131.25	122.72
2	B	158	VAL	C-N-CA	6.18	131.25	122.72
2	B	65	LEU	O-C-N	6.16	130.78	123.33
2	B	115	SER	O-C-N	6.10	129.38	123.04
1	A	14(E)	GLU	CB-CG-CD	6.03	122.85	112.60
2	B	173	ARG	N-CA-CB	5.99	119.79	110.44
2	B	75	ARG	CD-NE-CZ	5.92	132.69	124.40
2	B	115	SER	CA-C-O	-5.87	114.85	121.25
2	B	157	VAL	CA-C-O	-5.82	115.11	121.28
2	B	53	LEU	CA-C-O	-5.80	114.56	120.71
2	B	233	ARG	CD-NE-CZ	5.73	132.43	124.40
3	C	59	ILE	O-C-N	5.66	127.55	121.10
2	B	163	VAL	O-C-N	-5.65	117.11	122.98
2	B	203	SER	CA-C-O	5.62	126.01	120.17
2	B	130	LEU	CB-CA-C	5.57	120.74	111.83
2	B	51	TRP	O-C-N	5.54	129.80	123.31
2	B	226	GLY	O-C-N	5.54	130.91	123.11
2	B	165	ARG	CA-C-N	5.52	124.98	119.24
2	B	165	ARG	C-N-CA	5.52	124.98	119.24
2	B	68	ILE	N-CA-C	5.50	116.41	108.48
2	B	221(A)	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	B	175	ARG	CA-C-O	5.46	126.83	120.49
2	B	114	PHE	CA-CB-CG	-5.45	108.35	113.80
2	B	60(B)	PRO	CB-CA-C	5.43	117.54	110.92
2	B	163	VAL	CB-CA-C	5.41	119.66	110.95
2	B	66	VAL	N-CA-CB	-5.38	104.53	110.99
2	B	207	TRP	CA-C-O	-5.37	114.58	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186(B)	GLU	CB-CG-CD	5.33	121.67	112.60
2	B	187	ARG	CD-NE-CZ	-5.31	116.97	124.40
2	B	216	GLY	CA-C-N	-5.30	115.32	122.95
2	B	216	GLY	C-N-CA	-5.30	115.32	122.95
2	B	169	LYS	CA-CB-CG	5.26	124.62	114.10
2	B	54	THR	CA-CB-CG2	5.21	119.37	110.50
2	B	207	TRP	O-C-N	5.18	129.13	123.27
1	A	4	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	B	82	ILE	CB-CG1-CD1	5.18	124.68	113.80
2	B	80	GLU	CG-CD-OE2	-5.18	106.50	118.40
2	B	129(B)	SER	CA-C-O	-5.17	112.90	119.31
2	B	27	SER	O-C-N	-5.16	117.42	121.19
2	B	43	GLY	N-CA-C	-5.12	104.73	112.41
2	B	84	MET	N-CA-C	-5.12	101.93	110.17
2	B	83	SER	N-CA-CB	5.11	118.72	110.85
2	B	234	LEU	CA-C-N	5.11	127.64	120.28
2	B	234	LEU	C-N-CA	5.11	127.64	120.28
1	A	13	GLU	O-C-N	5.09	129.15	123.19
1	A	14(C)	GLU	CG-CD-OE1	-5.08	106.71	118.40
2	B	135	LYS	CA-C-N	5.08	128.26	122.67
2	B	135	LYS	C-N-CA	5.08	128.26	122.67
2	B	181	PHE	N-CA-C	-5.07	101.59	109.24
1	A	13	GLU	CA-C-O	-5.07	115.18	120.80
2	B	164	GLU	CA-C-N	5.06	128.46	120.97
2	B	164	GLU	C-N-CA	5.06	128.46	120.97
2	B	126	ARG	N-CA-CB	5.04	117.62	110.06
2	B	186(D)	LYS	N-CA-C	-5.04	99.41	108.48
2	B	36	LYS	N-CA-CB	5.02	119.03	110.50
2	B	232	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	PRO	Mainchain
2	B	122	CYS	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	2	0
2	B	1970	0	1922	100	0
3	C	63	0	43	8	0
4	B	2	0	0	0	0
5	B	35	0	33	5	0
6	A	8	0	0	1	0
6	B	121	0	0	8	0
6	C	5	0	0	2	0
All	All	2412	0	2201	107	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 24.

All (107) 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:236:LYS:HE3	2:B:236:LYS:H	1.08	1.15
2:B:195:SER:OG	5:B:1:0IV:C9	1.94	1.14
2:B:75:ARG:HA	2:B:75:ARG:NH1	1.64	1.11
2:B:236:LYS:HE3	2:B:236:LYS:N	1.80	0.95
2:B:43:GLY:HA3	6:B:564:HOH:O	1.66	0.94
2:B:236:LYS:H	2:B:236:LYS:CE	1.82	0.92
3:C:60:PRO:HG2	3:C:63:TYS:HE2	1.53	0.89
2:B:72:SER:OG	2:B:75:ARG:HG2	1.76	0.85
2:B:77(A):ARG:O	6:B:499:HOH:O	1.95	0.83
2:B:75:ARG:NH1	2:B:75:ARG:CA	2.41	0.83
2:B:85:LEU:HD13	2:B:106:MET:HE2	1.61	0.81
2:B:74:THR:O	6:B:450:HOH:O	1.97	0.81
2:B:151:GLN:NE2	6:B:557:HOH:O	2.16	0.78
2:B:71:HIS:CD2	2:B:154:VAL:HG22	2.21	0.76
2:B:178:ASP:HB3	2:B:233:ARG:HH11	1.51	0.75
2:B:85:LEU:CD1	2:B:106:MET:HE2	2.20	0.72
2:B:86:GLU:HB3	2:B:107:LYS:HG3	1.73	0.69
2:B:75:ARG:HH12	3:C:57:GLU:CB	2.07	0.67
3:C:59:ILE:HG23	6:C:537:HOH:O	1.95	0.66
2:B:178:ASP:CB	2:B:233:ARG:HH11	2.07	0.66
2:B:80:GLU:O	2:B:81:LYS:HD3	1.95	0.65
2:B:75:ARG:HH11	2:B:75:ARG:HB3	1.60	0.65
2:B:75:ARG:NH1	3:C:57:GLU:OE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLU:H	2:B:164:GLU:CD	2.03	0.65
2:B:35:ARG:HB2	2:B:41:LEU:HD13	1.78	0.64
2:B:242:ILE:O	2:B:246:GLY:N	2.29	0.64
2:B:109:LYS:HB3	6:B:572:HOH:O	1.99	0.63
2:B:187:ARG:NE	2:B:221:ASP:OD2	2.32	0.63
2:B:46:LEU:HD22	2:B:48:SER:O	1.99	0.63
2:B:165:ARG:NH2	2:B:177:THR:O	2.32	0.63
2:B:75:ARG:HH11	2:B:75:ARG:CB	2.13	0.61
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.06	0.61
2:B:215:TRP:CE3	5:B:1:OIV:H2	2.35	0.61
2:B:72:SER:OG	2:B:75:ARG:CG	2.49	0.60
2:B:50:ARG:NH1	2:B:108:LEU:O	2.34	0.60
2:B:50:ARG:HH11	2:B:107:LYS:HE2	1.65	0.59
2:B:236:LYS:HG2	2:B:237:TRP:H	1.67	0.59
2:B:195:SER:OG	5:B:1:OIV:O2	2.20	0.59
2:B:130:LEU:CD2	2:B:162:ILE:HD13	2.33	0.59
2:B:77(A):ARG:O	2:B:78:ASN:HB2	2.03	0.59
2:B:86:GLU:CD	2:B:107:LYS:HD3	2.28	0.58
2:B:71:HIS:CD2	2:B:154:VAL:CG2	2.86	0.58
2:B:107:LYS:HG3	2:B:107:LYS:O	2.03	0.58
3:C:60:PRO:HG2	3:C:63:TYS:CE2	2.29	0.57
2:B:36:LYS:HG2	2:B:65:LEU:HD22	1.86	0.57
2:B:130:LEU:CD2	2:B:162:ILE:CD1	2.83	0.56
2:B:35:ARG:HD3	2:B:39:GLU:OE2	2.05	0.56
2:B:165:ARG:O	2:B:169:LYS:HD3	2.06	0.56
2:B:50:ARG:HE	2:B:111:PRO:HD3	1.70	0.56
3:C:59:ILE:CG2	6:C:537:HOH:O	2.54	0.56
2:B:75:ARG:HH12	3:C:57:GLU:HB2	1.70	0.55
2:B:75:ARG:HH12	3:C:57:GLU:HB3	1.73	0.54
2:B:91:HIS:ND1	2:B:92:PRO:HD2	2.24	0.53
2:B:35:ARG:O	2:B:38:GLN:CA	2.57	0.53
2:B:123:LEU:HD12	6:B:503:HOH:O	2.08	0.53
2:B:195:SER:HG	5:B:1:OIV:C9	2.17	0.53
2:B:187:ARG:NH2	2:B:221:ASP:O	2.33	0.52
2:B:75:ARG:HA	2:B:75:ARG:HH11	1.67	0.52
2:B:236:LYS:N	2:B:236:LYS:CE	2.56	0.52
2:B:126:ARG:O	2:B:126:ARG:CG	2.58	0.52
2:B:32:MET:HG3	2:B:40:LEU:HD13	1.91	0.51
2:B:75:ARG:NH1	2:B:75:ARG:CB	2.72	0.50
2:B:165:ARG:N	2:B:166:PRO:HD2	2.27	0.50
2:B:124:PRO:O	2:B:235:LYS:NZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:HD22	2:B:162:ILE:HD13	1.93	0.49
2:B:87:LYS:HB3	2:B:89:TYR:CE1	2.48	0.49
2:B:35:ARG:NH1	2:B:39:GLU:OE2	2.37	0.49
2:B:17:VAL:O	2:B:188:GLY:HA2	2.13	0.48
2:B:32:MET:HG3	2:B:40:LEU:CD1	2.43	0.48
5:B:1:OIV:O2S	5:B:1:OIV:HB3	2.14	0.47
2:B:51:TRP:HZ2	2:B:246:GLY:HA3	1.80	0.47
2:B:35:ARG:CD	2:B:39:GLU:OE2	2.63	0.46
2:B:102:ASP:OD2	2:B:214:SER:OG	2.23	0.46
2:B:165:ARG:O	2:B:169:LYS:CD	2.64	0.46
2:B:46:LEU:CD2	2:B:48:SER:O	2.63	0.46
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.51	0.46
2:B:204(B):ASN:C	2:B:204(B):ASN:ND2	2.70	0.46
2:B:43:GLY:CA	6:B:564:HOH:O	2.43	0.45
2:B:130:LEU:HD23	2:B:130:LEU:HA	1.75	0.45
1:A:14(G):LEU:HD22	1:A:14(G):LEU:N	2.32	0.45
2:B:107:LYS:HE3	2:B:107:LYS:HB2	1.37	0.45
2:B:230:HIS:ND1	2:B:233:ARG:HG3	2.32	0.45
2:B:60(G):ASN:ND2	6:B:453:HOH:O	2.31	0.45
2:B:130:LEU:HD23	2:B:162:ILE:CD1	2.47	0.45
1:A:1(A):ASP:HB3	6:A:553:HOH:O	2.18	0.44
2:B:36:LYS:HE3	2:B:62:ASN:O	2.18	0.44
2:B:91:HIS:CG	2:B:92:PRO:HD2	2.52	0.44
2:B:129:ALA:HA	2:B:210:MET:HE1	2.01	0.43
2:B:86:GLU:HB3	2:B:107:LYS:CG	2.45	0.43
2:B:22:ALA:O	2:B:71:HIS:HE1	2.00	0.43
2:B:70:LYS:HE3	2:B:72:SER:O	2.18	0.43
2:B:33:LEU:CD2	2:B:64:LEU:HD22	2.48	0.43
2:B:84:MET:O	2:B:109:LYS:HB2	2.18	0.42
2:B:75:ARG:HG2	2:B:75:ARG:H	1.63	0.42
2:B:35:ARG:HB2	2:B:41:LEU:CD1	2.47	0.42
2:B:233:ARG:O	2:B:236:LYS:HD2	2.20	0.42
2:B:125:ASP:OD1	2:B:128:THR:HB	2.19	0.41
2:B:178:ASP:CB	2:B:233:ARG:NH1	2.79	0.41
2:B:211:GLY:HA2	2:B:229:THR:O	2.18	0.41
2:B:125:ASP:OD1	2:B:128:THR:CB	2.68	0.41
2:B:198:PRO:HB2	2:B:200:VAL:HG13	2.01	0.41
2:B:71:HIS:NE2	2:B:154:VAL:HG22	2.36	0.41
2:B:151:GLN:HA	2:B:152:PRO:HD3	1.86	0.41
2:B:188:GLY:O	2:B:189:ASP:HB2	2.21	0.41
2:B:87:LYS:HB3	2:B:89:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LYS:HE2	2:B:236:LYS:HB3	1.84	0.40
2:B:130:LEU:HG	2:B:210:MET:HE3	2.04	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	243/259 (94%)	232 (96%)	10 (4%)	1 (0%)	30	28
3	C	6/13 (46%)	6 (100%)	0	0	100	100
All	All	273/308 (89%)	261 (96%)	11 (4%)	1 (0%)	30	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	245	PHE

5.3.2 Protein sidechains [i](#)

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%)	21 (91%)	2 (9%)	9	7
2	B	205/225 (91%)	182 (89%)	23 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	4/10 (40%)	4 (100%)	0	100	100
All	All	232/266 (87%)	207 (89%)	25 (11%)	6	4

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	10	LYS
2	B	33	LEU
2	B	41	LEU
2	B	46	LEU
2	B	50	ARG
2	B	64	LEU
2	B	65	LEU
2	B	66	VAL
2	B	75	ARG
2	B	83	SER
2	B	87	LYS
2	B	90	ILE
2	B	107	LYS
2	B	129(B)	SER
2	B	129(C)	LEU
2	B	130	LEU
2	B	145	LYS
2	B	154	VAL
2	B	163	VAL
2	B	164	GLU
2	B	169	LYS
2	B	176	ILE
2	B	236	LYS
2	B	241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	57	HIS
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	0.81	0	15,22,24	1.51	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	C	63	3	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	63	TYS	O2-S-O1	2.27	121.01	112.24
3	C	63	TYS	CD1-CE1-CZ	-2.21	117.21	119.73
3	C	63	TYS	OH-S-O2	-2.12	101.10	107.56

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 [i](#)

There are no oligosaccharides 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	0IV	B	1	-	34,37,37	3.41	14 (41%)	47,51,51	3.75	24 (51%)

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	0IV	B	1	-	-	8/27/52/52	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	0IV	CB1-CA2	-9.28	1.42	1.53
5	B	1	0IV	C31-NE	8.45	1.62	1.47
5	B	1	0IV	C21-C11	6.43	1.69	1.53
5	B	1	0IV	CB1-CG1	-5.45	1.44	1.53
5	B	1	0IV	C8-N2	4.97	1.44	1.34
5	B	1	0IV	CD1-NE	-4.86	1.41	1.46
5	B	1	0IV	O2-C9	4.64	1.37	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	0IV	C21-C31	4.57	1.66	1.51
5	B	1	0IV	CZ-NH2	-3.77	1.25	1.34
5	B	1	0IV	CD1-CG1	3.18	1.57	1.52
5	B	1	0IV	S-N	3.05	1.66	1.61
5	B	1	0IV	CA-N	-2.92	1.41	1.46
5	B	1	0IV	CA1-C8	2.89	1.57	1.52
5	B	1	0IV	CA2-N2	-2.74	1.42	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	0IV	CA1-N1-C7	-12.80	108.03	119.77
5	B	1	0IV	C21-C11-CG1	-8.50	94.19	112.08
5	B	1	0IV	C8-CA1-N1	-6.90	95.55	113.22
5	B	1	0IV	CB1-CG1-C11	-6.73	96.04	111.71
5	B	1	0IV	O2S-S-N	-5.86	98.77	107.11
5	B	1	0IV	CB-CG-CD	5.62	118.14	110.75
5	B	1	0IV	CG1-CB1-CA2	5.42	121.81	114.52
5	B	1	0IV	C11-C21-C31	-4.59	104.72	110.75
5	B	1	0IV	O2S-S-O1S	4.26	125.30	119.34
5	B	1	0IV	O2-C9-CA2	4.12	135.36	124.77
5	B	1	0IV	C11-CG1-CD1	3.80	113.09	108.59
5	B	1	0IV	O-C7-N1	3.80	126.95	122.53
5	B	1	0IV	O2S-S-C	3.55	113.78	108.33
5	B	1	0IV	O1S-S-C	-3.52	102.93	108.33
5	B	1	0IV	C31-NE-CD1	-3.48	106.36	113.07
5	B	1	0IV	CB1-CA2-N2	-3.45	105.47	110.69
5	B	1	0IV	CG1-CD1-NE	3.33	116.96	111.27
5	B	1	0IV	O-C7-CA	-3.11	113.90	120.68
5	B	1	0IV	NH2-CZ-NE	3.10	123.09	118.02
5	B	1	0IV	CD1-NE-CZ	3.01	127.88	119.25
5	B	1	0IV	C-C1-C2	-2.99	116.96	120.56
5	B	1	0IV	C9-CA2-N2	2.79	114.88	109.50
5	B	1	0IV	O1-C8-N2	-2.76	118.28	122.95
5	B	1	0IV	CB1-CA2-C9	2.70	115.15	110.99

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	0IV	O2-C9-CA2-CB1
5	B	1	0IV	C9-CA2-CB1-CG1

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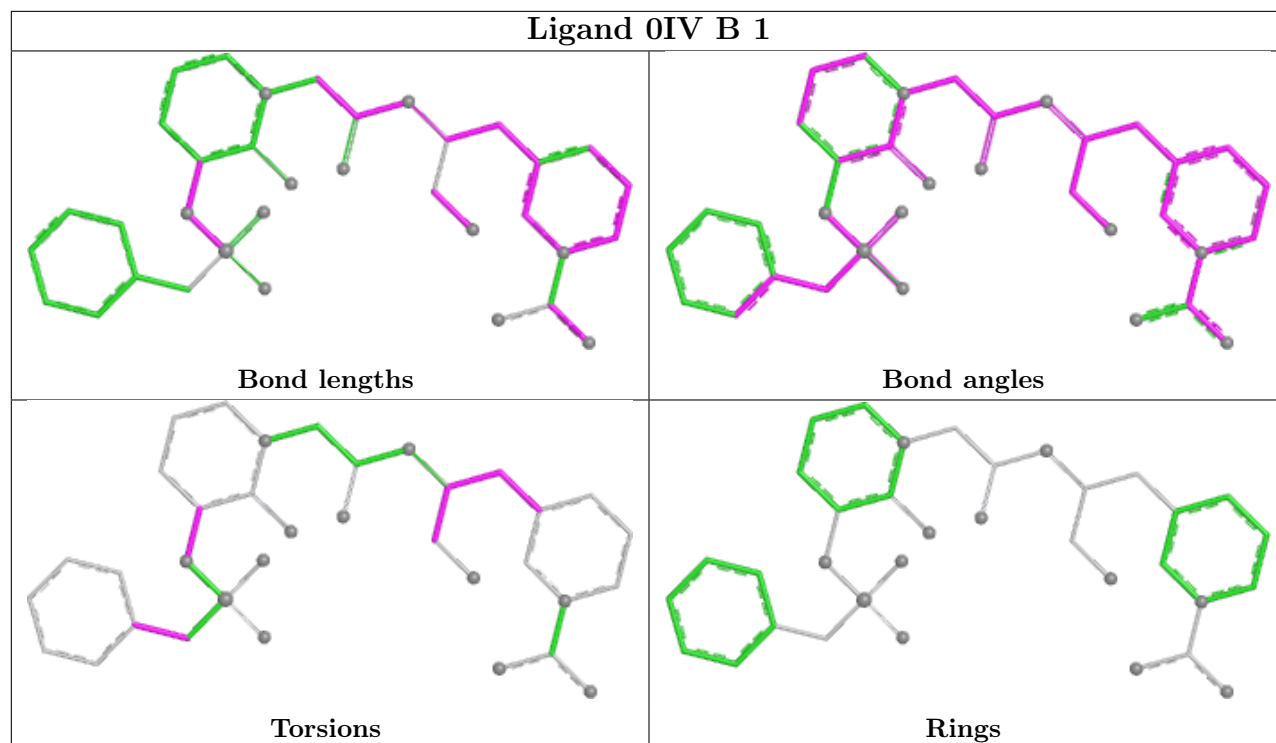
Mol	Chain	Res	Type	Atoms
5	B	1	0IV	CA2-CB1-CG1-C11
5	B	1	0IV	N2-CA2-CB1-CG1
5	B	1	0IV	CA2-CB1-CG1-CD1
5	B	1	0IV	CB-CA-N-S
5	B	1	0IV	C7-CA-N-S
5	B	1	0IV	S-C-C1-C6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	0IV	5	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.