



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:45 AM UTC

PDB ID : 1ZZZ / pdb_00001zzz
Title : Trypsin 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 : 1998-06-02
Resolution : 1.90 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)
Xtriage (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

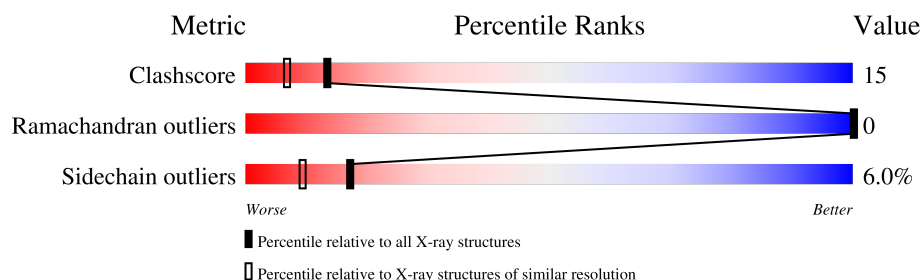
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	237	

2 Entry composition [i](#)

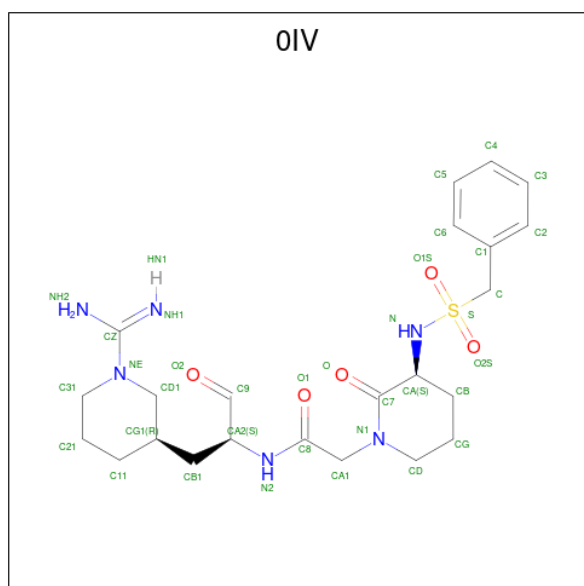
There are 4 unique types of molecules in this entry. The entry contains 1815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1629	1012	279	324	14	0	0	0

- Molecule 2 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).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	28	16	6	5	1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total 157	O 157	0	0

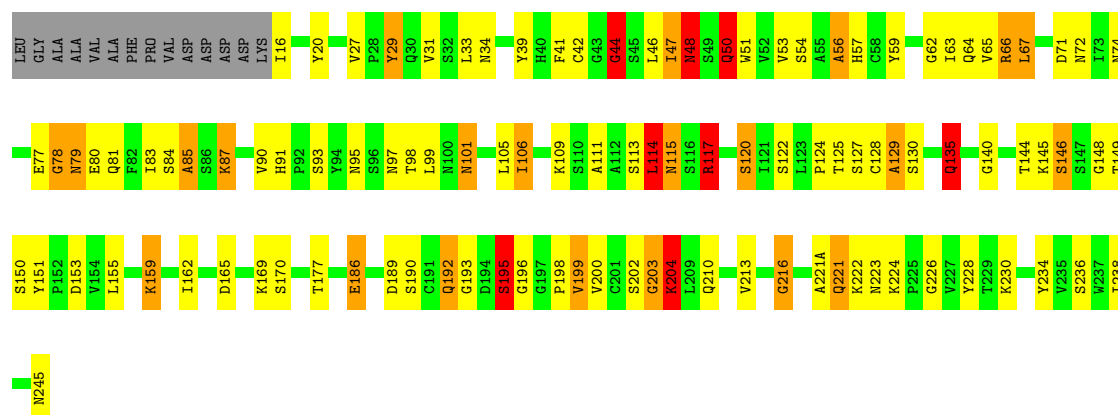
3 Residue-property plots

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: TRYPSIN

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.67Å 63.20Å 69.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90	Depositor
% Data completeness (in resolution range)	72.0 (7.00-1.90)	Depositor
R_{merge}	0.04	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	1815	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CA, 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	1.29	1/1660 (0.1%)	2.43	110/2250 (4.9%)

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	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLY	CA-C	5.08	1.57	1.51

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLN	OE1-CD-NE2	-12.23	110.37	122.60
1	A	151	TYR	CA-C-O	-10.85	110.76	119.66
1	A	204	LYS	CA-C-O	-9.70	110.24	121.68
1	A	50	GLN	OE1-CD-NE2	9.61	132.21	122.60
1	A	54	SER	CA-C-O	-8.23	112.58	120.56
1	A	48	ASN	CA-C-O	-8.12	112.53	121.05
1	A	117	ARG	CB-CA-C	-8.07	93.92	110.38
1	A	159	LYS	CA-C-O	-7.89	111.62	120.54
1	A	203	GLY	CA-C-O	-7.86	110.20	119.00
1	A	79	ASN	CA-C-O	-7.80	112.78	119.18
1	A	97	ASN	CA-CB-CG	-7.80	104.80	112.60
1	A	98	THR	CA-C-O	-7.75	110.20	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	SER	CB-CA-C	7.62	123.62	110.45
1	A	67	LEU	CA-C-O	-7.59	112.58	121.16
1	A	79	ASN	O-C-N	7.54	129.28	121.89
1	A	202	SER	CA-C-O	-7.37	113.03	121.65
1	A	66	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	A	117	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	A	135	GLN	CB-CG-CD	6.90	124.34	112.60
1	A	78	GLY	CA-C-N	-6.78	116.21	126.86
1	A	78	GLY	C-N-CA	-6.78	116.21	126.86
1	A	135	GLN	CG-CD-NE2	6.73	126.50	116.40
1	A	50	GLN	CA-CB-CG	-6.65	100.81	114.10
1	A	114	LEU	CA-C-N	6.63	134.29	122.08
1	A	114	LEU	C-N-CA	6.63	134.29	122.08
1	A	91	HIS	CA-CB-CG	-6.63	107.17	113.80
1	A	67	LEU	O-C-N	6.60	131.47	123.16
1	A	223	ASN	OD1-CG-ND2	6.60	129.20	122.60
1	A	170	SER	CA-C-N	6.53	129.56	120.29
1	A	170	SER	C-N-CA	6.53	129.56	120.29
1	A	98	THR	O-C-N	6.52	131.40	122.46
1	A	238	ILE	O-C-N	6.47	128.25	121.91
1	A	54	SER	O-C-N	6.42	130.27	122.88
1	A	106	ILE	O-C-N	6.41	130.13	123.20
1	A	80	GLU	CA-C-N	6.40	131.80	122.77
1	A	80	GLU	C-N-CA	6.40	131.80	122.77
1	A	189	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	148	GLY	N-CA-C	-6.38	103.23	112.17
1	A	170	SER	CA-C-O	-6.38	111.53	119.38
1	A	66	ARG	CA-C-O	-6.38	113.63	120.46
1	A	67	LEU	CD1-CG-CD2	-6.38	96.77	110.80
1	A	145	LYS	CB-CA-C	-6.35	97.95	109.38
1	A	57	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	162	ILE	O-C-N	6.22	129.72	122.81
1	A	42	CYS	CA-C-O	-6.18	114.83	121.38
1	A	200	VAL	CA-C-O	-6.17	113.91	120.39
1	A	62	GLY	CA-C-O	-6.17	112.18	119.46
1	A	226	GLY	CA-C-N	6.17	131.05	123.10
1	A	226	GLY	C-N-CA	6.17	131.05	123.10
1	A	198	PRO	CB-CA-C	-6.15	102.11	110.60
1	A	190	SER	CB-CA-C	6.14	120.57	109.83
1	A	84	SER	CA-C-N	-6.08	111.30	121.39
1	A	84	SER	C-N-CA	-6.08	111.30	121.39
1	A	146	SER	CB-CA-C	-6.07	99.02	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLY	N-CA-C	-6.03	101.45	110.38
1	A	71	ASP	CA-CB-CG	-6.02	106.58	112.60
1	A	48	ASN	N-CA-CB	5.99	120.31	110.97
1	A	20	TYR	CA-C-O	-5.97	114.66	121.58
1	A	165	ASP	CB-CA-C	5.96	122.11	110.67
1	A	109	LYS	CB-CG-CD	-5.95	97.61	111.30
1	A	221	GLN	CA-C-N	5.94	129.15	120.71
1	A	221	GLN	C-N-CA	5.94	129.15	120.71
1	A	210	GLN	CA-C-N	-5.92	115.20	121.48
1	A	210	GLN	C-N-CA	-5.92	115.20	121.48
1	A	236	SER	CA-CB-OG	-5.76	99.58	111.10
1	A	128	CYS	N-CA-CB	-5.69	101.97	110.17
1	A	115	ASN	CA-C-O	5.69	126.77	120.80
1	A	199	VAL	CB-CA-C	5.64	117.44	110.73
1	A	117	ARG	CA-C-O	-5.64	113.14	119.79
1	A	129	ALA	O-C-N	-5.62	116.45	122.85
1	A	72	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	50	GLN	CB-CG-CD	5.60	122.12	112.60
1	A	48	ASN	CB-CG-ND2	5.59	124.79	116.40
1	A	97	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	54	SER	CA-C-N	-5.57	113.91	122.87
1	A	54	SER	C-N-CA	-5.57	113.91	122.87
1	A	125	THR	N-CA-C	-5.56	106.50	113.72
1	A	63	ILE	O-C-N	5.54	129.27	122.95
1	A	85	ALA	N-CA-C	-5.52	102.30	110.48
1	A	41	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	140	GLY	CA-C-O	-5.47	116.43	121.63
1	A	39	TYR	O-C-N	5.43	128.84	123.46
1	A	169	LYS	CA-CB-CG	-5.40	103.30	114.10
1	A	177	THR	CA-CB-OG1	-5.38	101.52	109.60
1	A	34	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	A	189	ASP	O-C-N	5.36	128.61	123.04
1	A	127	SER	CA-CB-OG	-5.35	100.40	111.10
1	A	65	VAL	CA-C-O	-5.35	114.39	120.65
1	A	33	LEU	CA-C-O	-5.33	114.62	120.43
1	A	124	PRO	CA-C-O	5.33	128.90	122.08
1	A	125	THR	CA-C-O	5.32	124.91	119.05
1	A	196	GLY	CA-C-O	-5.31	113.94	119.20
1	A	56	ALA	N-CA-CB	5.27	117.87	110.12
1	A	165	ASP	CB-CG-OD1	5.27	130.52	118.40
1	A	192	GLN	CA-C-N	-5.26	117.19	123.44
1	A	192	GLN	C-N-CA	-5.26	117.19	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	SER	O-C-N	5.23	129.94	123.14
1	A	122	SER	O-C-N	5.22	128.75	122.79
1	A	222	LYS	CA-C-N	5.21	130.74	122.61
1	A	222	LYS	C-N-CA	5.21	130.74	122.61
1	A	83	ILE	CA-C-O	-5.20	115.02	120.27
1	A	210	GLN	CB-CG-CD	5.18	121.40	112.60
1	A	101	ASN	O-C-N	5.17	128.78	122.58
1	A	47	ILE	CA-CB-CG2	5.14	119.24	110.50
1	A	93	SER	CA-CB-OG	-5.12	100.85	111.10
1	A	135	GLN	CA-C-O	-5.07	115.09	120.92
1	A	221(A)	ALA	CA-C-O	-5.06	115.67	121.54
1	A	195	SER	CA-C-O	-5.05	115.98	121.44
1	A	222	LYS	CA-C-O	-5.04	115.65	121.19
1	A	170	SER	CB-CA-C	5.03	120.82	110.31

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ALA	Mainchain
1	A	117	ARG	Sidechain,Mainchain
1	A	120	SER	Mainchain
1	A	129	ALA	Mainchain
1	A	135	GLN	Mainchain
1	A	155	LEU	Mainchain
1	A	186	GLU	Mainchain
1	A	193	GLY	Mainchain
1	A	195	SER	Mainchain
1	A	204	LYS	Mainchain
1	A	213	VAL	Mainchain
1	A	216	GLY	Mainchain
1	A	29	TYR	Sidechain
1	A	44	GLY	Mainchain
1	A	48	ASN	Mainchain
1	A	77	GLU	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	1629	0	1588	48	0
2	A	28	0	26	6	0
3	A	1	0	0	0	0
4	A	157	0	0	9	0
All	All	1815	0	1614	48	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 15.

All (48) 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)
1:A:195:SER:OG	2:A:246:OIV:C9	1.81	1.27
1:A:67:LEU:HG	4:A:471:HOH:O	1.33	1.23
1:A:117:ARG:N	1:A:117:ARG:HD2	1.59	1.11
1:A:186:GLU:HG3	4:A:598:HOH:O	1.56	1.04
1:A:81:GLN:HE22	1:A:113:SER:H	1.15	0.93
1:A:48:ASN:HD22	1:A:50:GLN:H	1.18	0.91
1:A:67:LEU:CG	4:A:471:HOH:O	1.99	0.89
1:A:67:LEU:CD1	4:A:471:HOH:O	2.24	0.84
1:A:31:VAL:HG12	1:A:67:LEU:HD23	1.67	0.76
1:A:117:ARG:N	1:A:117:ARG:CD	2.49	0.70
1:A:81:GLN:NE2	1:A:113:SER:H	1.89	0.68
1:A:195:SER:OG	2:A:246:OIV:CA2	2.44	0.65
1:A:195:SER:OG	2:A:246:OIV:O2	2.17	0.63
1:A:64:GLN:NE2	1:A:66:ARG:HE	1.97	0.62
1:A:48:ASN:ND2	1:A:50:GLN:H	1.94	0.62
1:A:117:ARG:HD2	1:A:117:ARG:H	1.58	0.61
1:A:224:LYS:CE	4:A:626:HOH:O	2.48	0.61
1:A:195:SER:CB	2:A:246:OIV:C9	2.79	0.60
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.49	0.58
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.36	0.58
1:A:59:TYR:CD1	1:A:59:TYR:C	2.82	0.58
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.51	0.58
1:A:186:GLU:OE2	4:A:612:HOH:O	2.18	0.55
1:A:224:LYS:HE3	4:A:626:HOH:O	2.06	0.55
1:A:27:VAL:HG13	1:A:29:TYR:CZ	2.42	0.54
1:A:81:GLN:HE22	1:A:113:SER:N	1.96	0.53
1:A:230:LYS:NZ	4:A:460:HOH:O	2.25	0.51
1:A:47:ILE:C	1:A:120:SER:HB2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD13	1:A:53:VAL:HG23	1.93	0.50
1:A:16:ILE:O	1:A:144:THR:HA	2.11	0.49
1:A:78:GLY:O	1:A:79:ASN:HB2	2.12	0.49
1:A:204:LYS:HD2	1:A:204:LYS:N	2.26	0.49
1:A:195:SER:CB	2:A:246:OIV:O2	2.62	0.48
1:A:56:ALA:HB1	1:A:90:VAL:HG13	1.97	0.47
1:A:47:ILE:HD13	1:A:53:VAL:CG2	2.45	0.46
1:A:85:ALA:HB1	1:A:106:ILE:HG23	1.98	0.46
1:A:216:GLY:O	2:A:246:OIV:N	2.48	0.45
1:A:48:ASN:HD21	1:A:51:TRP:HD1	1.62	0.45
1:A:87:LYS:NZ	1:A:245:ASN:OD1	2.50	0.45
1:A:115:ASN:OD1	1:A:117:ARG:HB2	2.16	0.45
1:A:46:LEU:HD21	1:A:114:LEU:HD11	1.98	0.44
1:A:101:ASN:ND2	1:A:234:TYR:OH	2.44	0.43
1:A:203:GLY:C	1:A:204:LYS:HD2	2.44	0.42
1:A:46:LEU:O	1:A:120:SER:HA	2.20	0.42
1:A:221:GLN:HG3	4:A:481:HOH:O	2.19	0.42
1:A:199:VAL:HG21	1:A:228:TYR:CD2	2.55	0.41
1:A:31:VAL:HG22	1:A:44:GLY:C	2.45	0.40
1:A:95:ASN:O	1:A:99:LEU:N	2.50	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	221/237 (93%)	212 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	184/194 (95%)	173 (94%)	11 (6%)	17 9

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	50	GLN
1	A	87	LYS
1	A	105	LEU
1	A	114	LEU
1	A	135	GLN
1	A	146	SER
1	A	149	THR
1	A	159	LYS
1	A	192	GLN
1	A	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	ASN
1	A	50	GLN
1	A	64	GLN
1	A	81	GLN
1	A	97	ASN
1	A	100	ASN
1	A	101	ASN
1	A	135	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	0IV	A	246	-	25,29,37	3.03	13 (52%)	32,39,51	3.00	15 (46%)

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
2	0IV	A	246	-	-	8/21/46/52	0/2/2/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	246	0IV	CB1-CA2	-7.39	1.44	1.53
2	A	246	0IV	O2-C9	5.52	1.40	1.20
2	A	246	0IV	C8-N2	4.92	1.44	1.34
2	A	246	0IV	CA2-N2	-4.01	1.40	1.46
2	A	246	0IV	CA-N	-3.94	1.42	1.47
2	A	246	0IV	CD1-NE	-3.55	1.42	1.46
2	A	246	0IV	CA-C7	3.39	1.57	1.52
2	A	246	0IV	C31-NE	3.15	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	246	0IV	CB1-CG1	-2.99	1.48	1.53
2	A	246	0IV	CZ-NH2	-2.93	1.27	1.34
2	A	246	0IV	C21-C11	-2.55	1.46	1.53
2	A	246	0IV	CA1-N1	2.22	1.48	1.45
2	A	246	0IV	CA1-C8	2.10	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	246	0IV	C8-CA1-N1	-7.88	93.04	113.22
2	A	246	0IV	CB1-CA2-C9	7.40	122.39	110.99
2	A	246	0IV	CA1-N1-C7	-5.31	114.90	119.77
2	A	246	0IV	O1-C8-N2	-4.71	114.97	122.95
2	A	246	0IV	C11-C21-C31	-3.94	105.58	110.75
2	A	246	0IV	O2-C9-CA2	-3.93	114.67	124.77
2	A	246	0IV	CB-CG-CD	3.62	115.50	110.75
2	A	246	0IV	O-C7-N1	3.35	126.44	122.53
2	A	246	0IV	O-C7-CA	-3.35	113.38	120.68
2	A	246	0IV	C7-CA-N	3.07	115.57	110.16
2	A	246	0IV	CG-CB-CA	2.82	114.68	110.97
2	A	246	0IV	C9-CA2-N2	2.79	114.87	109.50
2	A	246	0IV	CB1-CA2-N2	-2.67	106.66	110.69
2	A	246	0IV	CA1-C8-N2	-2.11	110.52	115.70
2	A	246	0IV	CG1-CD1-NE	-2.01	107.84	111.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

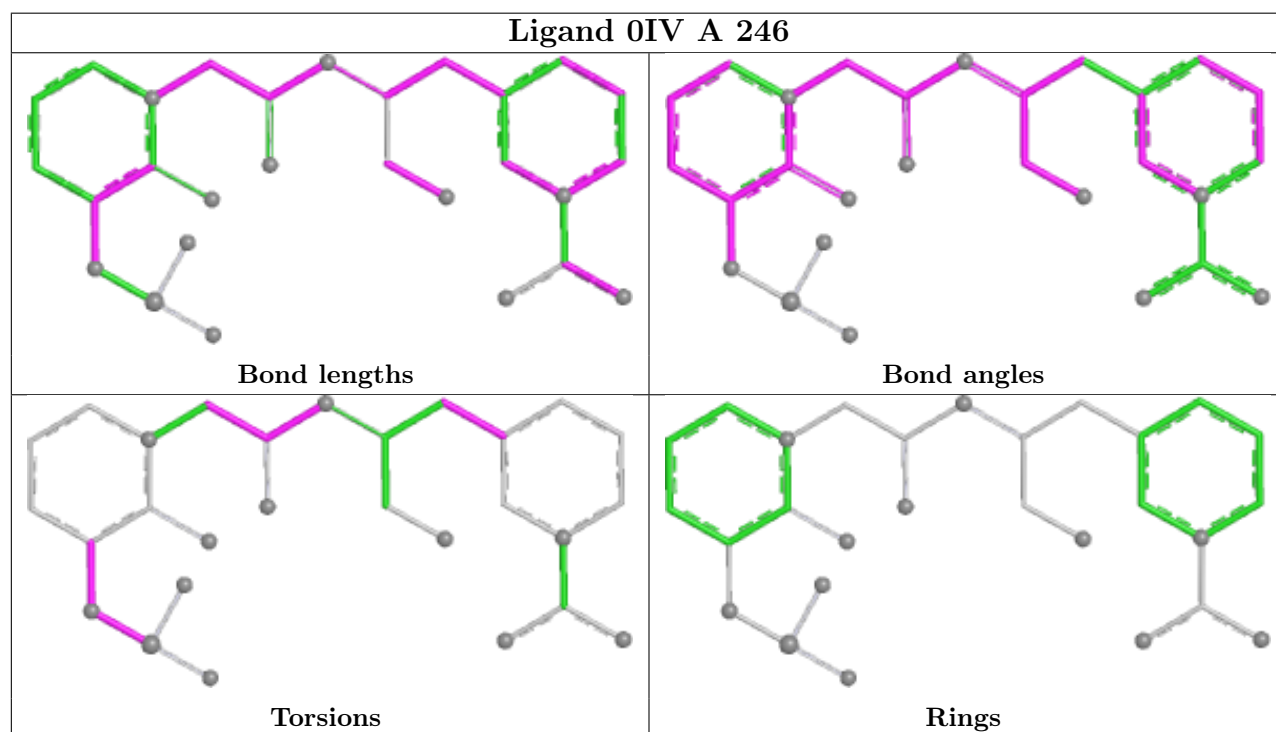
Mol	Chain	Res	Type	Atoms
2	A	246	0IV	CA-N-S-O1S
2	A	246	0IV	CA-N-S-O2S
2	A	246	0IV	CA2-CB1-CG1-C11
2	A	246	0IV	CA2-CB1-CG1-CD1
2	A	246	0IV	O1-C8-CA1-N1
2	A	246	0IV	CB-CA-N-S
2	A	246	0IV	CA1-C8-N2-CA2
2	A	246	0IV	C7-CA-N-S

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	246	OIV	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 [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.