



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 1GJ4 / pdb_00001gj4
Title : SELECTIVITY AT S1, H2O DISPLACEMENT, UPA, TPA, SER190/ALA190 PROTEASE, STRUCTURE-BASED DRUG DESIGN
Authors : Katz, B.A.; Sprengeler, P.A.; Luong, C.; Verner, E.; Spencer, J.R.; Breitenbucher, J.G.; Hui, H.; McGee, D.; Allen, D.; Martelli, A.; Mackman, R.L.
Deposited on : 2001-04-27
Resolution : 1.81 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

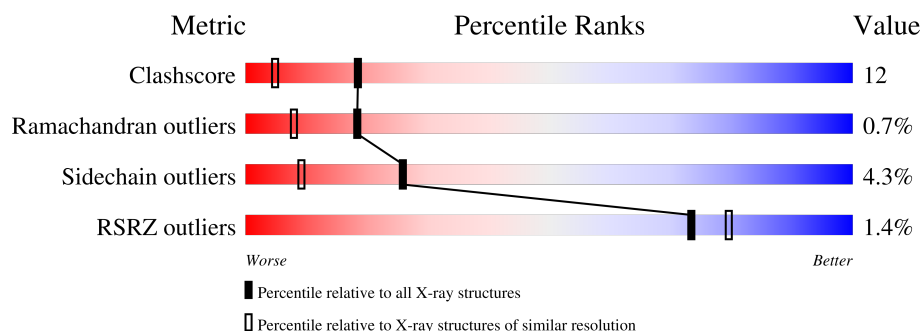
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	258	
3	I	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	132	H	410	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5591 atoms, of which 2910 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
1	L	28	Total	C	H	N	O	S	0	0	0
			460	145	229	37	48	1			

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	251	Total	C	H	N	O	S	0	4	0
			4087	1307	2039	362	363	16			

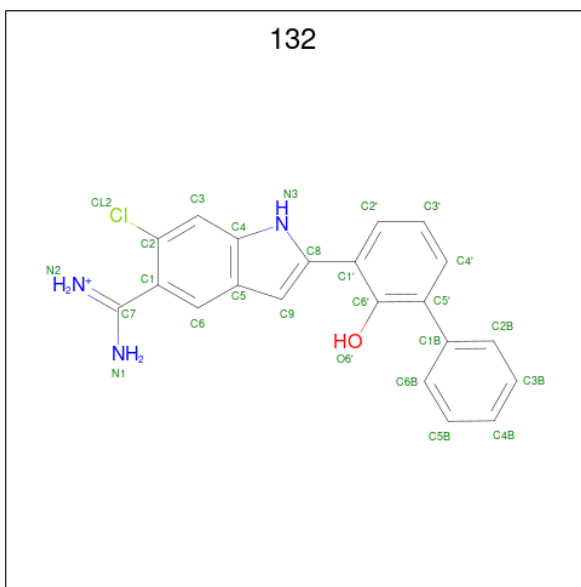
- Molecule 3 is a protein called ACETYL HIRUDIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	11	Total	C	H	N	O	S	0	0	0
			188	64	84	12	27	1			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is 6-CHLORO-2-(2-HYDROXY-BIPHENYL-3-YL)-1H-INDOLE-5-CARBOXYA MIDINE (CCD ID: 132) (formula: C₂₁H₁₇ClN₃O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	C	Cl	H	N	O	0	0
			42	21	1	16	3	1		

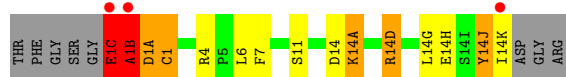
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	26	Total	H	O	0	0
			78	52	26		
6	H	223	Total	H	O	0	6
			675	450	225		
6	I	20	Total	H	O	0	0
			60	40	20		

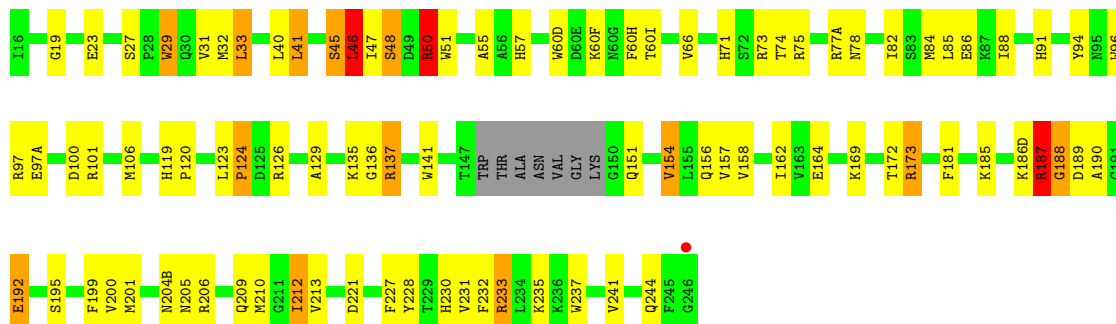
3 Residue-property plots [i](#)

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 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.

• Molecule 1: THROMBIN



• Molecule 2: THROMBIN



• Molecule 3: ACETYL HIRUDIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 72.09Å 72.84Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	7.00 – 1.81 7.00 – 1.81	Depositor EDS
% Data completeness (in resolution range)	59.1 (7.00-1.81) 57.9 (7.00-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.56Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.236 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYS, NA, 132

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	2.02	3/233 (1.3%)	1.85	6/310 (1.9%)
2	H	1.84	25/2117 (1.2%)	1.88	49/2856 (1.7%)
3	I	1.61	0/88	1.74	2/115 (1.7%)
All	All	1.85	28/2438 (1.1%)	1.87	57/3281 (1.7%)

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	L	0	1
2	H	0	8
All	All	0	9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	119	HIS	CG-ND1	-9.32	1.27	1.38
1	L	14(J)	TYR	CA-CB	9.31	1.65	1.52
2	H	230	HIS	CG-ND1	-8.96	1.28	1.38
2	H	27	SER	CA-CB	8.39	1.62	1.53
2	H	71	HIS	CG-ND1	-8.17	1.29	1.38
2	H	91	HIS	CD2-NE2	-7.04	1.30	1.37
2	H	57	HIS	CG-ND1	-6.91	1.30	1.38
2	H	91	HIS	CG-ND1	-6.69	1.30	1.38
2	H	237	TRP	NE1-CE2	-6.04	1.30	1.37
2	H	119	HIS	CD2-NE2	-6.00	1.31	1.37
1	L	1(B)	ALA	C-O	-5.98	1.16	1.24
2	H	231	VAL	CA-CB	5.88	1.60	1.54
2	H	29	TRP	NE1-CE2	-5.87	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	230	HIS	CD2-NE2	-5.75	1.31	1.37
2	H	96	TRP	NE1-CE2	-5.59	1.31	1.37
2	H	230	HIS	CA-CB	-5.46	1.45	1.52
2	H	60(D)	TRP	NE1-CE2	-5.43	1.31	1.37
1	L	1(B)	ALA	CA-C	-5.34	1.45	1.52
2	H	212	ILE	CA-CB	-5.29	1.47	1.55
2	H	156	GLN	N-CA	5.23	1.52	1.45
2	H	47	ILE	N-CA	5.19	1.51	1.46
2	H	192	GLU	CD-OE2	-5.17	1.15	1.25
2	H	71	HIS	CD2-NE2	-5.15	1.32	1.37
2	H	51	TRP	NE1-CE2	-5.15	1.31	1.37
2	H	57	HIS	CD2-NE2	-5.12	1.32	1.37
2	H	141	TRP	NE1-CE2	-5.10	1.31	1.37
2	H	75	ARG	CA-C	-5.09	1.46	1.52
2	H	55	ALA	CA-CB	-5.07	1.45	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	232	PHE	CA-CB-CG	-10.38	103.42	113.80
2	H	244	GLN	N-CA-C	-9.30	101.71	113.43
2	H	119	HIS	CA-CB-CG	-8.93	104.87	113.80
1	L	1(C)	GLU	CA-C-O	-8.83	105.79	120.80
3	I	56	PHE	CA-CB-CG	-8.56	105.23	113.80
1	L	14(J)	TYR	N-CA-C	8.48	124.02	111.81
1	L	14(A)	LYS	N-CA-C	8.42	122.65	112.38
2	H	151	GLN	N-CA-C	-8.12	96.34	109.58
2	H	181	PHE	CA-CB-CG	8.03	121.83	113.80
2	H	199	PHE	N-CA-C	-7.98	95.40	108.41
2	H	181	PHE	N-CA-C	-7.71	97.59	109.24
2	H	227	PHE	CA-CB-CG	-7.69	106.11	113.80
2	H	190	ALA	N-CA-C	-7.66	98.49	110.36
2	H	119	HIS	CE1-NE2-CD2	-7.61	101.39	109.00
2	H	230	HIS	CE1-NE2-CD2	-7.50	101.50	109.00
2	H	173	ARG	N-CA-C	-7.46	103.77	113.17
2	H	154	VAL	N-CA-CB	-7.17	100.43	112.47
2	H	33	LEU	N-CA-C	-6.96	97.38	108.73
2	H	71	HIS	CE1-NE2-CD2	-6.87	102.13	109.00
2	H	94	TYR	N-CA-C	-6.87	99.87	110.10
2	H	123	LEU	N-CA-C	-6.86	101.47	110.39
2	H	205	ASN	CA-CB-CG	-6.54	106.06	112.60
2	H	205	ASN	N-CA-C	6.17	120.11	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60(I)	THR	CA-CB-OG1	-6.14	100.39	109.60
2	H	86	GLU	N-CA-C	-6.14	104.52	112.68
2	H	84[A]	MET	N-CA-C	-6.03	101.27	110.14
2	H	84[B]	MET	N-CA-C	-6.03	101.27	110.14
2	H	173	ARG	CB-CA-C	-5.97	100.11	110.09
1	L	14	ASP	N-CA-C	-5.90	101.27	110.42
2	H	91	HIS	ND1-CG-CD2	5.90	112.00	106.10
2	H	74	THR	N-CA-C	5.83	120.52	113.17
2	H	48	SER	N-CA-C	-5.76	101.19	108.45
2	H	45	SER	CA-CB-OG	-5.71	99.68	111.10
1	L	4	ARG	N-CA-C	5.60	116.71	109.65
2	H	82	ILE	N-CA-CB	-5.59	103.70	111.41
2	H	158	VAL	N-CA-C	-5.59	100.43	108.42
2	H	97(A)	GLU	N-CA-C	5.58	119.65	111.34
2	H	19	GLY	N-CA-C	-5.57	101.96	112.10
2	H	188	GLY	CA-C-O	-5.56	116.77	121.66
2	H	162	ILE	N-CA-C	-5.54	101.67	109.21
2	H	23	GLU	N-CA-C	-5.52	101.58	110.14
3	I	57	GLU	N-CA-C	-5.49	101.59	110.32
1	L	7	PHE	CA-CB-CG	-5.42	108.38	113.80
2	H	186(D)	LYS	N-CA-C	-5.41	100.49	108.99
2	H	199	PHE	CA-CB-CG	-5.37	108.43	113.80
2	H	60(I)	THR	N-CA-CB	-5.36	102.23	111.55
2	H	124	PRO	CA-C-O	-5.34	115.10	122.15
2	H	230	HIS	ND1-CE1-NE2	5.30	113.70	108.40
2	H	71	HIS	CA-CB-CG	-5.30	108.50	113.80
2	H	185	LYS	N-CA-C	-5.26	102.56	110.24
2	H	136	GLY	N-CA-C	-5.24	103.44	111.10
2	H	50	ARG	CB-CA-C	-5.19	100.95	109.99
2	H	88	ILE	N-CA-C	-5.15	101.06	108.48
2	H	74	THR	CA-CB-OG1	-5.14	101.89	109.60
2	H	71	HIS	CG-CD2-NE2	5.10	112.30	107.20
2	H	100	ASP	N-CA-C	-5.09	102.16	110.20
2	H	46	LEU	N-CA-CB	-5.05	102.19	110.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	101	ARG	Sidechain
2	H	137	ARG	Sidechain
2	H	173	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	187	ARG	Sidechain
2	H	233	ARG	Sidechain
2	H	50	ARG	Sidechain
2	H	73	ARG	Sidechain
2	H	97	ARG	Sidechain
1	L	14(D)	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	L	231	229	231	15	0
2	H	2048	2039	2028	44	2
3	I	104	84	81	1	0
4	H	1	0	0	0	0
5	H	26	16	17	13	0
6	H	225	450	0	6	9
6	I	20	40	0	0	0
6	L	26	52	0	2	1
All	All	2681	2910	2357	57	9

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 12.

All (57) 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:H:77(A):ARG:O	6:H:413:HOH:O	1.70	1.08
2:H:33:LEU:HD21	2:H:106[B]:MET:HE1	1.47	0.97
2:H:60(F):LYS:HE2	5:H:410:132:H4'	1.50	0.92
2:H:60(F):LYS:HE2	5:H:410:132:C4B	2.01	0.89
2:H:60(F):LYS:CE	5:H:410:132:H4'	2.15	0.75
2:H:60(F):LYS:HE2	5:H:410:132:C5B	2.17	0.74
2:H:195:SER:OG	6:H:588:HOH:O	2.07	0.71
2:H:124:PRO:O	2:H:235:LYS:NZ	2.24	0.70
2:H:195:SER:OG	5:H:410:132:O6'	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:LEU:CD2	2:H:106[B]:MET:HE1	2.22	0.66
2:H:60(F):LYS:CE	5:H:410:132:C4B	2.74	0.65
1:L:14(D):ARG:HD2	6:L:560:HOH:O	1.98	0.64
1:L:1(C):GLU:OE2	2:H:120:PRO:HG3	1.98	0.62
3:I:58:GLU:H	3:I:58:GLU:CD	2.07	0.61
2:H:195:SER:CB	6:H:588:HOH:O	2.48	0.60
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.09	0.59
1:L:14(J):TYR:O	1:L:14(K):ILE:HG23	2.01	0.59
2:H:41:LEU:HD21	2:H:60(H):PHE:CE2	2.38	0.58
2:H:60(F):LYS:HE2	5:H:410:132:H5'	1.86	0.57
1:L:14(J):TYR:O	1:L:14(K):ILE:HG12	2.05	0.55
1:L:14(D):ARG:HB2	6:L:474:HOH:O	2.06	0.55
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.37	0.54
2:H:192:GLU:HG3	5:H:410:132:C2'	2.38	0.53
2:H:129:ALA:HA	2:H:210:MET:HE1	1.91	0.52
2:H:77(A):ARG:N	6:H:413:HOH:O	2.42	0.52
1:L:1(C):GLU:OE2	2:H:120:PRO:CG	2.57	0.52
1:L:1(C):GLU:O	1:L:1(A):ASP:N	2.41	0.50
1:L:1(C):GLU:OE1	1:L:1:CYS:N	2.44	0.50
2:H:60(F):LYS:NZ	5:H:410:132:H4'	2.26	0.50
2:H:233:ARG:NH2	6:H:500:HOH:O	2.45	0.50
2:H:60(F):LYS:NZ	5:H:410:132:C4B	2.75	0.49
2:H:200:VAL:HG12	2:H:209:GLN:HA	1.95	0.49
2:H:46:LEU:HD22	2:H:48:SER:O	2.12	0.48
1:L:1(B):ALA:C	2:H:206:ARG:HH12	2.21	0.48
1:L:14(G):LEU:N	1:L:14(G):LEU:CD2	2.80	0.45
2:H:29:TRP:O	2:H:45:SER:HA	2.17	0.45
2:H:85:LEU:HD13	2:H:106[A]:MET:HE2	2.00	0.44
1:L:1(B):ALA:O	2:H:206:ARG:NH1	2.49	0.43
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.73	0.43
2:H:195:SER:HB2	6:H:588:HOH:O	2.17	0.43
1:L:14(A):LYS:HB2	1:L:14(A):LYS:NZ	2.33	0.43
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.92	0.43
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.19	0.43
2:H:32:MET:HG3	2:H:40:LEU:HD13	2.00	0.43
1:L:14(J):TYR:C	1:L:14(K):ILE:HG12	2.45	0.42
1:L:14(D):ARG:HG2	1:L:14(H):GLU:CD	2.44	0.42
2:H:228:TYR:CD1	2:H:228:TYR:N	2.88	0.42
2:H:188:GLY:O	2:H:189:ASP:HB2	2.20	0.41
2:H:164:GLU:H	2:H:164:GLU:CD	2.29	0.41
2:H:135:LYS:O	2:H:201:MET:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:ARG:HG3	2:H:157:VAL:HG23	2.01	0.41
2:H:213:VAL:HG13	5:H:410:132:CL2	2.57	0.41
2:H:192:GLU:CG	5:H:410:132:C2'	2.99	0.41
2:H:212:ILE:O	2:H:228:TYR:HA	2.21	0.41
2:H:31:VAL:HG11	2:H:66:VAL:HG13	2.03	0.41
2:H:187:ARG:NH2	2:H:221:ASP:O	2.55	0.40
5:H:410:132:CL2	5:H:410:132:N2	2.72	0.40

All (9) 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	Interatomic distance (Å)	Clash overlap (Å)
6:H:414:HOH:H2	6:H:414:HOH:H2[2_555]	0.38	1.22
6:H:414:HOH:O	6:H:414:HOH:H2[2_555]	0.82	0.78
6:H:414:HOH:O	6:H:414:HOH:O[2_555]	1.64	0.56
6:H:413:HOH:H1	6:H:413:HOH:H2[2_555]	1.07	0.53
2:H:169:LYS:HE2	6:H:559:HOH:H1[2_656]	1.19	0.41
6:H:413:HOH:H1	6:H:413:HOH:H1[2_555]	1.27	0.33
2:H:172:THR:O	6:H:555:HOH:H2[4_546]	1.52	0.08
6:L:743:HOH:O	6:H:548:HOH:H1[3_455]	1.53	0.07
6:H:413:HOH:O	6:H:413:HOH:H1[2_555]	1.55	0.05

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	26/36 (72%)	24 (92%)	1 (4%)	1 (4%)	2	0
2	H	251/258 (97%)	227 (90%)	22 (9%)	2 (1%)	16	6
3	I	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	285/305 (93%)	257 (90%)	25 (9%)	3 (1%)	18	4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA
2	H	126[A]	ARG
2	H	126[B]	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	26/31 (84%)	21 (81%)	5 (19%)	1	0
2	H	223/224 (100%)	217 (97%)	6 (3%)	39	22
3	I	10/10 (100%)	10 (100%)	0	100	100
All	All	259/265 (98%)	248 (96%)	11 (4%)	26	10

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

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	1	CYS
1	L	6	LEU
1	L	11	SER
2	H	41	LEU
2	H	46	LEU
2	H	50	ARG
2	H	154	VAL
2	H	187	ARG
2	H	241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	204(B)	ASN

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Mol	Chain	Res	Type
3	I	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYS	I	63	3	15,16,17	2.23	2 (13%)	15,22,24	1.18	2 (13%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-S	-7.29	1.44	1.58
3	I	63	TYS	OH-CZ	-3.14	1.37	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	O2-S-O1	-2.83	101.31	112.24
3	I	63	TYS	OH-S-O1	2.40	114.87	107.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
5	132	H	410	-	29,29,29	2.71	12 (41%)	40,42,42	1.63	7 (17%)

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	132	H	410	-	-	3/11/12/12	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	410	132	C8-N3	-6.18	1.31	1.38
5	H	410	132	C5'-C1B	-5.68	1.39	1.49
5	H	410	132	C1-C7	-5.49	1.39	1.48
5	H	410	132	C4B-C3B	-4.41	1.28	1.38
5	H	410	132	C1'-C8	-3.90	1.40	1.47
5	H	410	132	C4-N3	-3.57	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	410	132	C5-C4	-3.33	1.35	1.41
5	H	410	132	C5B-C4B	3.23	1.45	1.38
5	H	410	132	C2-CL2	2.59	1.79	1.73
5	H	410	132	C5-C9	-2.56	1.36	1.44
5	H	410	132	C6-C5	-2.30	1.36	1.40
5	H	410	132	C1-C2	2.23	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	410	132	C6-C5-C4	5.42	122.48	119.13
5	H	410	132	C3-C2-C1	-3.76	118.51	121.59
5	H	410	132	C5B-C4B-C3B	3.32	124.41	119.87
5	H	410	132	C4B-C5B-C6B	-3.07	116.45	120.24
5	H	410	132	C4'-C5'-C6'	2.41	120.57	117.95
5	H	410	132	C3-C4-C5	-2.09	120.53	122.59
5	H	410	132	C5-C9-C8	-2.06	105.61	107.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	410	132	C6-C1-C7-N1
5	H	410	132	C2-C1-C7-N1
5	H	410	132	C6-C1-C7-N2

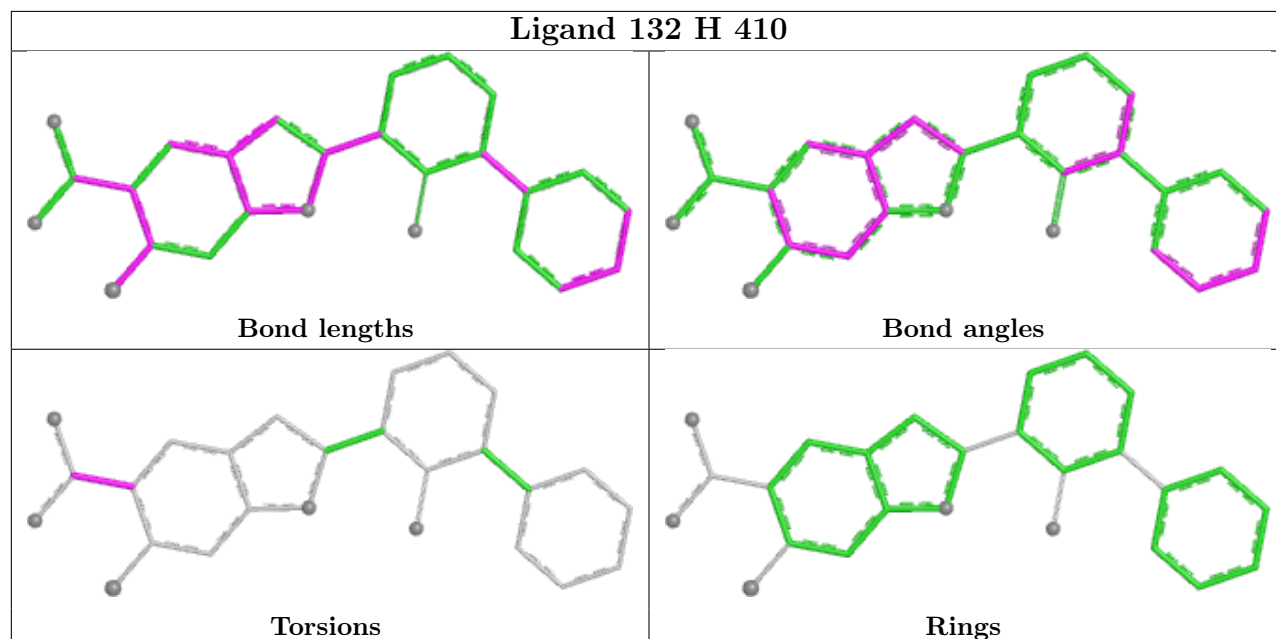
There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	410	132	13	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	28/36 (77%)	-0.25	3 (10%) 11 12	10, 21, 32, 45	5 (17%)
2	H	251/258 (97%)	-0.65	1 (0%) 88 91	4, 23, 42, 54	26 (10%)
3	I	10/11 (90%)	0.56	0 100 100	13, 36, 49, 51	4 (40%)
All	All	289/305 (94%)	-0.56	4 (1%) 73 79	4, 23, 43, 54	35 (12%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	14(K)	ILE	4.3
1	L	1(C)	GLU	3.9
2	H	246	GLY	3.7
1	L	1(B)	ALA	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYS	I	63	16/17	0.96	0.06	27,38,50,52	0

6.3 Carbohydrates

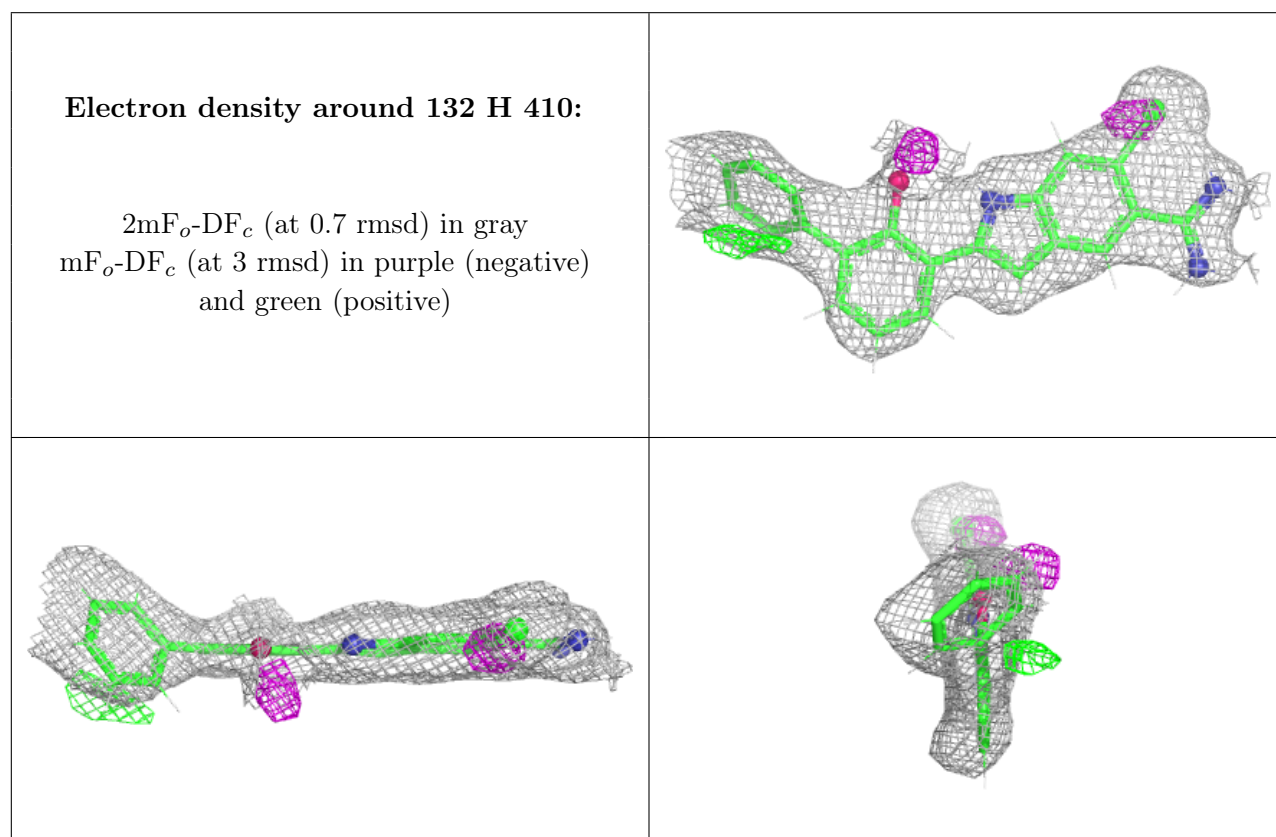
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	132	H	410	26/26	0.88	0.07	17,29,36,37	42
4	NA	H	409	1/1	0.91	0.05	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.