



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:00 PM UTC

PDB ID : 1A4W / pdb_00001a4w
Title : CRYSTAL STRUCTURES OF THROMBIN WITH THIAZOLE-CONTAINING INHIBITORS: PROBES OF THE S1' BINDING SITE
Authors : Matthews, J.H.; Krishnan, R.; Costanzo, M.J.; Maryanoff, B.E.; Tulinsky, A.
Deposited on : 1998-02-06
Resolution : 1.80 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

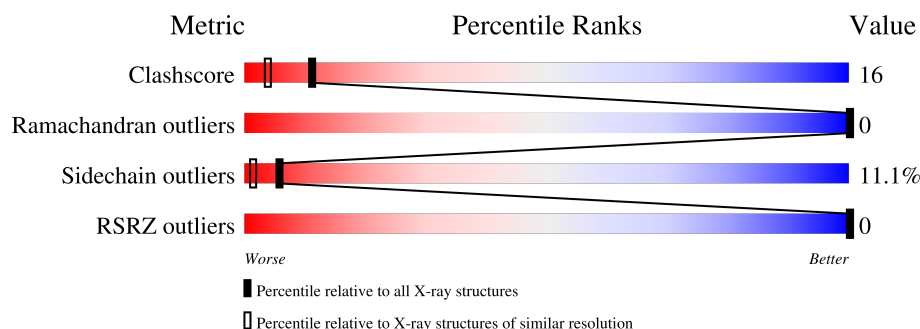
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	259	
3	I	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2439 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	26	Total	C	N	O	S	0	0	0
			203	127	31	44	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	248	Total	C	N	O	S	0	0	0
			1966	1255	345	352	14			

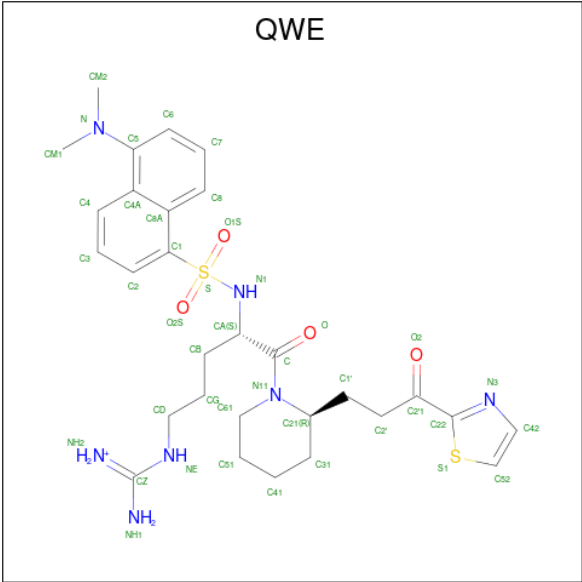
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			69	44	9	15	1			

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

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

- Molecule 5 is amino{[(4S)-4-({[5-(dimethylamino)naphthalen-1-yl]sulfonyl}amino)-5-oxo-5-{{(2R)-2-[3-oxo-3-(1,3-thiazol-2-yl)propyl]pip eridin-1-yl}pentyl]amino}methaniminium (CCD ID: QWE) (formula: C₂₉H₄₀N₇O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	S	0	0
			42	29	7	4	2		

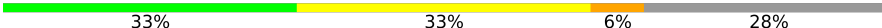
- Molecule 6 is water.

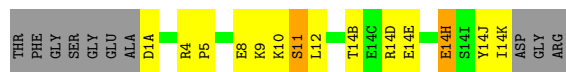
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	13	Total	O	0	0
			13	13		
6	H	138	Total	O	0	0
			138	138		
6	I	6	Total	O	0	0
			6	6		

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 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.

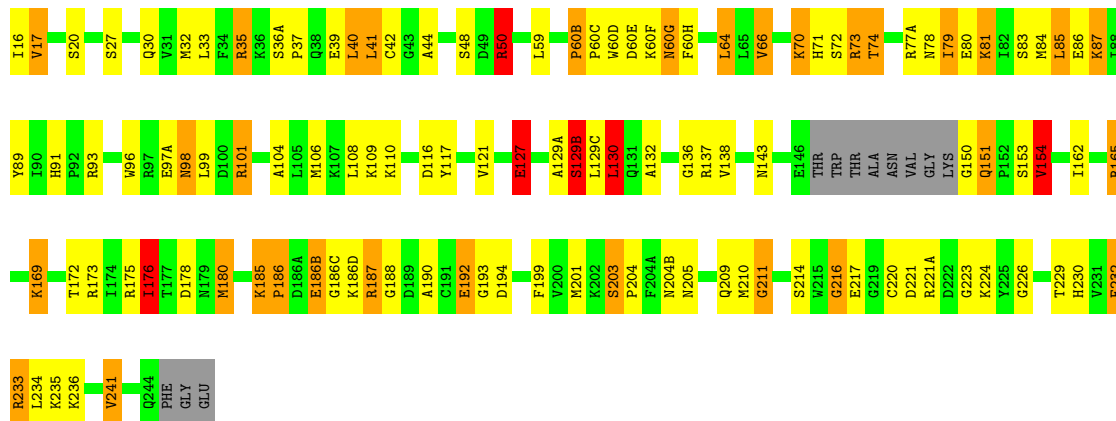
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



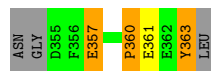
• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRUGEN

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.47Å 72.00Å 73.39Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	7.00 – 1.80 7.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	65.0 (7.00-1.80) 58.7 (7.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.155 , (Not available) 0.149 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.2	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2439	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: QWE, NA, 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	L	1.24	0/205	2.30	11/274 (4.0%)
2	H	1.30	1/2017 (0.0%)	2.16	84/2728 (3.1%)
3	I	0.82	0/54	2.27	2/72 (2.8%)
All	All	1.29	1/2276 (0.0%)	2.18	97/3074 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	GLY	N-CA	7.73	1.52	1.45

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	CD-NE-CZ	14.11	144.16	124.40
2	H	74	THR	N-CA-CB	-12.97	92.64	110.67
2	H	138	VAL	O-C-N	10.49	134.51	123.18
1	L	1(A)	ASP	CA-CB-CG	-10.12	102.48	112.60
2	H	74	THR	OG1-CB-CG2	9.80	128.90	109.30
1	L	11	SER	N-CA-CB	9.59	126.60	112.13
2	H	233	ARG	NE-CZ-NH2	-9.23	110.89	119.20
2	H	110	LYS	O-C-N	8.96	128.24	121.88
2	H	165	ARG	CD-NE-CZ	8.86	136.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60(F)	LYS	CA-CB-CG	8.58	131.26	114.10
2	H	221(A)	ARG	CA-C-O	-8.55	111.30	121.05
2	H	165	ARG	NE-CZ-NH1	8.49	129.99	121.50
2	H	193	GLY	N-CA-C	-8.33	104.77	114.69
2	H	101	ARG	NE-CZ-NH2	-8.24	111.78	119.20
2	H	35	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	L	11	SER	CA-C-O	-7.91	111.86	121.28
2	H	27	SER	CA-C-O	7.73	129.79	121.28
2	H	17	VAL	CA-C-O	7.71	128.81	120.57
2	H	30	GLN	OE1-CD-NE2	7.66	130.26	122.60
2	H	186(B)	GLU	N-CA-C	7.59	120.44	111.71
2	H	241	VAL	CA-CB-CG1	7.57	123.27	110.40
2	H	27	SER	O-C-N	-7.40	115.23	121.23
1	L	4	ARG	NE-CZ-NH2	7.31	125.78	119.20
2	H	154	VAL	N-CA-CB	-7.16	100.41	112.44
2	H	93	ARG	NE-CZ-NH1	7.16	128.66	121.50
2	H	132	ALA	CA-C-O	-7.12	113.32	121.15
2	H	42	CYS	O-C-N	7.00	129.84	123.26
2	H	154	VAL	CA-CB-CG1	6.80	121.96	110.40
2	H	79	ILE	O-C-N	6.70	126.94	121.85
2	H	232	PHE	CA-CB-CG	-6.66	107.14	113.80
2	H	60(B)	PRO	N-CA-C	6.61	118.76	110.70
1	L	8	GLU	O-C-N	6.50	129.01	122.12
2	H	180	MET	CA-C-O	-6.48	113.54	121.06
2	H	35	ARG	NH1-CZ-NH2	6.46	127.70	119.30
2	H	176	ILE	CB-CA-C	6.44	120.03	111.21
2	H	35	ARG	CD-NE-CZ	-6.37	115.48	124.40
2	H	60(H)	PHE	CA-CB-CG	-6.35	107.45	113.80
2	H	60(B)	PRO	CB-CA-C	6.32	118.62	110.92
2	H	138	VAL	CA-C-O	-6.24	113.37	120.67
2	H	186(B)	GLU	CG-CD-OE1	6.21	132.69	118.40
3	I	360	PRO	CA-C-O	6.21	128.42	121.34
2	H	70	LYS	N-CA-C	6.21	118.93	110.55
2	H	216	GLY	O-C-N	6.20	129.32	123.56
2	H	129(A)	ALA	CA-C-O	6.18	127.51	120.90
1	L	14(B)	THR	CA-C-O	-6.17	112.05	119.03
2	H	73	ARG	CA-C-O	6.14	126.93	120.42
2	H	127	GLU	CB-CG-CD	6.05	122.88	112.60
2	H	193	GLY	CA-C-O	-6.01	112.84	119.27
2	H	101	ARG	NE-CZ-NH1	6.01	127.51	121.50
2	H	121	VAL	CA-C-O	-5.97	114.45	121.80
2	H	130	LEU	CA-C-N	5.96	132.39	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	130	LEU	C-N-CA	5.96	132.39	122.73
2	H	129(B)	SER	N-CA-C	5.93	117.74	111.28
2	H	143	ASN	OD1-CG-ND2	5.92	128.52	122.60
2	H	220	CYS	CA-C-O	-5.89	113.01	120.20
2	H	44	ALA	CA-C-O	-5.88	114.84	121.25
1	L	14(K)	ILE	CA-C-O	-5.85	110.86	120.80
2	H	129(B)	SER	N-CA-CB	-5.82	101.57	110.12
2	H	241	VAL	N-CA-CB	5.80	119.29	110.58
2	H	39	GLU	O-C-N	5.79	129.70	123.56
2	H	117	TYR	O-C-N	5.76	129.43	122.35
2	H	153	SER	O-C-N	5.65	130.06	122.49
2	H	66	VAL	N-CA-CB	-5.63	104.62	111.21
2	H	173	ARG	N-CA-C	-5.60	106.50	113.38
2	H	186	PRO	CB-CA-C	5.59	120.93	112.21
2	H	85	LEU	O-C-N	5.58	129.72	123.19
2	H	235	LYS	CA-CB-CG	5.47	125.04	114.10
2	H	17	VAL	O-C-N	-5.47	116.96	123.03
2	H	50	ARG	N-CA-CB	-5.46	102.66	110.80
2	H	70	LYS	CA-C-O	5.46	128.26	121.81
2	H	205	ASN	OD1-CG-ND2	-5.46	117.14	122.60
2	H	172	THR	CA-C-O	-5.45	115.62	121.45
2	H	203	SER	O-C-N	5.43	126.72	121.28
2	H	226	GLY	O-C-N	5.42	128.49	122.96
2	H	185	LYS	CA-CB-CG	-5.39	103.31	114.10
2	H	192	GLU	CA-C-O	-5.39	115.26	121.19
2	H	116	ASP	CA-C-O	-5.32	112.84	119.38
2	H	234	LEU	CA-C-N	5.31	127.93	120.28
2	H	234	LEU	C-N-CA	5.31	127.93	120.28
1	L	9	LYS	CA-C-O	-5.31	112.14	119.05
2	H	74	THR	N-CA-C	5.30	120.75	113.97
2	H	173	ARG	CA-C-O	-5.28	113.13	119.15
2	H	27	SER	CB-CA-C	5.25	118.98	111.27
1	L	14(J)	TYR	CA-C-O	-5.25	116.34	122.37
1	L	14(E)	GLU	CB-CG-CD	5.24	121.50	112.60
2	H	190	ALA	N-CA-C	-5.23	103.78	110.53
2	H	104	ALA	CA-C-O	-5.21	115.16	120.99
2	H	209	GLN	CA-C-O	-5.20	115.51	120.92
2	H	96	TRP	O-C-N	5.20	129.63	122.46
3	I	357	GLU	CA-CB-CG	5.19	124.48	114.10
2	H	187	ARG	CD-NE-CZ	-5.15	117.19	124.40
2	H	143	ASN	CB-CG-ND2	-5.12	108.73	116.40
2	H	214	SER	O-C-N	-5.11	116.11	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	137	ARG	NE-CZ-NH1	5.11	126.61	121.50
2	H	44	ALA	O-C-N	5.09	128.34	123.04
1	L	14(H)	GLU	CA-C-O	-5.03	112.52	119.05
2	H	60(G)	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	151	GLN	Mainchain
2	H	20	SER	Mainchain
2	H	232	PHE	Sidechain
2	H	73	ARG	Sidechain

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	L	203	0	188	3	0
2	H	1966	0	1913	65	0
3	I	69	0	47	3	0
4	H	2	0	0	0	0
5	H	42	0	40	4	0
6	H	138	0	0	8	0
6	I	6	0	0	1	0
6	L	13	0	0	1	0
All	All	2439	0	2188	73	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 16.

All (73) 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:50:ARG:NH1	2:H:108:LEU:O	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:LEU:HD11	2:H:106:MET:HE1	1.54	0.88
2:H:186(C):GLY:O	2:H:186(D):LYS:HG3	1.78	0.82
2:H:60(E):ASP:OD2	6:H:513:HOH:O	2.04	0.75
2:H:169:LYS:HE3	6:H:412:HOH:O	1.92	0.69
2:H:97(A):GLU:OE1	6:H:493:HOH:O	2.10	0.68
2:H:204:PRO:O	6:H:517:HOH:O	2.12	0.67
2:H:98:ASN:H	2:H:98:ASN:HD22	1.43	0.67
2:H:80:GLU:O	2:H:81:LYS:HD3	1.96	0.66
2:H:175:ARG:NH1	6:H:519:HOH:O	2.10	0.65
2:H:186(C):GLY:O	2:H:186(D):LYS:CG	2.43	0.65
2:H:84:MET:HE3	2:H:109:LYS:HD3	1.80	0.64
3:I:360:PRO:HG2	3:I:363:TYS:HE2	1.80	0.63
2:H:17:VAL:O	2:H:188:GLY:HA2	1.99	0.62
2:H:178:ASP:O	2:H:233:ARG:HD2	1.98	0.62
2:H:165:ARG:NH2	2:H:180:MET:O	2.33	0.62
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.82	0.61
2:H:127:GLU:O	2:H:129(B):SER:HB2	2.02	0.60
2:H:87:LYS:HG3	2:H:89:TYR:OH	2.02	0.60
2:H:169:LYS:CE	6:H:412:HOH:O	2.50	0.59
2:H:70:LYS:HE3	2:H:72:SER:O	2.03	0.58
2:H:41:LEU:HD23	2:H:64:LEU:CD2	2.36	0.55
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	2.07	0.55
2:H:98:ASN:HD22	2:H:98:ASN:N	2.01	0.54
2:H:130:LEU:HD23	2:H:162:ILE:CD1	2.38	0.54
2:H:130:LEU:CD2	2:H:162:ILE:HD13	2.38	0.53
2:H:169:LYS:HG2	2:H:176:ILE:HG12	1.91	0.53
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.91	0.52
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.09	0.52
2:H:185:LYS:O	2:H:186(B):GLU:HB2	2.10	0.51
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.17	0.51
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.46	0.50
2:H:98:ASN:N	2:H:98:ASN:ND2	2.59	0.50
2:H:187:ARG:NH2	2:H:221:ASP:O	2.42	0.50
2:H:98:ASN:H	2:H:98:ASN:ND2	2.08	0.49
2:H:60(G):ASN:ND2	6:H:424:HOH:O	2.28	0.49
2:H:127:GLU:HG2	6:H:487:HOH:O	2.13	0.49
2:H:230:HIS:CG	2:H:233:ARG:HG3	2.48	0.48
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.44	0.48
2:H:150:GLY:C	2:H:151:GLN:HG2	2.39	0.48
2:H:35:ARG:HB2	2:H:41:LEU:CD1	2.44	0.47
1:L:12:LEU:HB3	6:L:473:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:GLU:OE1	2:H:224:LYS:NZ	2.42	0.46
2:H:41:LEU:HD23	2:H:64:LEU:HD22	1.98	0.46
2:H:150:GLY:O	2:H:151:GLN:HG2	2.15	0.46
2:H:16:ILE:N	2:H:194:ASP:OD2	2.48	0.45
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.28	0.45
2:H:169:LYS:HG2	2:H:176:ILE:CG1	2.47	0.45
2:H:36(A):SER:HA	2:H:37:PRO:C	2.42	0.45
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.97	0.45
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.31	0.45
2:H:87:LYS:HG3	2:H:89:TYR:HH	1.82	0.45
5:H:373:QWE:HM13	5:H:373:QWE:H4	1.98	0.44
2:H:80:GLU:C	2:H:81:LYS:HD3	2.42	0.44
5:H:373:QWE:H21	5:H:373:QWE:HA	1.78	0.44
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.81	0.43
2:H:60(D):TRP:HZ3	5:H:373:QWE:C52	2.32	0.43
2:H:186:PRO:HG3	2:H:223:GLY:H	1.82	0.43
1:L:5:PRO:O	1:L:10:LYS:HD2	2.19	0.43
2:H:216:GLY:O	5:H:373:QWE:N1	2.49	0.43
2:H:70:LYS:CE	2:H:72:SER:O	2.67	0.42
2:H:150:GLY:C	2:H:151:GLN:CG	2.91	0.42
3:I:363:TYS:C	6:I:435:HOH:O	2.65	0.42
3:I:361:GLU:C	3:I:363:TYS:N	2.75	0.42
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.55	0.42
2:H:230:HIS:ND1	2:H:233:ARG:HG3	2.35	0.42
2:H:186:PRO:HG3	2:H:223:GLY:N	2.34	0.41
2:H:211:GLY:HA2	2:H:229:THR:O	2.20	0.41
2:H:50:ARG:CZ	2:H:108:LEU:O	2.62	0.41
2:H:165:ARG:NH1	2:H:176:ILE:HD12	2.35	0.41
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.80	0.40
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.57	0.40
2:H:201:MET:SD	2:H:210:MET:HG3	2.61	0.40

There are no symmetry-related clashes.

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	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
2	H	244/259 (94%)	233 (96%)	11 (4%)	0	100	100
3	I	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	275/307 (90%)	262 (95%)	13 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	22/31 (71%)	21 (96%)	1 (4%)	24	12
2	H	208/225 (92%)	184 (88%)	24 (12%)	5	1
3	I	4/10 (40%)	3 (75%)	1 (25%)	0	0
All	All	234/266 (88%)	208 (89%)	26 (11%)	6	1

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

Mol	Chain	Res	Type
1	L	11	SER
2	H	40	LEU
2	H	41	LEU
2	H	48	SER
2	H	50	ARG
2	H	59	LEU
2	H	64	LEU
2	H	66	VAL
2	H	74	THR
2	H	79	ILE
2	H	81	LYS
2	H	83	SER
2	H	87	LYS

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Mol	Chain	Res	Type
2	H	98	ASN
2	H	99	LEU
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	154	VAL
2	H	169	LYS
2	H	176	ILE
2	H	192	GLU
2	H	236	LYS
2	H	241	VAL
3	I	357	GLU

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	98	ASN
2	H	156	GLN
2	H	204(B)	ASN

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	363	3	15,16,17	1.42	2 (13%)	15,22,24	1.58	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	I	363	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	363	TYS	OH-S	4.26	1.66	1.58
3	I	363	TYS	OH-CZ	-2.68	1.38	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	363	TYS	O2-S-O1	2.95	123.60	112.24
3	I	363	TYS	OH-S-O2	-2.66	99.46	107.56
3	I	363	TYS	OH-CZ-CE1	2.19	122.99	118.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	363	TYS	3	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	QWE	H	373	-	45,45,45	3.97	15 (33%)	59,63,63	2.90	23 (38%)

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	QWE	H	373	-	-	3/39/50/50	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	373	QWE	S-N1	17.92	1.91	1.61
5	H	373	QWE	C1-S	10.03	1.88	1.77
5	H	373	QWE	C21-N11	8.16	1.56	1.47
5	H	373	QWE	CM2-N	7.03	1.61	1.45
5	H	373	QWE	C61-N11	5.00	1.55	1.47
5	H	373	QWE	C41-C31	4.32	1.64	1.53
5	H	373	QWE	O1S-S	3.71	1.47	1.43
5	H	373	QWE	O2S-S	3.70	1.47	1.43
5	H	373	QWE	C1'-C21	-3.68	1.36	1.52
5	H	373	QWE	C-N11	3.61	1.42	1.34
5	H	373	QWE	C2-C1	3.52	1.42	1.37
5	H	373	QWE	C1-C8A	-2.94	1.38	1.43
5	H	373	QWE	C5-C4A	-2.63	1.37	1.42
5	H	373	QWE	C51-C41	2.63	1.61	1.51
5	H	373	QWE	C8-C8A	-2.47	1.37	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	373	QWE	O2S-S-C1	11.59	128.30	108.09
5	H	373	QWE	O2S-S-N1	-9.41	89.80	106.88
5	H	373	QWE	O1S-S-C1	-6.76	96.30	108.09
5	H	373	QWE	C61-N11-C21	5.71	123.12	115.24
5	H	373	QWE	CA-N1-S	-4.96	110.40	121.30
5	H	373	QWE	S1-C22-N3	3.89	118.05	114.37
5	H	373	QWE	C31-C21-N11	-3.86	104.55	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	373	QWE	CM1-N-C5	3.23	124.03	114.19
5	H	373	QWE	O2S-S-O1S	3.16	123.35	119.52
5	H	373	QWE	C52-S1-C22	-3.05	86.27	89.51
5	H	373	QWE	C1'-C21-N11	2.90	115.96	111.44
5	H	373	QWE	CM2-N-CM1	-2.87	106.97	116.18
5	H	373	QWE	C1'-C21-C31	-2.68	108.58	112.65
5	H	373	QWE	O-C-CA	-2.62	114.82	119.61
5	H	373	QWE	C1'-C2'-C2'1	-2.53	106.90	113.25
5	H	373	QWE	CM2-N-C5	2.48	121.74	114.19
5	H	373	QWE	C2-C1-C8A	2.46	123.70	120.95
5	H	373	QWE	C42-N3-C22	-2.31	106.86	109.83
5	H	373	QWE	C8-C8A-C4A	2.21	121.17	118.42
5	H	373	QWE	C-CA-N1	-2.16	105.25	110.80
5	H	373	QWE	CG-CD-NE	-2.05	106.44	112.20
5	H	373	QWE	C6-C5-N	-2.04	118.58	121.61
5	H	373	QWE	C3-C2-C1	-2.02	118.11	120.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	373	QWE	C21-C1'-C2'-C2'1
5	H	373	QWE	C2'-C2'1-C22-N3
5	H	373	QWE	O2-C2'1-C22-N3

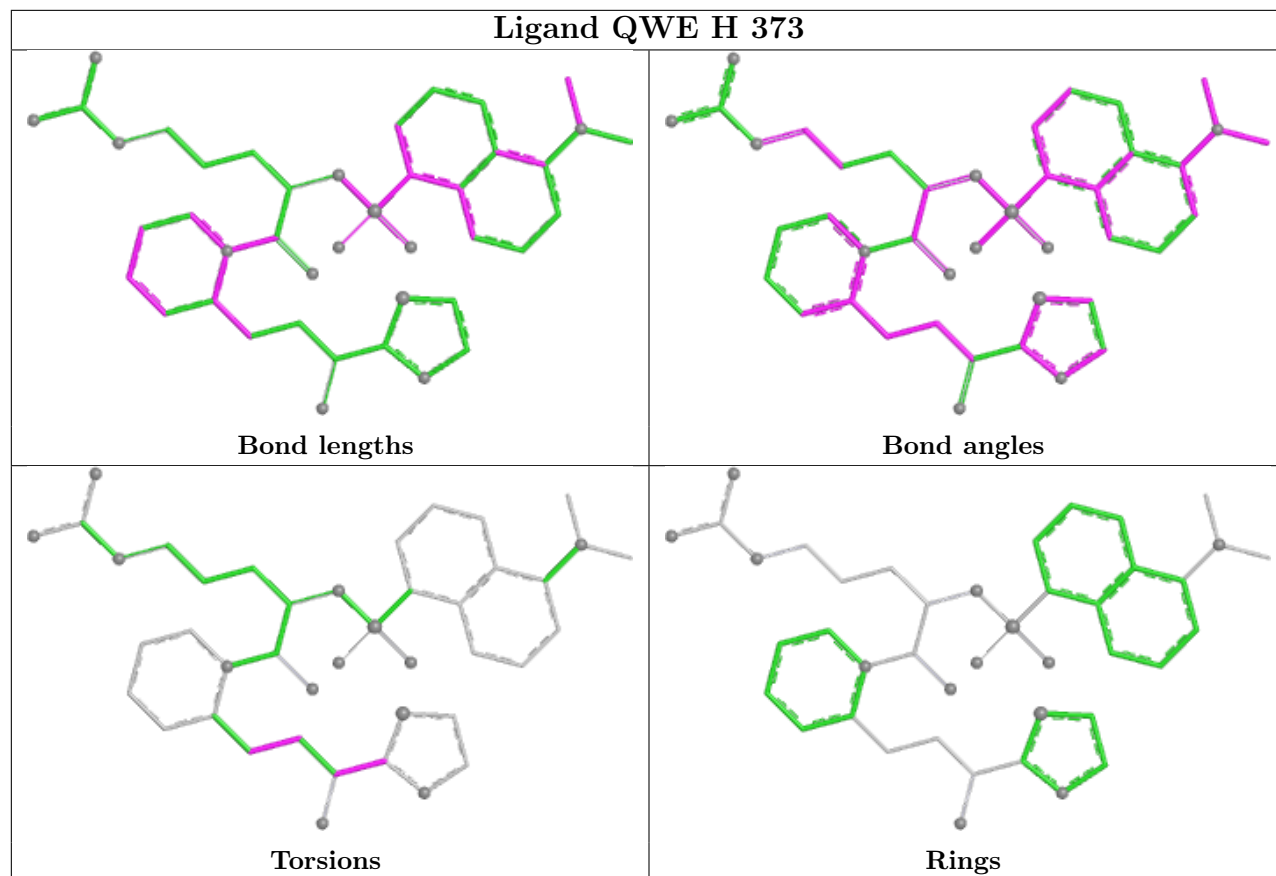
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	373	QWE	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	26/36 (72%)	-1.00	0 100 100	16, 23, 33, 40	0
2	H	248/259 (95%)	-0.95	0 100 100	14, 24, 39, 47	0
3	I	8/12 (66%)	-0.48	0 100 100	39, 43, 45, 45	0
All	All	282/307 (91%)	-0.94	0 100 100	14, 24, 41, 47	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	TYS	I	363	16/17	0.95	0.06	37,42,44,44	0

6.3 Carbohydrates [i](#)

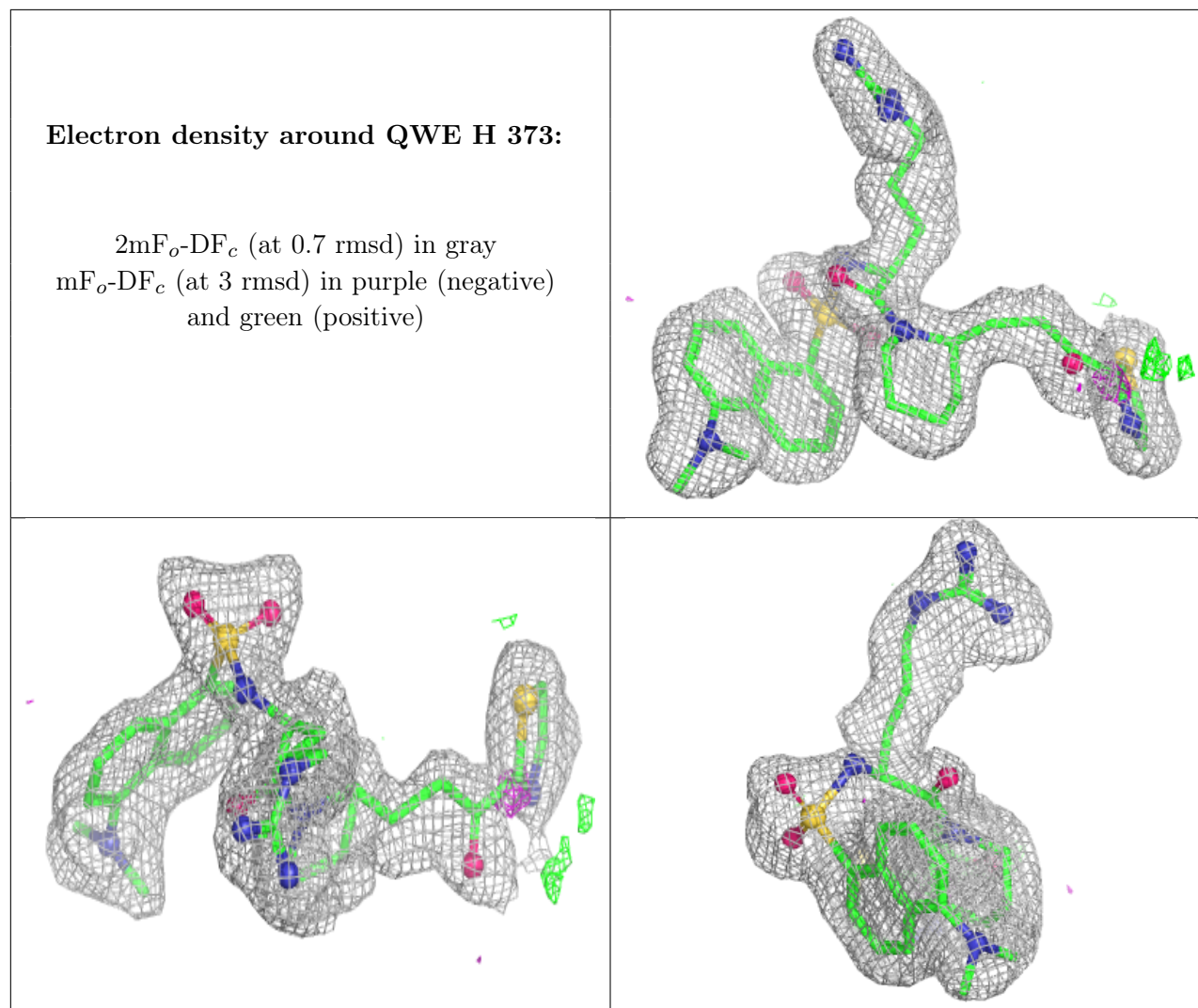
There are no oligosaccharides in this entry.

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	QWE	H	373	42/42	0.96	0.05	20,27,43,43	0
4	NA	H	542	1/1	0.98	0.03	24,24,24,24	1
4	NA	H	541	1/1	0.99	0.02	23,23,23,23	1

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 ⓘ

There are no such residues in this entry.