



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 3WTK / pdb_00003wtk
Title : Crystal Structure of Lymnaea stagnalis Acetylcholine-Binding Protein Q55R
Mutant Complexed with Thiachloprid
Authors : Okajima, T.; Ihara, M.; Yamashita, A.; Oda, T.; Matsuda, K.
Deposited on : 2014-04-11
Resolution : 2.69 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

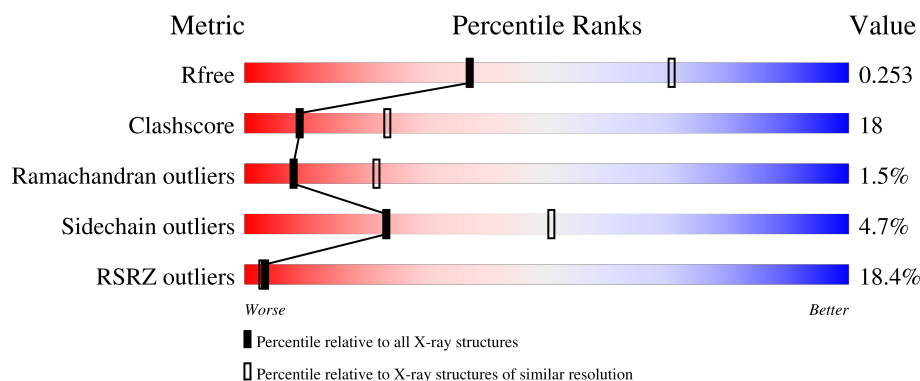
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	214	
1	B	214	
1	C	214	
1	D	214	
1	E	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8706 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1657	1033	287	332	5			
1	B	209	Total	C	N	O	S	0	0	0
			1666	1038	288	335	5			
1	C	208	Total	C	N	O	S	0	0	0
			1657	1033	287	332	5			
1	D	208	Total	C	N	O	S	0	1	0
			1665	1038	290	332	5			
1	E	208	Total	C	N	O	S	0	1	0
			1665	1038	290	332	5			

There are 35 discrepancies between the modelled and reference sequences:

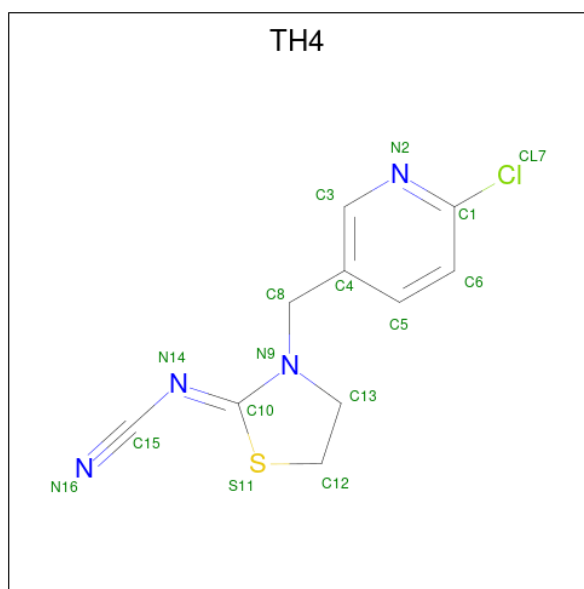
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP P58154
A	-2	ALA	-	expression tag	UNP P58154
A	-1	GLU	-	expression tag	UNP P58154
A	0	ALA	-	expression tag	UNP P58154
A	1	ALA	-	expression tag	UNP P58154
A	55	ARG	GLN	engineered mutation	UNP P58154
A	66	ASP	ASN	SEE REMARK 999	UNP P58154
B	-3	GLU	-	expression tag	UNP P58154
B	-2	ALA	-	expression tag	UNP P58154
B	-1	GLU	-	expression tag	UNP P58154
B	0	ALA	-	expression tag	UNP P58154
B	1	ALA	-	expression tag	UNP P58154
B	55	ARG	GLN	engineered mutation	UNP P58154
B	66	ASP	ASN	SEE REMARK 999	UNP P58154
C	-3	GLU	-	expression tag	UNP P58154
C	-2	ALA	-	expression tag	UNP P58154
C	-1	GLU	-	expression tag	UNP P58154
C	0	ALA	-	expression tag	UNP P58154
C	1	ALA	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
C	55	ARG	GLN	engineered mutation	UNP P58154
C	66	ASP	ASN	SEE REMARK 999	UNP P58154
D	-3	GLU	-	expression tag	UNP P58154
D	-2	ALA	-	expression tag	UNP P58154
D	-1	GLU	-	expression tag	UNP P58154
D	0	ALA	-	expression tag	UNP P58154
D	1	ALA	-	expression tag	UNP P58154
D	55	ARG	GLN	engineered mutation	UNP P58154
D	66	ASP	ASN	SEE REMARK 999	UNP P58154
E	-3	GLU	-	expression tag	UNP P58154
E	-2	ALA	-	expression tag	UNP P58154
E	-1	GLU	-	expression tag	UNP P58154
E	0	ALA	-	expression tag	UNP P58154
E	1	ALA	-	expression tag	UNP P58154
E	55	ARG	GLN	engineered mutation	UNP P58154
E	66	ASP	ASN	SEE REMARK 999	UNP P58154

- Molecule 2 is {(2Z)-3-[(6-chloropyridin-3-yl)methyl]-1,3-thiazolidin-2-ylidene}cyanamide (CCD ID: TH4) (formula: C₁₀H₉ClN₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	S	0	0
			16	10	1	4	1		
2	B	1	Total	C	Cl	N	S	0	0
			16	10	1	4	1		
2	C	1	Total	C	Cl	N	S	0	0
			16	10	1	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	Cl	N	S	
			16	10	1	4	1	
2	E	1	Total	C	Cl	N	S	
			16	10	1	4	1	

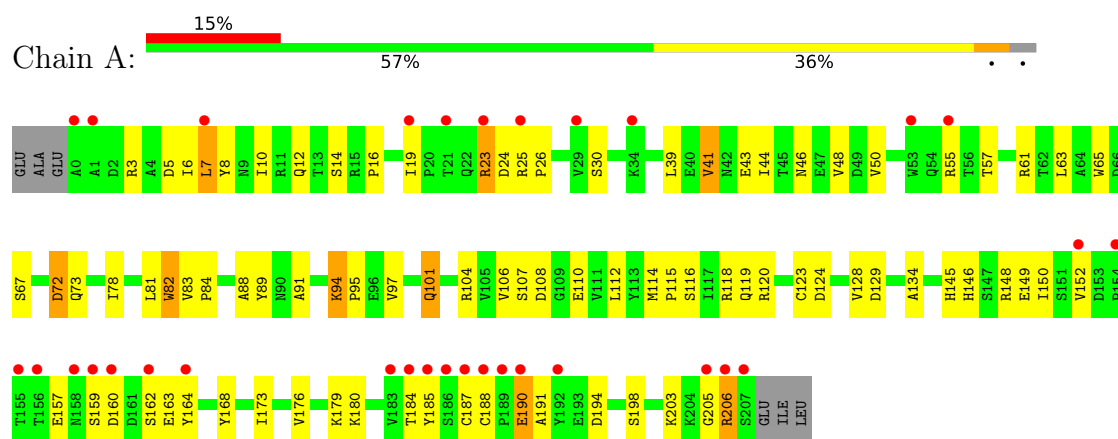
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O		
			57	57	0	0
3	B	56	Total	O		
			56	56	0	0
3	C	54	Total	O		
			54	54	0	0
3	D	66	Total	O		
			66	66	0	0
3	E	83	Total	O		
			83	83	0	0

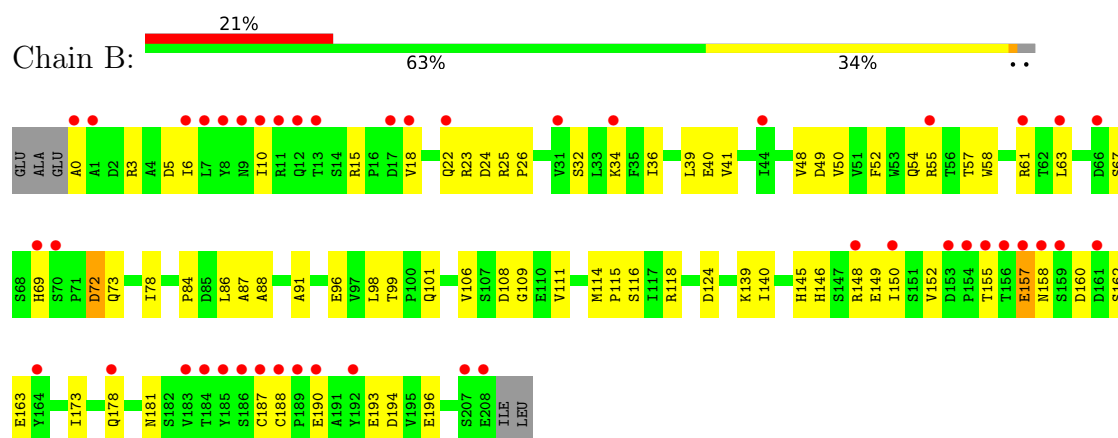
3 Residue-property plots [i](#)

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.

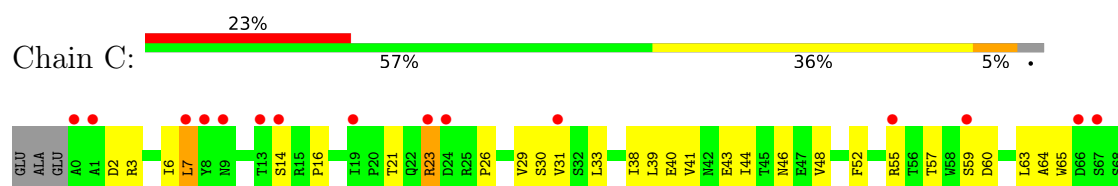
• Molecule 1: Acetylcholine-binding protein

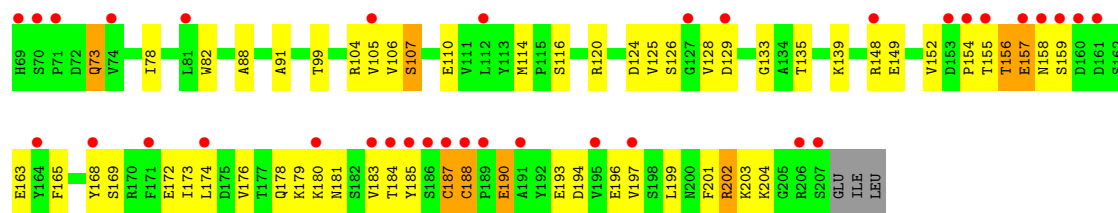


• Molecule 1: Acetylcholine-binding protein

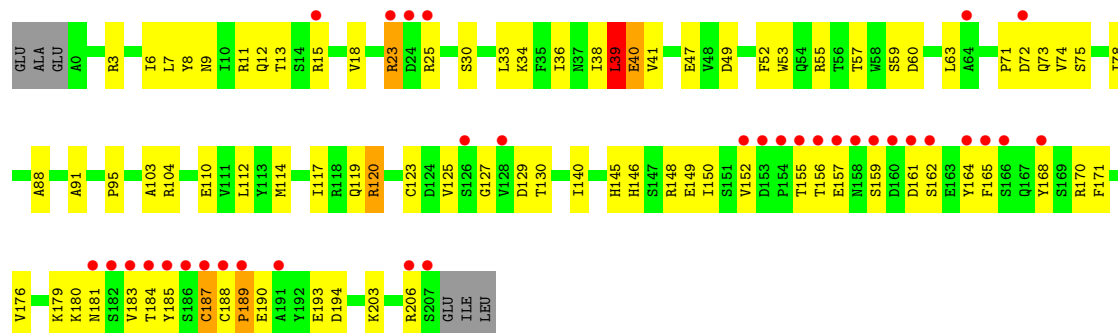


• Molecule 1: Acetylcholine-binding protein

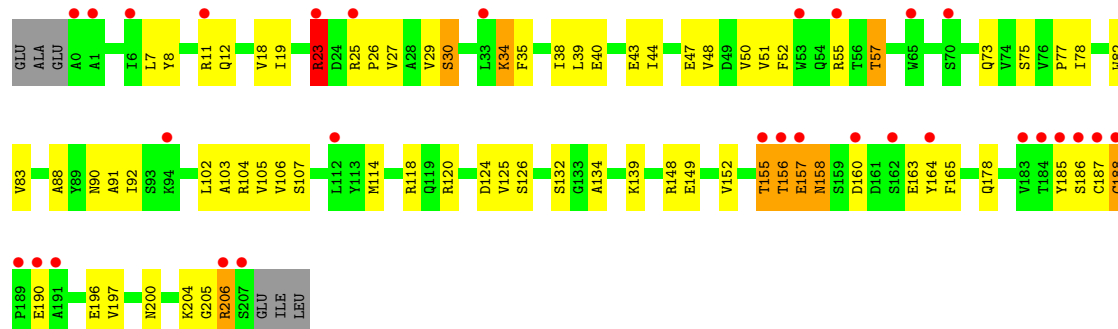




● Molecule 1: Acetylcholine-binding protein



● Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	74.53Å 74.53Å 350.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.60 – 2.69 39.60 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.60-2.69) 100.0 (39.60-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.60 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.200 , 0.274 0.261 , 0.253	Depositor DCC
R_{free} test set	2643 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: TH4

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	0.55	0/1693	0.93	6/2309 (0.3%)
1	B	0.50	0/1702	0.87	0/2321
1	C	0.52	0/1693	0.91	3/2309 (0.1%)
1	D	0.53	0/1704	0.91	3/2323 (0.1%)
1	E	0.54	0/1704	0.92	3/2323 (0.1%)
All	All	0.53	0/8496	0.91	15/11585 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ARG	N-CA-C	-9.03	99.48	110.31
1	E	82	TRP	N-CA-C	-6.65	98.79	109.96
1	D	117	ILE	N-CA-C	6.26	116.88	108.11
1	C	174	LEU	N-CA-C	-5.98	105.64	113.12
1	C	23	ARG	CB-CA-C	-5.89	109.79	116.63
1	A	44	ILE	N-CA-C	5.74	115.92	110.53
1	E	35	PHE	N-CA-C	5.64	118.19	110.24
1	C	31	VAL	N-CA-C	5.47	115.77	108.11
1	A	116	SER	N-CA-C	-5.46	100.80	109.76
1	A	25	ARG	N-CA-C	-5.39	103.28	110.07
1	E	23	ARG	CB-CA-C	-5.38	110.39	116.63
1	A	82	TRP	N-CA-C	-5.28	101.93	110.32
1	D	39	LEU	CB-CA-C	-5.15	108.96	116.53
1	A	124	ASP	N-CA-C	5.10	116.50	109.15
1	A	50	VAL	N-CA-C	5.01	117.22	108.95

There are no chirality outliers.

There are no planarity outliers.

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	1657	0	1601	61	0
1	B	1666	0	1607	56	0
1	C	1657	0	1601	73	0
1	D	1665	0	1614	67	0
1	E	1665	0	1614	61	0
2	A	16	0	9	1	0
2	B	16	0	9	0	0
2	C	16	0	9	1	0
2	D	16	0	9	1	0
2	E	16	0	9	1	0
3	A	57	0	0	4	0
3	B	56	0	0	4	0
3	C	54	0	0	8	0
3	D	66	0	0	6	0
3	E	83	0	0	2	0
All	All	8706	0	8082	301	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 18.

All (301) 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:B:160:ASP:HB3	1:B:163:GLU:HB2	1.49	0.95
1:A:160:ASP:HB3	1:A:163:GLU:HB2	1.54	0.90
1:B:55:ARG:HG3	1:B:114:MET:HE2	1.53	0.90
1:C:55:ARG:HB2	1:C:114:MET:HE2	1.53	0.89
1:D:47:GLU:HB3	1:D:120[B]:ARG:HH11	1.44	0.83
1:E:55:ARG:HA	1:E:114:MET:HG3	1.63	0.80
1:D:155:THR:HG22	1:D:157:GLU:HG2	1.62	0.80
1:D:123:CYS:HB2	3:D:441:HOH:O	1.82	0.79
1:E:8:TYR:O	1:E:12:GLN:HG2	1.84	0.78
1:E:30:SER:HB2	1:E:57:THR:HG22	1.66	0.76
1:D:34:LYS:HG2	3:D:453:HOH:O	1.87	0.74
1:D:55:ARG:HG3	1:D:114:MET:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HG2	1:C:196:GLU:HG2	1.71	0.72
1:E:206:ARG:HH11	1:E:206:ARG:HB2	1.54	0.71
1:E:139:LYS:HG2	1:E:196:GLU:HG2	1.71	0.71
1:D:146:HIS:CE1	1:D:148:ARG:HB2	2.26	0.71
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.26	0.70
1:B:145:HIS:HB2	1:B:150:ILE:HD12	1.74	0.69
1:C:3:ARG:O	1:C:7:LEU:HD12	1.92	0.69
1:A:88:ALA:HB3	1:A:91:ALA:HB2	1.74	0.68
1:D:39:LEU:O	1:D:41:VAL:HG23	1.94	0.68
1:A:14:SER:HB2	1:A:63:LEU:HD21	1.76	0.68
1:E:206:ARG:HB2	1:E:206:ARG:NH1	2.09	0.68
1:A:55:ARG:HA	1:A:114:MET:HG3	1.75	0.68
1:D:187:CYS:SG	1:D:188:CYS:N	2.67	0.67
1:A:94:LYS:HD2	1:B:96:GLU:HG3	1.76	0.67
1:A:3:ARG:HG3	1:A:3:ARG:HH11	1.60	0.67
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.76	0.66
1:A:187:CYS:SG	1:A:188:CYS:N	2.68	0.66
1:A:41:VAL:HG22	1:A:48:VAL:HG12	1.76	0.66
1:D:161:ASP:HB3	1:D:176:VAL:HG23	1.78	0.66
1:A:30:SER:OG	1:A:57:THR:HB	1.96	0.65
1:B:18:VAL:HG22	1:C:7:LEU:HD13	1.77	0.65
1:D:146:HIS:HE1	1:D:148:ARG:HB2	1.61	0.65
1:A:145:HIS:HB2	1:A:150:ILE:HD12	1.79	0.65
1:A:8:TYR:O	1:A:12:GLN:HG2	1.97	0.65
1:D:145:HIS:HB2	1:D:150:ILE:HD12	1.77	0.65
1:E:34:LYS:HG2	1:E:164:TYR:HD2	1.61	0.65
1:B:187:CYS:SG	1:B:188:CYS:N	2.70	0.65
1:C:44:ILE:HG22	1:D:170:ARG:HD3	1.79	0.64
1:D:72:ASP:HB3	3:D:447:HOH:O	1.97	0.64
1:E:34:LYS:HG2	1:E:164:TYR:CD2	2.33	0.64
1:D:95:PRO:HD3	1:D:119:GLN:NE2	2.12	0.64
1:C:44:ILE:HD12	3:C:411:HOH:O	1.97	0.64
1:E:178:GLN:HG2	1:E:197:VAL:HG13	1.80	0.64
1:C:78:ILE:HD12	3:C:452:HOH:O	1.98	0.63
1:C:152:VAL:HG22	1:C:193:GLU:HB3	1.79	0.63
1:E:55:ARG:HG3	1:E:114:MET:HE2	1.81	0.63
1:B:146:HIS:CE1	1:B:148:ARG:HB2	2.34	0.62
1:C:88:ALA:HB3	1:C:91:ALA:HB2	1.81	0.62
1:E:187:CYS:SG	1:E:188:CYS:N	2.73	0.62
1:B:78:ILE:HG23	1:B:101:GLN:O	2.00	0.61
1:D:185:TYR:HB3	1:E:164:TYR:OH	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:HG23	1:C:116:SER:HB3	1.82	0.61
1:A:10:ILE:HG23	1:A:63:LEU:HD22	1.82	0.60
1:B:146:HIS:HE1	1:B:148:ARG:HB2	1.66	0.60
1:C:60:ASP:OD2	1:C:63:LEU:HG	2.01	0.60
1:B:55:ARG:HA	1:B:114:MET:HG3	1.82	0.60
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.82	0.60
1:E:157:GLU:O	1:E:157:GLU:HG3	2.02	0.60
1:C:154:PRO:O	1:C:156:THR:N	2.35	0.59
1:C:178:GLN:HG2	1:C:197:VAL:HG22	1.84	0.59
1:D:129:ASP:OD1	1:D:203:LYS:HD3	2.02	0.59
1:E:40:GLU:HB3	1:E:120[B]:ARG:NH2	2.17	0.59
1:A:104:ARG:HH22	1:E:149:GLU:CD	2.11	0.59
1:D:39:LEU:HD12	1:D:39:LEU:N	2.18	0.59
1:E:155:THR:C	1:E:157:GLU:H	2.11	0.59
1:B:55:ARG:CG	1:B:114:MET:HE2	2.29	0.59
1:C:124:ASP:HB2	1:D:168:TYR:CD1	2.38	0.58
1:A:162:SER:HB3	1:A:173:ILE:HB	1.85	0.58
1:C:39:LEU:O	1:C:41:VAL:HG23	2.03	0.58
1:D:152:VAL:HG22	1:D:193:GLU:HB3	1.86	0.58
1:C:14:SER:HA	3:C:421:HOH:O	2.03	0.58
1:C:55:ARG:CB	1:C:114:MET:HE2	2.30	0.58
1:A:179:LYS:HE3	1:A:180:LYS:O	2.03	0.57
1:B:152:VAL:HG22	1:B:193:GLU:HB3	1.86	0.57
1:A:5:ASP:HA	3:A:421:HOH:O	2.04	0.57
1:C:183:VAL:HG12	1:C:184:THR:N	2.20	0.56
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.87	0.56
1:A:179:LYS:HG2	1:A:180:LYS:N	2.18	0.56
1:B:39:LEU:O	1:B:41:VAL:HG23	2.05	0.56
1:D:39:LEU:HD12	1:D:39:LEU:H	1.71	0.56
1:E:51:VAL:HG22	1:E:118:ARG:HG3	1.88	0.56
1:E:44:ILE:HD12	3:E:460:HOH:O	2.06	0.56
1:D:184:THR:HG22	1:D:185:TYR:H	1.71	0.56
1:A:12:GLN:HA	1:A:12:GLN:NE2	2.22	0.55
1:B:58:TRP:CZ2	1:B:111:VAL:HG11	2.41	0.55
1:B:139:LYS:HE2	1:B:194:ASP:OD2	2.07	0.55
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.71	0.55
1:B:32:SER:HA	1:B:178:GLN:HE22	1.69	0.55
1:D:40:GLU:HB3	1:D:120[B]:ARG:HH22	1.71	0.54
1:A:39:LEU:HD13	1:A:118:ARG:NH2	2.23	0.54
1:C:149:GLU:CD	1:D:104:ARG:HH22	2.15	0.54
1:B:6:ILE:O	1:B:10:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:O	1:D:40:GLU:C	2.50	0.54
1:C:188:CYS:HB3	1:C:190:GLU:OE2	2.08	0.54
1:C:157:GLU:O	1:C:157:GLU:HG2	2.06	0.54
1:D:72:ASP:CB	3:D:447:HOH:O	2.52	0.53
1:D:184:THR:HG22	1:D:185:TYR:N	2.23	0.53
1:C:184:THR:HG22	1:C:185:TYR:H	1.73	0.53
1:D:47:GLU:HB3	1:D:120[B]:ARG:NH1	2.18	0.53
1:A:12:GLN:HA	1:A:12:GLN:HE21	1.73	0.53
1:C:176:VAL:HG22	1:C:199:LEU:HD12	1.89	0.53
1:C:187:CYS:SG	1:C:188:CYS:N	2.82	0.53
1:B:99:THR:HG23	1:B:116:SER:HB3	1.90	0.53
1:C:185:TYR:HB3	1:D:164:TYR:OH	2.08	0.53
1:D:30:SER:OG	1:D:57:THR:HB	2.08	0.53
1:E:26:PRO:HB3	1:E:148:ARG:C	2.34	0.53
1:D:33:LEU:HD22	1:D:52:PHE:CD2	2.44	0.52
1:C:133:GLY:HA2	1:C:202:ARG:HB3	1.91	0.52
1:A:146:HIS:CE1	1:A:149:GLU:HG3	2.44	0.52
1:E:205:GLY:HA2	1:E:206:ARG:NH2	2.25	0.52
1:C:184:THR:HG22	1:C:185:TYR:N	2.24	0.52
1:E:75:SER:OG	1:E:104:ARG:NH1	2.42	0.52
1:B:155:THR:O	1:B:157:GLU:HG3	2.09	0.52
1:E:48:VAL:O	1:E:120[B]:ARG:HG3	2.10	0.52
1:E:92:ILE:HD11	1:E:120[B]:ARG:HG2	1.92	0.52
1:C:65:TRP:CZ3	1:C:107:SER:HA	2.45	0.52
1:D:120[A]:ARG:HH11	1:D:120[A]:ARG:HG2	1.75	0.52
1:E:7:LEU:HD11	1:E:11:ARG:NE	2.25	0.52
1:A:118:ARG:NH1	1:E:92:ILE:O	2.44	0.51
1:D:11:ARG:HG3	1:D:11:ARG:HH11	1.75	0.51
1:D:127:GLY:HA2	1:D:130:THR:HG23	1.92	0.51
1:E:38:ILE:HG13	1:E:165:PHE:CE1	2.45	0.51
1:B:67:SER:HB2	1:B:72:ASP:OD1	2.11	0.51
1:C:30:SER:OG	1:C:57:THR:HB	2.11	0.51
1:C:148:ARG:HH21	1:C:190:GLU:HB3	1.74	0.51
1:A:146:HIS:CE1	1:A:148:ARG:HB2	2.46	0.51
1:D:189:PRO:HG2	1:D:190:GLU:H	1.75	0.51
1:E:38:ILE:HG13	1:E:165:PHE:HE1	1.76	0.51
1:D:40:GLU:HB3	1:D:120[B]:ARG:NH2	2.26	0.51
1:A:159:SER:HA	3:A:407:HOH:O	2.11	0.50
1:E:155:THR:O	1:E:157:GLU:N	2.43	0.50
1:D:179:LYS:HG2	1:D:180:LYS:N	2.26	0.50
1:B:73:GLN:HE21	1:B:106:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:CA	1:E:114:MET:HG3	2.40	0.50
1:B:25:ARG:NE	3:B:411:HOH:O	2.41	0.50
1:E:47:GLU:HB2	1:E:120[B]:ARG:NH1	2.26	0.50
1:A:67:SER:OG	1:A:72:ASP:HB3	2.11	0.50
1:E:43:GLU:OE2	1:E:126:SER:HA	2.12	0.50
1:A:94:LYS:N	1:B:98:LEU:HD22	2.26	0.50
1:C:43:GLU:HB2	3:C:454:HOH:O	2.12	0.50
1:C:179:LYS:HG2	1:C:180:LYS:O	2.12	0.50
1:A:16:PRO:HA	1:A:82:TRP:HA	1.93	0.50
1:A:55:ARG:CA	1:A:114:MET:HG3	2.41	0.50
1:B:26:PRO:HB3	1:B:148:ARG:C	2.36	0.49
1:E:39:LEU:HD13	1:E:118:ARG:CZ	2.42	0.49
1:A:129:ASP:OD1	1:A:203:LYS:HE2	2.12	0.49
1:C:33:LEU:HD22	1:C:52:PHE:CD2	2.47	0.49
1:C:64:ALA:HA	1:C:107:SER:O	2.12	0.49
1:B:26:PRO:HB3	1:B:148:ARG:O	2.12	0.49
1:B:55:ARG:CA	1:B:114:MET:HG3	2.43	0.49
1:C:59:SER:HB2	1:C:110:GLU:OE2	2.12	0.49
1:E:134:ALA:O	1:E:200:ASN:HA	2.13	0.48
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.48	0.48
1:B:187:CYS:HB3	3:B:427:HOH:O	2.14	0.48
1:E:83:VAL:N	3:E:415:HOH:O	2.36	0.48
1:A:7:LEU:HD22	1:E:18:VAL:HG22	1.95	0.48
1:A:123:CYS:HB2	3:A:429:HOH:O	2.11	0.48
1:C:133:GLY:CA	1:C:202:ARG:HB3	2.43	0.48
1:C:152:VAL:HG23	1:C:152:VAL:O	2.13	0.48
1:E:134:ALA:O	1:E:200:ASN:ND2	2.36	0.48
1:C:43:GLU:OE2	1:C:126:SER:HA	2.13	0.48
1:C:135:THR:HA	1:C:199:LEU:O	2.14	0.48
1:C:39:LEU:O	1:C:40:GLU:C	2.57	0.48
1:C:57:THR:HG22	3:C:422:HOH:O	2.13	0.48
1:A:3:ARG:HH11	1:A:3:ARG:CG	2.27	0.48
1:A:16:PRO:HB3	1:A:81:LEU:O	2.13	0.47
1:C:2:ASP:O	1:C:6:ILE:HG13	2.14	0.47
1:B:3:ARG:HG3	1:B:3:ARG:HH11	1.79	0.47
1:C:157:GLU:O	1:C:157:GLU:CG	2.62	0.47
1:E:47:GLU:CB	1:E:120[B]:ARG:HH11	2.27	0.47
1:A:6:ILE:O	1:A:10:ILE:HG13	2.14	0.47
1:C:73:GLN:HG3	1:C:106:VAL:HG22	1.97	0.47
1:A:43:GLU:CD	1:A:43:GLU:H	2.23	0.47
1:A:65:TRP:CZ3	1:A:107:SER:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HB3	1:A:119:GLN:NE2	2.30	0.46
1:C:169:SER:HB3	3:C:432:HOH:O	2.15	0.46
1:E:23:ARG:HG3	1:E:25:ARG:NH2	2.30	0.46
1:C:65:TRP:CE3	1:C:107:SER:HA	2.51	0.46
1:B:39:LEU:HD12	1:B:118:ARG:NE	2.31	0.45
1:D:11:ARG:HG3	1:D:11:ARG:NH1	2.31	0.45
1:A:39:LEU:HD13	1:A:118:ARG:CZ	2.46	0.45
1:A:152:VAL:HG23	1:A:152:VAL:O	2.15	0.45
1:A:184:THR:OG1	1:A:191:ALA:HB2	2.15	0.45
1:D:125:VAL:HG12	1:D:125:VAL:O	2.16	0.45
1:C:169:SER:O	1:C:204:LYS:HD3	2.17	0.45
1:D:112:LEU:O	2:D:301:TH4:CL7	2.72	0.45
1:E:23:ARG:HG3	1:E:25:ARG:CZ	2.47	0.45
1:B:139:LYS:HE2	1:B:194:ASP:CG	2.41	0.45
1:D:38:ILE:HG13	1:D:165:PHE:HE1	1.81	0.45
1:D:162:SER:HB2	1:D:165:PHE:HB3	1.99	0.45
1:A:89:TYR:N	1:A:89:TYR:CD2	2.84	0.45
1:E:114:MET:HE1	2:E:301:TH4:C15	2.47	0.45
1:A:26:PRO:HB3	1:A:148:ARG:O	2.17	0.45
1:D:9:ASN:O	1:D:13:THR:HG23	2.17	0.45
1:B:22:GLN:OE1	1:B:22:GLN:HA	2.17	0.44
1:C:129:ASP:OD2	1:C:203:LYS:HE2	2.17	0.44
1:D:33:LEU:HD11	1:D:140:ILE:HD12	1.99	0.44
1:C:16:PRO:HA	1:C:82:TRP:HA	1.99	0.44
1:C:38:ILE:HG13	1:C:165:PHE:HE1	1.82	0.44
1:C:125:VAL:HG12	1:C:125:VAL:O	2.16	0.44
1:D:78:ILE:HG22	1:D:103:ALA:HB2	1.99	0.44
1:D:95:PRO:HD3	1:D:119:GLN:HE22	1.80	0.44
1:E:19:ILE:CG1	1:E:27:VAL:HG21	2.47	0.44
1:C:48:VAL:O	1:C:120:ARG:HA	2.18	0.44
1:D:171:PHE:N	1:D:171:PHE:CD1	2.85	0.44
1:C:159:SER:HB3	1:C:163:GLU:OE1	2.18	0.44
1:D:57:THR:OG1	1:D:112:LEU:HD13	2.17	0.44
1:D:155:THR:C	1:D:157:GLU:H	2.25	0.44
1:E:139:LYS:NZ	1:E:196:GLU:OE2	2.48	0.44
1:B:61:ARG:C	1:B:63:LEU:H	2.26	0.43
1:B:106:VAL:HB	1:B:108:ASP:OD1	2.18	0.43
1:D:183:VAL:HG23	1:D:194:ASP:OD2	2.18	0.43
1:A:19:ILE:HG23	1:A:19:ILE:O	2.18	0.43
1:C:152:VAL:HG21	1:C:194:ASP:HA	2.00	0.43
1:C:168:TYR:HA	3:C:423:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:VAL:HG21	1:D:194:ASP:CA	2.48	0.43
1:A:190:GLU:CD	1:A:190:GLU:H	2.25	0.43
1:C:29:VAL:O	1:C:152:VAL:HA	2.19	0.43
1:D:88:ALA:HB3	1:D:91:ALA:HB2	2.00	0.43
1:A:16:PRO:HA	1:A:82:TRP:CA	2.48	0.43
1:B:39:LEU:O	1:B:40:GLU:C	2.61	0.43
1:C:183:VAL:HG12	1:C:184:THR:H	1.82	0.43
1:D:3:ARG:HA	1:D:6:ILE:HD12	2.00	0.43
1:D:152:VAL:HG21	1:D:194:ASP:HA	2.01	0.43
1:B:15:ARG:HB3	1:B:15:ARG:NH1	2.34	0.43
1:B:84:PRO:HB2	1:B:86:LEU:HG	1.99	0.43
1:C:73:GLN:HA	1:C:105:VAL:O	2.19	0.43
1:C:172:GLU:O	1:C:201:PHE:HB2	2.19	0.43
1:E:158:ASN:HD22	1:E:158:ASN:HA	1.64	0.43
1:D:59:SER:HB3	1:D:110:GLU:OE2	2.18	0.43
1:B:139:LYS:HG3	1:B:196:GLU:HG2	2.00	0.43
1:E:155:THR:C	1:E:157:GLU:N	2.76	0.43
1:B:162:SER:HB3	1:B:173:ILE:HB	2.01	0.43
1:E:125:VAL:HG12	1:E:125:VAL:O	2.18	0.43
1:E:160:ASP:O	1:E:163:GLU:HB2	2.18	0.43
1:A:185:TYR:C	1:A:187:CYS:H	2.27	0.42
1:B:10:ILE:HG23	1:B:63:LEU:HD22	2.00	0.42
1:C:46:ASN:HA	1:C:125:VAL:HG23	2.01	0.42
1:D:75:SER:HA	1:D:103:ALA:O	2.19	0.42
1:D:149:GLU:CD	1:E:104:ARG:HH22	2.25	0.42
1:B:15:ARG:HB3	1:B:15:ARG:HH11	1.83	0.42
1:D:8:TYR:N	1:D:8:TYR:CD1	2.87	0.42
1:E:47:GLU:HB2	1:E:120[B]:ARG:HH11	1.85	0.42
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.54	0.42
1:C:125:VAL:HG12	1:C:128:VAL:HB	2.01	0.42
1:C:152:VAL:HG21	1:C:194:ASP:CA	2.50	0.42
1:D:23:ARG:HB2	1:D:23:ARG:HH11	1.84	0.42
1:E:106:VAL:HG12	1:E:107:SER:N	2.35	0.42
1:A:65:TRP:CE3	1:A:107:SER:HA	2.55	0.42
1:B:57:THR:O	1:B:58:TRP:HB3	2.19	0.42
1:E:29:VAL:O	1:E:152:VAL:HA	2.20	0.42
1:E:156:THR:O	1:E:158:ASN:N	2.53	0.42
1:C:26:PRO:HD3	3:C:447:HOH:O	2.19	0.42
1:C:114:MET:HE1	2:C:301:TH4:N16	2.35	0.42
1:D:7:LEU:O	1:D:11:ARG:HG2	2.19	0.42
1:D:49:ASP:HA	1:D:120[A]:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLU:CD	1:C:104:ARG:HH22	2.27	0.42
1:E:73:GLN:HA	1:E:105:VAL:O	2.19	0.42
1:A:83:VAL:HG13	1:A:84:PRO:HD2	2.01	0.42
1:D:15:ARG:HB3	1:D:18:VAL:HG23	2.01	0.42
1:D:60:ASP:HB3	1:D:63:LEU:HD12	2.02	0.41
1:E:160:ASP:HB3	1:E:163:GLU:HB2	2.01	0.41
1:D:73:GLN:O	1:D:74:VAL:HG13	2.19	0.41
1:E:78:ILE:HG22	1:E:103:ALA:HB2	2.02	0.41
1:B:36:ILE:HG12	1:B:52:PHE:HA	2.03	0.41
1:E:77:PRO:HA	1:E:102:LEU:HD23	2.02	0.41
1:A:108:ASP:OD2	1:A:110:GLU:HG2	2.20	0.41
1:B:34:LYS:HG2	3:B:453:HOH:O	2.21	0.41
1:B:106:VAL:O	1:B:109:GLY:N	2.49	0.41
1:E:40:GLU:HB3	1:E:120[B]:ARG:HH22	1.82	0.41
1:A:46:ASN:HB3	1:A:123:CYS:O	2.20	0.41
1:A:164:TYR:OH	1:E:185:TYR:HB3	2.21	0.41
1:B:22:GLN:O	1:B:23:ARG:HB2	2.20	0.41
1:B:152:VAL:HG21	1:B:194:ASP:HA	2.01	0.41
1:C:38:ILE:HD11	1:C:199:LEU:HD21	2.03	0.41
1:A:97:VAL:HG13	1:A:115:PRO:HB2	2.03	0.41
1:A:112:LEU:O	2:A:301:TH4:CL7	2.75	0.41
1:B:61:ARG:C	1:B:63:LEU:N	2.79	0.41
1:D:72:ASP:CG	3:D:447:HOH:O	2.63	0.41
1:A:10:ILE:HG23	1:A:63:LEU:CD2	2.48	0.41
1:A:176:VAL:HA	1:A:198:SER:O	2.21	0.41
1:B:5:ASP:O	1:B:6:ILE:C	2.64	0.41
1:B:87:ALA:O	1:B:140:ILE:HA	2.21	0.41
1:C:21:THR:HG22	1:C:23:ARG:O	2.21	0.41
1:C:194:ASP:OD1	1:C:194:ASP:C	2.63	0.41
1:D:71:PRO:HD3	3:D:411:HOH:O	2.21	0.41
1:A:73:GLN:CG	1:A:106:VAL:HG22	2.51	0.41
1:C:55:ARG:HH11	1:C:55:ARG:HG2	1.85	0.41
1:C:173:ILE:HG21	1:C:176:VAL:HG23	2.02	0.41
1:C:187:CYS:C	1:C:188:CYS:SG	3.04	0.41
1:E:50:VAL:HG12	1:E:52:PHE:HD1	1.85	0.41
1:A:128:VAL:N	1:A:134:ALA:HB2	2.36	0.40
1:E:90:ASN:OD1	1:E:90:ASN:N	2.54	0.40
1:A:78:ILE:HG12	1:A:101:GLN:HB3	2.02	0.40
1:B:0:ALA:HB1	1:B:69:HIS:O	2.22	0.40
1:B:15:ARG:NH1	3:B:403:HOH:O	2.54	0.40
1:B:54:GLN:O	1:B:115:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:HD3	3:A:445:HOH:O	2.22	0.40
1:D:36:ILE:HD11	1:D:53:TRP:CD2	2.57	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	206/214 (96%)	187 (91%)	17 (8%)	2 (1%)	12	32
1	B	207/214 (97%)	184 (89%)	22 (11%)	1 (0%)	24	48
1	C	206/214 (96%)	189 (92%)	14 (7%)	3 (2%)	8	22
1	D	207/214 (97%)	192 (93%)	10 (5%)	5 (2%)	4	12
1	E	207/214 (97%)	195 (94%)	8 (4%)	4 (2%)	6	17
All	All	1033/1070 (96%)	947 (92%)	71 (7%)	15 (2%)	8	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ASN
1	C	155	THR
1	C	156	THR
1	D	156	THR
1	D	187	CYS
1	D	206	ARG
1	E	156	THR
1	E	157	GLU
1	E	204	LYS
1	C	187	CYS
1	D	159	SER
1	D	189	PRO

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Mol	Chain	Res	Type
1	A	206	ARG
1	E	186	SER
1	A	205	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/197 (98%)	179 (93%)	13 (7%)	14	35
1	B	193/197 (98%)	186 (96%)	7 (4%)	31	60
1	C	192/197 (98%)	183 (95%)	9 (5%)	23	51
1	D	193/197 (98%)	186 (96%)	7 (4%)	31	60
1	E	193/197 (98%)	183 (95%)	10 (5%)	21	47
All	All	963/985 (98%)	917 (95%)	46 (5%)	23	50

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	23	ARG
1	A	24	ASP
1	A	41	VAL
1	A	61	ARG
1	A	72	ASP
1	A	94	LYS
1	A	101	GLN
1	A	120	ARG
1	A	157	GLU
1	A	190	GLU
1	A	194	ASP
1	A	206	ARG
1	B	24	ASP
1	B	49	ASP
1	B	50	VAL

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Mol	Chain	Res	Type
1	B	72	ASP
1	B	157	GLU
1	B	181	ASN
1	B	190	GLU
1	C	7	LEU
1	C	73	GLN
1	C	107	SER
1	C	157	GLU
1	C	158	ASN
1	C	181	ASN
1	C	188	CYS
1	C	190	GLU
1	C	202	ARG
1	D	12	GLN
1	D	23	ARG
1	D	39	LEU
1	D	40	GLU
1	D	120[A]	ARG
1	D	120[B]	ARG
1	D	181	ASN
1	E	23	ARG
1	E	30	SER
1	E	34	LYS
1	E	57	THR
1	E	132	SER
1	E	155	THR
1	E	158	ASN
1	E	188	CYS
1	E	190	GLU
1	E	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	22	GLN
1	A	54	GLN
1	A	101	GLN
1	A	119	GLN
1	A	146	HIS
1	A	158	ASN
1	A	200	ASN

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	178	GLN
1	C	9	ASN
1	C	54	GLN
1	C	73	GLN
1	C	158	ASN
1	C	200	ASN
1	D	69	HIS
1	D	119	GLN
1	D	158	ASN
1	E	69	HIS
1	E	158	ASN

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](#)

5 ligands are 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	$\# Z > 2$
2	TH4	D	301	-	17,17,17	2.25	3 (17%)	20,22,22	2.31	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TH4	A	301	-	17,17,17	2.16	4 (23%)	20,22,22	2.45	7 (35%)
2	TH4	E	301	-	17,17,17	2.37	4 (23%)	20,22,22	2.46	8 (40%)
2	TH4	B	301	-	17,17,17	2.24	3 (17%)	20,22,22	2.42	6 (30%)
2	TH4	C	301	-	17,17,17	2.18	4 (23%)	20,22,22	2.66	8 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TH4	D	301	-	-	0/6/17/17	0/2/2/2
2	TH4	A	301	-	-	0/6/17/17	0/2/2/2
2	TH4	E	301	-	-	0/6/17/17	0/2/2/2
2	TH4	B	301	-	-	0/6/17/17	0/2/2/2
2	TH4	C	301	-	-	0/6/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	TH4	C15-N14	-6.03	1.22	1.32
2	D	301	TH4	C15-N14	-5.79	1.23	1.32
2	A	301	TH4	C15-N14	-5.55	1.23	1.32
2	B	301	TH4	C15-N14	-5.43	1.23	1.32
2	E	301	TH4	C10-S11	-5.29	1.67	1.75
2	C	301	TH4	C10-S11	-5.23	1.67	1.75
2	B	301	TH4	C10-S11	-5.12	1.67	1.75
2	D	301	TH4	C10-S11	-5.10	1.67	1.75
2	A	301	TH4	C10-S11	-5.03	1.67	1.75
2	C	301	TH4	C15-N14	-4.94	1.24	1.32
2	E	301	TH4	C1-N2	3.55	1.40	1.32
2	B	301	TH4	C1-N2	2.97	1.38	1.32
2	A	301	TH4	C1-N2	2.79	1.38	1.32
2	D	301	TH4	C1-N2	2.71	1.38	1.32
2	C	301	TH4	C1-N2	2.67	1.38	1.32
2	C	301	TH4	C3-C4	2.17	1.43	1.38
2	A	301	TH4	C3-C4	2.11	1.43	1.38
2	E	301	TH4	C3-C4	2.04	1.43	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	TH4	C15-N14-C10	6.91	125.62	118.11
2	A	301	TH4	C15-N14-C10	6.39	125.05	118.11
2	B	301	TH4	C15-N14-C10	6.10	124.74	118.11
2	E	301	TH4	C15-N14-C10	5.54	124.14	118.11
2	D	301	TH4	C15-N14-C10	5.52	124.11	118.11
2	E	301	TH4	C3-N2-C1	4.66	121.93	116.33
2	B	301	TH4	C3-N2-C1	4.52	121.76	116.33
2	C	301	TH4	C3-N2-C1	4.45	121.67	116.33
2	D	301	TH4	C3-N2-C1	4.43	121.65	116.33
2	A	301	TH4	C3-N2-C1	4.30	121.50	116.33
2	C	301	TH4	C12-S11-C10	3.94	97.52	91.21
2	B	301	TH4	C12-S11-C10	3.92	97.48	91.21
2	D	301	TH4	C12-S11-C10	3.87	97.41	91.21
2	E	301	TH4	C12-S11-C10	3.64	97.03	91.21
2	A	301	TH4	C12-S11-C10	3.40	96.66	91.21
2	E	301	TH4	C6-C1-N2	-3.36	119.99	124.87
2	C	301	TH4	C6-C1-N2	-3.31	120.06	124.87
2	B	301	TH4	C6-C1-N2	-3.28	120.11	124.87
2	D	301	TH4	C6-C1-N2	-3.25	120.14	124.87
2	C	301	TH4	S11-C10-N9	-3.19	109.96	112.43
2	E	301	TH4	C4-C3-N2	-3.14	119.33	123.99
2	A	301	TH4	C6-C1-N2	-3.08	120.39	124.87
2	A	301	TH4	C4-C3-N2	-2.90	119.68	123.99
2	C	301	TH4	C4-C3-N2	-2.82	119.80	123.99
2	B	301	TH4	C4-C3-N2	-2.75	119.90	123.99
2	C	301	TH4	CL7-C1-N2	2.62	120.88	115.98
2	D	301	TH4	C4-C3-N2	-2.56	120.18	123.99
2	E	301	TH4	S11-C10-N9	-2.54	110.46	112.43
2	E	301	TH4	CL7-C1-N2	2.53	120.72	115.98
2	B	301	TH4	S11-C10-N9	-2.49	110.50	112.43
2	C	301	TH4	C5-C6-C1	2.40	119.77	117.36
2	A	301	TH4	CL7-C1-N2	2.40	120.48	115.98
2	D	301	TH4	S11-C10-N9	-2.38	110.58	112.43
2	A	301	TH4	S11-C10-N9	-2.34	110.61	112.43
2	E	301	TH4	C5-C6-C1	2.11	119.47	117.36

There are no chirality outliers.

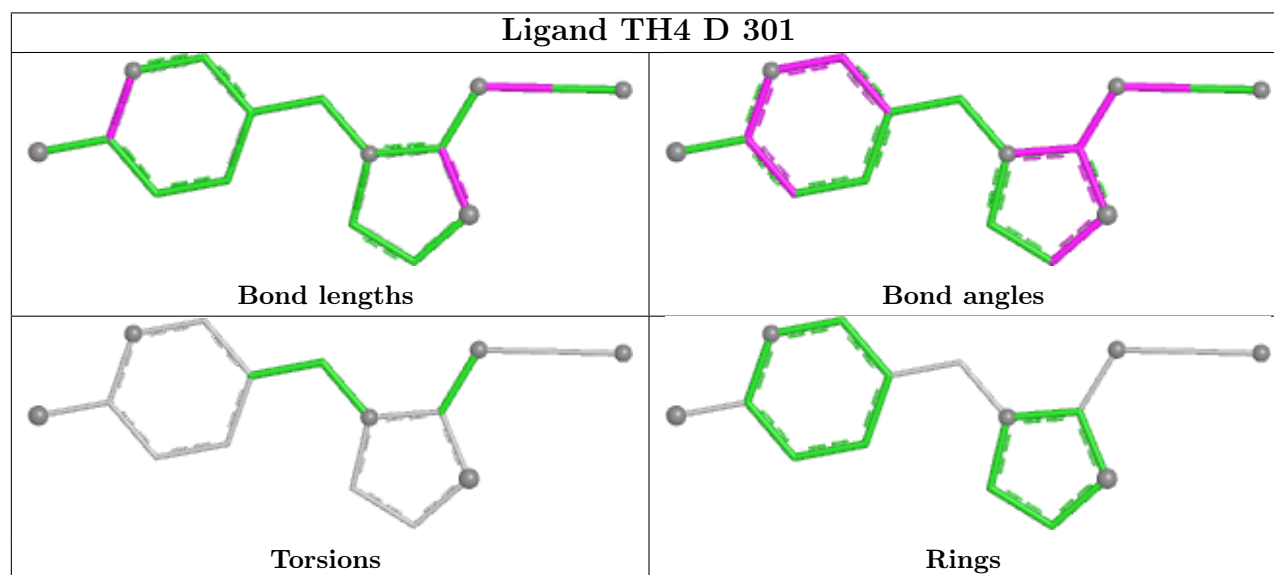
There are no torsion outliers.

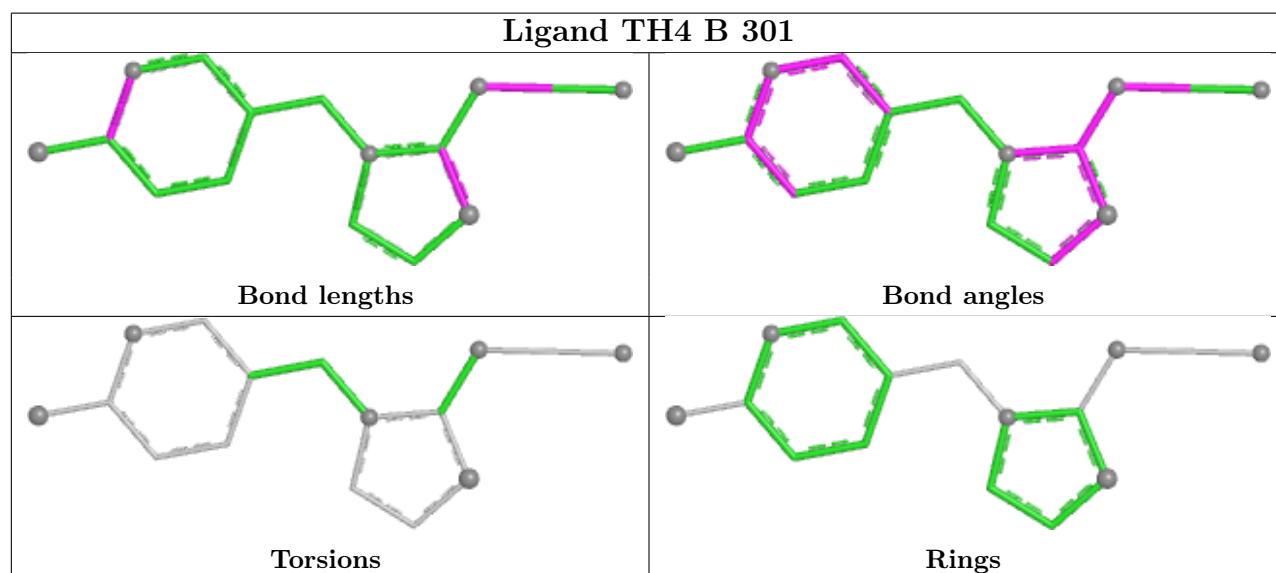
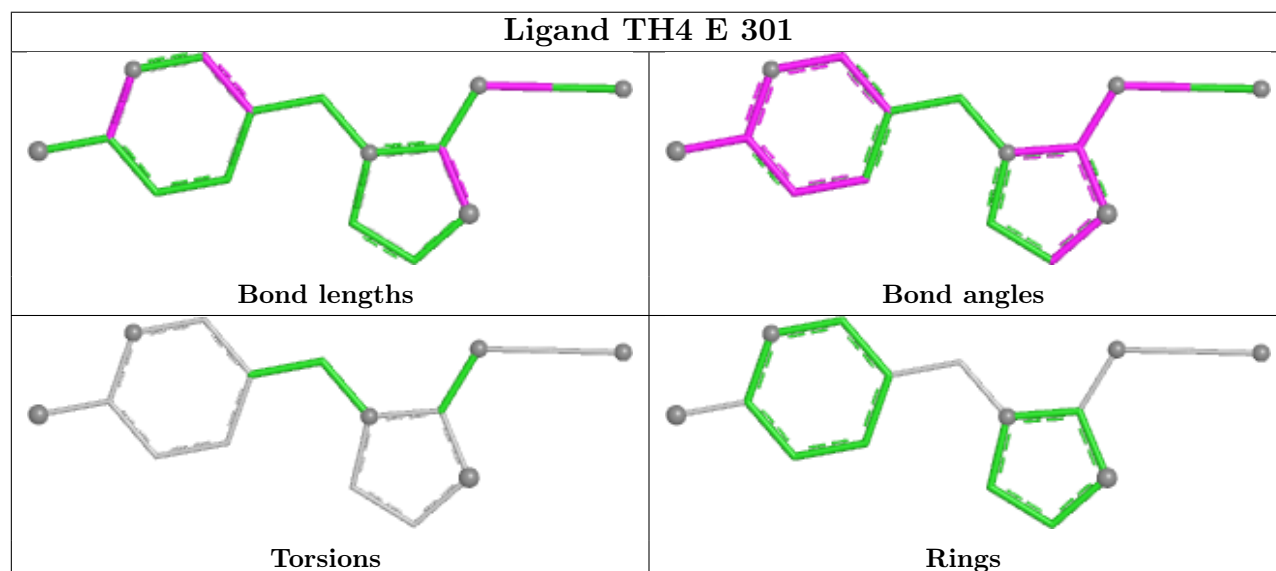
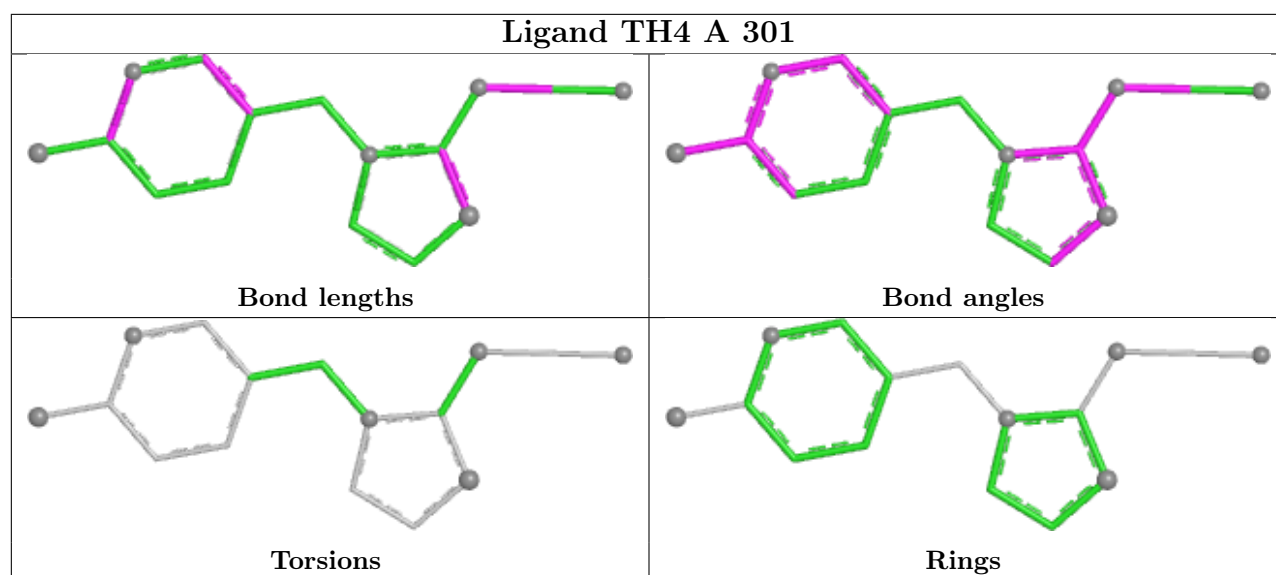
There are no ring outliers.

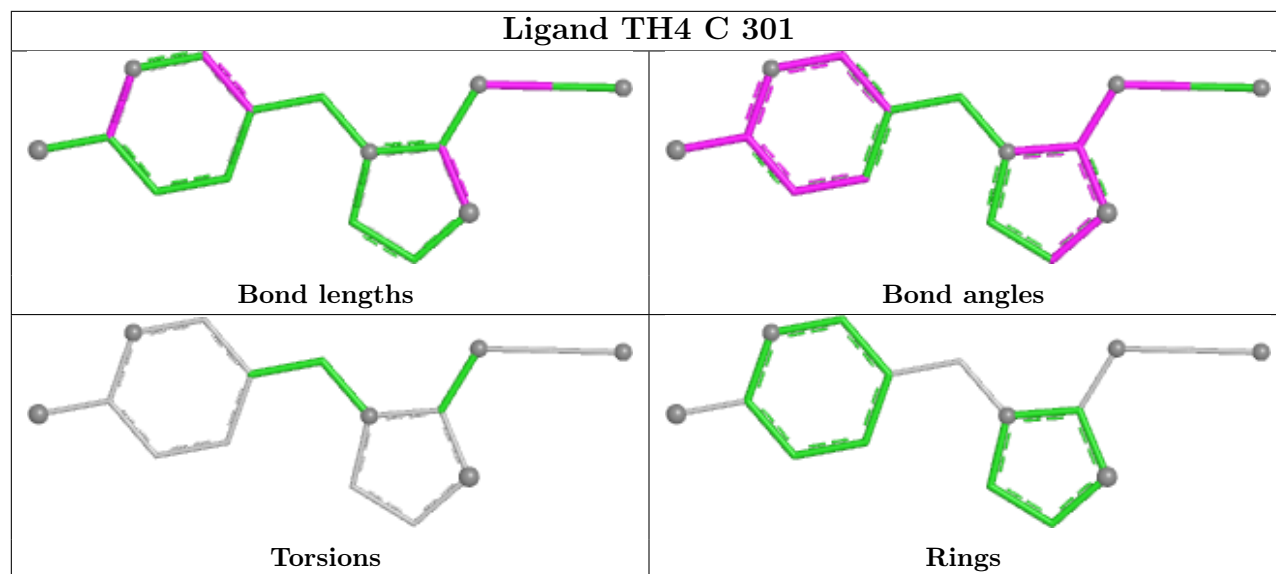
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	TH4	1	0
2	A	301	TH4	1	0
2	E	301	TH4	1	0
2	C	301	TH4	1	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	A	208/214 (97%)	1.08	32 (15%) 5 4	22, 42, 82, 93	0
1	B	209/214 (97%)	1.37	45 (21%) 2 2	24, 47, 81, 102	0
1	C	208/214 (97%)	1.41	50 (24%) 2 1	22, 47, 78, 91	0
1	D	208/214 (97%)	1.18	35 (16%) 4 3	16, 41, 89, 106	1 (0%)
1	E	208/214 (97%)	1.06	30 (14%) 6 5	15, 39, 78, 97	1 (0%)
All	All	1041/1070 (97%)	1.22	192 (18%) 3 3	15, 43, 82, 106	2 (0%)

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	SER	7.4
1	E	186	SER	6.8
1	A	185	TYR	6.7
1	D	185	TYR	6.3
1	E	187	CYS	6.2
1	B	185	TYR	5.8
1	B	187	CYS	5.5
1	A	189	PRO	5.4
1	E	189	PRO	5.3
1	C	1	ALA	5.0
1	A	186	SER	4.9
1	D	189	PRO	4.9
1	D	164	TYR	4.8
1	B	156	THR	4.7
1	E	185	TYR	4.6
1	E	188	CYS	4.5
1	C	187	CYS	4.4
1	B	189	PRO	4.4
1	A	164	TYR	4.4
1	E	164	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	187	CYS	4.3
1	D	182	SER	4.3
1	E	183	VAL	4.2
1	E	0	ALA	4.1
1	D	155	THR	4.1
1	C	188	CYS	3.9
1	B	63	LEU	3.8
1	D	24	ASP	3.8
1	C	158	ASN	3.8
1	C	185	TYR	3.8
1	D	160	ASP	3.7
1	D	188	CYS	3.7
1	A	25	ARG	3.6
1	D	181	ASN	3.6
1	E	156	THR	3.5
1	C	155	THR	3.5
1	B	6	ILE	3.5
1	D	187	CYS	3.4
1	A	158	ASN	3.4
1	C	9	ASN	3.4
1	B	164	TYR	3.4
1	D	207	SER	3.4
1	B	188	CYS	3.4
1	A	155	THR	3.3
1	D	183	VAL	3.3
1	A	188	CYS	3.3
1	B	184	THR	3.3
1	C	164	TYR	3.3
1	A	159	SER	3.2
1	C	207	SER	3.2
1	C	74	VAL	3.2
1	D	156	THR	3.2
1	B	192	TYR	3.2
1	A	207	SER	3.2
1	A	160	ASP	3.1
1	D	184	THR	3.1
1	C	0	ALA	3.1
1	D	186	SER	3.1
1	A	0	ALA	3.1
1	B	161	ASP	3.0
1	C	184	THR	3.0
1	C	183	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	3.0
1	A	192	TYR	3.0
1	D	128	VAL	3.0
1	B	158	ASN	3.0
1	A	53	TRP	2.9
1	B	0	ALA	2.9
1	A	154	PRO	2.9
1	E	55	ARG	2.9
1	A	190	GLU	2.9
1	B	159	SER	2.9
1	C	160	ASP	2.9
1	B	148	ARG	2.9
1	D	154	PRO	2.8
1	E	155	THR	2.8
1	B	31	VAL	2.8
1	B	12	GLN	2.8
1	C	159	SER	2.8
1	E	191	ALA	2.8
1	E	6	ILE	2.8
1	B	207	SER	2.8
1	E	53	TRP	2.8
1	D	158	ASN	2.8
1	C	191	ALA	2.8
1	B	190	GLU	2.8
1	B	155	THR	2.8
1	C	157	GLU	2.8
1	C	189	PRO	2.7
1	C	70	SER	2.7
1	C	161	ASP	2.7
1	C	55	ARG	2.7
1	B	154	PRO	2.7
1	B	18	VAL	2.7
1	C	71	PRO	2.7
1	E	162	SER	2.7
1	A	1	ALA	2.7
1	B	183	VAL	2.7
1	A	184	THR	2.7
1	C	153	ASP	2.7
1	B	44	ILE	2.6
1	C	8	TYR	2.6
1	D	165	PHE	2.6
1	E	184	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	8	TYR	2.6
1	C	23	ARG	2.6
1	A	55	ARG	2.6
1	D	157	GLU	2.6
1	C	154	PRO	2.6
1	B	17	ASP	2.5
1	A	205	GLY	2.5
1	D	191	ALA	2.5
1	E	190	GLU	2.5
1	B	10	ILE	2.5
1	C	19	ILE	2.5
1	D	161	ASP	2.5
1	D	168	TYR	2.5
1	C	171	PHE	2.5
1	A	34	LYS	2.4
1	B	11	ARG	2.4
1	C	14	SER	2.4
1	D	159	SER	2.4
1	C	105	VAL	2.4
1	B	13	THR	2.4
1	C	13	THR	2.4
1	D	162	SER	2.4
1	C	195	VAL	2.4
1	B	61	ARG	2.4
1	D	23	ARG	2.4
1	A	156	THR	2.4
1	C	59	SER	2.4
1	C	24	ASP	2.4
1	B	34	LYS	2.4
1	A	23	ARG	2.4
1	E	1	ALA	2.4
1	E	25	ARG	2.4
1	C	112	LEU	2.4
1	B	66	ASP	2.4
1	A	29	VAL	2.4
1	C	7	LEU	2.3
1	C	67	SER	2.3
1	A	206	ARG	2.3
1	B	1	ALA	2.3
1	B	69	HIS	2.3
1	B	70	SER	2.3
1	D	206	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	168	TYR	2.3
1	B	9	ASN	2.3
1	D	166	SER	2.3
1	A	183	VAL	2.3
1	B	157	GLU	2.2
1	E	23	ARG	2.2
1	D	72	ASP	2.2
1	D	126	SER	2.2
1	C	31	VAL	2.2
1	D	15	ARG	2.2
1	D	25	ARG	2.2
1	A	152	VAL	2.2
1	E	206	ARG	2.2
1	B	153	ASP	2.2
1	C	174	LEU	2.2
1	E	65	TRP	2.2
1	C	127	GLY	2.2
1	C	186	SER	2.2
1	C	197	VAL	2.2
1	E	207	SER	2.2
1	E	157	GLU	2.1
1	C	81	LEU	2.1
1	C	66	ASP	2.1
1	D	64	ALA	2.1
1	B	208	GLU	2.1
1	A	7	LEU	2.1
1	C	69	HIS	2.1
1	E	160	ASP	2.1
1	C	180	LYS	2.1
1	E	94	LYS	2.1
1	B	178	GLN	2.1
1	B	150	ILE	2.1
1	D	153	ASP	2.1
1	E	70	SER	2.1
1	E	11	ARG	2.1
1	A	19	ILE	2.1
1	D	152	VAL	2.1
1	C	129	ASP	2.0
1	C	206	ARG	2.0
1	A	21	THR	2.0
1	B	22	GLN	2.0
1	E	33	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	112	LEU	2.0
1	A	162	SER	2.0
1	B	55	ARG	2.0
1	C	148	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

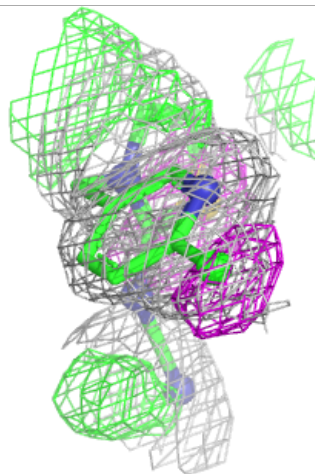
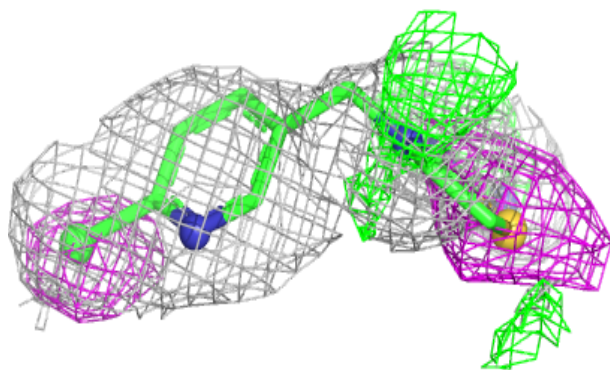
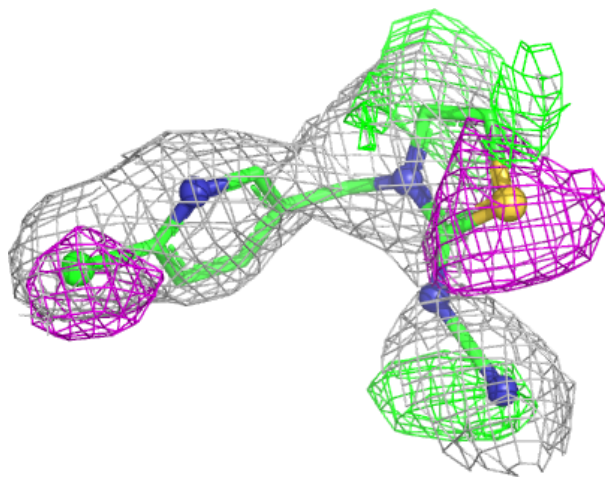
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	TH4	A	301	16/16	0.57	0.27	29,50,61,63	0
2	TH4	E	301	16/16	0.61	0.24	27,46,58,58	0
2	TH4	B	301	16/16	0.64	0.25	37,53,67,67	0
2	TH4	C	301	16/16	0.73	0.20	35,52,58,59	0
2	TH4	D	301	16/16	0.74	0.18	26,40,47,50	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.

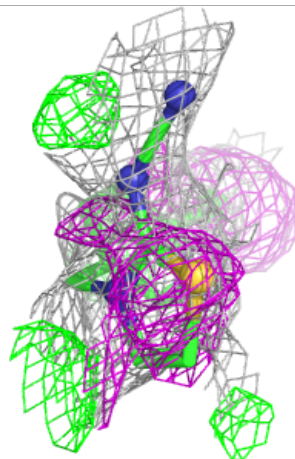
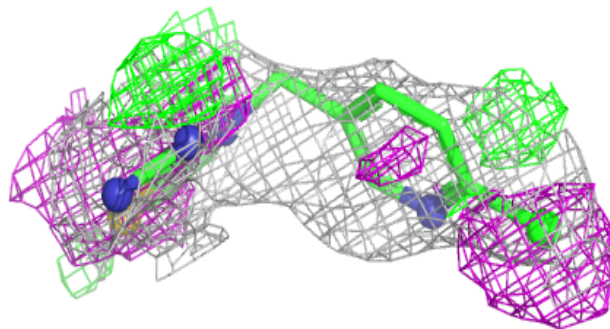
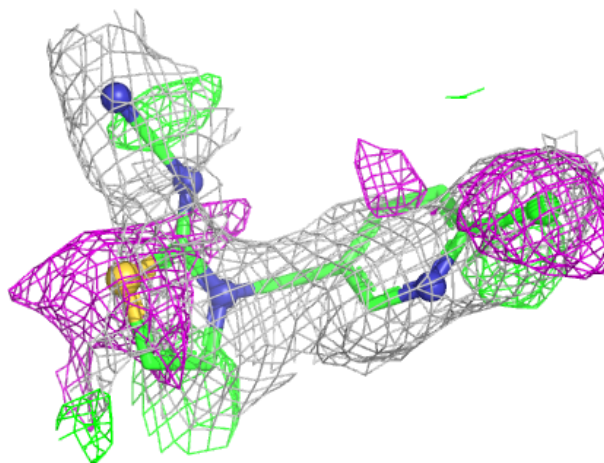
Electron density around TH4 A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



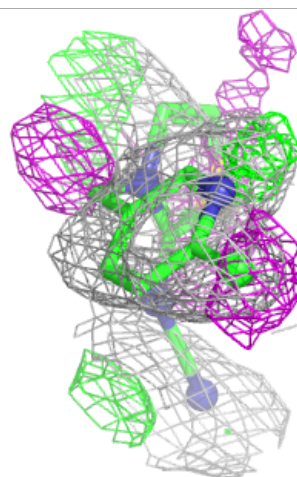
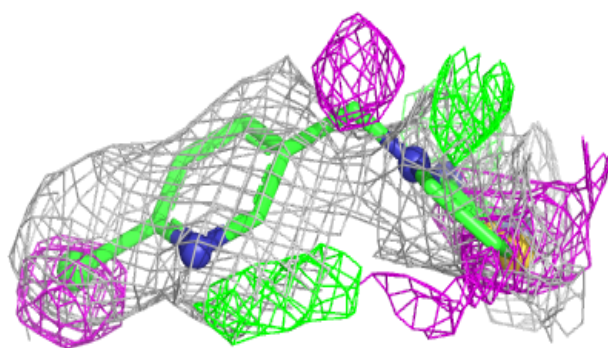
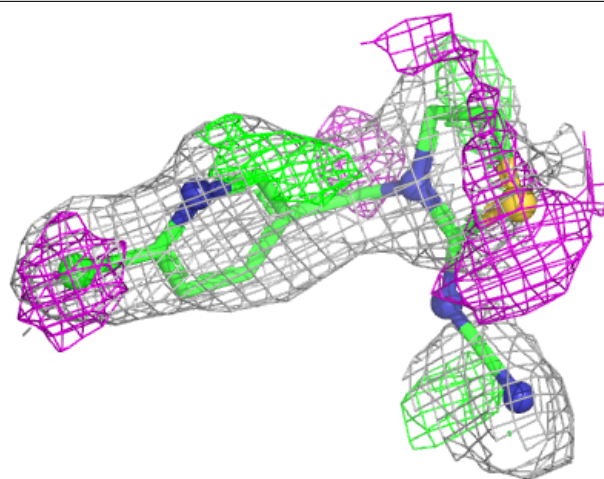
Electron density around TH4 E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



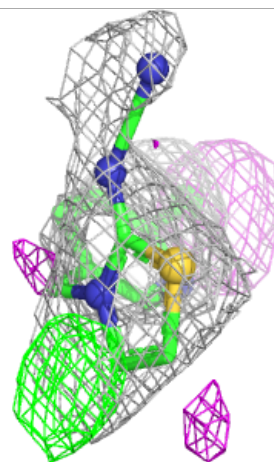
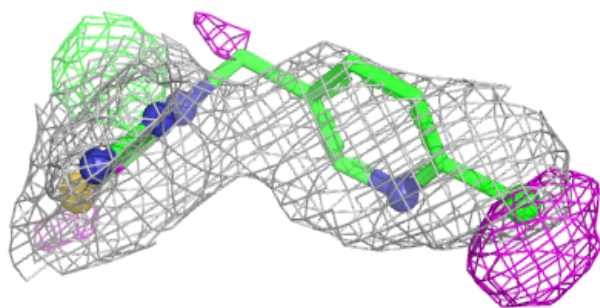
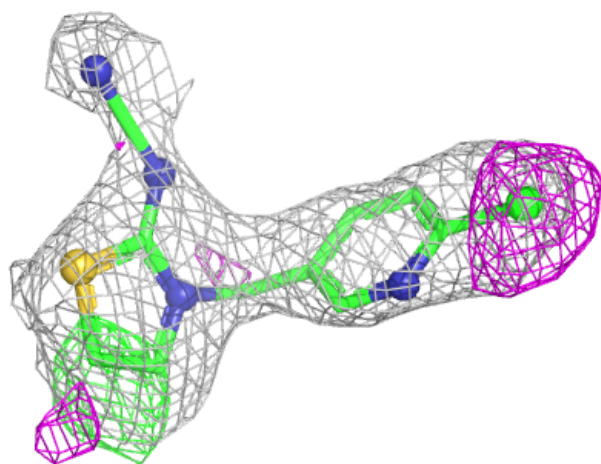
Electron density around TH4 B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



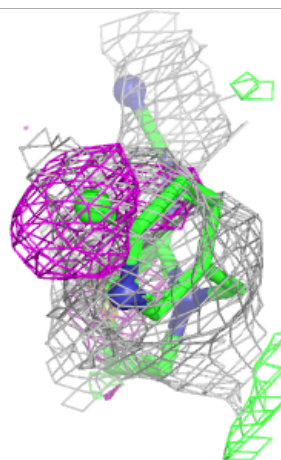
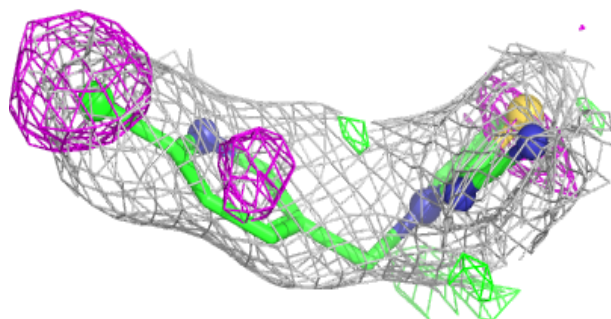
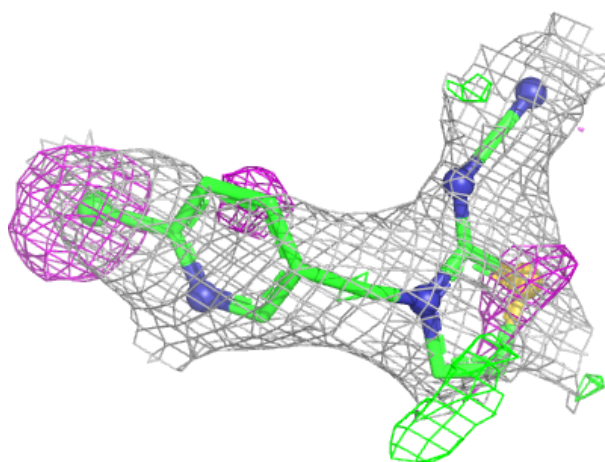
Electron density around TH4 C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TH4 D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.