



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 12:05 pm BST

PDB ID : 2CBQ
Title : Crystal structure of the neocarzinostatin 1Tes15 mutant bound to testosterone hemisuccinate.
Authors : Drevelle, A.; Graille, M.; Heyd, B.; Sorel, I.; Ulryck, N.; Pecorari, F.; Desmadril, M.; Van Tilbeurgh, H.; Minard, P.
Deposited on : 2006-01-06
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

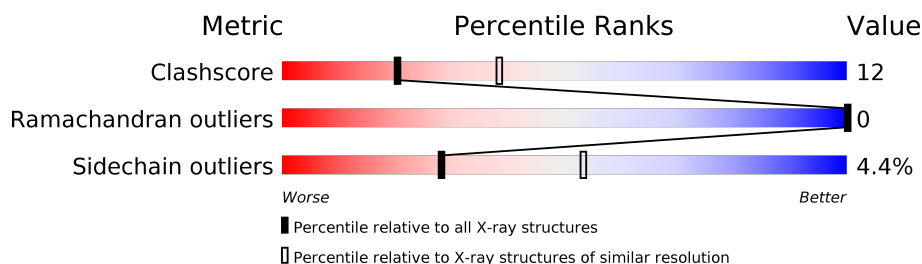
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	114	 75% 20% . .
1	B	114	 75% 22% ...
1	C	114	 75% 21% . .
1	D	114	 74% 24% . .
1	E	114	 75% 20% . . .
1	F	114	 75% 18% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5016 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 NEOCARZINOSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			
1	B	113	Total	C	N	O	S	0	0	0
			791	485	139	165	2			
1	C	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	D	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	E	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	F	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			

There are 42 discrepancies between the modelled and reference sequences:

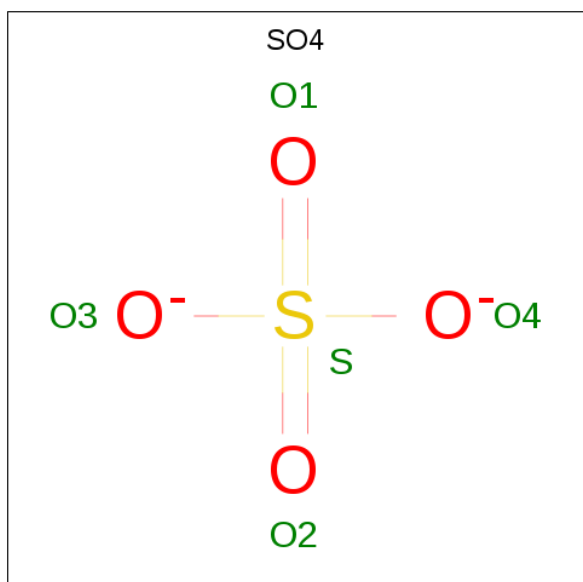
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	TRP	ASP	engineered mutation	UNP P0A3R9
A	35	TYR	GLY	engineered mutation	UNP P0A3R9
A	37	ARG	CYS	engineered mutation	UNP P0A3R9
A	39	ALA	TRP	engineered mutation	UNP P0A3R9
A	45	HIS	LEU	engineered mutation	UNP P0A3R9
A	47	SER	CYS	engineered mutation	UNP P0A3R9
A	52	LEU	PHE	engineered mutation	UNP P0A3R9
B	33	TRP	ASP	engineered mutation	UNP P0A3R9
B	35	TYR	GLY	engineered mutation	UNP P0A3R9
B	37	ARG	CYS	engineered mutation	UNP P0A3R9
B	39	ALA	TRP	engineered mutation	UNP P0A3R9
B	45	HIS	LEU	engineered mutation	UNP P0A3R9
B	47	SER	CYS	engineered mutation	UNP P0A3R9
B	52	LEU	PHE	engineered mutation	UNP P0A3R9
C	33	TRP	ASP	engineered mutation	UNP P0A3R9
C	35	TYR	GLY	engineered mutation	UNP P0A3R9
C	37	ARG	CYS	engineered mutation	UNP P0A3R9

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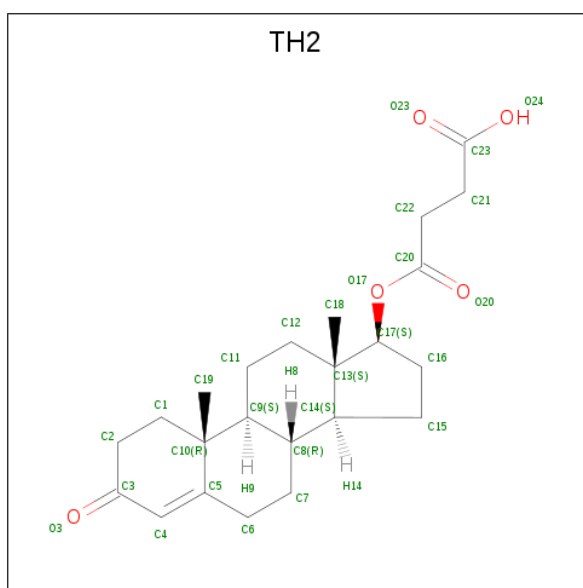
Chain	Residue	Modelled	Actual	Comment	Reference
C	39	ALA	TRP	engineered mutation	UNP P0A3R9
C	45	HIS	LEU	engineered mutation	UNP P0A3R9
C	47	SER	CYS	engineered mutation	UNP P0A3R9
C	52	LEU	PHE	engineered mutation	UNP P0A3R9
D	33	TRP	ASP	engineered mutation	UNP P0A3R9
D	35	TYR	GLY	engineered mutation	UNP P0A3R9
D	37	ARG	CYS	engineered mutation	UNP P0A3R9
D	39	ALA	TRP	engineered mutation	UNP P0A3R9
D	45	HIS	LEU	engineered mutation	UNP P0A3R9
D	47	SER	CYS	engineered mutation	UNP P0A3R9
D	52	LEU	PHE	engineered mutation	UNP P0A3R9
E	33	TRP	ASP	engineered mutation	UNP P0A3R9
E	35	TYR	GLY	engineered mutation	UNP P0A3R9
E	37	ARG	CYS	engineered mutation	UNP P0A3R9
E	39	ALA	TRP	engineered mutation	UNP P0A3R9
E	45	HIS	LEU	engineered mutation	UNP P0A3R9
E	47	SER	CYS	engineered mutation	UNP P0A3R9
E	52	LEU	PHE	engineered mutation	UNP P0A3R9
F	33	TRP	ASP	engineered mutation	UNP P0A3R9
F	35	TYR	GLY	engineered mutation	UNP P0A3R9
F	37	ARG	CYS	engineered mutation	UNP P0A3R9
F	39	ALA	TRP	engineered mutation	UNP P0A3R9
F	45	HIS	LEU	engineered mutation	UNP P0A3R9
F	47	SER	CYS	engineered mutation	UNP P0A3R9
F	52	LEU	PHE	engineered mutation	UNP P0A3R9

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is TESTOSTERONE HEMISUCCINATE (three-letter code: TH2) (formula: $C_{23}H_{32}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 23 5	0	0
3	A	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	C	1	Total C O 28 23 5	0	0
3	D	1	Total C O 28 23 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			28	23	5		
3	F	1	Total	C	O	0	0
			28	23	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	17	Total	O	0	0
			17	17		
4	C	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	14	Total	O	0	0
			14	14		
4	F	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NEOCARZINOSTATIN

Chain A: 



• Molecule 1: NEOCARZINOSTATIN

Chain B: 



• Molecule 1: NEOCARZINOSTATIN

Chain C: 



• Molecule 1: NEOCARZINOSTATIN

Chain D: 



• Molecule 1: NEOCARZINOSTATIN

Chain E: 



• Molecule 1: NEOCARZINOSTATIN

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.98 Å 97.83 Å 129.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 25.51 – 1.28	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.60) 42.5 (25.51-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 1.28 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.257 0.777 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.67$, $\langle L^2 \rangle = 0.55$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.30	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8852e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SO4, TH2

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	0.35	0/787	0.64	0/1078
1	B	0.38	0/806	0.64	1/1104 (0.1%)
1	C	0.43	1/795 (0.1%)	0.68	1/1089 (0.1%)
1	D	0.42	1/795 (0.1%)	0.66	1/1089 (0.1%)
1	E	0.41	1/795 (0.1%)	0.67	2/1089 (0.2%)
1	F	0.36	0/787	0.63	0/1078
All	All	0.39	3/4765 (0.1%)	0.66	5/6527 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	ASN	CG-OD1	5.51	1.36	1.24
1	D	113	ASN	CG-OD1	5.50	1.36	1.24
1	E	113	ASN	CG-OD1	5.47	1.35	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	D	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	C	113	ASN	OD1-CG-ND2	-6.87	106.11	121.90
1	E	52	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	52	LEU	CA-CB-CG	5.47	127.87	115.30

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	773	0	731	21	0
1	B	791	0	744	24	0
1	C	781	0	737	23	0
1	D	781	0	737	16	0
1	E	781	0	737	22	0
1	F	773	0	731	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	56	0	62	3	0
3	B	56	0	62	1	0
3	C	28	0	31	0	0
3	D	28	0	31	0	0
3	E	28	0	31	0	0
3	F	28	0	31	0	0
4	A	15	0	0	0	0
4	B	17	0	0	1	0
4	C	17	0	0	2	0
4	D	17	0	0	0	0
4	E	14	0	0	0	0
4	F	7	0	0	0	0
All	All	5016	0	4665	119	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 12.

All (119) 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:C:37:ARG:HE	1:C:94:GLN:HE21	1.17	0.92
1:D:35:TYR:HB3	1:D:52:LEU:HD23	1.53	0.90
3:A:1115:TH2:H6C2	1:F:20:LYS:HB2	1.53	0.88
3:B:1117:TH2:H6C2	1:C:20:LYS:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:NE	1:E:94:GLN:HE21	1.86	0.74
1:E:82:ARG:HG3	1:E:82:ARG:HH11	1.55	0.70
1:B:34:VAL:HG22	1:B:97:LEU:CD1	2.21	0.69
1:A:87:ASP:OD2	1:A:89:THR:HB	1.93	0.69
1:E:39:ALA:HA	1:E:45:HIS:HD2	1.58	0.69
1:A:52:LEU:HD22	1:A:53:SER:H	1.60	0.66
1:C:55:VAL:HG22	1:C:63:ALA:HB1	1.79	0.65
1:C:37:ARG:NE	1:C:94:GLN:HE21	1.92	0.64
1:B:34:VAL:HG22	1:B:97:LEU:HD12	1.79	0.64
1:E:37:ARG:CZ	1:E:94:GLN:HE21	2.12	0.63
1:F:82:ARG:HG2	1:F:82:ARG:NH1	2.14	0.63
1:C:34:VAL:HG23	1:C:54:SER:HA	1.80	0.62
1:E:39:ALA:HA	1:E:45:HIS:CD2	2.34	0.62
1:B:74:GLU:HG3	1:B:82:ARG:NH1	2.15	0.61
1:E:40:VAL:HB	1:E:83:TRP:CZ2	2.34	0.61
1:D:87:ASP:OD2	1:D:89:THR:HB	2.01	0.61
1:B:93:CYS:HB2	4:B:2014:HOH:O	2.00	0.61
1:C:35:TYR:HB3	1:C:52:LEU:HD23	1.84	0.60
1:F:82:ARG:HG2	1:F:82:ARG:HH11	1.69	0.58
1:C:99:ASP:OD2	1:C:103:ASN:HB2	2.04	0.57
1:A:48:ASN:HB2	1:A:73:PHE:CD1	2.39	0.57
1:E:82:ARG:HG3	1:E:82:ARG:NH1	2.20	0.56
1:B:10:SER:O	1:B:110:ILE:HA	2.05	0.56
1:E:52:LEU:HD13	1:E:53:SER:N	2.19	0.56
1:D:7:VAL:HG21	1:D:95:VAL:HB	1.87	0.55
1:C:74:GLU:OE1	1:C:82:ARG:NE	2.40	0.55
1:A:41:ASP:HB3	1:A:44:VAL:HB	1.89	0.54
1:B:34:VAL:HG22	1:B:97:LEU:HD11	1.88	0.54
1:A:52:LEU:HD13	1:A:53:SER:N	2.22	0.54
1:B:48:ASN:HB2	1:B:73:PHE:CD1	2.42	0.54
1:B:20:LYS:NZ	1:B:22:ALA:HB2	2.23	0.54
1:C:58:ASP:HB2	4:C:2010:HOH:O	2.08	0.54
1:C:48:ASN:HB2	1:C:73:PHE:CD1	2.44	0.53
1:D:52:LEU:HD13	1:D:52:LEU:C	2.28	0.53
1:A:33:TRP:CE3	1:A:52:LEU:HD21	2.43	0.53
1:F:82:ARG:HH11	1:F:82:ARG:CG	2.23	0.52
1:F:76:PHE:CE1	1:F:82:ARG:HG3	2.45	0.52
1:F:94:GLN:OE1	1:F:107:GLY:HA3	2.09	0.52
1:C:33:TRP:CE3	1:C:52:LEU:HD11	2.45	0.52
1:C:37:ARG:HH21	1:C:94:GLN:NE2	2.08	0.51
1:A:33:TRP:CZ2	1:C:80:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:CZ	1:E:94:GLN:NE2	2.72	0.51
1:A:52:LEU:C	1:A:52:LEU:HD13	2.31	0.51
1:E:48:ASN:HB2	1:E:73:PHE:CD1	2.45	0.51
1:C:37:ARG:HE	1:C:94:GLN:NE2	1.97	0.50
1:C:52:LEU:HD13	1:C:53:SER:N	2.27	0.50
1:D:80:GLY:HA2	1:E:33:TRP:CZ2	2.47	0.50
1:A:52:LEU:HD22	1:A:53:SER:N	2.26	0.49
1:F:97:LEU:HD23	1:F:105:PRO:HG3	1.94	0.49
1:F:7:VAL:HG12	1:F:9:PRO:O	2.13	0.49
1:E:52:LEU:HD13	1:E:52:LEU:C	2.32	0.49
1:B:35:TYR:CD2	1:B:35:TYR:N	2.80	0.48
1:A:5:ALA:HB2	1:A:105:PRO:HG3	1.94	0.48
1:B:72:SER:HA	1:B:86:VAL:O	2.13	0.48
1:E:87:ASP:OD2	1:E:89:THR:HB	2.14	0.48
1:E:7:VAL:HG21	1:E:95:VAL:HB	1.96	0.48
1:E:35:TYR:CD2	1:E:35:TYR:N	2.82	0.48
1:A:33:TRP:HE3	1:A:52:LEU:HD21	1.78	0.47
1:A:33:TRP:CH2	1:C:80:GLY:HA2	2.50	0.47
1:F:57:ALA:HB1	1:F:61:GLY:HA2	1.97	0.47
1:C:52:LEU:C	1:C:52:LEU:HD13	2.36	0.46
1:A:47:SER:HB2	3:A:1114:TH2:O3	2.15	0.46
1:B:52:LEU:HD22	1:B:53:SER:N	2.31	0.46
1:E:71:ARG:HH21	1:E:71:ARG:HB2	1.80	0.45
1:A:77:LEU:HD12	1:A:81:THR:HB	1.97	0.45
1:B:40:VAL:O	1:B:41:ASP:HB2	2.15	0.45
1:B:27:GLN:O	1:B:30:THR:HB	2.16	0.45
1:C:55:VAL:CG2	1:C:63:ALA:HB1	2.46	0.45
1:D:34:VAL:HG12	1:D:67:LEU:HD22	1.98	0.45
1:A:7:VAL:O	1:A:10:SER:HB3	2.15	0.45
1:B:112:PHE:CD1	1:B:112:PHE:N	2.84	0.45
1:F:41:ASP:OD1	1:F:42:THR:N	2.47	0.45
1:D:74:GLU:OE1	1:D:82:ARG:NE	2.37	0.45
1:D:5:ALA:HB2	1:D:105:PRO:HG3	1.99	0.44
1:A:21:VAL:O	1:A:64:SER:HA	2.17	0.44
1:A:80:GLY:HA2	1:C:33:TRP:CZ2	2.53	0.44
1:E:57:ALA:HB1	1:E:61:GLY:HA2	1.99	0.44
1:B:52:LEU:HD22	1:B:53:SER:H	1.82	0.44
1:B:33:TRP:CE3	1:B:52:LEU:HD21	2.53	0.43
1:C:7:VAL:HG12	1:C:9:PRO:O	2.17	0.43
1:F:8:THR:HA	1:F:9:PRO:C	2.37	0.43
1:D:33:TRP:CZ2	1:E:80:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ASN:HB2	1:E:73:PHE:CG	2.54	0.43
1:B:35:TYR:HB3	1:B:52:LEU:HD23	2.00	0.43
1:D:48:ASN:ND2	1:D:51:ASP:HB2	2.34	0.43
1:B:33:TRP:CZ3	1:B:52:LEU:HD11	2.54	0.43
1:E:37:ARG:NH1	1:E:45:HIS:ND1	2.66	0.43
1:A:112:PHE:N	1:A:112:PHE:CD1	2.86	0.43
1:D:41:ASP:HB3	1:D:44:VAL:CG2	2.49	0.43
1:A:47:SER:O	1:A:75:GLY:HA2	2.19	0.42
1:E:72:SER:HA	1:E:86:VAL:O	2.19	0.42
1:C:36:GLN:HB2	4:C:2005:HOH:O	2.19	0.42
1:B:20:LYS:HZ3	1:B:22:ALA:HB2	1.84	0.42
1:C:82:ARG:HH22	1:C:84:GLY:HA2	1.85	0.42
1:C:5:ALA:HA	1:C:22:ALA:O	2.19	0.42
1:B:9:PRO:HG2	1:B:13:LEU:CD2	2.50	0.41
1:B:97:LEU:HB3	1:B:105:PRO:HD2	2.02	0.41
1:F:49:PRO:HA	1:F:52:LEU:HB2	2.02	0.41
1:E:82:ARG:CG	1:E:82:ARG:NH1	2.83	0.41
1:F:17:THR:O	1:F:69:VAL:HG22	2.20	0.41
1:D:2:ALA:HA	1:D:3:PRO:HD3	1.89	0.41
1:F:9:PRO:HG2	1:F:13:LEU:CD2	2.50	0.41
1:F:74:GLU:CD	1:F:82:ARG:NH1	2.73	0.41
1:B:5:ALA:HB2	1:B:105:PRO:HG3	2.03	0.41
1:F:55:VAL:HG22	1:F:63:ALA:HB1	2.03	0.41
1:A:5:ALA:HA	1:A:22:ALA:O	2.20	0.41
1:D:94:GLN:OE1	1:D:107:GLY:HA3	2.21	0.41
1:D:17:THR:O	1:D:69:VAL:HG22	2.20	0.41
1:D:48:ASN:HB2	1:D:73:PHE:CD1	2.56	0.41
1:D:35:TYR:N	1:D:35:TYR:CD2	2.88	0.41
1:F:112:PHE:N	1:F:112:PHE:CD1	2.89	0.41
1:F:35:TYR:HB3	1:F:52:LEU:HD23	2.02	0.40
1:A:35:TYR:CD2	3:A:1114:TH2:H6C1	2.57	0.40
1:B:33:TRP:O	1:B:97:LEU:HA	2.20	0.40
1:B:33:TRP:CZ2	1:F:80:GLY:HA2	2.57	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	A	109/114 (96%)	106 (97%)	3 (3%)	0	100	100
1	B	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
1	C	110/114 (96%)	104 (94%)	6 (6%)	0	100	100
1	D	110/114 (96%)	105 (96%)	5 (4%)	0	100	100
1	E	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
1	F	109/114 (96%)	105 (96%)	4 (4%)	0	100	100
All	All	659/684 (96%)	634 (96%)	25 (4%)	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	A	79/81 (98%)	75 (95%)	4 (5%)	24	46
1	B	81/81 (100%)	78 (96%)	3 (4%)	34	60
1	C	80/81 (99%)	78 (98%)	2 (2%)	47	73
1	D	80/81 (99%)	77 (96%)	3 (4%)	33	59
1	E	80/81 (99%)	75 (94%)	5 (6%)	18	36
1	F	79/81 (98%)	75 (95%)	4 (5%)	24	46
All	All	479/486 (99%)	458 (96%)	21 (4%)	28	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	52	LEU
1	A	79	ASP
1	A	97	LEU
1	B	20	LYS
1	B	52	LEU
1	B	71	ARG
1	C	55	VAL
1	C	113	ASN
1	D	52	LEU
1	D	55	VAL
1	D	79	ASP
1	E	52	LEU
1	E	55	VAL
1	E	71	ARG
1	E	97	LEU
1	E	113	ASN
1	F	8	THR
1	F	52	LEU
1	F	55	VAL
1	F	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	94	GLN
1	C	94	GLN
1	D	45	HIS
1	E	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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
3	TH2	B	1117	-	28,31,31	1.67	9 (32%)	45,48,48	2.09	11 (24%)
3	TH2	C	1115	-	28,31,31	1.63	7 (25%)	45,48,48	1.98	10 (22%)
3	TH2	B	1116	-	28,31,31	1.65	6 (21%)	45,48,48	1.97	10 (22%)
2	SO4	E	1114	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	B	1115	-	4,4,4	0.30	0	6,6,6	0.16	0
3	TH2	F	1114	-	28,31,31	1.56	8 (28%)	45,48,48	2.00	9 (20%)
3	TH2	A	1114	-	28,31,31	1.63	7 (25%)	45,48,48	2.03	12 (26%)
3	TH2	D	1114	-	28,31,31	1.66	7 (25%)	45,48,48	2.03	11 (24%)
2	SO4	F	1113	-	4,4,4	0.25	0	6,6,6	0.10	0
3	TH2	A	1115	-	28,31,31	1.66	9 (32%)	45,48,48	2.02	10 (22%)
2	SO4	A	1113	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	C	1114	-	4,4,4	0.26	0	6,6,6	0.13	0
3	TH2	E	1115	-	28,31,31	1.61	8 (28%)	45,48,48	2.05	11 (24%)

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	TH2	B	1117	-	-	6/7/67/67	0/4/4/4
3	TH2	C	1115	-	-	5/7/67/67	0/4/4/4
3	TH2	B	1116	-	-	3/7/67/67	0/4/4/4
3	TH2	D	1114	-	-	5/7/67/67	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TH2	A	1114	-	-	2/7/67/67	0/4/4/4
3	TH2	A	1115	-	-	3/7/67/67	0/4/4/4
3	TH2	F	1114	-	-	6/7/67/67	0/4/4/4
3	TH2	E	1115	-	-	6/7/67/67	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1114	TH2	C10-C5	3.43	1.59	1.52
3	D	1114	TH2	C10-C5	3.34	1.59	1.52
3	B	1117	TH2	C10-C5	3.24	1.59	1.52
3	C	1115	TH2	C10-C5	3.20	1.59	1.52
3	B	1116	TH2	C10-C5	3.06	1.58	1.52
3	A	1115	TH2	C10-C5	2.93	1.58	1.52
3	B	1116	TH2	O17-C17	-2.80	1.41	1.46
3	D	1114	TH2	C11-C9	2.73	1.58	1.53
3	E	1115	TH2	C16-C17	2.73	1.59	1.53
3	F	1114	TH2	C10-C5	2.71	1.58	1.52
3	A	1114	TH2	O17-C17	-2.66	1.41	1.46
3	E	1115	TH2	C10-C5	2.56	1.57	1.52
3	E	1115	TH2	O17-C17	-2.55	1.42	1.46
3	B	1117	TH2	C11-C9	2.54	1.58	1.53
3	A	1115	TH2	C16-C17	2.52	1.59	1.53
3	C	1115	TH2	C11-C9	2.50	1.58	1.53
3	E	1115	TH2	C8-C9	2.50	1.58	1.53
3	A	1114	TH2	C11-C9	2.50	1.57	1.53
3	B	1117	TH2	C8-C9	2.47	1.58	1.53
3	F	1114	TH2	O17-C17	-2.46	1.42	1.46
3	D	1114	TH2	C16-C17	2.46	1.59	1.53
3	A	1115	TH2	C4-C5	2.45	1.38	1.34
3	B	1117	TH2	C16-C17	2.44	1.59	1.53
3	F	1114	TH2	C10-C9	2.42	1.60	1.56
3	D	1114	TH2	C7-C8	2.41	1.57	1.53
3	B	1116	TH2	C11-C9	2.40	1.57	1.53
3	B	1116	TH2	O17-C20	-2.40	1.27	1.34
3	B	1116	TH2	C16-C17	2.39	1.58	1.53
3	C	1115	TH2	O17-C17	-2.38	1.42	1.46
3	A	1115	TH2	C8-C9	2.37	1.58	1.53
3	A	1115	TH2	C1-C10	2.36	1.58	1.54
3	D	1114	TH2	C8-C9	2.36	1.58	1.53
3	E	1115	TH2	O17-C20	-2.36	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1117	TH2	C7-C8	2.31	1.57	1.53
3	F	1114	TH2	C7-C8	2.31	1.57	1.53
3	A	1115	TH2	C13-C17	2.29	1.57	1.53
3	A	1115	TH2	C11-C9	2.29	1.57	1.53
3	B	1117	TH2	C4-C5	2.28	1.37	1.34
3	A	1114	TH2	O17-C20	-2.28	1.27	1.34
3	F	1114	TH2	C16-C17	2.27	1.58	1.53
3	D	1114	TH2	O17-C17	-2.22	1.42	1.46
3	A	1114	TH2	C8-C9	2.20	1.57	1.53
3	A	1115	TH2	C10-C9	2.20	1.59	1.56
3	A	1114	TH2	C10-C9	2.17	1.59	1.56
3	D	1114	TH2	C1-C10	2.15	1.58	1.54
3	E	1115	TH2	C1-C10	2.12	1.58	1.54
3	E	1115	TH2	C4-C5	2.12	1.37	1.34
3	B	1116	TH2	C10-C9	2.11	1.59	1.56
3	E	1115	TH2	C11-C9	2.11	1.57	1.53
3	C	1115	TH2	C10-C9	2.11	1.59	1.56
3	F	1114	TH2	O17-C20	-2.11	1.28	1.34
3	C	1115	TH2	C16-C17	2.09	1.58	1.53
3	B	1117	TH2	O17-C17	-2.08	1.42	1.46
3	F	1114	TH2	C8-C9	2.06	1.57	1.53
3	B	1117	TH2	O17-C20	-2.05	1.28	1.34
3	C	1115	TH2	O3-C3	-2.05	1.19	1.23
3	F	1114	TH2	C1-C10	2.05	1.58	1.54
3	A	1115	TH2	O17-C20	-2.04	1.28	1.34
3	A	1114	TH2	C16-C17	2.03	1.58	1.53
3	B	1117	TH2	O3-C3	-2.01	1.19	1.23
3	C	1115	TH2	C7-C8	2.00	1.57	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1115	TH2	O17-C17-C16	5.89	125.74	111.07
3	B	1117	TH2	O17-C17-C16	5.50	124.76	111.07
3	B	1117	TH2	C17-O17-C20	5.42	128.13	117.92
3	E	1115	TH2	C17-O17-C20	5.33	127.95	117.92
3	A	1115	TH2	O17-C17-C16	5.25	124.15	111.07
3	F	1114	TH2	O17-C17-C16	5.24	124.12	111.07
3	A	1114	TH2	O17-C17-C13	5.22	123.53	111.09
3	B	1116	TH2	O17-C17-C16	5.21	124.05	111.07
3	D	1114	TH2	O17-C17-C13	5.17	123.42	111.09
3	D	1114	TH2	O17-C17-C16	5.08	123.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1114	TH2	O17-C17-C13	5.00	123.01	111.09
3	A	1115	TH2	C17-O17-C20	5.00	127.33	117.92
3	C	1115	TH2	C17-O17-C20	4.93	127.20	117.92
3	A	1115	TH2	O17-C17-C13	4.90	122.76	111.09
3	B	1117	TH2	O17-C17-C13	4.84	122.62	111.09
3	C	1115	TH2	O17-C17-C13	4.80	122.54	111.09
3	C	1115	TH2	O17-C17-C16	4.80	123.02	111.07
3	E	1115	TH2	C11-C9-C10	-4.70	106.89	113.08
3	A	1114	TH2	O17-C17-C16	4.70	122.78	111.07
3	B	1116	TH2	C17-O17-C20	4.59	126.56	117.92
3	A	1114	TH2	C17-O17-C20	4.47	126.33	117.92
3	B	1116	TH2	O17-C17-C13	4.44	121.67	111.09
3	F	1114	TH2	C17-O17-C20	4.44	126.27	117.92
3	D	1114	TH2	C17-O17-C20	4.42	126.24	117.92
3	B	1116	TH2	C11-C9-C10	-4.37	107.32	113.08
3	B	1117	TH2	C11-C9-C10	-4.34	107.37	113.08
3	D	1114	TH2	C11-C9-C10	-4.32	107.38	113.08
3	A	1114	TH2	C11-C9-C10	-4.31	107.40	113.08
3	C	1115	TH2	C11-C9-C10	-4.30	107.41	113.08
3	A	1115	TH2	C11-C9-C10	-4.30	107.42	113.08
3	F	1114	TH2	C11-C9-C10	-4.24	107.50	113.08
3	D	1114	TH2	C12-C11-C9	-3.90	106.36	113.11
3	B	1117	TH2	C12-C11-C9	-3.77	106.58	113.11
3	E	1115	TH2	O17-C17-C13	3.74	120.00	111.09
3	A	1115	TH2	C12-C11-C9	-3.66	106.78	113.11
3	A	1114	TH2	C12-C11-C9	-3.65	106.79	113.11
3	F	1114	TH2	C12-C11-C9	-3.59	106.89	113.11
3	E	1115	TH2	C12-C11-C9	-3.57	106.93	113.11
3	B	1116	TH2	C12-C11-C9	-3.42	107.19	113.11
3	A	1114	TH2	O17-C20-O20	3.39	131.89	123.70
3	C	1115	TH2	O17-C20-O20	3.31	131.69	123.70
3	C	1115	TH2	C12-C11-C9	-3.31	107.39	113.11
3	E	1115	TH2	O17-C20-O20	3.25	131.55	123.70
3	B	1117	TH2	O17-C20-O20	3.21	131.45	123.70
3	B	1116	TH2	O17-C20-O20	3.11	131.21	123.70
3	A	1115	TH2	C16-C17-C13	-3.06	102.00	105.21
3	B	1117	TH2	C16-C17-C13	-3.03	102.03	105.21
3	A	1115	TH2	O17-C20-O20	2.98	130.91	123.70
3	C	1115	TH2	C16-C17-C13	-2.94	102.12	105.21
3	D	1114	TH2	C16-C17-C13	-2.88	102.19	105.21
3	F	1114	TH2	O17-C20-O20	2.86	130.62	123.70
3	F	1114	TH2	C16-C17-C13	-2.86	102.21	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1117	TH2	C18-C13-C14	2.85	117.03	111.71
3	A	1114	TH2	C16-C17-C13	-2.85	102.22	105.21
3	E	1115	TH2	C16-C17-C13	-2.83	102.24	105.21
3	D	1114	TH2	O17-C20-O20	2.78	130.41	123.70
3	F	1114	TH2	C18-C13-C14	2.77	116.88	111.71
3	D	1114	TH2	C18-C13-C14	2.73	116.81	111.71
3	B	1116	TH2	C16-C17-C13	-2.69	102.38	105.21
3	A	1115	TH2	C18-C13-C14	2.60	116.57	111.71
3	A	1114	TH2	C9-C10-C5	-2.56	105.64	109.65
3	A	1114	TH2	O20-C20-C22	-2.53	113.85	123.73
3	B	1117	TH2	O20-C20-C22	-2.52	113.90	123.73
3	F	1114	TH2	O20-C20-C22	-2.51	113.96	123.73
3	D	1114	TH2	O20-C20-C22	-2.47	114.11	123.73
3	B	1116	TH2	O20-C20-C22	-2.41	114.33	123.73
3	A	1115	TH2	C9-C10-C5	-2.41	105.88	109.65
3	A	1114	TH2	C18-C13-C14	2.34	116.08	111.71
3	A	1115	TH2	O20-C20-C22	-2.34	114.62	123.73
3	C	1115	TH2	O20-C20-C22	-2.30	114.74	123.73
3	E	1115	TH2	O20-C20-C22	-2.30	114.77	123.73
3	E	1115	TH2	C18-C13-C14	2.29	115.99	111.71
3	D	1114	TH2	C9-C10-C5	-2.29	106.06	109.65
3	B	1116	TH2	C18-C13-C14	2.29	115.98	111.71
3	C	1115	TH2	C9-C10-C5	-2.25	106.13	109.65
3	E	1115	TH2	C9-C10-C5	-2.21	106.19	109.65
3	A	1114	TH2	C22-C21-C23	-2.18	109.02	112.67
3	B	1117	TH2	C9-C10-C5	-2.17	106.25	109.65
3	C	1115	TH2	C15-C16-C17	2.17	108.30	104.69
3	E	1115	TH2	C19-C10-C9	-2.15	109.12	111.68
3	B	1117	TH2	C19-C10-C9	-2.15	109.12	111.68
3	B	1116	TH2	C15-C16-C17	2.06	108.13	104.69
3	A	1114	TH2	C15-C16-C17	2.04	108.08	104.69
3	D	1114	TH2	C19-C10-C9	-2.01	109.28	111.68

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1117	TH2	C16-C17-O17-C20
3	C	1115	TH2	C22-C20-O17-C17
3	B	1116	TH2	C16-C17-O17-C20
3	F	1114	TH2	C16-C17-O17-C20
3	A	1114	TH2	C22-C20-O17-C17

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Mol	Chain	Res	Type	Atoms
3	D	1114	TH2	C16-C17-O17-C20
3	A	1115	TH2	C23-C21-C22-C20
3	E	1115	TH2	C16-C17-O17-C20
3	E	1115	TH2	C23-C21-C22-C20
3	C	1115	TH2	O20-C20-O17-C17
3	B	1116	TH2	C22-C20-O17-C17
3	E	1115	TH2	C22-C20-O17-C17
3	A	1114	TH2	O20-C20-O17-C17
3	E	1115	TH2	O20-C20-O17-C17
3	C	1115	TH2	C16-C17-O17-C20
3	B	1117	TH2	C22-C20-O17-C17
3	F	1114	TH2	C22-C20-O17-C17
3	D	1114	TH2	C22-C20-O17-C17
3	A	1115	TH2	C22-C20-O17-C17
3	B	1116	TH2	O20-C20-O17-C17
3	A	1115	TH2	O20-C20-O17-C17
3	B	1117	TH2	O20-C20-O17-C17
3	F	1114	TH2	O20-C20-O17-C17
3	D	1114	TH2	O20-C20-O17-C17
3	F	1114	TH2	C23-C21-C22-C20
3	F	1114	TH2	O17-C20-C22-C21
3	E	1115	TH2	O17-C20-C22-C21
3	B	1117	TH2	O17-C20-C22-C21
3	D	1114	TH2	O17-C20-C22-C21
3	E	1115	TH2	O20-C20-C22-C21
3	B	1117	TH2	O20-C20-C22-C21
3	F	1114	TH2	O20-C20-C22-C21
3	B	1117	TH2	C23-C21-C22-C20
3	C	1115	TH2	O17-C20-C22-C21
3	C	1115	TH2	O20-C20-C22-C21
3	D	1114	TH2	O20-C20-C22-C21

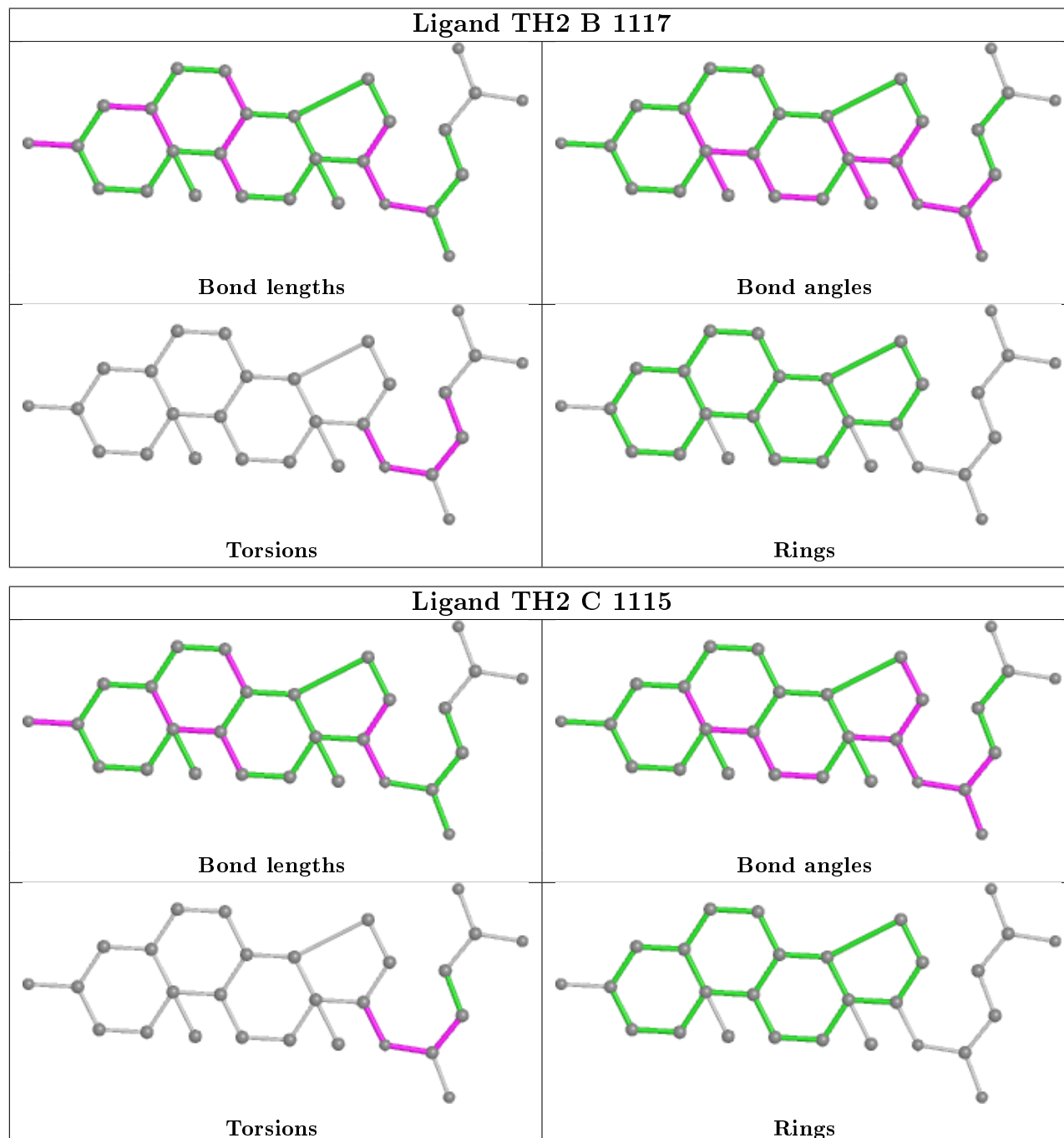
There are no ring outliers.

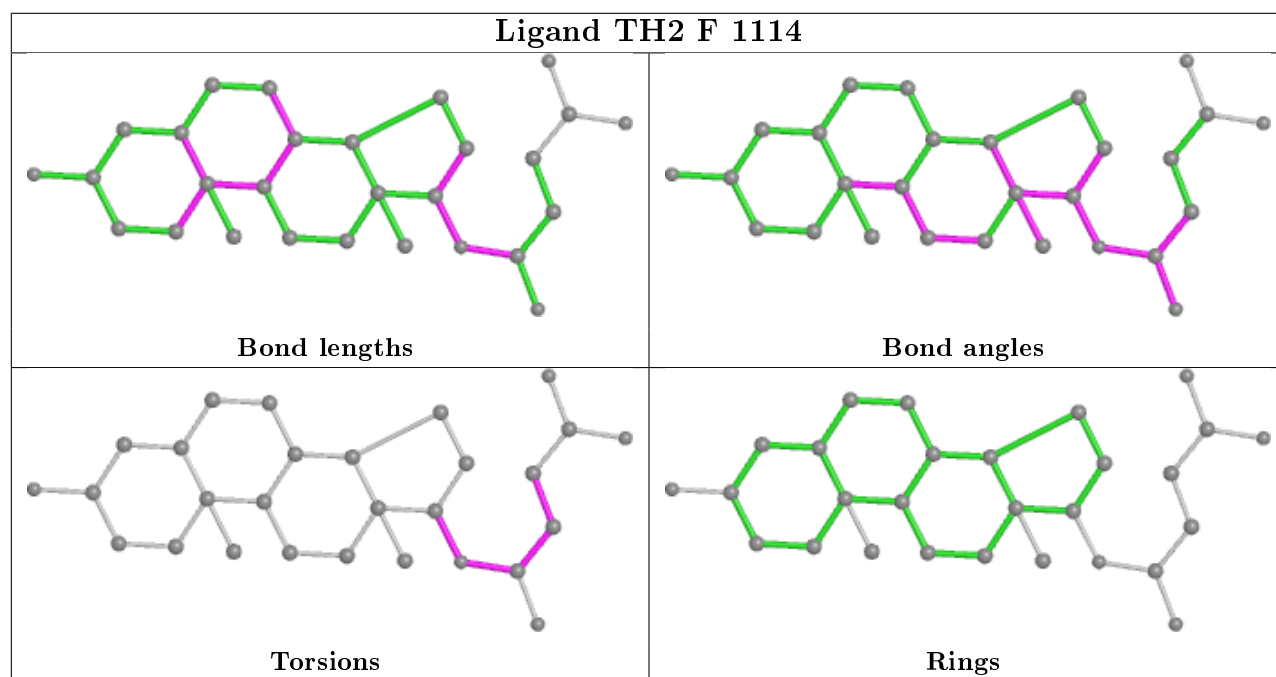
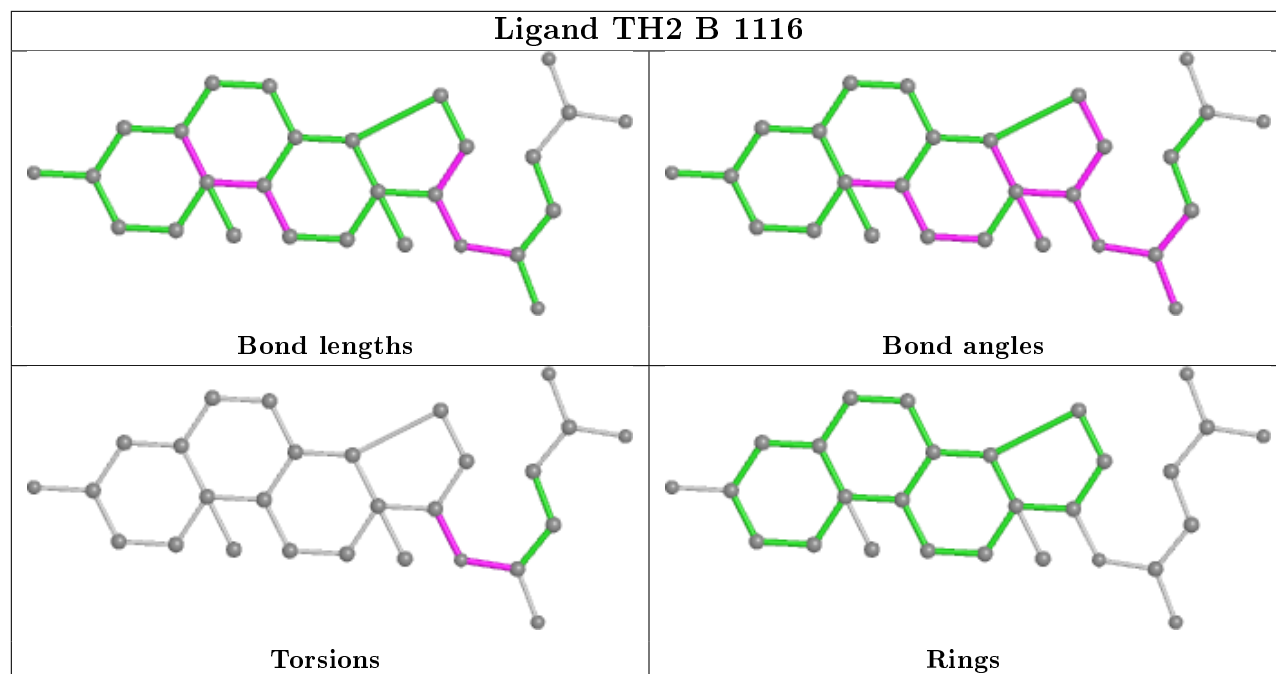
3 monomers are involved in 4 short contacts:

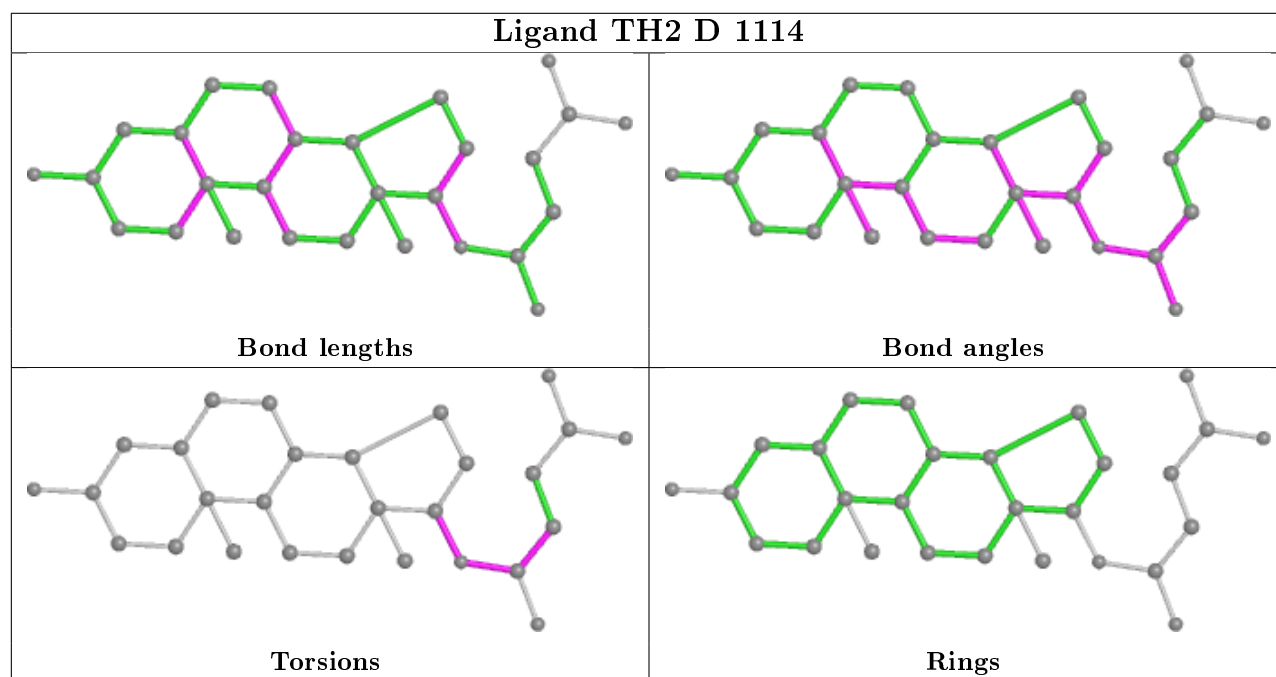
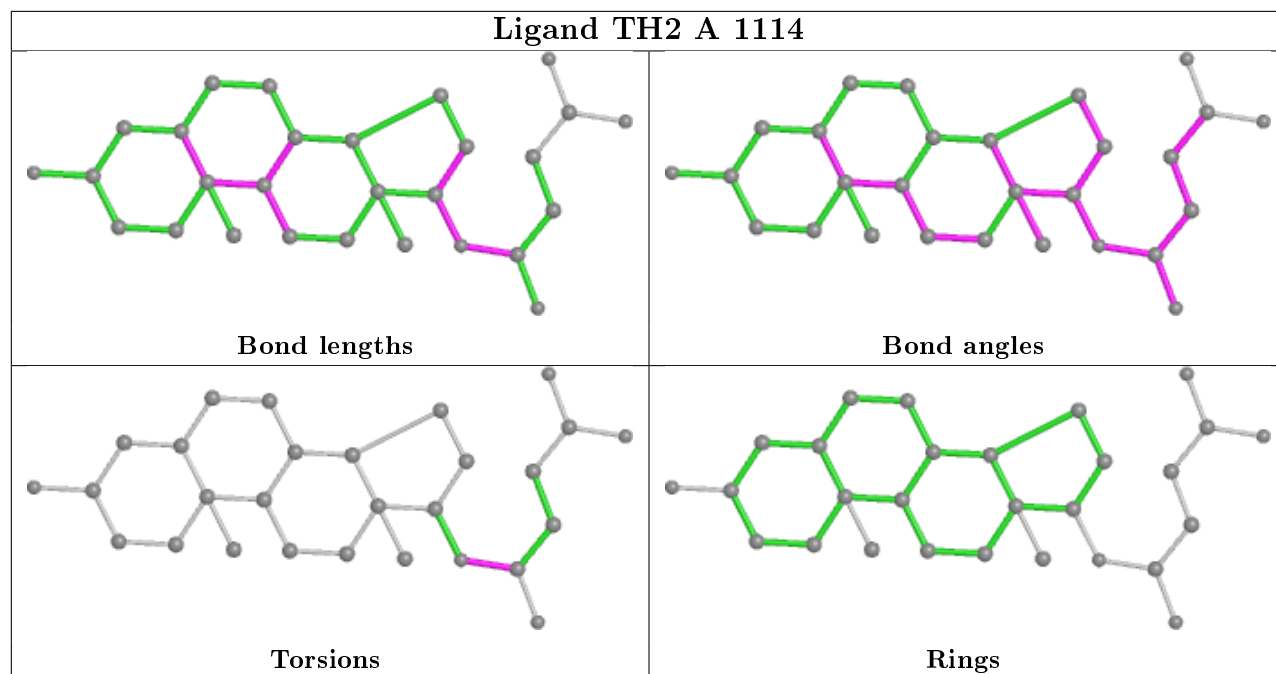
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1117	TH2	1	0
3	A	1114	TH2	2	0
3	A	1115	TH2	1	0

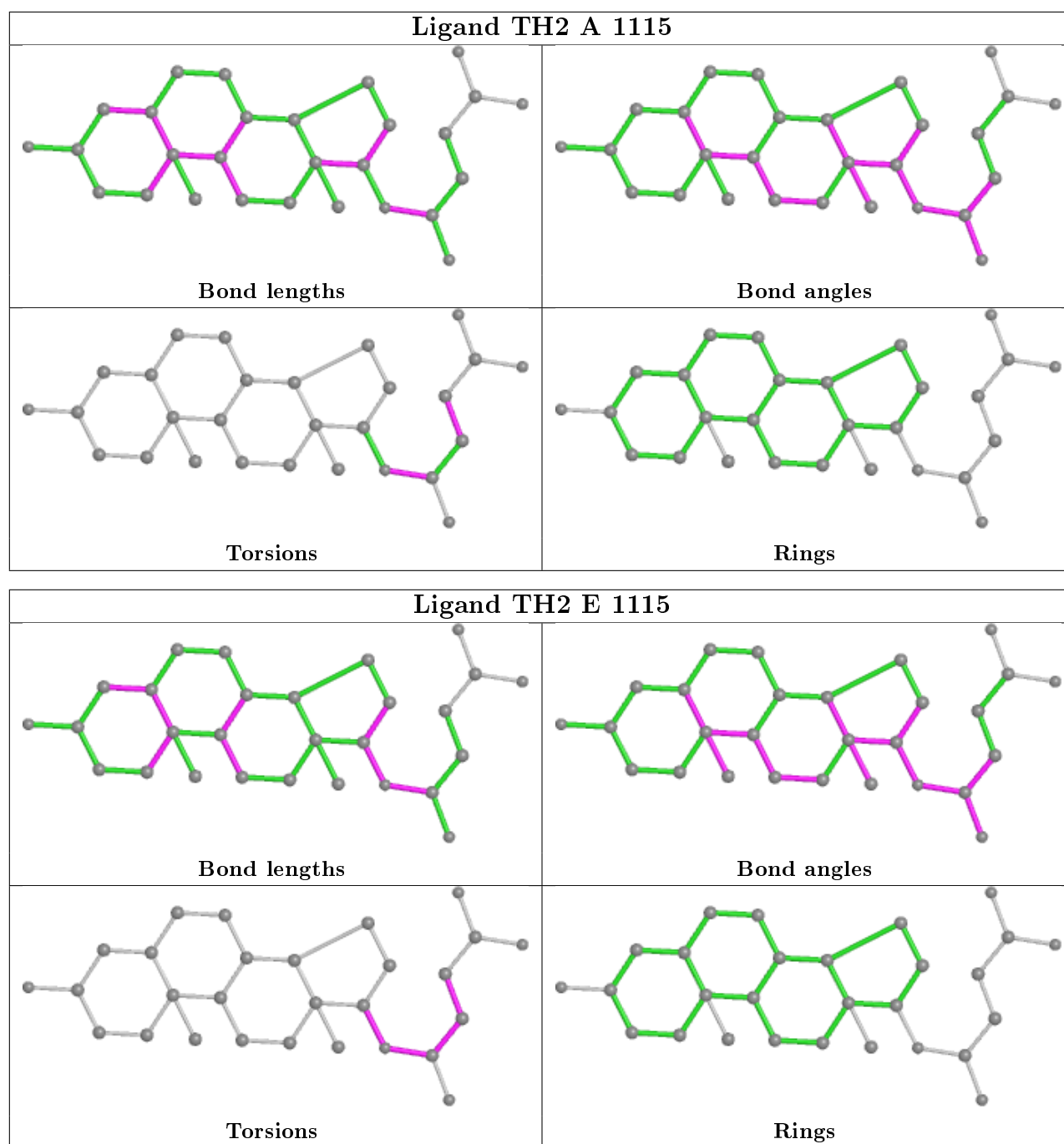
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

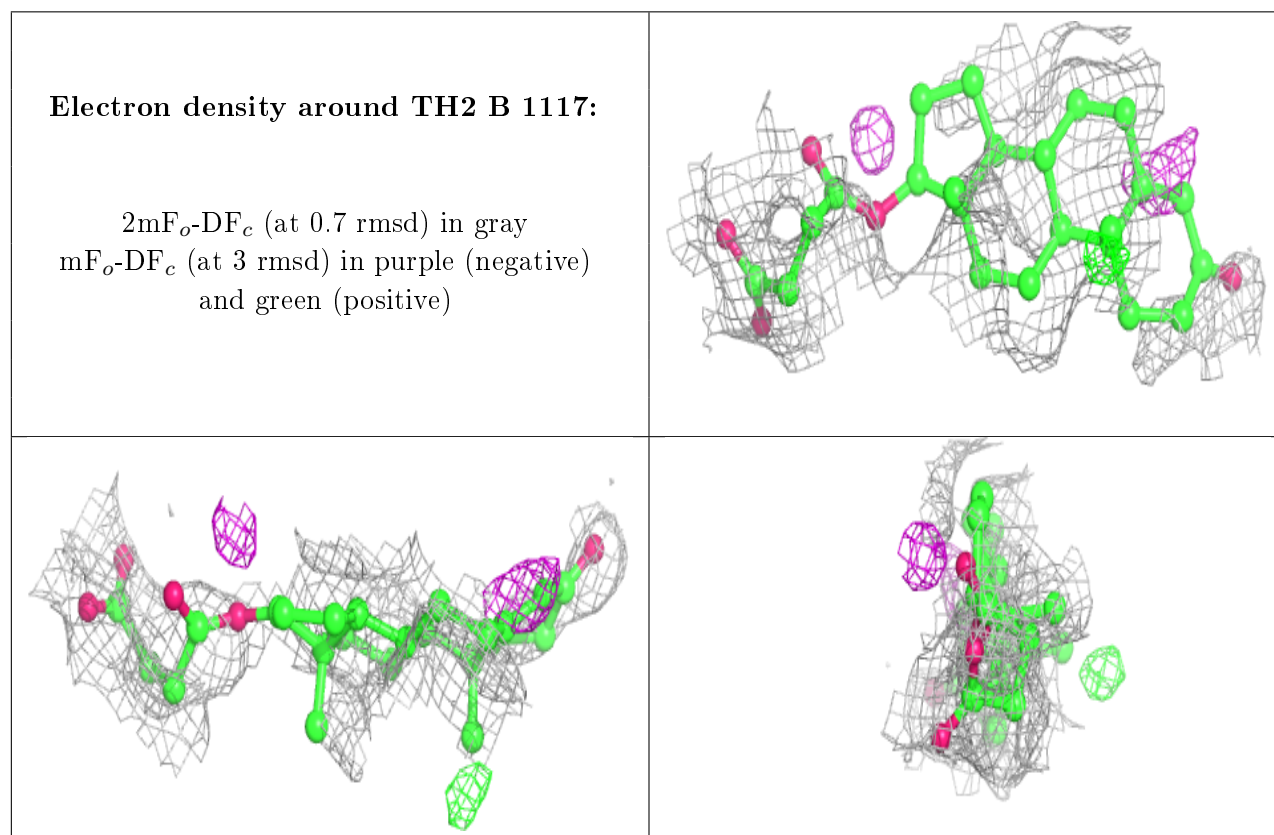
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

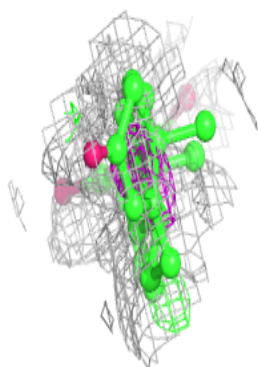
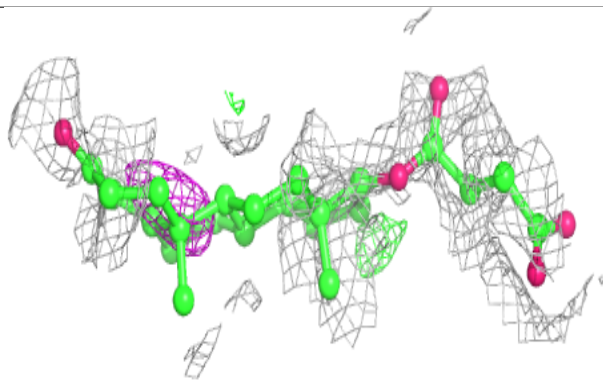
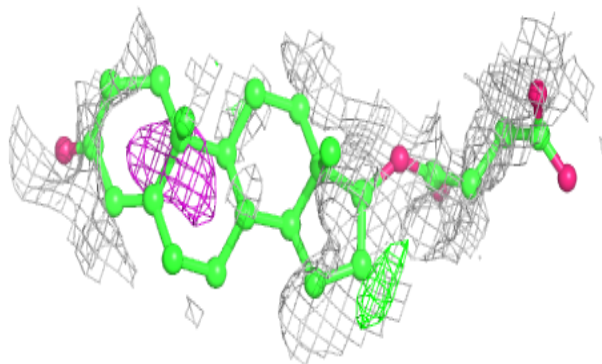
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

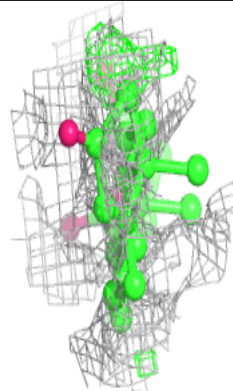
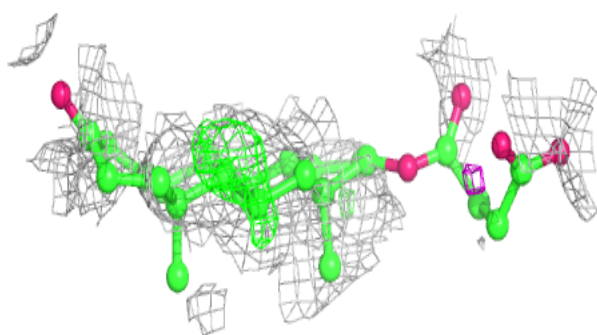
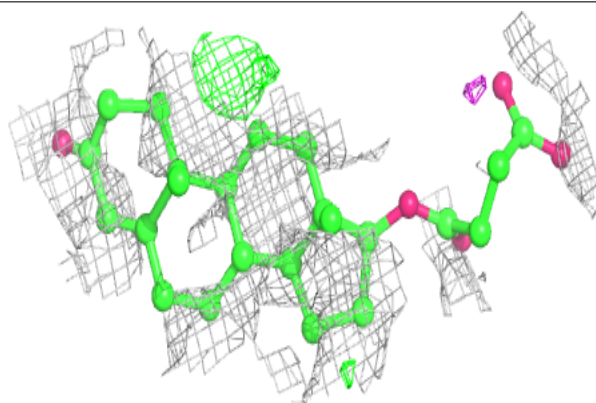


Electron density around TH2 C 1115:

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

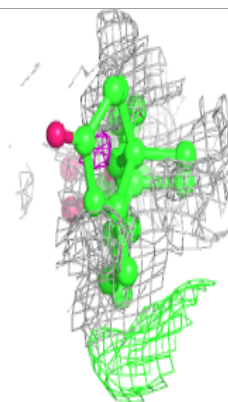
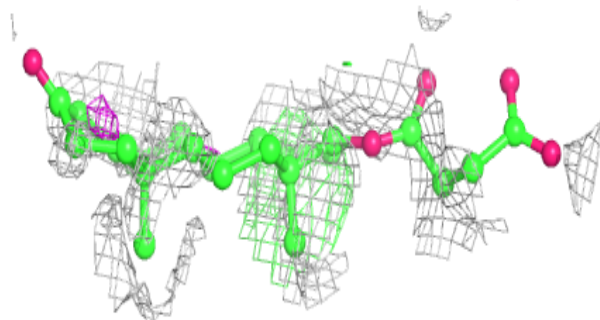
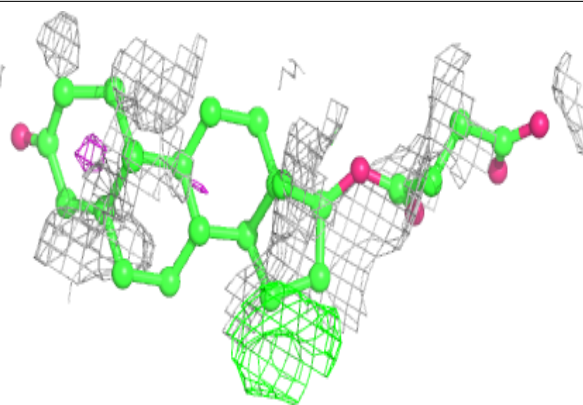
**Electron density around TH2 B 1116:**

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

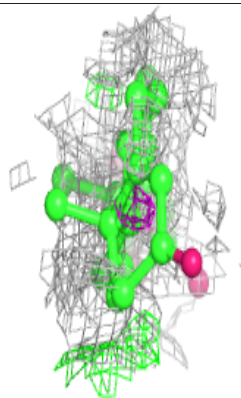
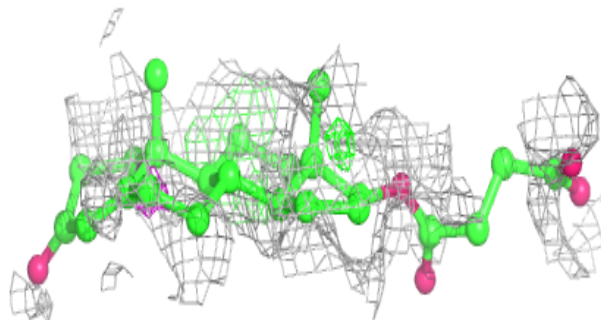
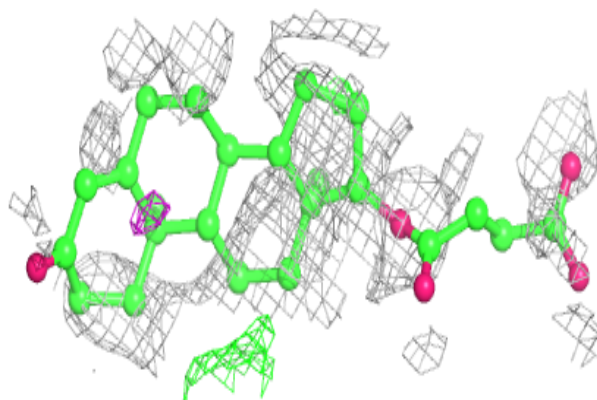


Electron density around TH2 F 1114:

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

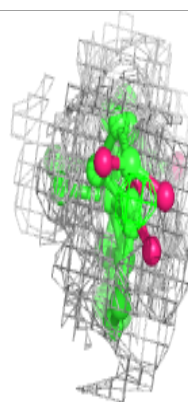
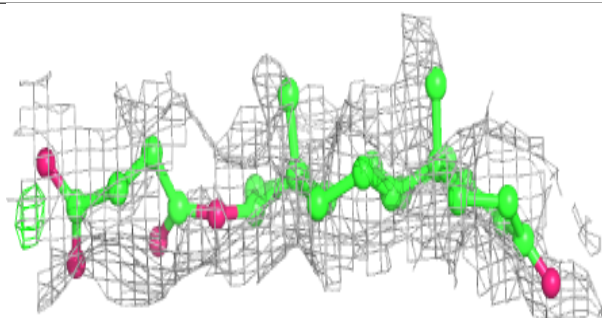
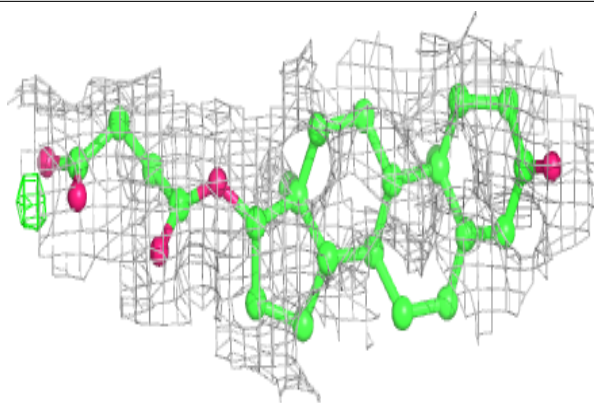
**Electron density around TH2 A 1114:**

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

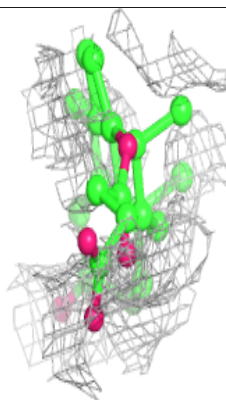
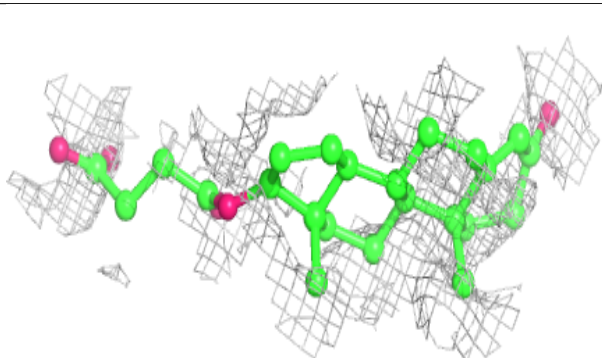
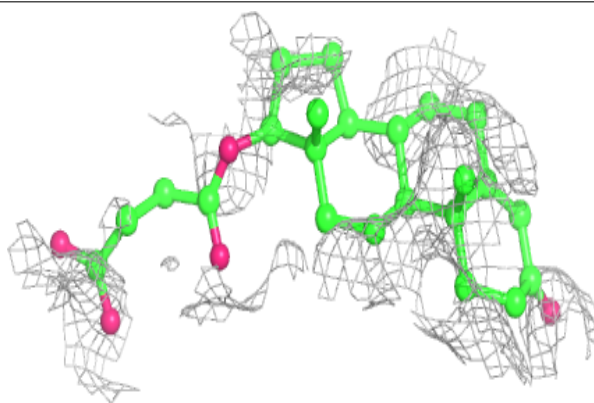


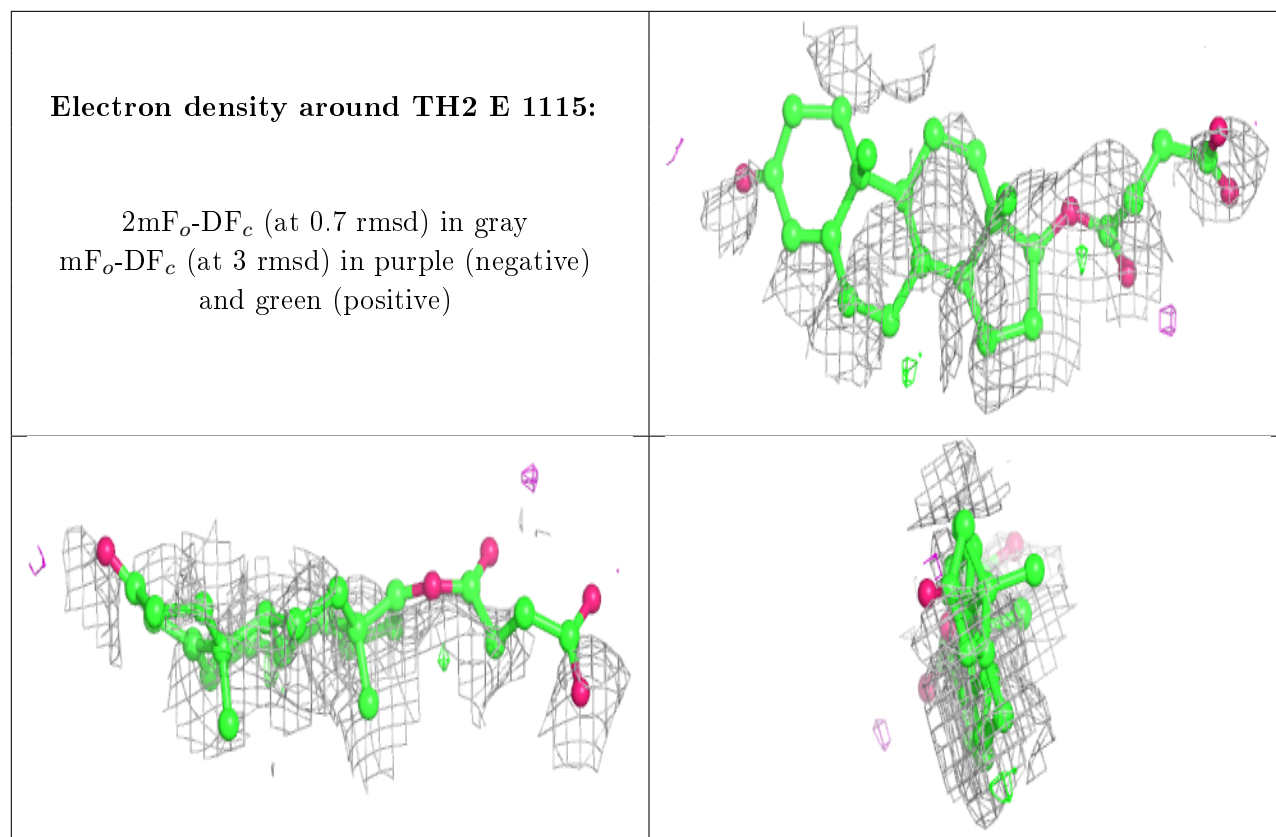
Electron density around TH2 D 1114:

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

**Electron density around TH2 A 1115:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.