



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2026 – 05:34 pm BST

PDB ID : 9T7M / pdb_00009t7m
Title : Crystallographic structure of Clostridioides difficile CspA protein in complex with Taurocholate at 2.9 angstrom resolution
Authors : Alcorlo, M.; Mayor-Luna, C.; Hermoso, J.
Deposited on : 2025-11-11
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
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

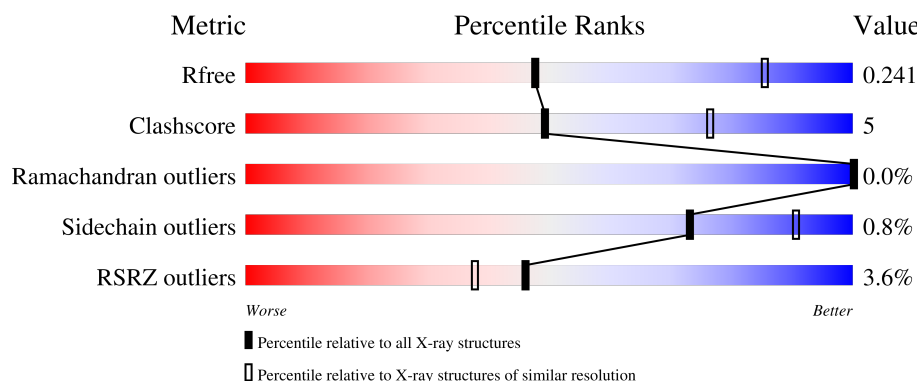
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	548	 2% 86% 14%
1	B	548	 4% 87% 12% .
1	C	548	 3% 86% 13% .
1	D	548	 4% 86% 13% .
1	E	548	 4% 83% 15% .

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Mol	Chain	Length	Quality of chain
1	F	548	<div><div></div><div>4%</div><div>83%</div><div>17%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25491 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.

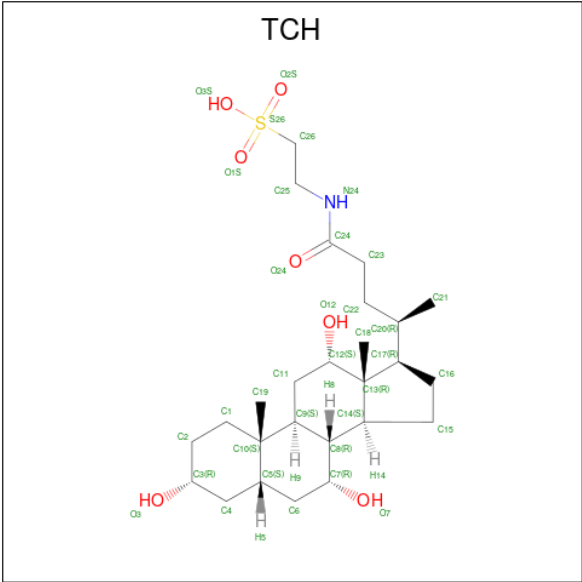
- Molecule 1 is a protein called Subtilisin-like serine germination related protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	540	Total	C	N	O	S	0	0	0
			4167	2639	692	825	11			
1	A	548	Total	C	N	O	S	0	0	0
			4228	2678	701	838	11			
1	B	546	Total	C	N	O	S	0	0	0
			4212	2668	699	834	11			
1	C	543	Total	C	N	O	S	0	0	0
			4192	2660	694	827	11			
1	D	542	Total	C	N	O	S	0	0	0
			4184	2654	693	826	11			
1	F	548	Total	C	N	O	S	0	0	0
			4228	2678	701	838	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1133	LEU	-	expression tag	UNP A0AB74Q767
E	1134	ASP	-	expression tag	UNP A0AB74Q767
A	1133	LEU	-	expression tag	UNP A0AB74Q767
A	1134	ASP	-	expression tag	UNP A0AB74Q767
B	1133	LEU	-	expression tag	UNP A0AB74Q767
B	1134	ASP	-	expression tag	UNP A0AB74Q767
C	1133	LEU	-	expression tag	UNP A0AB74Q767
C	1134	ASP	-	expression tag	UNP A0AB74Q767
D	1133	LEU	-	expression tag	UNP A0AB74Q767
D	1134	ASP	-	expression tag	UNP A0AB74Q767
F	1133	LEU	-	expression tag	UNP A0AB74Q767
F	1134	ASP	-	expression tag	UNP A0AB74Q767

- Molecule 2 is TAUROCHOLIC ACID (CCD ID: TCH) (formula: C₂₆H₄₅NO₇S) (labeled as "Ligand of Interest" by depositor).

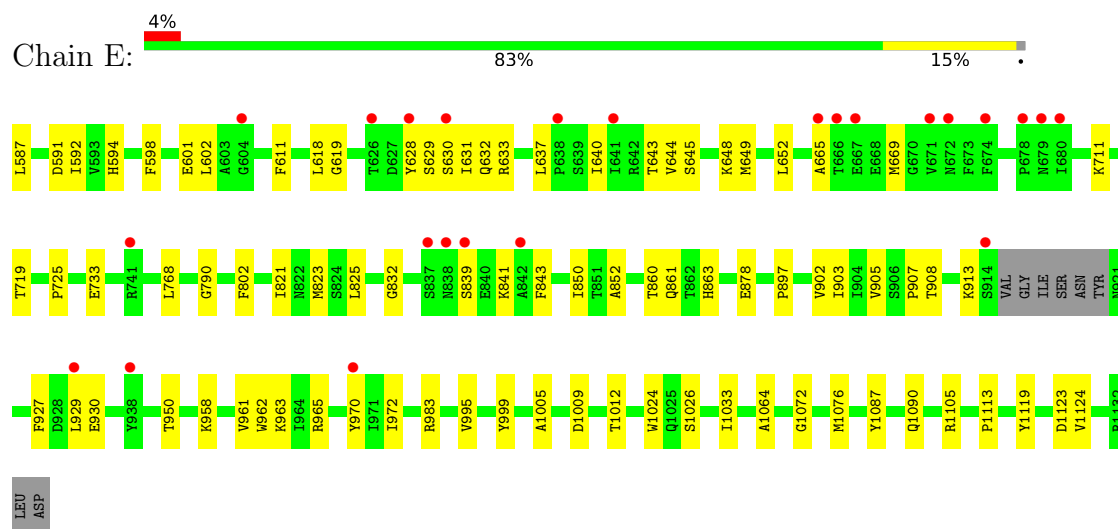


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	C	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	C	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	D	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	F	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
2	F	1	Total	C	N	O	S	0	0
			35	26	1	7	1		

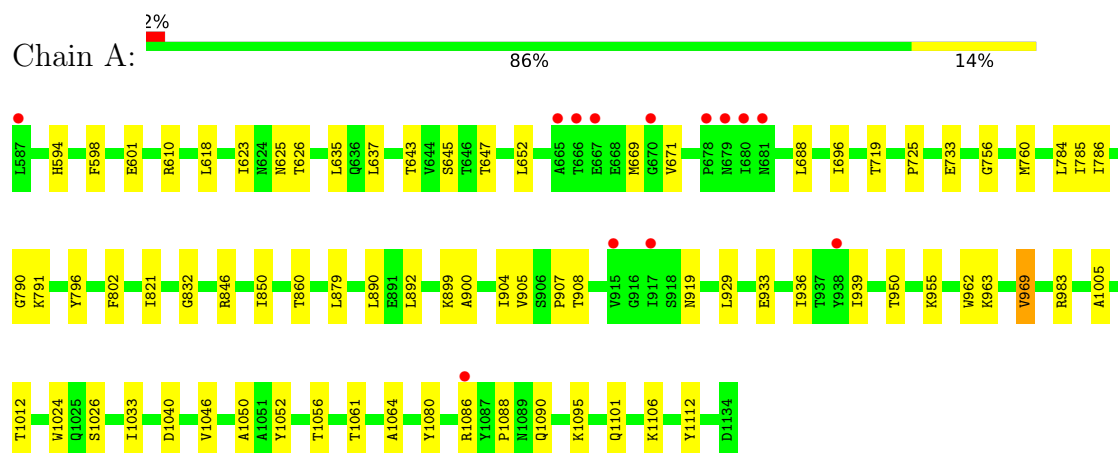
3 Residue-property plots

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.

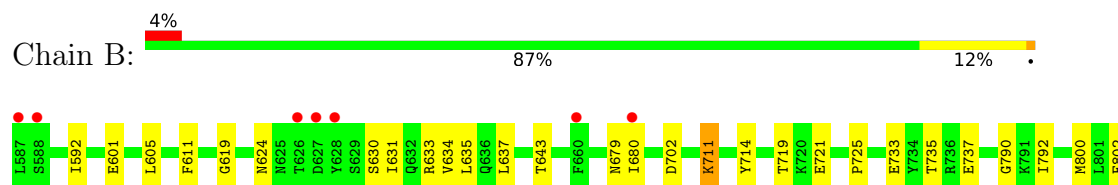
- Molecule 1: Subtilisin-like serine germination related protease

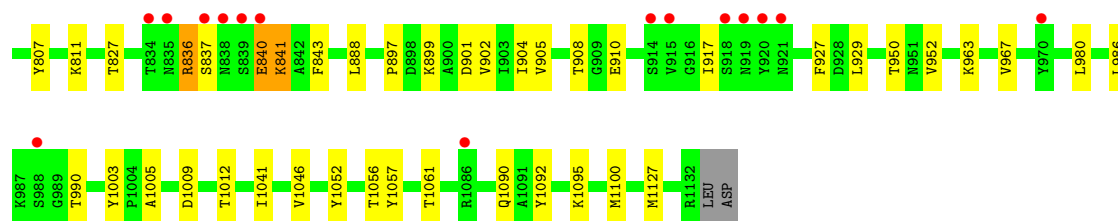


- Molecule 1: Subtilisin-like serine germination related protease

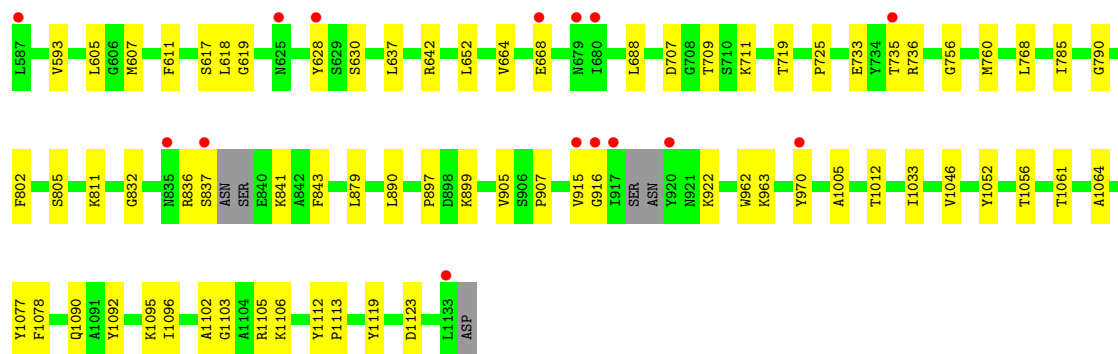
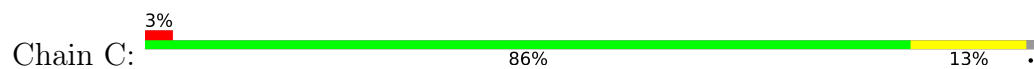


- Molecule 1: Subtilisin-like serine germination related protease

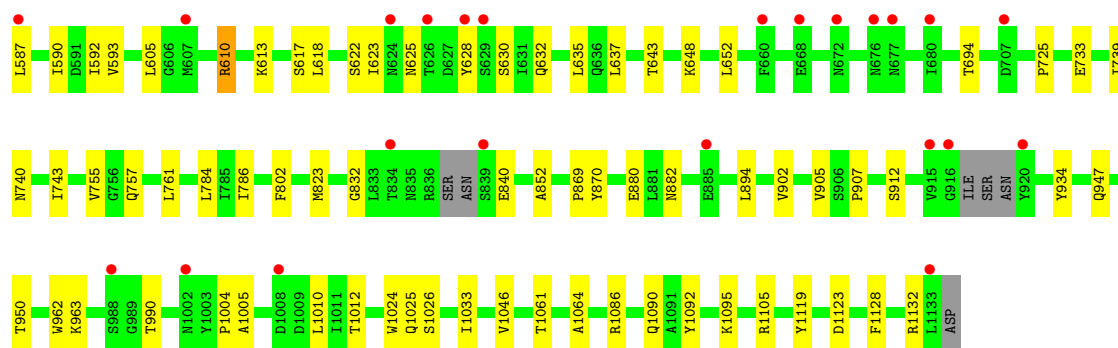
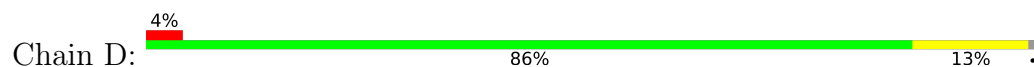




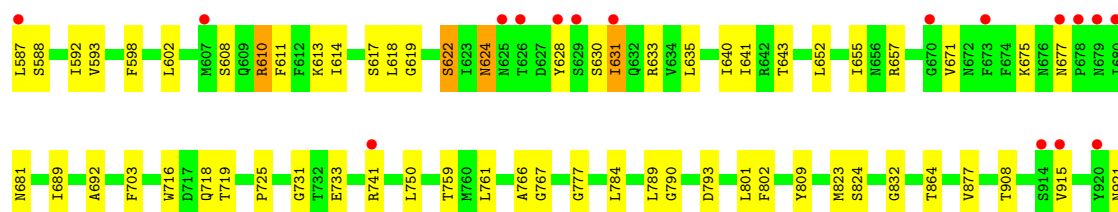
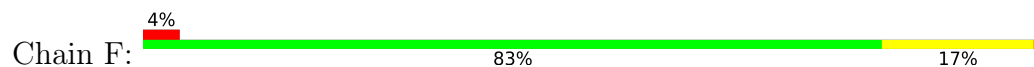
- Molecule 1: Subtilisin-like serine germination related protease

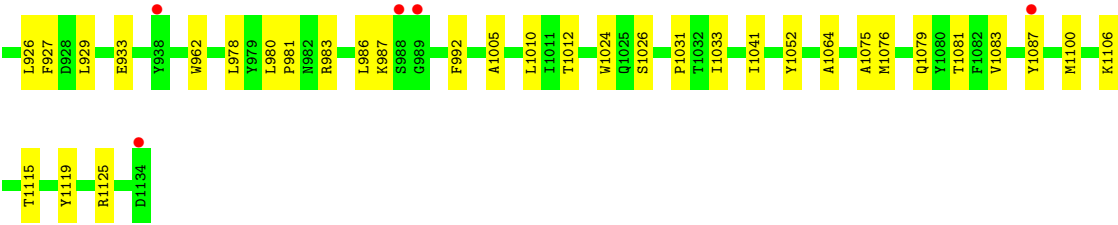


- Molecule 1: Subtilisin-like serine germination related protease



- Molecule 1: Subtilisin-like serine germination related protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.24Å 158.63Å 188.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.87 – 2.90 28.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.87-2.90) 99.8 (28.87-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.205 , 0.241 0.205 , 0.241	Depositor DCC
R_{free} test set	4712 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25491	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TCH

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	0.12	0/4312	0.32	0/5859
1	B	0.18	0/4296	0.34	0/5837
1	C	0.11	0/4274	0.29	0/5804
1	D	0.13	0/4266	0.34	0/5793
1	E	0.12	0/4249	0.30	0/5771
1	F	0.14	0/4312	0.31	0/5859
All	All	0.14	0/25709	0.32	0/34923

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	836	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4228	0	4146	40	0
1	B	4212	0	4131	43	0
1	C	4192	0	4118	48	0
1	D	4184	0	4107	40	0
1	E	4167	0	4087	50	0
1	F	4228	0	4146	57	0
2	A	35	0	45	0	0
2	B	35	0	45	3	0
2	C	70	0	90	3	0
2	D	35	0	45	1	0
2	E	35	0	45	1	0
2	F	70	0	90	2	0
All	All	25491	0	25095	271	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 5.

All (271) 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:642:ARG:HE	1:C:837:SER:HB3	1.50	0.76
1:E:725:PRO:HG3	1:E:733:GLU:HB2	1.68	0.74
1:C:668:GLU:HG2	1:C:1105:ARG:HH12	1.52	0.74
1:B:802:PHE:HB2	2:B:1201:TCH:H26A	1.73	0.71
1:F:801:LEU:HD21	1:F:823:MET:HE1	1.72	0.70
1:A:1090:GLN:HG2	1:A:1095:LYS:HD2	1.73	0.69
1:B:840:GLU:HA	2:B:1201:TCH:H2	1.74	0.69
1:B:908:THR:HG21	1:B:929:LEU:HD22	1.74	0.69
1:C:905:VAL:HB	1:C:963:LYS:HB2	1.74	0.68
1:A:899:LYS:HB2	1:A:969:VAL:HG22	1.78	0.65
1:B:792:ILE:HG13	1:B:800:MET:HE3	1.79	0.65
1:E:839:SER:HB2	1:C:841:LYS:HE2	1.78	0.64
1:B:635:LEU:HD22	1:B:643:THR:HG21	1.79	0.63
1:F:630:SER:HA	1:F:633:ARG:HD3	1.79	0.63
1:E:601:GLU:HB3	1:E:637:LEU:HD22	1.81	0.62
1:E:802:PHE:HB2	2:E:1201:TCH:H26	1.82	0.62
1:B:899:LYS:NZ	1:B:917:ILE:HG12	2.15	0.61
1:F:610:ARG:HG2	1:F:622:SER:HB2	1.83	0.60
1:F:725:PRO:HG3	1:F:733:GLU:HB2	1.83	0.60
1:A:635:LEU:HD22	1:A:643:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:PRO:HG3	1:C:733:GLU:HB2	1.83	0.60
1:B:592:ILE:HG12	1:B:643:THR:HG22	1.83	0.60
1:F:618:LEU:HD22	1:F:802:PHE:HD2	1.66	0.60
1:D:652:LEU:HB2	1:D:1064:ALA:HB2	1.84	0.60
1:B:905:VAL:HB	1:B:963:LYS:HB2	1.83	0.60
1:A:652:LEU:HB2	1:A:1064:ALA:HB2	1.83	0.59
1:D:740:ASN:HA	1:D:743:ILE:HD12	1.85	0.59
1:B:1090:GLN:HA	1:B:1095:LYS:HD3	1.85	0.58
1:F:598:PHE:CZ	1:F:602:LEU:HD12	2.37	0.58
1:A:933:GLU:HB2	1:A:955:LYS:HB2	1.85	0.58
1:D:905:VAL:HB	1:D:963:LYS:HB2	1.84	0.58
1:D:1090:GLN:HA	1:D:1095:LYS:HD3	1.85	0.58
1:F:692:ALA:HB1	1:F:789:LEU:HD21	1.86	0.58
1:E:630:SER:HA	1:E:633:ARG:HG3	1.85	0.57
1:B:725:PRO:HG3	1:B:733:GLU:HB2	1.85	0.57
1:F:915:VAL:HG12	1:F:921:ASN:HD21	1.68	0.57
1:D:1005:ALA:HB1	1:D:1012:THR:HG23	1.87	0.57
1:E:930:GLU:HB3	1:E:958:LYS:HG3	1.86	0.56
1:A:618:LEU:HD22	1:A:802:PHE:HD2	1.70	0.56
1:F:1005:ALA:HB1	1:F:1012:THR:HG23	1.87	0.56
1:C:688:LEU:HD13	1:C:785:ILE:HD11	1.88	0.56
1:F:983:ARG:HH21	1:F:986:LEU:HB3	1.70	0.56
1:E:591:ASP:HB2	1:E:644:VAL:HG23	1.88	0.56
1:E:903:ILE:HD12	1:E:965:ARG:HD2	1.88	0.56
1:D:1092:TYR:HB2	1:D:1095:LYS:HD2	1.88	0.56
1:F:593:VAL:HG12	1:F:641:ILE:HB	1.88	0.56
1:A:908:THR:HG21	1:A:929:LEU:HD22	1.88	0.56
1:A:1046:VAL:HA	1:A:1061:THR:HG23	1.88	0.55
1:D:725:PRO:HG3	1:D:733:GLU:HB2	1.87	0.55
1:C:1052:TYR:HB3	1:C:1056:THR:HG23	1.88	0.55
1:A:905:VAL:HB	1:A:963:LYS:HB2	1.88	0.55
1:D:840:GLU:HA	2:D:1201:TCH:H2	1.89	0.55
1:A:1052:TYR:HB3	1:A:1056:THR:HG23	1.88	0.55
1:F:652:LEU:HB2	1:F:1064:ALA:HB2	1.88	0.55
1:E:908:THR:HG21	1:E:929:LEU:HD13	1.89	0.54
1:B:902:VAL:HG21	1:B:950:THR:HG21	1.89	0.54
1:F:987:LYS:H	1:F:987:LYS:HD2	1.72	0.54
1:C:719:THR:HG22	1:C:790:GLY:HA2	1.88	0.54
1:A:1005:ALA:HB1	1:A:1012:THR:HG23	1.89	0.53
1:C:618:LEU:HD22	1:C:802:PHE:HD2	1.72	0.53
1:F:761:LEU:HD11	1:F:1064:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:GLU:HG3	2:B:1201:TCH:H9	1.91	0.53
1:F:671:VAL:HG13	1:F:1076:MET:HE1	1.90	0.53
1:D:902:VAL:HG21	1:D:950:THR:HG21	1.91	0.52
1:B:601:GLU:HB3	1:B:637:LEU:HD22	1.91	0.52
1:D:694:THR:HG21	1:D:755:VAL:HB	1.90	0.52
1:E:861:GLN:HG2	1:E:995:VAL:HG11	1.92	0.52
1:B:1092:TYR:HB2	1:B:1095:LYS:HD2	1.92	0.52
1:F:980:LEU:HD22	1:F:986:LEU:HD21	1.92	0.52
1:B:1005:ALA:HB1	1:B:1012:THR:HG23	1.92	0.51
1:C:652:LEU:HB2	1:C:1064:ALA:HB2	1.91	0.51
1:A:601:GLU:HB3	1:A:637:LEU:HD22	1.93	0.51
1:D:618:LEU:HD22	1:D:802:PHE:HD2	1.75	0.50
1:B:719:THR:HG22	1:B:790:GLY:HA2	1.92	0.50
1:B:836:ARG:H	1:B:841:LYS:HZ3	1.58	0.50
1:D:1046:VAL:HA	1:D:1061:THR:HG23	1.94	0.50
1:F:587:LEU:HD21	1:F:793:ASP:HB2	1.94	0.50
1:F:1041:ILE:HD13	1:F:1100:MET:HB3	1.93	0.50
1:E:878:GLU:OE1	1:E:961:VAL:HG11	2.12	0.49
1:C:707:ASP:HB2	1:C:709:THR:HG23	1.94	0.49
1:D:832:GLY:HA2	1:D:1033:ILE:HD11	1.94	0.49
1:B:1046:VAL:HA	1:B:1061:THR:HG23	1.94	0.49
1:D:610:ARG:HB2	1:D:622:SER:H	1.77	0.49
1:F:981:PRO:HB2	1:F:986:LEU:HD13	1.95	0.49
1:D:823:MET:HE2	1:D:1004:PRO:HG3	1.95	0.49
1:E:821:ILE:HB	1:E:850:ILE:HG12	1.94	0.49
1:F:631:ILE:HD12	1:F:631:ILE:H	1.77	0.49
1:E:592:ILE:HG13	1:E:643:THR:HG22	1.94	0.49
1:C:841:LYS:HD2	1:C:843:PHE:HE2	1.78	0.48
1:B:910:GLU:HB2	1:B:927:PHE:CD1	2.48	0.48
1:C:836:ARG:NH2	2:C:1201:TCH:H39	2.28	0.48
1:E:832:GLY:HA2	1:E:1033:ILE:HD11	1.93	0.48
1:E:1119:TYR:CE2	1:C:897:PRO:HD3	2.48	0.48
1:B:904:ILE:HD11	1:B:952:VAL:HG13	1.95	0.48
1:F:927:PHE:CE2	1:F:962:TRP:HZ3	2.31	0.48
1:F:1081:THR:HG22	1:F:1087:TYR:HD2	1.78	0.48
1:C:1103:GLY:O	1:C:1123:ASP:HB3	2.14	0.48
1:F:766:ALA:HB3	1:F:784:LEU:HD21	1.95	0.48
1:A:1080:TYR:CZ	1:A:1086:ARG:HG2	2.49	0.48
1:D:1105:ARG:HG3	1:D:1123:ASP:HB2	1.95	0.48
1:C:802:PHE:HB2	2:C:1201:TCH:O1S	2.14	0.47
1:E:1087:TYR:HB3	1:E:1090:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:784:LEU:HD22	1:D:786:ILE:HD11	1.96	0.47
1:E:611:PHE:CZ	1:E:619:GLY:HA3	2.49	0.47
1:C:593:VAL:HA	1:C:617:SER:O	2.14	0.47
1:F:635:LEU:HD11	2:F:1202:TCH:H1	1.97	0.47
1:E:665:ALA:O	1:E:669:MET:HG2	2.14	0.47
1:D:894:LEU:O	1:D:947:GLN:HB2	2.14	0.47
1:E:1105:ARG:HH11	1:E:1123:ASP:HB2	1.80	0.47
1:C:607:MET:SD	1:C:630:SER:HB3	2.55	0.47
1:C:756:GLY:O	1:C:760:MET:HG3	2.15	0.47
1:D:1005:ALA:HA	1:D:1010:LEU:HD11	1.96	0.47
1:E:970:TYR:OH	1:E:972:ILE:HD11	2.14	0.47
1:B:630:SER:HA	1:B:633:ARG:HE	1.79	0.47
1:F:602:LEU:HD22	1:F:608:SER:OG	2.14	0.47
1:F:613:LYS:HB2	1:F:613:LYS:HE3	1.65	0.47
1:B:1052:TYR:HB3	1:B:1056:THR:HG23	1.97	0.46
1:C:1106:LYS:HB3	1:C:1112:TYR:CE1	2.51	0.46
1:E:594:HIS:HB2	1:E:598:PHE:HB2	1.96	0.46
1:D:757:GLN:HE21	1:D:761:LEU:HD11	1.80	0.46
1:F:767:GLY:H	1:F:777:GLY:HA3	1.79	0.46
1:E:905:VAL:HB	1:E:963:LYS:HB2	1.96	0.46
1:A:784:LEU:HB3	1:A:786:ILE:HD13	1.97	0.46
1:B:735:THR:HG23	1:B:737:GLU:H	1.80	0.46
1:A:610:ARG:NH2	1:A:626:THR:HG23	2.30	0.46
1:D:590:ILE:HD11	1:D:623:ILE:HD11	1.96	0.46
1:C:605:LEU:HD11	1:C:637:LEU:HD21	1.98	0.46
1:A:594:HIS:HB2	1:A:598:PHE:HB2	1.98	0.46
1:F:832:GLY:HA2	1:F:1033:ILE:HD11	1.98	0.46
1:F:864:THR:HG21	1:F:877:VAL:HG11	1.98	0.46
1:C:841:LYS:HD2	1:C:843:PHE:CE2	2.51	0.46
1:A:892:LEU:HB3	1:A:950:THR:HB	1.98	0.46
1:C:899:LYS:HD3	1:C:970:TYR:CE2	2.51	0.46
1:C:1090:GLN:HA	1:C:1095:LYS:HD3	1.97	0.46
1:E:649:MET:HB3	1:E:825:LEU:HB3	1.98	0.45
1:C:711:LYS:HE3	1:C:768:LEU:HG	1.98	0.45
1:E:970:TYR:HE2	1:C:1102:ALA:HA	1.82	0.45
1:C:1113:PRO:HG3	1:C:1119:TYR:CE2	2.51	0.45
1:F:1125:ARG:HE	1:F:1125:ARG:HB3	1.64	0.45
1:E:652:LEU:HB2	1:E:1064:ALA:HB2	1.99	0.45
1:A:669:MET:HE2	1:A:671:VAL:HG21	1.99	0.45
1:B:836:ARG:O	1:B:836:ARG:HD3	2.17	0.45
1:C:879:LEU:HD22	1:C:890:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:ILE:HD12	1:F:619:GLY:HA2	1.98	0.45
1:A:645:SER:O	1:A:647:THR:HG23	2.17	0.45
1:A:719:THR:HG22	1:A:790:GLY:HA2	1.98	0.45
1:A:907:PRO:HD3	1:A:962:TRP:CD2	2.51	0.45
1:C:811:LYS:HA	1:C:811:LYS:HD3	1.77	0.45
1:A:904:ILE:HG13	1:A:936:ILE:HD11	1.98	0.45
1:F:1005:ALA:HA	1:F:1010:LEU:HD11	1.99	0.45
1:C:1077:TYR:CE1	1:C:1096:ILE:HG12	2.52	0.44
1:F:655:ILE:HD13	1:F:1052:TYR:HE1	1.81	0.44
1:C:1092:TYR:HB2	1:C:1095:LYS:HD2	1.99	0.44
1:B:910:GLU:HB2	1:B:927:PHE:HD1	1.82	0.44
1:B:1127:MET:HE2	1:B:1127:MET:HB3	1.84	0.44
1:D:628:TYR:C	1:D:630:SER:H	2.25	0.44
1:A:832:GLY:HA2	1:A:1033:ILE:HD11	2.00	0.44
1:D:587:LEU:HD23	1:D:648:LYS:HG2	2.00	0.44
1:F:628:TYR:C	1:F:630:SER:H	2.26	0.44
1:F:703:PHE:HE2	1:F:759:THR:HG23	1.81	0.44
1:E:637:LEU:HB2	1:E:640:ILE:HD13	2.00	0.44
1:A:900:ALA:HA	1:A:969:VAL:HG13	1.99	0.44
1:E:631:ILE:HG13	1:E:632:GLN:N	2.32	0.44
1:A:688:LEU:HD13	1:A:785:ILE:HD11	1.99	0.44
1:B:605:LEU:HD11	1:B:637:LEU:HD21	1.99	0.44
1:B:702:ASP:OD2	1:B:1057:TYR:OH	2.34	0.44
1:B:897:PRO:HD3	1:D:1119:TYR:CE2	2.53	0.44
1:C:733:GLU:OE2	1:C:811:LYS:HE3	2.18	0.44
1:B:631:ILE:O	1:B:634:VAL:HG22	2.18	0.43
1:C:1092:TYR:O	1:C:1096:ILE:HG13	2.18	0.43
1:E:841:LYS:HD2	1:E:843:PHE:CE2	2.53	0.43
1:A:791:LYS:HE2	1:A:796:TYR:CZ	2.53	0.43
1:D:912:SER:HB2	1:D:934:TYR:CZ	2.54	0.43
1:E:839:SER:HB2	1:C:841:LYS:CE	2.46	0.43
1:E:1005:ALA:HB1	1:E:1012:THR:HG23	2.01	0.43
1:F:823:MET:HE3	1:F:823:MET:HB3	1.75	0.43
1:E:907:PRO:HD3	1:E:962:TRP:CD2	2.53	0.43
1:B:714:TYR:HB3	1:B:807:TYR:OH	2.18	0.43
1:D:605:LEU:HD11	1:D:637:LEU:HD11	2.00	0.43
1:F:657:ARG:HD2	1:F:657:ARG:HA	1.73	0.43
1:F:671:VAL:HG12	1:F:675:LYS:HD2	2.01	0.43
1:E:587:LEU:HD23	1:E:648:LYS:HG2	2.00	0.43
1:A:821:ILE:HB	1:A:850:ILE:HG12	1.99	0.43
1:B:811:LYS:HA	1:B:811:LYS:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ARG:HH22	1:A:625:ASN:H	1.65	0.43
1:D:739:ILE:HG22	1:D:743:ILE:HD11	2.01	0.43
1:F:635:LEU:HA	1:F:640:ILE:HD12	2.01	0.43
1:E:711:LYS:HE3	1:E:768:LEU:HG	2.00	0.42
1:E:970:TYR:CE2	1:C:1102:ALA:HA	2.53	0.42
1:E:1113:PRO:HG3	1:E:1119:TYR:CE2	2.53	0.42
1:F:809:TYR:CE2	2:F:1201:TCH:H6A	2.54	0.42
1:F:1106:LYS:HE2	1:F:1119:TYR:O	2.19	0.42
1:A:860:THR:HB	1:A:983:ARG:HB2	2.00	0.42
1:E:863:HIS:CE1	1:E:999:TYR:HB2	2.54	0.42
1:E:897:PRO:HD3	1:C:1119:TYR:CE2	2.54	0.42
1:C:832:GLY:HA2	1:C:1033:ILE:HD11	2.01	0.42
1:A:846:ARG:HD2	1:A:1088:PRO:O	2.20	0.42
1:B:611:PHE:CZ	1:B:619:GLY:HA3	2.54	0.42
1:B:1041:ILE:HD13	1:B:1100:MET:HB3	2.00	0.42
1:F:1024:TRP:CH2	1:F:1026:SER:HB2	2.54	0.42
1:E:618:LEU:HD22	1:E:802:PHE:HD2	1.84	0.42
1:E:860:THR:HB	1:E:983:ARG:HB2	2.02	0.42
1:D:632:GLN:HA	1:D:635:LEU:HG	2.01	0.42
1:F:1031:PRO:HD3	1:F:1115:THR:HG21	2.02	0.42
1:D:869:PRO:HB2	1:D:870:TYR:CD2	2.54	0.42
1:F:741:ARG:HH22	1:F:750:LEU:HD21	1.84	0.42
1:E:823:MET:HB2	1:E:852:ALA:HA	2.01	0.42
1:E:913:LYS:HB3	1:E:913:LYS:HE2	1.92	0.42
1:A:1106:LYS:HB3	1:A:1112:TYR:CE1	2.55	0.42
1:C:907:PRO:HD3	1:C:962:TRP:CD2	2.54	0.42
1:B:929:LEU:HD23	1:B:929:LEU:O	2.20	0.42
1:C:735:THR:HG22	1:C:736:ARG:N	2.35	0.42
1:D:1024:TRP:CH2	1:D:1026:SER:HB2	2.54	0.42
1:F:1079:GLN:HA	1:F:1083:VAL:HB	2.01	0.42
1:B:679:ASN:O	1:B:680:ILE:HD13	2.19	0.41
1:D:1086:ARG:HA	1:D:1086:ARG:HD3	1.81	0.41
1:F:593:VAL:HA	1:F:617:SER:O	2.20	0.41
1:F:611:PHE:CE1	1:F:619:GLY:HA3	2.55	0.41
1:E:927:PHE:HB3	1:E:930:GLU:OE1	2.20	0.41
1:A:1040:ASP:HB3	1:A:1101:GLN:HE21	1.85	0.41
1:C:915:VAL:HG12	1:C:916:GLY:N	2.34	0.41
1:D:592:ILE:HG12	1:D:643:THR:HG22	2.02	0.41
1:E:1024:TRP:CH2	1:E:1026:SER:HB2	2.55	0.41
1:C:760:MET:HE2	1:C:760:MET:HB3	1.96	0.41
1:D:623:ILE:O	1:D:623:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:902:VAL:HG21	1:E:950:THR:HG21	2.02	0.41
1:D:1128:PHE:O	1:D:1132:ARG:HG2	2.21	0.41
1:E:843:PHE:CE1	1:E:1009:ASP:HA	2.55	0.41
1:A:725:PRO:HB3	1:A:733:GLU:HB2	2.03	0.41
1:A:760:MET:HE2	1:A:1050:ALA:HB3	2.03	0.41
1:B:827:THR:HG23	1:B:1003:TYR:HB3	2.02	0.41
1:E:719:THR:HG22	1:E:790:GLY:HA2	2.03	0.41
1:A:623:ILE:HG22	1:A:623:ILE:O	2.21	0.41
1:B:711:LYS:HB2	1:B:711:LYS:HE2	1.81	0.41
1:D:610:ARG:HH12	1:D:625:ASN:HB2	1.86	0.41
1:D:823:MET:HB2	1:D:852:ALA:HA	2.02	0.41
1:A:696:ILE:HG22	1:A:786:ILE:HG21	2.03	0.41
1:F:716:TRP:CE2	1:F:718:GLN:HG2	2.56	0.41
1:F:978:LEU:HD23	1:F:992:PHE:CZ	2.55	0.41
1:C:1005:ALA:HB1	1:C:1012:THR:HG23	2.02	0.41
1:D:587:LEU:HD23	1:D:648:LYS:HE2	2.02	0.41
1:D:907:PRO:HD3	1:D:962:TRP:CD2	2.56	0.41
1:F:635:LEU:HD22	1:F:643:THR:HG21	2.02	0.41
1:F:718:GLN:HA	1:F:731:GLY:HA3	2.03	0.41
1:F:908:THR:HG21	1:F:929:LEU:HD22	2.02	0.41
1:E:628:TYR:HD1	1:E:631:ILE:HD11	1.85	0.41
1:A:756:GLY:O	1:A:760:MET:HG3	2.21	0.41
1:A:919:ASN:O	1:A:939:ILE:HA	2.21	0.41
1:B:901:ASP:HB2	1:B:967:VAL:HG13	2.03	0.40
1:C:611:PHE:CZ	1:C:619:GLY:HA3	2.56	0.40
1:C:1078:PHE:HD1	1:C:1078:PHE:HA	1.78	0.40
1:D:593:VAL:HA	1:D:617:SER:O	2.21	0.40
1:D:880:GLU:O	1:D:990:THR:HA	2.21	0.40
1:F:588:SER:OG	1:F:624:ASN:N	2.54	0.40
1:F:592:ILE:HD12	1:F:611:PHE:HE2	1.86	0.40
1:E:628:TYR:CG	1:E:629:SER:N	2.89	0.40
1:E:930:GLU:O	1:E:958:LYS:HE2	2.21	0.40
1:A:1024:TRP:CH2	1:A:1026:SER:HB2	2.56	0.40
1:B:980:LEU:HB3	1:B:986:LEU:HD11	2.04	0.40
1:C:1046:VAL:HA	1:C:1061:THR:HG23	2.03	0.40
1:F:926:LEU:HD12	1:F:933:GLU:HG3	2.01	0.40
1:B:888:LEU:HD11	1:B:990:THR:HG21	2.02	0.40
1:C:628:TYR:OH	1:C:922:LYS:HD3	2.21	0.40
1:C:805:SER:CB	2:C:1201:TCH:H37	2.51	0.40
1:A:879:LEU:HD22	1:A:890:LEU:HD11	2.03	0.40
1:B:843:PHE:CE1	1:B:1009:ASP:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:PRO:HD3	1:C:962:TRP:CE3	2.57	0.40
1:E:1072:GLY:O	1:E:1076:MET:HG3	2.21	0.40
1:B:735:THR:HG23	1:B:737:GLU:N	2.36	0.40
1:F:689:ILE:HD11	1:F:1075:ALA:HB2	2.03	0.40
1:F:719:THR:HG23	1:F:790:GLY:HA2	2.03	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	546/548 (100%)	534 (98%)	12 (2%)	0	100	100
1	B	544/548 (99%)	532 (98%)	11 (2%)	1 (0%)	43	72
1	C	537/548 (98%)	533 (99%)	4 (1%)	0	100	100
1	D	536/548 (98%)	522 (97%)	14 (3%)	0	100	100
1	E	536/548 (98%)	524 (98%)	12 (2%)	0	100	100
1	F	546/548 (100%)	529 (97%)	17 (3%)	0	100	100
All	All	3245/3288 (99%)	3174 (98%)	70 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	837	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/457 (100%)	456 (100%)	1 (0%)	87	96
1	B	455/457 (100%)	450 (99%)	5 (1%)	65	88
1	C	452/457 (99%)	451 (100%)	1 (0%)	87	96
1	D	451/457 (99%)	447 (99%)	4 (1%)	70	90
1	E	450/457 (98%)	447 (99%)	3 (1%)	76	92
1	F	457/457 (100%)	450 (98%)	7 (2%)	57	84
All	All	2722/2742 (99%)	2701 (99%)	21 (1%)	73	90

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

Mol	Chain	Res	Type
1	E	602	LEU
1	E	645	SER
1	E	1124	VAL
1	A	969	VAL
1	B	624	ASN
1	B	711	LYS
1	B	721	GLU
1	B	840	GLU
1	B	841	LYS
1	C	664	VAL
1	D	610	ARG
1	D	613	LYS
1	D	882	ASN
1	D	1025	GLN
1	F	610	ARG
1	F	622	SER
1	F	624	ASN
1	F	631	ILE
1	F	677	ASN
1	F	681	ASN
1	F	824	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	757	GLN

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Mol	Chain	Res	Type
1	E	822	ASN
1	E	977	ASN
1	E	982	ASN
1	A	636	GLN
1	A	822	ASN
1	A	835	ASN
1	A	947	GLN
1	A	977	ASN
1	A	1047	ASN
1	A	1094	GLN
1	B	624	ASN
1	B	681	ASN
1	B	947	GLN
1	B	1007	GLN
1	C	752	GLN
1	C	947	GLN
1	C	977	ASN
1	C	1109	ASN
1	D	672	ASN
1	D	681	ASN
1	D	746	ASN
1	D	822	ASN
1	D	977	ASN
1	F	822	ASN
1	F	835	ASN
1	F	882	ASN
1	F	921	ASN
1	F	951	ASN
1	F	977	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	TCH	C	1201	-	38,38,38	0.52	0	59,60,60	1.17	4 (6%)
2	TCH	F	1202	-	38,38,38	0.51	1 (2%)	59,60,60	0.64	1 (1%)
2	TCH	E	1201	-	38,38,38	0.47	0	59,60,60	0.56	0
2	TCH	C	1202	-	38,38,38	0.48	1 (2%)	59,60,60	0.57	0
2	TCH	B	1201	-	38,38,38	0.47	0	59,60,60	0.63	1 (1%)
2	TCH	D	1201	-	38,38,38	0.47	0	59,60,60	0.55	0
2	TCH	A	1201	-	38,38,38	0.47	0	59,60,60	0.62	0
2	TCH	F	1201	-	38,38,38	0.48	0	59,60,60	0.52	0

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	TCH	C	1201	-	-	2/16/81/81	0/4/4/4
2	TCH	F	1202	-	-	9/16/81/81	0/4/4/4
2	TCH	E	1201	-	-	4/16/81/81	0/4/4/4
2	TCH	C	1202	-	-	8/16/81/81	0/4/4/4
2	TCH	B	1201	-	-	8/16/81/81	0/4/4/4
2	TCH	D	1201	-	-	6/16/81/81	0/4/4/4
2	TCH	A	1201	-	-	4/16/81/81	0/4/4/4
2	TCH	F	1201	-	-	2/16/81/81	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1202	TCH	O3S-S26	2.07	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1202	TCH	O3S-S26	2.02	1.54	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	TCH	C5-C6-C7	4.94	119.91	114.46
2	C	1201	TCH	C6-C5-C10	3.31	116.17	112.66
2	C	1201	TCH	C9-C10-C5	3.15	113.00	108.58
2	F	1202	TCH	C13-C17-C20	2.47	122.44	119.50
2	C	1201	TCH	C5-C4-C3	2.35	116.21	112.76
2	B	1201	TCH	C16-C17-C13	-2.35	101.25	103.55

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1201	TCH	C25-C26-S26-O1S
2	A	1201	TCH	C25-C26-S26-O1S
2	B	1201	TCH	N24-C25-C26-S26
2	C	1201	TCH	N24-C25-C26-S26
2	C	1202	TCH	C23-C24-N24-C25
2	C	1202	TCH	O24-C24-N24-C25
2	C	1202	TCH	N24-C25-C26-S26
2	C	1202	TCH	C25-C26-S26-O2S
2	C	1202	TCH	C25-C26-S26-O3S
2	D	1201	TCH	C23-C24-N24-C25
2	D	1201	TCH	O24-C24-N24-C25
2	D	1201	TCH	C25-C26-S26-O3S
2	F	1202	TCH	N24-C25-C26-S26
2	C	1202	TCH	C21-C20-C22-C23
2	F	1202	TCH	C13-C17-C20-C22
2	D	1201	TCH	C20-C22-C23-C24
2	C	1201	TCH	C21-C20-C22-C23
2	A	1201	TCH	C21-C20-C22-C23
2	F	1201	TCH	C21-C20-C22-C23
2	C	1202	TCH	C17-C20-C22-C23
2	F	1202	TCH	C16-C17-C20-C21
2	F	1202	TCH	C16-C17-C20-C22
2	E	1201	TCH	C21-C20-C22-C23
2	A	1201	TCH	C25-C26-S26-O3S
2	B	1201	TCH	C13-C17-C20-C21
2	B	1201	TCH	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
2	E	1201	TCH	C25-C26-S26-O3S
2	F	1202	TCH	C17-C20-C22-C23
2	B	1201	TCH	C16-C17-C20-C22
2	B	1201	TCH	C21-C20-C22-C23
2	B	1201	TCH	C16-C17-C20-C21
2	E	1201	TCH	C25-C26-S26-O2S
2	A	1201	TCH	C25-C26-S26-O2S
2	B	1201	TCH	C25-C26-S26-O1S
2	C	1202	TCH	C25-C26-S26-O1S
2	D	1201	TCH	C25-C26-S26-O1S
2	D	1201	TCH	C25-C26-S26-O2S
2	F	1201	TCH	C25-C26-S26-O1S
2	F	1202	TCH	C22-C23-C24-O24
2	F	1202	TCH	C22-C23-C24-N24
2	B	1201	TCH	O24-C24-N24-C25
2	F	1202	TCH	C13-C17-C20-C21
2	F	1202	TCH	C21-C20-C22-C23

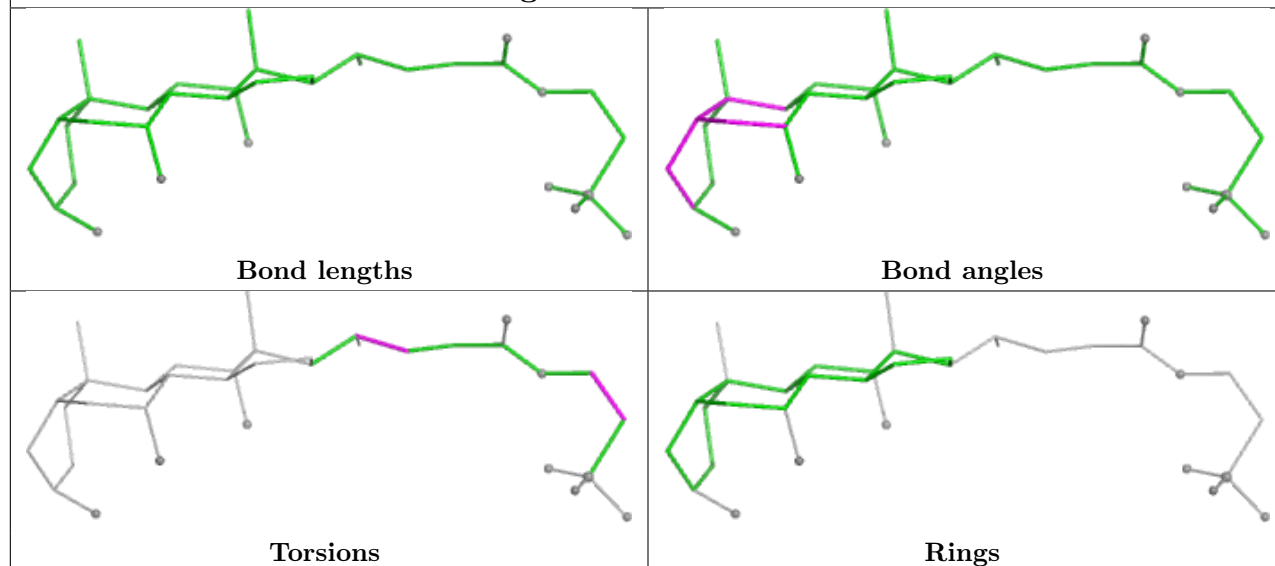
There are no ring outliers.

6 monomers are involved in 10 short contacts:

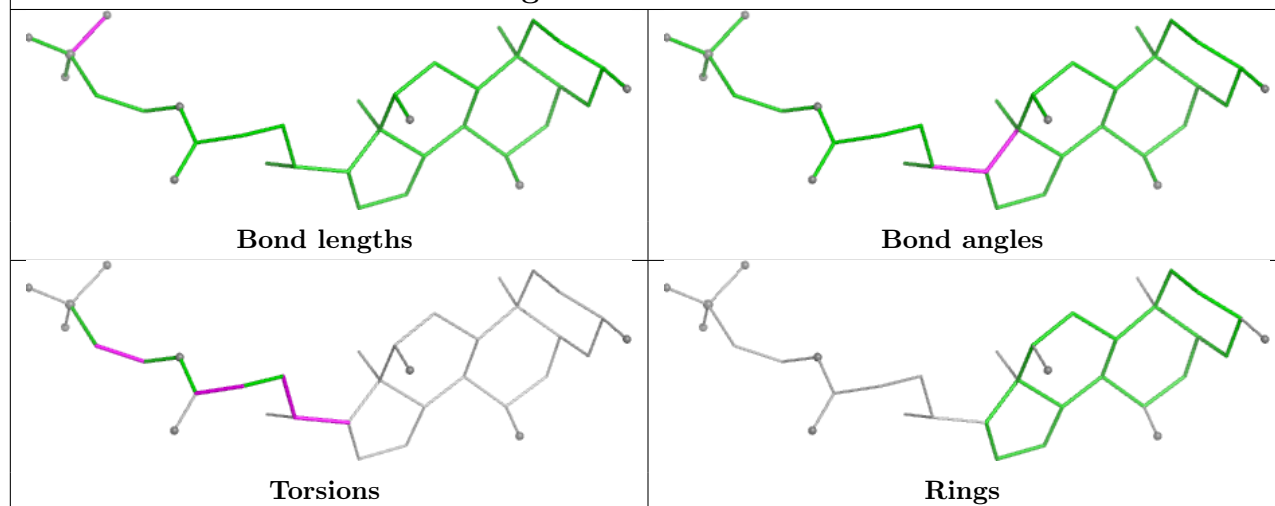
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	TCH	3	0
2	F	1202	TCH	1	0
2	E	1201	TCH	1	0
2	B	1201	TCH	3	0
2	D	1201	TCH	1	0
2	F	1201	TCH	1	0

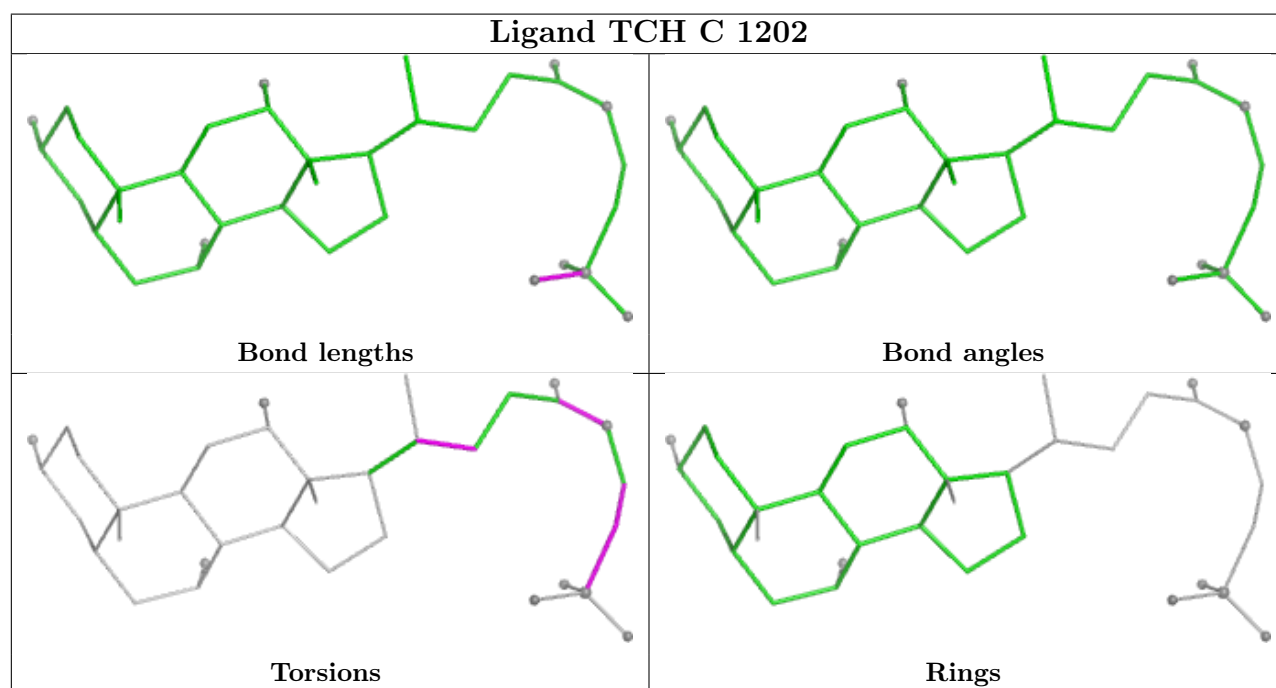
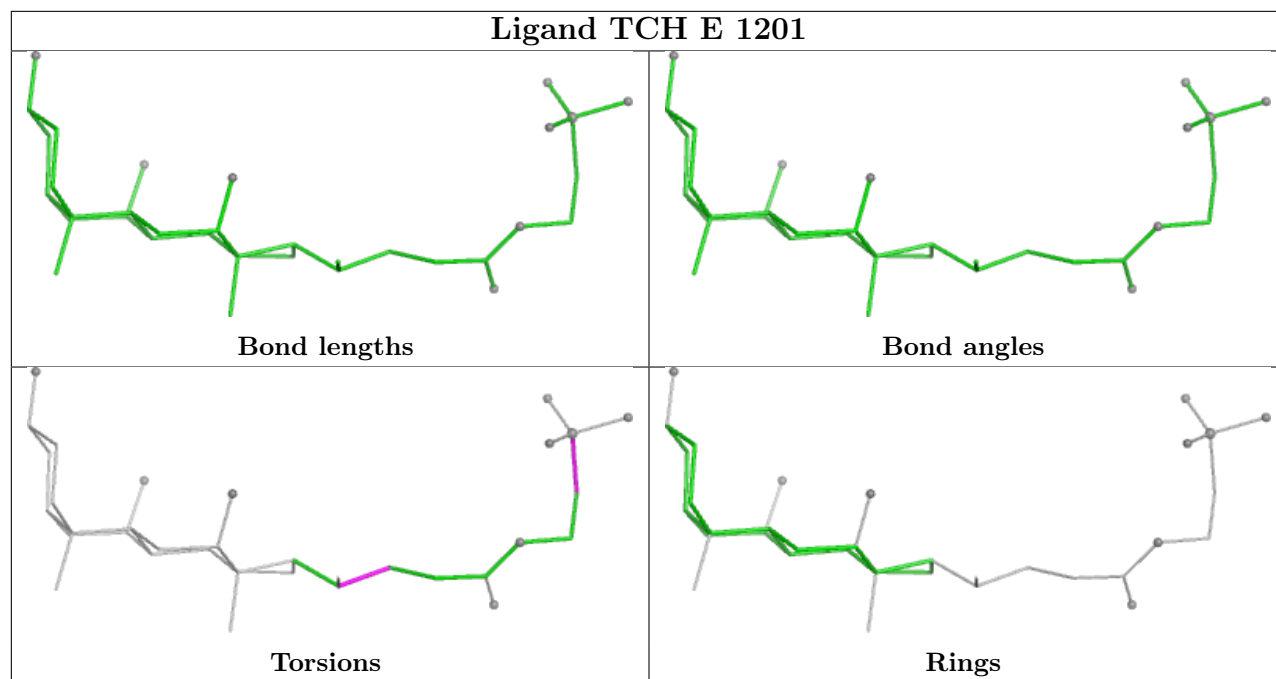
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

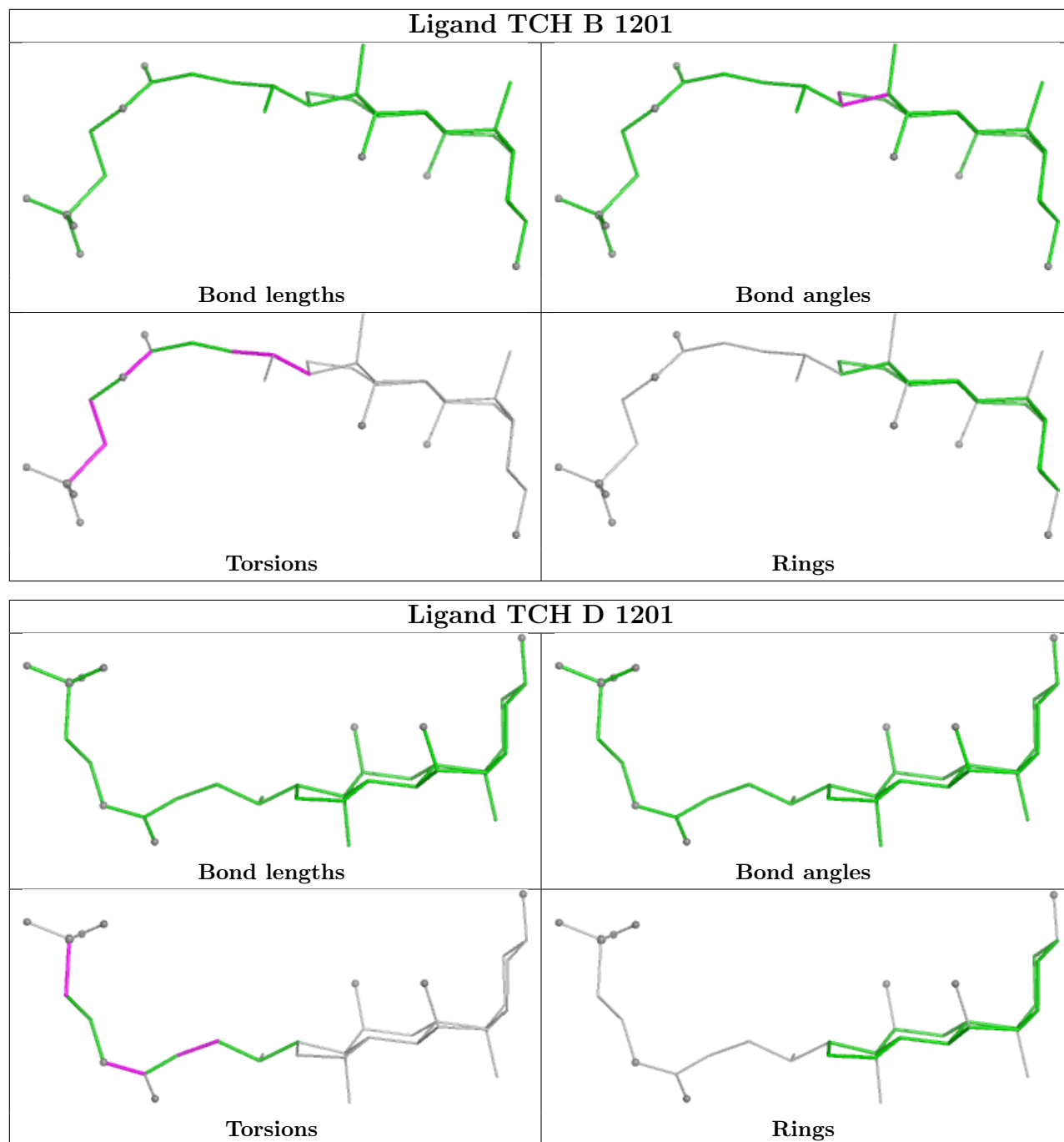
Ligand TCH C 1201

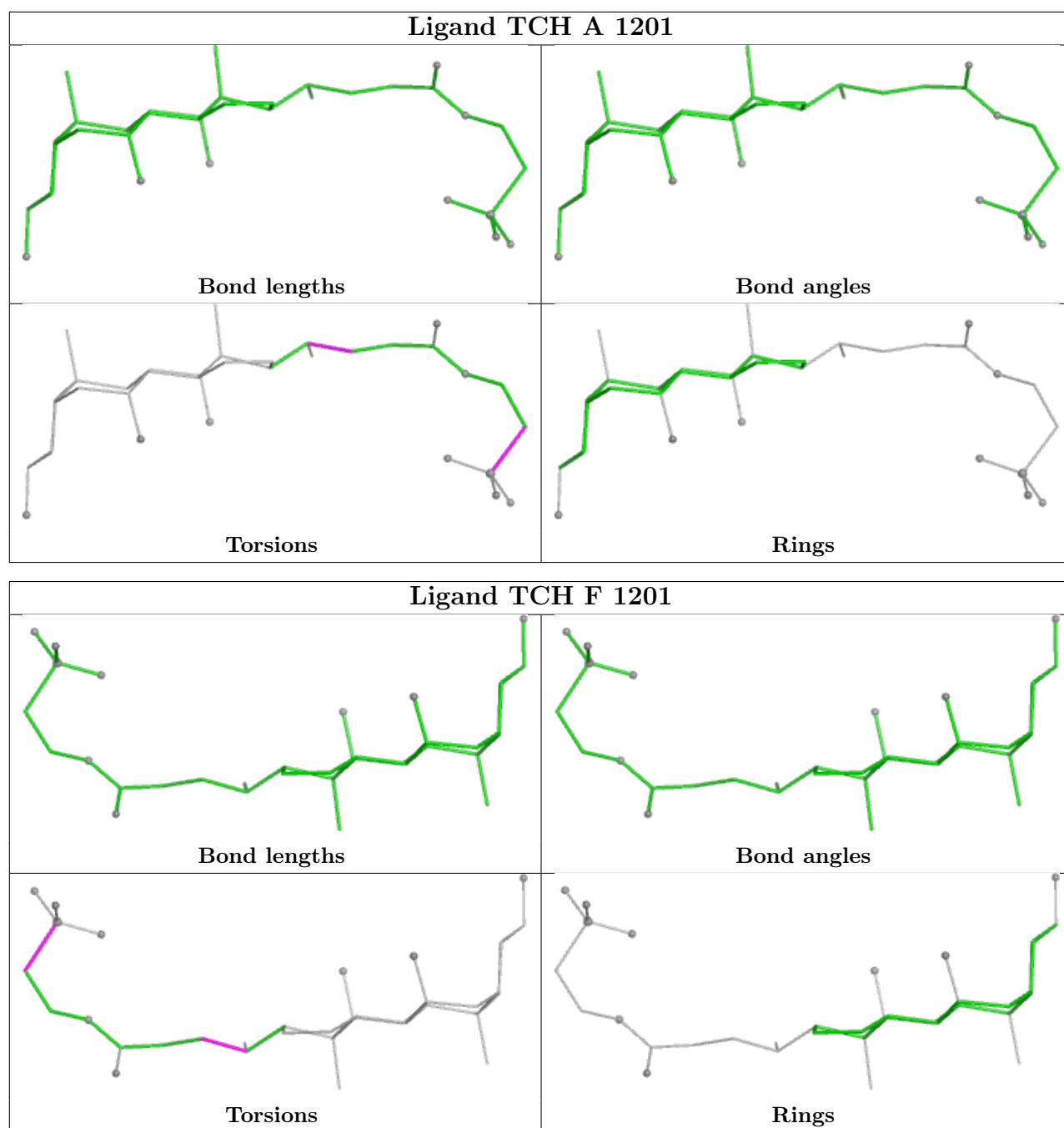


Ligand TCH F 1202









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	548/548 (100%)	-0.11	13 (2%) 59 50	27, 38, 70, 129	0
1	B	546/548 (99%)	0.13	22 (4%) 42 34	33, 52, 91, 150	0
1	C	543/548 (99%)	0.10	15 (2%) 55 46	37, 52, 78, 131	0
1	D	542/548 (98%)	0.23	23 (4%) 40 32	36, 55, 104, 146	0
1	E	540/548 (98%)	0.09	24 (4%) 39 30	27, 43, 111, 172	0
1	F	548/548 (100%)	0.36	22 (4%) 42 34	41, 64, 107, 138	0
All	All	3267/3288 (99%)	0.13	119 (3%) 46 38	27, 51, 98, 172	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	ALA	7.2
1	D	916	GLY	6.3
1	D	915	VAL	5.9
1	C	920	TYR	5.6
1	A	666	THR	5.0
1	C	916	GLY	5.0
1	D	1133	LEU	5.0
1	D	834	THR	4.8
1	B	915	VAL	4.6
1	C	915	VAL	4.4
1	F	680	ILE	4.1
1	B	660	PHE	4.1
1	B	919	ASN	4.1
1	A	915	VAL	3.6
1	D	660	PHE	3.4
1	D	626	THR	3.4
1	C	917	ILE	3.4
1	A	679	ASN	3.4
1	F	587	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	918	SER	3.2
1	B	839	SER	3.1
1	D	707	ASP	3.1
1	D	628	TYR	3.1
1	B	920	TYR	3.1
1	F	628	TYR	3.1
1	B	838	ASN	3.1
1	F	607	MET	3.0
1	F	625	ASN	2.9
1	E	837	SER	2.9
1	F	626	THR	2.9
1	B	1086	ARG	2.9
1	E	638	PRO	2.9
1	A	667	GLU	2.9
1	D	668	GLU	2.9
1	F	915	VAL	2.9
1	B	680	ILE	2.8
1	A	1086	ARG	2.8
1	A	917	ILE	2.7
1	F	989	GLY	2.7
1	E	680	ILE	2.7
1	E	914	SER	2.7
1	C	970	TYR	2.7
1	C	735	THR	2.7
1	F	629	SER	2.7
1	E	929	LEU	2.7
1	A	681	ASN	2.7
1	E	641	ILE	2.6
1	E	666	THR	2.6
1	E	672	ASN	2.6
1	D	839	SER	2.6
1	B	628	TYR	2.6
1	D	920	TYR	2.6
1	B	835	ASN	2.6
1	B	834	THR	2.6
1	B	626	THR	2.6
1	C	679	ASN	2.6
1	D	885	GLU	2.5
1	C	837	SER	2.5
1	F	670	GLY	2.5
1	E	679	ASN	2.5
1	C	680	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	627	ASP	2.5
1	B	988	SER	2.5
1	D	988	SER	2.5
1	C	628	TYR	2.5
1	C	625	ASN	2.5
1	E	671	VAL	2.4
1	E	741	ARG	2.4
1	F	920	TYR	2.4
1	A	938	TYR	2.4
1	D	680	ILE	2.4
1	E	626	THR	2.4
1	A	587	LEU	2.4
1	D	624	ASN	2.3
1	F	679	ASN	2.3
1	B	840	GLU	2.3
1	E	839	SER	2.3
1	D	607	MET	2.3
1	E	938	TYR	2.3
1	B	587	LEU	2.3
1	F	631	ILE	2.3
1	B	588	SER	2.3
1	E	842	ALA	2.3
1	E	970	TYR	2.3
1	A	678	PRO	2.2
1	E	667	GLU	2.2
1	B	921	ASN	2.2
1	D	1002	ASN	2.2
1	A	680	ILE	2.2
1	F	988	SER	2.2
1	D	677	ASN	2.2
1	F	678	PRO	2.2
1	B	837	SER	2.2
1	E	838	ASN	2.1
1	F	1134	ASP	2.1
1	E	628	TYR	2.1
1	F	1087	TYR	2.1
1	D	672	ASN	2.1
1	E	678	PRO	2.1
1	A	670	GLY	2.1
1	C	587	LEU	2.1
1	D	587	LEU	2.1
1	E	665	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	914	SER	2.1
1	C	1133	LEU	2.1
1	B	970	TYR	2.1
1	F	938	TYR	2.1
1	C	835	ASN	2.1
1	F	677	ASN	2.1
1	E	674	PHE	2.1
1	D	629	SER	2.0
1	E	604	GLY	2.0
1	F	741	ARG	2.0
1	C	668	GLU	2.0
1	E	630	SER	2.0
1	B	914	SER	2.0
1	D	676	ASN	2.0
1	F	673	PHE	2.0
1	D	1008	ASP	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.

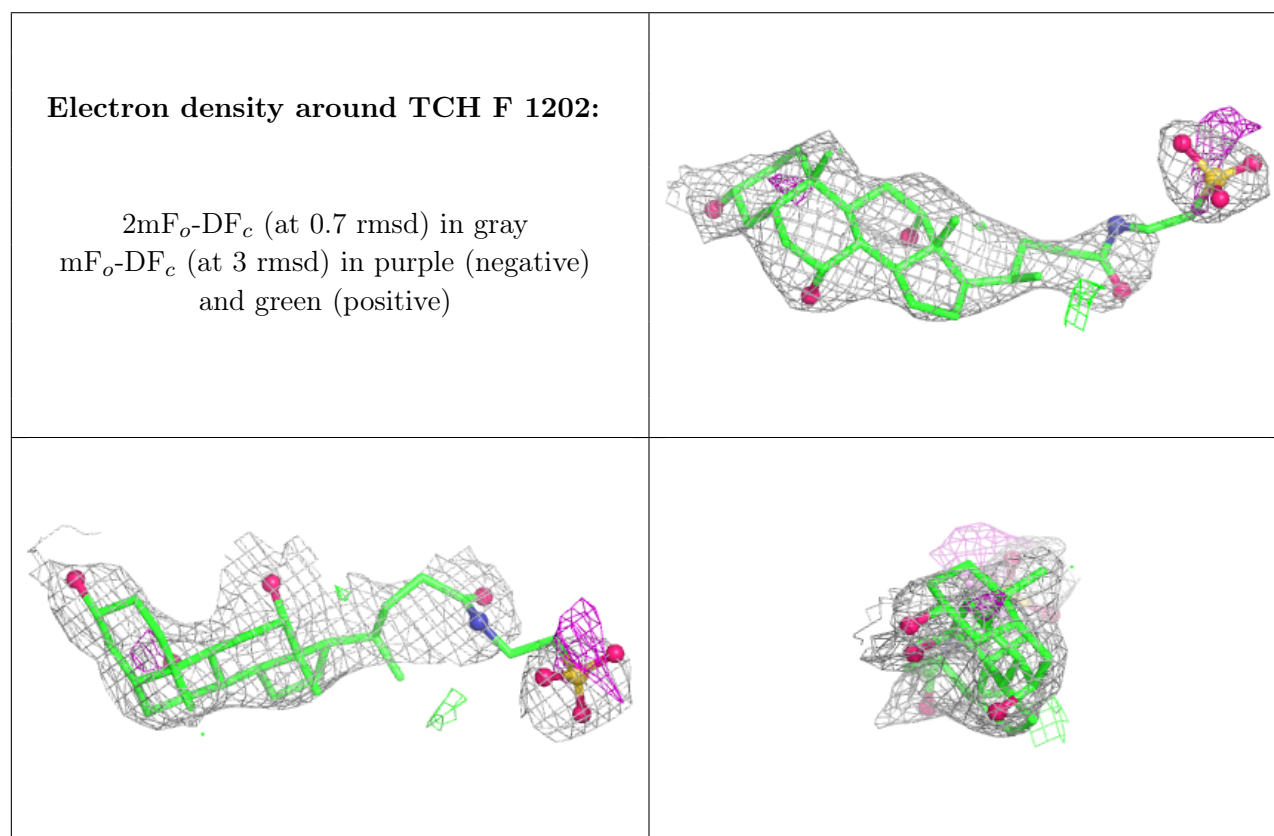
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TCH	F	1202	35/35	0.72	0.17	71,78,99,105	0
2	TCH	C	1202	35/35	0.73	0.18	67,79,90,95	0
2	TCH	C	1201	35/35	0.80	0.15	57,71,87,95	0
2	TCH	B	1201	35/35	0.82	0.16	58,69,84,90	0
2	TCH	E	1201	35/35	0.85	0.14	49,63,79,84	0
2	TCH	D	1201	35/35	0.86	0.13	53,67,82,93	0
2	TCH	F	1201	35/35	0.92	0.10	50,56,62,67	0

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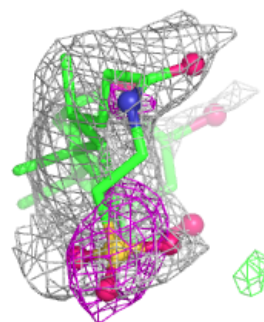
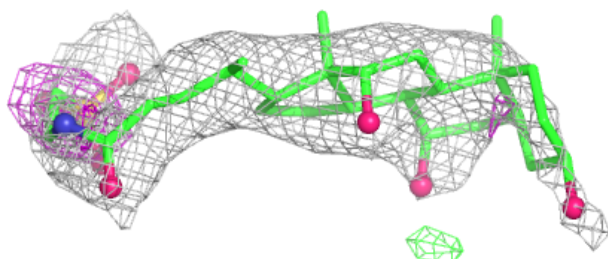
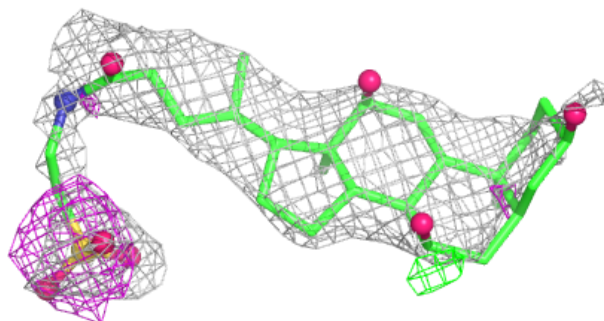
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TCH	A	1201	35/35	0.93	0.10	34,41,48,54	0

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.

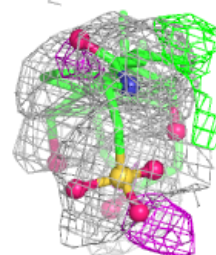
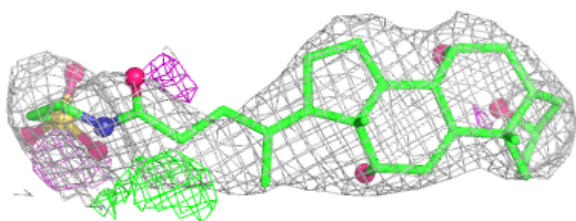
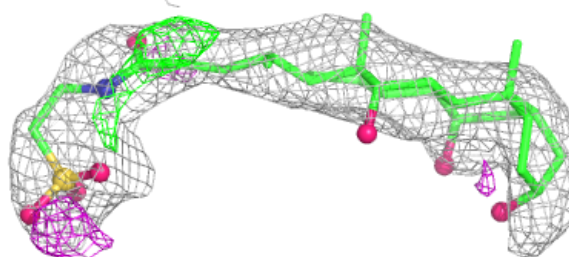


Electron density around TCH C 1202:

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

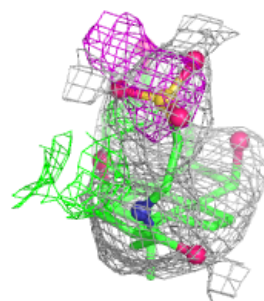
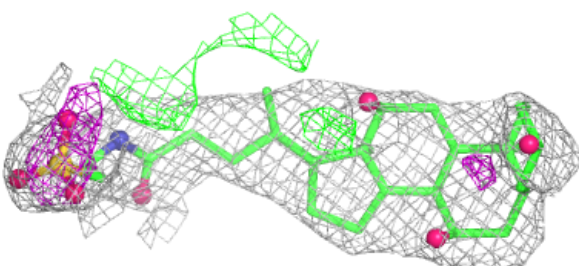
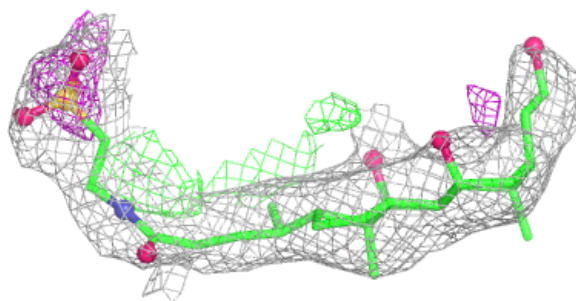
**Electron density around TCH C 1201:**

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

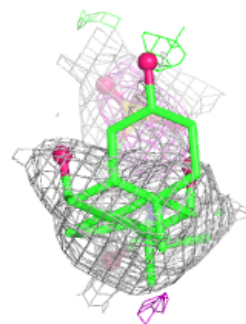
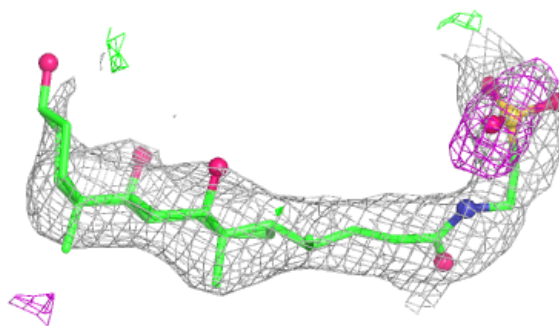


Electron density around TCH B 1201:

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

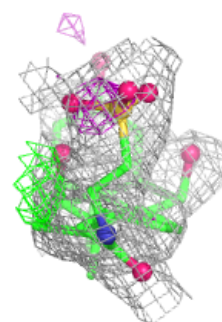
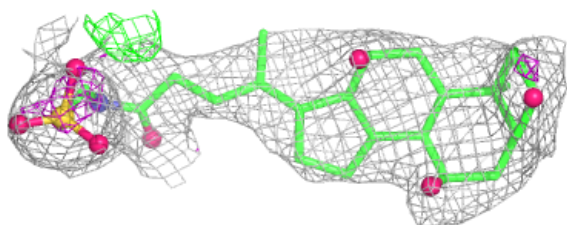
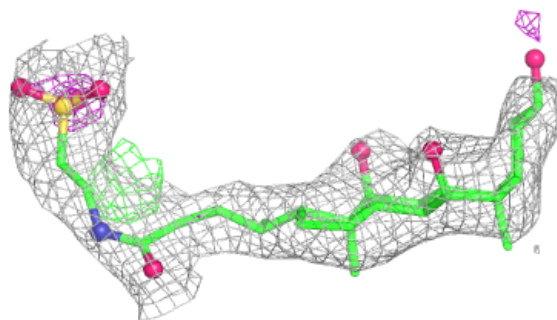
**Electron density around TCH E 1201:**

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

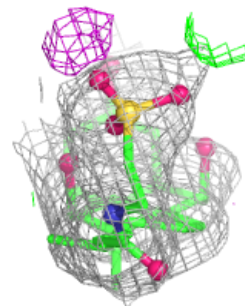
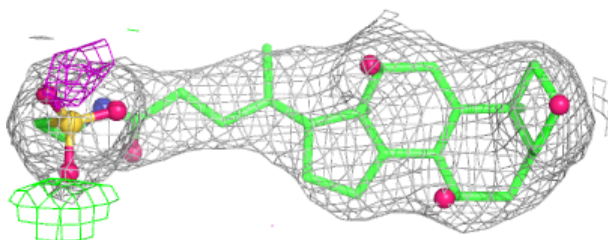


Electron density around TCH D 1201:

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

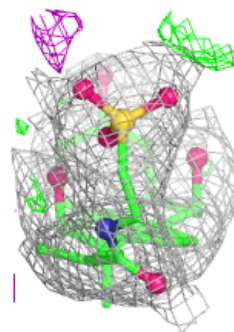
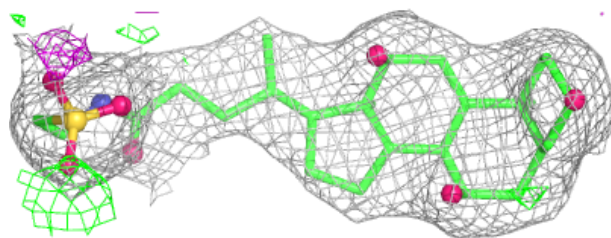
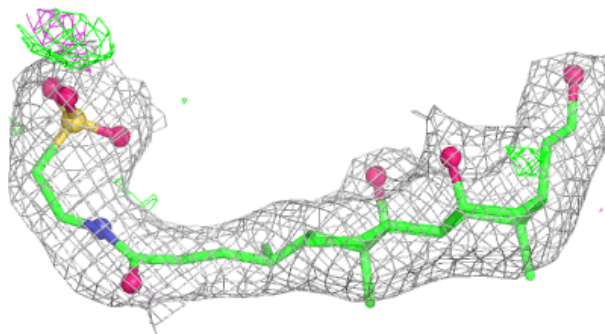
**Electron density around TCH F 1201:**

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



Electron density around TCH A 1201:

$2mF_o-DF_c$ (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.