



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 AM UTC

PDB ID : 4FR4 / pdb_00004fr4
Title : Crystal structure of human serine/threonine-protein kinase 32A (YANK1)
Authors : Chaikuad, A.; Elkins, J.M.; Krojer, T.; Mahajan, P.; Goubin, S.; Szklarz, M.; Tumber, A.; Wang, J.; Savitsky, P.; Shrestha, B.; Daga, N.; Picaud, S.; Fedorov, O.; Allerston, C.K.; Latwiel, S.V.A.; Vollmar, M.; Canning, P.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2012-06-26
Resolution : 2.29 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)

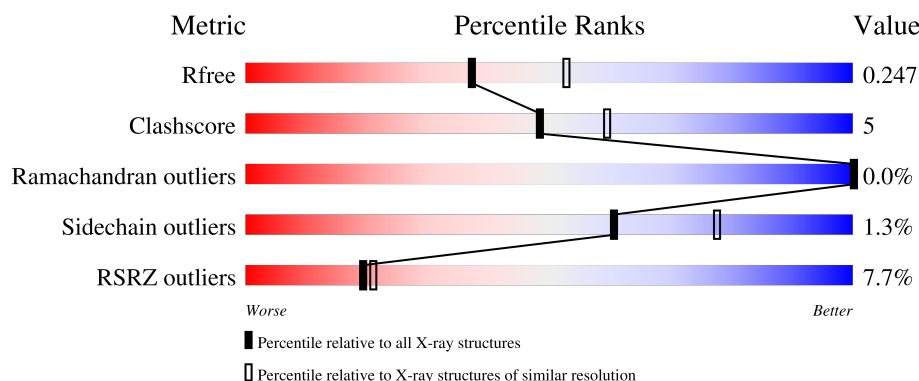
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	384	5% 81% 10% 9%
1	B	384	7% 78% 12% 9%
1	C	384	6% 79% 11% 10%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	384	8% 81% 9% 10%
1	E	384	8% 81% 8% 11%
1	F	384	8% 80% 10% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18277 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.

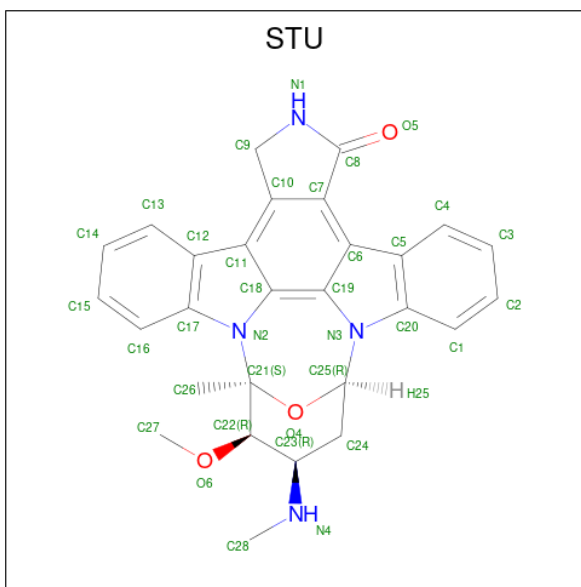
- Molecule 1 is a protein called Serine/threonine-protein kinase 32A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	7	0
			2871	1830	493	527	21			
1	B	350	Total	C	N	O	S	0	6	0
			2873	1831	490	531	21			
1	C	344	Total	C	N	O	S	0	6	0
			2833	1805	484	522	22			
1	D	346	Total	C	N	O	S	0	5	0
			2825	1806	477	521	21			
1	E	342	Total	C	N	O	S	0	6	0
			2810	1792	475	522	21			
1	F	346	Total	C	N	O	S	0	5	0
			2820	1800	478	522	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q8WU08
A	0	MET	-	expression tag	UNP Q8WU08
B	-1	SER	-	expression tag	UNP Q8WU08
B	0	MET	-	expression tag	UNP Q8WU08
C	-1	SER	-	expression tag	UNP Q8WU08
C	0	MET	-	expression tag	UNP Q8WU08
D	-1	SER	-	expression tag	UNP Q8WU08
D	0	MET	-	expression tag	UNP Q8WU08
E	-1	SER	-	expression tag	UNP Q8WU08
E	0	MET	-	expression tag	UNP Q8WU08
F	-1	SER	-	expression tag	UNP Q8WU08
F	0	MET	-	expression tag	UNP Q8WU08

- Molecule 2 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		
2	C	1	Total	C	N	O	0	0
			35	28	4	3		
2	D	1	Total	C	N	O	0	0
			35	28	4	3		
2	E	1	Total	C	N	O	0	0
			35	28	4	3		
2	F	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	B	167	Total O 167 167	0	0
4	C	172	Total O 172 172	0	0
4	D	144	Total O 144 144	0	0

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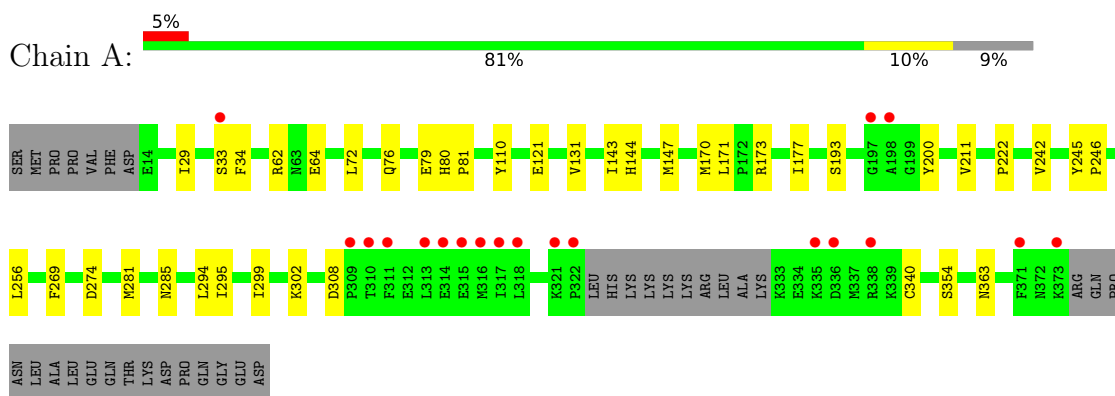
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	163	Total 163	O 163	0	0
4	F	173	Total 173	O 173	0	0

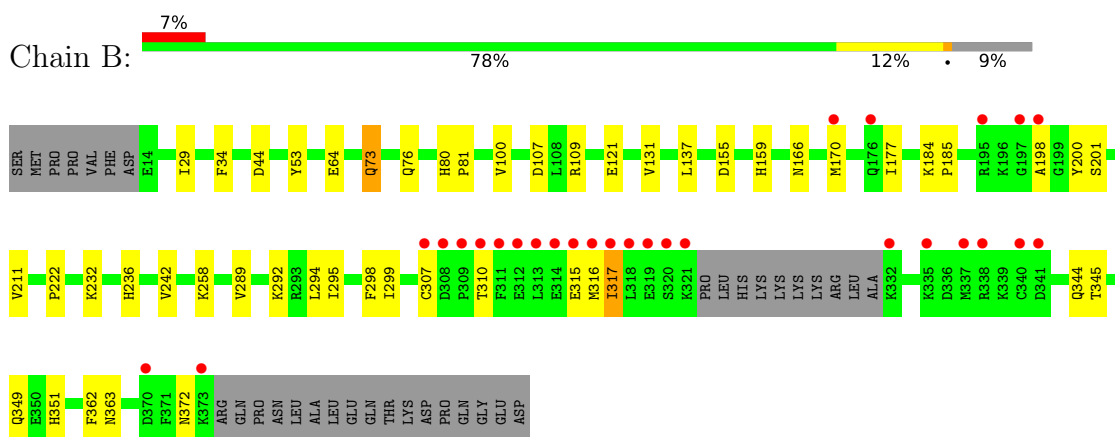
3 Residue-property plots

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.

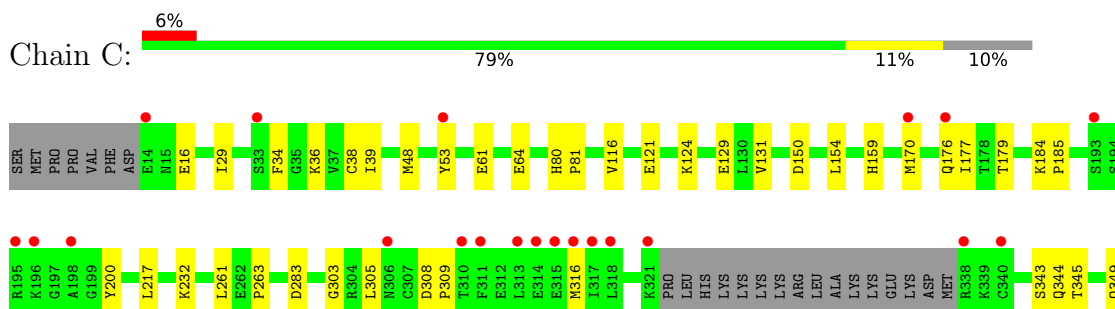
• Molecule 1: Serine/threonine-protein kinase 32A

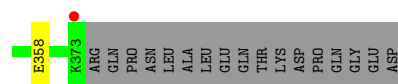


• Molecule 1: Serine/threonine-protein kinase 32A

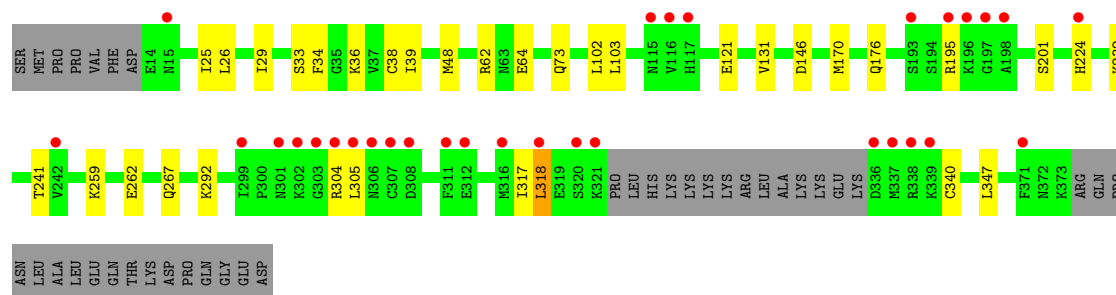
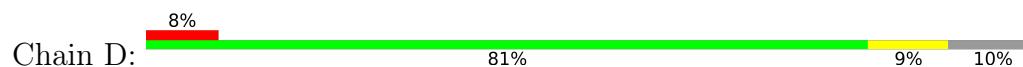


• Molecule 1: Serine/threonine-protein kinase 32A

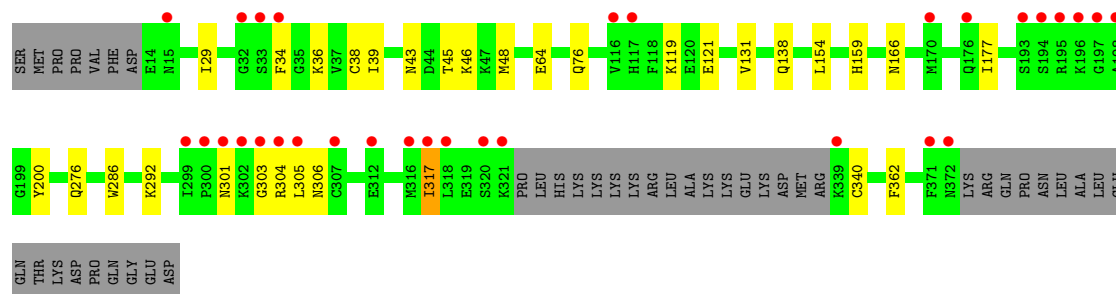
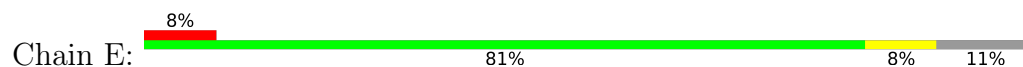




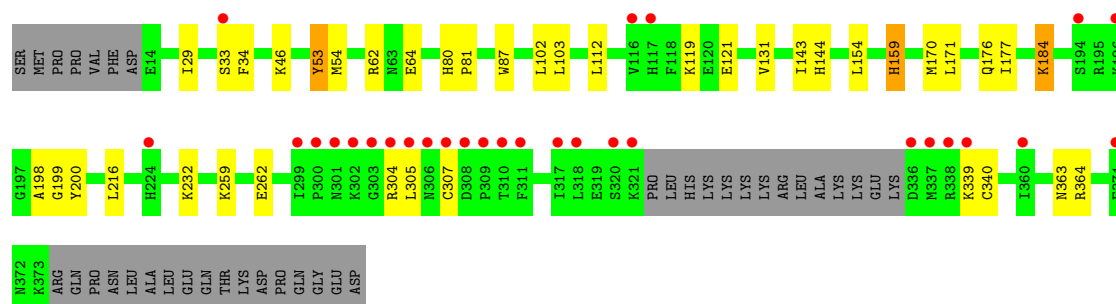
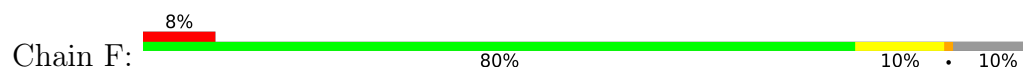
• Molecule 1: Serine/threonine-protein kinase 32A



• Molecule 1: Serine/threonine-protein kinase 32A



• Molecule 1: Serine/threonine-protein kinase 32A



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	154.11Å 154.11Å 112.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.44 – 2.29 50.44 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.44-2.29) 95.7 (50.44-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.244 0.207 , 0.247	Depositor DCC
R_{free} test set	6741 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.000 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18277	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 26.77 % 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 2.4797e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: STU, EDO

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	1.10	4/2958 (0.1%)	0.75	0/3997
1	B	1.09	5/2956 (0.2%)	0.73	0/3992
1	C	1.08	1/2916 (0.0%)	0.72	0/3939
1	D	0.99	0/2906	0.71	0/3928
1	E	1.04	0/2892	0.72	0/3908
1	F	1.06	4/2900 (0.1%)	0.74	0/3920
All	All	1.06	14/17528 (0.1%)	0.73	0/23684

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	HIS	CG-CD2	5.88	1.42	1.35
1	F	159	HIS	CG-CD2	5.69	1.42	1.35
1	F	53	TYR	CA-C	-5.66	1.45	1.52
1	B	236	HIS	CG-CD2	5.42	1.41	1.35
1	F	144	HIS	CG-ND1	-5.36	1.32	1.38
1	C	303	GLY	N-CA	5.27	1.49	1.44
1	A	110	TYR	C-O	-5.26	1.18	1.24
1	B	53	TYR	CA-C	-5.24	1.46	1.52
1	B	351	HIS	ND1-CE1	5.23	1.37	1.32
1	B	100	VAL	CA-C	5.13	1.57	1.52
1	A	144	HIS	CG-ND1	-5.09	1.32	1.38
1	A	354	SER	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	184	LYS	N-CA	5.09	1.51	1.46
1	A	79	GLU	C-O	-5.05	1.18	1.23

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	315	GLU	Peptide

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	2871	0	2779	26	0
1	B	2873	0	2777	40	0
1	C	2833	0	2749	31	0
1	D	2825	0	2724	30	0
1	E	2810	0	2720	22	0
1	F	2820	0	2715	31	0
2	A	35	0	26	5	0
2	B	35	0	26	4	0
2	C	35	0	26	4	0
2	D	35	0	26	5	0
2	E	35	0	26	4	0
2	F	35	0	26	3	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	12	0	18	0	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
4	A	184	0	0	8	0
4	B	167	0	0	7	0
4	C	172	0	0	9	0
4	D	144	0	0	7	0
4	E	163	0	0	7	0
4	F	173	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18277	0	16668	185	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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:STU:H261	2:B:401:STU:H16	1.52	0.91
2:C:401:STU:H261	2:C:401:STU:H16	1.56	0.86
2:E:401:STU:H261	2:E:401:STU:H16	1.61	0.83
2:A:401:STU:H261	2:A:401:STU:H16	1.58	0.82
2:D:401:STU:H261	2:D:401:STU:H16	1.63	0.80
1:D:26:LEU:HD13	1:D:318:LEU:HD22	1.68	0.74
2:F:401:STU:H261	2:F:401:STU:H16	1.69	0.73
1:D:224[A]:HIS:ND1	4:D:639:HOH:O	2.22	0.72
1:C:232:LYS:NZ	4:C:617:HOH:O	2.27	0.68
1:B:289:VAL:HG22	1:B:294:LEU:HD12	1.77	0.65
1:B:34:PHE:CZ	1:B:64:GLU:HG3	2.32	0.65
1:B:73[A]:GLN:OE1	1:B:170:MET:HE1	1.96	0.65
1:C:150:ASP:O	2:C:401:STU:H272	1.97	0.65
1:E:34:PHE:CZ	1:E:64:GLU:HG3	2.32	0.63
1:C:34:PHE:CZ	1:C:64:GLU:HG3	2.34	0.63
1:B:307:CYS:SG	1:F:307:CYS:CB	2.87	0.62
1:B:292:LYS:HA	4:B:578:HOH:O	1.99	0.62
1:E:39:ILE:HD13	1:E:317:ILE:HG21	1.81	0.61
1:A:193[A]:SER:OG	4:A:658:HOH:O	2.16	0.61
4:A:638:HOH:O	1:F:232:LYS:HE2	2.00	0.61
1:E:43:ASN:HB2	4:E:545:HOH:O	1.99	0.61
1:A:34:PHE:CZ	1:A:64:GLU:HG3	2.36	0.60
1:D:34:PHE:CZ	1:D:64:GLU:HG3	2.36	0.60
1:D:73:GLN:OE1	1:D:170:MET:HE1	2.02	0.59
1:F:34:PHE:CZ	1:F:64:GLU:HG3	2.38	0.59
1:A:64:GLU:OE2	4:A:677:HOH:O	2.16	0.58
1:B:198:ALA:HB1	4:B:643:HOH:O	2.03	0.57
1:B:232:LYS:HG2	4:B:650:HOH:O	2.05	0.56
1:A:170:MET:HG2	4:A:633:HOH:O	2.06	0.56
2:B:401:STU:H261	2:B:401:STU:C16	2.23	0.56
1:C:38[B]:CYS:SG	1:C:53:TYR:HE2	2.29	0.56
1:E:76:GLN:HG2	1:E:362:PHE:CG	2.41	0.55
1:B:298:PHE:O	1:B:299:ILE:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:MET:HG2	4:F:642:HOH:O	2.05	0.55
1:B:316:MET:HE2	4:C:534:HOH:O	2.07	0.55
1:B:201:SER:HB3	4:B:577:HOH:O	2.06	0.54
1:D:241:THR:HG21	4:D:641:HOH:O	2.07	0.54
1:E:304:ARG:O	1:E:305:LEU:CB	2.56	0.54
1:D:26:LEU:CD1	1:D:318:LEU:HD22	2.38	0.54
1:B:211:VAL:HG13	1:B:222:PRO:HD2	1.91	0.53
1:F:304:ARG:O	1:F:305:LEU:CB	2.56	0.53
2:C:401:STU:H261	2:C:401:STU:C16	2.26	0.53
1:D:262[B]:GLU:HG2	1:D:267:GLN:HB2	1.89	0.53
1:D:304:ARG:O	1:D:305:LEU:CB	2.57	0.53
1:F:184:LYS:HE3	4:F:518:HOH:O	2.09	0.53
1:E:76:GLN:HG2	1:E:362:PHE:CD2	2.44	0.52
2:B:401:STU:C16	2:B:401:STU:C26	2.87	0.52
1:A:143:ILE:HD11	1:A:171:LEU:HD22	1.92	0.52
1:D:292:LYS:NZ	4:D:549:HOH:O	2.29	0.52
1:F:259:LYS:CE	4:F:635:HOH:O	2.58	0.51
1:C:343:SER:HB2	1:D:347:LEU:CD1	2.40	0.51
1:E:29:ILE:HD12	2:E:401:STU:C5	2.40	0.51
2:F:401:STU:H261	2:F:401:STU:C16	2.40	0.51
1:B:258:LYS:NZ	4:B:653:HOH:O	2.43	0.51
1:E:34:PHE:CZ	1:E:64:GLU:CG	2.95	0.50
1:A:299:ILE:HB	4:A:679:HOH:O	2.12	0.50
1:C:179:THR:HG23	4:C:618:HOH:O	2.12	0.50
1:B:44:ASP:HA	1:F:46:LYS:HG2	1.94	0.50
1:C:184:LYS:HE3	4:C:599:HOH:O	2.10	0.50
1:A:269:PHE:CD1	1:A:274:ASP:HB3	2.47	0.49
1:E:36:LYS:HD2	1:E:38[A]:CYS:SG	2.52	0.49
2:D:401:STU:H273	2:D:401:STU:C17	2.43	0.49
1:F:177:ILE:HG22	1:F:200:TYR:O	2.12	0.49
1:C:34:PHE:CZ	1:C:64:GLU:CG	2.95	0.49
2:E:401:STU:H261	2:E:401:STU:C16	2.32	0.49
1:A:302:LYS:NZ	4:A:669:HOH:O	2.45	0.49
1:B:34:PHE:CZ	1:B:64:GLU:CG	2.95	0.49
1:B:166:ASN:ND2	4:B:633:HOH:O	2.21	0.49
1:A:302:LYS:HE3	1:A:308:ASP:OD2	2.12	0.48
1:B:372:ASN:ND2	1:D:195:ARG:HA	2.28	0.48
1:A:256:LEU:HD22	1:A:281:MET:HE2	1.96	0.48
1:B:344:GLN:HG3	1:B:345:THR:N	2.29	0.48
1:E:36:LYS:HG2	4:E:572:HOH:O	2.13	0.48
1:A:34:PHE:CZ	1:A:64:GLU:CG	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HG13	1:A:222:PRO:HD2	1.96	0.48
1:A:294:LEU:HD22	1:F:62:ARG:NH2	2.28	0.47
1:F:143:ILE:HD11	1:F:171:LEU:HD22	1.96	0.47
1:C:36:LYS:HD2	1:C:38[A]:CYS:SG	2.53	0.47
1:C:344:GLN:HG3	1:C:345:THR:N	2.29	0.47
1:C:176[B]:GLN:NE2	4:C:553:HOH:O	2.45	0.47
1:E:34:PHE:CE2	1:E:64:GLU:HG3	2.49	0.47
2:C:401:STU:C16	2:C:401:STU:C26	2.92	0.47
1:D:34:PHE:CZ	1:D:64:GLU:CG	2.98	0.47
1:A:295:ILE:HD13	1:A:295:ILE:N	2.29	0.47
1:D:36:LYS:HD2	1:D:38[B]:CYS:SG	2.55	0.47
1:D:146:ASP:HA	4:D:527:HOH:O	2.14	0.47
1:C:116:VAL:HA	4:C:641:HOH:O	2.14	0.46
1:F:154:LEU:HA	1:F:159:HIS:O	2.15	0.46
1:F:80:HIS:CG	1:F:81:PRO:HD2	2.51	0.46
1:B:73[A]:GLN:OE1	1:B:170:MET:CE	2.61	0.46
1:F:102:LEU:C	1:F:103:LEU:HD22	2.39	0.46
1:F:176:GLN:CD	1:F:199:GLY:HA3	2.40	0.46
2:A:401:STU:C16	2:A:401:STU:C26	2.94	0.46
1:D:29:ILE:HD12	2:D:401:STU:C5	2.46	0.46
1:F:198:ALA:HB1	4:F:609:HOH:O	2.15	0.46
1:C:261:LEU:O	1:C:263:PRO:HD3	2.16	0.46
1:E:166:ASN:HB3	4:E:628:HOH:O	2.15	0.46
1:A:173:ARG:NE	4:A:631:HOH:O	2.48	0.45
1:C:34:PHE:CE2	1:C:64:GLU:HG3	2.50	0.45
1:B:177:ILE:HG22	1:B:200:TYR:O	2.16	0.45
1:B:34:PHE:CE2	1:B:64:GLU:HG3	2.51	0.45
1:B:242:VAL:O	1:B:242:VAL:HG23	2.16	0.45
1:B:310:THR:HG22	1:C:358:GLU:CD	2.42	0.45
1:A:72:LEU:O	1:A:76:GLN:HG3	2.17	0.45
1:E:301:ASN:OD1	1:E:303:GLY:N	2.49	0.45
1:B:76:GLN:HG2	1:B:362:PHE:CD2	2.52	0.45
1:C:343:SER:HB3	1:D:347:LEU:HD12	1.98	0.44
1:D:102:LEU:C	1:D:103:LEU:HD22	2.42	0.44
1:A:29:ILE:HD12	2:A:401:STU:C5	2.48	0.44
1:F:53:TYR:C	1:F:54:MET:HG3	2.42	0.44
1:B:295:ILE:N	1:B:295:ILE:HD13	2.32	0.44
2:A:401:STU:H16	2:A:401:STU:C26	2.40	0.44
1:F:87:TRP:CE3	1:F:364:ARG:HB3	2.53	0.44
1:C:343:SER:CB	1:D:347:LEU:HD12	2.48	0.44
1:A:177:ILE:HG22	1:A:200:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:HG21	1:E:48:MET:HE2	2.00	0.44
1:E:154:LEU:HA	1:E:159:HIS:O	2.18	0.44
1:A:80:HIS:CG	1:A:81:PRO:HD2	2.53	0.43
1:F:339:LYS:HD2	4:F:670:HOH:O	2.18	0.43
1:B:44:ASP:HA	1:F:46:LYS:CG	2.48	0.43
1:F:34:PHE:CZ	1:F:64:GLU:CG	3.01	0.43
1:C:217:LEU:HD22	4:C:591:HOH:O	2.17	0.43
1:A:34:PHE:CE2	1:A:64:GLU:HG3	2.54	0.43
1:A:299:ILE:HG21	4:A:683:HOH:O	2.19	0.43
1:B:289:VAL:CG2	1:B:294:LEU:HD12	2.45	0.43
1:D:232:LYS:HG2	4:D:612:HOH:O	2.19	0.43
1:F:363:ASN:OD1	1:F:363:ASN:C	2.60	0.43
1:B:242:VAL:O	1:B:242:VAL:CG2	2.67	0.43
1:D:34:PHE:CE2	1:D:64:GLU:HG3	2.54	0.42
2:D:401:STU:C16	2:D:401:STU:C26	2.96	0.42
1:E:306:ASN:N	4:E:517:HOH:O	2.52	0.42
1:C:232:LYS:HG2	4:C:550:HOH:O	2.20	0.42
1:D:39:ILE:HD13	1:D:317:ILE:HG21	2.01	0.42
1:E:45:THR:O	1:E:46:LYS:HB2	2.19	0.42
1:C:80:HIS:CG	1:C:81:PRO:HD2	2.54	0.42
1:D:176:GLN:NE2	4:D:634:HOH:O	2.46	0.42
1:B:294:LEU:HD22	1:D:62:ARG:NH2	2.35	0.42
2:A:401:STU:H273	2:A:401:STU:C17	2.50	0.42
1:B:317:ILE:HG22	1:C:170:MET:HB3	2.01	0.42
1:F:29:ILE:HD12	2:F:401:STU:C5	2.49	0.42
1:A:363:ASN:OD1	1:A:363:ASN:C	2.63	0.42
1:B:184:LYS:N	1:B:185:PRO:HD2	2.33	0.42
1:C:177:ILE:HG22	1:C:200:TYR:O	2.19	0.42
1:E:276:GLN:HG2	1:E:286:TRP:NE1	2.35	0.41
1:F:262:GLU:HB3	4:F:636:HOH:O	2.19	0.41
1:B:80:HIS:CG	1:B:81:PRO:HD2	2.55	0.41
1:C:184:LYS:N	1:C:185:PRO:HD2	2.35	0.41
1:F:119:LYS:HD3	4:F:662:HOH:O	2.20	0.41
1:A:285:ASN:OD1	1:A:285:ASN:C	2.62	0.41
1:A:33:SER:HB2	1:A:62:ARG:HH12	1.85	0.41
1:B:76:GLN:HG2	1:B:362:PHE:CG	2.56	0.41
1:C:39:ILE:HG21	1:C:48:MET:HE2	2.02	0.41
1:E:138:GLN:HB2	4:E:520:HOH:O	2.19	0.41
1:A:245:TYR:O	1:A:246:PRO:C	2.63	0.41
1:D:262[B]:GLU:HG2	1:D:267:GLN:CB	2.51	0.41
1:F:112:LEU:HD21	1:F:216:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLU:OE2	1:C:159:HIS:ND1	2.43	0.41
1:D:201:SER:HB3	4:D:581:HOH:O	2.21	0.41
1:B:294:LEU:HD22	1:D:62:ARG:HH22	1.85	0.41
2:E:401:STU:C16	2:E:401:STU:C26	2.98	0.41
1:A:147:MET:HE3	1:A:147:MET:HB3	1.94	0.41
1:B:155:ASP:OD1	1:B:155:ASP:C	2.64	0.41
1:C:154:LEU:HA	1:C:159:HIS:O	2.21	0.41
1:E:119:LYS:HE3	4:E:650:HOH:O	2.20	0.41
1:E:177:ILE:HG22	1:E:200:TYR:O	2.21	0.41
1:D:39:ILE:HG21	1:D:48:MET:HE2	2.03	0.41
1:B:107:ASP:OD2	1:B:109:ARG:HB3	2.21	0.40
1:D:25:ILE:HG23	1:D:38[A]:CYS:SG	2.61	0.40
1:D:259:LYS:HD2	1:D:259:LYS:HA	1.98	0.40
1:B:258:LYS:HE2	4:B:653:HOH:O	2.21	0.40
1:B:363:ASN:OD1	1:B:363:ASN:C	2.65	0.40
1:C:29:ILE:HG22	1:C:305:LEU:HD21	2.02	0.40
1:F:34:PHE:CE2	1:F:64:GLU:HG3	2.55	0.40
1:B:29:ILE:HD12	2:B:401:STU:C5	2.51	0.40
1:C:124:LYS:NZ	1:C:283:ASP:OD1	2.46	0.40
2:D:401:STU:H261	2:D:401:STU:C16	2.34	0.40
1:D:33:SER:HB2	1:D:62:ARG:HH12	1.86	0.40
1:F:33:SER:HB2	1:F:62:ARG:HH12	1.87	0.40
1:F:103:LEU:HD22	1:F:103:LEU:N	2.37	0.40
1:B:44:ASP:CB	1:F:46:LYS:HE2	2.52	0.40
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.94	0.40
1:C:16:GLU:HA	4:C:567:HOH:O	2.22	0.40
1:C:61:GLU:OE2	1:F:119:LYS:NZ	2.53	0.40
1:C:308:ASP:HA	1:C:309:PRO:HD3	1.92	0.40
1:E:292:LYS:HA	4:E:612:HOH:O	2.21	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	353/384 (92%)	332 (94%)	21 (6%)	0	100	100
1	B	352/384 (92%)	334 (95%)	17 (5%)	1 (0%)	36	46
1	C	346/384 (90%)	326 (94%)	20 (6%)	0	100	100
1	D	347/384 (90%)	325 (94%)	22 (6%)	0	100	100
1	E	344/384 (90%)	324 (94%)	20 (6%)	0	100	100
1	F	347/384 (90%)	326 (94%)	21 (6%)	0	100	100
All	All	2089/2304 (91%)	1967 (94%)	121 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	ILE

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	315/355 (89%)	311 (99%)	4 (1%)	61	77
1	B	315/355 (89%)	310 (98%)	5 (2%)	55	73
1	C	314/355 (88%)	310 (99%)	4 (1%)	61	77
1	D	309/355 (87%)	305 (99%)	4 (1%)	61	77
1	E	311/355 (88%)	307 (99%)	4 (1%)	61	77
1	F	308/355 (87%)	305 (99%)	3 (1%)	68	82
All	All	1872/2130 (88%)	1848 (99%)	24 (1%)	61	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	A	131	VAL
1	A	242	VAL
1	A	340	CYS

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Mol	Chain	Res	Type
1	B	73[A]	GLN
1	B	73[B]	GLN
1	B	121	GLU
1	B	131	VAL
1	B	349	GLN
1	C	121	GLU
1	C	131	VAL
1	C	316	MET
1	C	349	GLN
1	D	121	GLU
1	D	131	VAL
1	D	318	LEU
1	D	340	CYS
1	E	121	GLU
1	E	131	VAL
1	E	317	ILE
1	E	340	CYS
1	F	121	GLU
1	F	131	VAL
1	F	340	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	115	ASN
1	A	236	HIS
1	A	349	GLN
1	B	349	GLN
1	B	356	GLN
1	C	73	GLN
1	C	76	GLN
1	C	166	ASN
1	C	251	GLN
1	C	271	GLN
1	C	349	GLN
1	C	356	GLN
1	E	166	ASN
1	F	73	GLN
1	F	115	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 ⓘ

14 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	EDO	C	404	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	B	403	-	3,3,3	0.77	0	2,2,2	0.17	0
3	EDO	C	403	-	3,3,3	0.57	0	2,2,2	0.29	0
2	STU	F	401	-	39,42,42	2.64	16 (41%)	50,68,68	2.76	17 (34%)
3	EDO	E	402	-	3,3,3	0.57	0	2,2,2	0.33	0
3	EDO	A	402	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	F	402	-	3,3,3	0.53	0	2,2,2	0.24	0
3	EDO	B	402	-	3,3,3	0.84	0	2,2,2	0.42	0
3	EDO	C	402	-	3,3,3	0.62	0	2,2,2	0.07	0
2	STU	C	401	-	39,42,42	2.64	11 (28%)	50,68,68	2.69	17 (34%)
2	STU	D	401	-	39,42,42	2.55	13 (33%)	50,68,68	2.74	17 (34%)
2	STU	E	401	-	39,42,42	2.62	13 (33%)	50,68,68	2.77	17 (34%)
2	STU	A	401	-	39,42,42	2.64	13 (33%)	50,68,68	2.62	16 (32%)
2	STU	B	401	-	39,42,42	2.76	16 (41%)	50,68,68	2.58	16 (32%)

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	EDO	C	404	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	C	403	-	-	1/1/1/1	-
2	STU	F	401	-	-	0/4/42/42	-
3	EDO	E	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	F	402	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
2	STU	C	401	-	-	1/4/42/42	-
2	STU	D	401	-	-	0/4/42/42	-
2	STU	E	401	-	-	0/4/42/42	-
2	STU	A	401	-	-	1/4/42/42	-
2	STU	B	401	-	-	0/4/42/42	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	STU	C9-C10	-7.78	1.43	1.50
2	C	401	STU	C9-C10	-7.59	1.43	1.50
2	A	401	STU	C9-C10	-7.27	1.44	1.50
2	E	401	STU	C9-C10	-6.83	1.44	1.50
2	B	401	STU	C9-C10	-6.67	1.44	1.50
2	C	401	STU	C25-N3	6.53	1.51	1.45
2	D	401	STU	C11-C10	5.98	1.51	1.40
2	D	401	STU	C9-C10	-5.92	1.45	1.50
2	B	401	STU	C18-N2	-5.82	1.33	1.40
2	B	401	STU	C11-C10	5.77	1.51	1.40
2	A	401	STU	C11-C10	5.73	1.51	1.40
2	B	401	STU	C9-N1	5.68	1.51	1.45
2	E	401	STU	C6-C7	5.62	1.50	1.40
2	F	401	STU	C11-C10	5.48	1.50	1.40
2	D	401	STU	C6-C7	5.33	1.50	1.40
2	F	401	STU	C18-N2	-5.32	1.34	1.40
2	A	401	STU	C25-N3	5.31	1.50	1.45
2	D	401	STU	C5-C20	5.12	1.48	1.41
2	E	401	STU	C5-C20	5.05	1.48	1.41
2	C	401	STU	C11-C10	5.01	1.50	1.40
2	E	401	STU	C22-C23	-4.89	1.48	1.53
2	C	401	STU	C9-N1	4.82	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	STU	C18-N2	-4.79	1.34	1.40
2	B	401	STU	C5-C20	4.75	1.48	1.41
2	A	401	STU	C5-C20	4.67	1.48	1.41
2	C	401	STU	C6-C7	4.66	1.49	1.40
2	F	401	STU	C6-C7	4.59	1.48	1.40
2	B	401	STU	C6-C7	4.55	1.48	1.40
2	E	401	STU	C18-N2	-4.42	1.35	1.40
2	E	401	STU	C9-N1	4.37	1.50	1.45
2	A	401	STU	C18-N2	-4.32	1.35	1.40
2	E	401	STU	C19-C18	4.15	1.49	1.40
2	E	401	STU	C11-C10	4.10	1.48	1.40
2	B	401	STU	C22-C23	-4.04	1.48	1.53
2	C	401	STU	C19-C18	4.03	1.49	1.40
2	A	401	STU	C6-C7	4.01	1.47	1.40
2	F	401	STU	C19-C18	3.93	1.49	1.40
2	D	401	STU	C12-C17	3.90	1.47	1.41
2	C	401	STU	C12-C17	3.89	1.47	1.41
2	A	401	STU	C9-N1	3.86	1.49	1.45
2	F	401	STU	C5-C20	3.85	1.46	1.41
2	F	401	STU	C25-N3	3.63	1.48	1.45
2	D	401	STU	C25-N3	3.62	1.48	1.45
2	A	401	STU	C19-C18	3.61	1.48	1.40
2	D	401	STU	C19-C18	3.58	1.48	1.40
2	B	401	STU	C25-N3	3.53	1.48	1.45
2	B	401	STU	C19-C18	3.50	1.48	1.40
2	C	401	STU	C18-N2	-3.49	1.36	1.40
2	F	401	STU	C12-C17	3.46	1.46	1.41
2	E	401	STU	C12-C17	3.42	1.46	1.41
2	C	401	STU	C22-C23	-3.38	1.49	1.53
2	F	401	STU	C22-C23	-3.23	1.49	1.53
2	A	401	STU	C7-C10	3.23	1.45	1.39
2	C	401	STU	C5-C20	3.18	1.45	1.41
2	A	401	STU	C26-C21	3.13	1.55	1.51
2	D	401	STU	C9-N1	3.09	1.48	1.45
2	A	401	STU	C22-C23	-3.07	1.49	1.53
2	E	401	STU	C25-N3	3.04	1.48	1.45
2	E	401	STU	C7-C10	3.03	1.44	1.39
2	A	401	STU	C12-C17	2.92	1.45	1.41
2	F	401	STU	C9-N1	2.91	1.48	1.45
2	B	401	STU	C13-C12	-2.75	1.35	1.40
2	F	401	STU	C26-C21	2.74	1.54	1.51
2	D	401	STU	C7-C10	2.73	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	STU	C17-N2	-2.69	1.37	1.40
2	B	401	STU	C23-N4	-2.55	1.44	1.47
2	B	401	STU	C5-C6	-2.51	1.40	1.46
2	B	401	STU	O5-C8	2.46	1.29	1.23
2	E	401	STU	O5-C8	2.42	1.29	1.23
2	B	401	STU	C12-C17	2.39	1.44	1.41
2	D	401	STU	O5-C8	2.30	1.28	1.23
2	D	401	STU	C8-N1	2.29	1.37	1.35
2	F	401	STU	C5-C6	-2.26	1.41	1.46
2	C	401	STU	C26-C21	2.26	1.54	1.51
2	E	401	STU	C26-C21	2.26	1.54	1.51
2	D	401	STU	C5-C6	-2.17	1.41	1.46
2	F	401	STU	C14-C15	2.13	1.42	1.38
2	B	401	STU	C7-C10	2.09	1.43	1.39
2	F	401	STU	C24-C23	-2.09	1.50	1.53
2	A	401	STU	C5-C6	-2.08	1.42	1.46
2	B	401	STU	C17-N2	-2.07	1.38	1.40
2	F	401	STU	O6-C22	2.03	1.46	1.42

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	STU	C12-C17-N2	-7.83	103.79	108.94
2	D	401	STU	C12-C17-N2	-7.22	104.19	108.94
2	A	401	STU	C11-C10-C7	-7.06	116.60	121.25
2	C	401	STU	C12-C17-N2	-6.93	104.38	108.94
2	A	401	STU	C12-C17-N2	-6.88	104.42	108.94
2	B	401	STU	C12-C17-N2	-6.87	104.42	108.94
2	E	401	STU	C11-C10-C7	-6.82	116.76	121.25
2	E	401	STU	C9-C10-C7	6.76	112.37	109.88
2	D	401	STU	C11-C10-C7	-6.66	116.86	121.25
2	C	401	STU	C28-N4-C23	6.42	122.06	114.39
2	E	401	STU	C12-C17-N2	-6.37	104.75	108.94
2	F	401	STU	C28-N4-C23	6.27	121.88	114.39
2	B	401	STU	C9-C10-C7	6.17	112.15	109.88
2	F	401	STU	C11-C10-C7	-6.07	117.25	121.25
2	C	401	STU	C11-C10-C7	-5.95	117.33	121.25
2	F	401	STU	C18-N2-C17	5.88	114.48	107.37
2	D	401	STU	C28-N4-C23	5.88	121.41	114.39
2	D	401	STU	C9-C10-C7	5.66	111.96	109.88
2	B	401	STU	C11-C10-C7	-5.56	117.59	121.25
2	E	401	STU	C6-C7-C10	5.40	124.53	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	STU	C16-C17-N2	5.35	138.25	130.22
2	E	401	STU	C28-N4-C23	5.33	120.75	114.39
2	A	401	STU	C18-N2-C17	5.21	113.67	107.37
2	B	401	STU	C28-N4-C23	5.21	120.61	114.39
2	F	401	STU	C16-C17-N2	5.18	138.00	130.22
2	C	401	STU	C9-C10-C7	5.12	111.76	109.88
2	E	401	STU	C16-C17-N2	5.12	137.90	130.22
2	B	401	STU	C16-C17-N2	5.10	137.87	130.22
2	D	401	STU	C16-C17-N2	5.02	137.76	130.22
2	D	401	STU	C10-C7-C8	-4.99	103.91	108.09
2	E	401	STU	C10-C7-C8	-4.97	103.93	108.09
2	B	401	STU	C18-N2-C17	4.97	113.37	107.37
2	C	401	STU	C18-N2-C17	4.96	113.36	107.37
2	E	401	STU	C18-N2-C17	4.94	113.33	107.37
2	A	401	STU	C28-N4-C23	4.89	120.22	114.39
2	A	401	STU	C6-C7-C10	4.80	124.11	120.76
2	F	401	STU	C6-C7-C10	4.79	124.10	120.76
2	A	401	STU	C16-C17-N2	4.78	137.40	130.22
2	D	401	STU	C18-N2-C17	4.73	113.08	107.37
2	C	401	STU	C6-C7-C10	4.57	123.95	120.76
2	A	401	STU	C9-C10-C7	4.46	111.52	109.88
2	F	401	STU	C9-C10-C7	4.37	111.49	109.88
2	F	401	STU	C9-N1-C8	-4.23	110.00	113.86
2	C	401	STU	C9-N1-C8	-4.15	110.07	113.86
2	B	401	STU	C7-C8-N1	4.07	110.26	106.38
2	E	401	STU	C7-C8-N1	4.07	110.26	106.38
2	A	401	STU	C9-C10-C11	4.03	131.79	128.73
2	C	401	STU	C7-C8-N1	3.98	110.17	106.38
2	A	401	STU	C10-C7-C8	-3.98	104.76	108.09
2	E	401	STU	C16-C17-C12	-3.93	117.00	121.59
2	B	401	STU	C6-C7-C10	3.83	123.43	120.76
2	D	401	STU	C9-N1-C8	-3.74	110.45	113.86
2	F	401	STU	C7-C8-N1	3.74	109.94	106.38
2	D	401	STU	C7-C8-N1	3.73	109.94	106.38
2	D	401	STU	C6-C7-C10	3.69	123.33	120.76
2	B	401	STU	C9-N1-C8	-3.68	110.50	113.86
2	F	401	STU	C10-C7-C8	-3.68	105.01	108.09
2	C	401	STU	C10-C7-C8	-3.66	105.03	108.09
2	B	401	STU	C10-C7-C8	-3.63	105.05	108.09
2	C	401	STU	C16-C17-C12	-3.62	117.36	121.59
2	E	401	STU	C9-N1-C8	-3.54	110.63	113.86
2	A	401	STU	C4-C5-C20	3.53	123.32	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	STU	C1-C20-C5	-3.50	117.50	121.59
2	B	401	STU	C13-C12-C17	3.47	123.25	119.24
2	F	401	STU	C1-C20-C5	-3.46	117.54	121.59
2	F	401	STU	C4-C5-C20	3.38	123.15	119.24
2	A	401	STU	C1-C20-C5	-3.38	117.63	121.59
2	B	401	STU	C16-C17-C12	-3.34	117.68	121.59
2	F	401	STU	C9-C10-C11	3.23	131.18	128.73
2	D	401	STU	C9-C10-C11	3.22	131.18	128.73
2	B	401	STU	C1-C20-C5	-3.05	118.02	121.59
2	D	401	STU	C16-C17-C12	-3.04	118.04	121.59
2	A	401	STU	C7-C8-N1	3.01	109.25	106.38
2	D	401	STU	C4-C5-C20	2.98	122.68	119.24
2	A	401	STU	C16-C17-C12	-2.97	118.12	121.59
2	C	401	STU	C13-C12-C17	2.96	122.66	119.24
2	C	401	STU	C4-C5-C20	2.96	122.66	119.24
2	F	401	STU	C16-C17-C12	-2.93	118.16	121.59
2	C	401	STU	C9-C10-C11	2.83	130.88	128.73
2	E	401	STU	C13-C12-C17	2.83	122.51	119.24
2	D	401	STU	C1-C20-C5	-2.81	118.31	121.59
2	F	401	STU	C13-C12-C17	2.78	122.46	119.24
2	E	401	STU	C1-C20-C5	-2.76	118.36	121.59
2	D	401	STU	C13-C12-C17	2.75	122.41	119.24
2	E	401	STU	C9-C10-C11	2.74	130.81	128.73
2	F	401	STU	C1-C20-N3	2.65	134.25	129.73
2	A	401	STU	C1-C20-N3	2.55	134.09	129.73
2	C	401	STU	C1-C20-N3	2.51	134.00	129.73
2	E	401	STU	C1-C20-N3	2.45	133.91	129.73
2	B	401	STU	C1-C20-N3	2.43	133.87	129.73
2	B	401	STU	C4-C5-C20	2.42	122.03	119.24
2	D	401	STU	O5-C8-N1	-2.37	122.72	125.35
2	A	401	STU	C9-N1-C8	-2.34	111.73	113.86
2	A	401	STU	C13-C12-C17	2.31	121.91	119.24
2	E	401	STU	O5-C8-C7	-2.24	125.23	128.47
2	D	401	STU	C1-C20-N3	2.20	133.48	129.73
2	B	401	STU	O5-C8-N1	-2.11	123.00	125.35
2	C	401	STU	O5-C8-N1	-2.09	123.03	125.35
2	E	401	STU	C4-C5-C20	2.08	121.65	119.24
2	F	401	STU	O5-C8-C7	-2.08	125.45	128.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	EDO	O1-C1-C2-O2
2	C	401	STU	C24-C23-N4-C28
3	C	404	EDO	O1-C1-C2-O2
3	A	402	EDO	O1-C1-C2-O2
3	C	403	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2
3	E	402	EDO	O1-C1-C2-O2
3	B	403	EDO	O1-C1-C2-O2
2	A	401	STU	C24-C23-N4-C28

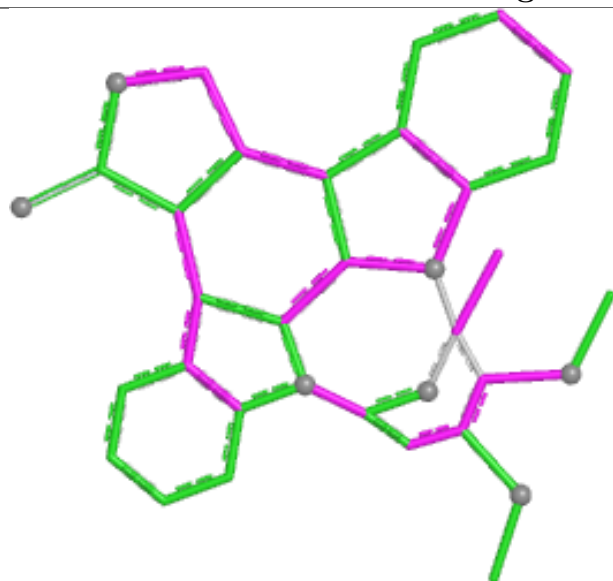
There are no ring outliers.

6 monomers are involved in 25 short contacts:

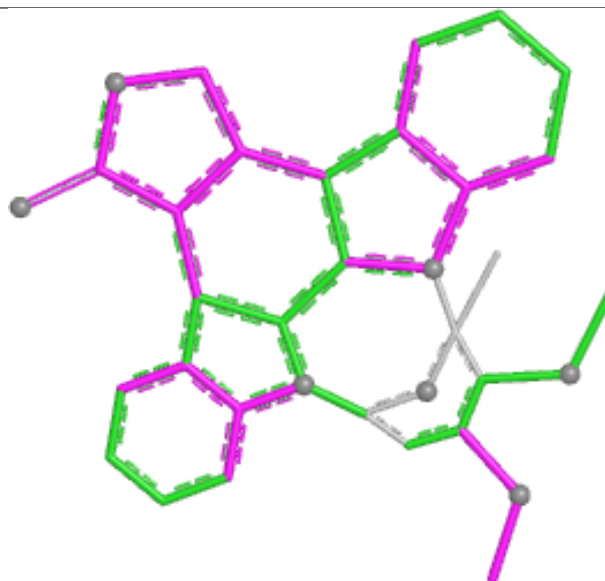
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	STU	3	0
2	C	401	STU	4	0
2	D	401	STU	5	0
2	E	401	STU	4	0
2	A	401	STU	5	0
2	B	401	STU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

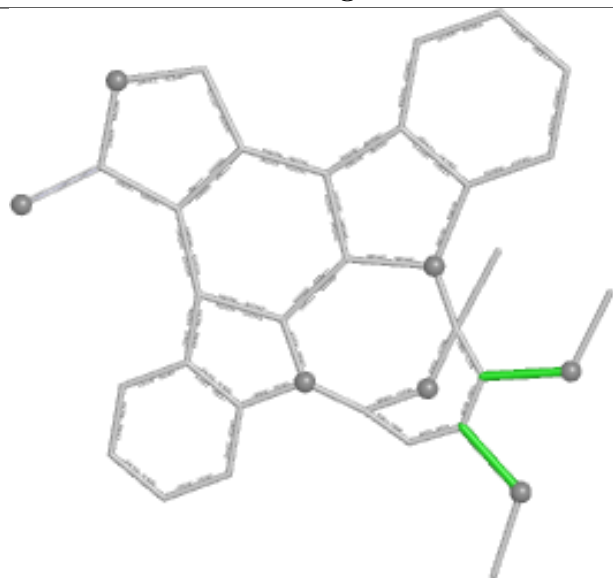
Ligand STU F 401



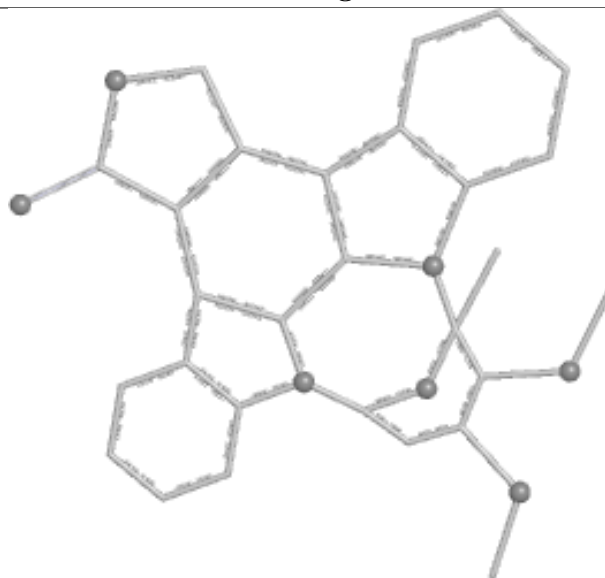
Bond lengths



Bond angles

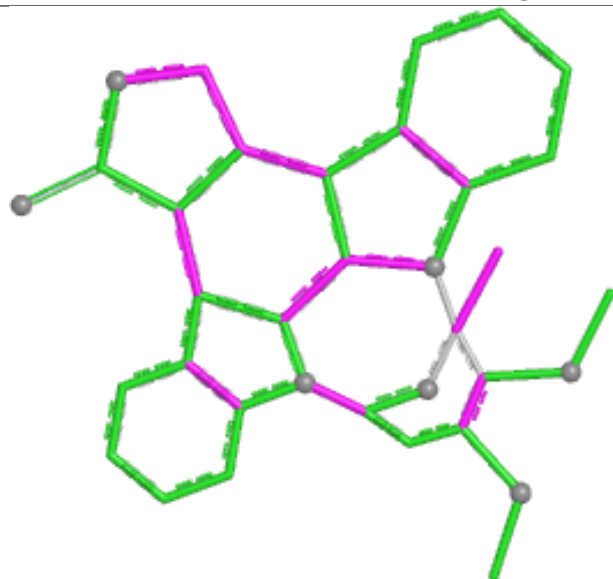


Torsions

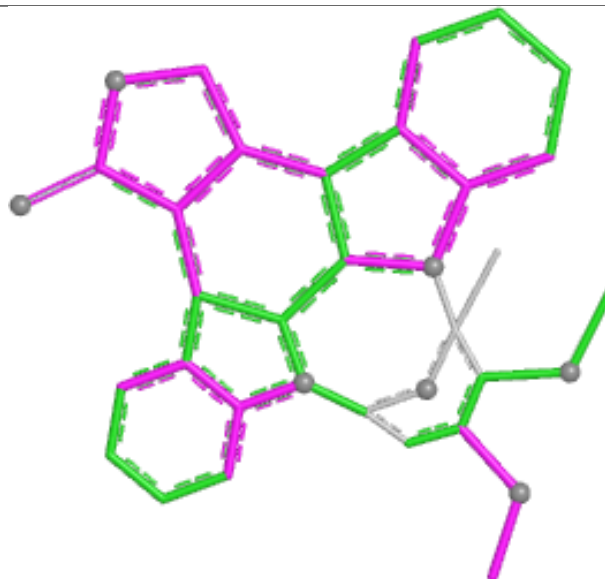


Rings

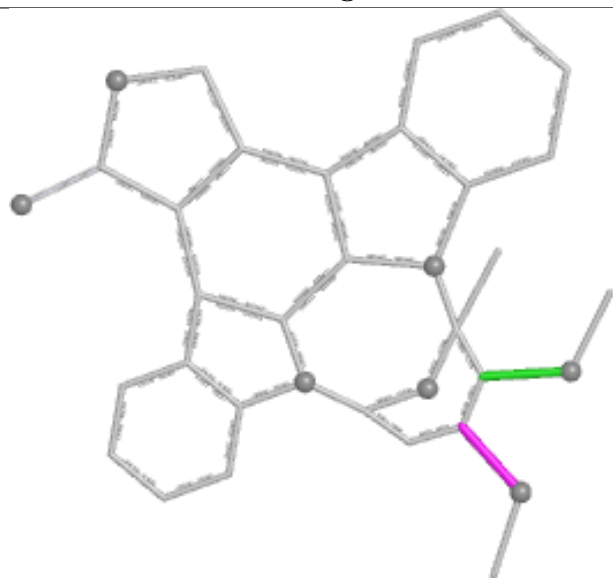
Ligand STU C 401



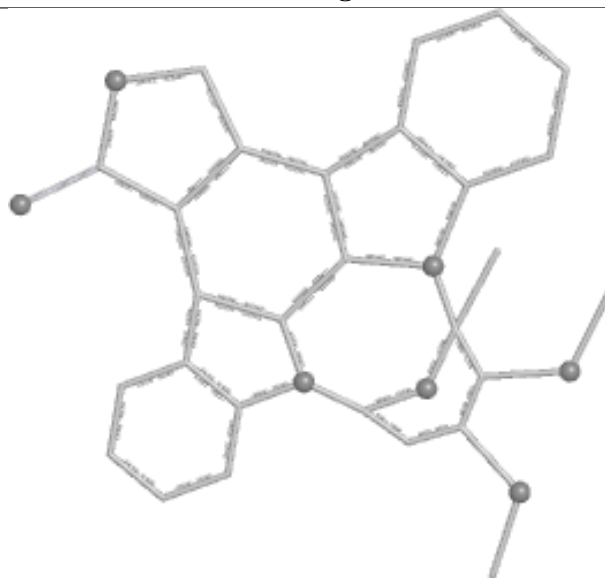
Bond lengths



Bond angles

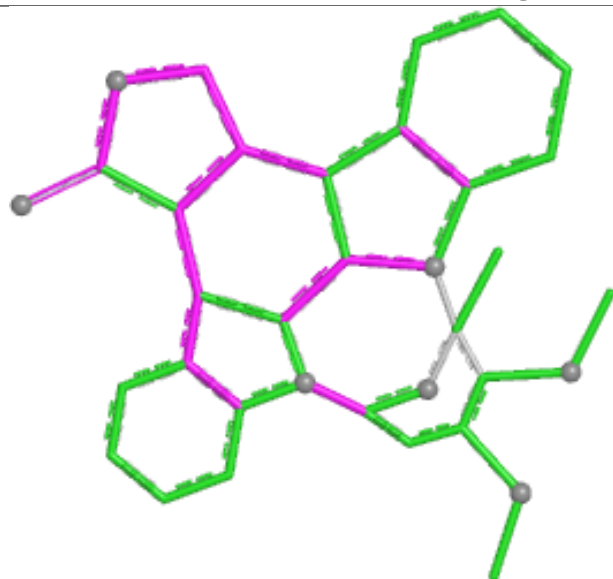


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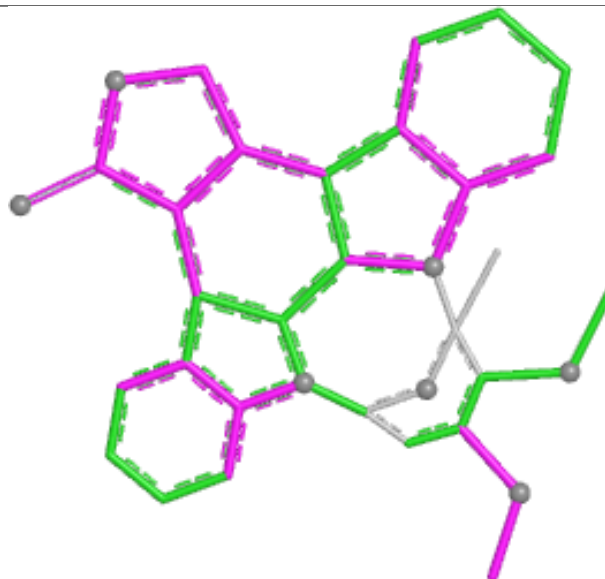


Rings

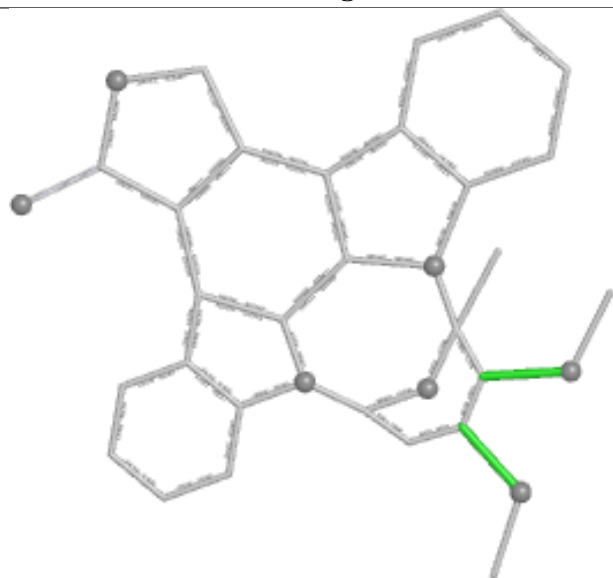
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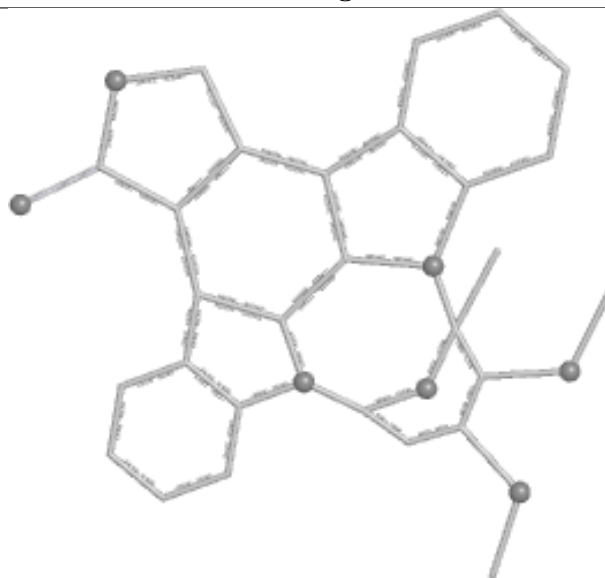
Bond lengths



Bond angles

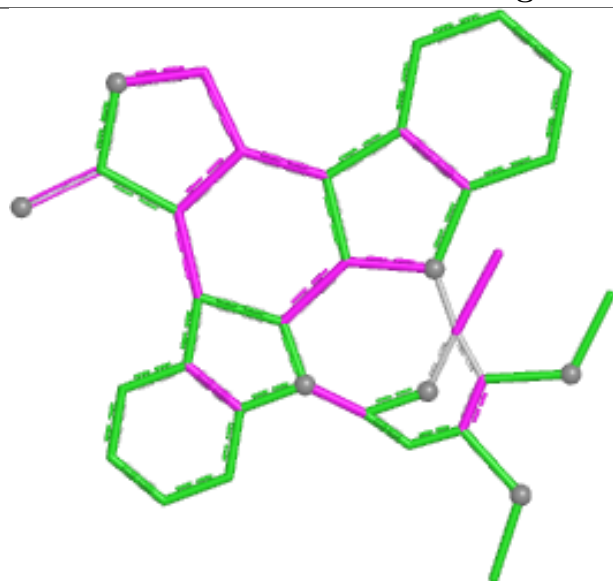


Torsions

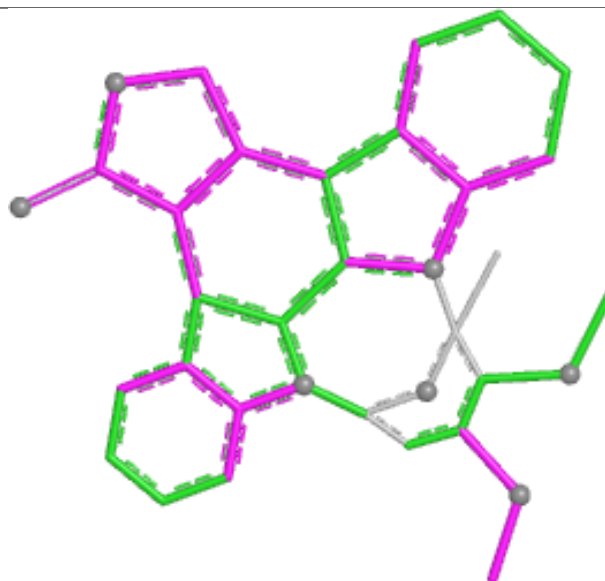


Rings

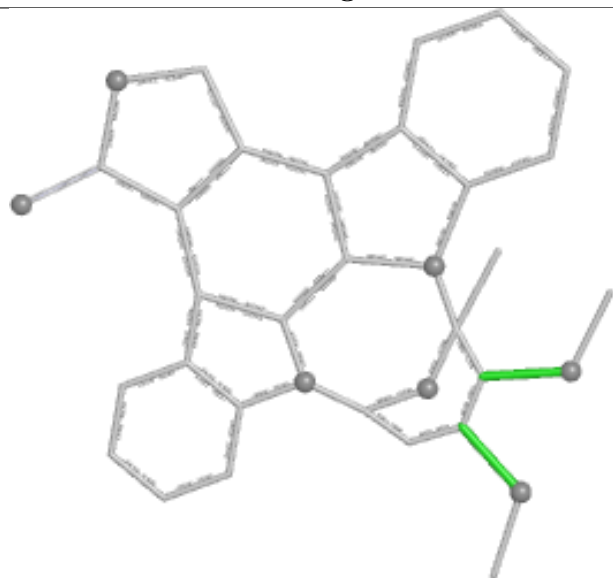
Ligand STU E 401



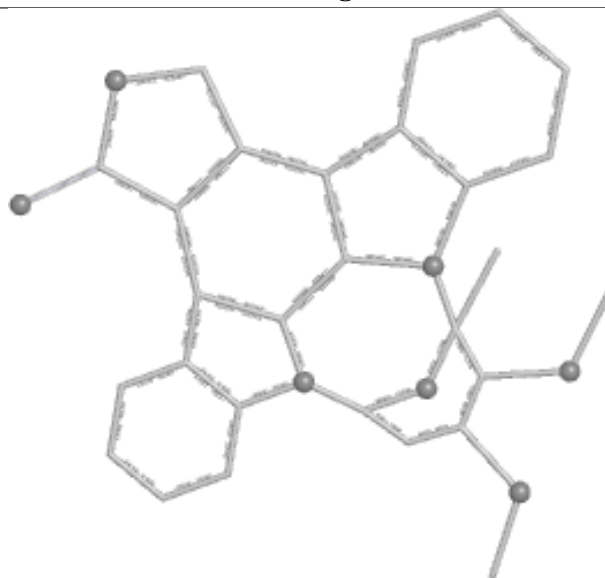
Bond lengths



Bond angles

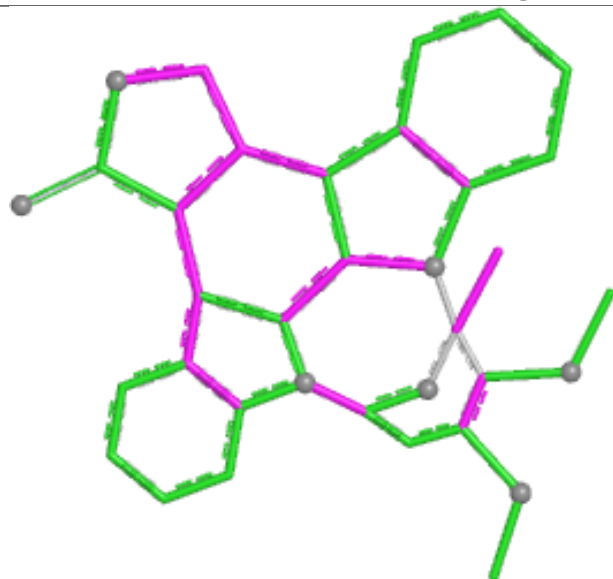


Torsions

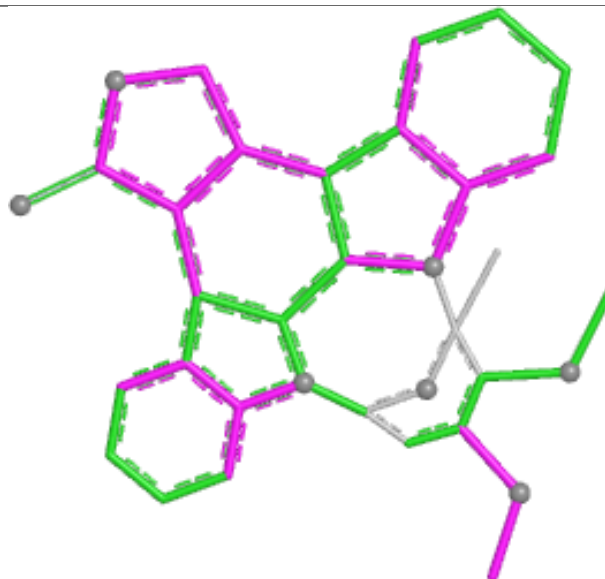


Rings

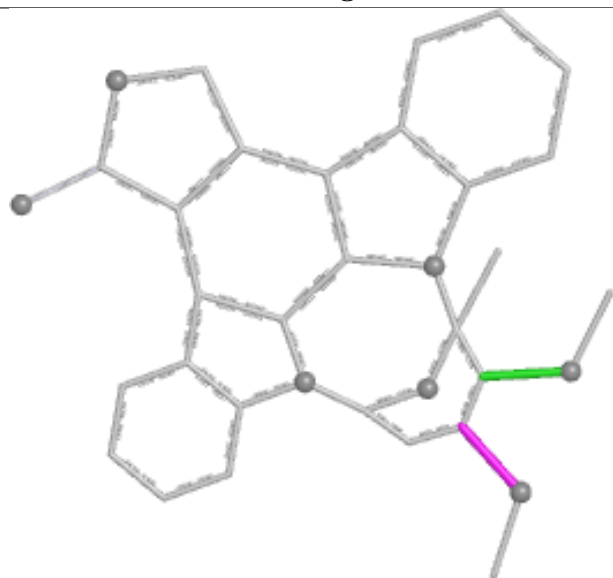
Ligand STU A 401



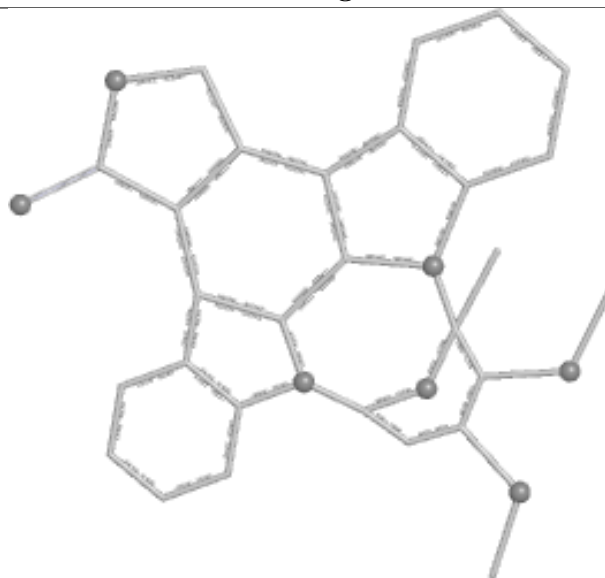
Bond lengths



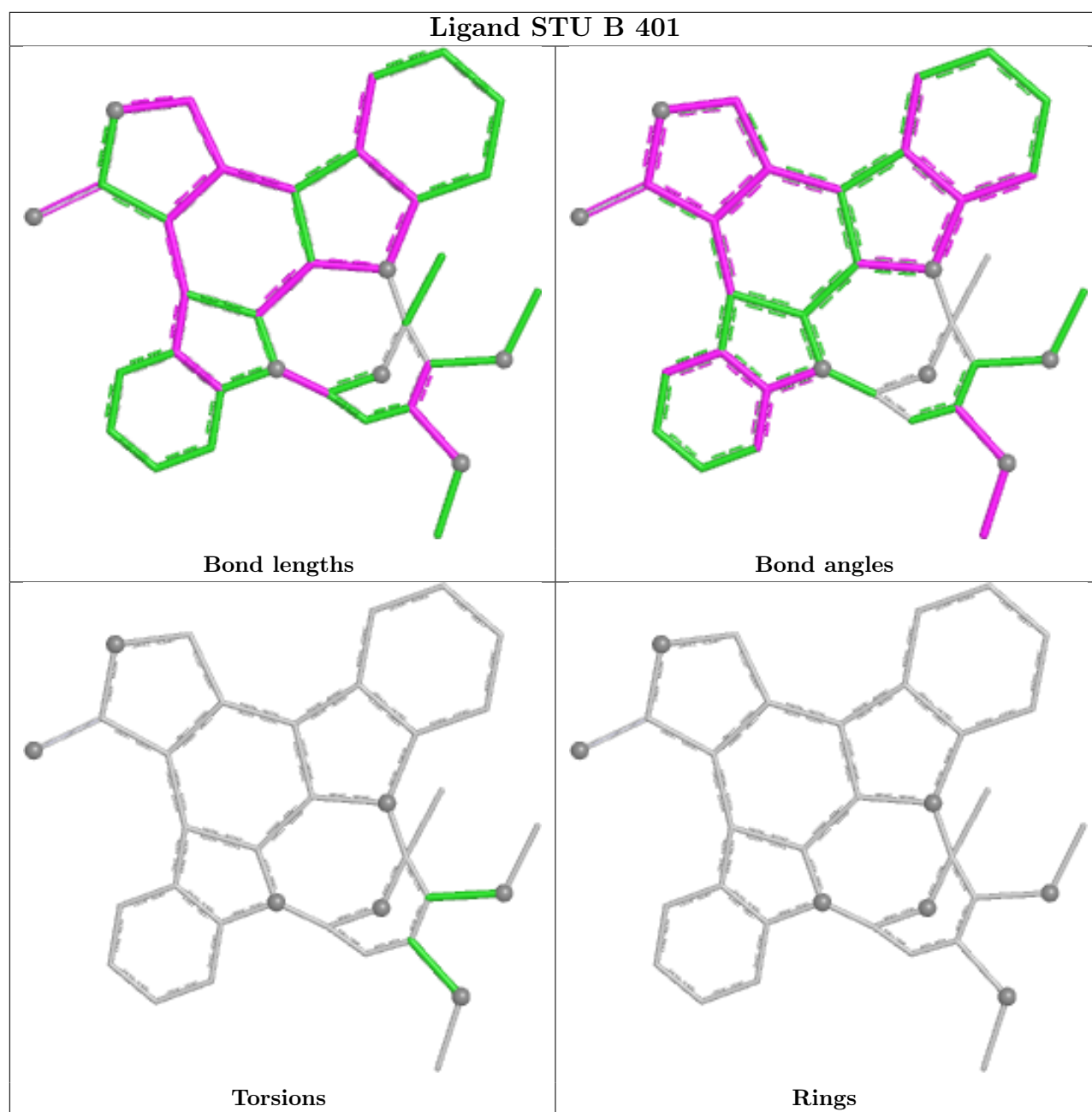
Bond angles



Torsions



Rings



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	350/384 (91%)	-0.10	19 (5%)	31	33	16, 35, 99, 134	7 (2%)
1	B	350/384 (91%)	0.04	28 (8%)	18	20	18, 37, 106, 148	6 (1%)
1	C	344/384 (89%)	-0.02	22 (6%)	25	27	17, 37, 89, 131	6 (1%)
1	D	346/384 (90%)	0.30	31 (8%)	15	16	24, 46, 103, 128	5 (1%)
1	E	342/384 (89%)	0.21	31 (9%)	15	16	18, 41, 93, 124	6 (1%)
1	F	346/384 (90%)	0.11	29 (8%)	17	18	18, 39, 98, 136	5 (1%)
All	All	2078/2304 (90%)	0.09	160 (7%)	19	21	16, 39, 97, 148	35 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	304	ARG	5.9
1	A	316	MET	5.6
1	D	305	LEU	5.3
1	A	322	PRO	5.1
1	A	313	LEU	5.0
1	F	300	PRO	4.8
1	E	195	ARG	4.7
1	E	305	LEU	4.6
1	D	303	GLY	4.5
1	B	321	LYS	4.5
1	F	305	LEU	4.5
1	B	314	GLU	4.4
1	E	304	ARG	4.3
1	F	301	ASN	4.3
1	A	315	GLU	4.3
1	B	313	LEU	4.3
1	B	311	PHE	4.3
1	B	198	ALA	4.2
1	D	304	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	317	ILE	4.1
1	F	302	LYS	4.1
1	C	314	GLU	4.0
1	F	307	CYS	4.0
1	E	302	LYS	4.0
1	D	336	ASP	4.0
1	B	310	THR	3.9
1	A	311	PHE	3.8
1	B	332	LYS	3.7
1	F	337	MET	3.6
1	B	308	ASP	3.6
1	E	303	GLY	3.6
1	F	339	LYS	3.6
1	F	303	GLY	3.6
1	A	309	PRO	3.6
1	D	338	ARG	3.6
1	B	317	ILE	3.6
1	B	370	ASP	3.5
1	D	299	ILE	3.5
1	C	198	ALA	3.5
1	E	198	ALA	3.5
1	B	309	PRO	3.4
1	F	321	LYS	3.4
1	B	316	MET	3.4
1	B	318	LEU	3.4
1	B	315	GLU	3.4
1	A	321	LYS	3.4
1	E	307	CYS	3.4
1	E	321	LYS	3.4
1	E	193[A]	SER	3.3
1	B	197	GLY	3.3
1	B	307	CYS	3.3
1	D	307	CYS	3.3
1	D	117[A]	HIS	3.3
1	F	336	ASP	3.2
1	C	318	LEU	3.2
1	E	33	SER	3.2
1	F	311	PHE	3.1
1	D	195	ARG	3.1
1	B	373	LYS	3.1
1	A	314	GLU	3.0
1	C	373	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	317	ILE	3.0
1	B	176[A]	GLN	3.0
1	C	311	PHE	2.9
1	D	311	PHE	2.9
1	B	320	SER	2.9
1	D	337	MET	2.9
1	C	306	ASN	2.9
1	A	318	LEU	2.9
1	B	338	ARG	2.9
1	F	318	LEU	2.9
1	F	338	ARG	2.9
1	F	299	ILE	2.9
1	F	310	THR	2.9
1	F	317	ILE	2.9
1	E	301	ASN	2.8
1	D	198	ALA	2.8
1	B	195	ARG	2.8
1	A	310	THR	2.8
1	E	372	ASN	2.7
1	E	320	SER	2.7
1	F	33	SER	2.7
1	D	339	LYS	2.7
1	E	196	LYS	2.7
1	B	335	LYS	2.7
1	C	321	LYS	2.7
1	C	195	ARG	2.7
1	D	318	LEU	2.7
1	E	117	HIS	2.7
1	E	116	VAL	2.7
1	D	321	LYS	2.7
1	F	309	PRO	2.6
1	D	224[A]	HIS	2.6
1	D	306	ASN	2.6
1	E	197	GLY	2.6
1	C	193[A]	SER	2.6
1	C	316	MET	2.6
1	C	315	GLU	2.6
1	A	198	ALA	2.6
1	D	301	ASN	2.6
1	F	116	VAL	2.6
1	A	33	SER	2.6
1	B	319	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	318	LEU	2.5
1	E	15	ASN	2.5
1	E	339	LYS	2.5
1	A	335	LYS	2.5
1	E	300	PRO	2.5
1	E	371	PHE	2.5
1	C	338	ARG	2.5
1	D	116	VAL	2.5
1	E	316	MET	2.5
1	E	299	ILE	2.4
1	F	308	ASP	2.4
1	C	176[A]	GLN	2.4
1	E	317	ILE	2.4
1	D	316	MET	2.4
1	D	312	GLU	2.4
1	B	340	CYS	2.4
1	B	170	MET	2.4
1	F	306	ASN	2.4
1	D	197	GLY	2.4
1	E	194	SER	2.4
1	F	320	SER	2.4
1	E	34	PHE	2.4
1	F	371	PHE	2.4
1	A	336	ASP	2.3
1	C	53	TYR	2.3
1	D	320	SER	2.3
1	E	176[A]	GLN	2.3
1	D	115	ASN	2.3
1	D	308	ASP	2.3
1	C	170	MET	2.3
1	F	224[A]	HIS	2.3
1	D	371	PHE	2.3
1	B	341	ASP	2.3
1	C	33	SER	2.3
1	E	312	GLU	2.3
1	D	193[A]	SER	2.2
1	C	313	LEU	2.2
1	B	337	MET	2.2
1	D	196	LYS	2.2
1	F	360	ILE	2.2
1	C	14	GLU	2.2
1	E	170	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	196	LYS	2.2
1	D	302	LYS	2.2
1	A	197	GLY	2.2
1	A	338	ARG	2.1
1	D	15	ASN	2.1
1	A	371	PHE	2.1
1	F	194	SER	2.1
1	A	373	LYS	2.1
1	E	32	GLY	2.1
1	F	196	LYS	2.0
1	C	310	THR	2.0
1	B	312	GLU	2.0
1	D	242	VAL	2.0
1	C	340	CYS	2.0
1	F	117	HIS	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(Å ²)	Q<0.9
3	EDO	F	402	4/4	0.80	0.18	61,62,65,65	0
3	EDO	B	402	4/4	0.82	0.16	40,42,42,48	0
3	EDO	C	402	4/4	0.84	0.21	55,56,58,60	0
3	EDO	E	402	4/4	0.87	0.18	42,50,52,53	0
3	EDO	A	402	4/4	0.88	0.14	55,55,56,56	0
3	EDO	C	403	4/4	0.95	0.07	37,40,44,46	0
3	EDO	C	404	4/4	0.95	0.07	39,43,46,50	0
2	STU	E	401	35/35	0.95	0.07	31,36,43,44	0

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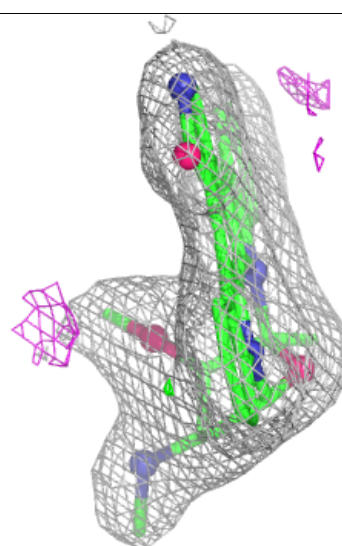
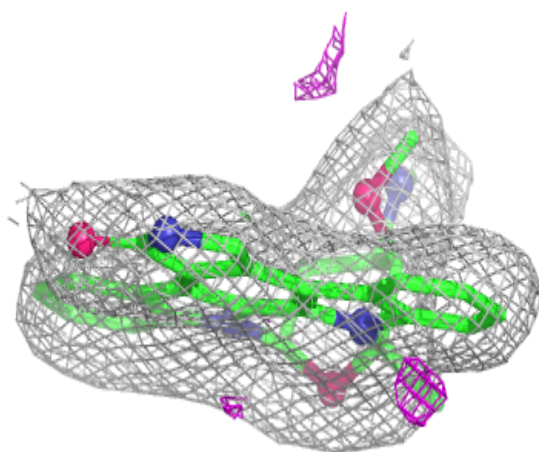
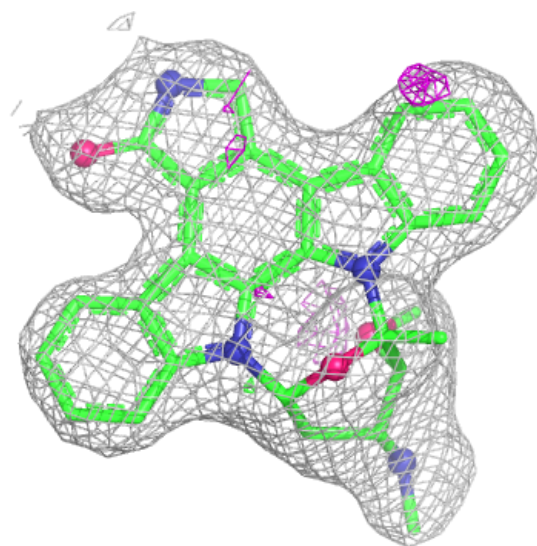
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	STU	D	401	35/35	0.95	0.08	25,35,40,42	0
2	STU	F	401	35/35	0.96	0.06	25,29,35,37	0
3	EDO	B	403	4/4	0.97	0.05	29,30,35,36	0
2	STU	C	401	35/35	0.97	0.06	23,27,31,33	0
2	STU	B	401	35/35	0.97	0.05	20,23,26,30	0
2	STU	A	401	35/35	0.98	0.05	16,22,24,25	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.

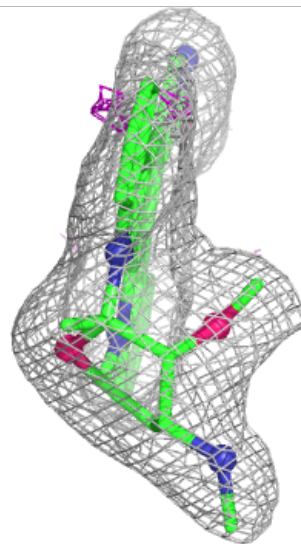
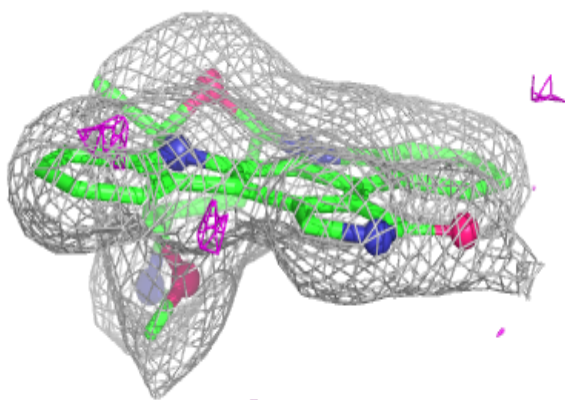
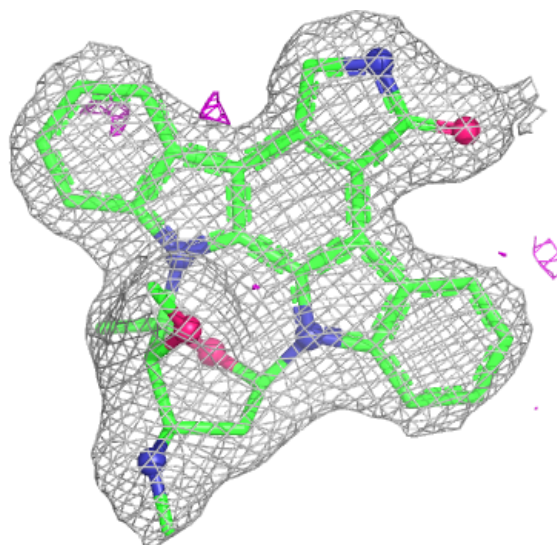
Electron density around STU E 401:

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



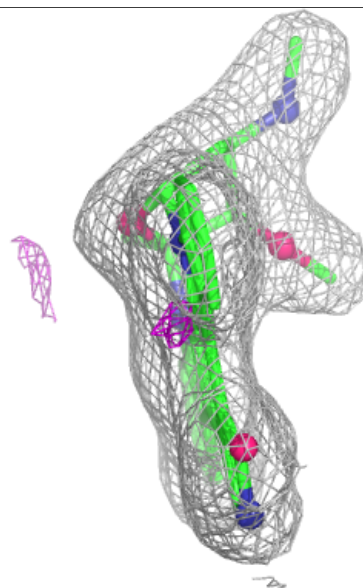
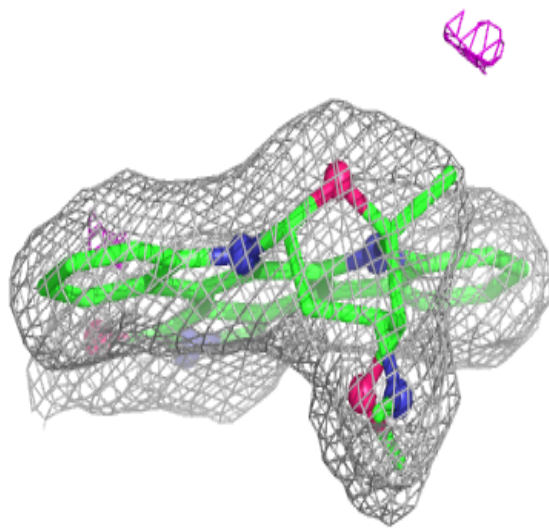
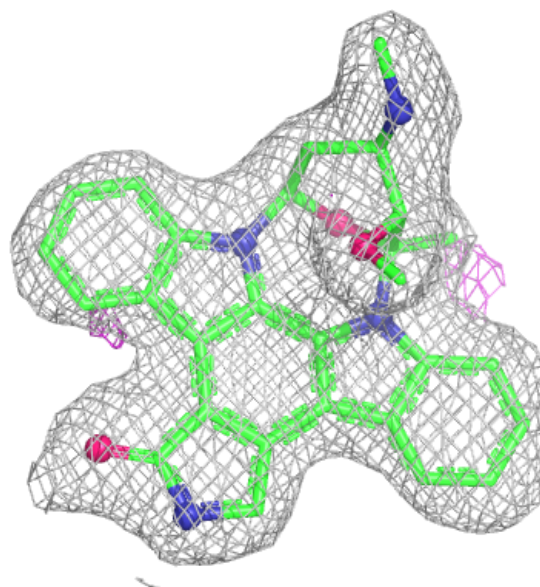
Electron density around STU D 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



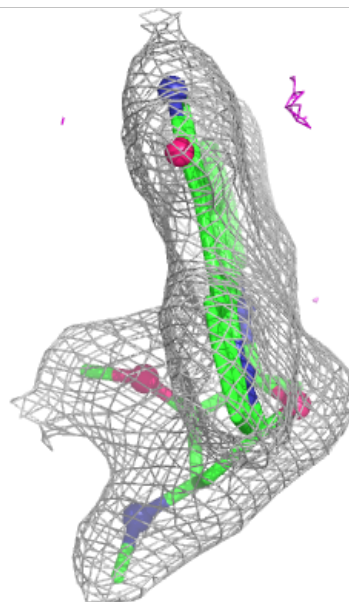
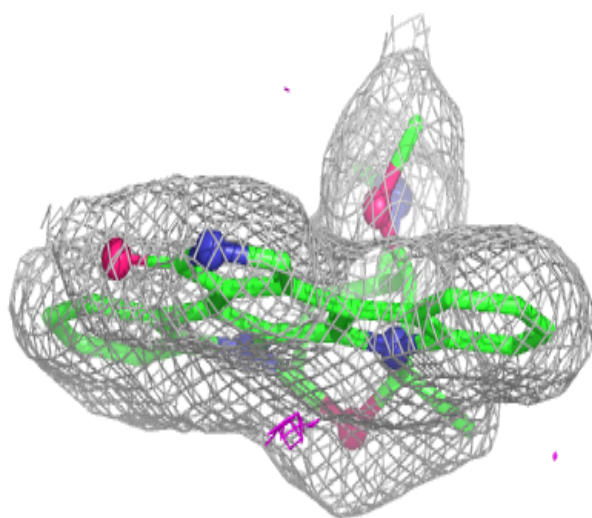
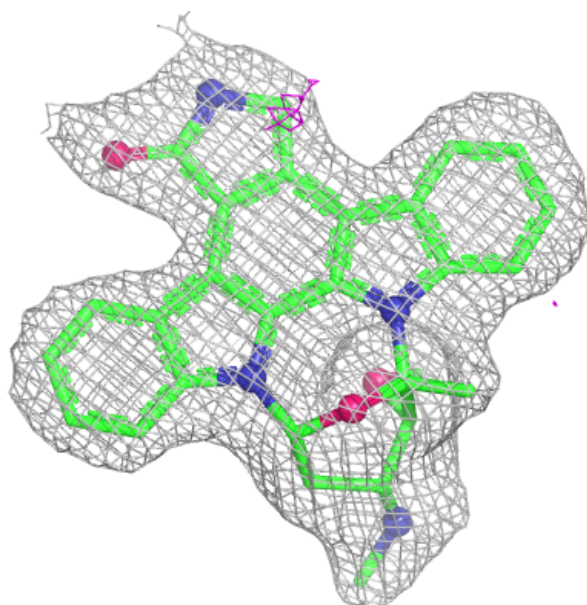
Electron density around STU F 401:

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and green (positive)



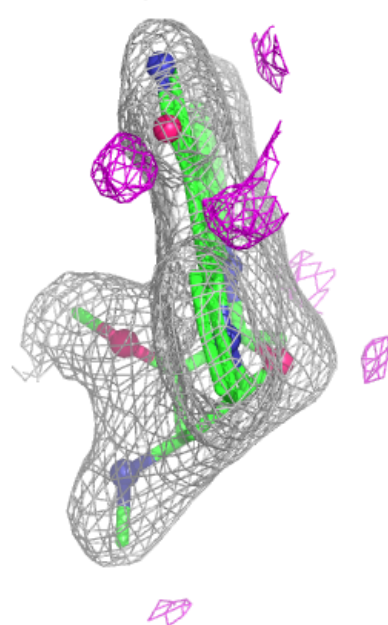
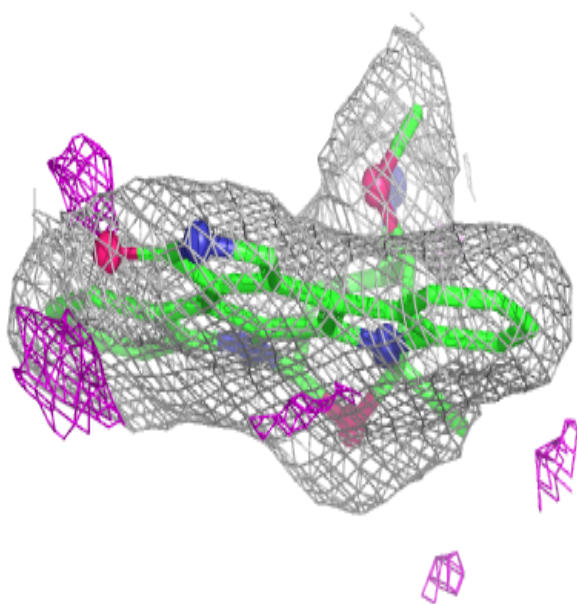
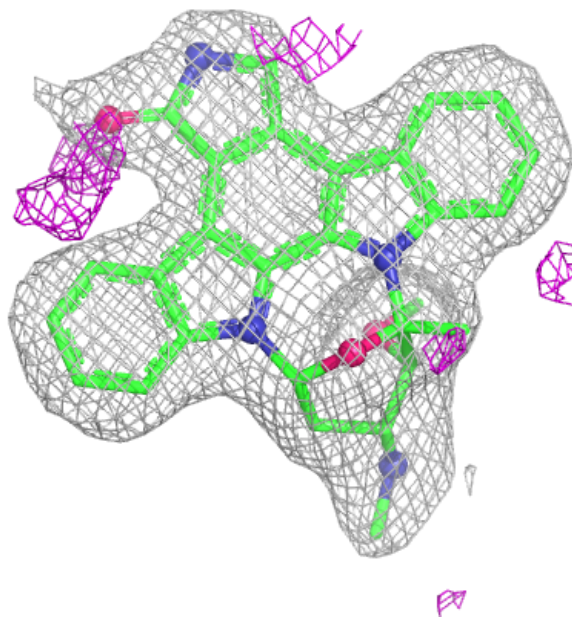
Electron density around STU C 401:

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and green (positive)



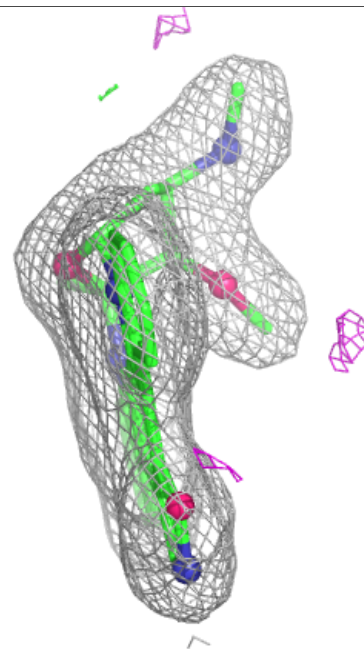
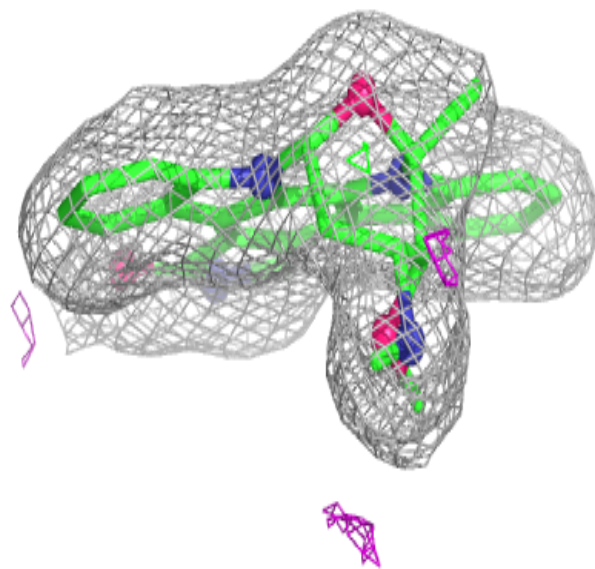
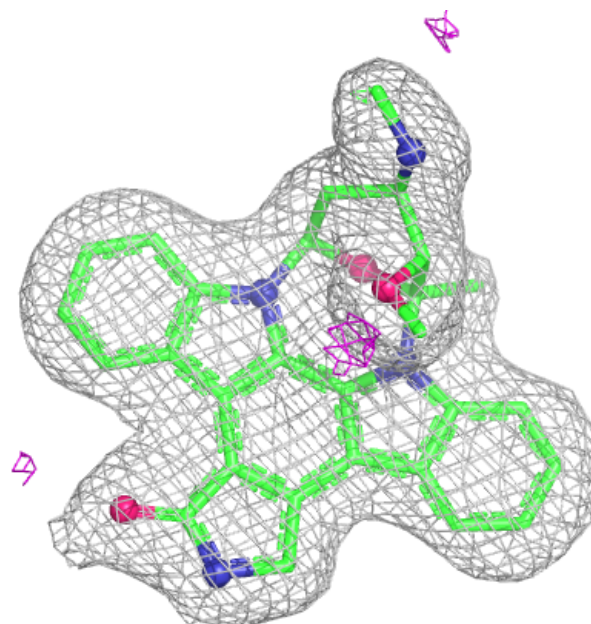
Electron density around STU B 401:

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



Electron density around STU A 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.