



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 2GCD / pdb_00002gcd
Title : TAO2 kinase domain-staurosporine structure
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Deposited on : 2006-03-14
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

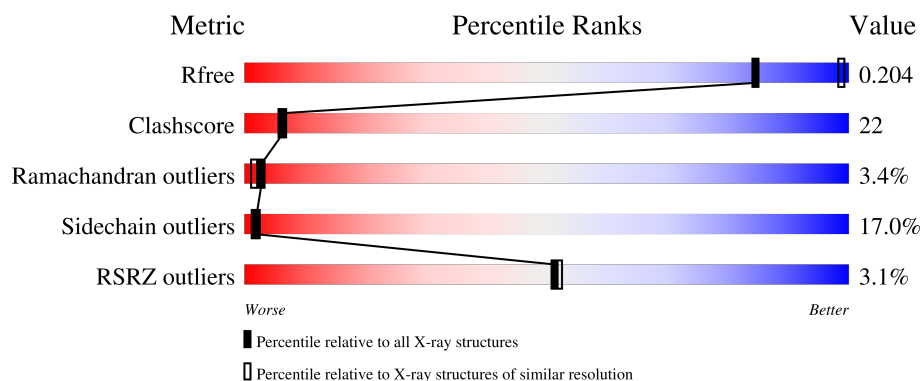
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

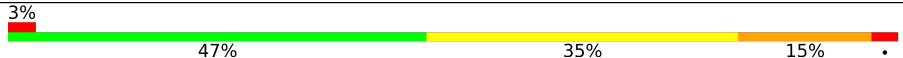
The reported resolution of this entry is 2.55 Å.

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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	309	
1	B	309	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	B	181	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5327 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.

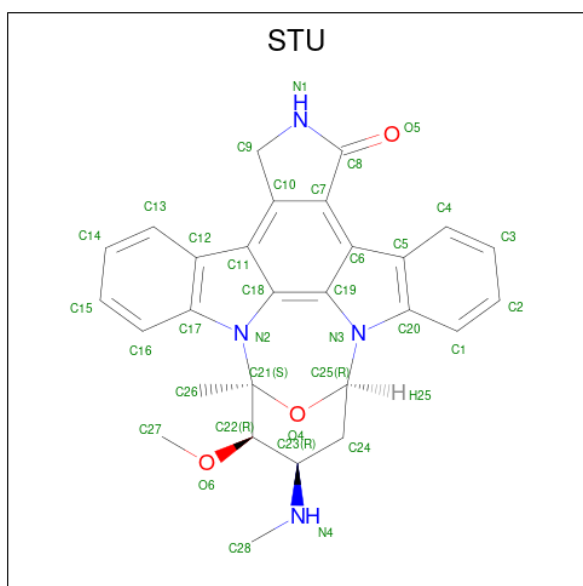
- Molecule 1 is a protein called Serine/threonine-protein kinase TAO2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			
1	B	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SEP	SER	modified residue	UNP Q9JLS3
B	181	SEP	SER	modified residue	UNP Q9JLS3

- 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		

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

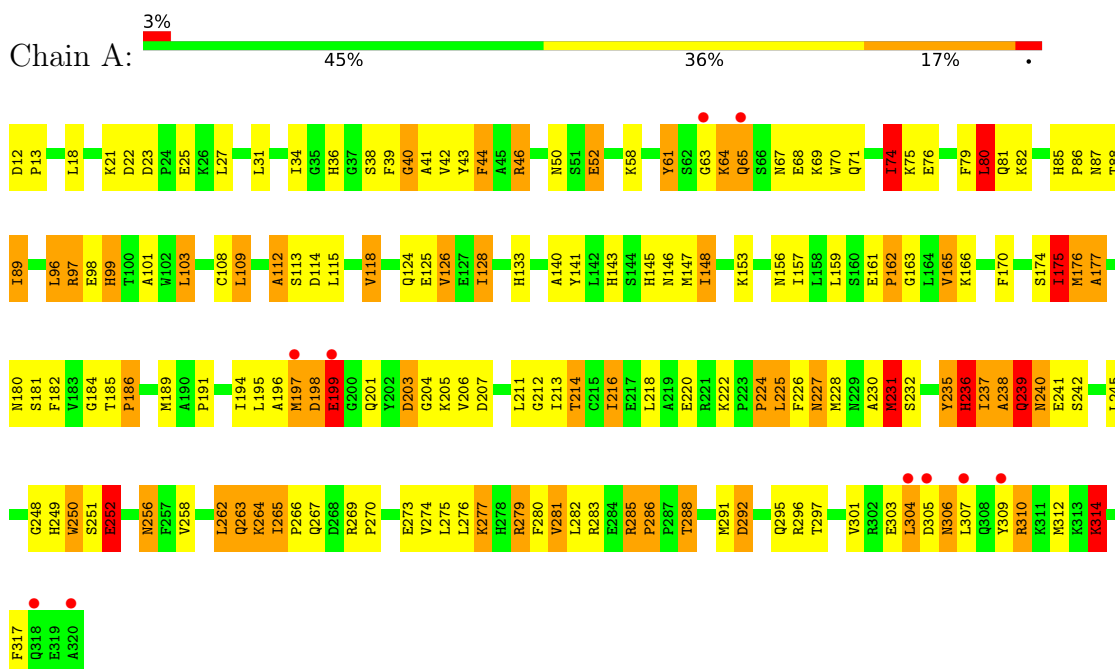
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	135	Total	O	0	0
			135	135		

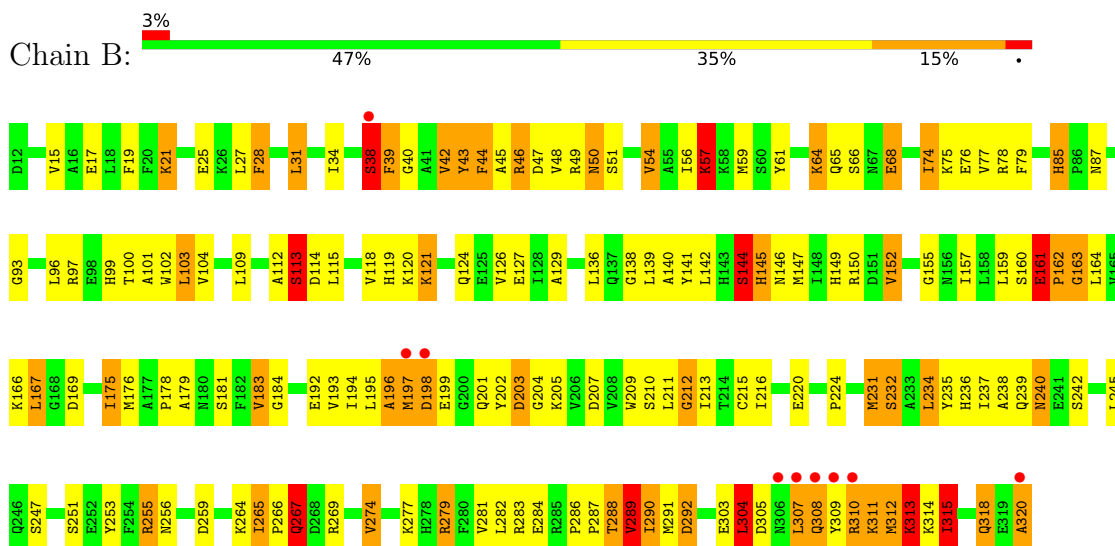
3 Residue-property plots

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 TAO2



• Molecule 1: Serine/threonine-protein kinase TAO2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.02Å 186.02Å 94.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	160.13 – 2.55 160.13 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (160.13-2.55) 92.2 (160.13-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.261 0.195 , 0.204	Depositor DCC
R_{free} test set	1548 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.87	50/2538 (2.0%)	1.71	37/3428 (1.1%)
1	B	1.93	46/2538 (1.8%)	1.78	45/3428 (1.3%)
All	All	1.90	96/5076 (1.9%)	1.75	82/6856 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ILE	CA-CB	-9.57	1.42	1.54
1	A	101	ALA	CA-CB	-8.75	1.40	1.53
1	B	101	ALA	CA-CB	-8.66	1.39	1.53
1	A	237	ILE	CA-CB	7.92	1.63	1.54
1	B	240	ASN	CA-C	-7.86	1.43	1.52
1	A	211	LEU	C-O	7.73	1.33	1.24
1	A	112	ALA	C-O	-7.62	1.14	1.24
1	B	213	ILE	N-CA	-7.58	1.37	1.46
1	B	77	VAL	CA-CB	-7.57	1.45	1.54
1	A	240	ASN	C-O	-7.52	1.14	1.24
1	A	252	GLU	CG-CD	7.46	1.70	1.52
1	B	157	ILE	CA-CB	-7.44	1.44	1.54
1	A	42	VAL	N-CA	-7.38	1.37	1.46
1	B	49	ARG	C-O	-7.21	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	GLU	N-CA	7.07	1.55	1.45
1	B	289	VAL	CA-CB	-7.06	1.44	1.54
1	B	256	ASN	C-O	6.92	1.32	1.24
1	A	265	ILE	CA-CB	6.83	1.60	1.53
1	A	88	THR	CA-CB	-6.82	1.40	1.53
1	B	193	VAL	CA-C	-6.63	1.44	1.52
1	A	235	TYR	CA-CB	6.57	1.64	1.53
1	A	214	THR	C-O	6.50	1.32	1.24
1	A	186	PRO	N-CA	6.41	1.55	1.47
1	A	239	GLN	C-O	-6.41	1.16	1.24
1	A	41	ALA	C-O	-6.40	1.15	1.23
1	A	213	ILE	CA-CB	-6.39	1.45	1.54
1	B	104	VAL	CA-CB	-6.38	1.46	1.54
1	B	136	LEU	C-O	6.37	1.31	1.24
1	B	152	VAL	C-O	-6.32	1.17	1.24
1	A	140	ALA	CA-CB	-6.26	1.43	1.53
1	A	274	VAL	C-O	6.22	1.31	1.24
1	B	59	MET	C-O	-6.21	1.16	1.24
1	A	74	ILE	CA-CB	-6.21	1.46	1.54
1	B	93	GLY	C-O	-6.19	1.17	1.23
1	A	263	GLN	C-O	-6.10	1.16	1.24
1	A	212	GLY	C-O	6.07	1.31	1.23
1	B	184	GLY	C-O	-6.06	1.17	1.23
1	A	80	LEU	C-O	-6.03	1.17	1.24
1	A	68	GLU	CA-CB	6.00	1.62	1.53
1	B	224	PRO	C-O	-5.93	1.16	1.24
1	B	267	GLN	CA-C	-5.92	1.44	1.52
1	A	128	ILE	CA-CB	-5.83	1.46	1.54
1	A	175	ILE	CG1-CD1	5.83	1.74	1.51
1	B	212	GLY	C-O	5.79	1.30	1.23
1	A	279	ARG	C-O	5.78	1.31	1.24
1	B	15	VAL	CA-CB	-5.73	1.48	1.54
1	A	307	LEU	N-CA	5.72	1.53	1.46
1	A	101	ALA	C-O	-5.71	1.17	1.24
1	B	28	PHE	CA-C	-5.69	1.45	1.52
1	A	68	GLU	N-CA	5.65	1.53	1.46
1	B	192	GLU	CB-CG	-5.65	1.35	1.52
1	B	199	GLU	CA-C	5.64	1.59	1.53
1	A	211	LEU	CA-C	5.56	1.60	1.52
1	A	250	TRP	C-O	5.54	1.30	1.23
1	B	42	VAL	N-CA	-5.54	1.39	1.46
1	A	68	GLU	CB-CG	5.53	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	ASN	CA-C	5.53	1.59	1.53
1	B	216	ILE	C-O	5.52	1.30	1.24
1	B	232	SER	N-CA	-5.51	1.39	1.46
1	A	199	GLU	CA-CB	5.49	1.59	1.52
1	A	175	ILE	C-O	-5.48	1.17	1.24
1	B	307	LEU	N-CA	5.47	1.53	1.46
1	B	237	ILE	CA-C	5.46	1.59	1.52
1	A	281	VAL	CA-CB	-5.44	1.46	1.54
1	A	98	GLU	CG-CD	5.42	1.65	1.52
1	A	165	VAL	CA-C	-5.42	1.46	1.52
1	A	225	LEU	N-CA	5.39	1.53	1.46
1	B	42	VAL	CA-CB	5.39	1.61	1.54
1	B	140	ALA	C-O	5.38	1.30	1.24
1	B	265	ILE	CA-CB	5.35	1.60	1.54
1	B	207	ASP	CA-C	-5.34	1.45	1.52
1	A	256	ASN	N-CA	5.32	1.52	1.46
1	A	191	PRO	C-O	5.32	1.31	1.24
1	B	259	ASP	C-O	5.31	1.30	1.24
1	A	216	ILE	CA-CB	-5.29	1.48	1.54
1	B	194	ILE	C-O	-5.25	1.18	1.24
1	A	265	ILE	CA-C	5.23	1.57	1.53
1	A	52	GLU	CA-C	5.23	1.59	1.52
1	B	57	LYS	CB-CG	5.23	1.68	1.52
1	A	231	MET	CB-CG	5.22	1.68	1.52
1	A	281	VAL	N-CA	-5.18	1.39	1.46
1	B	202	TYR	N-CA	5.18	1.52	1.46
1	A	46	ARG	CA-C	-5.16	1.46	1.52
1	A	157	ILE	CA-CB	-5.13	1.47	1.53
1	B	44	PHE	CA-C	5.13	1.59	1.52
1	B	234	LEU	CA-C	-5.11	1.46	1.52
1	B	49	ARG	CA-C	-5.11	1.46	1.52
1	A	240	ASN	CA-C	-5.10	1.46	1.52
1	B	203	ASP	N-CA	-5.09	1.39	1.46
1	A	118	VAL	CA-CB	5.09	1.60	1.54
1	B	315	ILE	CA-CB	5.07	1.61	1.54
1	B	76	GLU	C-O	5.06	1.29	1.24
1	B	210	SER	C-O	-5.06	1.17	1.24
1	A	199	GLU	CG-CD	5.06	1.64	1.52
1	B	292	ASP	N-CA	5.05	1.52	1.46
1	B	308	GLN	N-CA	5.03	1.52	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	LYS	CA-C-N	-10.72	109.42	120.03
1	B	121	LYS	C-N-CA	-10.72	109.42	120.03
1	A	252	GLU	N-CA-C	-10.06	100.42	112.89
1	B	242	SER	CA-C-N	9.27	129.83	119.92
1	B	242	SER	C-N-CA	9.27	129.83	119.92
1	A	184	GLY	N-CA-C	-8.83	97.84	110.46
1	B	21	LYS	N-CA-C	-8.00	103.53	113.38
1	A	222	LYS	CA-C-N	-7.95	112.19	120.38
1	A	222	LYS	C-N-CA	-7.95	112.19	120.38
1	B	286	PRO	CA-C-N	-7.66	111.62	120.89
1	B	286	PRO	C-N-CA	-7.66	111.62	120.89
1	A	113	SER	CB-CA-C	-7.60	98.64	110.81
1	A	224	PRO	CA-C-N	-7.53	115.04	126.86
1	A	224	PRO	C-N-CA	-7.53	115.04	126.86
1	A	236	HIS	N-CA-C	7.18	118.80	110.97
1	B	224	PRO	CA-C-N	-7.14	111.01	122.66
1	B	224	PRO	C-N-CA	-7.14	111.01	122.66
1	B	140	ALA	N-CA-C	-7.12	103.46	111.07
1	B	78	ARG	N-CA-C	-7.11	103.58	111.82
1	B	265	ILE	CA-C-N	-7.09	110.97	119.84
1	B	265	ILE	C-N-CA	-7.09	110.97	119.84
1	A	65	GLN	N-CA-C	6.81	119.94	108.23
1	A	265	ILE	N-CA-C	6.75	113.70	107.56
1	A	248	GLY	N-CA-C	-6.72	97.26	113.18
1	B	144	SER	CA-CB-OG	-6.64	97.81	111.10
1	A	249	HIS	N-CA-C	6.59	120.77	112.87
1	B	113	SER	N-CA-C	6.54	120.12	111.75
1	B	85	HIS	CA-C-N	-6.52	112.98	119.56
1	B	85	HIS	C-N-CA	-6.52	112.98	119.56
1	A	156	ASN	N-CA-C	-6.47	104.70	112.59
1	B	129	ALA	N-CA-C	-6.46	103.74	111.69
1	B	48	VAL	N-CA-C	-6.40	103.09	111.09
1	B	17	GLU	N-CA-C	6.38	119.04	111.71
1	B	192	GLU	CB-CA-C	-6.35	100.20	110.74
1	B	152	VAL	N-CA-CB	6.21	117.94	110.31
1	A	99	HIS	N-CA-C	6.18	120.06	111.90
1	A	41	ALA	N-CA-C	6.17	119.59	110.46
1	A	64	LYS	N-CA-C	-6.17	102.15	111.34
1	B	21	LYS	CB-CA-C	6.14	120.34	109.65
1	B	56	ILE	CA-C-N	-6.07	114.55	123.05
1	B	56	ILE	C-N-CA	-6.07	114.55	123.05
1	B	54	VAL	N-CA-CB	-6.00	103.42	112.35
1	A	40	GLY	CA-C-N	-5.96	112.35	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLY	C-N-CA	-5.96	112.35	122.67
1	A	274	VAL	N-CA-C	5.96	116.62	110.36
1	A	143	HIS	N-CA-C	-5.93	104.90	111.36
1	B	43	TYR	N-CA-C	5.93	119.07	109.40
1	A	262	LEU	N-CA-C	5.93	120.51	113.16
1	A	230	ALA	N-CA-C	5.84	117.64	111.28
1	A	286	PRO	CA-C-N	-5.80	113.70	119.56
1	A	286	PRO	C-N-CA	-5.80	113.70	119.56
1	A	280	PHE	CA-C-O	5.71	127.01	120.90
1	A	89	ILE	CG1-CB-CG2	-5.60	93.91	110.70
1	B	242	SER	N-CA-C	-5.57	102.60	110.29
1	B	234	LEU	N-CA-C	-5.52	105.17	111.07
1	B	292	ASP	N-CA-C	5.50	118.03	111.71
1	B	179	ALA	N-CA-C	-5.42	101.28	109.85
1	B	27	LEU	CA-C-N	-5.42	114.16	122.62
1	B	27	LEU	C-N-CA	-5.42	114.16	122.62
1	A	176	MET	N-CA-C	5.41	117.21	108.34
1	A	18	LEU	N-CA-C	5.39	121.61	114.12
1	B	320	ALA	N-CA-C	5.36	126.02	111.00
1	A	292	ASP	N-CA-C	5.36	117.12	111.28
1	B	207	ASP	N-CA-C	-5.34	105.50	112.23
1	B	274	VAL	N-CA-C	5.34	115.54	110.42
1	A	126	VAL	CB-CA-C	-5.30	105.18	111.97
1	A	61	TYR	N-CA-C	-5.30	104.25	111.56
1	A	177	ALA	N-CA-C	-5.29	102.51	110.24
1	B	198	ASP	N-CA-C	5.28	120.09	111.37
1	B	183	VAL	N-CA-CB	-5.28	102.52	111.23
1	B	145	HIS	CA-C-N	-5.24	115.45	123.47
1	B	145	HIS	C-N-CA	-5.24	115.45	123.47
1	A	317	PHE	N-CA-C	5.23	117.66	111.33
1	A	207	ASP	N-CA-C	-5.15	106.15	112.90
1	A	68	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	69	LYS	N-CA-C	5.13	117.26	111.11
1	B	231	MET	CA-C-N	-5.12	111.97	120.68
1	B	231	MET	C-N-CA	-5.12	111.97	120.68
1	A	264	LYS	CD-CE-NZ	5.10	128.21	111.90
1	B	245	LEU	N-CA-C	-5.09	102.86	110.23
1	B	287	PRO	CB-CA-C	5.07	116.81	110.27
1	B	204	GLY	N-CA-C	5.07	120.03	114.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	MET	Peptide
1	B	196	ALA	Peptide
1	B	313	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2468	116	0
1	B	2490	0	2469	96	0
2	A	35	0	26	3	0
2	B	35	0	26	7	0
3	A	142	0	0	14	0
3	B	135	0	0	6	0
All	All	5327	0	4989	221	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 22.

All (221) 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:A:175:ILE:CD1	1:A:175:ILE:CG1	1.74	1.58
2:B:500:STU:H261	2:B:500:STU:H16	1.23	1.10
1:A:65:GLN:HE21	1:A:67:ASN:HB2	1.16	1.08
1:A:65:GLN:NE2	1:A:67:ASN:HB2	1.73	1.02
1:B:46:ARG:HG2	1:B:46:ARG:HH11	1.25	0.98
1:A:114:ASP:HB3	1:A:312:MET:HE1	1.44	0.97
1:B:79:PHE:CZ	1:B:147:MET:HE2	2.02	0.95
1:A:85:HIS:CD2	1:A:87:ASN:H	1.86	0.93
1:A:203:ASP:HB3	1:A:205:LYS:H	1.32	0.92
1:B:79:PHE:CE1	1:B:147:MET:HE2	2.04	0.92
1:A:85:HIS:HD2	1:A:87:ASN:H	1.13	0.92
1:A:65:GLN:HE21	1:A:67:ASN:CB	1.84	0.90
1:A:96:LEU:O	1:A:97:ARG:HD3	1.72	0.89
1:A:279:ARG:HG2	3:A:420:HOH:O	1.72	0.88
1:A:175:ILE:HD12	1:A:175:ILE:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:HIS:CD2	1:A:285:ARG:HH22	1.92	0.87
1:B:85:HIS:HD2	1:B:87:ASN:H	1.22	0.86
1:A:118:VAL:HG23	1:A:312:MET:HE2	1.57	0.86
1:B:85:HIS:CD2	1:B:87:ASN:H	1.96	0.83
1:B:39:PHE:CD1	1:B:40:GLY:N	2.46	0.83
1:A:175:ILE:CD1	1:A:175:ILE:H	1.93	0.81
1:A:108:CYS:HB3	1:A:159:LEU:O	1.80	0.81
1:B:235:TYR:CE1	1:B:239:GLN:HG3	2.16	0.80
2:B:500:STU:H16	2:B:500:STU:C26	2.08	0.80
1:B:96:LEU:C	1:B:96:LEU:HD23	2.09	0.78
1:B:61:TYR:CE2	1:B:99:HIS:HA	2.19	0.78
1:A:175:ILE:HD12	1:A:175:ILE:H	1.48	0.76
2:B:500:STU:H261	2:B:500:STU:C16	2.04	0.75
1:A:89:ILE:O	1:A:89:ILE:HG22	1.86	0.75
1:A:175:ILE:CD1	1:A:175:ILE:N	2.50	0.75
1:B:61:TYR:CZ	1:B:99:HIS:HA	2.22	0.74
1:B:288:THR:HB	1:B:292:ASP:OD2	1.87	0.73
1:A:161:GLU:HA	1:A:162:PRO:C	2.14	0.73
1:A:306:ASN:OD1	1:A:309:TYR:HB2	1.90	0.72
1:A:124:GLN:HG2	3:A:461:HOH:O	1.90	0.72
1:B:68:GLU:N	1:B:68:GLU:CD	2.48	0.71
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.01	0.71
1:A:36:HIS:HE1	3:A:518:HOH:O	1.73	0.70
1:B:161:GLU:HA	1:B:162:PRO:C	2.17	0.69
1:A:240:ASN:O	1:A:264:LYS:HE3	1.93	0.69
1:B:68:GLU:CD	1:B:68:GLU:H	2.01	0.68
2:B:500:STU:H273	2:B:500:STU:C17	2.23	0.68
1:A:12:ASP:N	1:A:13:PRO:HD2	2.09	0.67
1:A:85:HIS:HD2	1:A:87:ASN:N	1.91	0.67
1:B:196:ALA:C	1:B:197:MET:O	2.36	0.67
1:B:96:LEU:HD23	1:B:97:ARG:N	2.10	0.67
1:B:310:ARG:HH21	1:B:311:LYS:HD3	1.60	0.67
1:A:238:ALA:O	1:A:264:LYS:NZ	2.23	0.67
1:B:265:ILE:O	1:B:266:PRO:C	2.34	0.67
1:A:79:PHE:CE1	1:A:147:MET:HE2	2.30	0.66
1:A:50:ASN:OD1	1:A:52:GLU:HB2	1.96	0.65
1:B:312:MET:HE3	1:B:312:MET:HA	1.78	0.65
1:A:224:PRO:O	1:A:225:LEU:CB	2.41	0.65
1:B:176:MET:HE2	1:B:178:PRO:O	1.97	0.65
1:A:194:ILE:O	1:A:197:MET:HG3	1.98	0.64
1:A:23:ASP:HB2	1:A:97:ARG:NH2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:CZ	1:A:310:ARG:HA	2.29	0.63
1:A:114:ASP:CB	1:A:312:MET:HE1	2.24	0.62
1:A:133:HIS:HD2	1:A:285:ARG:HH22	1.46	0.61
1:B:145:HIS:O	1:B:146:ASN:CB	2.46	0.61
1:A:270:PRO:HG2	1:A:275:LEU:HD11	1.83	0.60
1:B:46:ARG:HG2	1:B:46:ARG:NH1	2.05	0.60
1:A:180:ASN:ND2	3:A:510:HOH:O	2.32	0.60
1:A:270:PRO:HG3	1:A:275:LEU:HD21	1.83	0.60
1:A:224:PRO:O	1:A:225:LEU:HB2	2.01	0.60
1:A:89:ILE:O	1:A:89:ILE:CG2	2.47	0.59
1:A:203:ASP:HB3	1:A:205:LYS:N	2.13	0.59
1:A:231:MET:HB2	3:A:404:HOH:O	2.02	0.59
1:A:196:ALA:C	1:A:198:ASP:O	2.46	0.59
1:A:288:THR:HB	1:A:292:ASP:OD2	2.03	0.58
1:B:318:GLN:HB3	3:B:580:HOH:O	2.03	0.58
1:A:43:TYR:CE1	1:A:58:LYS:HG3	2.39	0.58
1:A:182:PHE:CE1	1:A:189:MET:HE1	2.38	0.58
1:B:114:ASP:O	1:B:118:VAL:HG23	2.03	0.58
1:A:203:ASP:CB	1:A:205:LYS:H	2.11	0.57
1:B:145:HIS:O	1:B:146:ASN:HB2	2.04	0.57
2:B:500:STU:C26	2:B:500:STU:C16	2.73	0.57
1:A:231:MET:HG3	3:A:418:HOH:O	2.04	0.57
1:B:79:PHE:HE1	1:B:147:MET:HG2	1.70	0.57
1:B:209:TRP:C	1:B:209:TRP:CD1	2.83	0.57
1:B:31:LEU:HD22	1:B:45:ALA:HB2	1.87	0.56
1:A:270:PRO:CG	1:A:275:LEU:HD21	2.36	0.56
1:B:161:GLU:HA	1:B:162:PRO:O	2.05	0.56
1:B:312:MET:HE2	1:B:315:ILE:CD1	2.35	0.56
1:A:236:HIS:O	1:A:240:ASN:HB2	2.06	0.56
1:A:227:ASN:HD22	1:A:227:ASN:C	2.13	0.56
1:B:46:ARG:HH21	1:B:320:ALA:HB2	1.71	0.55
1:B:212:GLY:O	1:B:215:CYS:HB2	2.06	0.55
1:A:304:LEU:HD22	1:A:310:ARG:HD2	1.88	0.55
1:B:39:PHE:HD1	1:B:40:GLY:N	2.03	0.55
1:B:238:ALA:O	1:B:264:LYS:NZ	2.40	0.55
1:A:228:MET:HE2	1:A:232:SER:HB3	1.87	0.55
1:A:25:GLU:HG3	3:A:470:HOH:O	2.07	0.54
1:A:34:ILE:HA	1:A:314:LYS:HD3	1.89	0.54
2:A:400:STU:H261	2:A:400:STU:H16	1.90	0.54
1:B:236:HIS:HB3	3:B:543:HOH:O	2.07	0.54
1:B:96:LEU:C	1:B:96:LEU:CD2	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG2	1:A:80:LEU:HD22	1.90	0.54
1:B:113:SER:HB3	1:B:155:GLY:HA2	1.90	0.54
1:B:79:PHE:CE1	1:B:147:MET:HG2	2.42	0.54
1:B:46:ARG:CG	1:B:46:ARG:NH1	2.65	0.53
1:A:85:HIS:CD2	1:A:86:PRO:HD2	2.43	0.53
1:A:205:LYS:HE2	1:A:269:ARG:O	2.08	0.53
1:A:146:ASN:ND2	1:A:177:ALA:HB3	2.24	0.53
1:A:70:TRP:CZ2	1:A:74:ILE:HD11	2.43	0.53
1:A:235:TYR:CE1	1:A:239:GLN:HG3	2.44	0.53
1:B:175:ILE:HD12	1:B:176:MET:H	1.73	0.53
1:B:43:TYR:CD1	1:B:43:TYR:N	2.78	0.52
1:B:267:GLN:N	1:B:267:GLN:OE1	2.41	0.52
1:B:282:LEU:O	1:B:283:ARG:C	2.53	0.52
1:A:231:MET:CG	3:A:418:HOH:O	2.56	0.52
1:A:185:THR:O	1:A:189:MET:HG3	2.10	0.52
1:A:258:VAL:CG1	1:A:262:LEU:HD12	2.39	0.52
1:B:19:PHE:CD2	1:B:96:LEU:HB2	2.45	0.51
1:B:119:HIS:O	1:B:120:LYS:HB2	2.10	0.51
1:A:214:THR:O	1:A:218:LEU:HG	2.10	0.51
1:A:44:PHE:C	1:A:44:PHE:CD2	2.89	0.51
1:A:310:ARG:HA	1:A:310:ARG:NE	2.25	0.51
1:A:277:LYS:O	1:A:282:LEU:HD12	2.10	0.51
1:B:100:THR:O	1:B:102:TRP:HD1	1.94	0.51
1:A:79:PHE:CZ	1:A:147:MET:HE2	2.46	0.50
1:B:103:LEU:HD23	1:B:103:LEU:N	2.27	0.50
1:B:85:HIS:HD2	1:B:87:ASN:N	2.00	0.50
1:B:65:GLN:O	1:B:66:SER:C	2.55	0.50
1:A:235:TYR:CD1	1:A:239:GLN:HG3	2.47	0.50
1:B:239:GLN:C	1:B:240:ASN:HD22	2.20	0.50
1:A:196:ALA:O	1:A:198:ASP:O	2.30	0.49
1:B:203:ASP:OD1	1:B:203:ASP:C	2.54	0.49
1:A:241:GLU:HG2	1:A:242:SER:H	1.76	0.49
1:A:114:ASP:HB3	1:A:312:MET:CE	2.31	0.49
1:B:308:GLN:HB2	1:B:309:TYR:CD2	2.47	0.49
1:B:39:PHE:CG	1:B:57:LYS:HE3	2.47	0.49
1:B:160:SER:O	1:B:163:GLY:HA2	2.12	0.49
1:A:79:PHE:HE2	1:A:170:PHE:CD2	2.31	0.48
1:B:220:GLU:OE1	3:B:553:HOH:O	2.20	0.48
1:A:258:VAL:HG12	1:A:262:LEU:HD12	1.94	0.48
1:B:149:HIS:O	1:B:150:ARG:HB2	2.13	0.48
1:A:273:GLU:O	1:A:276:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:N	1:B:159:LEU:HD22	2.29	0.48
1:A:245:LEU:HD13	1:A:250:TRP:CD1	2.49	0.48
1:B:247:SER:O	1:B:255:ARG:NH2	2.47	0.48
1:A:252:GLU:OE2	1:A:256:ASN:HB2	2.14	0.47
1:A:266:PRO:HB2	1:A:267:GLN:OE1	2.13	0.47
1:A:197:MET:C	1:A:198:ASP:O	2.57	0.47
1:A:282:LEU:O	1:A:283:ARG:C	2.58	0.47
1:A:147:MET:HG3	3:A:494:HOH:O	2.15	0.47
2:A:400:STU:O5	2:A:400:STU:H4	2.15	0.47
1:A:34:ILE:CA	1:A:314:LYS:HD3	2.45	0.46
1:A:301:VAL:O	1:A:304:LEU:HB2	2.16	0.46
1:B:290:ILE:HD13	1:B:290:ILE:HA	1.59	0.46
1:A:205:LYS:NZ	3:A:416:HOH:O	2.34	0.46
1:B:163:GLY:HA3	1:B:290:ILE:HG22	1.98	0.46
1:B:47:ASP:O	1:B:51:SER:N	2.49	0.46
1:A:97:ARG:HD2	1:A:97:ARG:HA	1.92	0.46
1:A:216:ILE:O	1:A:220:GLU:N	2.46	0.46
1:B:61:TYR:CE2	1:B:99:HIS:CA	2.95	0.46
1:A:279:ARG:CG	3:A:420:HOH:O	2.43	0.46
1:B:112:ALA:O	1:B:115:LEU:HB2	2.16	0.45
1:B:141:TYR:O	1:B:144:SER:HB2	2.16	0.45
1:A:279:ARG:NE	3:A:420:HOH:O	2.49	0.45
1:B:74:ILE:O	1:B:75:LYS:C	2.59	0.45
1:B:68:GLU:N	1:B:68:GLU:OE2	2.50	0.45
1:A:61:TYR:CE2	1:A:99:HIS:HA	2.51	0.45
1:B:50:ASN:O	1:B:51:SER:HB2	2.16	0.45
1:B:61:TYR:CE2	1:B:99:HIS:C	2.95	0.45
1:B:166:LYS:NZ	3:B:600:HOH:O	2.50	0.45
1:B:304:LEU:HD21	1:B:310:ARG:NH1	2.32	0.45
1:A:23:ASP:HB2	1:A:97:ARG:HH21	1.82	0.45
1:A:75:LYS:NZ	1:A:175:ILE:HD11	2.31	0.45
1:B:312:MET:HE2	1:B:315:ILE:HD11	1.99	0.44
1:A:252:GLU:OE2	1:A:279:ARG:NH1	2.43	0.44
1:B:100:THR:O	1:B:102:TRP:CD1	2.70	0.44
1:B:169:ASP:C	1:B:169:ASP:OD1	2.58	0.44
1:A:279:ARG:HG2	1:A:279:ARG:H	1.53	0.44
1:B:288:THR:O	1:B:289:VAL:C	2.60	0.44
1:B:312:MET:HA	1:B:312:MET:CE	2.46	0.43
1:A:153:LYS:HA	1:A:214:THR:OG1	2.18	0.43
1:A:296:ARG:HB2	3:A:482:HOH:O	2.18	0.43
1:B:38:SER:CB	3:B:535:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLN:NE2	1:B:68:GLU:HG2	2.34	0.43
1:A:109:LEU:N	1:A:109:LEU:CD2	2.82	0.43
1:A:125:GLU:HA	1:A:128:ILE:HD12	2.00	0.43
1:B:205:LYS:HE2	1:B:269:ARG:O	2.19	0.43
1:B:235:TYR:CZ	1:B:239:GLN:HG3	2.53	0.43
2:B:500:STU:H1	2:B:500:STU:H25	1.84	0.43
1:A:198:ASP:CG	1:A:199:GLU:H	2.26	0.43
1:A:228:MET:HE2	1:A:232:SER:CB	2.48	0.43
1:B:163:GLY:HA3	1:B:290:ILE:CG2	2.49	0.43
1:A:112:ALA:O	1:A:115:LEU:HB2	2.18	0.42
1:A:285:ARG:O	1:A:286:PRO:C	2.60	0.42
1:A:148:ILE:HG23	1:A:204:GLY:HA2	2.01	0.42
1:B:28:PHE:HA	1:B:46:ARG:O	2.20	0.42
1:A:103:LEU:N	1:A:103:LEU:HD23	2.33	0.42
1:A:263:GLN:HA	1:A:263:GLN:OE1	2.19	0.42
1:B:34:ILE:HG12	1:B:42:VAL:O	2.20	0.42
1:A:141:TYR:CE1	1:A:145:HIS:HE1	2.38	0.42
1:A:265:ILE:HA	1:A:265:ILE:HD13	1.70	0.42
2:A:400:STU:H22	3:A:411:HOH:O	2.19	0.42
1:B:79:PHE:CE1	1:B:147:MET:CE	2.89	0.42
1:B:138:GLY:HA3	1:B:167:LEU:HD22	2.02	0.41
1:B:161:GLU:N	3:B:521:HOH:O	2.38	0.41
1:B:96:LEU:O	1:B:97:ARG:HG2	2.20	0.41
1:A:176:MET:HG3	1:A:177:ALA:O	2.20	0.41
1:A:185:THR:O	1:A:186:PRO:C	2.62	0.41
1:A:297:THR:O	1:A:301:VAL:HG23	2.21	0.41
1:A:161:GLU:CA	1:A:162:PRO:C	2.88	0.41
1:B:313:LYS:HE3	1:B:313:LYS:HB3	1.90	0.41
1:A:175:ILE:CD1	1:A:175:ILE:CB	2.82	0.41
1:B:141:TYR:O	1:B:142:LEU:C	2.60	0.41
1:A:39:PHE:CD1	1:A:40:GLY:N	2.88	0.40
1:A:79:PHE:CE2	1:A:170:PHE:CD2	3.09	0.40
1:B:274:VAL:O	1:B:277:LYS:HB2	2.22	0.40
1:B:307:LEU:O	1:B:313:LYS:HG3	2.21	0.40
1:A:85:HIS:CG	1:A:86:PRO:CD	3.05	0.40
1:B:34:ILE:HD12	2:B:500:STU:C5	2.52	0.40
1:A:252:GLU:OE1	1:A:279:ARG:NH1	2.53	0.40
1:B:124:GLN:HB2	1:B:127:GLU:HG3	2.04	0.40
1:A:85:HIS:CG	1:A:86:PRO:HD2	2.57	0.40
1:B:139:LEU:HG	1:B:167:LEU:HD21	2.03	0.40
1:B:234:LEU:HA	1:B:234:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TYR:CD2	1:B:279:ARG:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/309 (99%)	269 (88%)	26 (8%)	11 (4%)	2	1
1	B	306/309 (99%)	266 (87%)	30 (10%)	10 (3%)	3	2
All	All	612/618 (99%)	535 (87%)	56 (9%)	21 (3%)	3	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	251	SER
1	B	39	PHE
1	B	64	LYS
1	B	162	PRO
1	B	197	MET
1	B	304	LEU
1	B	314	LYS
1	A	238	ALA
1	A	239	GLN
1	B	50	ASN
1	A	226	PHE
1	B	38	SER
1	A	203	ASP
1	A	303	GLU
1	A	314	LYS
1	A	63	GLY

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Mol	Chain	Res	Type
1	A	163	GLY
1	B	289	VAL
1	B	163	GLY
1	A	162	PRO

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	268/268 (100%)	225 (84%)	43 (16%)	2	2
1	B	268/268 (100%)	220 (82%)	48 (18%)	2	1
All	All	536/536 (100%)	445 (83%)	91 (17%)	2	2

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	ASP
1	A	27	LEU
1	A	31	LEU
1	A	38	SER
1	A	44	PHE
1	A	46	ARG
1	A	64	LYS
1	A	71	GLN
1	A	74	ILE
1	A	80	LEU
1	A	81	GLN
1	A	82	LYS
1	A	96	LEU
1	A	97	ARG
1	A	103	LEU
1	A	109	LEU
1	A	126	VAL
1	A	148	ILE

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	166	LYS
1	A	174	SER
1	A	175	ILE
1	A	195	LEU
1	A	199	GLU
1	A	201	GLN
1	A	206	VAL
1	A	227	ASN
1	A	231	MET
1	A	236	HIS
1	A	237	ILE
1	A	239	GLN
1	A	252	GLU
1	A	277	LYS
1	A	281	VAL
1	A	285	ARG
1	A	288	THR
1	A	291	MET
1	A	295	GLN
1	A	304	LEU
1	A	305	ASP
1	A	310	ARG
1	A	314	LYS
1	B	21	LYS
1	B	25	GLU
1	B	31	LEU
1	B	38	SER
1	B	44	PHE
1	B	46	ARG
1	B	54	VAL
1	B	57	LYS
1	B	64	LYS
1	B	68	GLU
1	B	74	ILE
1	B	103	LEU
1	B	109	LEU
1	B	113	SER
1	B	121	LYS
1	B	126	VAL
1	B	144	SER
1	B	152	VAL

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Mol	Chain	Res	Type
1	B	161	GLU
1	B	164	LEU
1	B	167	LEU
1	B	175	ILE
1	B	183	VAL
1	B	195	LEU
1	B	198	ASP
1	B	201	GLN
1	B	211	LEU
1	B	231	MET
1	B	232	SER
1	B	251	SER
1	B	255	ARG
1	B	267	GLN
1	B	279	ARG
1	B	281	VAL
1	B	284	GLU
1	B	288	THR
1	B	289	VAL
1	B	290	ILE
1	B	291	MET
1	B	303	GLU
1	B	304	LEU
1	B	305	ASP
1	B	310	ARG
1	B	311	LYS
1	B	312	MET
1	B	313	LYS
1	B	315	ILE
1	B	318	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	81	GLN
1	A	85	HIS
1	A	90	GLN
1	A	133	HIS
1	A	145	HIS
1	A	227	ASN
1	A	236	HIS

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Mol	Chain	Res	Type
1	B	36	HIS
1	B	71	GLN
1	B	85	HIS
1	B	239	GLN
1	B	240	ASN
1	B	308	GLN
1	B	318	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	SEP	B	181	1	8,9,10	1.81	3 (37%)	7,12,14	3.57	4 (57%)
1	SEP	A	181	1	8,9,10	1.98	3 (37%)	7,12,14	3.19	3 (42%)

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
1	SEP	B	181	1	-	5/6/8/10	-
1	SEP	A	181	1	-	2/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	SEP	P-O1P	4.11	1.63	1.50
1	B	181	SEP	P-O1P	2.97	1.59	1.50
1	B	181	SEP	P-O3P	2.46	1.64	1.54
1	A	181	SEP	O-C	2.43	1.29	1.20
1	B	181	SEP	P-O2P	2.33	1.63	1.54
1	A	181	SEP	P-O2P	2.28	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	SEP	O3P-P-OG	-6.54	89.63	106.67
1	B	181	SEP	O2P-P-OG	-5.73	91.72	106.67
1	B	181	SEP	O3P-P-O2P	5.49	128.38	107.80
1	A	181	SEP	OG-CB-CA	-4.07	104.19	108.14
1	B	181	SEP	OG-P-O1P	3.71	116.46	106.44
1	A	181	SEP	O3P-P-O1P	2.82	121.82	110.83
1	B	181	SEP	OG-CB-CA	-2.76	105.45	108.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	181	SEP	N-CA-CB-OG
1	A	181	SEP	C-CA-CB-OG
1	B	181	SEP	N-CA-CB-OG
1	B	181	SEP	C-CA-CB-OG
1	B	181	SEP	CB-OG-P-O1P
1	B	181	SEP	CB-OG-P-O2P
1	B	181	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	STU	A	400	-	39,42,42	1.92	11 (28%)	50,68,68	2.24	16 (32%)
2	STU	B	500	-	39,42,42	3.46	20 (51%)	50,68,68	3.06	19 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	A	400	-	-	1/4/42/42	-
2	STU	B	500	-	-	2/4/42/42	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	STU	C13-C12	8.54	1.53	1.40
2	B	500	STU	C3-C4	7.48	1.51	1.38
2	B	500	STU	C17-N2	-6.43	1.32	1.40
2	B	500	STU	C15-C16	6.43	1.49	1.38
2	B	500	STU	C14-C15	5.49	1.50	1.38
2	B	500	STU	C1-C20	4.83	1.47	1.39
2	B	500	STU	C19-N3	-4.69	1.31	1.39
2	A	400	STU	C22-C23	4.62	1.57	1.53
2	B	500	STU	C5-C20	4.59	1.48	1.41
2	B	500	STU	C2-C1	4.30	1.46	1.38
2	B	500	STU	C28-N4	4.19	1.57	1.46
2	A	400	STU	C8-N1	3.94	1.38	1.35
2	B	500	STU	C22-C23	3.62	1.56	1.53
2	A	400	STU	C9-N1	3.60	1.49	1.45
2	B	500	STU	C9-N1	3.49	1.49	1.45
2	A	400	STU	C23-N4	3.42	1.51	1.47
2	A	400	STU	C9-C10	3.41	1.53	1.50
2	B	500	STU	C24-C25	3.41	1.58	1.51
2	B	500	STU	C11-C10	-3.40	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	STU	C3-C2	3.19	1.45	1.38
2	A	400	STU	C26-C21	3.17	1.55	1.51
2	A	400	STU	C19-N3	-2.85	1.34	1.39
2	B	500	STU	O4-C25	2.81	1.47	1.43
2	B	500	STU	C16-C17	2.76	1.43	1.39
2	A	400	STU	C2-C1	2.63	1.43	1.38
2	A	400	STU	C28-N4	2.62	1.53	1.46
2	B	500	STU	C23-N4	2.55	1.50	1.47
2	A	400	STU	O6-C22	2.33	1.46	1.42
2	B	500	STU	C9-C10	2.18	1.52	1.50
2	B	500	STU	C7-C8	-2.08	1.42	1.49
2	A	400	STU	C4-C5	2.03	1.43	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	STU	O5-C8-N1	9.41	135.81	125.35
2	B	500	STU	O5-C8-C7	-8.74	115.80	128.47
2	B	500	STU	C1-C20-C5	5.99	128.61	121.59
2	A	400	STU	C9-C10-C7	-5.65	107.81	109.88
2	B	500	STU	C9-C10-C7	5.36	111.85	109.88
2	B	500	STU	C20-N3-C25	-5.27	113.97	127.45
2	B	500	STU	C12-C17-N2	5.24	112.39	108.94
2	A	400	STU	C28-N4-C23	-4.96	108.46	114.39
2	B	500	STU	C2-C1-C20	-4.73	108.74	118.28
2	A	400	STU	C4-C5-C20	4.55	124.49	119.24
2	B	500	STU	C3-C2-C1	4.39	125.66	120.24
2	A	400	STU	C9-C10-C11	4.04	131.80	128.73
2	B	500	STU	C10-C9-N1	-3.93	97.93	101.75
2	B	500	STU	C3-C4-C5	-3.83	113.88	120.23
2	A	400	STU	C9-N1-C8	-3.79	110.41	113.86
2	B	500	STU	C19-N3-C25	3.70	135.03	123.02
2	B	500	STU	C1-C20-N3	-3.65	123.53	129.73
2	A	400	STU	C27-O6-C22	-3.55	108.46	114.46
2	A	400	STU	C6-C7-C10	-3.35	118.43	120.76
2	A	400	STU	C3-C2-C1	3.29	124.29	120.24
2	A	400	STU	C3-C4-C5	-3.27	114.81	120.23
2	A	400	STU	C13-C12-C17	3.22	122.96	119.24
2	A	400	STU	C16-C17-C12	-3.13	117.93	121.59
2	A	400	STU	C18-C19-N3	3.04	132.00	129.42
2	B	500	STU	C18-C19-N3	-2.96	126.91	129.42
2	B	500	STU	C16-C17-C12	-2.89	118.21	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	STU	C20-N3-C25	-2.77	120.36	127.45
2	B	500	STU	C11-C12-C17	-2.71	103.76	106.49
2	B	500	STU	C15-C14-C13	-2.64	116.98	120.24
2	A	400	STU	C7-C6-C19	2.52	122.26	118.04
2	A	400	STU	C10-C9-N1	2.48	104.16	101.75
2	A	400	STU	C7-C8-N1	2.45	108.72	106.38
2	B	500	STU	C19-N3-C20	2.35	111.00	107.90
2	B	500	STU	C6-C5-C20	-2.26	104.21	106.49
2	B	500	STU	C7-C8-N1	2.06	108.34	106.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	STU	C22-C23-N4-C28
2	A	400	STU	C24-C23-N4-C28
2	B	500	STU	C24-C23-N4-C28

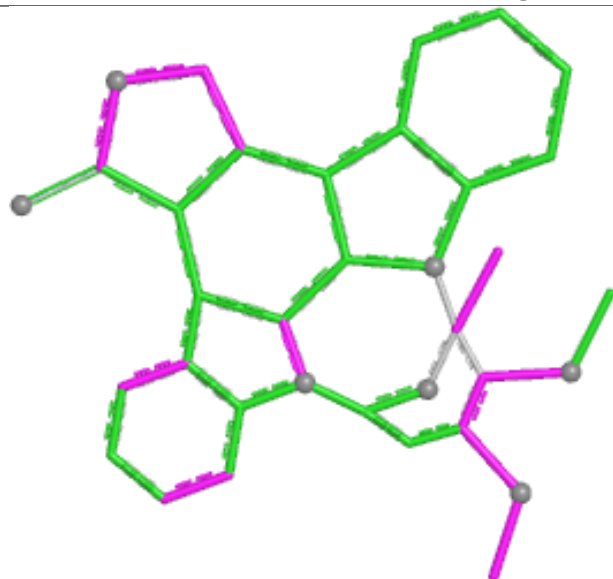
There are no ring outliers.

2 monomers are involved in 10 short contacts:

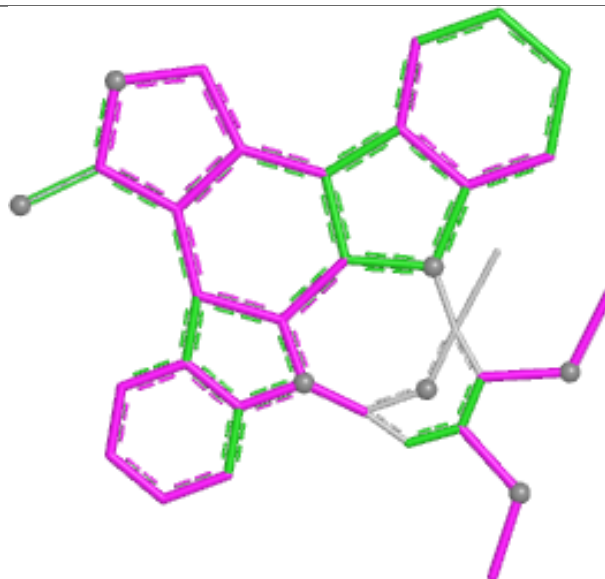
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	STU	3	0
2	B	500	STU	7	0

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.

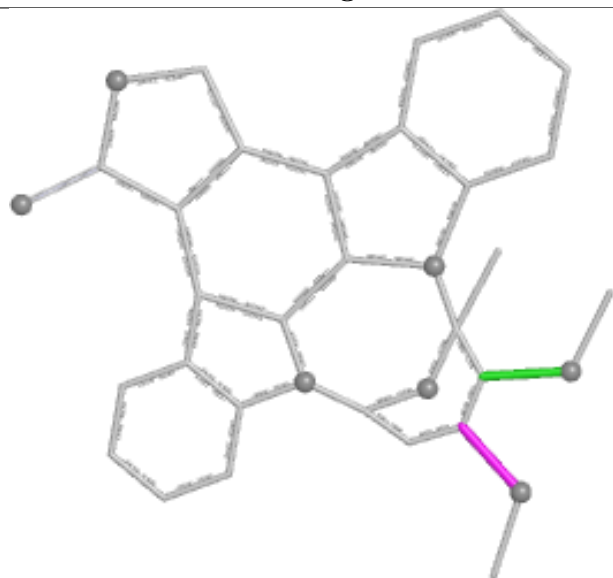
Ligand STU A 400



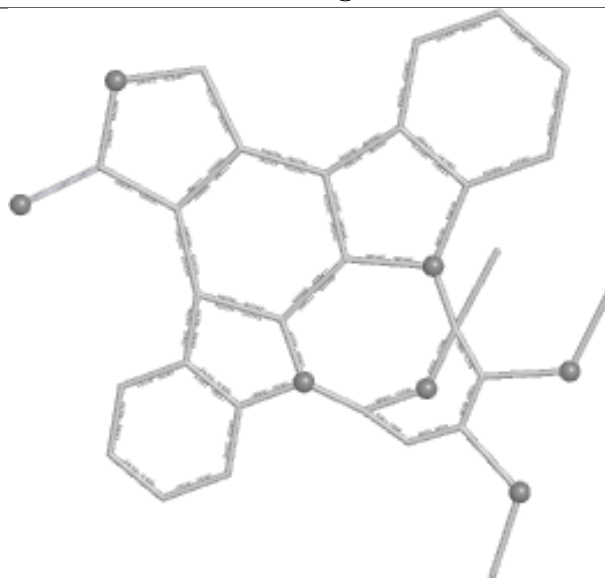
Bond lengths



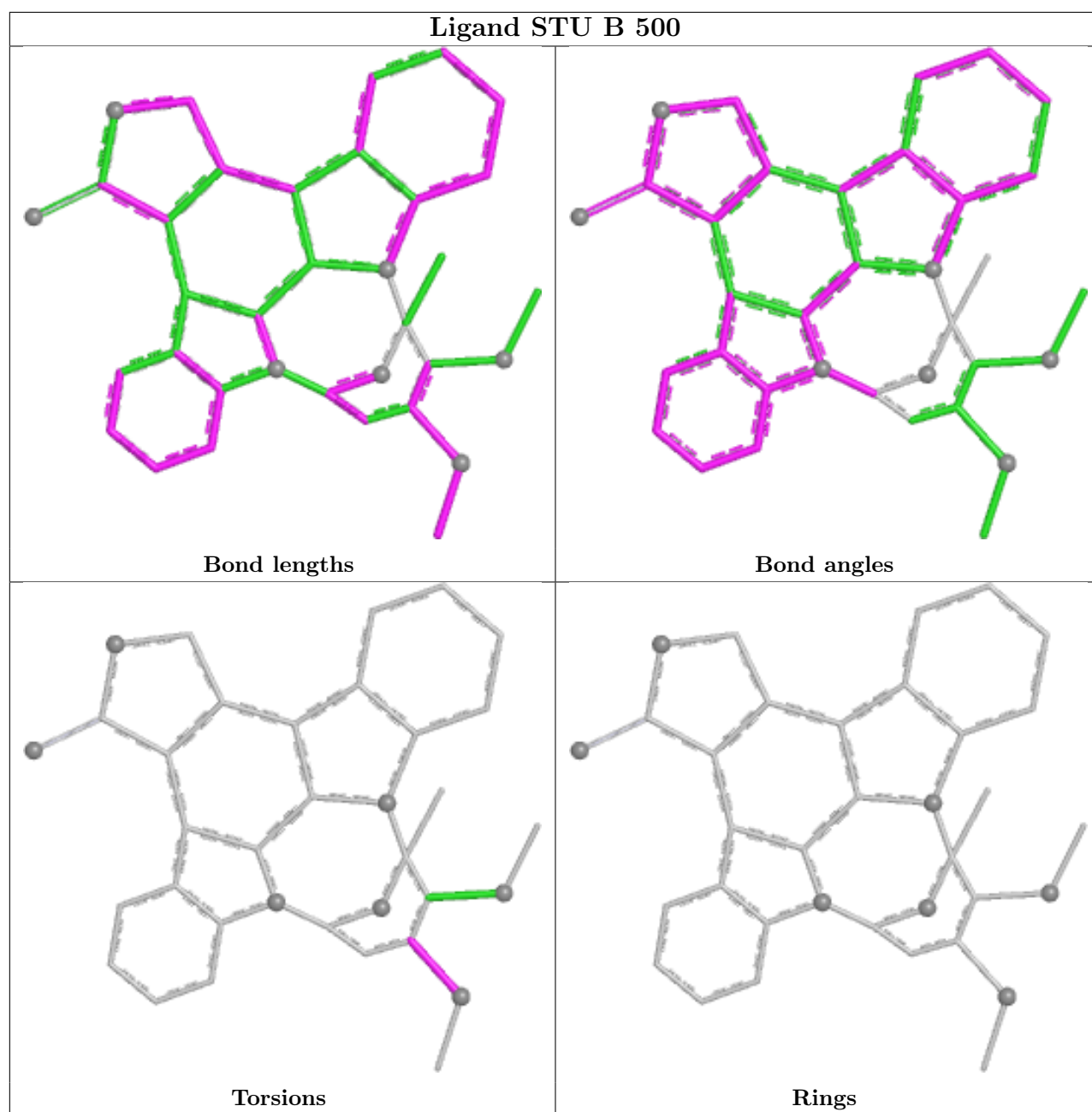
Bond angles



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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/309 (99%)	-0.29	10 (3%) 50 51	15, 37, 83, 117	0
1	B	308/309 (99%)	-0.34	9 (2%) 53 55	16, 37, 84, 113	0
All	All	616/618 (99%)	-0.32	19 (3%) 51 52	15, 37, 84, 117	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	LEU	5.4
1	A	307	LEU	4.8
1	B	309	TYR	4.4
1	A	63	GLY	4.0
1	B	197	MET	3.4
1	B	308	GLN	3.2
1	A	320	ALA	2.8
1	A	309	TYR	2.7
1	A	304	LEU	2.6
1	B	320	ALA	2.5
1	B	306	ASN	2.5
1	B	38	SER	2.2
1	B	198	ASP	2.2
1	A	65	GLN	2.1
1	A	318	GLN	2.1
1	A	199	GLU	2.1
1	A	197	MET	2.1
1	A	305	ASP	2.1
1	B	310	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	181	10/11	0.97	0.05	36,37,40,46	0
1	SEP	B	181	10/11	0.97	0.05	33,37,41,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

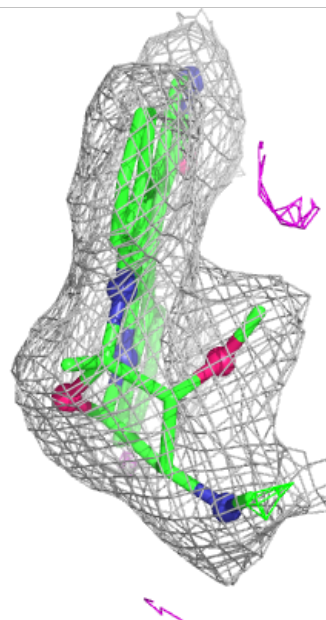
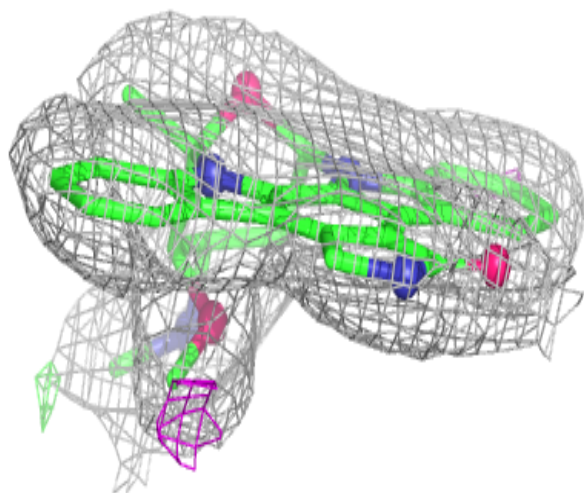
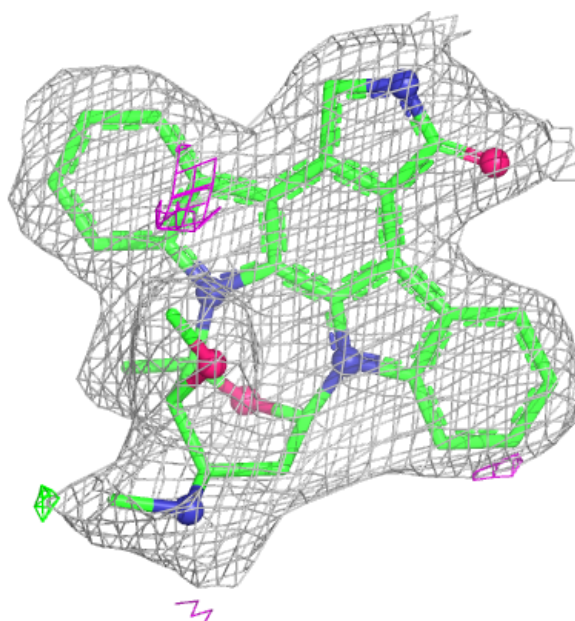
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	STU	B	500	35/35	0.96	0.06	18,22,24,29	0
2	STU	A	400	35/35	0.97	0.05	27,29,34,40	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.

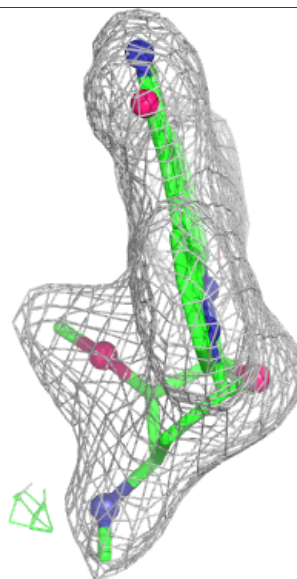
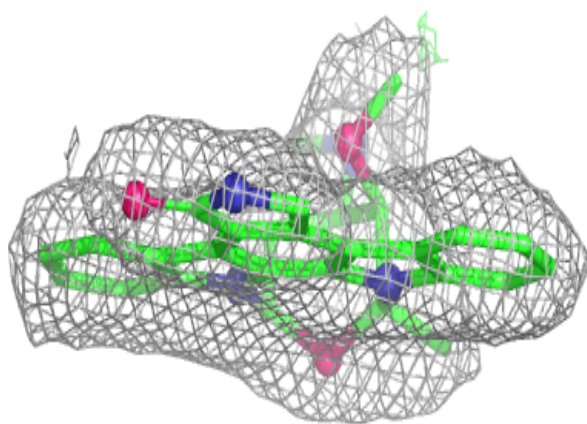
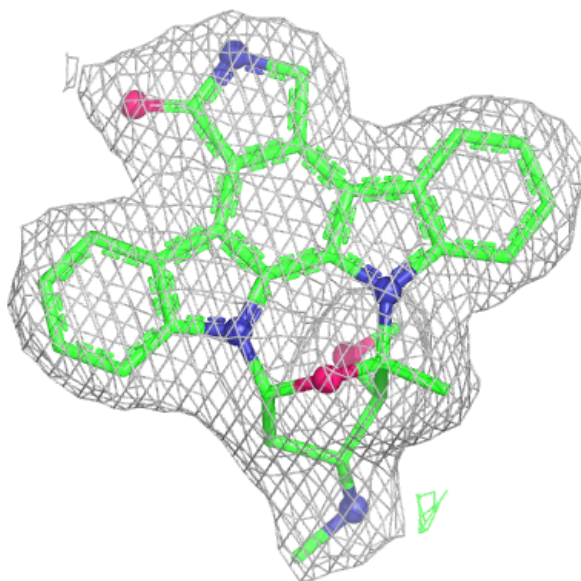
Electron density around STU B 500:

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



Electron density around STU A 400:

$2mF_o-DF_c$ (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.