



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:00 AM UTC

PDB ID : 8DSM / pdb_00008dsm
Title : Human NAMPT in complex with inhibitor ZN-4-3
Authors : Ratia, K.; Xiong, R.; Shen, Z.; Thatcher, G.R.
Deposited on : 2022-07-22
Resolution : 2.75 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

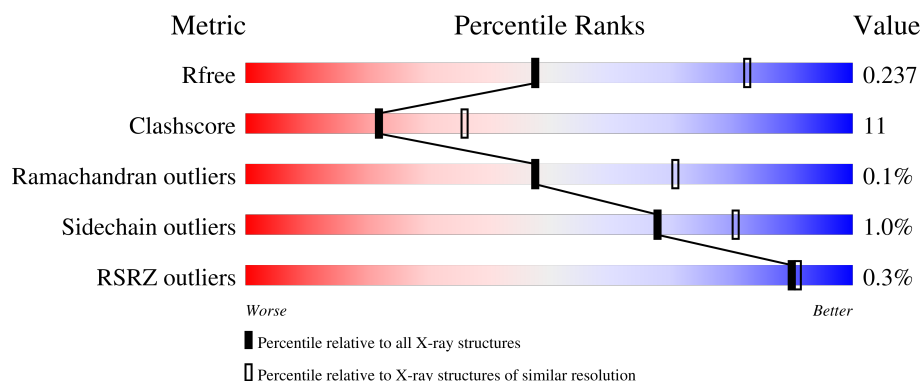
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	499	 76% 16% • 6%
1	B	499	 75% 18% • 6%
1	C	499	 69% 23% • 6%
1	D	499	 73% 19% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15222 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3723	2395	615	706	7			
1	B	469	Total	C	N	O	S	0	0	0
			3738	2404	617	710	7			
1	C	468	Total	C	N	O	S	0	0	0
			3730	2397	616	710	7			
1	D	469	Total	C	N	O	S	0	0	0
			3738	2404	617	710	7			

There are 32 discrepancies between the modelled and reference sequences:

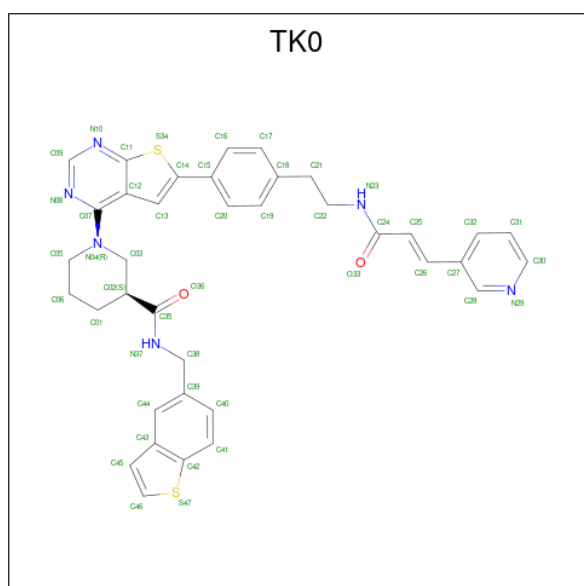
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag	UNP P43490
A	499	HIS	-	expression tag	UNP P43490
B	492	LEU	-	expression tag	UNP P43490
B	493	GLU	-	expression tag	UNP P43490
B	494	HIS	-	expression tag	UNP P43490
B	495	HIS	-	expression tag	UNP P43490
B	496	HIS	-	expression tag	UNP P43490
B	497	HIS	-	expression tag	UNP P43490
B	498	HIS	-	expression tag	UNP P43490
B	499	HIS	-	expression tag	UNP P43490
C	492	LEU	-	expression tag	UNP P43490
C	493	GLU	-	expression tag	UNP P43490
C	494	HIS	-	expression tag	UNP P43490
C	495	HIS	-	expression tag	UNP P43490
C	496	HIS	-	expression tag	UNP P43490

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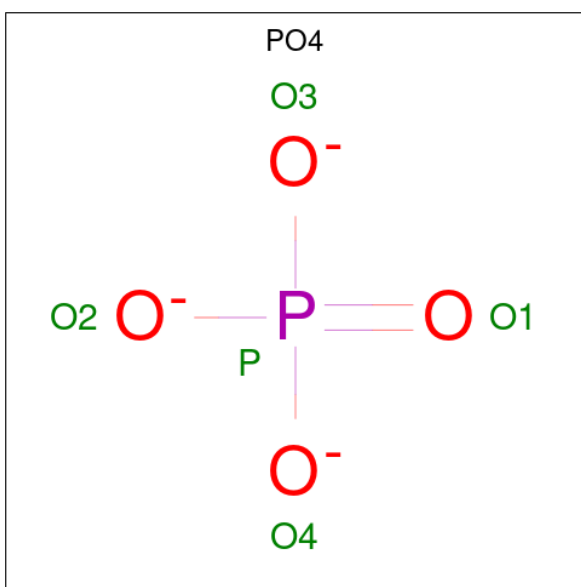
Chain	Residue	Modelled	Actual	Comment	Reference
C	497	HIS	-	expression tag	UNP P43490
C	498	HIS	-	expression tag	UNP P43490
C	499	HIS	-	expression tag	UNP P43490
D	492	LEU	-	expression tag	UNP P43490
D	493	GLU	-	expression tag	UNP P43490
D	494	HIS	-	expression tag	UNP P43490
D	495	HIS	-	expression tag	UNP P43490
D	496	HIS	-	expression tag	UNP P43490
D	497	HIS	-	expression tag	UNP P43490
D	498	HIS	-	expression tag	UNP P43490
D	499	HIS	-	expression tag	UNP P43490

- Molecule 2 is (3S)-N-[(1-benzothiophen-5-yl)methyl]-1-[6-(4-{2-[(2E)-3-(pyridin-3-yl)prop-2-enamido]ethyl}phenyl)thieno[2,3-d]pyrimidin-4-yl]piperidine-3-carboxamide (CCD ID: TK0) (formula: C₃₇H₃₄N₆O₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			47	37	6	2	2		
2	B	1	Total	C	N	O	S	0	0
			47	37	6	2	2		
2	C	1	Total	C	N	O	S	0	0
			47	37	6	2	2		
2	D	1	Total	C	N	O	S	0	0
			47	37	6	2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

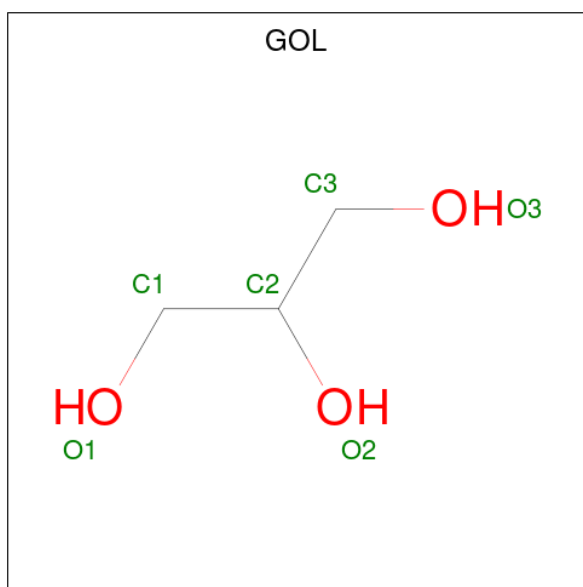


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

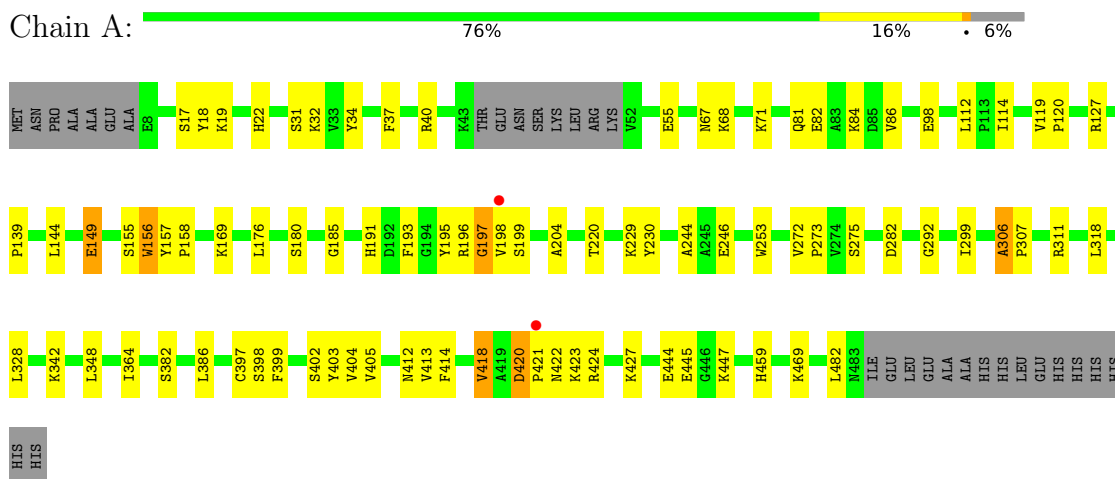
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	15	Total	O	0	0
			15	15		
6	C	8	Total	O	0	0
			8	8		
6	D	16	Total	O	0	0
			16	16		

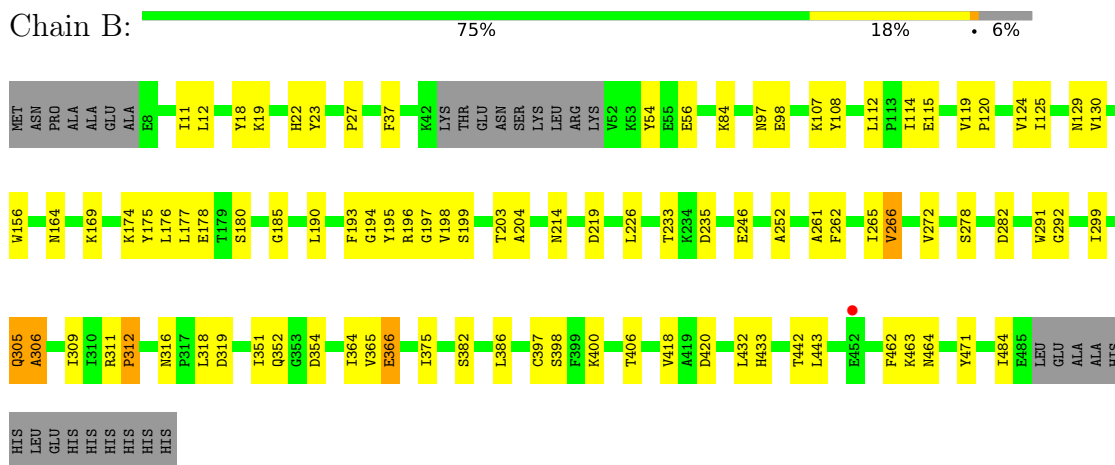
3 Residue-property plots

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: Nicotinamide phosphoribosyltransferase

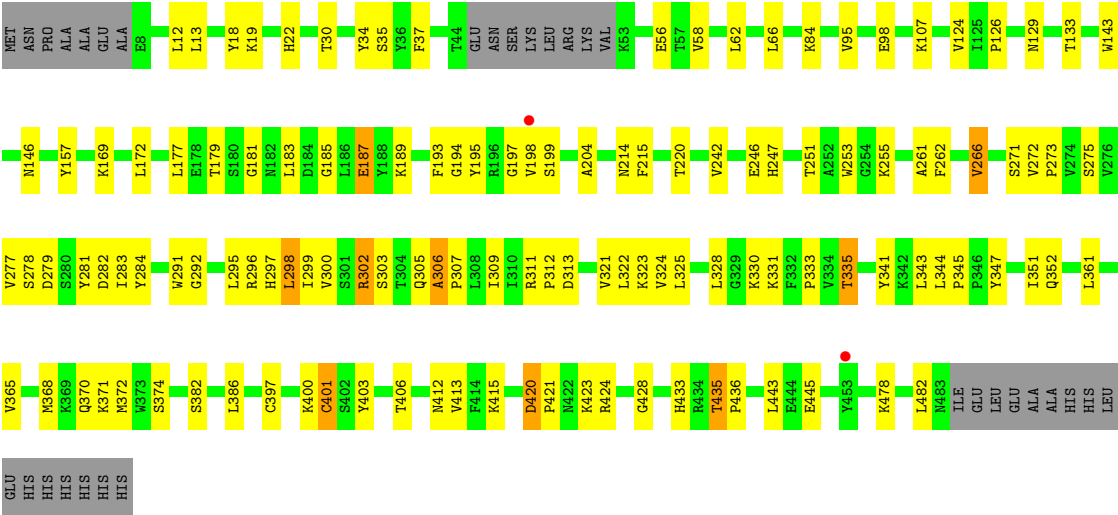


• Molecule 1: Nicotinamide phosphoribosyltransferase

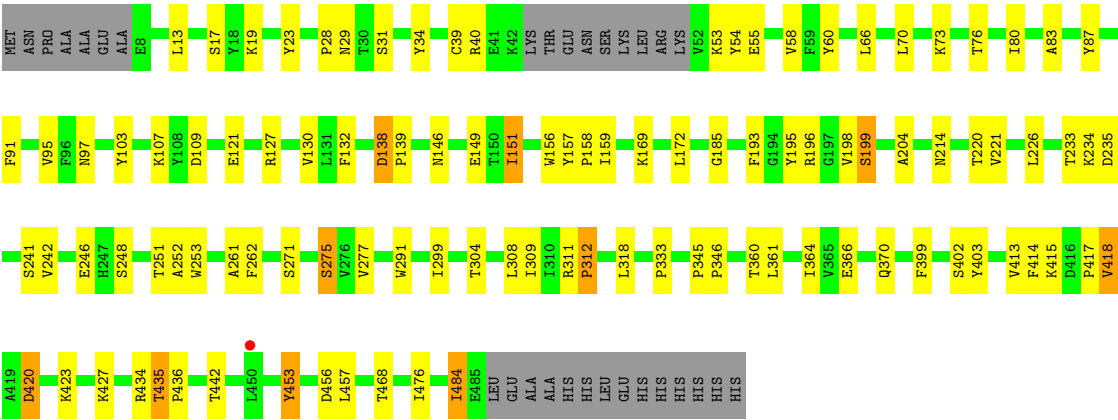


• Molecule 1: Nicotinamide phosphoribosyltransferase





● Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.99Å 94.42Å 246.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.09 – 2.75 20.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.09-2.75) 99.6 (20.09-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.75Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.194 , 0.238 0.197 , 0.237	Depositor DCC
R_{free} test set	2773 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15222	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: TK0, CL, GOL, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/3811	0.71	10/5168 (0.2%)
1	B	0.42	0/3826	0.72	7/5188 (0.1%)
1	C	0.43	1/3818 (0.0%)	0.76	13/5177 (0.3%)
1	D	0.43	0/3826	0.82	14/5188 (0.3%)
All	All	0.42	1/15281 (0.0%)	0.75	44/20721 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	275	SER	N-CA	-6.00	1.38	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	SER	N-CA-C	8.05	120.05	111.28
1	A	306	ALA	CA-C-N	7.41	127.86	120.52
1	A	306	ALA	C-N-CA	7.41	127.86	120.52
1	D	435	THR	CA-C-N	6.82	126.62	119.05
1	D	435	THR	C-N-CA	6.82	126.62	119.05
1	A	197	GLY	N-CA-C	6.81	120.90	112.73
1	B	306	ALA	CA-C-N	6.73	126.91	120.31
1	B	306	ALA	C-N-CA	6.73	126.91	120.31
1	C	107	LYS	N-CA-C	6.61	118.28	111.14
1	D	107	LYS	N-CA-C	6.59	118.54	111.36
1	D	453	TYR	N-CA-C	6.41	118.34	111.36
1	D	199	SER	N-CA-C	6.18	118.02	111.28
1	C	199	SER	N-CA-C	6.04	117.87	111.28
1	A	156	TRP	N-CA-C	-6.00	104.73	111.28
1	D	31	SER	N-CA-C	5.90	117.80	111.36
1	C	292	GLY	N-CA-C	5.77	120.16	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	420	ASP	CA-C-N	5.76	125.12	118.85
1	D	420	ASP	C-N-CA	5.76	125.12	118.85
1	D	53	LYS	N-CA-C	5.75	117.55	111.28
1	D	138	ASP	CA-C-N	5.74	125.42	119.05
1	D	138	ASP	C-N-CA	5.74	125.42	119.05
1	C	420	ASP	CA-C-N	5.58	124.93	118.85
1	C	420	ASP	C-N-CA	5.58	124.93	118.85
1	C	435	THR	CA-C-N	5.56	125.22	119.05
1	C	435	THR	C-N-CA	5.56	125.22	119.05
1	A	299	ILE	N-CA-C	5.43	116.16	110.62
1	B	197	GLY	N-CA-C	5.41	119.22	112.73
1	C	306	ALA	CA-C-N	5.40	125.60	120.31
1	C	306	ALA	C-N-CA	5.40	125.60	120.31
1	B	292	GLY	N-CA-C	5.39	119.67	112.77
1	B	420	ASP	CA-C-N	5.35	124.68	118.85
1	B	420	ASP	C-N-CA	5.35	124.68	118.85
1	A	420	ASP	CA-C-N	5.31	124.64	118.85
1	A	420	ASP	C-N-CA	5.31	124.64	118.85
1	C	266	VAL	N-CA-C	5.27	116.04	110.72
1	C	194	GLY	N-CA-C	5.18	123.98	115.34
1	D	271	SER	N-CA-C	5.17	119.27	112.92
1	A	40	ARG	N-CA-C	5.15	117.70	110.23
1	A	292	GLY	N-CA-C	5.15	119.36	112.77
1	B	194	GLY	N-CA-C	5.12	123.89	115.34
1	C	302	ARG	N-CA-C	5.10	117.62	110.23
1	D	468	THR	N-CA-C	5.09	116.91	111.36
1	D	40	ARG	N-CA-C	5.04	117.73	110.28
1	A	229	LYS	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3723	0	3677	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3738	0	3696	71	0
1	C	3730	0	3683	115	0
1	D	3738	0	3696	88	0
2	A	47	0	0	4	0
2	B	47	0	0	2	0
2	C	47	0	0	9	0
2	D	47	0	0	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	2	0	0	2	0
4	C	1	0	0	1	0
5	A	6	0	8	0	0
5	D	12	0	16	1	0
6	A	25	0	0	1	0
6	B	15	0	0	1	0
6	C	8	0	0	1	0
6	D	16	0	0	1	0
All	All	15222	0	14776	319	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 11.

All (319) 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:D:151:ILE:H	1:D:151:ILE:HD12	1.28	0.97
1:D:484:ILE:H	1:D:484:ILE:HD12	1.30	0.94
1:C:187:GLU:O	1:C:215:PHE:HD2	1.51	0.92
1:B:198:VAL:HG21	1:B:204:ALA:HB2	1.53	0.90
1:C:420:ASP:OD2	1:C:423:LYS:HG3	1.71	0.90
1:B:305:GLN:N	1:B:305:GLN:OE1	2.09	0.85
1:C:262:PHE:CD2	1:C:291:TRP:CZ2	2.67	0.81
1:A:420:ASP:OD2	1:A:423:LYS:HG3	1.80	0.81
1:C:413:VAL:HG11	1:D:252:ALA:HA	1.61	0.81
1:C:187:GLU:O	1:C:215:PHE:CD2	2.33	0.81
1:D:333:PRO:O	1:D:345:PRO:HD3	1.82	0.79
1:C:291:TRP:HE3	1:C:299:ILE:HD11	1.49	0.78
1:C:335:THR:HG23	1:C:343:LEU:HB3	1.67	0.76
1:C:478:LYS:O	1:C:478:LYS:HD3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:O	1:B:266:VAL:HG22	1.85	0.76
4:A:504:CL:CL	1:B:311:ARG:NH2	2.56	0.76
1:D:151:ILE:HD12	1:D:151:ILE:N	2.02	0.75
1:D:193:PHE:CZ	2:D:501:TK0:C25	2.69	0.75
1:C:187:GLU:H	1:C:187:GLU:CD	1.96	0.74
1:D:138:ASP:OD1	1:D:139:PRO:HD2	1.87	0.74
1:D:484:ILE:H	1:D:484:ILE:CD1	2.02	0.73
1:D:484:ILE:HD12	1:D:484:ILE:N	2.03	0.73
1:A:19:LYS:HE3	1:A:149:GLU:HG2	1.71	0.72
1:C:295:LEU:O	1:C:299:ILE:HG13	1.89	0.72
1:A:81:GLN:HG3	1:C:282:ASP:OD2	1.90	0.71
1:C:284:TYR:CE1	1:C:323:LYS:HD2	2.26	0.70
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.26	0.70
1:B:272:VAL:C	1:B:306:ALA:HB1	2.16	0.70
1:D:151:ILE:H	1:D:151:ILE:CD1	2.04	0.70
1:A:414:PHE:CE2	1:A:427:LYS:HE3	2.26	0.70
1:C:246:GLU:OE2	1:D:146:ASN:ND2	2.20	0.70
1:A:149:GLU:HB2	1:A:399:PHE:CD1	2.27	0.69
1:C:433:HIS:CD2	1:C:443:LEU:HD23	2.27	0.69
1:D:291:TRP:CE3	1:D:299:ILE:HD11	2.28	0.69
1:C:433:HIS:HD2	1:C:443:LEU:HD23	1.57	0.68
1:B:226:LEU:C	1:B:226:LEU:HD23	2.18	0.68
1:C:478:LYS:HD3	1:C:478:LYS:C	2.18	0.68
1:C:242:VAL:HG22	2:C:501:TK0:C21	2.23	0.68
1:D:435:THR:HB	1:D:436:PRO:HD2	1.76	0.67
1:D:23:TYR:CE1	1:D:97:ASN:HB2	2.29	0.67
1:C:296:ARG:O	1:C:300:VAL:HG23	1.95	0.67
1:B:176:LEU:O	1:B:180:SER:HB3	1.94	0.67
1:A:193:PHE:CE2	2:A:501:TK0:C26	2.78	0.67
1:D:34:TYR:HB3	1:D:403:TYR:HB3	1.76	0.67
1:B:107:LYS:HD3	1:B:108:TYR:CZ	2.31	0.65
1:C:187:GLU:N	1:C:187:GLU:OE1	2.30	0.65
1:C:198:VAL:HG21	1:C:204:ALA:HB2	1.79	0.65
1:D:55:GLU:H	1:D:55:GLU:CD	2.05	0.65
1:B:130:VAL:H	1:B:442:THR:HG21	1.61	0.64
1:C:262:PHE:HD2	1:C:291:TRP:CZ2	2.14	0.64
1:A:413:VAL:HG11	1:B:252:ALA:HA	1.78	0.64
1:D:198:VAL:HG21	1:D:204:ALA:HB2	1.78	0.64
1:D:435:THR:HG22	1:D:453:TYR:CE2	2.33	0.64
1:A:193:PHE:CZ	2:A:501:TK0:C26	2.80	0.64
1:C:172:LEU:HD13	1:C:189:LYS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD23	1:B:226:LEU:O	1.99	0.63
1:C:253:TRP:CG	1:C:261:ALA:HB2	2.32	0.63
1:C:37:PHE:CZ	1:C:397:CYS:HB3	2.34	0.63
1:A:19:LYS:CE	1:A:149:GLU:HG2	2.28	0.62
1:A:196:ARG:HG2	6:A:611:HOH:O	1.97	0.62
1:C:193:PHE:CZ	2:C:501:TK0:C25	2.83	0.62
1:A:19:LYS:HE3	1:A:149:GLU:CG	2.30	0.61
1:B:174:LYS:O	1:B:178:GLU:HG3	2.01	0.61
1:C:321:VAL:HG23	1:C:352:GLN:HE21	1.66	0.61
1:D:66:LEU:HD23	1:D:70:LEU:HD12	1.83	0.61
1:C:291:TRP:CE3	1:C:299:ILE:HD11	2.33	0.61
1:C:322:LEU:HD22	1:C:371:LYS:HD2	1.83	0.61
1:C:341:TYR:CD1	1:C:372:MET:HA	2.36	0.61
1:D:253:TRP:CG	1:D:261:ALA:HB2	2.36	0.61
1:C:413:VAL:HG12	1:D:251:THR:O	2.01	0.60
1:A:197:GLY:O	1:B:156:TRP:CZ2	2.55	0.60
1:D:291:TRP:HE3	1:D:299:ILE:HD11	1.67	0.59
1:A:17:SER:HB2	1:B:219:ASP:CG	2.27	0.59
1:D:414:PHE:HB3	1:D:427:LYS:HG2	1.85	0.59
1:A:19:LYS:NZ	1:A:149:GLU:HG2	2.17	0.59
1:C:185:GLY:HA3	2:C:501:TK0:C09	2.33	0.59
1:C:307:PRO:HG3	2:C:501:TK0:C38	2.32	0.59
1:D:275:SER:HB2	1:D:309:ILE:HB	1.85	0.59
1:C:282:ASP:HA	1:D:418:VAL:HG12	1.84	0.58
1:D:103:TYR:CE2	1:D:138:ASP:OD2	2.56	0.58
1:D:55:GLU:OE2	1:D:55:GLU:N	2.20	0.58
1:D:435:THR:HG22	1:D:453:TYR:HE2	1.68	0.58
1:A:112:LEU:HD22	1:A:144:LEU:HD21	1.85	0.58
1:B:107:LYS:HD3	1:B:108:TYR:CE2	2.39	0.58
1:C:283:ILE:CD1	1:C:312:PRO:HB3	2.34	0.58
1:B:11:ILE:HG23	1:B:12:LEU:HD12	1.85	0.58
1:C:273:PRO:HG3	1:C:306:ALA:HA	1.86	0.57
1:C:157:TYR:CG	1:D:199:SER:HB2	2.40	0.57
1:C:330:LYS:HG2	1:C:331:LYS:HE2	1.87	0.57
1:C:187:GLU:O	1:C:215:PHE:HB3	2.05	0.57
1:D:304:THR:HG23	1:D:346:PRO:HB2	1.87	0.57
1:C:177:LEU:O	1:C:181:GLY:N	2.38	0.57
1:A:418:VAL:HG12	1:B:282:ASP:HA	1.87	0.56
1:C:197:GLY:O	1:D:156:TRP:CZ2	2.58	0.56
1:D:60:TYR:O	1:D:158:PRO:HB2	2.05	0.56
1:C:197:GLY:O	1:D:156:TRP:HZ2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LYS:HG2	1:D:417:PRO:HD3	1.86	0.56
1:D:435:THR:HB	1:D:436:PRO:CD	2.34	0.56
1:C:277:VAL:HA	1:C:311:ARG:HB3	1.88	0.56
1:C:34:TYR:HB3	1:C:403:TYR:HB3	1.87	0.56
1:D:456:ASP:OD1	1:D:457:LEU:N	2.39	0.56
1:B:177:LEU:HD22	1:B:484:ILE:HD11	1.87	0.55
1:C:361:LEU:O	1:C:365:VAL:HG22	2.06	0.55
1:B:261:ALA:O	1:B:265:ILE:HG13	2.06	0.55
1:D:434:ARG:HB2	1:D:434:ARG:NH2	2.21	0.55
1:A:185:GLY:HA3	2:A:501:TK0:C09	2.37	0.55
1:C:335:THR:HG21	1:C:343:LEU:HD22	1.87	0.55
1:B:193:PHE:CZ	2:B:501:TK0:C25	2.90	0.54
1:C:247:HIS:NE2	1:D:415:LYS:HE3	2.23	0.54
1:A:199:SER:HB2	1:B:203:THR:OG1	2.07	0.54
1:D:226:LEU:HD23	1:D:226:LEU:C	2.33	0.54
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.43	0.54
1:D:103:TYR:HE2	1:D:138:ASP:OD2	1.90	0.54
1:B:318:LEU:HD13	1:B:364:ILE:HA	1.90	0.54
1:D:172:LEU:HD21	1:D:361:LEU:HD11	1.90	0.53
1:C:30:THR:OG1	1:C:406:THR:HG22	2.09	0.53
1:D:13:LEU:HD21	1:D:83:ALA:HA	1.91	0.53
1:A:198:VAL:HG21	1:A:204:ALA:HB2	1.90	0.53
1:D:149:GLU:HG3	1:D:399:PHE:CD1	2.44	0.53
1:C:262:PHE:CE2	1:C:291:TRP:CZ2	2.97	0.52
1:D:39:CYS:O	1:D:127:ARG:HG3	2.09	0.52
1:A:318:LEU:HD13	1:A:364:ILE:HA	1.90	0.52
1:C:169:LYS:HD2	1:C:214:ASN:HB3	1.91	0.52
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.90	0.52
1:B:27:PRO:HB2	1:B:406:THR:HG21	1.91	0.52
1:D:138:ASP:OD1	1:D:139:PRO:CD	2.55	0.52
1:D:193:PHE:CE2	2:D:501:TK0:C25	2.93	0.52
1:B:198:VAL:HG21	1:B:204:ALA:CB	2.33	0.51
1:B:84:LYS:CE	1:B:98:GLU:OE2	2.58	0.51
1:C:273:PRO:HB3	1:C:307:PRO:HD2	1.91	0.51
1:A:197:GLY:O	1:B:156:TRP:HZ2	1.93	0.51
1:A:55:GLU:O	1:A:127:ARG:HG2	2.10	0.51
1:B:12:LEU:HD12	1:B:12:LEU:N	2.25	0.51
1:C:56:GLU:HB2	1:C:124:VAL:HG12	1.93	0.51
1:A:328:LEU:HD13	1:A:348:LEU:HD21	1.93	0.51
1:B:398:SER:OG	1:B:400:LYS:NZ	2.43	0.51
1:C:335:THR:CG2	1:C:343:LEU:HD22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:SER:OG	1:D:242:VAL:N	2.44	0.51
1:A:84:LYS:HE2	1:A:98:GLU:OE1	2.10	0.51
1:A:311:ARG:NH2	4:A:503:CL:CL	2.75	0.51
1:B:119:VAL:HG21	1:B:125:ILE:HD11	1.92	0.51
1:A:272:VAL:C	1:A:306:ALA:HB1	2.37	0.50
1:C:400:LYS:HE2	1:C:415:LYS:HD3	1.93	0.50
4:C:503:CL:CL	1:D:311:ARG:NH2	2.81	0.50
1:C:242:VAL:CG2	2:C:501:TK0:C21	2.89	0.50
1:C:177:LEU:HD13	1:C:183:LEU:HG	1.91	0.50
1:C:415:LYS:O	1:C:424:ARG:HA	2.11	0.50
1:A:414:PHE:CD2	1:A:427:LYS:HG2	2.47	0.50
1:B:84:LYS:HE2	1:B:98:GLU:OE2	2.11	0.50
1:C:169:LYS:HG2	1:C:482:LEU:HD11	1.93	0.50
1:D:28:PRO:O	1:D:29:ASN:HB2	2.12	0.50
1:B:291:TRP:CE3	1:B:299:ILE:HD11	2.46	0.50
1:B:352:GLN:HE21	1:B:354:ASP:H	1.60	0.49
1:B:432:LEU:HD12	1:B:442:THR:HG22	1.93	0.49
1:C:300:VAL:HG13	1:C:347:TYR:CZ	2.47	0.49
1:C:382:SER:HB3	1:C:386:LEU:HB2	1.94	0.49
1:C:247:HIS:O	1:C:251:THR:HG23	2.12	0.49
1:D:234:LYS:NZ	6:D:602:HOH:O	2.45	0.49
1:C:95:VAL:HG22	1:C:95:VAL:O	2.12	0.49
1:A:412:ASN:ND2	1:A:445:GLU:HG2	2.28	0.49
1:C:18:TYR:OH	1:D:196:ARG:NH2	2.45	0.49
1:D:132:PHE:C	1:D:132:PHE:CD1	2.91	0.49
1:C:195:TYR:CG	1:C:220:THR:HG23	2.48	0.48
1:C:478:LYS:C	1:C:478:LYS:CD	2.86	0.48
1:A:18:TYR:CE2	1:B:246:GLU:HB3	2.48	0.48
1:C:19:LYS:HA	1:C:22:HIS:ND1	2.28	0.48
1:A:156:TRP:CD2	1:A:157:TYR:N	2.81	0.48
1:A:273:PRO:HG3	1:A:307:PRO:HD2	1.95	0.48
1:C:341:TYR:HD1	1:C:372:MET:HA	1.78	0.48
1:B:226:LEU:C	1:B:226:LEU:CD2	2.86	0.48
1:C:177:LEU:O	1:C:181:GLY:HA2	2.14	0.48
1:C:277:VAL:HG13	1:C:277:VAL:O	2.11	0.48
1:B:84:LYS:CE	1:B:98:GLU:CD	2.87	0.48
1:B:115:GLU:HA	1:B:462:PHE:O	2.14	0.48
1:C:253:TRP:CD1	1:C:261:ALA:HB2	2.49	0.48
1:C:272:VAL:C	1:C:306:ALA:HB1	2.38	0.47
1:C:297:HIS:CD2	1:C:298:LEU:HD12	2.49	0.47
1:C:305:GLN:HA	1:C:305:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:PHE:CD2	1:D:291:TRP:CZ2	3.02	0.47
1:A:246:GLU:HB3	1:B:18:TYR:CE2	2.48	0.47
1:C:335:THR:CG2	1:C:343:LEU:CD2	2.93	0.47
3:C:502:PO4:O2	5:D:503:GOL:H31	2.13	0.47
1:C:401:CYS:SG	1:C:413:VAL:HG21	2.54	0.47
1:B:365:VAL:HG12	1:B:375:ILE:HD12	1.97	0.47
1:A:67:ASN:O	1:A:71:LYS:HG2	2.14	0.47
1:A:149:GLU:HB2	1:A:399:PHE:CE1	2.49	0.47
1:A:282:ASP:HA	1:B:418:VAL:HG12	1.95	0.47
1:B:23:TYR:CE1	1:B:97:ASN:HB2	2.50	0.47
1:C:247:HIS:CD2	1:D:415:LYS:HE3	2.50	0.47
1:C:435:THR:HB	1:C:436:PRO:HD2	1.97	0.47
1:A:402:SER:HA	1:A:413:VAL:O	2.15	0.47
1:C:34:TYR:OH	1:C:133:THR:HG21	2.15	0.47
1:C:343:LEU:HD23	1:C:344:LEU:O	2.14	0.47
1:D:402:SER:HA	1:D:413:VAL:O	2.15	0.47
1:A:82:GLU:O	1:A:86:VAL:HG23	2.15	0.47
1:C:282:ASP:HA	1:D:418:VAL:CG1	2.45	0.47
1:A:382:SER:HB3	1:A:386:LEU:HB2	1.96	0.47
1:B:382:SER:HB3	1:B:386:LEU:HB2	1.98	0.46
1:D:19:LYS:NZ	1:D:149:GLU:OE1	2.37	0.46
1:A:253:TRP:CG	1:B:27:PRO:HG3	2.51	0.46
1:B:233:THR:HG23	1:B:235:ASP:O	2.15	0.46
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.50	0.46
1:A:253:TRP:CD2	1:B:27:PRO:HG3	2.50	0.46
1:C:193:PHE:CZ	2:C:501:TK0:C26	2.98	0.46
1:C:412:ASN:ND2	1:C:428:GLY:HA3	2.30	0.46
1:D:87:TYR:O	1:D:91:PHE:HB2	2.15	0.46
1:A:459:HIS:HD2	1:A:469:LYS:HE3	1.80	0.46
1:A:31:SER:HB2	1:A:139:PRO:HB3	1.97	0.46
1:B:185:GLY:HA3	2:B:501:TK0:C09	2.45	0.46
1:C:13:LEU:O	1:D:221:VAL:HG23	2.16	0.46
1:C:146:ASN:ND2	1:D:248:SER:CB	2.79	0.46
1:D:58:VAL:O	1:D:159:ILE:HG23	2.15	0.46
1:D:169:LYS:HD2	1:D:214:ASN:HB3	1.97	0.45
1:D:193:PHE:CZ	2:D:501:TK0:C26	2.99	0.45
1:B:311:ARG:HA	1:B:312:PRO:HD3	1.72	0.45
1:C:412:ASN:ND2	1:C:445:GLU:HG2	2.31	0.45
1:D:434:ARG:HB2	1:D:434:ARG:HH21	1.81	0.45
1:A:155:SER:C	1:A:158:PRO:HD2	2.42	0.45
1:A:195:TYR:CG	1:A:220:THR:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:THR:O	1:D:80:ILE:HG13	2.16	0.45
1:C:35:SER:HA	1:C:401:CYS:HA	1.99	0.45
1:C:37:PHE:HZ	1:C:397:CYS:HB3	1.80	0.45
1:C:193:PHE:CE2	2:C:501:TK0:C25	3.00	0.45
1:B:129:ASN:HA	1:B:442:THR:HG21	1.98	0.45
1:C:279:ASP:OD2	1:C:313:ASP:HB3	2.16	0.45
1:A:114:ILE:HG12	1:A:144:LEU:HD23	1.99	0.45
2:A:501:TK0:C31	1:B:18:TYR:CE1	2.99	0.45
1:D:311:ARG:HA	1:D:312:PRO:HD3	1.76	0.45
1:A:68:LYS:HB2	1:A:230:TYR:CE1	2.52	0.45
1:B:316:ASN:HB3	1:B:319:ASP:HB2	1.98	0.45
1:C:278:SER:O	1:C:283:ILE:HA	2.17	0.45
1:B:169:LYS:HD2	1:B:214:ASN:HB3	1.99	0.45
1:B:433:HIS:CD2	1:B:443:LEU:HD12	2.51	0.45
1:C:309:ILE:HG22	1:C:351:ILE:HG22	1.98	0.45
1:A:156:TRP:CG	1:A:157:TYR:N	2.84	0.44
1:C:341:TYR:HB2	1:C:374:SER:HB2	1.99	0.44
1:A:176:LEU:O	1:A:180:SER:HB3	2.16	0.44
1:B:195:TYR:CD1	1:B:204:ALA:HB1	2.52	0.44
1:D:157:TYR:HB3	1:D:158:PRO:HD3	1.99	0.44
1:B:291:TRP:HE3	1:B:299:ILE:HD11	1.81	0.44
1:D:23:TYR:CD1	1:D:97:ASN:HB2	2.53	0.44
1:C:420:ASP:HA	1:C:421:PRO:HD3	1.84	0.44
1:D:121:GLU:O	1:D:476:ILE:HG12	2.17	0.44
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.53	0.44
1:C:179:THR:HB	1:C:374:SER:HA	2.00	0.44
1:A:404:VAL:HG11	1:B:252:ALA:HB1	2.00	0.44
1:B:309:ILE:HG22	1:B:351:ILE:HG22	2.00	0.44
1:C:412:ASN:HD22	1:C:445:GLU:HG2	1.82	0.44
1:C:370:GLN:NE2	6:C:603:HOH:O	2.49	0.43
1:D:54:TYR:O	1:D:127:ARG:NH1	2.51	0.43
1:A:422:ASN:C	1:A:424:ARG:H	2.26	0.43
1:C:172:LEU:HD13	1:C:189:LYS:CB	2.48	0.43
1:C:333:PRO:O	1:C:345:PRO:HD3	2.18	0.43
1:D:318:LEU:HD12	1:D:318:LEU:O	2.18	0.43
1:D:233:THR:HG23	1:D:235:ASP:O	2.18	0.43
1:A:253:TRP:CD1	1:A:253:TRP:N	2.85	0.43
1:C:62:LEU:O	1:C:66:LEU:HG	2.18	0.43
1:A:18:TYR:OH	1:B:196:ARG:NH2	2.47	0.43
1:A:155:SER:O	1:A:158:PRO:HG2	2.18	0.43
1:A:253:TRP:CD1	1:A:253:TRP:H	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TRP:CD1	1:C:143:TRP:H	2.36	0.43
1:B:84:LYS:HE2	1:B:98:GLU:CD	2.43	0.43
1:C:187:GLU:O	1:C:215:PHE:CB	2.67	0.43
1:A:191:HIS:CD2	1:A:193:PHE:HE1	2.36	0.43
1:B:112:LEU:O	1:B:464:ASN:HA	2.19	0.43
1:A:119:VAL:HG12	1:A:120:PRO:HD2	2.00	0.42
1:A:444:GLU:O	1:A:447:LYS:HG3	2.18	0.42
1:C:84:LYS:NZ	1:C:98:GLU:OE1	2.52	0.42
1:C:325:LEU:HD11	1:C:368:MET:HE3	2.00	0.42
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.86	0.42
1:D:157:TYR:HB3	1:D:158:PRO:CD	2.49	0.42
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.76	0.42
1:B:54:TYR:OH	1:B:164:ASN:OD1	2.25	0.42
1:C:324:VAL:O	1:C:328:LEU:HG	2.20	0.42
1:D:185:GLY:HA3	2:D:501:TK0:C09	2.50	0.42
1:B:12:LEU:N	1:B:12:LEU:CD1	2.83	0.42
1:C:242:VAL:HG21	2:C:501:TK0:C17	2.49	0.42
1:C:266:VAL:HG23	1:C:302:ARG:NH2	2.35	0.42
1:B:114:ILE:O	1:B:463:LYS:HA	2.20	0.42
1:C:12:LEU:HD12	1:C:12:LEU:N	2.35	0.42
1:C:126:PRO:O	1:C:129:ASN:ND2	2.38	0.42
1:C:413:VAL:CG1	1:D:251:THR:O	2.67	0.42
1:D:17:SER:O	1:D:91:PHE:HZ	2.03	0.42
1:D:420:ASP:OD2	1:D:423:LYS:HG3	2.20	0.42
1:A:32:LYS:HB3	1:A:405:VAL:HB	2.02	0.41
1:A:195:TYR:CD1	1:A:220:THR:HG23	2.55	0.41
1:A:459:HIS:CD2	1:A:469:LYS:HE3	2.55	0.41
1:D:195:TYR:CD1	1:D:220:THR:HG23	2.55	0.41
1:A:195:TYR:CD1	1:A:204:ALA:HB1	2.55	0.41
1:D:130:VAL:HG12	1:D:442:THR:CG2	2.50	0.41
1:D:360:THR:O	1:D:364:ILE:HG13	2.20	0.41
1:C:177:LEU:O	1:C:181:GLY:CA	2.69	0.41
1:C:255:LYS:HA	1:C:281:TYR:CZ	2.55	0.41
1:D:277:VAL:O	1:D:277:VAL:HG13	2.20	0.41
1:A:84:LYS:HE2	1:A:98:GLU:CD	2.45	0.41
1:A:342:LYS:HE2	1:A:342:LYS:HB2	1.70	0.41
1:A:398:SER:HB2	3:A:502:PO4:O4	2.21	0.41
1:B:278:SER:HA	6:B:603:HOH:O	2.21	0.41
1:A:156:TRP:CD2	1:A:156:TRP:C	2.98	0.41
1:A:169:LYS:HG2	1:A:482:LEU:HD11	2.01	0.41
1:C:18:TYR:CE2	1:D:246:GLU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:TYR:CZ	1:D:97:ASN:HB2	2.56	0.41
1:B:120:PRO:HB3	1:B:471:TYR:CE2	2.56	0.41
1:D:73:LYS:HG3	1:D:109:ASP:O	2.21	0.41
1:D:366:GLU:O	1:D:370:GLN:HG3	2.20	0.41
1:A:244:ALA:CB	1:A:275:SER:HB3	2.50	0.41
1:D:55:GLU:CD	1:D:55:GLU:N	2.76	0.41
1:A:420:ASP:HA	1:A:421:PRO:HD3	1.86	0.40
1:B:56:GLU:HB2	1:B:124:VAL:HG12	2.03	0.40
1:B:84:LYS:HE3	1:B:98:GLU:OE1	2.20	0.40
1:C:193:PHE:CE2	2:C:501:TK0:C28	3.04	0.40
1:D:23:TYR:OH	1:D:95:VAL:O	2.36	0.40
1:A:156:TRP:CE3	1:A:157:TYR:HA	2.56	0.40
1:B:175:TYR:OH	1:B:366:GLU:HG2	2.21	0.40
1:C:195:TYR:CD2	1:C:220:THR:HG23	2.56	0.40
1:C:255:LYS:HA	1:C:281:TYR:CE2	2.56	0.40
1:D:130:VAL:HG12	1:D:442:THR:HG23	2.03	0.40
1:A:156:TRP:C	1:A:156:TRP:CE3	3.00	0.40
1:A:253:TRP:CD1	1:B:27:PRO:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/499 (93%)	458 (99%)	6 (1%)	0	100	100
1	B	465/499 (93%)	457 (98%)	7 (2%)	1 (0%)	43	64
1	C	464/499 (93%)	461 (99%)	3 (1%)	0	100	100
1	D	465/499 (93%)	457 (98%)	7 (2%)	1 (0%)	43	64
All	All	1858/1996 (93%)	1833 (99%)	23 (1%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	PRO
1	D	312	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/438 (93%)	404 (100%)	2 (0%)	81	89
1	B	409/438 (93%)	405 (99%)	4 (1%)	68	81
1	C	408/438 (93%)	402 (98%)	6 (2%)	57	74
1	D	409/438 (93%)	404 (99%)	5 (1%)	63	78
All	All	1632/1752 (93%)	1615 (99%)	17 (1%)	68	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	GLU
1	A	418	VAL
1	B	199	SER
1	B	266	VAL
1	B	305	GLN
1	B	366	GLU
1	C	58	VAL
1	C	187	GLU
1	C	298	LEU
1	C	303	SER
1	C	335	THR
1	C	401	CYS
1	D	151	ILE
1	D	275	SER
1	D	308	LEU
1	D	418	VAL
1	D	484	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	214	ASN
1	A	412	ASN
1	B	22	HIS
1	B	154	GLN
1	B	396	ASN
1	C	214	ASN
1	C	305	GLN
1	C	396	ASN
1	D	297	HIS
1	D	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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	PO4	A	502	-	4,4,4	0.90	0	6,6,6	0.42	0
2	TK0	B	501	-	53,53,53	1.44	7 (13%)	69,73,73	2.31	24 (34%)
2	TK0	A	501	-	53,53,53	1.81	12 (22%)	69,73,73	2.33	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	502	-	4,4,4	0.83	0	6,6,6	0.87	0
5	GOL	D	504	-	5,5,5	1.20	0	5,5,5	0.92	0
5	GOL	D	503	-	5,5,5	0.91	0	5,5,5	1.07	1 (20%)
2	TK0	C	501	-	53,53,53	2.00	16 (30%)	69,73,73	2.40	22 (31%)
3	PO4	D	502	-	4,4,4	0.79	0	6,6,6	0.54	0
2	TK0	D	501	-	53,53,53	1.71	13 (24%)	69,73,73	2.32	25 (36%)
5	GOL	A	505	-	5,5,5	1.25	0	5,5,5	0.98	0
3	PO4	B	502	-	4,4,4	0.84	0	6,6,6	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TK0	B	501	-	-	5/28/38/38	0/7/7/7
2	TK0	A	501	-	-	9/28/38/38	0/7/7/7
5	GOL	D	503	-	-	0/4/4/4	-
2	TK0	C	501	-	-	13/28/38/38	0/7/7/7
2	TK0	D	501	-	-	5/28/38/38	0/7/7/7
5	GOL	A	505	-	-	4/4/4/4	-
5	GOL	D	504	-	-	4/4/4/4	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	TK0	C24-N23	4.98	1.44	1.34
2	A	501	TK0	C24-N23	4.50	1.43	1.34
2	A	501	TK0	C07-N04	4.47	1.48	1.37
2	C	501	TK0	C07-N04	4.39	1.48	1.37
2	D	501	TK0	C24-N23	4.30	1.43	1.34
2	D	501	TK0	C07-N04	4.09	1.47	1.37
2	B	501	TK0	C07-N04	3.81	1.47	1.37
2	C	501	TK0	C03-C02	3.74	1.59	1.53
2	A	501	TK0	C03-C02	3.67	1.59	1.53
2	B	501	TK0	C24-N23	3.57	1.41	1.34
2	C	501	TK0	C35-N37	3.27	1.41	1.33
2	C	501	TK0	C38-C39	3.15	1.58	1.51
2	A	501	TK0	C03-N04	3.08	1.52	1.46
2	C	501	TK0	C15-C14	3.05	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TK0	C35-N37	2.92	1.40	1.33
2	C	501	TK0	C12-C07	2.91	1.46	1.42
2	A	501	TK0	C09-N08	2.90	1.39	1.33
2	C	501	TK0	C03-N04	2.90	1.51	1.46
2	B	501	TK0	C38-C39	2.90	1.57	1.51
2	D	501	TK0	C09-N08	2.85	1.39	1.33
2	C	501	TK0	C05-N04	2.78	1.51	1.46
2	D	501	TK0	C35-N37	2.75	1.40	1.33
2	C	501	TK0	C09-N08	2.74	1.38	1.33
2	D	501	TK0	C15-C14	2.72	1.52	1.47
2	D	501	TK0	C11-S34	2.65	1.78	1.74
2	D	501	TK0	C17-C16	2.63	1.43	1.38
2	A	501	TK0	C05-N04	2.62	1.51	1.46
2	C	501	TK0	C20-C19	2.61	1.43	1.38
2	B	501	TK0	C35-N37	2.55	1.39	1.33
2	A	501	TK0	C20-C19	2.52	1.42	1.38
2	D	501	TK0	C38-C39	2.50	1.57	1.51
2	A	501	TK0	C15-C14	2.46	1.52	1.47
2	B	501	TK0	C17-C16	2.45	1.42	1.38
2	B	501	TK0	C12-C11	-2.42	1.38	1.41
2	A	501	TK0	C38-C39	2.41	1.56	1.51
2	B	501	TK0	C09-N08	2.40	1.38	1.33
2	C	501	TK0	C02-C35	2.37	1.55	1.51
2	A	501	TK0	C12-C07	2.37	1.46	1.42
2	C	501	TK0	C11-S34	2.25	1.78	1.74
2	C	501	TK0	C17-C16	2.23	1.42	1.38
2	D	501	TK0	C05-N04	2.15	1.50	1.46
2	D	501	TK0	C03-C02	2.14	1.56	1.53
2	D	501	TK0	C12-C07	2.13	1.45	1.42
2	C	501	TK0	C38-N37	2.13	1.50	1.46
2	D	501	TK0	C14-S34	2.12	1.80	1.75
2	D	501	TK0	C16-C15	2.12	1.42	1.39
2	A	501	TK0	C11-S34	2.09	1.77	1.74
2	C	501	TK0	C25-C24	2.01	1.52	1.48

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	TK0	C02-C35-N37	9.12	127.66	115.99
2	B	501	TK0	C02-C35-N37	8.86	127.32	115.99
2	A	501	TK0	C02-C35-N37	8.61	127.01	115.99
2	D	501	TK0	C02-C35-N37	7.60	125.71	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	TK0	C12-C11-S34	-5.38	108.82	111.56
2	D	501	TK0	C38-N37-C35	5.37	129.67	122.29
2	C	501	TK0	C20-C15-C16	-5.33	111.78	118.57
2	D	501	TK0	C20-C15-C16	-5.32	111.80	118.57
2	B	501	TK0	C20-C15-C16	-5.27	111.86	118.57
2	A	501	TK0	C20-C15-C16	-5.25	111.89	118.57
2	B	501	TK0	C12-C11-S34	-5.20	108.91	111.56
2	A	501	TK0	C12-C11-S34	-5.13	108.95	111.56
2	C	501	TK0	C12-C11-S34	-5.08	108.97	111.56
2	C	501	TK0	C25-C24-N23	4.79	125.58	115.07
2	A	501	TK0	C25-C24-N23	4.77	125.52	115.07
2	D	501	TK0	C25-C24-N23	4.53	125.00	115.07
2	A	501	TK0	C38-N37-C35	4.33	128.24	122.29
2	C	501	TK0	C38-N37-C35	4.22	128.08	122.29
2	C	501	TK0	O36-C35-C02	-3.96	116.07	122.19
2	D	501	TK0	C19-C20-C15	3.96	125.03	120.80
2	B	501	TK0	C38-N37-C35	3.95	127.71	122.29
2	B	501	TK0	C25-C24-N23	3.92	123.65	115.07
2	B	501	TK0	C19-C20-C15	3.88	124.94	120.80
2	A	501	TK0	O33-C24-N23	-3.80	116.33	122.29
2	C	501	TK0	C09-N08-C07	3.78	121.07	111.83
2	D	501	TK0	C13-C14-S34	-3.78	104.07	111.78
2	B	501	TK0	O36-C35-C02	-3.77	116.37	122.19
2	C	501	TK0	C13-C14-S34	-3.74	104.15	111.78
2	B	501	TK0	C13-C14-S34	-3.73	104.17	111.78
2	D	501	TK0	O33-C24-N23	-3.72	116.45	122.29
2	A	501	TK0	O36-C35-C02	-3.71	116.46	122.19
2	A	501	TK0	C09-N08-C07	3.70	120.86	111.83
2	C	501	TK0	O33-C24-N23	-3.68	116.51	122.29
2	A	501	TK0	C13-C14-S34	-3.66	104.31	111.78
2	B	501	TK0	O33-C24-N23	-3.58	116.67	122.29
2	D	501	TK0	C09-N08-C07	3.56	120.52	111.83
2	B	501	TK0	C09-N08-C07	3.55	120.51	111.83
2	C	501	TK0	C19-C20-C15	3.46	124.49	120.80
2	C	501	TK0	C32-C27-C28	-3.33	113.65	117.07
2	D	501	TK0	O36-C35-C02	-3.27	117.14	122.19
2	A	501	TK0	C19-C20-C15	3.21	124.22	120.80
2	C	501	TK0	O36-C35-N37	-3.17	116.27	122.98
2	B	501	TK0	O36-C35-N37	-3.16	116.30	122.98
2	A	501	TK0	C17-C16-C15	3.15	124.17	120.80
2	D	501	TK0	C32-C27-C28	-3.15	113.84	117.07
2	A	501	TK0	C12-C07-N08	-3.11	116.98	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	TK0	C12-C07-N08	-3.10	116.99	122.53
2	C	501	TK0	C19-C18-C17	-3.10	113.63	118.23
2	C	501	TK0	C17-C16-C15	3.07	124.08	120.80
2	B	501	TK0	C32-C27-C28	-3.07	113.92	117.07
2	A	501	TK0	O36-C35-N37	-3.05	116.53	122.98
2	A	501	TK0	C32-C27-C28	-3.00	113.99	117.07
2	D	501	TK0	C19-C18-C17	-2.97	113.82	118.23
2	B	501	TK0	C12-C07-N08	-2.97	117.24	122.53
2	D	501	TK0	C12-C07-N08	-2.92	117.32	122.53
2	B	501	TK0	C19-C18-C17	-2.92	113.89	118.23
2	A	501	TK0	C19-C18-C17	-2.90	113.92	118.23
2	D	501	TK0	C16-C15-C14	2.81	125.81	121.12
2	D	501	TK0	O36-C35-N37	-2.76	117.14	122.98
2	C	501	TK0	N10-C09-N08	-2.63	124.61	128.58
2	B	501	TK0	C16-C15-C14	2.58	125.43	121.12
2	B	501	TK0	N10-C09-N08	-2.55	124.72	128.58
2	D	501	TK0	C17-C16-C15	2.54	123.51	120.80
2	A	501	TK0	N10-C09-N08	-2.54	124.74	128.58
2	D	501	TK0	N10-C09-N08	-2.49	124.81	128.58
2	B	501	TK0	C17-C16-C15	2.49	123.46	120.80
2	B	501	TK0	C03-N04-C07	2.44	127.26	118.91
2	A	501	TK0	C20-C15-C14	2.41	125.14	121.12
2	B	501	TK0	C22-N23-C24	2.41	125.93	122.46
2	B	501	TK0	C01-C06-C05	2.37	113.87	110.75
2	D	501	TK0	C01-C06-C05	2.37	113.87	110.75
2	B	501	TK0	C44-C43-C45	-2.28	126.76	133.20
2	D	501	TK0	C44-C43-C45	-2.27	126.78	133.20
2	A	501	TK0	C44-C43-C45	-2.27	126.78	133.20
2	C	501	TK0	C22-C21-C18	2.26	117.94	112.83
2	D	501	TK0	C03-N04-C07	2.24	126.58	118.91
2	B	501	TK0	C22-C21-C18	2.23	117.87	112.83
2	D	501	TK0	C15-C14-S34	2.22	123.11	119.70
2	C	501	TK0	C44-C43-C45	-2.21	126.97	133.20
2	C	501	TK0	C15-C14-C13	2.19	134.26	128.43
2	D	501	TK0	C22-C21-C18	2.19	117.77	112.83
2	C	501	TK0	O33-C24-C25	-2.19	117.91	122.95
2	A	501	TK0	C22-C21-C18	2.19	117.76	112.83
2	A	501	TK0	C03-N04-C07	2.13	126.19	118.91
5	D	503	GOL	C3-C2-C1	-2.10	104.09	111.80
2	A	501	TK0	O33-C24-C25	-2.09	118.14	122.95
2	D	501	TK0	C22-N23-C24	2.06	125.42	122.46
2	B	501	TK0	C45-C46-S47	-2.06	109.67	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	TK0	C20-C15-C14	2.05	124.55	121.12
2	B	501	TK0	C42-S47-C46	2.04	95.41	91.37
2	D	501	TK0	C42-S47-C46	2.03	95.38	91.37
2	D	501	TK0	C45-C46-S47	-2.01	109.76	113.90
2	C	501	TK0	C45-C46-S47	-2.01	109.77	113.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TK0	C03-C02-C35-N37
2	B	501	TK0	C18-C21-C22-N23
2	C	501	TK0	C12-C07-N04-C03
2	C	501	TK0	N08-C07-N04-C03
2	C	501	TK0	C18-C21-C22-N23
2	D	501	TK0	C03-C02-C35-N37
2	D	501	TK0	C18-C21-C22-N23
2	D	501	TK0	N23-C24-C25-C26
5	A	505	GOL	O1-C1-C2-C3
5	D	504	GOL	O1-C1-C2-C3
5	D	504	GOL	C1-C2-C3-O3
2	C	501	TK0	C39-C38-N37-C35
2	A	501	TK0	C25-C26-C27-C28
2	A	501	TK0	C25-C26-C27-C32
2	A	501	TK0	N08-C07-N04-C03
2	D	501	TK0	O33-C24-C25-C26
2	B	501	TK0	N23-C24-C25-C26
2	C	501	TK0	N23-C24-C25-C26
2	A	501	TK0	C12-C07-N04-C03
5	A	505	GOL	O1-C1-C2-O2
2	C	501	TK0	O33-C24-C25-C26
2	B	501	TK0	C01-C02-C35-N37
2	A	501	TK0	O33-C24-C25-C26
2	B	501	TK0	O33-C24-C25-C26
2	A	501	TK0	N23-C24-C25-C26
2	C	501	TK0	C13-C14-C15-C16
2	A	501	TK0	C03-C02-C35-O36
5	A	505	GOL	C1-C2-C3-O3
2	C	501	TK0	S34-C14-C15-C20
2	C	501	TK0	C13-C14-C15-C20
5	D	504	GOL	O1-C1-C2-O2
5	D	504	GOL	O2-C2-C3-O3

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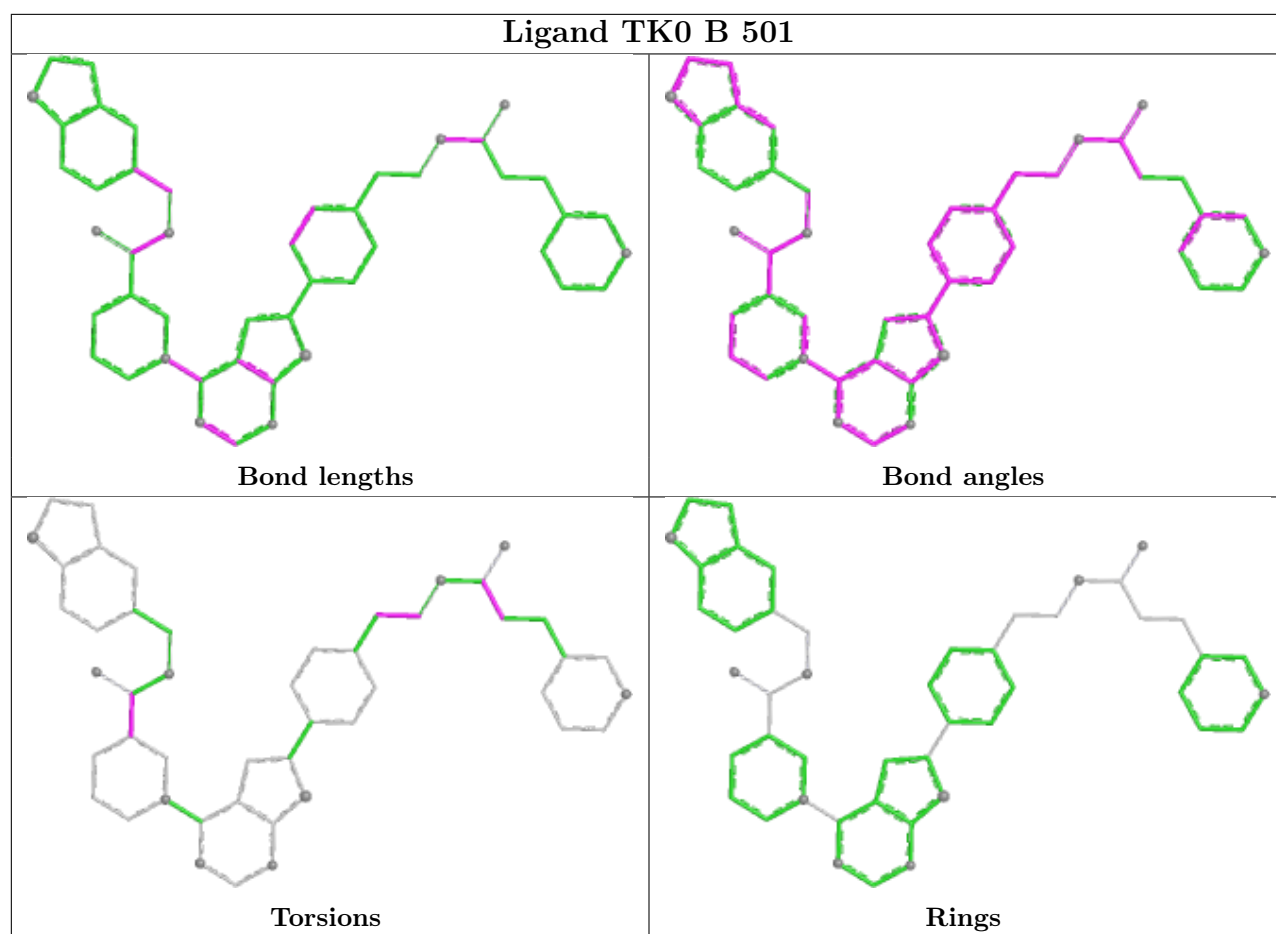
Mol	Chain	Res	Type	Atoms
2	D	501	TK0	C03-C02-C35-O36
2	B	501	TK0	C01-C02-C35-O36
2	C	501	TK0	S34-C14-C15-C16
5	A	505	GOL	O2-C2-C3-O3
2	C	501	TK0	C01-C02-C35-N37
2	C	501	TK0	C01-C02-C35-O36
2	A	501	TK0	C18-C21-C22-N23
2	C	501	TK0	C12-C07-N04-C05

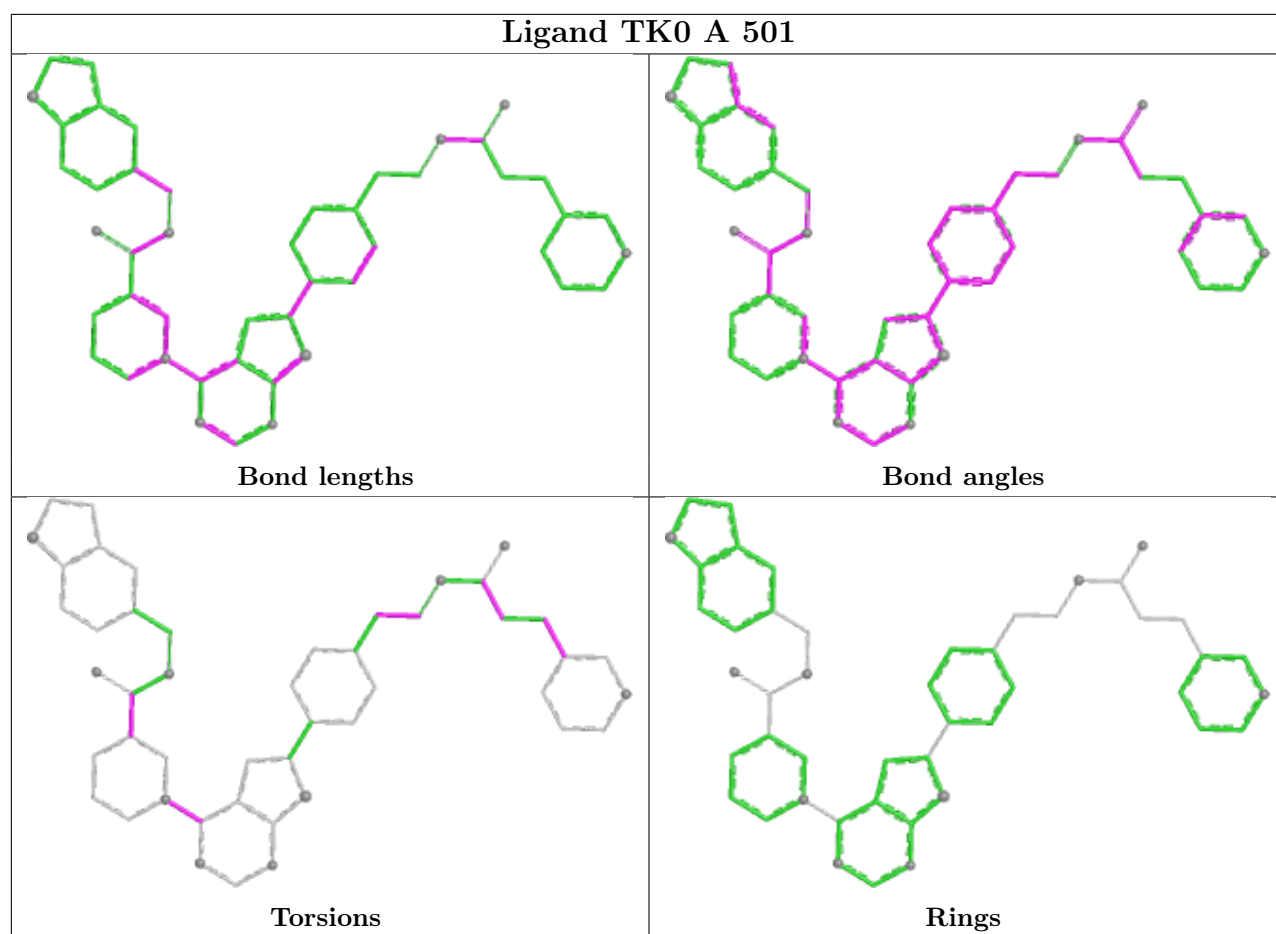
There are no ring outliers.

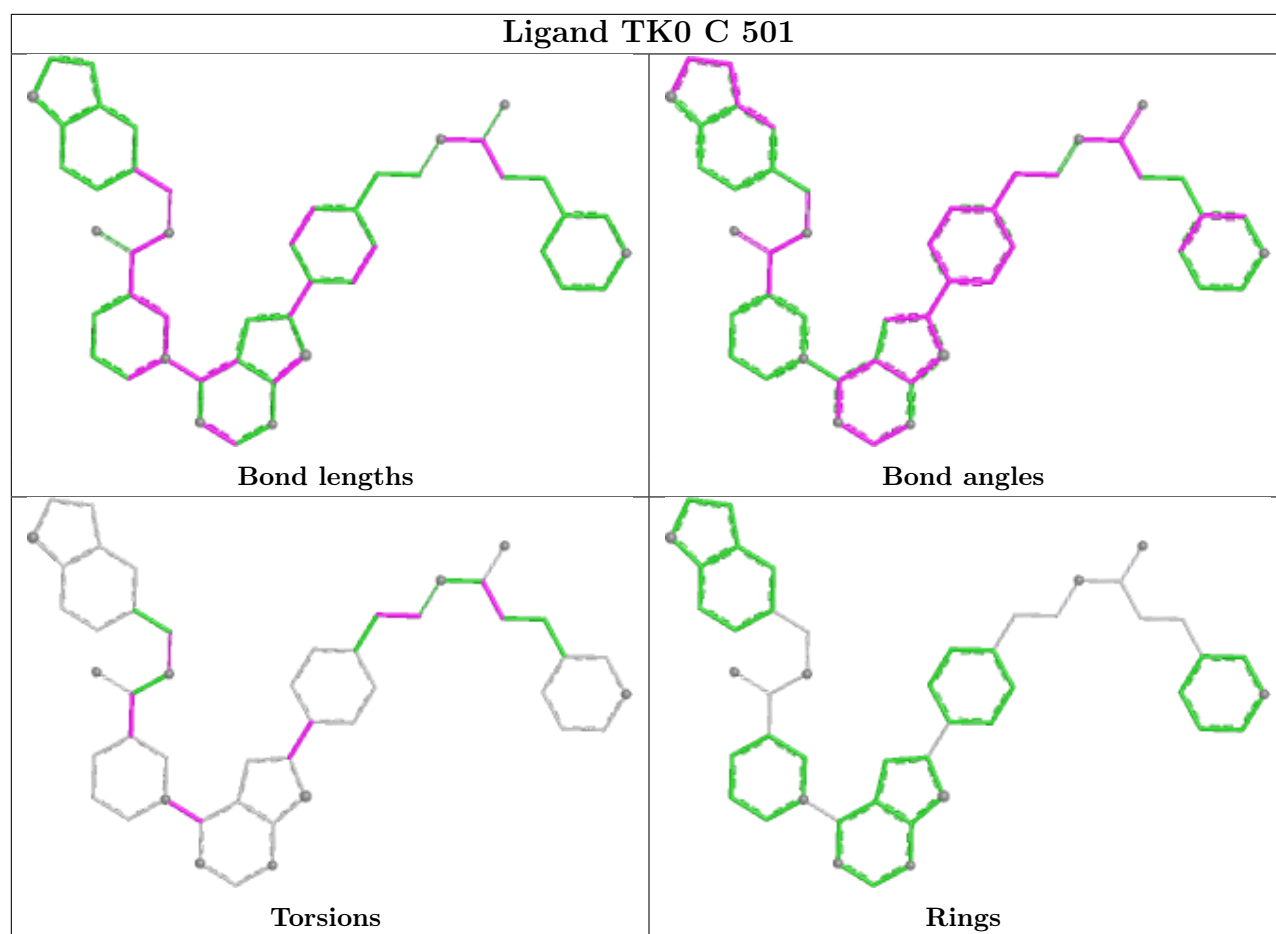
7 monomers are involved in 21 short contacts:

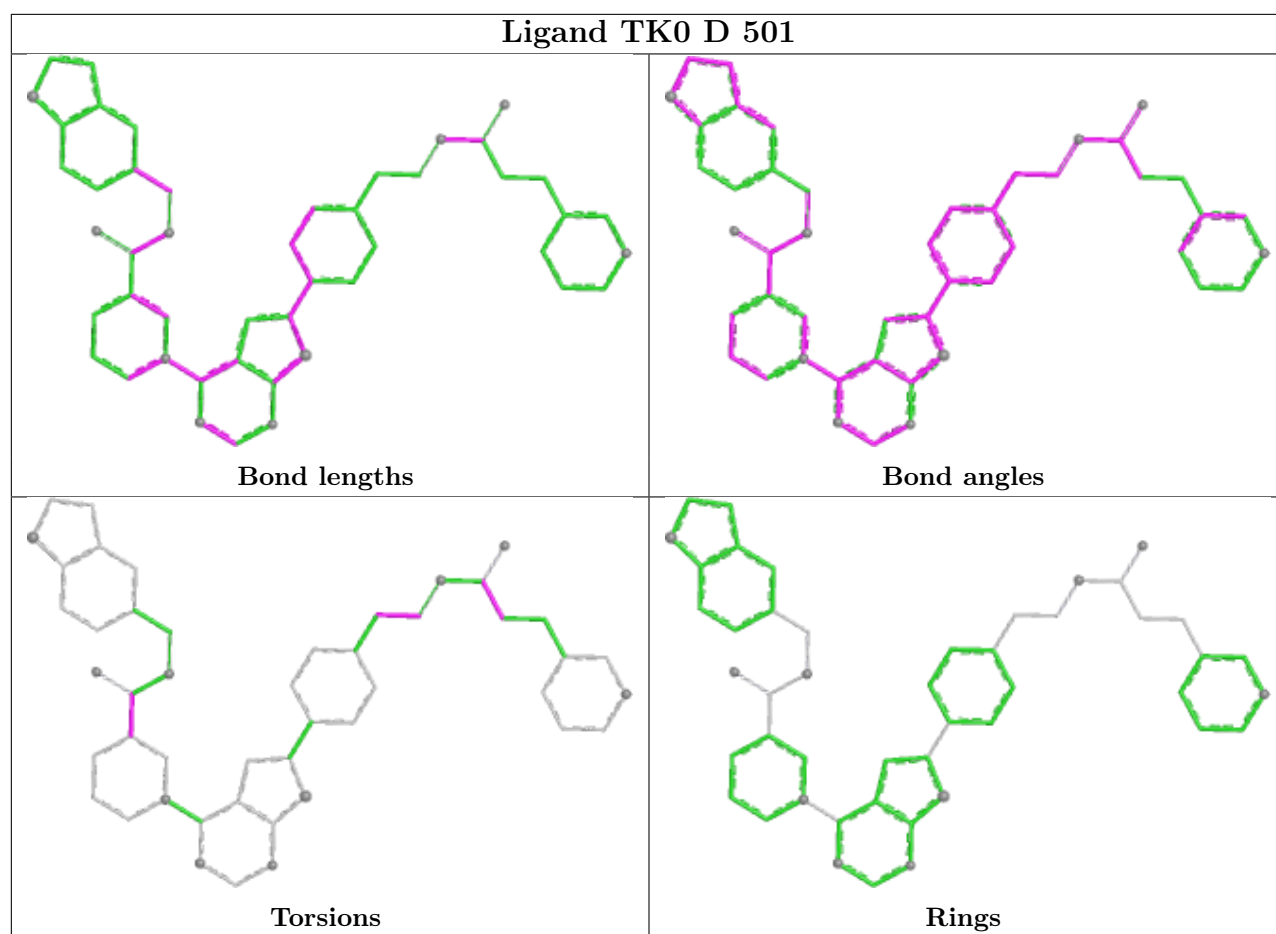
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PO4	1	0
2	B	501	TK0	2	0
2	A	501	TK0	4	0
3	C	502	PO4	1	0
5	D	503	GOL	1	0
2	C	501	TK0	9	0
2	D	501	TK0	4	0

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.









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	468/499 (93%)	-0.47	2 (0%) 88 89	36, 52, 73, 81	0
1	B	469/499 (93%)	-0.47	1 (0%) 91 92	39, 54, 71, 93	0
1	C	468/499 (93%)	-0.26	2 (0%) 88 89	46, 65, 86, 95	0
1	D	469/499 (93%)	-0.37	1 (0%) 91 92	44, 58, 80, 102	0
All	All	1874/1996 (93%)	-0.39	6 (0%) 90 91	36, 57, 81, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	450	LEU	2.7
1	C	453	TYR	2.4
1	A	421	PRO	2.3
1	A	198	VAL	2.2
1	B	452	GLU	2.1
1	C	198	VAL	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,

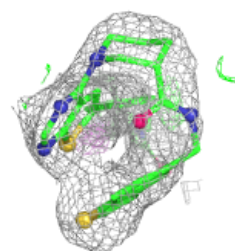
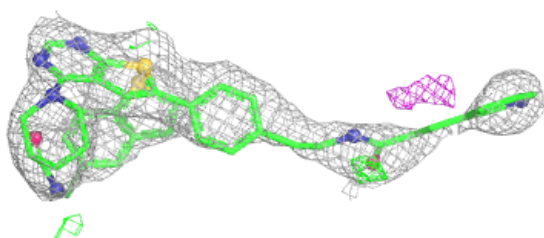
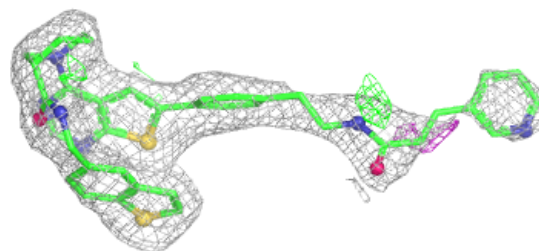
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	505	6/6	0.83	0.12	50,60,61,62	0
5	GOL	D	503	6/6	0.84	0.11	47,61,67,70	0
5	GOL	D	504	6/6	0.84	0.10	62,68,71,75	0
2	TK0	C	501	47/47	0.88	0.10	65,78,86,90	0
2	TK0	A	501	47/47	0.88	0.12	41,56,68,70	0
2	TK0	B	501	47/47	0.90	0.10	38,56,65,71	0
2	TK0	D	501	47/47	0.90	0.11	43,52,61,65	0
3	PO4	D	502	5/5	0.90	0.08	59,72,75,75	0
4	CL	A	504	1/1	0.92	0.10	60,60,60,60	0
3	PO4	C	502	5/5	0.94	0.07	61,65,67,71	0
3	PO4	A	502	5/5	0.94	0.07	58,64,65,68	0
4	CL	C	503	1/1	0.96	0.09	54,54,54,54	0
4	CL	A	503	1/1	0.98	0.06	57,57,57,57	0
3	PO4	B	502	5/5	0.98	0.07	41,46,53,55	0

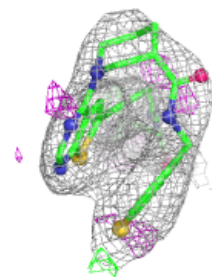
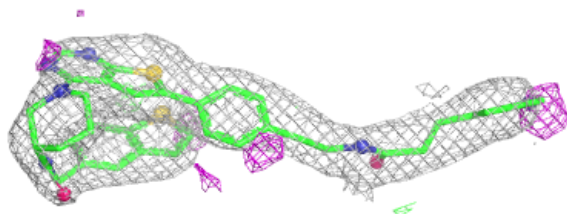
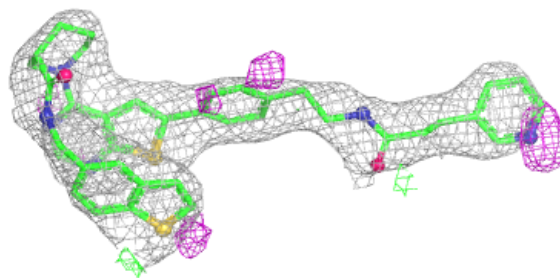
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TK0 C 501:

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

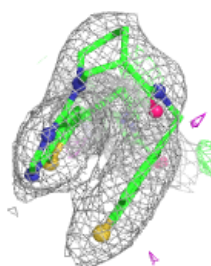
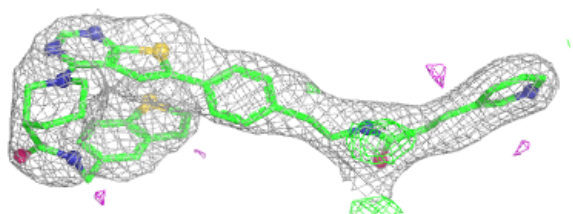
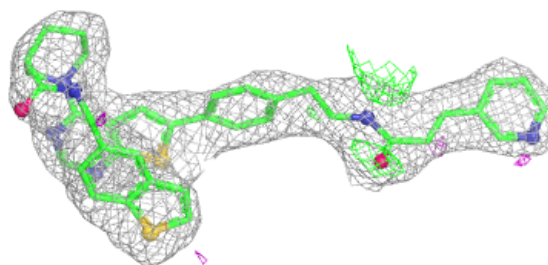
**Electron density around TK0 A 501:**

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

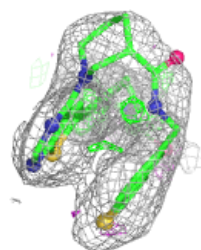
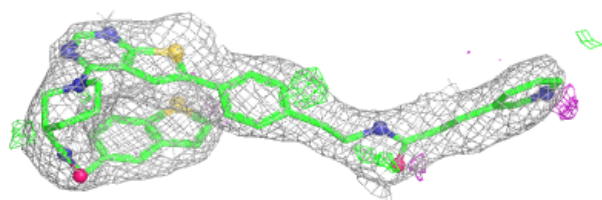
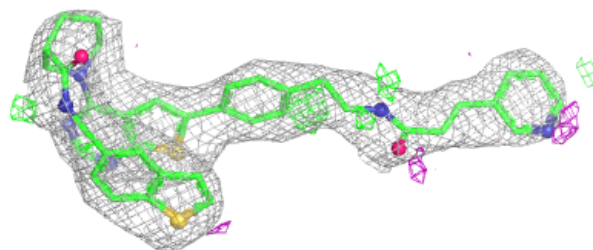


Electron density around TK0 B 501:

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

**Electron density around TK0 D 501:**

$2mF_o-DF_c$ (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.