



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 12:02 PM EDT

PDB ID : 8DTJ
Title : Human NAMPT in complex with small molecule activator ZN-43-S
Authors : Ratia, K.; Xiong, R.; Shen, Z.; Thatcher, G.R.
Deposited on : 2022-07-25
Resolution : 2.12 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

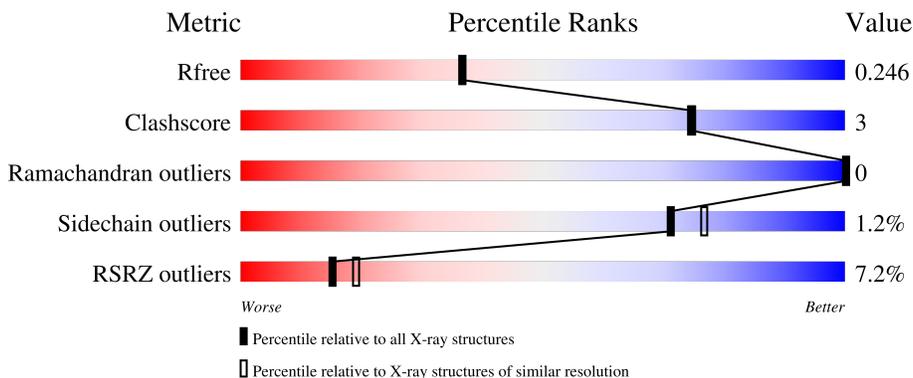
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	
1	B	499	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7985 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.

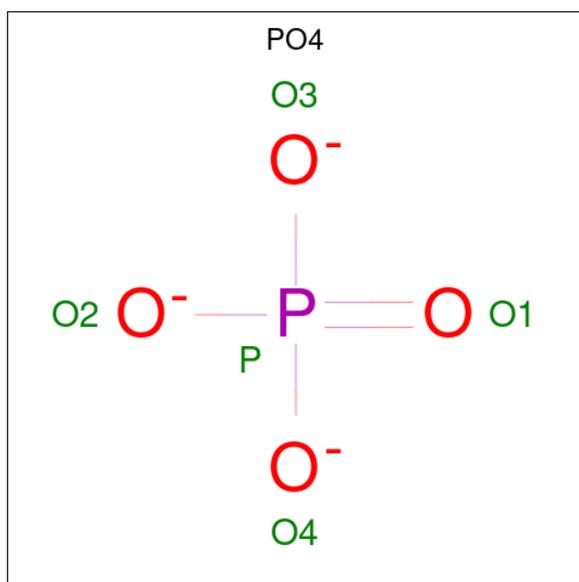
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	Total	C	N	O	S	0	0	0
			3757	2414	619	717	7			
1	B	468	Total	C	N	O	S	0	0	0
			3716	2389	611	709	7			

There are 16 discrepancies between the modelled and reference sequences:

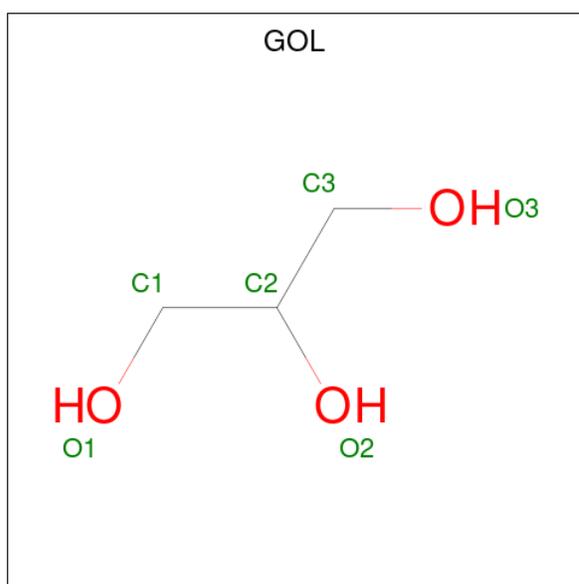
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



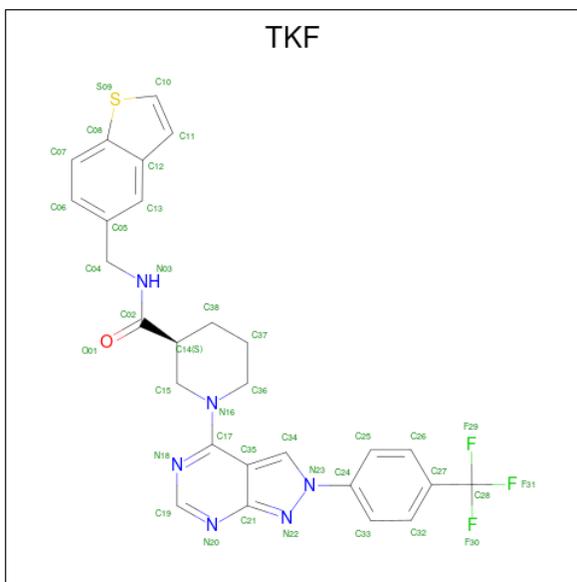
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is (3S)-N-[(1-benzothiophen-5-yl)methyl]-1-{2-[4-(trifluoromethyl)phenyl]-2H-pyrazolo[3,4-d]pyrimidin-4-yl}piperidine-3-carboxamide (three-letter code: TKF) (formula: C₂₇H₂₃F₃N₆OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	F	N	O	S	0	0
			38	27	3	6	1	1		
4	B	1	Total	C	F	N	O	S	0	0
			38	27	3	6	1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	200	Total	O	0	0
			200	200		
6	B	207	Total	O	0	0
			207	207		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.50Å 107.48Å 83.40Å 90.00° 96.64° 90.00°	Depositor
Resolution (Å)	19.67 – 2.12 19.69 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.67-2.12) 98.6 (19.69-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.11Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.216 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	2965 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7985	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, GOL, TKF

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	0.29	0/3845	0.49	0/5215
1	B	0.28	0/3804	0.46	0/5165
All	All	0.28	0/7649	0.47	0/10380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3757	0	3702	22	0
1	B	3716	0	3648	25	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	2	0
3	B	12	0	16	1	0
4	A	38	0	0	3	0
4	B	38	0	0	3	0
5	B	1	0	0	0	0
6	A	200	0	0	2	0
6	B	207	0	0	6	0
All	All	7985	0	7374	48	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 3.

All (48) 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:B:424:ARG:NH1	6:B:1304:HOH:O	2.32	0.63
1:A:172:LEU:HD21	1:A:361:LEU:HD11	1.81	0.62
1:B:259:LYS:NZ	6:B:1306:HOH:O	2.34	0.59
1:A:236:PRO:HD2	6:A:1141:HOH:O	2.02	0.58
1:B:469:LYS:NZ	3:B:1202:GOL:O2	2.37	0.56
1:B:185:GLY:HA3	4:B:1204:TKF:N18	2.21	0.56
1:B:414:PHE:HB3	1:B:427:LYS:HG2	1.88	0.55
3:A:1002:GOL:O3	3:A:1002:GOL:O1	2.20	0.54
1:B:187:GLU:H	1:B:187:GLU:CD	2.11	0.53
1:A:299:ILE:HD12	1:A:308:LEU:HD22	1.90	0.53
1:A:169:LYS:HG2	1:A:482:LEU:HD11	1.91	0.52
1:A:246:GLU:HG3	1:A:248:SER:H	1.74	0.51
4:A:1003:TKF:C34	4:A:1003:TKF:C36	2.89	0.51
1:B:172:LEU:HD21	1:B:361:LEU:HD11	1.92	0.51
1:B:246:GLU:HG3	1:B:248:SER:H	1.76	0.50
1:B:400:LYS:NZ	1:B:415:LYS:HE2	2.26	0.50
1:A:415:LYS:NZ	1:B:247:HIS:CE1	2.79	0.50
1:B:185:GLY:HA3	4:B:1204:TKF:C19	2.42	0.49
1:A:196:ARG:HD3	6:B:1308:HOH:O	2.12	0.48
1:A:435:THR:HB	1:A:436:PRO:HD2	1.95	0.48
1:B:169:LYS:HG2	1:B:482:LEU:HD11	1.95	0.48
1:A:259:LYS:HE3	1:A:294:ASP:HB3	1.96	0.47
1:A:185:GLY:HA3	4:A:1003:TKF:C19	2.45	0.47
1:A:435:THR:HB	1:A:436:PRO:CD	2.45	0.47
1:A:415:LYS:HZ2	1:B:247:HIS:CE1	2.33	0.46
1:A:224:LEU:CD2	1:A:238:PRO:HG2	2.44	0.46
1:B:299:ILE:HD12	1:B:308:LEU:HD22	1.96	0.46
1:A:185:GLY:HA3	4:A:1003:TKF:N18	2.31	0.46
1:B:405:VAL:HA	1:B:410:GLY:HA2	1.98	0.46
1:B:424:ARG:HE	1:B:424:ARG:HB3	1.45	0.46
4:B:1204:TKF:C34	4:B:1204:TKF:C36	2.93	0.46
1:B:272:VAL:C	1:B:306:ALA:HB1	2.35	0.46
1:A:224:LEU:HD22	1:A:238:PRO:HG2	1.99	0.45
1:B:102:ASN:ND2	6:B:1313:HOH:O	2.48	0.44
1:A:342:LYS:NZ	6:A:1102:HOH:O	2.34	0.44
1:B:433:HIS:HA	1:B:457:LEU:HD13	2.00	0.43
1:B:114:ILE:HD13	1:B:136:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLN:NE2	6:B:1317:HOH:O	2.47	0.42
1:A:434:ARG:HH12	3:A:1002:GOL:H12	1.84	0.42
1:A:34:TYR:HB3	1:A:403:TYR:HB3	2.01	0.42
1:B:259:LYS:HD2	1:B:294:ASP:HB3	2.01	0.42
1:B:415:LYS:NZ	6:B:1330:HOH:O	2.54	0.41
1:A:282:ASP:HB3	1:A:285:ASN:HB3	2.01	0.41
1:A:212:LEU:HD13	1:A:238:PRO:HB2	2.02	0.40
1:B:40:ARG:HB2	1:B:396:ASN:HB3	2.04	0.40
1:A:77:LYS:HD3	1:A:77:LYS:HA	1.89	0.40
1:B:177:LEU:HD22	1:B:484:ILE:HD11	2.02	0.40
1:A:487:GLU:H	1:A:487:GLU:HG2	1.71	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	468/499 (94%)	459 (98%)	9 (2%)	0	100	100
1	B	464/499 (93%)	455 (98%)	9 (2%)	0	100	100
All	All	932/998 (93%)	914 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	410/438 (94%)	406 (99%)	4 (1%)	76	81
1	B	405/438 (92%)	399 (98%)	6 (2%)	65	70
All	All	815/876 (93%)	805 (99%)	10 (1%)	71	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	195	TYR
1	A	219	ASP
1	A	289	LYS
1	B	18	TYR
1	B	195	TYR
1	B	219	ASP
1	B	289	LYS
1	B	305	GLN
1	B	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	396	ASN
1	B	305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	GOL	B	1203	-	5,5,5	0.88	0	5,5,5	0.99	0
2	PO4	A	1001	-	4,4,4	1.01	0	6,6,6	0.45	0
4	TKF	A	1003	-	42,43,43	2.19	13 (30%)	45,63,63	2.26	18 (40%)
2	PO4	B	1201	-	4,4,4	0.99	0	6,6,6	0.43	0
3	GOL	B	1202	-	5,5,5	0.83	0	5,5,5	1.04	0
4	TKF	B	1204	-	42,43,43	2.08	13 (30%)	45,63,63	2.30	15 (33%)
3	GOL	A	1002	-	5,5,5	0.19	0	5,5,5	0.23	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
3	GOL	B	1203	-	-	0/4/4/4	-
4	TKF	A	1003	-	-	6/23/33/33	1/6/6/6
3	GOL	B	1202	-	-	4/4/4/4	-
4	TKF	B	1204	-	-	7/23/33/33	0/6/6/6
3	GOL	A	1002	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TKF	C19-N18	5.04	1.43	1.33
4	A	1003	TKF	C17-N16	5.03	1.52	1.37
4	A	1003	TKF	C15-C14	4.63	1.60	1.53
4	B	1204	TKF	C19-N18	4.58	1.42	1.33
4	B	1204	TKF	C02-N03	4.51	1.43	1.33
4	B	1204	TKF	C17-N16	4.51	1.50	1.37
4	A	1003	TKF	C21-N20	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TKF	C02-N03	3.75	1.41	1.33
4	B	1204	TKF	C21-N20	3.58	1.42	1.37
4	A	1003	TKF	C24-N23	3.37	1.53	1.44
4	A	1003	TKF	C21-N22	3.24	1.39	1.34
4	B	1204	TKF	C34-N23	3.20	1.40	1.36
4	B	1204	TKF	C24-N23	3.11	1.52	1.44
4	B	1204	TKF	C04-C05	3.11	1.58	1.51
4	A	1003	TKF	C15-N16	3.04	1.52	1.46
4	B	1204	TKF	C21-N22	3.04	1.39	1.34
4	A	1003	TKF	C34-N23	2.90	1.40	1.36
4	A	1003	TKF	C14-C02	2.86	1.56	1.51
4	B	1204	TKF	C36-N16	2.83	1.51	1.46
4	B	1204	TKF	C15-C14	2.81	1.57	1.53
4	A	1003	TKF	C36-N16	2.74	1.51	1.46
4	B	1204	TKF	C14-C02	2.71	1.56	1.51
4	A	1003	TKF	C04-C05	2.45	1.56	1.51
4	B	1204	TKF	C15-N16	2.16	1.50	1.46
4	B	1204	TKF	C08-S09	2.12	1.75	1.74
4	A	1003	TKF	C07-C06	2.04	1.40	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1204	TKF	C14-C02-N03	7.68	125.96	115.99
4	A	1003	TKF	C14-C02-N03	6.47	124.38	115.99
4	A	1003	TKF	C04-N03-C02	5.70	130.54	122.34
4	B	1204	TKF	C33-C24-N23	4.95	123.48	119.15
4	B	1204	TKF	O01-C02-C14	-4.41	116.38	122.12
4	B	1204	TKF	C04-N03-C02	4.34	128.59	122.34
4	A	1003	TKF	C33-C24-N23	4.31	122.92	119.15
4	A	1003	TKF	N18-C17-N16	4.18	125.82	116.99
4	B	1204	TKF	N18-C17-N16	3.77	124.95	116.99
4	A	1003	TKF	C10-S09-C08	3.58	95.46	91.55
4	A	1003	TKF	C33-C24-C25	-3.52	116.12	121.33
4	B	1204	TKF	C33-C24-C25	-3.44	116.23	121.33
4	B	1204	TKF	C10-S09-C08	3.30	95.16	91.55
4	A	1003	TKF	O01-C02-C14	-3.30	117.82	122.12
4	A	1003	TKF	C34-N23-N22	-3.18	109.48	112.72
4	B	1204	TKF	C34-N23-N22	-3.15	109.51	112.72
4	A	1003	TKF	C11-C12-C13	-2.71	126.84	136.62
4	B	1204	TKF	C11-C12-C13	-2.68	126.93	136.62
4	B	1204	TKF	C07-C08-S09	2.57	130.00	125.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TKF	C07-C08-S09	2.53	129.91	125.07
4	B	1204	TKF	O01-C02-N03	-2.49	117.65	122.99
4	B	1204	TKF	F29-C28-C27	2.46	118.33	112.93
4	A	1003	TKF	O01-C02-N03	-2.42	117.80	122.99
4	B	1204	TKF	C38-C37-C36	2.30	114.08	110.85
4	A	1003	TKF	C35-C17-N16	-2.29	116.52	120.97
4	A	1003	TKF	C15-N16-C17	2.29	127.03	119.06
4	A	1003	TKF	F29-C28-C27	2.16	117.66	112.93
4	A	1003	TKF	C35-C17-N18	-2.14	117.65	122.64
4	B	1204	TKF	C35-C17-N18	-2.10	117.76	122.64
4	B	1204	TKF	C26-C25-C24	2.09	122.10	119.07
4	A	1003	TKF	C38-C37-C36	2.06	113.74	110.85
4	A	1003	TKF	C25-C24-N23	2.06	120.95	119.15
4	A	1003	TKF	C32-C33-C24	2.01	122.00	119.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	O1-C1-C2-O2
3	B	1202	GOL	O1-C1-C2-C3
4	A	1003	TKF	C35-C17-N16-C36
4	A	1003	TKF	N18-C17-N16-C36
4	A	1003	TKF	C33-C24-N23-C34
4	B	1204	TKF	C35-C17-N16-C36
4	B	1204	TKF	N18-C17-N16-C36
4	A	1003	TKF	N03-C02-C14-C15
4	B	1204	TKF	N03-C02-C14-C38
4	A	1003	TKF	O01-C02-C14-C15
4	A	1003	TKF	C25-C24-N23-C34
3	A	1002	GOL	O1-C1-C2-C3
3	B	1202	GOL	C1-C2-C3-O3
3	B	1202	GOL	O1-C1-C2-O2
4	B	1204	TKF	O01-C02-C14-C38
3	B	1202	GOL	O2-C2-C3-O3
4	B	1204	TKF	C25-C24-N23-N22
4	B	1204	TKF	C25-C24-N23-C34
4	B	1204	TKF	C33-C24-N23-C34

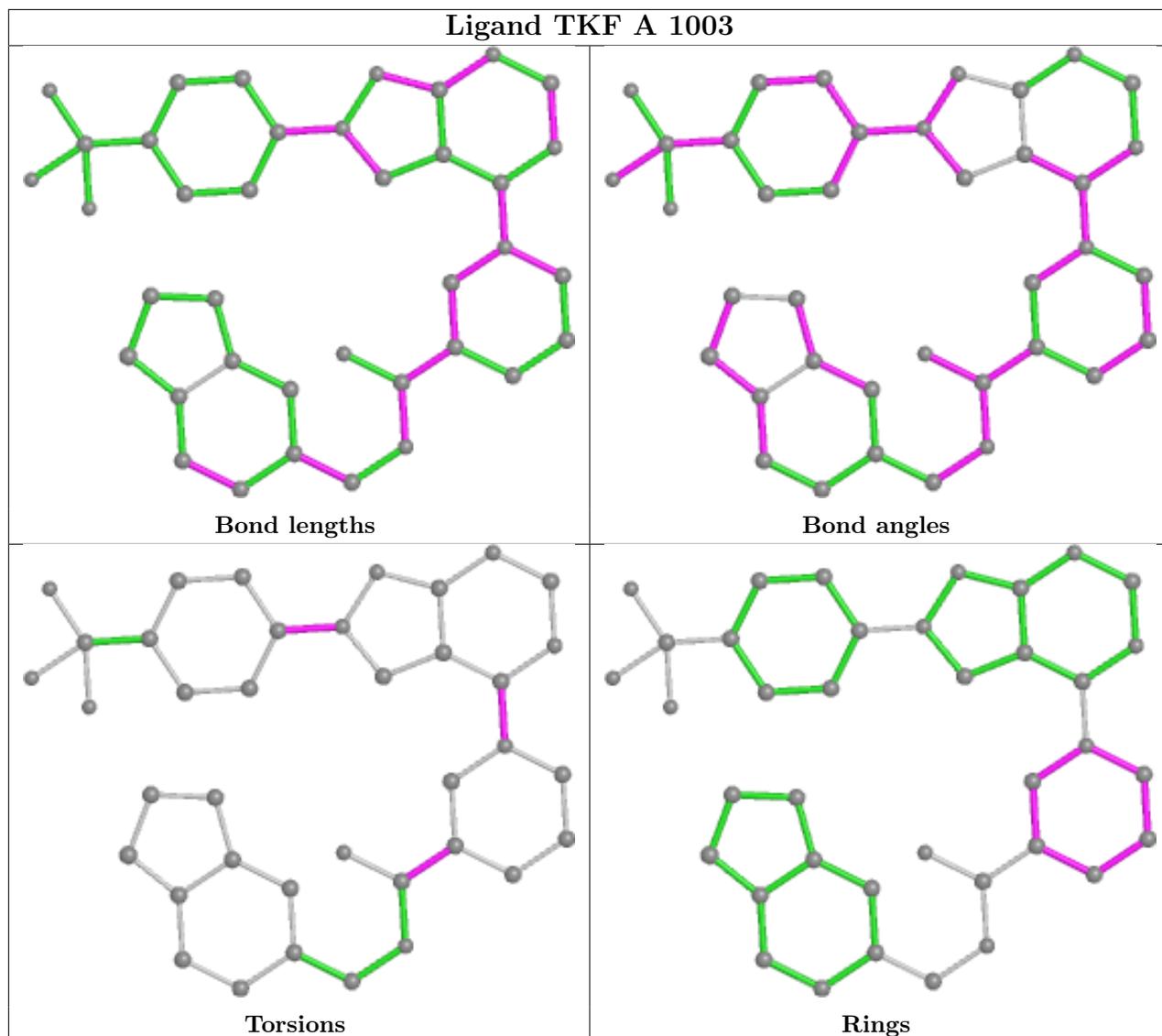
All (1) ring outliers are listed below:

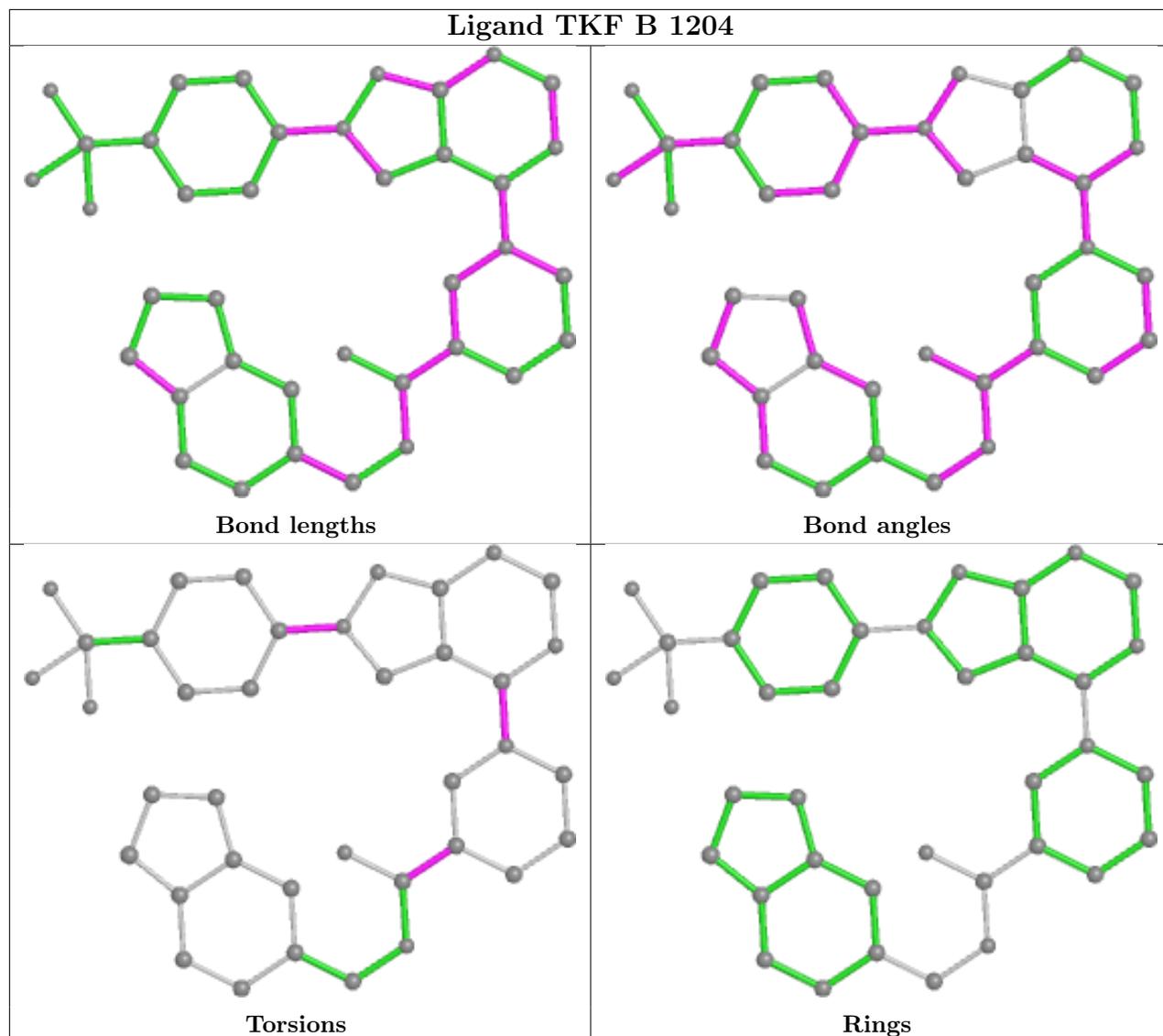
Mol	Chain	Res	Type	Atoms
4	A	1003	TKF	C14-C15-C36-C37-C38-N16

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	TKF	3	0
3	B	1202	GOL	1	0
4	B	1204	TKF	3	0
3	A	1002	GOL	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	472/499 (94%)	0.60	36 (7%) 13 17	24, 35, 53, 75	0
1	B	468/499 (93%)	0.60	32 (6%) 17 21	22, 35, 53, 68	0
All	All	940/998 (94%)	0.60	68 (7%) 15 19	22, 35, 53, 75	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	PRO	5.7
1	B	236	PRO	5.1
1	A	409	LEU	4.9
1	A	236	PRO	4.9
1	B	422	ASN	4.8
1	B	52	VAL	4.7
1	B	484	ILE	4.5
1	A	52	VAL	4.4
1	B	424	ARG	4.2
1	A	422	ASN	4.1
1	B	355	GLY	3.8
1	A	424	ARG	3.7
1	A	237	VAL	3.7
1	A	486	LEU	3.5
1	A	421	PRO	3.5
1	A	487	GLU	3.4
1	B	101	TRP	3.4
1	B	409	LEU	3.4
1	A	488	ALA	3.3
1	A	238	PRO	3.2
1	B	375	ILE	3.2
1	A	485	GLU	3.1
1	B	12	LEU	3.0
1	A	62	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	418	VAL	2.9
1	A	418	VAL	2.9
1	B	62	LEU	2.9
1	B	486	LEU	2.9
1	A	451	GLU	2.9
1	A	95	VAL	2.8
1	B	393	ASP	2.8
1	B	451	GLU	2.8
1	B	485	GLU	2.7
1	B	305	GLN	2.7
1	B	233	THR	2.6
1	A	305	GLN	2.6
1	B	450	LEU	2.6
1	A	18	TYR	2.5
1	B	78	GLU	2.4
1	A	235	ASP	2.4
1	A	365	VAL	2.4
1	A	375	ILE	2.4
1	B	291	TRP	2.4
1	B	23	TYR	2.3
1	A	8	GLU	2.3
1	A	483	ASN	2.3
1	B	185	GLY	2.3
1	B	483	ASN	2.3
1	B	271	SER	2.3
1	B	419	ALA	2.3
1	A	271	SER	2.3
1	A	458	LEU	2.2
1	A	438	GLY	2.2
1	B	449	ASP	2.2
1	A	393	ASP	2.2
1	B	448	GLY	2.2
1	A	108	TYR	2.2
1	B	407	ASN	2.2
1	A	268	GLN	2.1
1	A	266	VAL	2.1
1	A	435	THR	2.1
1	A	94	ASP	2.1
1	A	454	GLY	2.1
1	B	29	ASN	2.1
1	A	256	ASP	2.1
1	A	239	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	2.0
1	A	432	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

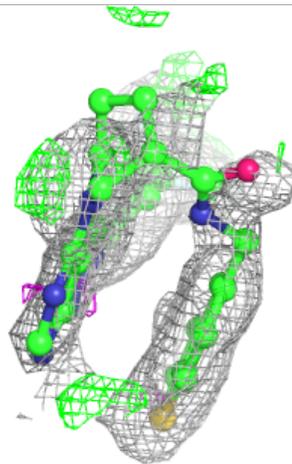
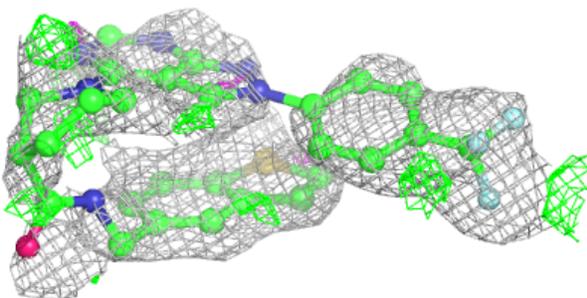
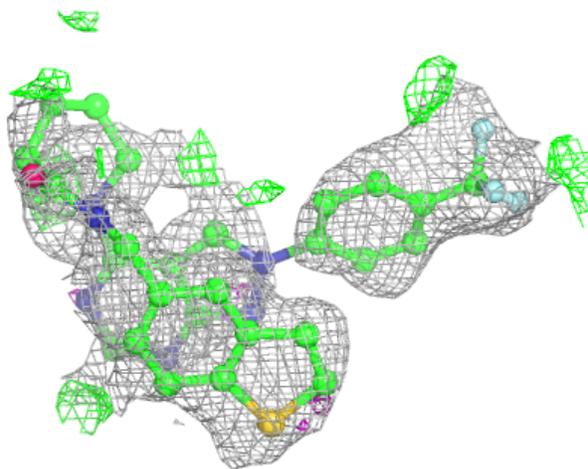
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

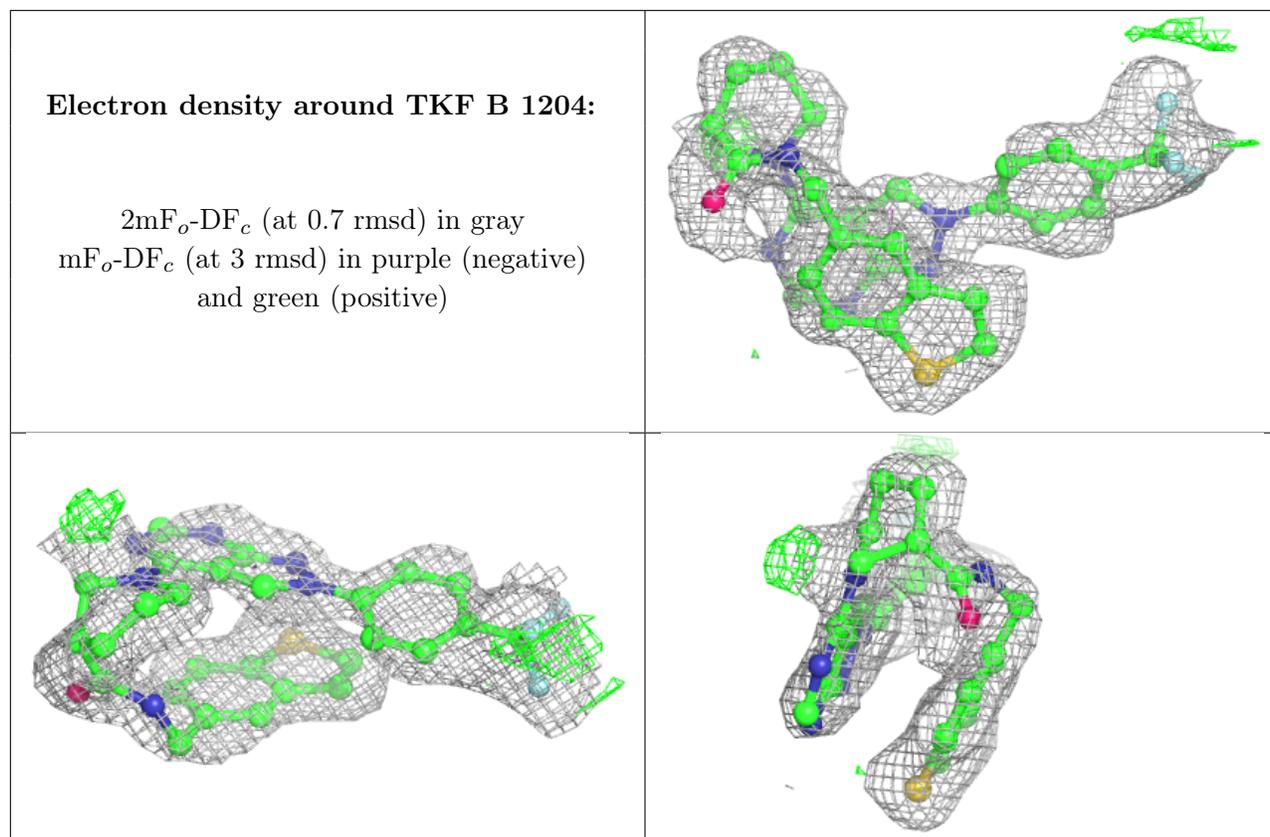
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TKF	A	1003	38/38	0.69	0.29	29,41,51,55	38
4	TKF	B	1204	38/38	0.76	0.23	26,41,50,56	38
3	GOL	B	1202	6/6	0.77	0.33	38,43,49,50	0
3	GOL	B	1203	6/6	0.83	0.12	37,44,48,53	0
2	PO4	B	1201	5/5	0.83	0.25	40,44,50,53	5
2	PO4	A	1001	5/5	0.83	0.29	49,53,54,56	5
3	GOL	A	1002	6/6	0.85	0.12	36,38,43,44	0
5	CL	B	1205	1/1	0.90	0.06	58,58,58,58	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 TKF A 1003:

$2mF_o-DF_c$ (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.