



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:42 AM EDT

PDB ID : 6RKY / pdb_00006rky
Title : STRUCTURE OF ESTER-HYDROLASE EH1AB1 FROM THE METAGENOME OF LAKE ARREO COMPLEXED WITH A DERIVATIVE OF BIPYRIDINE PHOSPHONATE
Authors : Cea-Rama, I.; Sanz-Aparicio, J.
Deposited on : 2019-04-30
Resolution : 2.79 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

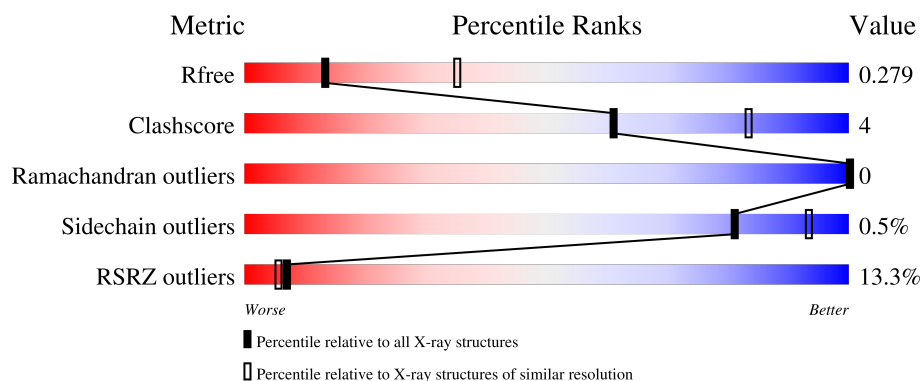
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	329	8% 87% 8% .
1	B	329	7% 87% 9% .
1	C	329	23% 85% 10% .
1	D	329	14% 87% 8% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9764 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 EH1AB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2385	1500	419	455	11			
1	B	315	Total	C	N	O	S	0	0	0
			2385	1500	419	455	11			
1	C	315	Total	C	N	O	S	0	0	0
			2385	1500	419	455	11			
1	D	315	Total	C	N	O	S	0	0	0
			2385	1500	419	455	11			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



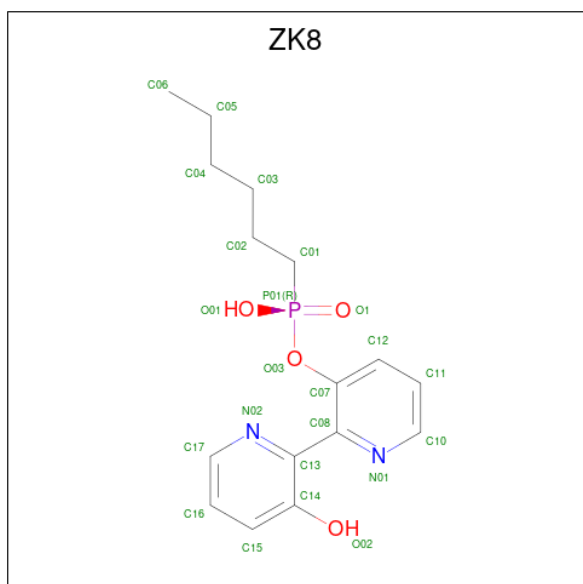
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is hexyl-[2-(3-oxidanylpiperidin-2-yl)piperidin-3-yl]oxy-phosphinic acid (CCD ID: ZK8) (formula: C₁₆H₂₁N₂O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	16	2	3	1		
3	B	1	Total	C	N	O	P	0	0
			22	16	2	3	1		
3	C	1	Total	C	N	O	P	0	0
			22	16	2	3	1		
3	D	1	Total	C	N	O	P	0	0
			22	16	2	3	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

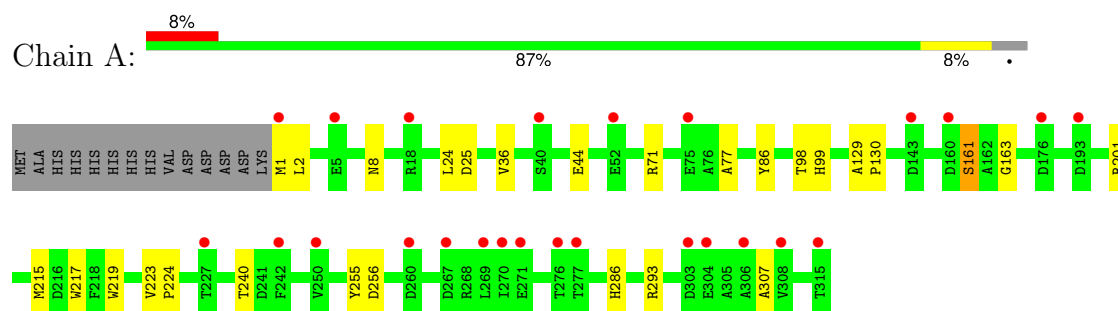
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	14	Total	O	0	0
			14	14		
5	C	19	Total	O	0	0
			19	19		
5	D	23	Total	O	0	0
			23	23		

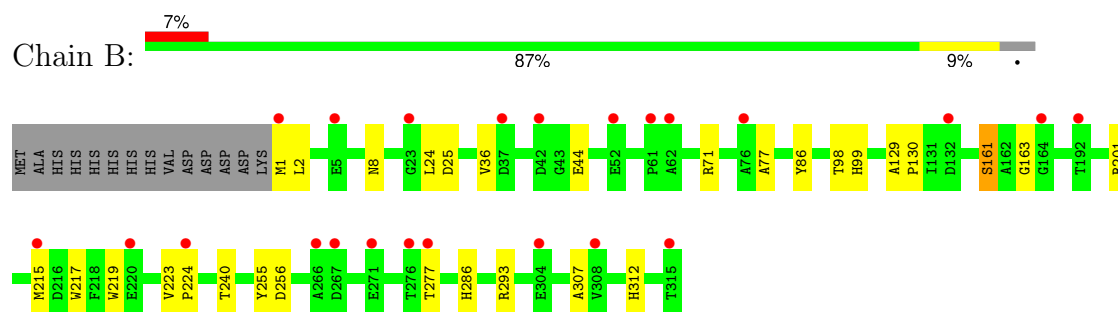
3 Residue-property plots [i](#)

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.

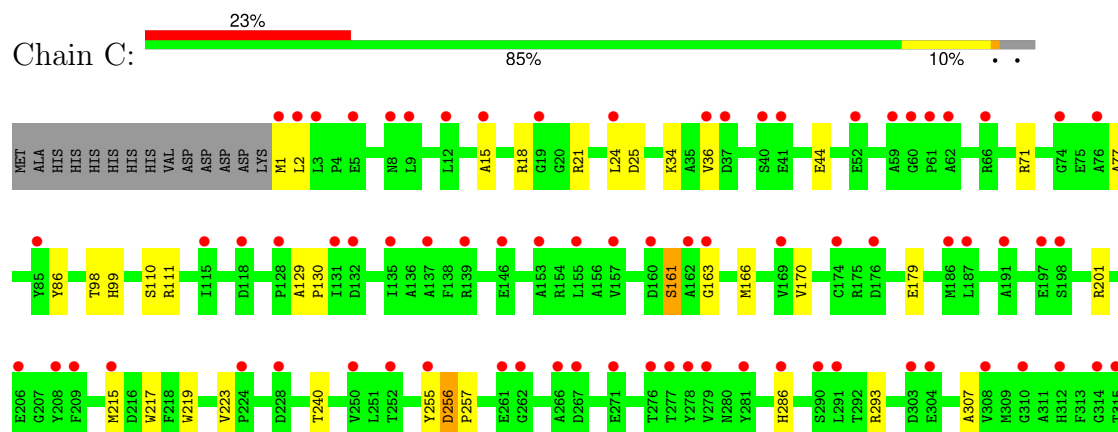
• Molecule 1: EH1AB1



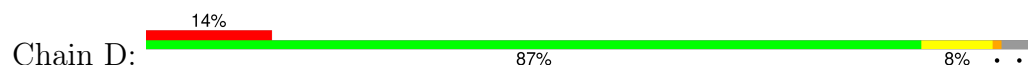
• Molecule 1: EH1AB1

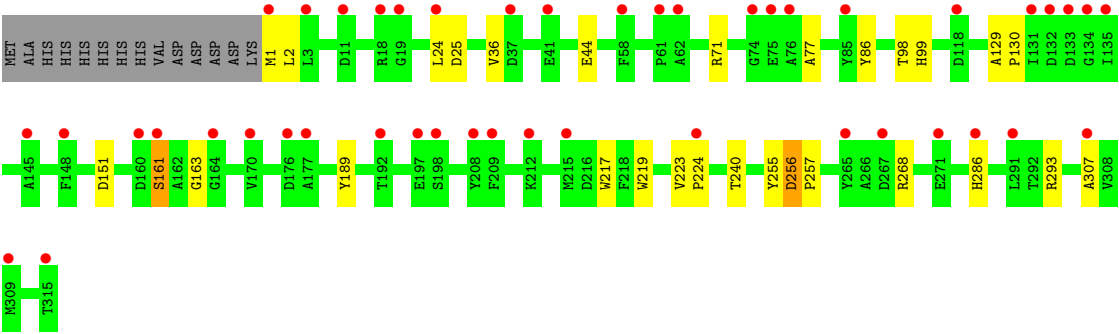


• Molecule 1: EH1AB1



• Molecule 1: EH1AB1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.77Å 201.92Å 90.64Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	49.08 – 2.79 49.08 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.08-2.79) 99.1 (49.08-2.79)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.239 , 0.276 0.241 , 0.279	Depositor DCC
R_{free} test set	1823 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9764	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3736e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ZK8, GOL

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	1.03	0/2443	1.45	3/3318 (0.1%)
1	B	1.04	0/2443	1.45	4/3318 (0.1%)
1	C	1.05	0/2443	1.46	3/3318 (0.1%)
1	D	1.06	0/2443	1.47	6/3318 (0.2%)
All	All	1.05	0/9772	1.45	16/13272 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	TYR	CB-CA-C	8.82	117.46	111.20
1	C	256	ASP	CB-CA-C	5.69	117.75	110.13
1	C	161	SER	CA-CB-OG	5.68	122.46	111.10
1	D	161	SER	CA-CB-OG	5.65	122.39	111.10
1	A	161	SER	CA-CB-OG	5.58	122.27	111.10
1	B	161	SER	CA-CB-OG	5.57	122.24	111.10
1	D	151	ASP	CA-C-N	5.38	127.75	120.38
1	D	151	ASP	C-N-CA	5.38	127.75	120.38
1	D	256	ASP	CB-CA-C	5.26	117.17	110.13
1	B	161	SER	N-CA-CB	5.25	119.35	110.49
1	B	256	ASP	CB-CA-C	5.20	117.09	110.13
1	A	161	SER	N-CA-CB	5.16	119.21	110.49
1	D	161	SER	N-CA-CB	5.12	119.14	110.49
1	C	161	SER	N-CA-CB	5.10	119.11	110.49
1	A	256	ASP	CB-CA-C	5.10	116.96	110.13
1	B	277	THR	CA-CB-OG1	-5.10	101.96	109.60

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	2385	0	2297	20	0
1	B	2385	0	2297	21	0
1	C	2385	0	2297	22	0
1	D	2385	0	2297	18	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	12	0	16	0	0
3	A	22	0	0	1	0
3	B	22	0	0	1	0
3	C	22	0	0	1	0
3	D	22	0	0	1	0
4	C	21	0	30	1	0
4	D	7	0	10	0	0
5	A	16	0	0	0	0
5	B	14	0	0	1	0
5	C	19	0	0	1	0
5	D	23	0	0	1	0
All	All	9764	0	9276	80	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 4.

All (80) 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:307:ALA:HB1	1:D:307:ALA:HB1	1.38	1.02
1:A:307:ALA:HB1	1:C:307:ALA:HB1	1.45	0.99
1:B:161:SER:HB3	1:B:286:HIS:CE1	2.26	0.71
1:C:161:SER:HB3	1:C:286:HIS:CE1	2.26	0.71
1:A:161:SER:HB3	1:A:286:HIS:CE1	2.26	0.69
1:D:161:SER:HB3	1:D:286:HIS:CE1	2.27	0.69
3:C:406:ZK8:O03	3:C:406:ZK8:O02	2.16	0.64
3:B:402:ZK8:O03	3:B:402:ZK8:O02	2.16	0.63
3:A:402:ZK8:O03	3:A:402:ZK8:O02	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:404:ZK8:O03	3:D:404:ZK8:O02	2.16	0.63
1:B:312:HIS:NE2	5:B:502:HOH:O	2.32	0.58
1:D:268:ARG:HG2	5:D:507:HOH:O	2.01	0.58
1:B:161:SER:HB3	1:B:286:HIS:HE1	1.69	0.58
1:A:98:THR:OG1	1:A:99:HIS:HD2	1.87	0.58
1:D:44:GLU:O	1:D:293:ARG:NH1	2.37	0.57
1:B:24:LEU:HD13	1:B:36:VAL:HG21	1.86	0.57
1:B:98:THR:OG1	1:B:99:HIS:HD2	1.87	0.57
1:D:98:THR:OG1	1:D:99:HIS:HD2	1.87	0.57
1:A:24:LEU:HD13	1:A:36:VAL:HG21	1.86	0.57
1:A:1:MET:HB2	1:A:255:TYR:OH	2.05	0.56
1:C:44:GLU:O	1:C:293:ARG:NH1	2.38	0.56
1:A:44:GLU:O	1:A:293:ARG:NH1	2.39	0.56
1:C:98:THR:OG1	1:C:99:HIS:HD2	1.87	0.56
1:B:44:GLU:O	1:B:293:ARG:NH1	2.39	0.56
1:D:161:SER:HB3	1:D:286:HIS:HE1	1.71	0.55
1:A:161:SER:HB3	1:A:286:HIS:HE1	1.68	0.55
1:A:8:ASN:HD22	1:B:8:ASN:ND2	2.05	0.55
1:A:219:TRP:CZ2	1:A:223:VAL:HG21	2.42	0.55
1:C:161:SER:HB3	1:C:286:HIS:HE1	1.70	0.55
1:C:219:TRP:CZ2	1:C:223:VAL:HG21	2.43	0.54
1:C:1:MET:HB2	1:C:255:TYR:OH	2.07	0.54
1:D:219:TRP:CZ2	1:D:223:VAL:HG21	2.42	0.54
1:D:1:MET:HB2	1:D:255:TYR:OH	2.09	0.53
1:A:8:ASN:ND2	1:B:8:ASN:HD22	2.07	0.53
1:B:219:TRP:CZ2	1:B:223:VAL:HG21	2.44	0.53
1:B:1:MET:HB2	1:B:255:TYR:OH	2.09	0.52
1:C:110:SER:O	1:C:111:ARG:HB2	2.08	0.52
1:A:24:LEU:HD13	1:A:36:VAL:CG2	2.40	0.51
1:A:71:ARG:NH2	1:A:77:ALA:O	2.44	0.51
1:C:25:ASP:HA	1:C:217:TRP:CD1	2.46	0.50
1:B:71:ARG:NH2	1:B:77:ALA:O	2.43	0.50
1:D:25:ASP:HA	1:D:217:TRP:CD1	2.47	0.49
1:A:25:ASP:HA	1:A:217:TRP:CD1	2.47	0.49
1:B:24:LEU:HD13	1:B:36:VAL:CG2	2.42	0.49
1:B:25:ASP:HA	1:B:217:TRP:CD1	2.48	0.49
1:C:24:LEU:HD13	1:C:36:VAL:HG21	1.95	0.49
1:A:8:ASN:HD22	1:B:8:ASN:HD22	1.59	0.48
1:D:86:TYR:O	1:D:163:GLY:HA3	2.14	0.48
1:D:71:ARG:NH2	1:D:77:ALA:O	2.44	0.48
1:A:86:TYR:O	1:A:163:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:O	1:B:163:GLY:HA3	2.14	0.47
1:C:1:MET:HG3	1:C:2:LEU:H	1.79	0.47
1:A:219:TRP:CE2	1:A:223:VAL:HG21	2.50	0.47
1:C:86:TYR:O	1:C:163:GLY:HA3	2.14	0.47
1:D:219:TRP:CE2	1:D:223:VAL:HG21	2.50	0.47
1:C:71:ARG:NH2	1:C:77:ALA:O	2.47	0.47
1:C:179:GLU:OE2	4:C:405:PEG:C2	2.63	0.47
1:A:1:MET:HG3	1:A:2:LEU:H	1.80	0.46
1:D:24:LEU:HD13	1:D:36:VAL:HG21	1.96	0.46
1:B:219:TRP:CE2	1:B:223:VAL:HG21	2.51	0.46
1:C:219:TRP:CE2	1:C:223:VAL:HG21	2.50	0.46
1:D:24:LEU:HD13	1:D:36:VAL:CG2	2.46	0.46
1:C:129:ALA:HB3	1:C:130:PRO:HD3	1.98	0.46
1:A:129:ALA:HB3	1:A:130:PRO:HD3	1.98	0.46
1:D:129:ALA:HB3	1:D:130:PRO:HD3	1.97	0.46
1:B:1:MET:HG3	1:B:2:LEU:H	1.82	0.45
1:B:129:ALA:HB3	1:B:130:PRO:HD3	1.98	0.45
1:C:24:LEU:HD13	1:C:36:VAL:CG2	2.46	0.45
1:C:201:ARG:NH1	1:C:215:MET:HE3	2.31	0.45
1:C:21:ARG:HD3	5:C:508:HOH:O	2.16	0.45
1:D:1:MET:HG3	1:D:2:LEU:H	1.83	0.43
1:D:223:VAL:HA	1:D:224:PRO:HD2	1.91	0.43
1:A:223:VAL:HA	1:A:224:PRO:HD2	1.92	0.43
1:C:15:ALA:HA	1:C:18:ARG:NH1	2.33	0.43
1:A:201:ARG:NH1	1:A:215:MET:HE3	2.35	0.42
1:D:256:ASP:O	1:D:257:PRO:C	2.63	0.41
1:C:256:ASP:O	1:C:257:PRO:C	2.63	0.41
1:B:201:ARG:NH1	1:B:215:MET:HE3	2.36	0.41
1:B:223:VAL:HA	1:B:224:PRO:HD2	1.92	0.41
1:C:166:MET:O	1:C:170:VAL:HG23	2.20	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	313/329 (95%)	296 (95%)	17 (5%)	0	100	100
1	B	313/329 (95%)	299 (96%)	14 (4%)	0	100	100
1	C	313/329 (95%)	298 (95%)	15 (5%)	0	100	100
1	D	313/329 (95%)	299 (96%)	14 (4%)	0	100	100
All	All	1252/1316 (95%)	1192 (95%)	60 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	238/251 (95%)	237 (100%)	1 (0%)	84	94
1	B	238/251 (95%)	237 (100%)	1 (0%)	84	94
1	C	238/251 (95%)	236 (99%)	2 (1%)	73	90
1	D	238/251 (95%)	237 (100%)	1 (0%)	84	94
All	All	952/1004 (95%)	947 (100%)	5 (0%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	THR
1	B	240	THR
1	C	34	LYS
1	C	240	THR
1	D	240	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	286	HIS
1	A	297	GLN
1	B	8	ASN
1	B	99	HIS
1	B	286	HIS
1	C	99	HIS
1	C	286	HIS
1	C	297	GLN
1	D	99	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	C	404	-	6,6,6	0.35	0	5,5,5	0.28	0
2	GOL	C	402	-	5,5,5	0.15	0	5,5,5	0.30	0
2	GOL	D	402	-	5,5,5	0.18	0	5,5,5	0.52	0
4	PEG	D	403	-	6,6,6	0.32	0	5,5,5	0.20	0
2	GOL	B	401	-	5,5,5	0.10	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZK8	B	402	1	19,23,24	2.32	3 (15%)	22,29,32	4.78	11 (50%)
2	GOL	A	401	-	5,5,5	0.15	0	5,5,5	0.41	0
2	GOL	C	401	-	5,5,5	0.10	0	5,5,5	0.36	0
3	ZK8	D	404	1	19,23,24	2.37	3 (15%)	22,29,32	4.81	11 (50%)
2	GOL	D	401	-	5,5,5	0.13	0	5,5,5	0.33	0
3	ZK8	A	402	1	19,23,24	2.33	3 (15%)	22,29,32	4.77	11 (50%)
3	ZK8	C	406	1	19,23,24	2.41	3 (15%)	22,29,32	4.80	11 (50%)
4	PEG	C	403	-	6,6,6	0.20	0	5,5,5	0.11	0
4	PEG	C	405	-	6,6,6	0.33	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
4	PEG	C	404	-	-	2/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
2	GOL	D	402	-	-	3/4/4/4	-
4	PEG	D	403	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
3	ZK8	B	402	1	-	8/10/14/16	0/2/2/2
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
3	ZK8	D	404	1	-	9/10/14/16	0/2/2/2
2	GOL	D	401	-	-	1/4/4/4	-
3	ZK8	A	402	1	-	8/10/14/16	0/2/2/2
3	ZK8	C	406	1	-	8/10/14/16	0/2/2/2
4	PEG	C	403	-	-	3/4/4/4	-
4	PEG	C	405	-	-	1/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	406	ZK8	C08-C13	-8.45	1.36	1.49
3	A	402	ZK8	C08-C13	-8.38	1.36	1.49
3	D	404	ZK8	C08-C13	-8.38	1.36	1.49
3	B	402	ZK8	C08-C13	-8.37	1.36	1.49
3	D	404	ZK8	O03-C07	3.74	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	406	ZK8	O02-C14	3.70	1.43	1.36
3	C	406	ZK8	O03-C07	3.69	1.46	1.40
3	A	402	ZK8	O03-C07	3.54	1.46	1.40
3	D	404	ZK8	O02-C14	3.41	1.43	1.36
3	B	402	ZK8	O03-C07	3.38	1.45	1.40
3	B	402	ZK8	O02-C14	3.18	1.42	1.36
3	A	402	ZK8	O02-C14	3.08	1.42	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	406	ZK8	C07-C08-N01	-11.79	112.63	121.69
3	D	404	ZK8	C07-C08-N01	-11.64	112.74	121.69
3	B	402	ZK8	C07-C08-N01	-11.61	112.77	121.69
3	A	402	ZK8	C07-C08-N01	-11.60	112.78	121.69
3	D	404	ZK8	C10-N01-C08	9.18	134.76	116.84
3	B	402	ZK8	C10-N01-C08	9.16	134.72	116.84
3	C	406	ZK8	C10-N01-C08	9.16	134.72	116.84
3	D	404	ZK8	C17-N02-C13	9.15	134.71	116.84
3	A	402	ZK8	C10-N01-C08	9.13	134.67	116.84
3	C	406	ZK8	C17-N02-C13	9.10	134.61	116.84
3	B	402	ZK8	C17-N02-C13	9.07	134.55	116.84
3	A	402	ZK8	C17-N02-C13	9.02	134.44	116.84
3	D	404	ZK8	C14-C13-N02	-7.32	111.34	121.19
3	B	402	ZK8	C14-C13-N02	-7.32	111.35	121.19
3	A	402	ZK8	C14-C13-N02	-7.27	111.41	121.19
3	C	406	ZK8	C14-C13-N02	-7.25	111.44	121.19
3	B	402	ZK8	C11-C10-N01	-6.79	112.68	123.42
3	D	404	ZK8	C11-C10-N01	-6.78	112.69	123.42
3	A	402	ZK8	C11-C10-N01	-6.69	112.83	123.42
3	C	406	ZK8	C11-C10-N01	-6.69	112.83	123.42
3	D	404	ZK8	C16-C17-N02	-6.46	113.19	123.42
3	C	406	ZK8	C16-C17-N02	-6.35	113.37	123.42
3	A	402	ZK8	C16-C17-N02	-6.34	113.39	123.42
3	B	402	ZK8	C16-C17-N02	-6.24	113.54	123.42
3	C	406	ZK8	C07-C08-C13	4.31	127.99	121.78
3	D	404	ZK8	C07-C08-C13	4.30	127.98	121.78
3	A	402	ZK8	C14-C13-C08	4.25	127.61	121.69
3	B	402	ZK8	C14-C13-C08	4.22	127.56	121.69
3	C	406	ZK8	C14-C13-C08	4.17	127.50	121.69
3	B	402	ZK8	C07-C08-C13	4.15	127.76	121.78
3	D	404	ZK8	C14-C13-C08	4.14	127.45	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ZK8	C07-C08-C13	4.11	127.71	121.78
3	D	404	ZK8	C08-C13-N02	3.30	121.20	114.82
3	B	402	ZK8	C08-C13-N02	3.23	121.08	114.82
3	C	406	ZK8	C08-C13-N02	3.21	121.04	114.82
3	A	402	ZK8	C08-C13-N02	3.18	120.97	114.82
3	A	402	ZK8	C15-C14-C13	2.75	120.54	118.30
3	D	404	ZK8	C15-C14-C13	2.66	120.47	118.30
3	B	402	ZK8	C15-C14-C13	2.59	120.41	118.30
3	A	402	ZK8	C13-C08-N01	2.42	119.50	114.82
3	B	402	ZK8	C13-C08-N01	2.40	119.47	114.82
3	C	406	ZK8	C15-C14-C13	2.40	120.25	118.30
3	C	406	ZK8	C13-C08-N01	2.35	119.38	114.82
3	D	404	ZK8	C13-C08-N01	2.30	119.28	114.82

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GOL	O1-C1-C2-C3
2	C	401	GOL	C1-C2-C3-O3
2	D	402	GOL	C1-C2-C3-O3
3	A	402	ZK8	C07-C08-C13-C14
3	A	402	ZK8	N01-C08-C13-N02
3	A	402	ZK8	P01-C01-C02-C03
3	B	402	ZK8	C07-C08-C13-C14
3	B	402	ZK8	N01-C08-C13-N02
3	B	402	ZK8	P01-C01-C02-C03
3	C	406	ZK8	C07-C08-C13-C14
3	C	406	ZK8	N01-C08-C13-N02
3	C	406	ZK8	P01-C01-C02-C03
3	D	404	ZK8	C07-C08-C13-C14
3	D	404	ZK8	N01-C08-C13-N02
3	D	404	ZK8	P01-C01-C02-C03
2	B	401	GOL	O1-C1-C2-O2
4	C	405	PEG	O1-C1-C2-O2
4	C	403	PEG	O2-C3-C4-O4
2	A	401	GOL	O1-C1-C2-C3
2	C	402	GOL	C1-C2-C3-O3
4	D	403	PEG	O2-C3-C4-O4
2	C	401	GOL	O2-C2-C3-O3
3	D	404	ZK8	C02-C03-C04-C05
3	B	402	ZK8	C02-C03-C04-C05

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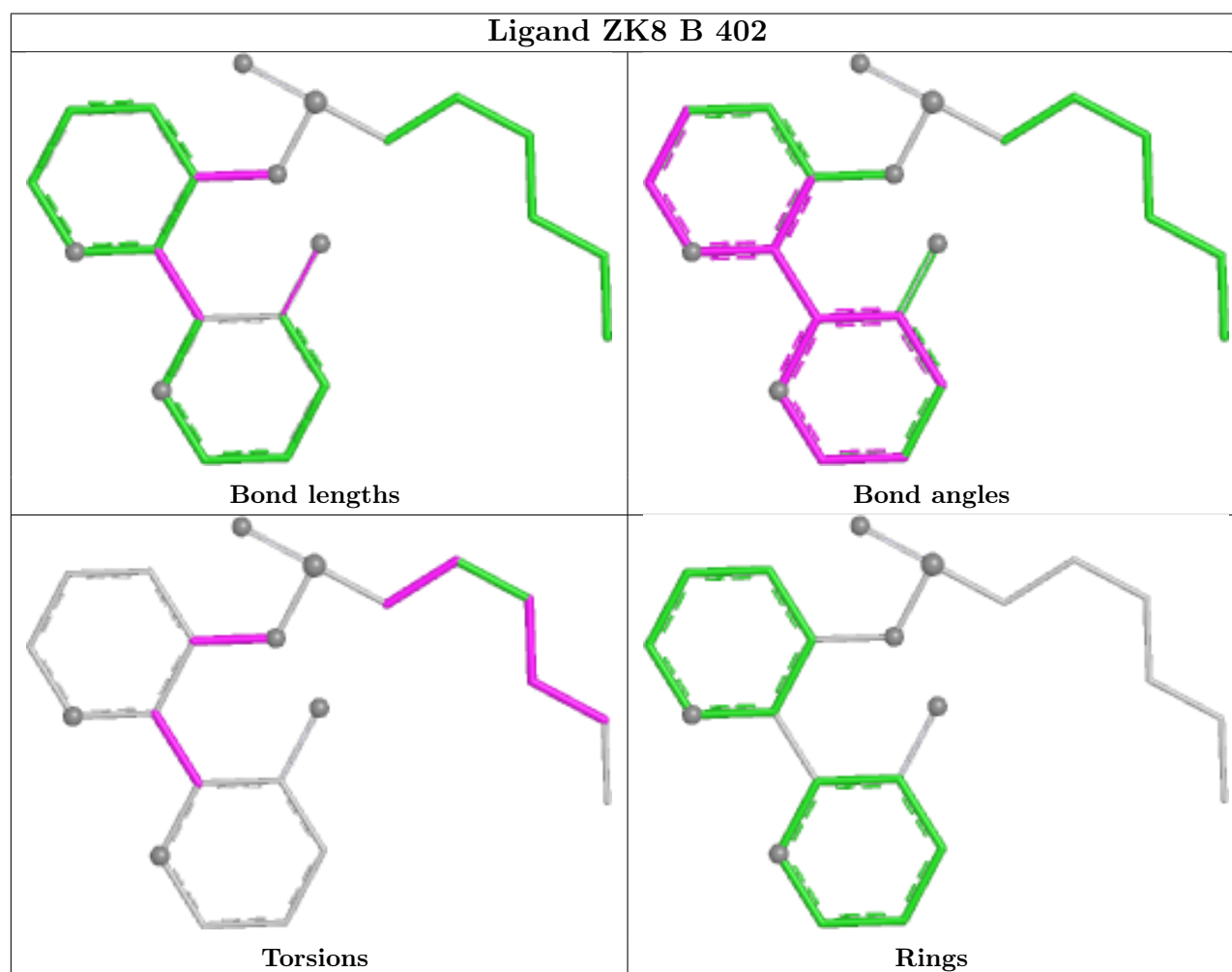
Mol	Chain	Res	Type	Atoms
3	C	406	ZK8	C02-C03-C04-C05
3	A	402	ZK8	C02-C03-C04-C05
2	A	401	GOL	O1-C1-C2-O2
4	D	403	PEG	O1-C1-C2-O2
4	C	403	PEG	O1-C1-C2-O2
2	D	402	GOL	O1-C1-C2-C3
4	C	404	PEG	O1-C1-C2-O2
3	C	406	ZK8	C03-C04-C05-C06
3	B	402	ZK8	C03-C04-C05-C06
3	D	404	ZK8	C03-C04-C05-C06
3	A	402	ZK8	C03-C04-C05-C06
3	A	402	ZK8	C12-C07-O03-P01
3	B	402	ZK8	C12-C07-O03-P01
3	C	406	ZK8	C12-C07-O03-P01
3	D	404	ZK8	C12-C07-O03-P01
4	C	403	PEG	C4-C3-O2-C2
2	C	402	GOL	O2-C2-C3-O3
2	C	402	GOL	O1-C1-C2-C3
2	D	402	GOL	O2-C2-C3-O3
4	C	404	PEG	C4-C3-O2-C2
2	C	402	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
3	D	404	ZK8	C08-C07-O03-P01
3	A	402	ZK8	N01-C08-C13-C14
3	A	402	ZK8	C07-C08-C13-N02
3	B	402	ZK8	N01-C08-C13-C14
3	B	402	ZK8	C07-C08-C13-N02
3	C	406	ZK8	N01-C08-C13-C14
3	C	406	ZK8	C07-C08-C13-N02
3	D	404	ZK8	N01-C08-C13-C14
3	D	404	ZK8	C07-C08-C13-N02

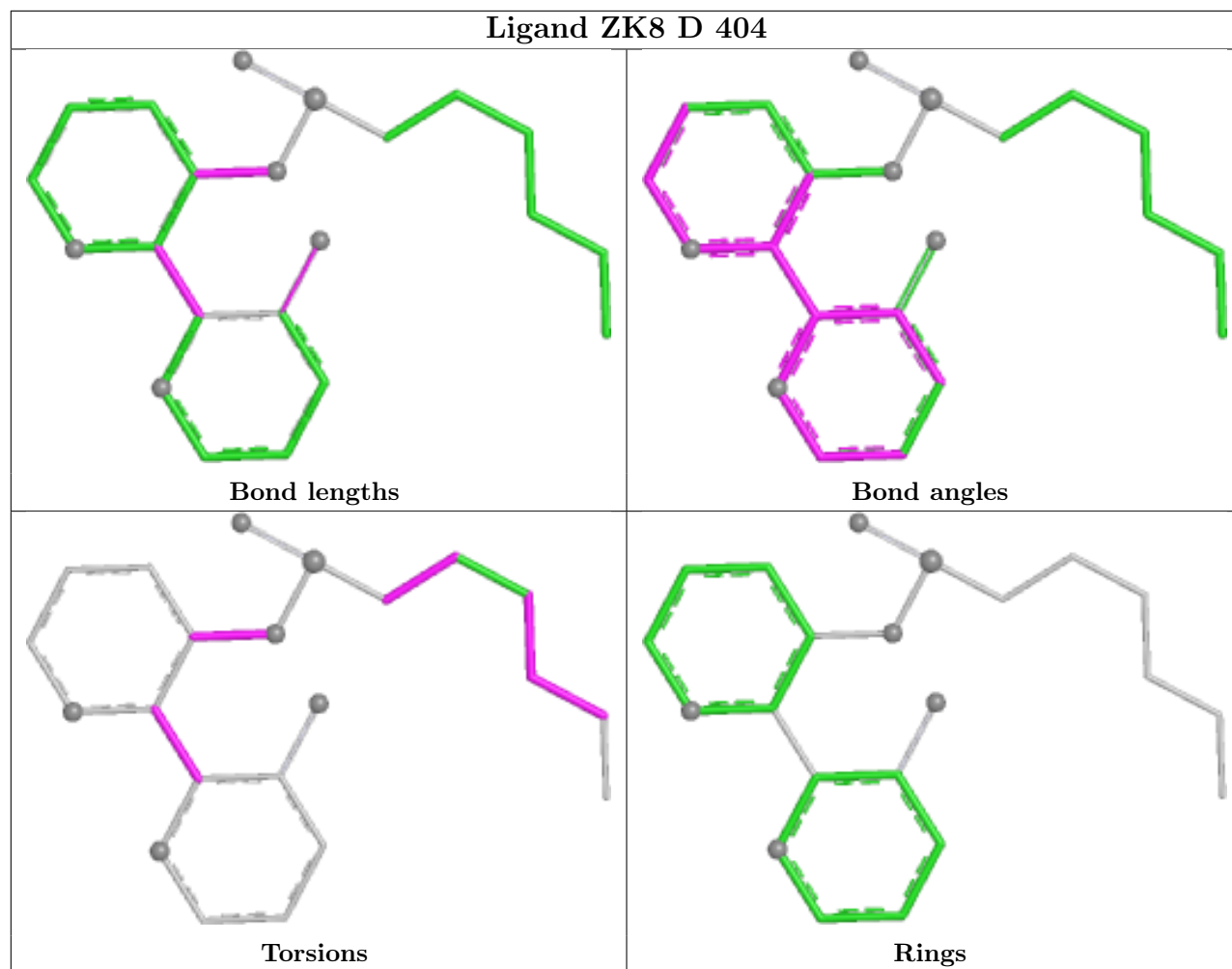
There are no ring outliers.

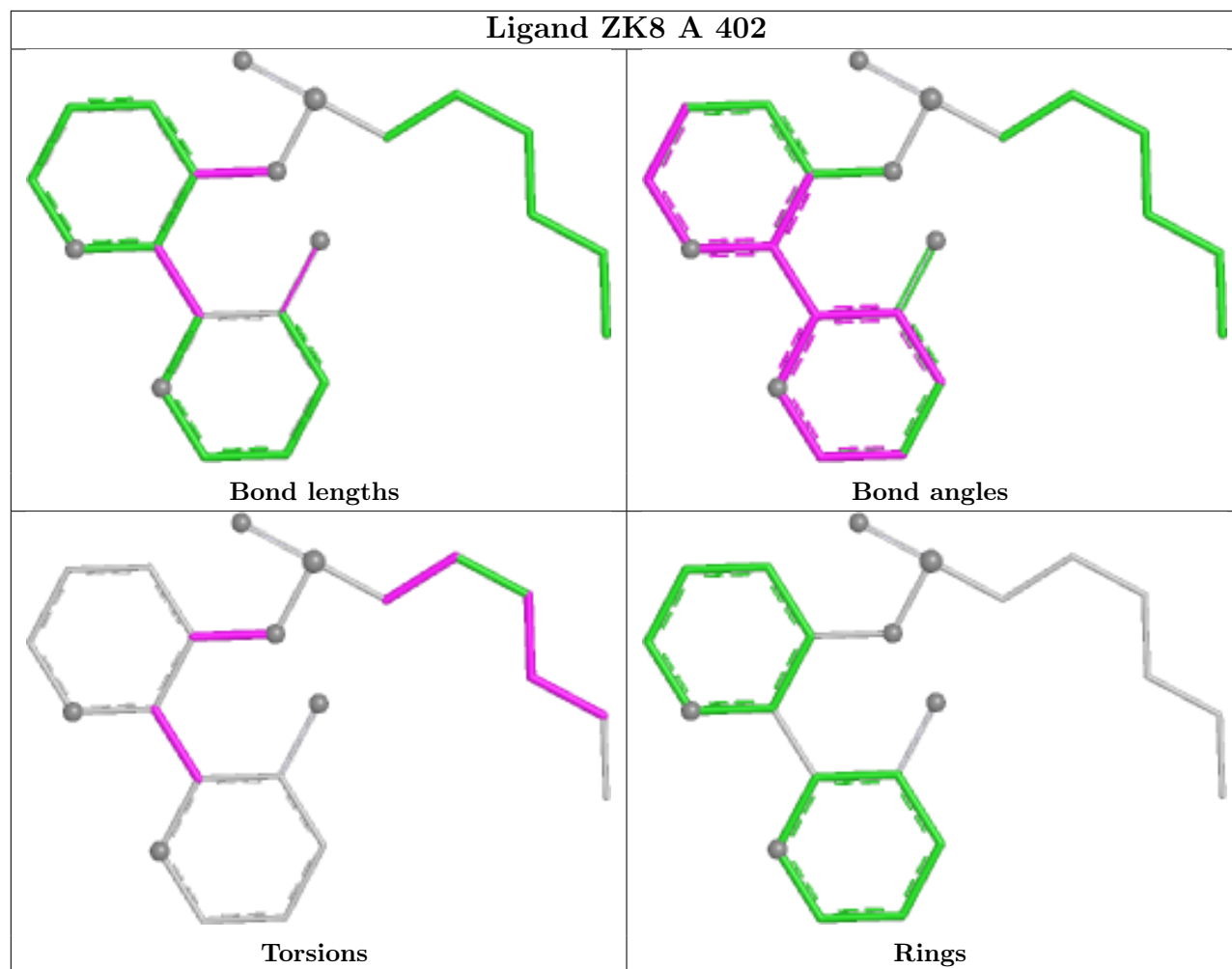
5 monomers are involved in 5 short contacts:

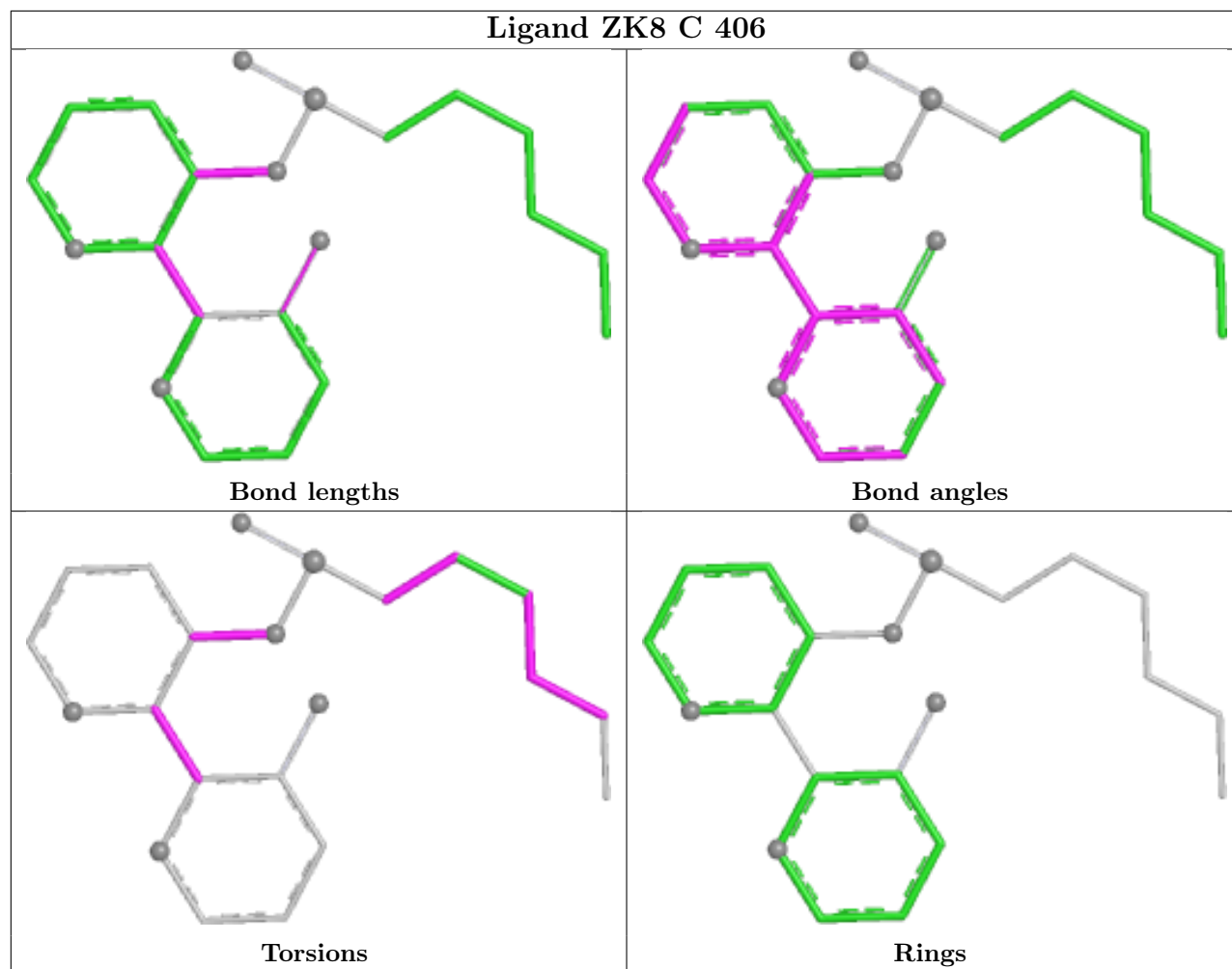
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	ZK8	1	0
3	D	404	ZK8	1	0
3	A	402	ZK8	1	0
3	C	406	ZK8	1	0
4	C	405	PEG	1	0

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









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	315/329 (95%)	0.84	25 (7%) 18 13	25, 46, 74, 103	0
1	B	315/329 (95%)	0.86	23 (7%) 21 15	25, 47, 77, 111	0
1	C	315/329 (95%)	1.38	75 (23%) 2 1	32, 52, 90, 110	0
1	D	315/329 (95%)	1.12	45 (14%) 6 5	25, 48, 77, 116	0
All	All	1260/1316 (95%)	1.05	168 (13%) 7 5	25, 48, 80, 116	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	THR	5.6
1	A	271	GLU	5.3
1	A	267	ASP	4.8
1	A	304	GLU	4.7
1	C	310	GLY	4.5
1	C	8	ASN	4.3
1	C	40	SER	4.3
1	D	209	PHE	4.3
1	D	75	GLU	4.2
1	B	267	ASP	4.2
1	C	19	GLY	4.2
1	C	209	PHE	4.1
1	C	315	THR	4.1
1	D	315	THR	3.9
1	C	176	ASP	3.7
1	C	277	THR	3.7
1	C	276	THR	3.7
1	C	137	ALA	3.6
1	D	161	SER	3.6
1	C	250	VAL	3.5
1	C	37	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	278	TYR	3.4
1	C	271	GLU	3.4
1	A	276	THR	3.4
1	C	262	GLY	3.3
1	C	314	GLY	3.3
1	B	1	MET	3.3
1	D	37	ASP	3.3
1	C	160	ASP	3.2
1	D	197	GLU	3.2
1	A	52	GLU	3.1
1	C	157	VAL	3.1
1	C	1	MET	3.0
1	C	59	ALA	3.0
1	B	308	VAL	3.0
1	D	177	ALA	3.0
1	C	304	GLU	2.9
1	C	61	PRO	2.9
1	C	266	ALA	2.9
1	B	52	GLU	2.9
1	C	131	ILE	2.9
1	D	164	GLY	2.9
1	D	131	ILE	2.9
1	C	132	ASP	2.9
1	C	155	LEU	2.8
1	C	224	PRO	2.8
1	A	193	ASP	2.8
1	D	307	ALA	2.8
1	C	303	ASP	2.8
1	A	306	ALA	2.8
1	D	198	SER	2.8
1	D	11	ASP	2.8
1	C	146	GLU	2.8
1	C	197	GLU	2.8
1	A	303	ASP	2.7
1	C	128	PRO	2.7
1	D	24	LEU	2.7
1	B	271	GLU	2.7
1	B	37	ASP	2.7
1	A	18	ARG	2.7
1	A	75	GLU	2.7
1	A	308	VAL	2.7
1	A	227	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	132	ASP	2.7
1	C	12	LEU	2.6
1	C	52	GLU	2.6
1	A	270	ILE	2.6
1	C	115	ILE	2.6
1	C	41	GLU	2.6
1	C	162	ALA	2.6
1	D	3	LEU	2.6
1	C	208	TYR	2.6
1	C	153	ALA	2.6
1	A	40	SER	2.5
1	A	250	VAL	2.5
1	B	42	ASP	2.5
1	C	24	LEU	2.5
1	C	291	LEU	2.5
1	D	271	GLU	2.5
1	D	134	GLY	2.5
1	C	62	ALA	2.5
1	A	143	ASP	2.5
1	D	132	ASP	2.5
1	D	176	ASP	2.5
1	D	1	MET	2.5
1	B	304	GLU	2.5
1	D	41	GLU	2.5
1	B	61	PRO	2.5
1	B	215	MET	2.5
1	B	62	ALA	2.5
1	C	252	THR	2.4
1	D	18	ARG	2.4
1	A	176	ASP	2.4
1	A	5	GLU	2.4
1	C	74	GLY	2.4
1	A	315	THR	2.4
1	B	277	THR	2.4
1	D	133	ASP	2.4
1	D	215	MET	2.4
1	C	60	GLY	2.4
1	C	308	VAL	2.4
1	A	260	ASP	2.4
1	B	224	PRO	2.4
1	D	224	PRO	2.4
1	C	36	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	2	LEU	2.4
1	A	277	THR	2.4
1	C	312	HIS	2.4
1	D	160	ASP	2.4
1	D	212	LYS	2.4
1	B	76	ALA	2.4
1	D	145	ALA	2.4
1	C	85	TYR	2.3
1	C	281	TYR	2.3
1	B	315	THR	2.3
1	C	174	CYS	2.3
1	D	170	VAL	2.3
1	D	61	PRO	2.3
1	D	19	GLY	2.3
1	C	15	ALA	2.3
1	C	76	ALA	2.3
1	D	148	PHE	2.3
1	C	206	GLU	2.2
1	C	290	SER	2.2
1	C	163	GLY	2.2
1	C	267	ASP	2.2
1	D	267	ASP	2.2
1	C	9	LEU	2.2
1	C	135	ILE	2.2
1	D	135	ILE	2.2
1	C	186	MET	2.2
1	C	215	MET	2.2
1	C	66	ARG	2.2
1	B	220	GLU	2.1
1	C	5	GLU	2.1
1	D	265	TYR	2.1
1	B	164	GLY	2.1
1	A	160	ASP	2.1
1	C	169	VAL	2.1
1	C	228	ASP	2.1
1	A	242	PHE	2.1
1	D	118	ASP	2.1
1	C	198	SER	2.1
1	C	191	ALA	2.1
1	D	62	ALA	2.1
1	B	5	GLU	2.1
1	D	192	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	3	LEU	2.1
1	D	58	PHE	2.1
1	D	76	ALA	2.1
1	C	187	LEU	2.1
1	C	286	HIS	2.1
1	C	255	TYR	2.1
1	C	279	VAL	2.1
1	C	118	ASP	2.0
1	D	309	MET	2.0
1	B	23	GLY	2.0
1	D	74	GLY	2.0
1	D	85	TYR	2.0
1	C	139	ARG	2.0
1	C	261	GLU	2.0
1	B	266	ALA	2.0
1	A	1	MET	2.0
1	B	192	THR	2.0
1	A	269	LEU	2.0
1	D	291	LEU	2.0
1	D	286	HIS	2.0
1	D	208	TYR	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($\text{\AA}^2$)	Q<0.9
2	GOL	C	401	6/6	0.64	0.23	82,86,90,92	0
4	PEG	C	404	7/7	0.66	0.21	65,75,81,82	0

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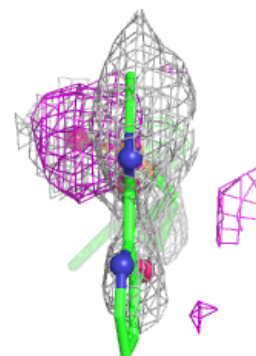
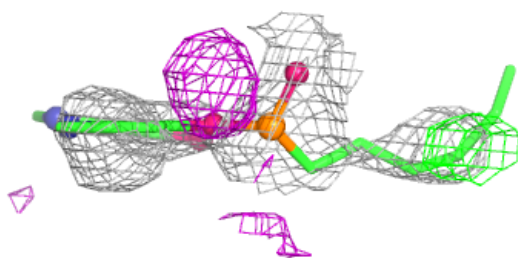
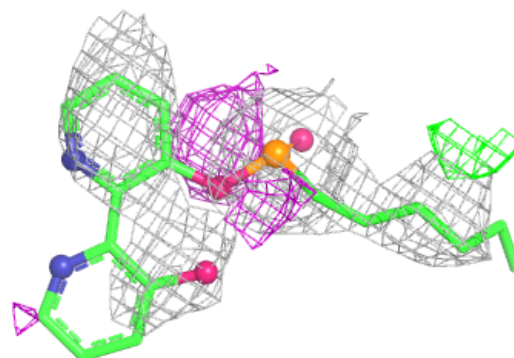
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	C	403	7/7	0.67	0.21	69,76,81,83	0
2	GOL	D	402	6/6	0.69	0.21	56,61,66,67	0
3	ZK8	D	404	22/23	0.70	0.33	68,101,129,134	0
3	ZK8	C	406	22/23	0.71	0.33	66,113,135,139	0
4	PEG	D	403	7/7	0.74	0.17	56,63,67,69	0
4	PEG	C	405	7/7	0.75	0.15	47,52,58,59	0
2	GOL	C	402	6/6	0.76	0.14	51,61,65,65	0
3	ZK8	B	402	22/23	0.77	0.30	63,112,129,140	0
3	ZK8	A	402	22/23	0.78	0.30	70,120,150,157	0
2	GOL	A	401	6/6	0.80	0.24	64,80,83,83	0
2	GOL	B	401	6/6	0.82	0.17	72,73,77,86	0
2	GOL	D	401	6/6	0.85	0.16	68,74,75,78	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.

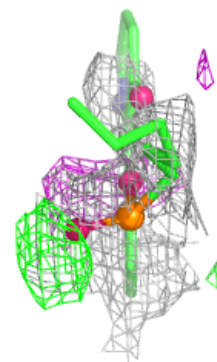
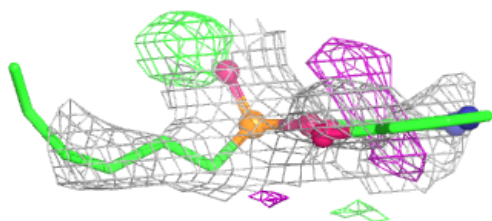
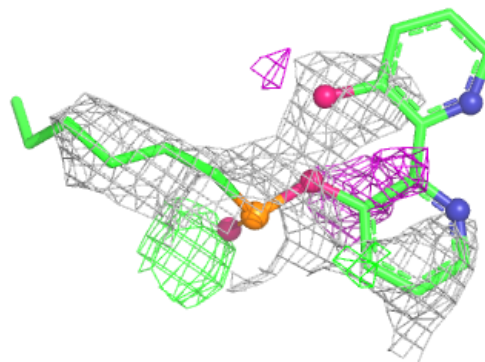
Electron density around ZK8 D 404:

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

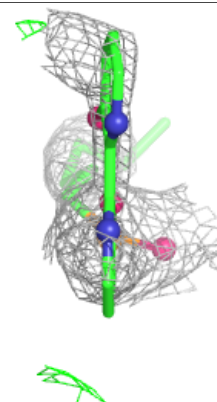
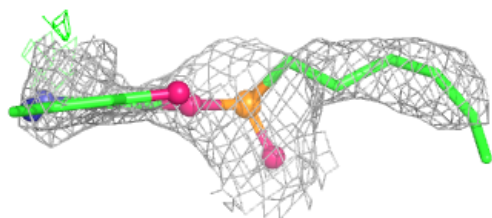
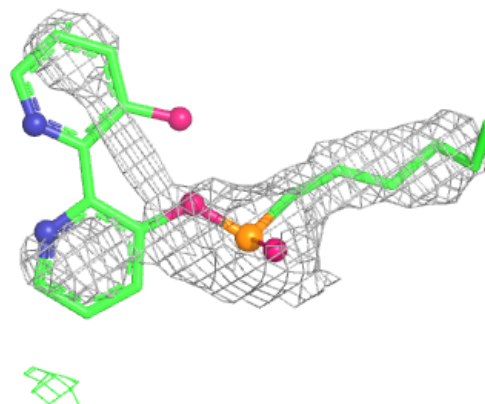


Electron density around ZK8 C 406:

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

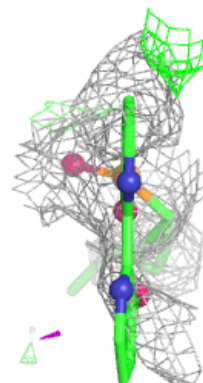
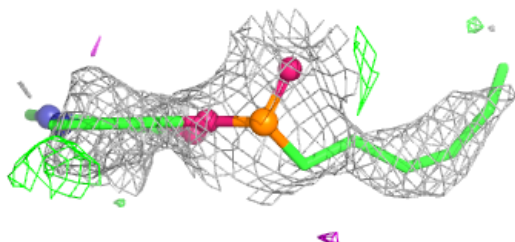
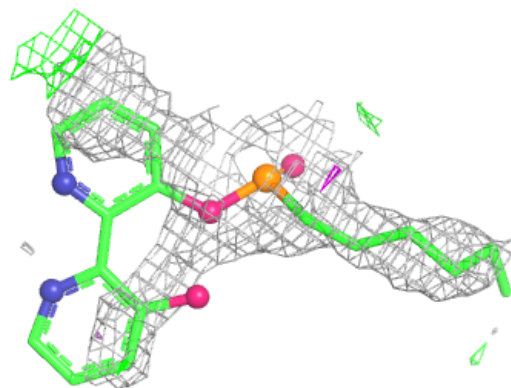
**Electron density around ZK8 B 402:**

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



Electron density around ZK8 A 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.