



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:27 AM UTC

PDB ID : 4RKD / pdb_00004rkd
Title : Psychrophilic aromatic amino acids aminotransferase from Psychrobacter sp.
B6 cocrystalized with aspartic acid
Authors : Bujacz, A.; Rutkiewicz-Krotewicz, M.; Bujacz, G.; Nowakowska-Sapota, K.;
Turkiewicz, M.
Deposited on : 2014-10-12
Resolution : 2.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

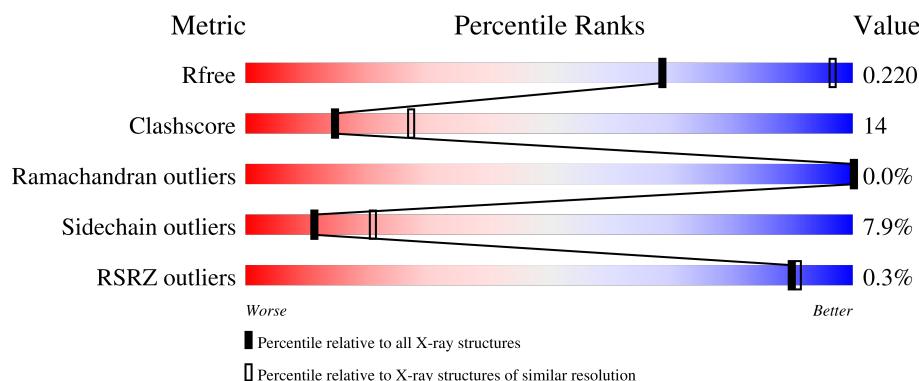
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	398	% 67% 29% .
1	B	398	% 67% 29% .
1	C	398	67% 28% 5%
1	D	398	63% 33% .

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Mol	Chain	Length	Quality of chain
1	E	398	 % 66% 30% •
1	F	398	 73% 23% •
1	G	398	 63% 33% •
1	H	398	 75% 22% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLP	B	401	-	X	-	-
4	KET	E	404[B]	-	-	X	-
6	PMP	D	401	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25951 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.

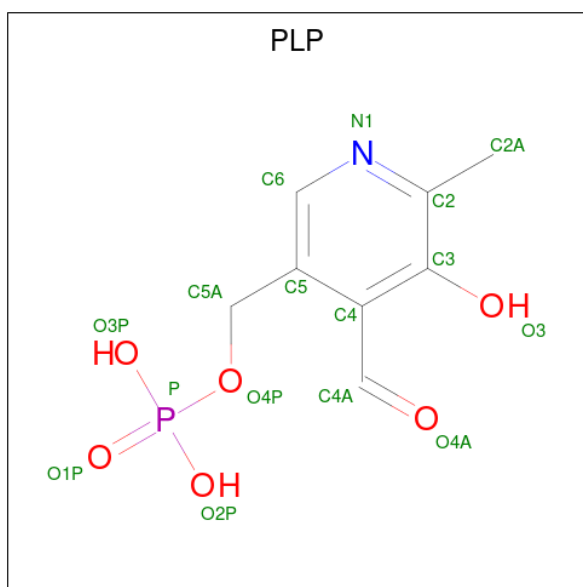
- Molecule 1 is a protein called Aromatic amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	2	0
			3115	1981	520	592	22			
1	B	398	Total	C	N	O	S	0	5	0
			3137	1994	524	597	22			
1	C	398	Total	C	N	O	S	0	2	0
			3110	1977	516	595	22			
1	D	398	Total	C	N	O	S	0	0	0
			3101	1971	516	592	22			
1	E	398	Total	C	N	O	S	0	3	0
			3121	1985	520	594	22			
1	F	398	Total	C	N	O	S	0	3	0
			3118	1981	517	598	22			
1	G	398	Total	C	N	O	S	0	2	0
			3117	1981	522	592	22			
1	H	398	Total	C	N	O	S	0	2	0
			3113	1979	518	594	22			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



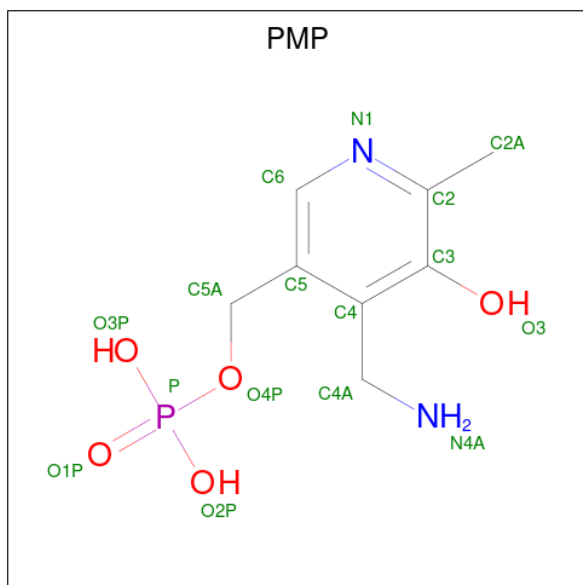
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (CCD ID: KET) (formula: C₁₂H₁₆N₂O₉P).

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
6	H	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	142	Total	O	0	0
			142	142		
7	C	83	Total	O	0	0
			83	83		
7	D	119	Total	O	0	0
			119	119		
7	E	84	Total	O	0	0
			84	84		
7	F	96	Total	O	0	0
			96	96		

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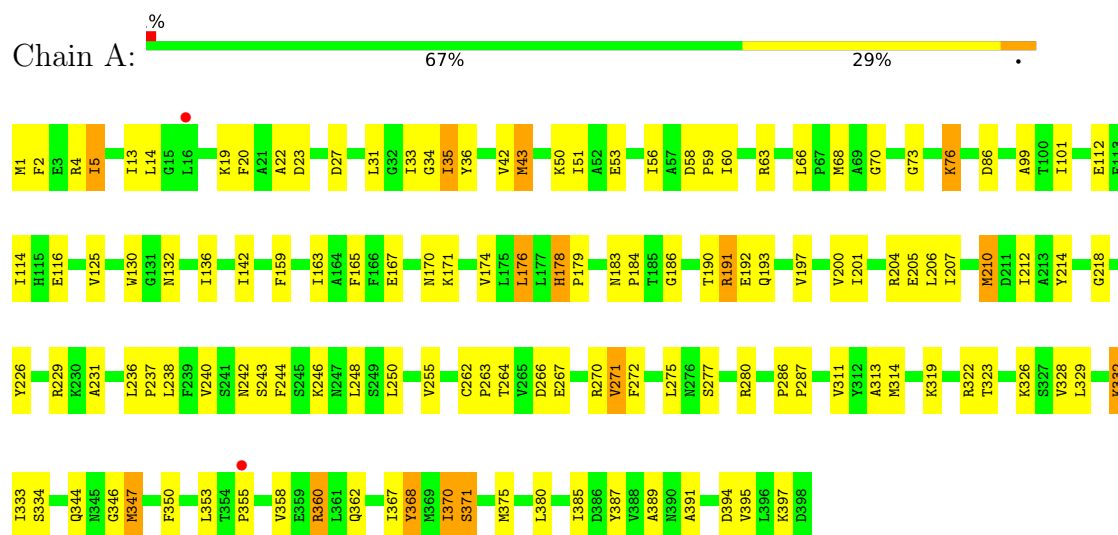
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	70	Total 70	O 70	0	0
7	H	122	Total 122	O 122	0	0

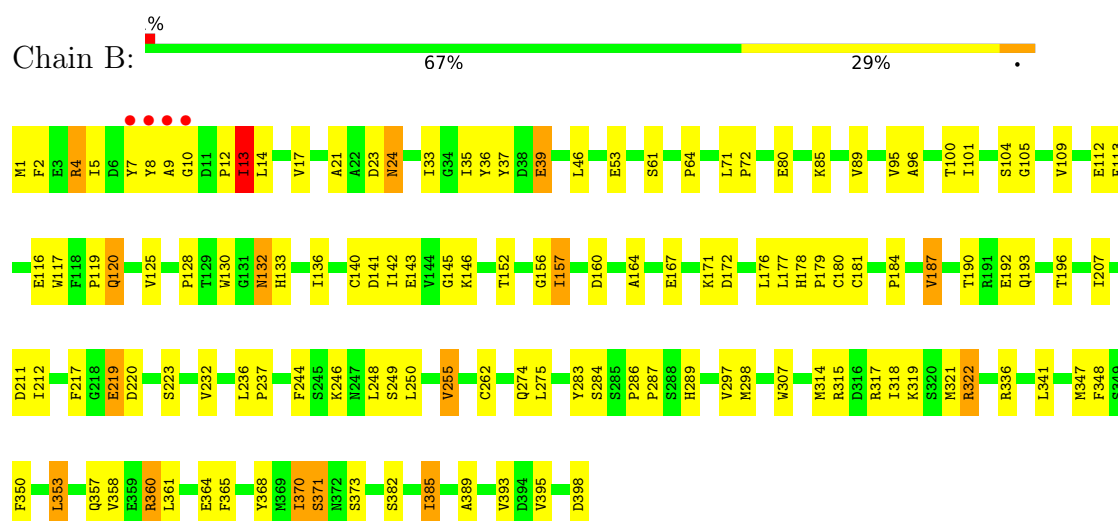
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Aromatic amino acid aminotransferase

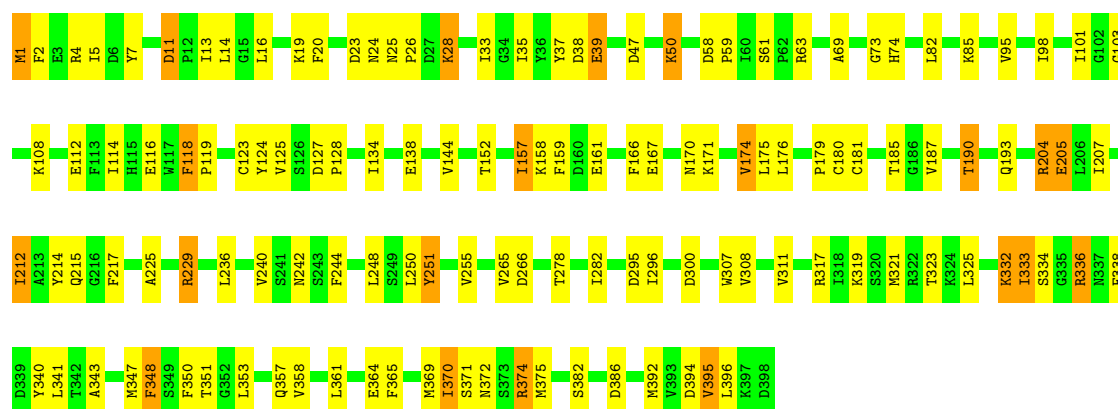


- Molecule 1: Aromatic amino acid aminotransferase



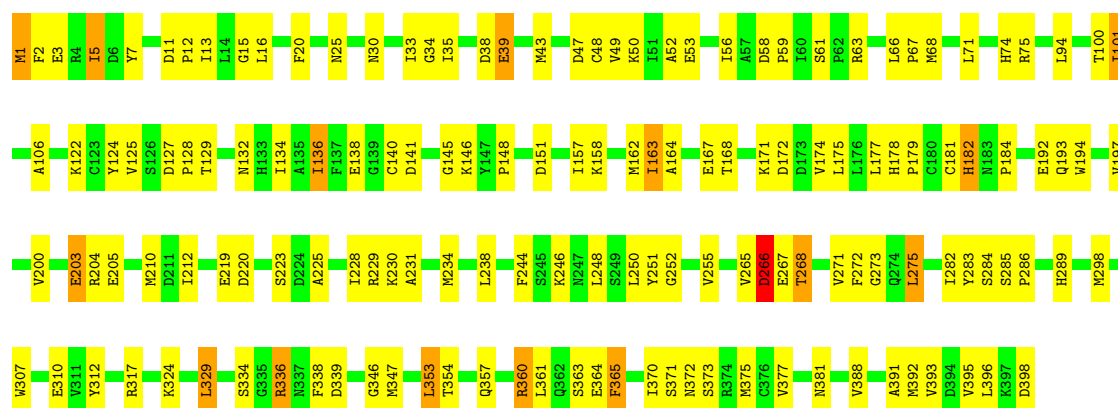
- Molecule 1: Aromatic amino acid aminotransferase





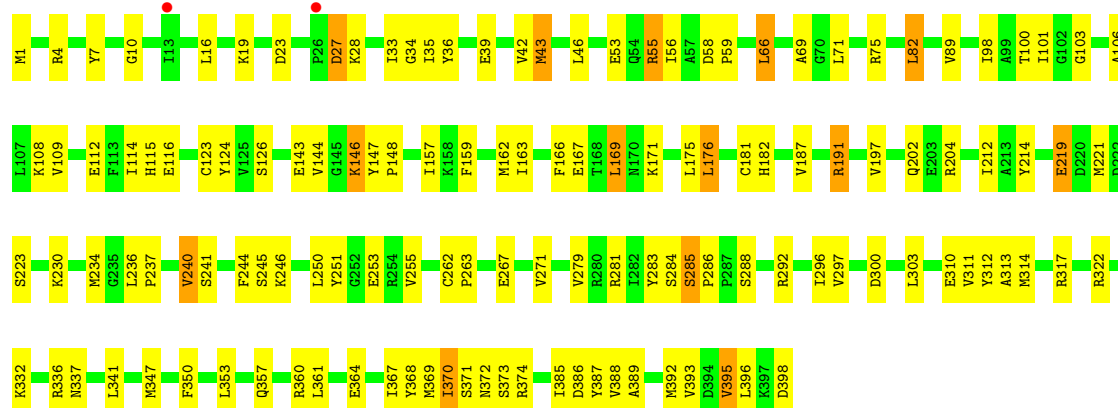
- Molecule 1: Aromatic amino acid aminotransferase

Chain D: 63% 33% .



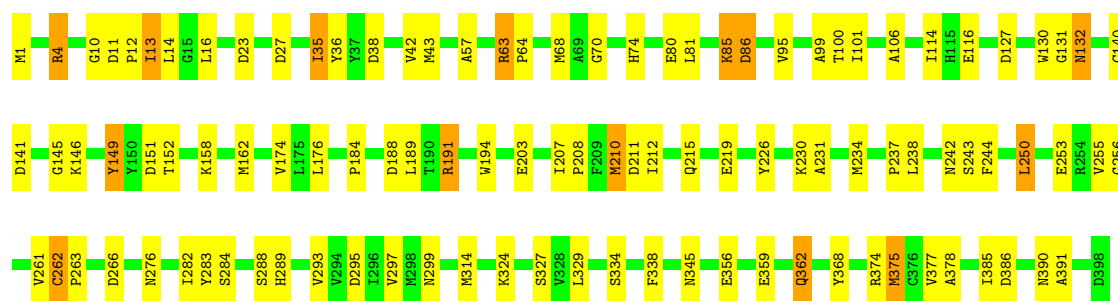
- Molecule 1: Aromatic amino acid aminotransferase

Chain E: 66% 30% .



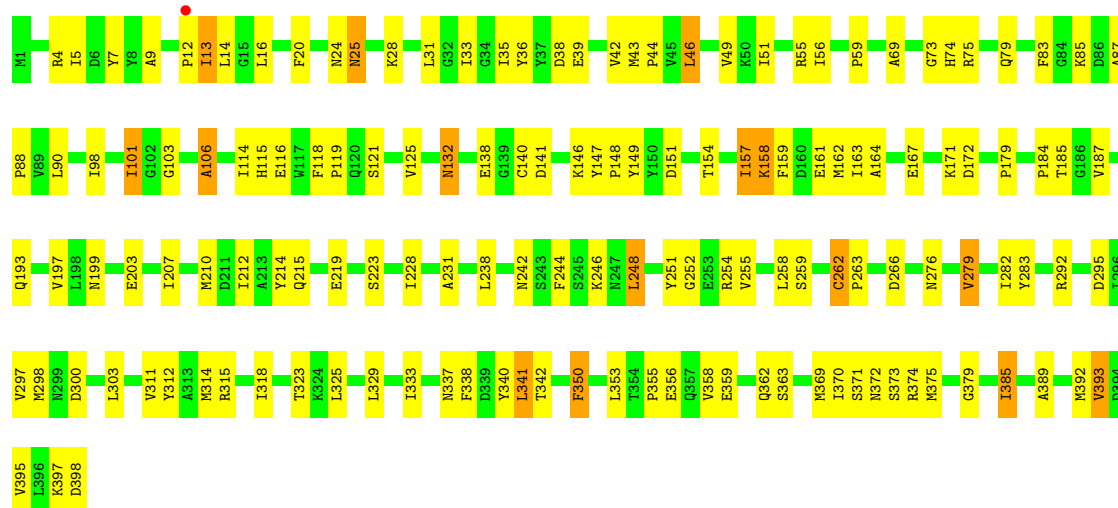
- Molecule 1: Aromatic amino acid aminotransferase

Chain F: 73% 23% .



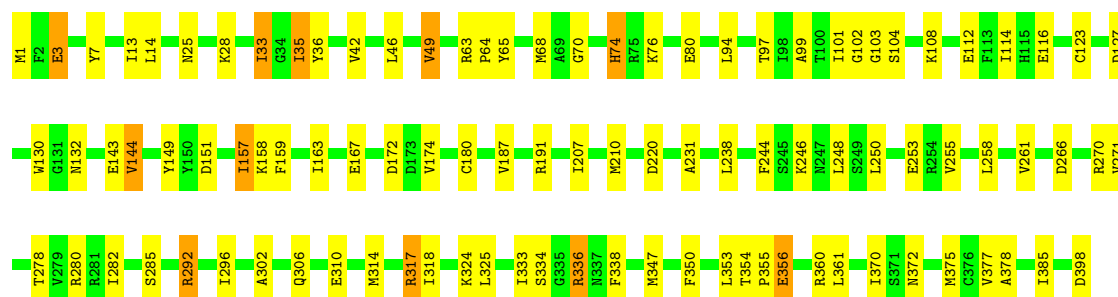
• Molecule 1: Aromatic amino acid aminotransferase

Chain G: 63% 33% .



• Molecule 1: Aromatic amino acid aminotransferase

Chain H: 75% 22% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.25Å 103.23Å 165.78Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	45.74 – 2.76 45.74 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.74-2.76) 97.4 (45.74-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.222 0.173 , 0.220	Depositor DCC
R_{free} test set	3862 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25951	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 43.05 % 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 1.8670e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, PMP, KET, MG, OAA

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	1.09	0/3190	1.36	22/4321 (0.5%)
1	B	1.22	5/3218 (0.2%)	1.38	16/4358 (0.4%)
1	C	1.09	2/3185 (0.1%)	1.32	15/4316 (0.3%)
1	D	1.26	3/3170 (0.1%)	1.41	24/4296 (0.6%)
1	E	1.11	1/3199 (0.0%)	1.32	18/4333 (0.4%)
1	F	1.14	0/3193	1.34	16/4328 (0.4%)
1	G	1.03	0/3192	1.30	18/4324 (0.4%)
1	H	1.16	1/3185 (0.0%)	1.31	12/4315 (0.3%)
All	All	1.14	12/25532 (0.0%)	1.34	141/34591 (0.4%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	ARG	CA-C	6.59	1.61	1.52
1	C	236	LEU	CA-C	6.14	1.60	1.53
1	E	240	VAL	CA-C	-5.84	1.45	1.52
1	H	302	ALA	CA-C	5.75	1.60	1.52
1	B	145	GLY	N-CA	5.64	1.50	1.44

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	285	SER	CA-C-N	11.94	128.26	119.66
1	E	285	SER	C-N-CA	11.94	128.26	119.66
1	D	285	SER	CA-C-N	9.54	126.53	119.66
1	D	285	SER	C-N-CA	9.54	126.53	119.66
1	A	43	MET	CA-C-N	-9.46	110.63	120.85

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	3115	0	3059	93	0
1	B	3137	0	3081	98	0
1	C	3110	0	3044	93	0
1	D	3101	0	3036	100	0
1	E	3121	0	3065	110	0
1	F	3118	0	3047	67	0
1	G	3117	0	3062	97	0
1	H	3113	0	3053	63	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	6	2	0
3	C	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	6	2	0
4	A	24	0	12	5	0
4	E	24	0	11	12	0
4	G	24	0	12	3	0
5	C	9	0	2	1	0
5	E	9	0	2	0	0
6	D	16	0	11	8	0
6	H	16	0	11	3	0
7	A	102	0	0	6	0
7	B	142	0	0	16	0
7	C	83	0	0	6	0
7	D	119	0	0	6	0
7	E	84	0	0	13	0
7	F	96	0	0	4	0
7	G	70	0	0	5	0
7	H	122	0	0	5	0
All	All	25951	0	24540	689	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 14.

The worst 5 of 689 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:246:LYS:HE3	6:D:401:PMP:N4A	1.44	1.29
1:D:246:LYS:CE	6:D:401:PMP:HNA2	1.56	1.17
1:G:246:LYS:HZ1	4:G:402:KET:H4A	1.15	1.09
1:D:33:ILE:HG13	1:D:35:ILE:HG12	1.37	1.07
1:C:11:ASP:HB2	1:C:14:LEU:HB2	1.32	1.06

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	398/398 (100%)	377 (95%)	21 (5%)	0	100	100
1	B	401/398 (101%)	383 (96%)	18 (4%)	0	100	100
1	C	398/398 (100%)	374 (94%)	23 (6%)	1 (0%)	36	56
1	D	396/398 (100%)	377 (95%)	19 (5%)	0	100	100
1	E	399/398 (100%)	373 (94%)	26 (6%)	0	100	100
1	F	399/398 (100%)	380 (95%)	19 (5%)	0	100	100
1	G	398/398 (100%)	372 (94%)	26 (6%)	0	100	100
1	H	398/398 (100%)	371 (93%)	27 (7%)	0	100	100
All	All	3187/3184 (100%)	3007 (94%)	179 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/337 (101%)	307 (91%)	32 (9%)	8	16
1	B	342/337 (102%)	317 (93%)	25 (7%)	13	24
1	C	339/337 (101%)	305 (90%)	34 (10%)	7	14
1	D	337/337 (100%)	310 (92%)	27 (8%)	11	20
1	E	340/337 (101%)	315 (93%)	25 (7%)	13	24
1	F	340/337 (101%)	316 (93%)	24 (7%)	13	25
1	G	339/337 (101%)	311 (92%)	28 (8%)	10	19
1	H	339/337 (101%)	320 (94%)	19 (6%)	19	36
All	All	2715/2696 (101%)	2501 (92%)	214 (8%)	11	21

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	365	PHE
1	F	4	ARG
1	H	42	VAL
1	E	35	ILE
1	E	212	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	24	ASN
1	G	345	ASN
1	G	74	HIS
1	G	276	ASN
1	H	24	ASN

5.3.3 RNA ⓘ

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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	PLP	C	402	1	15,15,16	4.12	4 (26%)	21,22,23	2.75	9 (42%)
3	PLP	B	401	1	15,15,16	3.34	4 (26%)	21,22,23	2.93	11 (52%)
5	OAA	E	403	-	8,8,8	2.47	2 (25%)	8,10,10	1.74	3 (37%)
3	PLP	E	402[A]	1	15,15,16	3.29	4 (26%)	21,22,23	1.71	3 (14%)
4	KET	E	404[B]	-	22,24,24	1.28	1 (4%)	21,34,34	2.76	5 (23%)
6	PMP	D	401	-	16,16,16	2.86	3 (18%)	22,23,23	1.79	4 (18%)
4	KET	A	403[B]	-	22,24,24	1.32	3 (13%)	21,34,34	1.90	5 (23%)
6	PMP	H	401	-	16,16,16	3.87	4 (25%)	22,23,23	1.91	6 (27%)
4	KET	G	402	-	22,24,24	1.50	5 (22%)	21,34,34	2.83	9 (42%)
3	PLP	A	402[A]	1	15,15,16	3.43	3 (20%)	21,22,23	1.73	7 (33%)
5	OAA	C	403	-	8,8,8	2.26	1 (12%)	8,10,10	1.82	3 (37%)
3	PLP	F	401	1	15,15,16	4.01	3 (20%)	21,22,23	2.22	6 (28%)

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	PLP	C	402	1	-	3/6/6/8	0/1/1/1
3	PLP	B	401	1	-	3/6/6/8	0/1/1/1
5	OAA	E	403	-	-	3/8/8/8	-
3	PLP	E	402[A]	1	-	5/6/6/8	0/1/1/1
4	KET	E	404[B]	-	-	11/18/19/19	0/1/1/1
6	PMP	D	401	-	-	4/8/8/8	0/1/1/1
4	KET	A	403[B]	-	-	7/18/19/19	0/1/1/1
6	PMP	H	401	-	-	7/8/8/8	0/1/1/1
4	KET	G	402	-	-	6/18/19/19	0/1/1/1
3	PLP	A	402[A]	1	-	2/6/6/8	0/1/1/1
5	OAA	C	403	-	-	5/8/8/8	-
3	PLP	F	401	1	-	2/6/6/8	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	PLP	C5-C4	11.70	1.53	1.40
6	H	401	PMP	C3-C2	11.62	1.53	1.41
3	B	401	PLP	C3-C2	10.35	1.51	1.41
3	C	402	PLP	C3-C2	9.74	1.51	1.41
3	C	402	PLP	C5-C4	9.32	1.51	1.40

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404[B]	KET	CA-N-C4A	10.26	139.33	117.01
4	G	402	KET	CA-N-C4A	7.61	133.57	117.01
3	B	401	PLP	C6-C5-C4	6.57	123.48	118.10
3	C	402	PLP	C6-C5-C4	6.45	123.38	118.10
3	B	401	PLP	C5A-C5-C4	-6.06	110.68	122.64

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402[A]	PLP	C4-C5-C5A-O4P
3	A	402[A]	PLP	C6-C5-C5A-O4P
3	B	401	PLP	C5A-O4P-P-O1P
3	B	401	PLP	C5A-O4P-P-O2P
3	B	401	PLP	C5A-O4P-P-O3P

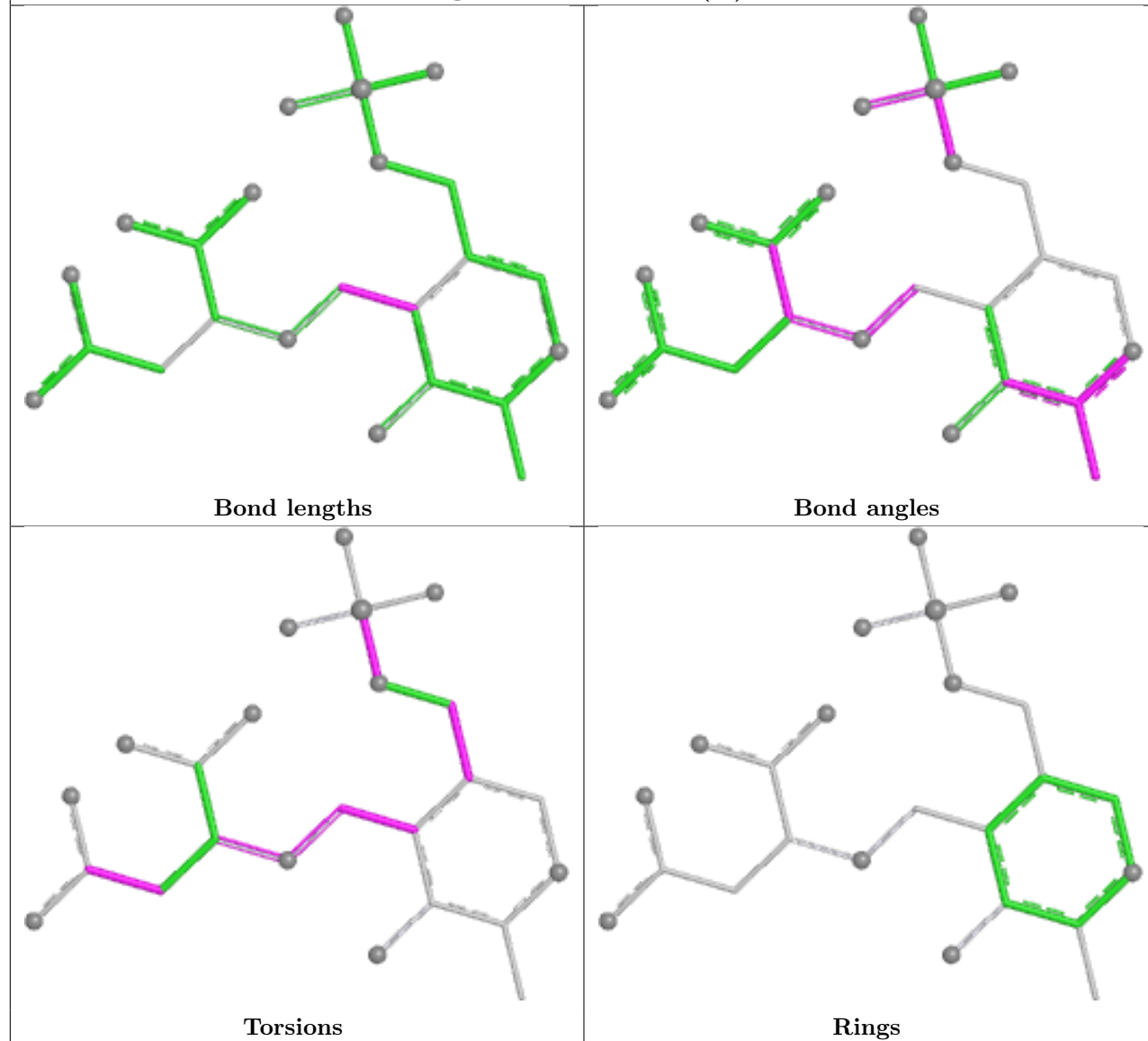
There are no ring outliers.

11 monomers are involved in 38 short contacts:

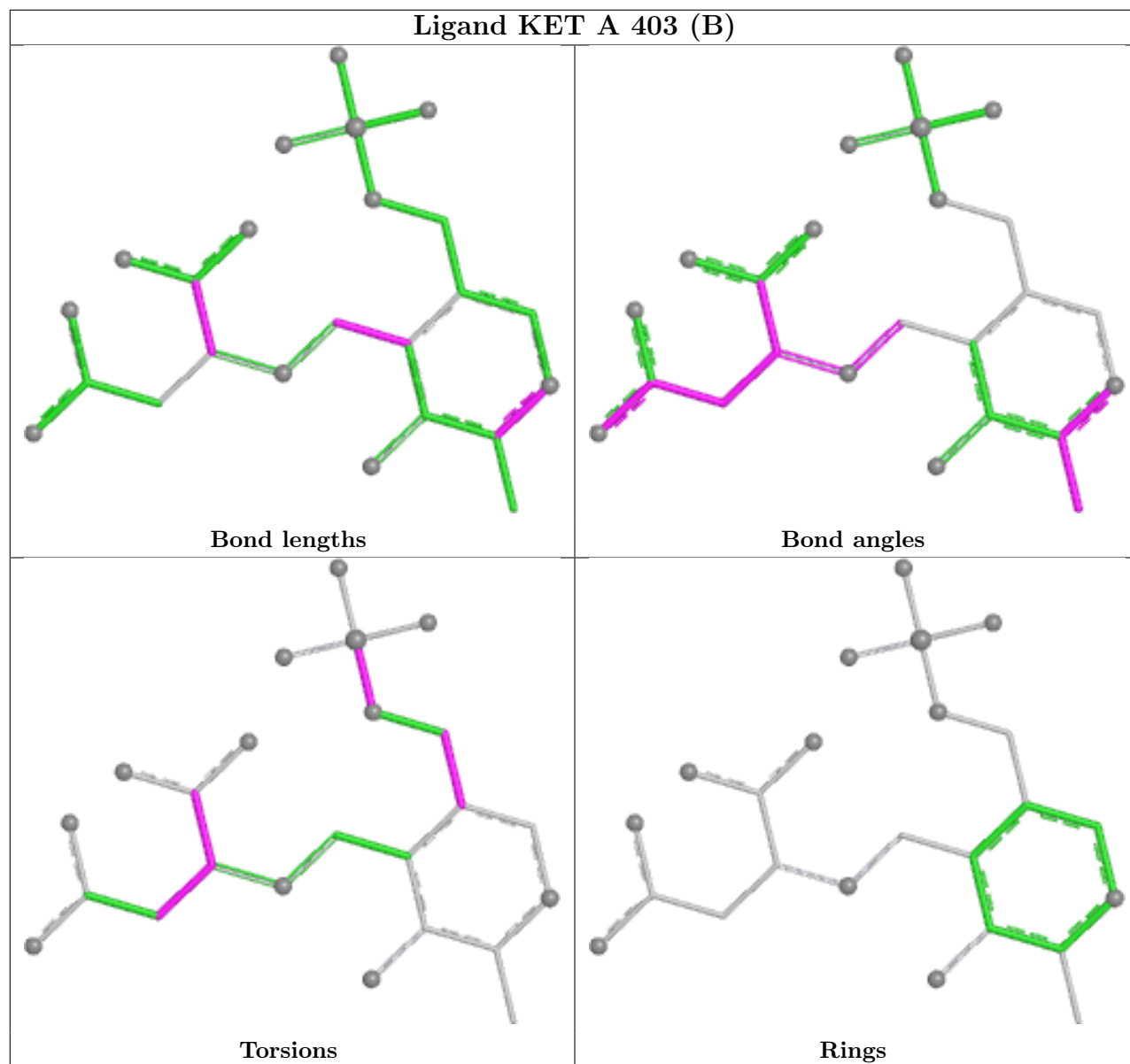
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	PLP	1	0
3	B	401	PLP	2	0
3	E	402[A]	PLP	1	0
4	E	404[B]	KET	12	0
6	D	401	PMP	8	0
4	A	403[B]	KET	5	0
6	H	401	PMP	3	0
4	G	402	KET	3	0
3	A	402[A]	PLP	1	0
5	C	403	OAA	1	0
3	F	401	PLP	2	0

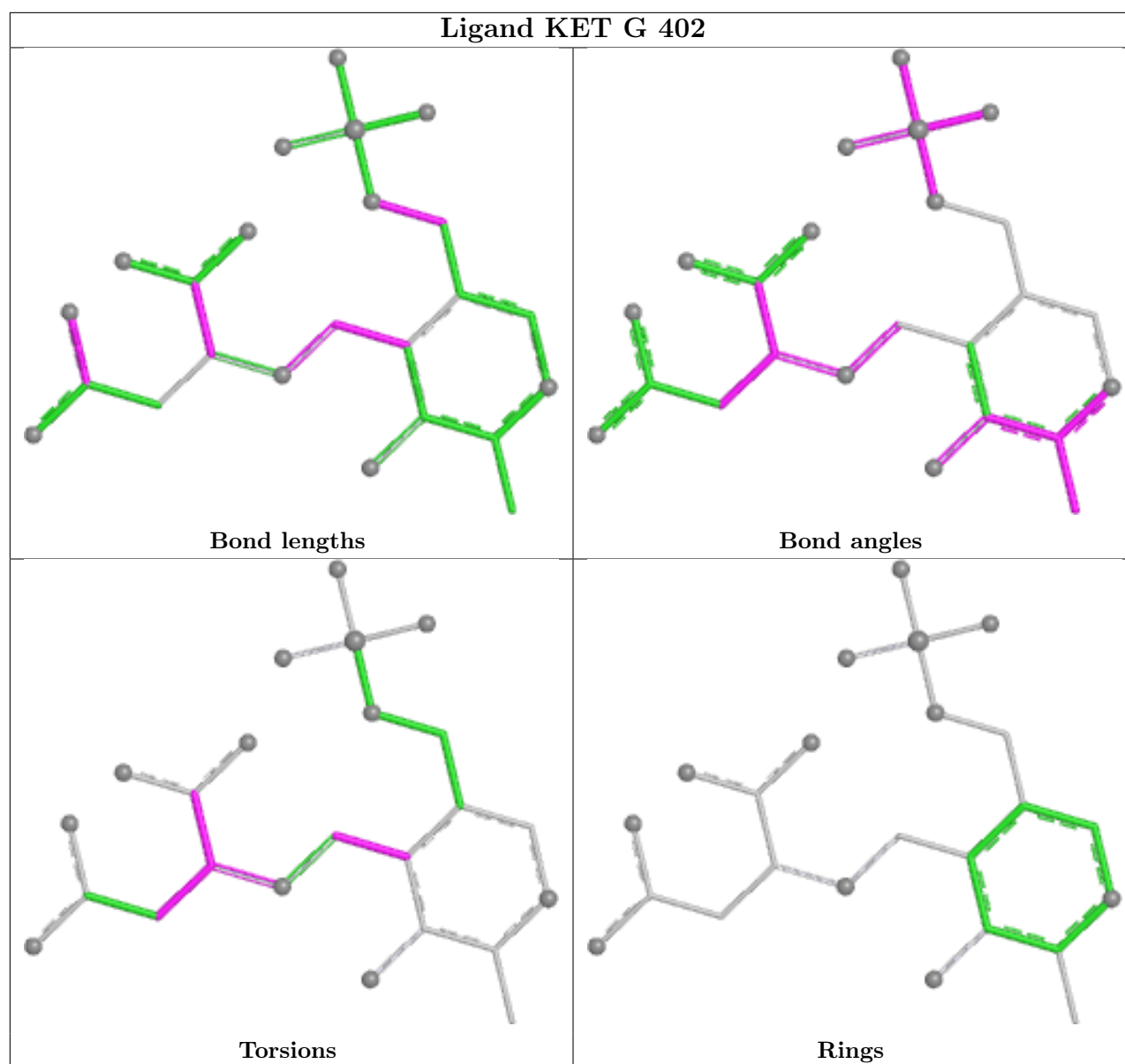
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand KET E 404 (B)



Ligand KET A 403 (B)





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	398/398 (100%)	-0.34	2 (0%) 87 87	13, 36, 94, 128	2 (0%)
1	B	398/398 (100%)	-0.55	4 (1%) 79 79	13, 31, 64, 114	5 (1%)
1	C	398/398 (100%)	-0.31	0 100 100	22, 42, 86, 130	2 (0%)
1	D	398/398 (100%)	-0.63	0 100 100	17, 29, 55, 99	0
1	E	398/398 (100%)	-0.35	2 (0%) 87 87	18, 37, 89, 123	3 (0%)
1	F	398/398 (100%)	-0.53	0 100 100	17, 34, 61, 94	3 (0%)
1	G	398/398 (100%)	-0.25	1 (0%) 90 91	19, 45, 85, 112	2 (0%)
1	H	398/398 (100%)	-0.58	0 100 100	15, 31, 66, 93	2 (0%)
All	All	3184/3184 (100%)	-0.44	9 (0%) 90 91	13, 35, 78, 130	19 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	12	PRO	3.0
1	B	7	TYR	2.8
1	B	9	ALA	2.7
1	A	16	LEU	2.7
1	B	8	TYR	2.1

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 ⓘ

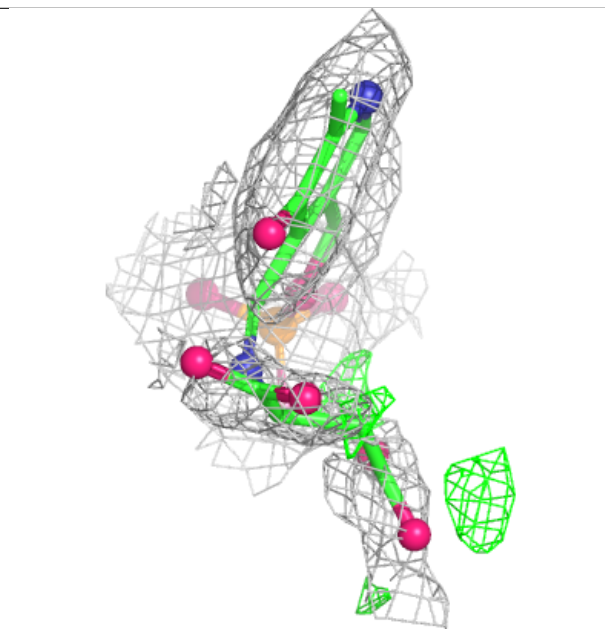
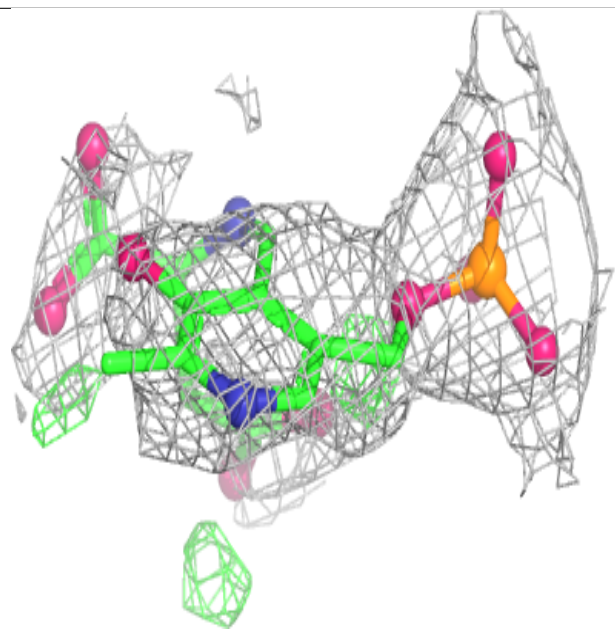
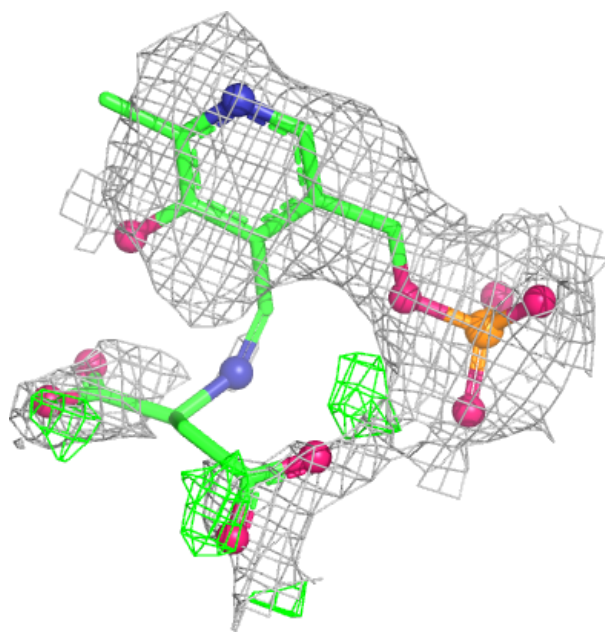
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	OAA	C	403	9/9	0.85	0.14	26,28,31,32	9
4	KET	E	404[B]	24/24	0.87	0.15	24,38,42,44	24
5	OAA	E	403	9/9	0.90	0.12	20,24,27,27	9
4	KET	A	403[B]	24/24	0.95	0.09	9,12,13,14	24
3	PLP	E	402[A]	15/16	0.96	0.11	30,61,71,71	15
3	PLP	A	402[A]	15/16	0.97	0.07	34,39,43,50	15
4	KET	G	402	24/24	0.97	0.08	27,45,90,102	0
3	PLP	C	402	15/16	0.98	0.07	21,35,46,48	0
2	MG	C	401	1/1	0.98	0.03	25,25,25,25	0
3	PLP	F	401	15/16	0.98	0.06	21,25,30,30	0
3	PLP	B	401	15/16	0.98	0.06	18,26,35,38	0
6	PMP	D	401	16/16	0.98	0.06	19,28,34,35	0
6	PMP	H	401	16/16	0.98	0.05	22,29,35,36	0
2	MG	A	401	1/1	0.99	0.05	15,15,15,15	0
2	MG	E	401	1/1	0.99	0.03	13,13,13,13	0
2	MG	G	401	1/1	1.00	0.01	19,19,19,19	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.

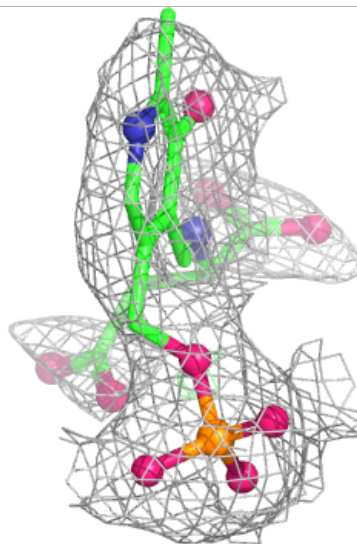
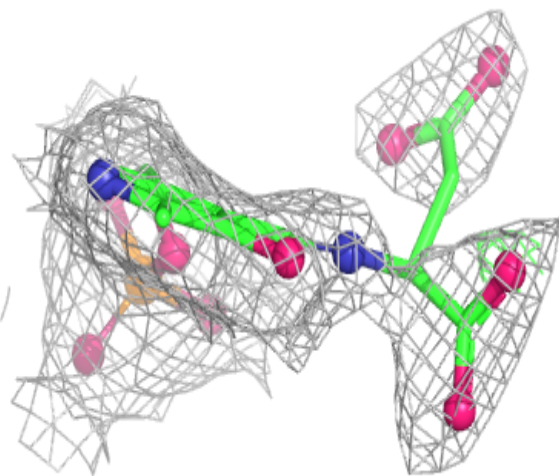
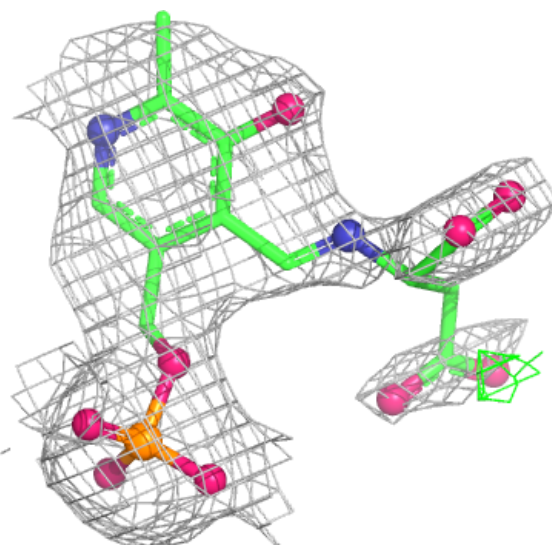
Electron density around KET E 404 (B):

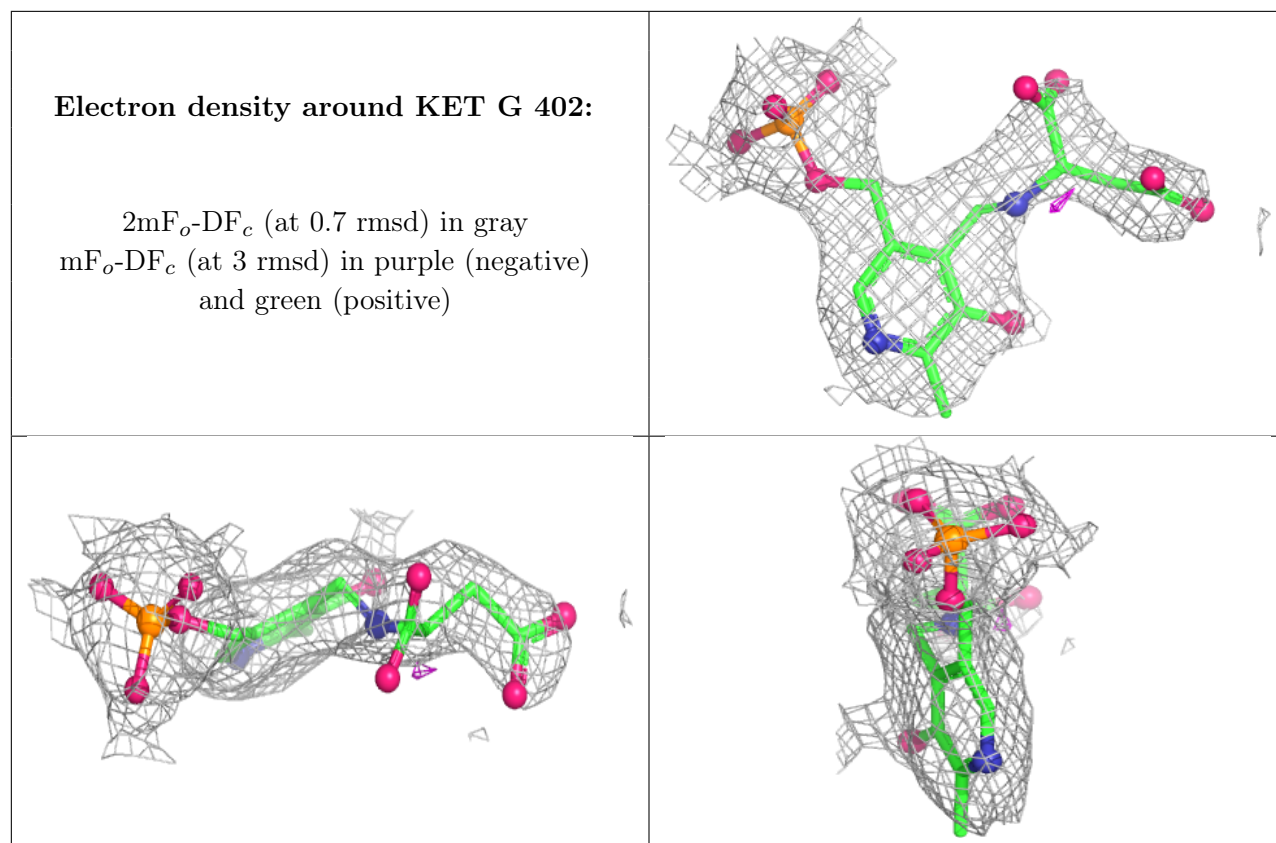
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KET A 403 (B):

$2mF_o-DF_c$ (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.