



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:44 PM UTC

PDB ID : 5QRD / pdb_00005qrd
Title : PanDDA analysis group deposition – Crystal Structure of human ALAS2A in complex with Z1328968520
Authors : Bezerra, G.A.; Foster, W.; Bailey, H.; Shrestha, L.; Krojer, T.; Talon, R.; Brandao-Neto, J.; Douangamath, A.; Nicola, B.B.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Brennan, P.E.; Yue, W.W.
Deposited on : 2019-05-22
Resolution : 1.76 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](#) ①) 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

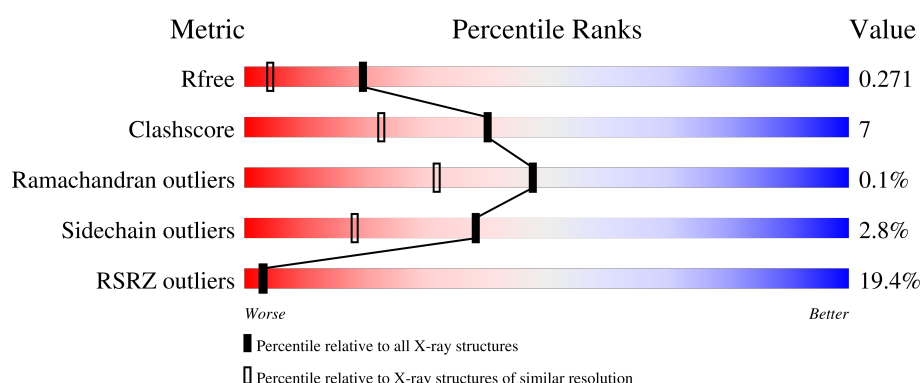
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	469	23% 79% 12% • 9%
1	B	469	13% 76% 14% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6919 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 5-aminolevulinate synthase, erythroid-specific, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	428	Total	C	N	O	S	0	1	0
			3302	2102	577	601	22			
1	A	429	Total	C	N	O	S	0	1	0
			3322	2114	587	599	22			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	MET	-	initiating methionine	UNP P22557
B	120	GLY	-	expression tag	UNP P22557
B	121	HIS	-	expression tag	UNP P22557
B	122	HIS	-	expression tag	UNP P22557
B	123	HIS	-	expression tag	UNP P22557
B	124	HIS	-	expression tag	UNP P22557
B	125	HIS	-	expression tag	UNP P22557
B	126	HIS	-	expression tag	UNP P22557
B	127	SER	-	expression tag	UNP P22557
B	128	SER	-	expression tag	UNP P22557
B	129	GLY	-	expression tag	UNP P22557
B	130	VAL	-	expression tag	UNP P22557
B	131	ASP	-	expression tag	UNP P22557
B	132	LEU	-	expression tag	UNP P22557
B	133	GLY	-	expression tag	UNP P22557
B	134	THR	-	expression tag	UNP P22557
B	135	GLU	-	expression tag	UNP P22557
B	136	ASN	-	expression tag	UNP P22557
B	137	LEU	-	expression tag	UNP P22557
B	138	TYR	-	expression tag	UNP P22557
B	139	PHE	-	expression tag	UNP P22557
B	140	GLN	-	expression tag	UNP P22557
B	141	SER	-	expression tag	UNP P22557
B	142	MET	-	expression tag	UNP P22557
B	221	VAL	ALA	conflict	UNP P22557

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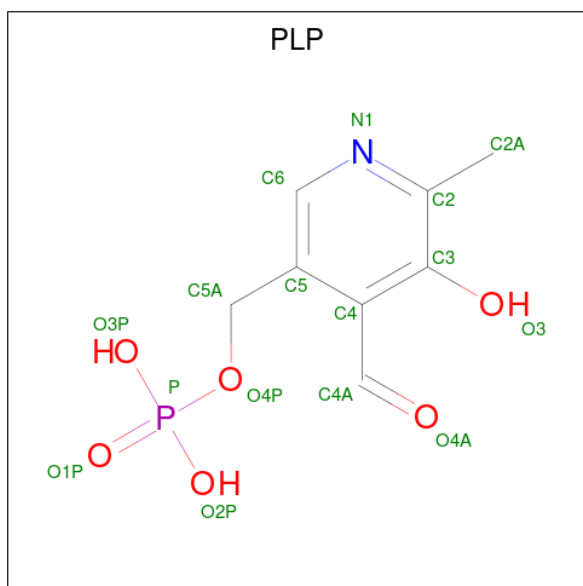
Chain	Residue	Modelled	Actual	Comment	Reference
B	579	GLY	-	expression tag	UNP P22557
B	580	PRO	-	expression tag	UNP P22557
B	581	GLN	-	expression tag	UNP P22557
B	582	TYR	-	expression tag	UNP P22557
B	583	VAL	-	expression tag	UNP P22557
B	584	THR	-	expression tag	UNP P22557
B	585	THR	-	expression tag	UNP P22557
B	586	TYR	-	expression tag	UNP P22557
B	587	ALA	-	expression tag	UNP P22557
A	119	MET	-	initiating methionine	UNP P22557
A	120	GLY	-	expression tag	UNP P22557
A	121	HIS	-	expression tag	UNP P22557
A	122	HIS	-	expression tag	UNP P22557
A	123	HIS	-	expression tag	UNP P22557
A	124	HIS	-	expression tag	UNP P22557
A	125	HIS	-	expression tag	UNP P22557
A	126	HIS	-	expression tag	UNP P22557
A	127	SER	-	expression tag	UNP P22557
A	128	SER	-	expression tag	UNP P22557
A	129	GLY	-	expression tag	UNP P22557
A	130	VAL	-	expression tag	UNP P22557
A	131	ASP	-	expression tag	UNP P22557
A	132	LEU	-	expression tag	UNP P22557
A	133	GLY	-	expression tag	UNP P22557
A	134	THR	-	expression tag	UNP P22557
A	135	GLU	-	expression tag	UNP P22557
A	136	ASN	-	expression tag	UNP P22557
A	137	LEU	-	expression tag	UNP P22557
A	138	TYR	-	expression tag	UNP P22557
A	139	PHE	-	expression tag	UNP P22557
A	140	GLN	-	expression tag	UNP P22557
A	141	SER	-	expression tag	UNP P22557
A	142	MET	-	expression tag	UNP P22557
A	221	VAL	ALA	conflict	UNP P22557
A	579	GLY	-	expression tag	UNP P22557
A	580	PRO	-	expression tag	UNP P22557
A	581	GLN	-	expression tag	UNP P22557
A	582	TYR	-	expression tag	UNP P22557
A	583	VAL	-	expression tag	UNP P22557
A	584	THR	-	expression tag	UNP P22557
A	585	THR	-	expression tag	UNP P22557
A	586	TYR	-	expression tag	UNP P22557

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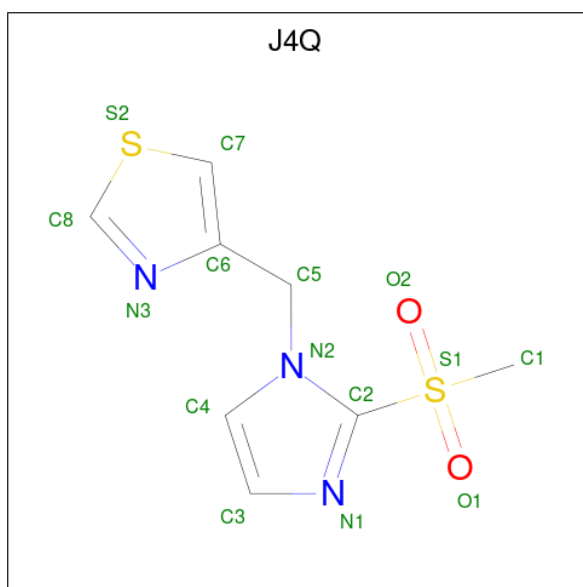
Chain	Residue	Modelled	Actual	Comment	Reference
A	587	ALA	-	expression tag	UNP P22557

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is 4-[(2-methylsulfonylimidazol-1-yl)methyl]-1,3-thiazole (CCD ID: J4Q) (formula: $C_8H_9N_3O_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	3	2	2		

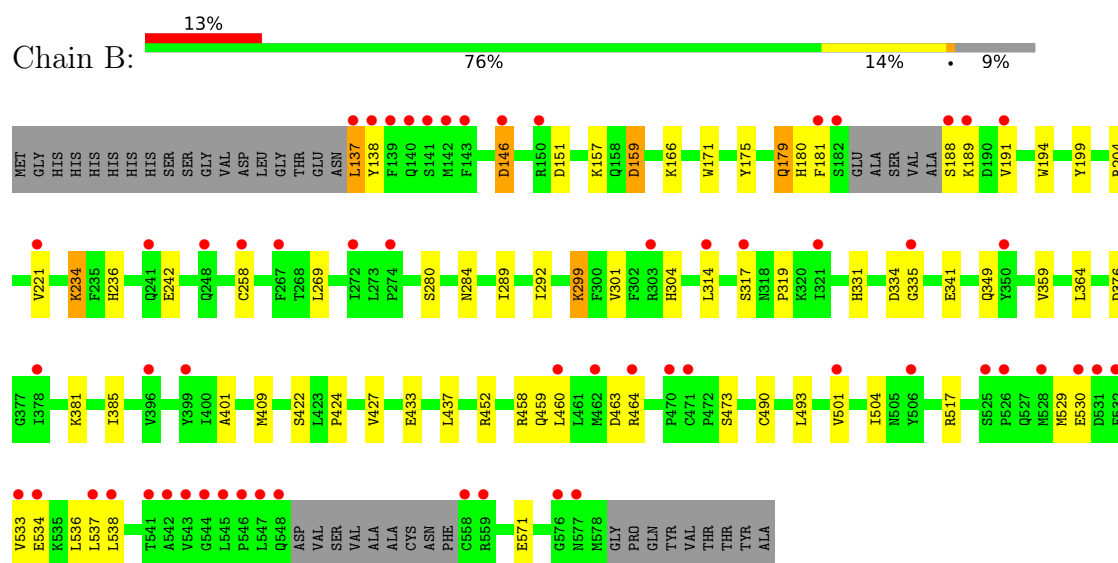
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	130	Total	O	0	0
			130	130		
4	A	118	Total	O	0	0
			118	118		

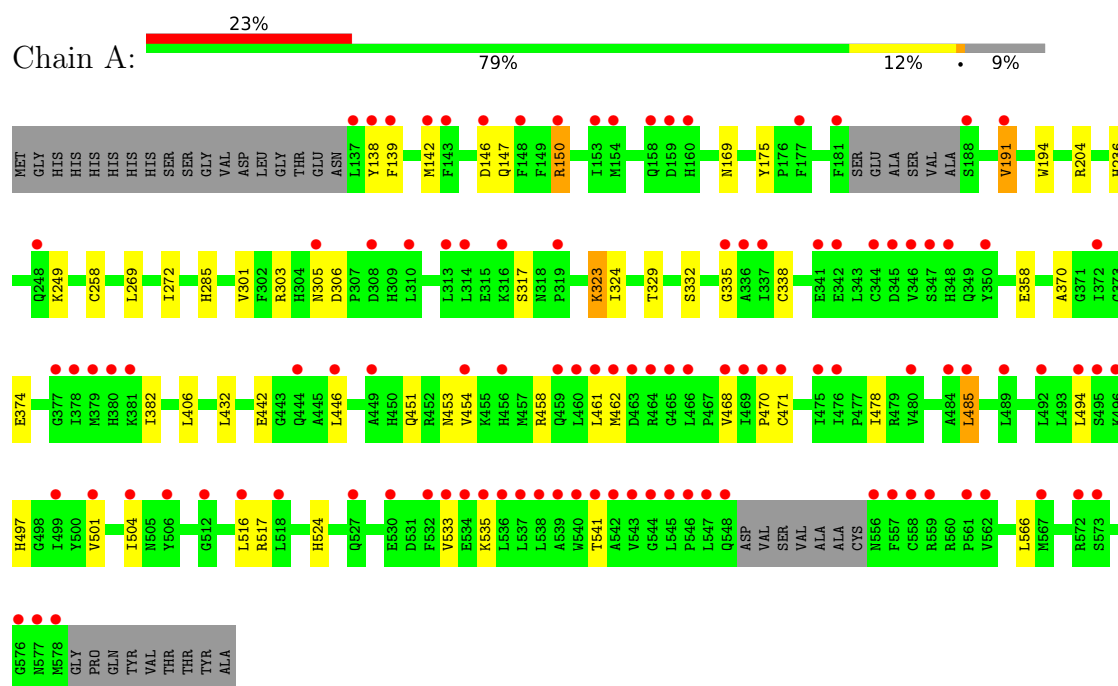
3 Residue-property plots [i](#)

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: 5-aminolevulinate synthase, erythroid-specific, mitochondrial



- Molecule 1: 5-aminolevulinate synthase, erythroid-specific, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.97Å 108.83Å 76.08Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	80.88 – 1.76 80.88 – 1.76	Depositor EDS
% Data completeness (in resolution range)	82.6 (80.88-1.76) 83.2 (80.88-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.225 , 0.255 (Not available) , 0.271	Depositor DCC
R_{free} test set	4815 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: J4Q, PLP

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	1.08	1/3403 (0.0%)	1.43	4/4608 (0.1%)
1	B	1.07	0/3381	1.39	4/4580 (0.1%)
All	All	1.08	1/6784 (0.0%)	1.41	8/9188 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	HIS	CE1-NE2	5.36	1.38	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	TYR	CA-C-N	5.78	128.97	120.82
1	A	138	TYR	C-N-CA	5.78	128.97	120.82
1	A	285	HIS	CA-C-N	5.34	127.70	120.38
1	A	285	HIS	C-N-CA	5.34	127.70	120.38
1	B	179	GLN	CB-CA-C	-5.31	101.09	109.80
1	B	159	ASP	CB-CA-C	-5.30	100.49	110.67
1	B	376	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	427	VAL	N-CA-C	-5.00	105.61	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	LEU	Peptide

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	3322	0	3215	41	0
1	B	3302	0	3192	48	1
2	A	16	0	7	2	0
2	B	16	0	7	2	0
3	B	15	0	0	0	0
4	A	118	0	0	1	0
4	B	130	0	0	8	0
All	All	6919	0	6421	87	1

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 7.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:O	1:A:471:CYS:HB3	1.82	0.79
1:B:349:GLN:OE1	4:B:701:HOH:O	2.07	0.72
1:B:335:GLY:CA	4:B:731:HOH:O	2.38	0.71
1:B:242:GLU:OE2	4:B:702:HOH:O	2.09	0.69
1:A:497:HIS:ND1	1:A:535:LYS:HE2	2.08	0.69
2:B:601:PLP:O3P	4:B:703:HOH:O	2.10	0.68
1:B:171:TRP:CZ2	1:B:179:GLN:HG3	2.29	0.67
1:A:470:PRO:O	1:A:471:CYS:SG	2.49	0.67
1:A:175:TYR:HB2	1:A:204:ARG:HD2	1.77	0.66
1:A:147:GLN:OE1	1:A:150:ARG:NH1	2.29	0.65
1:B:180:HIS:HE1	4:B:747:HOH:O	1.79	0.64
1:A:461:LEU:HD21	1:A:478:ILE:HD11	1.79	0.64
1:B:335:GLY:HA2	4:B:731:HOH:O	1.98	0.64
1:B:175:TYR:HB2	1:B:204:ARG:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:CD2	1:A:478:ILE:HD11	2.28	0.63
1:B:258:CYS:HB3	2:B:601:PLP:O4P	1.99	0.61
1:A:269:LEU:HB3	1:A:324:ILE:HD11	1.83	0.61
1:A:470:PRO:C	1:A:471:CYS:SG	2.84	0.60
1:A:504:ILE:HD13	1:A:517:ARG:HB2	1.85	0.58
1:B:460:LEU:O	1:B:464:ARG:HG2	2.03	0.58
1:B:166:LYS:HE3	1:B:490:CYS:SG	2.44	0.58
1:B:221:VAL:O	1:B:424:PRO:HB3	2.04	0.57
1:A:303:ARG:HD2	1:A:306:ASP:OD2	2.05	0.56
1:A:194:TRP:HB2	1:A:501:VAL:CG1	2.35	0.56
1:A:146:ASP:O	1:A:150:ARG:HG2	2.06	0.55
1:A:249:LYS:NZ	1:A:382:ILE:O	2.39	0.55
1:B:284:ASN:O	1:B:289:ILE:HD11	2.06	0.54
1:B:341:GLU:OE1	1:B:381:LYS:NZ	2.39	0.54
1:A:504:ILE:CD1	1:A:517:ARG:HB2	2.37	0.54
1:A:317:SER:OG	1:A:323:LYS:HE2	2.07	0.54
1:B:171:TRP:CZ2	1:B:179:GLN:CG	2.90	0.54
1:B:335:GLY:C	4:B:731:HOH:O	2.50	0.54
1:A:504:ILE:CD1	1:A:517:ARG:CB	2.86	0.53
1:B:175:TYR:CB	1:B:204:ARG:HD2	2.39	0.53
1:B:194:TRP:HB2	1:B:501:VAL:CG1	2.39	0.53
1:B:299:LYS:NZ	1:B:571:GLU:OE1	2.42	0.53
1:A:458:ARG:HG2	1:A:462:MET:HE2	1.91	0.53
1:B:194:TRP:HB2	1:B:501:VAL:HG13	1.90	0.52
1:B:319:PRO:O	1:A:142:MET:HB3	2.09	0.52
1:B:137:LEU:HD12	1:B:137:LEU:N	2.25	0.52
1:B:331:HIS:HB3	1:B:334:ASP:OD1	2.11	0.51
1:B:304:HIS:NE2	1:B:334:ASP:OD2	2.43	0.51
1:A:370:ALA:HB3	1:A:374:GLU:HB2	1.92	0.51
1:A:329:THR:OG1	1:A:358:GLU:OE1	2.26	0.50
1:B:504:ILE:CD1	1:B:517:ARG:HB2	2.42	0.50
1:A:453:ASN:ND2	1:A:524:HIS:O	2.45	0.50
1:A:194:TRP:HB2	1:A:501:VAL:HG12	1.95	0.49
1:A:305:ASN:OD1	1:A:338:CYS:HB2	2.12	0.48
1:B:452:ARG:NH1	4:B:708:HOH:O	2.47	0.48
1:B:269:LEU:HD23	1:B:409:MET:HE1	1.96	0.48
1:B:234:LYS:HG2	1:A:169:ASN:ND2	2.29	0.47
1:B:280:SER:O	1:B:301:VAL:HA	2.15	0.47
1:A:504:ILE:CD1	1:A:517:ARG:HB3	2.45	0.46
1:B:181:PHE:CE2	1:B:188:SER:HB2	2.50	0.46
1:A:406:LEU:C	1:A:406:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:MET:O	1:B:533:VAL:HG23	2.16	0.45
1:B:534:GLU:O	1:B:538:LEU:HD23	2.17	0.45
1:B:464:ARG:HB3	1:B:537:LEU:HD11	1.97	0.44
1:B:504:ILE:HD12	1:B:517:ARG:HB2	1.99	0.44
1:B:504:ILE:CD1	1:B:517:ARG:CB	2.96	0.44
1:A:332:SER:HB3	2:A:601:PLP:H2A1	1.99	0.44
1:A:191:VAL:HG21	1:A:494:LEU:CD1	2.47	0.44
1:B:199:TYR:CD2	1:B:364:LEU:HD11	2.52	0.43
1:B:459:GLN:NE2	1:B:463:ASP:OD1	2.52	0.43
1:A:194:TRP:HB2	1:A:501:VAL:HG13	1.99	0.43
1:B:236:HIS:NE2	1:B:422:SER:OG	2.49	0.43
1:A:301:VAL:HG11	1:A:566:LEU:O	2.18	0.43
1:A:305:ASN:OD1	1:A:338:CYS:CB	2.66	0.43
1:B:493:LEU:HD13	1:B:501:VAL:CG2	2.49	0.43
1:A:303:ARG:NH1	4:A:708:HOH:O	2.52	0.42
1:A:451:GLN:O	1:A:454:VAL:HG12	2.19	0.42
1:A:461:LEU:HD12	1:A:533:VAL:CG1	2.49	0.42
1:B:292:ILE:CG2	1:B:299:LYS:HG3	2.49	0.42
1:A:269:LEU:HB3	1:A:324:ILE:CD1	2.49	0.42
1:B:458:ARG:NH2	1:B:473:SER:O	2.53	0.42
1:B:171:TRP:CE2	1:B:179:GLN:HG3	2.54	0.42
1:B:314:LEU:O	1:B:317:SER:OG	2.35	0.41
1:B:349:GLN:HA	1:A:139:PHE:CD1	2.55	0.41
1:A:442:GLU:O	1:A:446:LEU:HD23	2.20	0.41
1:B:284:ASN:O	1:B:289:ILE:CD1	2.69	0.41
1:B:433:GLU:O	1:B:437:LEU:HG	2.19	0.41
1:A:175:TYR:HB2	1:A:204:ARG:CD	2.49	0.41
1:B:493:LEU:HD21	1:B:536:LEU:HA	2.03	0.41
1:A:485:LEU:HD13	1:A:485:LEU:HA	1.91	0.41
1:B:385:ILE:CG2	1:B:401:ALA:HB3	2.51	0.40
1:A:258:CYS:HB3	2:A:601:PLP:O4P	2.21	0.40
1:B:292:ILE:HG21	1:B:299:LYS:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:CD1	1:B:151:ASP:OD2[2_656]	2.05	0.15

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	424/469 (90%)	410 (97%)	14 (3%)	0	100	100
1	B	423/469 (90%)	409 (97%)	13 (3%)	1 (0%)	43	27
All	All	847/938 (90%)	819 (97%)	27 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	ASP

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	347/396 (88%)	338 (97%)	9 (3%)	40	20
1	B	345/396 (87%)	335 (97%)	10 (3%)	37	17
All	All	692/792 (87%)	673 (97%)	19 (3%)	38	19

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	TYR
1	B	146	ASP
1	B	157	LYS
1	B	159	ASP
1	B	189	LYS

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Mol	Chain	Res	Type
1	B	191	VAL
1	B	234	LYS
1	B	299	LYS
1	B	359	VAL
1	B	530	GLU
1	A	150	ARG
1	A	191	VAL
1	A	272	ILE
1	A	323	LYS
1	A	432	LEU
1	A	468	VAL
1	A	485	LEU
1	A	516	LEU
1	A	541	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	HIS
1	B	459	GLN
1	B	502	GLN
1	A	502	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 ⓘ

3 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	$\# Z > 2$
3	J4Q	B	602	-	15,16,16	1.88	3 (20%)	15,23,23	1.04	2 (13%)
2	PLP	B	601	-	16,16,16	1.00	1 (6%)	20,23,23	1.30	3 (15%)
2	PLP	A	601	-	16,16,16	1.02	2 (12%)	20,23,23	0.86	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	J4Q	B	602	-	-	2/9/10/10	0/2/2/2
2	PLP	B	601	-	-	1/8/8/8	0/1/1/1
2	PLP	A	601	-	-	1/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	J4Q	C2-N1	5.45	1.35	1.32
3	B	602	J4Q	C2-S1	3.97	1.81	1.78
2	A	601	PLP	P-O4P	2.83	1.69	1.60
2	B	601	PLP	P-O4P	2.69	1.68	1.60
3	B	602	J4Q	C6-N3	-2.37	1.32	1.38
2	A	601	PLP	C3-C2	2.03	1.43	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLP	C3-C4-C4A	-2.75	116.06	119.84
2	B	601	PLP	O4P-C5A-C5	2.59	114.21	109.36
2	B	601	PLP	O3P-P-O2P	2.23	116.17	107.80
3	B	602	J4Q	S1-C2-N1	2.02	125.52	122.59
3	B	602	J4Q	C7-S2-C8	-2.02	86.97	89.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

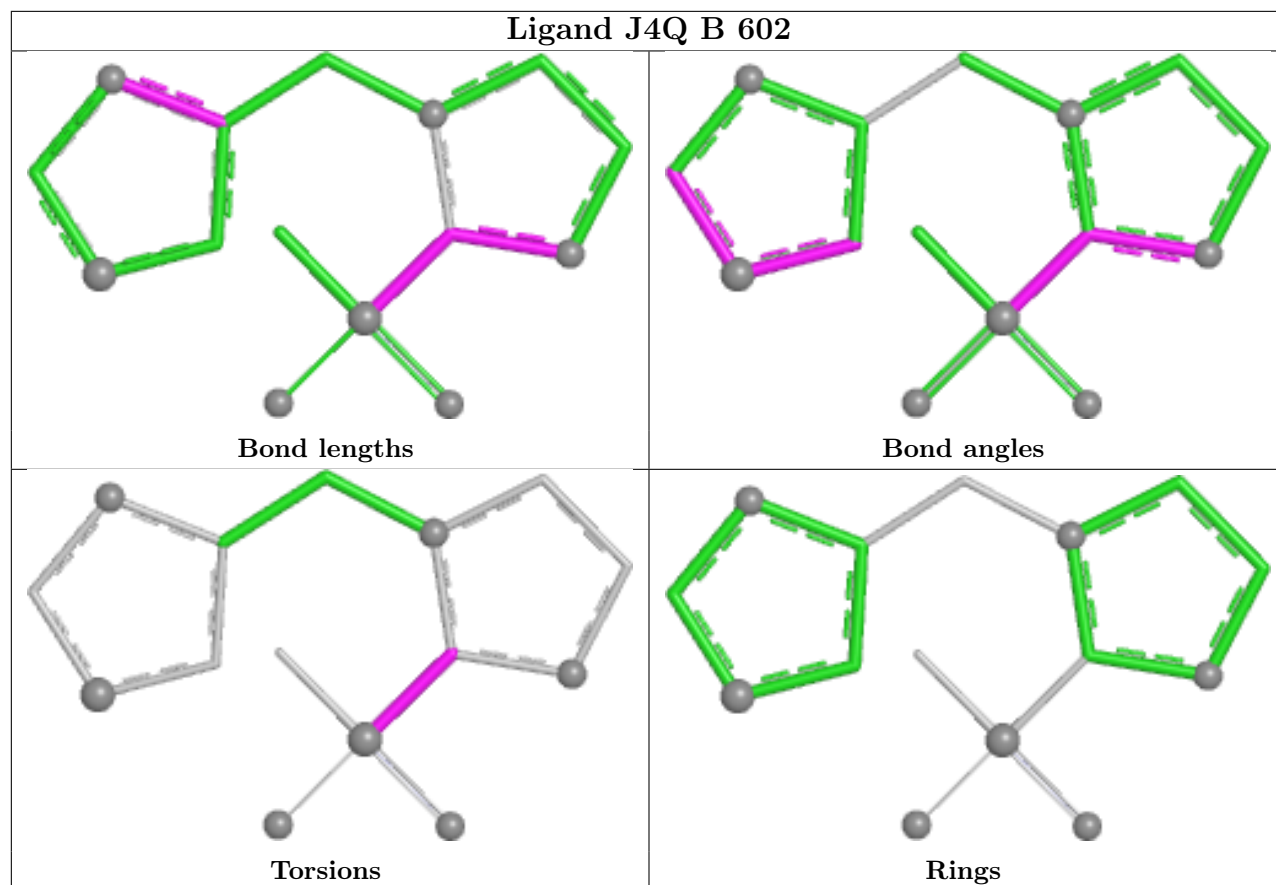
Mol	Chain	Res	Type	Atoms
3	B	602	J4Q	N1-C2-S1-C1
2	B	601	PLP	C5A-O4P-P-O1P
2	A	601	PLP	C5A-O4P-P-O2P
3	B	602	J4Q	N2-C2-S1-O1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLP	2	0
2	A	601	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.



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	429/469 (91%)	1.42	107 (24%) 2 2	9, 33, 58, 100	5 (1%)
1	B	428/469 (91%)	1.06	59 (13%) 6 7	8, 30, 49, 77	9 (2%)
All	All	857/938 (91%)	1.24	166 (19%) 3 3	8, 31, 53, 100	14 (1%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	PHE	15.5
1	A	506	TYR	14.2
1	B	267	PHE	12.4
1	A	143	PHE	12.4
1	B	532	PHE	11.7
1	A	380[A]	HIS	11.4
1	B	248[A]	GLN	11.3
1	B	143	PHE	11.2
1	B	350	TYR	11.0
1	B	139	PHE	10.7
1	B	399	TYR	10.6
1	A	177	PHE	10.3
1	A	181	PHE	8.7
1	B	531	ASP	8.5
1	A	137	LEU	7.5
1	A	139	PHE	6.6
1	B	138	TYR	6.5
1	B	558	CYS	6.4
1	A	545	LEU	6.1
1	A	537	LEU	5.9
1	A	547	LEU	5.7
1	B	137	LEU	5.5
1	A	470	PRO	5.4
1	B	471	CYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	VAL	5.3
1	A	548	GLN	5.0
1	B	538	LEU	4.9
1	B	547	LEU	4.6
1	A	543	VAL	4.6
1	A	540	TRP	4.5
1	B	545	LEU	4.4
1	A	466	LEU	4.3
1	B	221	VAL	4.3
1	A	346	VAL	4.3
1	A	577	ASN	4.2
1	A	538	LEU	4.2
1	A	378	ILE	4.1
1	A	556	ASN	4.1
1	B	541	THR	4.1
1	B	577	ASN	3.9
1	A	468	VAL	3.8
1	B	548	GLN	3.8
1	A	535	LYS	3.7
1	A	541	THR	3.7
1	A	471	CYS	3.7
1	A	562	VAL	3.7
1	B	303	ARG	3.7
1	A	578	MET	3.6
1	B	559	ARG	3.6
1	A	546	PRO	3.6
1	B	533	VAL	3.6
1	A	465	GLY	3.5
1	A	480	VAL	3.5
1	A	576	GLY	3.5
1	B	506	TYR	3.5
1	A	536	LEU	3.4
1	A	533	VAL	3.4
1	A	558	CYS	3.4
1	A	462	MET	3.4
1	B	546	PRO	3.4
1	A	336	ALA	3.3
1	B	460	LEU	3.3
1	A	542	ALA	3.3
1	B	321	ILE	3.3
1	B	526	PRO	3.3
1	A	492	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	469	ILE	3.2
1	A	154	MET	3.2
1	A	335	GLY	3.2
1	A	544	GLY	3.2
1	A	459	GLN	3.1
1	A	561	PRO	3.1
1	B	537	LEU	3.1
1	A	188	SER	3.1
1	A	159	ASP	3.1
1	A	377	GLY	3.0
1	A	138	TYR	3.0
1	B	542	ALA	3.0
1	A	527	GLN	3.0
1	A	454	VAL	3.0
1	A	461	LEU	3.0
1	A	449	ALA	3.0
1	A	539	ALA	3.0
1	A	463	ASP	2.9
1	B	534	GLU	2.9
1	B	181	PHE	2.9
1	A	518	LEU	2.8
1	A	345	ASP	2.8
1	A	153	ILE	2.8
1	A	464	ARG	2.8
1	A	148	PHE	2.8
1	A	485	LEU	2.8
1	B	335	GLY	2.8
1	B	140	GLN	2.7
1	B	470	PRO	2.7
1	A	158	GLN	2.7
1	A	314	LEU	2.7
1	B	191	VAL	2.7
1	B	396	VAL	2.7
1	A	456	HIS	2.6
1	A	446	LEU	2.6
1	A	341	GLU	2.6
1	A	484	ALA	2.6
1	B	188	SER	2.6
1	B	530	GLU	2.6
1	A	475	ILE	2.6
1	A	573	SER	2.6
1	A	512	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	310	LEU	2.6
1	A	460	LEU	2.6
1	B	142	MET	2.5
1	A	337	ILE	2.5
1	B	544	GLY	2.5
1	A	534	GLU	2.5
1	B	274	PRO	2.5
1	A	499	ILE	2.5
1	B	462	MET	2.5
1	A	305	ASN	2.4
1	B	146	ASP	2.4
1	A	160	HIS	2.4
1	A	348	HIS	2.4
1	A	381	LYS	2.4
1	A	516	LEU	2.4
1	A	316	LYS	2.4
1	B	258	CYS	2.4
1	A	532	PHE	2.4
1	A	146	ASP	2.4
1	B	464	ARG	2.3
1	A	308	ASP	2.3
1	A	494	LEU	2.3
1	B	576	GLY	2.3
1	A	342	GLU	2.3
1	B	543	VAL	2.3
1	A	344	CYS	2.3
1	B	241	GLN	2.2
1	A	489	LEU	2.2
1	B	182	SER	2.2
1	B	525	SER	2.2
1	B	317	SER	2.2
1	B	378	ILE	2.2
1	A	476	ILE	2.2
1	A	572	ARG	2.2
1	A	319	PRO	2.2
1	B	272	ILE	2.2
1	B	141	SER	2.2
1	A	501	VAL	2.1
1	A	313	LEU	2.1
1	A	142	MET	2.1
1	A	150	ARG	2.1
1	A	372	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	189	LYS	2.1
1	A	530	GLU	2.1
1	A	444	GLN	2.1
1	A	559	ARG	2.1
1	A	496	LYS	2.1
1	A	350	TYR	2.1
1	A	504	ILE	2.1
1	B	528	MET	2.0
1	A	567	MET	2.0
1	B	150	ARG	2.0
1	B	501	VAL	2.0
1	B	314	LEU	2.0
1	A	248	GLN	2.0
1	A	379	MET	2.0
1	A	347	SER	2.0
1	A	495	SER	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](#)

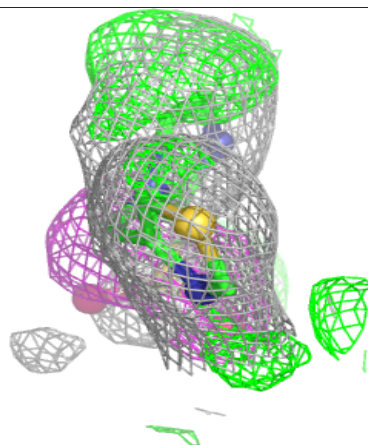
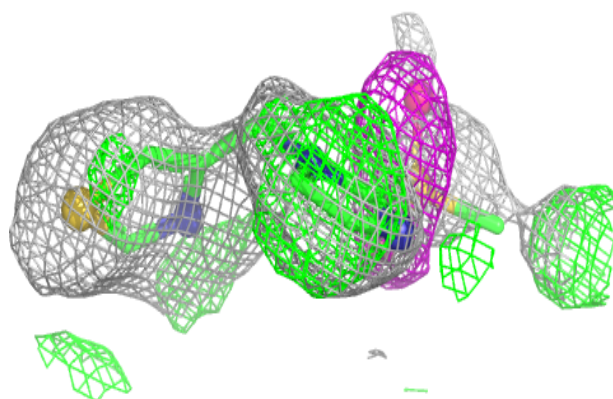
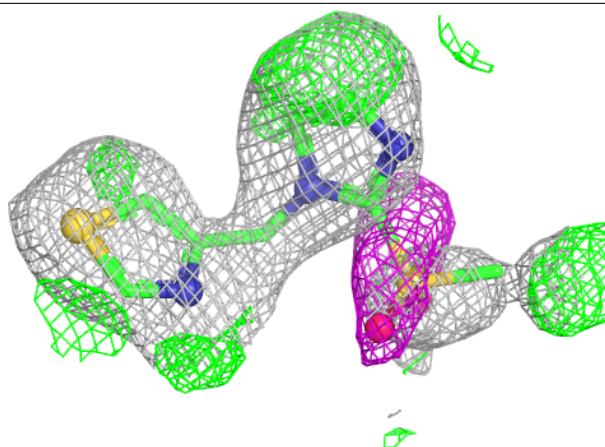
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	J4Q	B	602	15/15	0.63	0.32	38,41,56,58	15
2	PLP	B	601	16/16	0.86	0.13	24,31,34,42	0
2	PLP	A	601	16/16	0.90	0.12	27,32,37,51	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 J4Q B 602:

$2mF_o - DF_c$ (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.