



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:08 pm BST

PDB ID : 6B76
Title : Crystal Structure of human NAMPT in complex with NVP-LVR596
Authors : Weihofen, W.A.; Thigale, S.
Deposited on : 2017-10-03
Resolution : 2.44 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 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 : 2.11
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) : 2.11

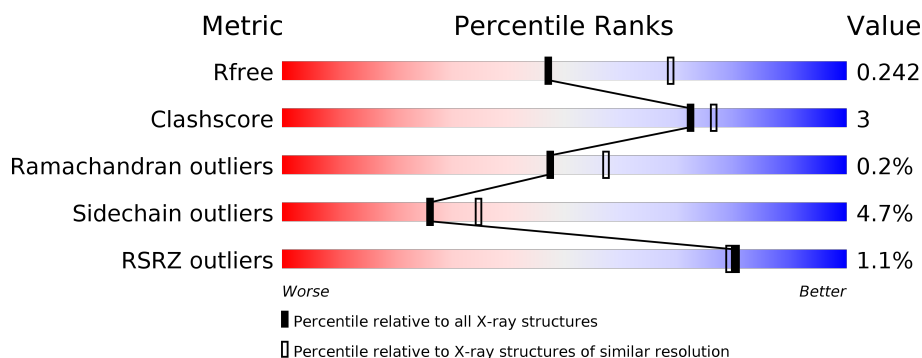
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on 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	501	<div> <div>83%</div> <div>10% • 6%</div> </div>
1	B	501	<div> <div>84%</div> <div>9% 7%</div> </div>
1	C	501	<div> <div>%</div> <div>81% 12% • 6%</div> </div>
1	D	501	<div> <div>3%</div> <div>79% 14% • 6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16057 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3763	2421	622	713	7			
1	B	468	Total	C	N	O	S	0	0	0
			3743	2408	619	709	7			
1	C	469	Total	C	N	O	S	0	0	0
			3754	2415	620	712	7			
1	D	471	Total	C	N	O	S	0	0	0
			3768	2423	623	715	7			

There are 40 discrepancies between the modelled and reference sequences:

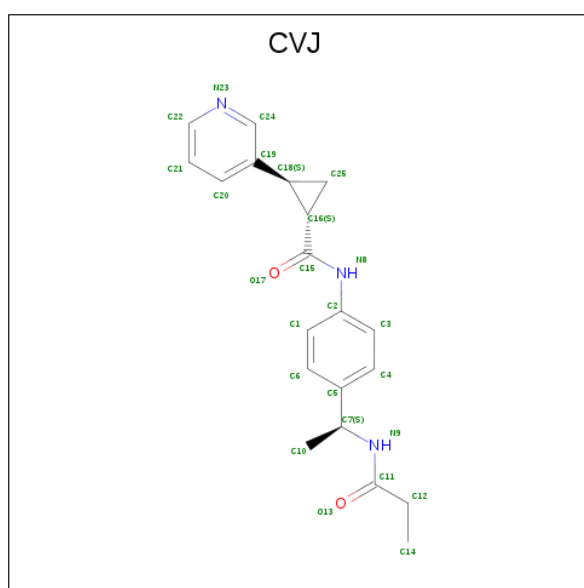
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag	UNP P43490
A	499	HIS	-	expression tag	UNP P43490
A	500	HIS	-	expression tag	UNP P43490
A	501	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
B	500	HIS	-	expression tag	UNP P43490
B	501	HIS	-	expression tag	UNP P43490
C	492	LEU	-	expression tag	UNP P43490

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP P43490
C	494	HIS	-	expression tag	UNP P43490
C	495	HIS	-	expression tag	UNP P43490
C	496	HIS	-	expression tag	UNP P43490
C	497	HIS	-	expression tag	UNP P43490
C	498	HIS	-	expression tag	UNP P43490
C	499	HIS	-	expression tag	UNP P43490
C	500	HIS	-	expression tag	UNP P43490
C	501	HIS	-	expression tag	UNP P43490
D	492	LEU	-	expression tag	UNP P43490
D	493	GLU	-	expression tag	UNP P43490
D	494	HIS	-	expression tag	UNP P43490
D	495	HIS	-	expression tag	UNP P43490
D	496	HIS	-	expression tag	UNP P43490
D	497	HIS	-	expression tag	UNP P43490
D	498	HIS	-	expression tag	UNP P43490
D	499	HIS	-	expression tag	UNP P43490
D	500	HIS	-	expression tag	UNP P43490
D	501	HIS	-	expression tag	UNP P43490

- Molecule 2 is (1S,2S)-N-{4-[(1S)-1-(propanoylamino)ethyl]phenyl}-2-(pyridin-3-yl)cyclopropane-1-carboxamide (three-letter code: CVJ) (formula: C₂₀H₂₃N₃O₂) (labeled as "Ligand of Interest" by author).



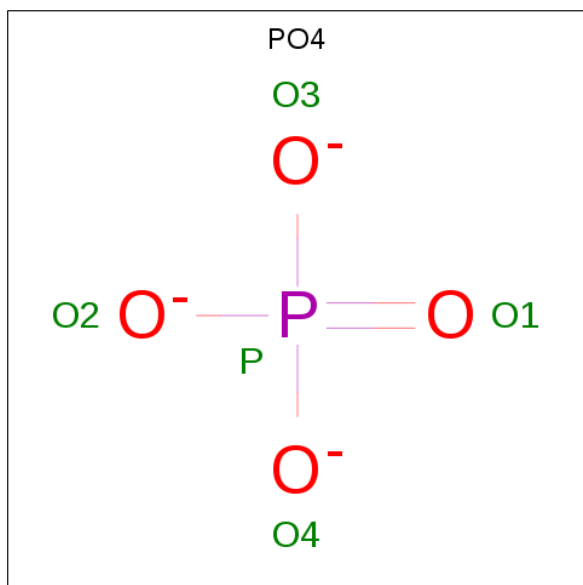
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			25	20	3	2		
2	C	1	Total	C	N	O	0	0
			25	20	3	2		
2	D	1	Total	C	N	O	0	0
			25	20	3	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

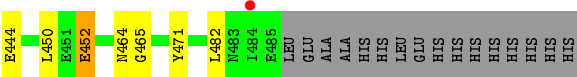
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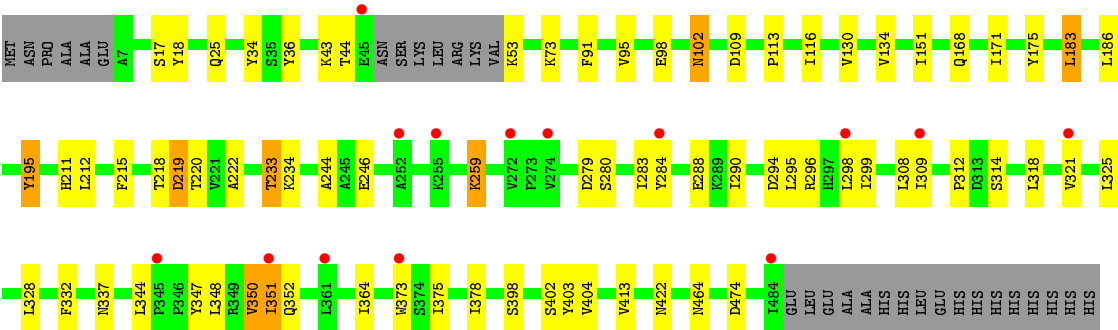
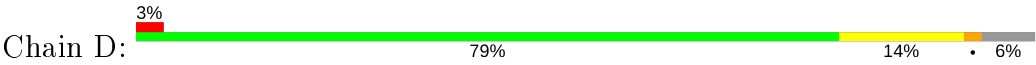
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	224	Total	O	0	0
			224	224		
4	C	185	Total	O	0	0
			185	185		
4	D	170	Total	O	0	0
			170	170		



● Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.87Å 96.83Å 248.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.15 – 2.44 124.15 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (124.15-2.44) 100.0 (124.15-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.179 , 0.233 0.184 , 0.242	Depositor DCC
R_{free} test set	4070 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16057	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: PO4, CVJ

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	0.51	0/3851	0.70	0/5216
1	B	0.50	0/3831	0.69	0/5190
1	C	0.52	0/3842	0.70	0/5205
1	D	0.51	0/3856	0.70	0/5223
All	All	0.51	0/15380	0.70	0/20834

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	3763	0	3746	24	0
1	B	3743	0	3723	17	0
1	C	3754	0	3733	31	0
1	D	3768	0	3749	37	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
4	A	295	0	0	1	0
4	B	224	0	0	0	0
4	C	185	0	0	1	0
4	D	170	0	0	1	0
All	All	16057	0	14951	102	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 (102) 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:C:63:GLN:HE22	1:C:471:TYR:H	1.35	0.73
1:A:63:GLN:HE22	1:A:471:TYR:H	1.37	0.71
1:C:33:VAL:H	1:C:136:ASN:HD21	1.38	0.70
1:D:299:ILE:HD12	1:D:308:LEU:HD22	1.74	0.69
1:C:245:ALA:HA	1:D:25:GLN:HE22	1.62	0.65
1:C:316:ASN:HD22	1:C:319:ASP:H	1.43	0.64
1:C:412:ASN:HB3	1:C:427:LYS:HB3	1.81	0.63
1:A:245:ALA:HA	1:B:25:GLN:HE22	1.69	0.58
1:A:32:LYS:HA	1:A:136:ASN:HD21	1.68	0.58
1:C:321:VAL:HG23	1:C:352:GLN:HE21	1.69	0.58
1:A:224:LEU:HD22	1:A:238:PRO:HD2	1.87	0.57
1:A:299:ILE:HD12	1:A:308:LEU:HD22	1.87	0.57
1:C:112:LEU:O	1:C:464:ASN:HA	2.06	0.55
1:C:18:TYR:CE2	1:D:246:GLU:HB3	2.41	0.55
1:B:362:GLN:O	1:B:366:GLU:HB2	2.07	0.55
1:D:318:LEU:HD13	1:D:364:ILE:HA	1.89	0.54
1:A:310:ILE:HD12	1:A:348:LEU:HD11	1.88	0.54
1:D:350:VAL:HB	1:D:378:ILE:HD12	1.90	0.54
1:D:259:LYS:HE2	1:D:294:ASP:HB3	1.89	0.54
1:D:344:LEU:HD22	1:D:348:LEU:HD23	1.89	0.54
1:B:12:LEU:HD23	1:B:96:PHE:HZ	1.75	0.52
1:C:18:TYR:HB2	1:D:244:ALA:HB3	1.92	0.52
1:B:264:HIS:O	1:B:268:GLN:HG2	2.11	0.51
1:B:312:PRO:HD2	1:B:351:ILE:O	2.11	0.50
1:D:321:VAL:HG23	1:D:352:GLN:HE21	1.75	0.50
1:D:290:ILE:HA	1:D:294:ASP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.93	0.49
1:D:34:TYR:HB3	1:D:403:TYR:HB3	1.94	0.49
1:C:382:SER:HB3	1:C:386:LEU:HB2	1.94	0.49
1:D:279:ASP:HB3	1:D:283:ILE:HB	1.95	0.49
1:A:328:LEU:HD22	1:A:348:LEU:HD21	1.96	0.48
1:A:316:ASN:HD22	1:A:319:ASP:H	1.61	0.48
1:A:13:LEU:HD21	1:A:83:ALA:HA	1.95	0.48
1:D:113:PRO:HA	1:D:464:ASN:HD22	1.79	0.48
1:D:17:SER:O	1:D:91:PHE:HZ	1.97	0.48
1:B:299:ILE:HD12	1:B:308:LEU:HD22	1.95	0.47
1:A:168:GLN:HA	1:A:171:ILE:HD12	1.96	0.47
1:D:183:LEU:HG	1:D:186:LEU:HD22	1.95	0.47
1:C:58:VAL:HG22	1:C:124:VAL:HG22	1.97	0.47
1:D:299:ILE:HG22	1:D:347:TYR:HD1	1.80	0.46
1:D:233:THR:HG22	1:D:474:ASP:OD1	2.14	0.46
1:A:183:LEU:HD11	1:A:484:ILE:HG12	1.98	0.46
1:C:116:ILE:HG12	1:C:134:VAL:HG22	1.97	0.46
1:C:18:TYR:HE2	1:D:246:GLU:HB3	1.81	0.46
1:D:168:GLN:HA	1:D:171:ILE:HD12	1.97	0.46
1:B:17:SER:O	1:B:91:PHE:HZ	1.98	0.46
1:C:58:VAL:CG2	1:C:166:ARG:HD2	2.46	0.46
1:C:169:LYS:HD2	1:C:214:ASN:HB3	1.98	0.46
1:C:120:PRO:O	1:C:123:PHE:HB2	2.16	0.46
1:A:318:LEU:HD11	1:A:367:GLY:HA3	1.99	0.45
1:A:136:ASN:H	1:A:136:ASN:HD22	1.64	0.45
1:D:325:LEU:HB3	1:D:373:TRP:CE2	2.52	0.45
1:C:465:GLY:HA2	4:C:714:HOH:O	2.17	0.45
1:C:170:LYS:HG3	1:C:482:LEU:HD22	1.98	0.45
1:D:284:TYR:O	1:D:288:GLU:HB2	2.17	0.45
1:C:31:SER:HB2	1:C:139:PRO:HB3	1.99	0.44
1:C:430:LEU:HD23	1:C:444:GLU:HA	1.98	0.44
1:B:63:GLN:HB3	1:B:231:TYR:CE1	2.52	0.44
1:D:195:TYR:CD2	1:D:220:THR:HA	2.53	0.44
1:C:413:VAL:HA	4:D:724:HOH:O	2.17	0.44
1:A:117:LYS:HA	1:A:459:HIS:O	2.17	0.44
1:C:450:LEU:HB3	1:C:452:GLU:HG3	2.00	0.44
1:A:466:LYS:HD3	1:A:468:THR:HG22	2.00	0.43
1:D:116:ILE:HG12	1:D:134:VAL:HG22	2.00	0.43
1:D:175:TYR:HB3	1:D:375:ILE:HG13	2.01	0.43
1:A:172:LEU:HD21	1:A:361:LEU:HD11	2.01	0.43
1:D:73:LYS:HG3	1:D:109:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:OG	1:A:433:HIS:HE1	2.00	0.43
1:C:20:VAL:HA	1:C:147:TRP:CZ3	2.53	0.43
1:D:183:LEU:HD12	1:D:183:LEU:HA	1.91	0.43
1:D:211:HIS:CE1	1:D:215:PHE:CD2	3.07	0.43
1:A:8:GLU:HB2	4:A:1043:HOH:O	2.17	0.43
1:A:252:ALA:HA	1:B:413:VAL:HG11	2.01	0.43
1:B:55:GLU:H	1:B:55:GLU:HG2	1.57	0.42
1:D:36:TYR:HB2	1:D:130:VAL:HG23	2.01	0.42
1:C:286:ALA:HA	1:C:290:ILE:HD12	2.01	0.42
1:C:318:LEU:HD13	1:C:364:ILE:HA	2.01	0.42
1:A:40:ARG:HD2	1:A:422:ASN:O	2.20	0.42
1:D:43:LYS:HA	1:D:422:ASN:HD21	1.84	0.42
1:C:112:LEU:HD22	1:C:144:LEU:HD21	2.02	0.42
1:D:113:PRO:HA	1:D:464:ASN:ND2	2.34	0.42
1:D:312:PRO:HD2	1:D:351:ILE:O	2.20	0.42
1:B:366:GLU:O	1:B:370:GLN:HG2	2.21	0.41
1:B:120:PRO:O	1:B:123:PHE:HB2	2.20	0.41
1:D:295:LEU:HD22	1:D:298:LEU:HD12	2.02	0.41
1:B:34:TYR:HB3	1:B:403:TYR:HB3	2.02	0.41
1:C:299:ILE:HD12	1:C:308:LEU:HD22	2.01	0.41
1:C:403:TYR:HB2	1:C:428:GLY:HA2	2.03	0.41
1:D:328:LEU:O	1:D:332:PHE:HB2	2.21	0.41
1:D:98:GLU:O	1:D:102:ASN:HB2	2.21	0.41
1:B:443:LEU:HD23	1:B:448:GLY:HA2	2.03	0.41
1:C:248:SER:O	1:C:252:ALA:HB2	2.21	0.41
1:A:63:GLN:NE2	1:A:471:TYR:H	2.12	0.40
1:C:33:VAL:H	1:C:136:ASN:ND2	2.12	0.40
1:D:212:LEU:HD11	1:D:218:THR:HG21	2.03	0.40
1:D:402:SER:HA	1:D:413:VAL:O	2.21	0.40
1:B:134:VAL:HG21	1:B:152:LEU:HD13	2.02	0.40
1:B:336:GLU:HG2	1:B:340:GLY:HA2	2.03	0.40
1:B:370:GLN:H	1:B:370:GLN:HG2	1.61	0.40
1:A:302:ARG:HB2	1:A:347:TYR:HB2	2.04	0.40
1:A:316:ASN:ND2	1:A:319:ASP:H	2.19	0.40
1:C:16:ASP:HA	1:D:219:ASP:O	2.21	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	466/501 (93%)	454 (97%)	12 (3%)	0	100	100
1	B	464/501 (93%)	450 (97%)	14 (3%)	0	100	100
1	C	465/501 (93%)	446 (96%)	19 (4%)	0	100	100
1	D	467/501 (93%)	439 (94%)	25 (5%)	3 (1%)	25	29
All	All	1862/2004 (93%)	1789 (96%)	70 (4%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	D	337	ASN
1	D	95	VAL

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	414/440 (94%)	394 (95%)	20 (5%)	25	34
1	B	411/440 (93%)	388 (94%)	23 (6%)	21	27
1	C	413/440 (94%)	398 (96%)	15 (4%)	35	46
1	D	414/440 (94%)	395 (95%)	19 (5%)	27	35
All	All	1652/1760 (94%)	1575 (95%)	77 (5%)	26	35

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	18	TYR
1	A	77	LYS
1	A	81	GLN
1	A	102	ASN
1	A	151	ILE
1	A	195	TYR
1	A	219	ASP
1	A	237	VAL
1	A	248	SER
1	A	259	LYS
1	A	278	SER
1	A	279	ASP
1	A	280	SER
1	A	294	ASP
1	A	316	ASN
1	A	318	LEU
1	A	335	THR
1	A	409	LEU
1	A	424	ARG
1	B	8	GLU
1	B	18	TYR
1	B	53	LYS
1	B	55	GLU
1	B	94	ASP
1	B	107	LYS
1	B	183	LEU
1	B	195	TYR
1	B	219	ASP
1	B	234	LYS
1	B	235	ASP
1	B	255	LYS
1	B	303	SER
1	B	305	GLN
1	B	326	GLU
1	B	361	LEU
1	B	370	GLN
1	B	409	LEU
1	B	411	ILE
1	B	435	THR
1	B	441	VAL
1	B	451	GLU
1	B	484	ILE

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Mol	Chain	Res	Type
1	C	18	TYR
1	C	19	LYS
1	C	21	THR
1	C	51	LYS
1	C	52	VAL
1	C	106	GLU
1	C	136	ASN
1	C	151	ILE
1	C	195	TYR
1	C	219	ASP
1	C	272	VAL
1	C	303	SER
1	C	398	SER
1	C	409	LEU
1	C	452	GLU
1	D	18	TYR
1	D	44	THR
1	D	53	LYS
1	D	102	ASN
1	D	151	ILE
1	D	183	LEU
1	D	195	TYR
1	D	219	ASP
1	D	233	THR
1	D	234	LYS
1	D	259	LYS
1	D	280	SER
1	D	296	ARG
1	D	309	ILE
1	D	314	SER
1	D	350	VAL
1	D	351	ILE
1	D	398	SER
1	D	404	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	129	ASN
1	A	136	ASN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	316	ASN
1	A	433	HIS
1	A	439	ASN
1	A	464	ASN
1	A	483	ASN
1	B	25	GLN
1	B	164	ASN
1	B	168	GLN
1	B	439	ASN
1	B	464	ASN
1	C	63	GLN
1	C	136	ASN
1	C	164	ASN
1	C	305	GLN
1	C	316	ASN
1	C	352	GLN
1	C	362	GLN
1	C	464	ASN
1	D	25	GLN
1	D	164	ASN
1	D	168	GLN
1	D	352	GLN
1	D	422	ASN
1	D	464	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	PO4	C	602	-	4,4,4	2.55	2 (50%)	6,6,6	0.86	0
2	CVJ	D	601	-	27,27,27	1.22	1 (3%)	37,37,37	1.02	2 (5%)
2	CVJ	B	601	-	27,27,27	1.32	3 (11%)	37,37,37	1.24	4 (10%)
3	PO4	B	604	-	4,4,4	2.49	1 (25%)	6,6,6	0.56	0
3	PO4	A	602	-	4,4,4	2.47	1 (25%)	6,6,6	0.86	0
3	PO4	D	602	-	4,4,4	1.90	0	6,6,6	0.75	0
3	PO4	D	603	-	4,4,4	2.51	1 (25%)	6,6,6	0.58	0
3	PO4	B	603	-	4,4,4	2.09	2 (50%)	6,6,6	0.57	0
3	PO4	C	603	-	4,4,4	2.52	1 (25%)	6,6,6	0.53	0
3	PO4	A	603	-	4,4,4	2.49	2 (50%)	6,6,6	0.79	0
3	PO4	C	604	-	4,4,4	2.53	1 (25%)	6,6,6	0.30	0
2	CVJ	C	601	-	27,27,27	1.14	1 (3%)	37,37,37	1.13	4 (10%)
2	CVJ	A	601	-	27,27,27	1.28	1 (3%)	37,37,37	1.17	4 (10%)
3	PO4	B	602	-	4,4,4	2.50	1 (25%)	6,6,6	0.43	0
3	PO4	A	604	-	4,4,4	2.49	1 (25%)	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CVJ	B	601	-	-	8/22/27/27	0/3/3/3
2	CVJ	A	601	-	-	8/22/27/27	0/3/3/3
2	CVJ	D	601	-	-	6/22/27/27	0/3/3/3
2	CVJ	C	601	-	-	6/22/27/27	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	PO4	P-O1	4.26	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	PO4	P-O1	4.20	1.60	1.50
3	C	604	PO4	P-O1	4.17	1.60	1.50
3	B	602	PO4	P-O1	4.16	1.60	1.50
3	B	604	PO4	P-O1	4.15	1.60	1.50
3	D	603	PO4	P-O1	4.14	1.60	1.50
3	A	603	PO4	P-O1	4.12	1.60	1.50
3	A	604	PO4	P-O1	4.12	1.60	1.50
3	A	602	PO4	P-O1	4.09	1.60	1.50
2	B	601	CVJ	C25-C18	2.52	1.54	1.50
2	D	601	CVJ	C25-C18	2.46	1.54	1.50
2	A	601	CVJ	C25-C18	2.41	1.54	1.50
3	B	603	PO4	P-O1	2.38	1.56	1.50
2	B	601	CVJ	C20-C19	2.26	1.42	1.39
2	C	601	CVJ	C25-C18	2.25	1.54	1.50
3	C	602	PO4	P-O3	2.04	1.60	1.54
2	B	601	CVJ	C6-C5	2.03	1.42	1.39
3	A	603	PO4	P-O2	2.03	1.60	1.54
3	B	603	PO4	P-O3	2.03	1.60	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	CVJ	C19-C18-C16	-3.73	113.73	120.54
2	C	601	CVJ	C22-N23-C24	3.00	122.03	116.85
2	B	601	CVJ	C22-N23-C24	2.98	122.00	116.85
2	A	601	CVJ	C22-N23-C24	2.90	121.86	116.85
2	B	601	CVJ	C19-C24-N23	-2.81	119.72	124.14
2	D	601	CVJ	C22-N23-C24	2.80	121.70	116.85
2	C	601	CVJ	C19-C24-N23	-2.47	120.27	124.14
2	A	601	CVJ	O13-C11-N9	2.35	126.92	122.95
2	C	601	CVJ	C19-C18-C16	-2.32	116.31	120.54
2	B	601	CVJ	O17-C15-C16	-2.18	119.10	121.73
2	A	601	CVJ	C7-N9-C11	2.16	125.99	122.90
2	D	601	CVJ	C19-C24-N23	-2.15	120.77	124.14
2	A	601	CVJ	C19-C24-N23	-2.09	120.86	124.14
2	C	601	CVJ	C20-C19-C24	2.09	119.10	116.88

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CVJ	C16-C18-C19-C24

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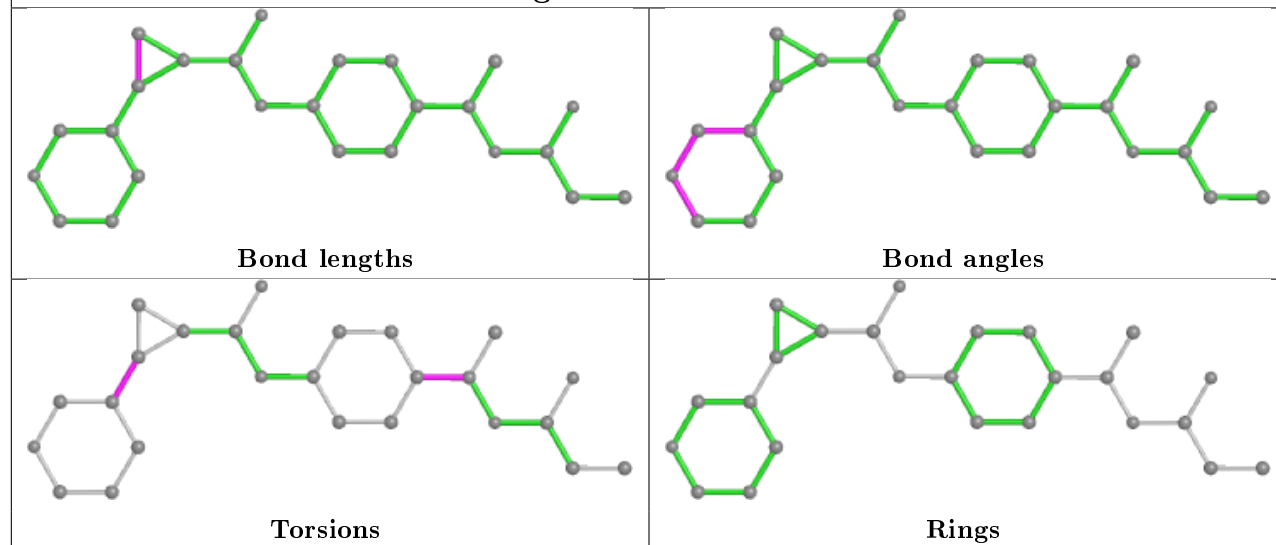
Mol	Chain	Res	Type	Atoms
2	C	601	CVJ	C16-C18-C19-C20
2	D	601	CVJ	C16-C18-C19-C24
2	B	601	CVJ	C16-C18-C19-C24
2	C	601	CVJ	C16-C18-C19-C24
2	D	601	CVJ	C16-C18-C19-C20
2	B	601	CVJ	C16-C18-C19-C20
2	A	601	CVJ	C16-C18-C19-C20
2	D	601	CVJ	C25-C18-C19-C24
2	B	601	CVJ	C25-C18-C19-C24
2	C	601	CVJ	C25-C18-C19-C24
2	A	601	CVJ	C25-C18-C19-C24
2	A	601	CVJ	C25-C18-C19-C20
2	B	601	CVJ	C25-C18-C19-C20
2	C	601	CVJ	C25-C18-C19-C20
2	C	601	CVJ	C6-C5-C7-N9
2	D	601	CVJ	C25-C18-C19-C20
2	B	601	CVJ	O13-C11-C12-C14
2	A	601	CVJ	C6-C5-C7-N9
2	D	601	CVJ	C6-C5-C7-N9
2	D	601	CVJ	C4-C5-C7-N9
2	C	601	CVJ	C4-C5-C7-N9
2	B	601	CVJ	N9-C11-C12-C14
2	B	601	CVJ	C6-C5-C7-N9
2	A	601	CVJ	O13-C11-C12-C14
2	A	601	CVJ	N9-C11-C12-C14
2	B	601	CVJ	C4-C5-C7-N9
2	A	601	CVJ	C4-C5-C7-N9

There are no ring outliers.

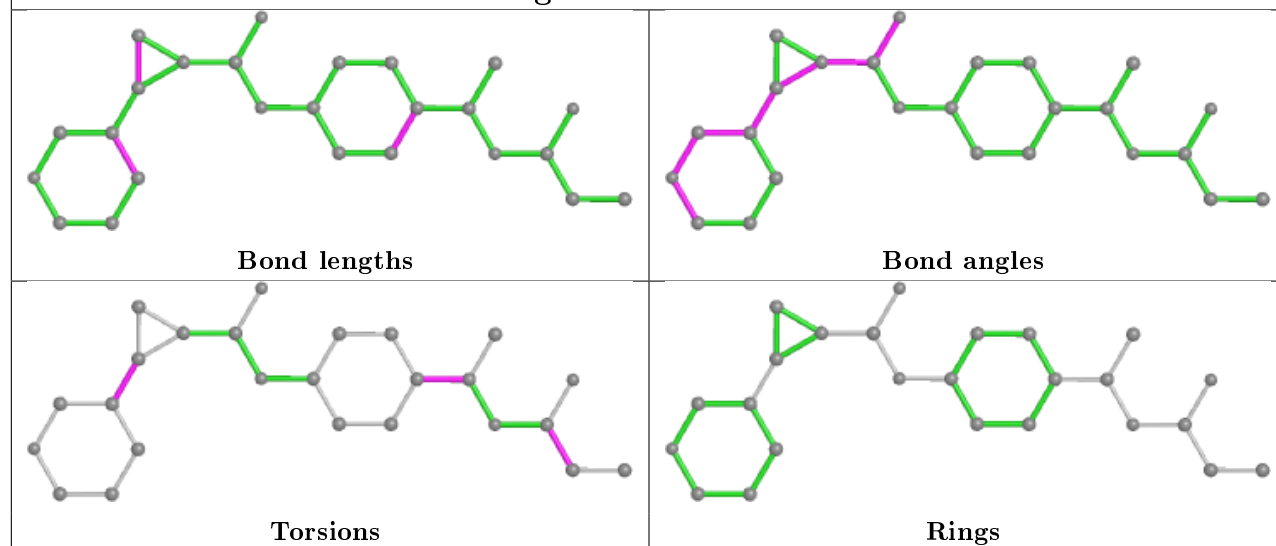
No monomer is involved in short contacts.

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.

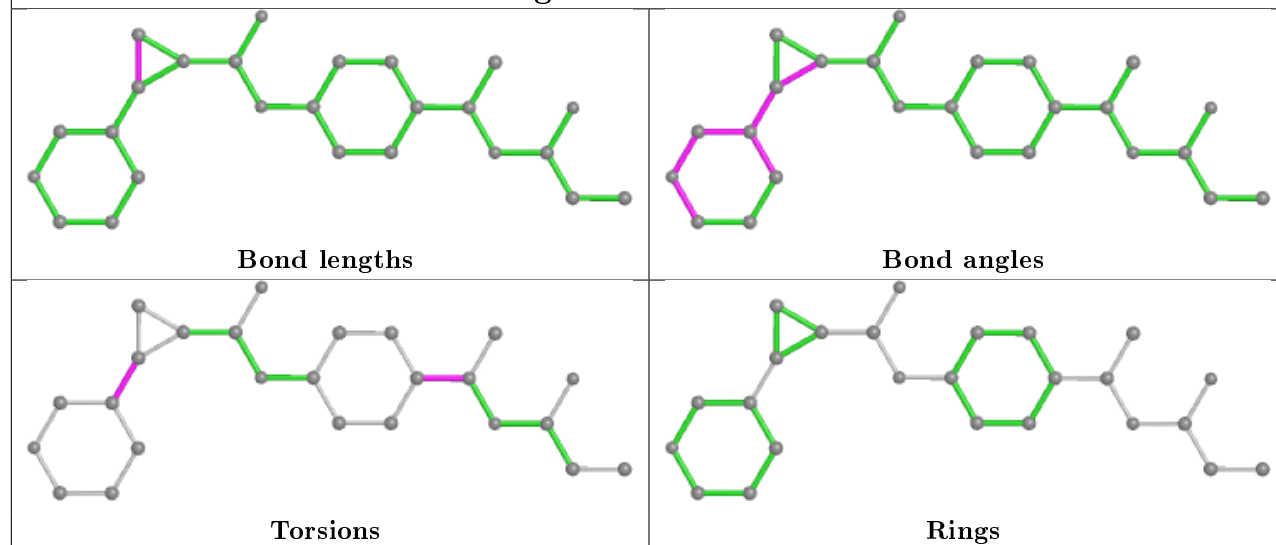
Ligand CVJ D 601

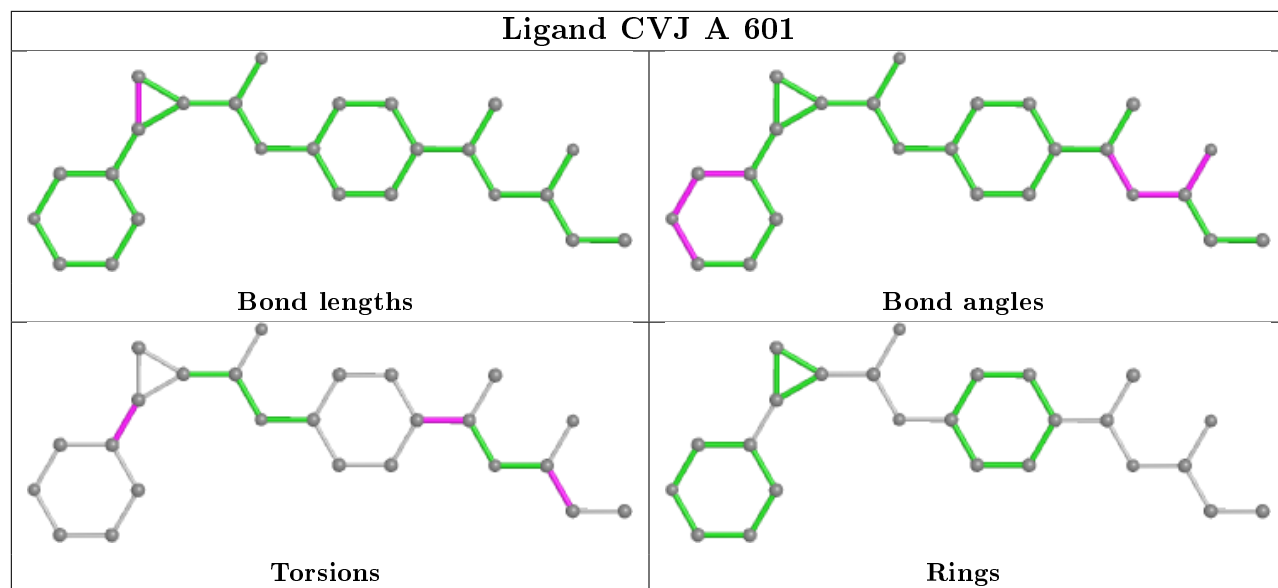


Ligand CVJ B 601



Ligand CVJ C 601





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	470/501 (93%)	-0.36	1 (0%) 95 95	28, 45, 80, 124	0
1	B	468/501 (93%)	-0.42	1 (0%) 95 95	28, 54, 82, 113	0
1	C	469/501 (93%)	-0.15	5 (1%) 80 79	36, 57, 89, 124	0
1	D	471/501 (94%)	-0.01	14 (2%) 50 46	38, 64, 99, 143	0
All	All	1878/2004 (93%)	-0.24	21 (1%) 80 79	28, 55, 90, 143	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	TYR	6.0
1	D	484	ILE	3.7
1	D	45	GLU	3.5
1	D	272	VAL	3.1
1	D	284	TYR	3.1
1	D	252	ALA	3.0
1	A	484	ILE	2.9
1	C	411	ILE	2.9
1	C	484	ILE	2.9
1	D	361	LEU	2.7
1	D	309	ILE	2.7
1	D	373	TRP	2.5
1	D	298	LEU	2.5
1	D	255	LYS	2.4
1	D	351	ILE	2.4
1	C	410	GLY	2.4
1	D	274	VAL	2.3
1	D	345	PRO	2.3
1	C	151	ILE	2.2
1	C	426	LYS	2.2
1	D	321	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

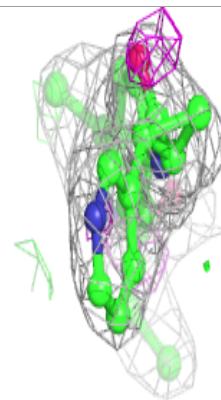
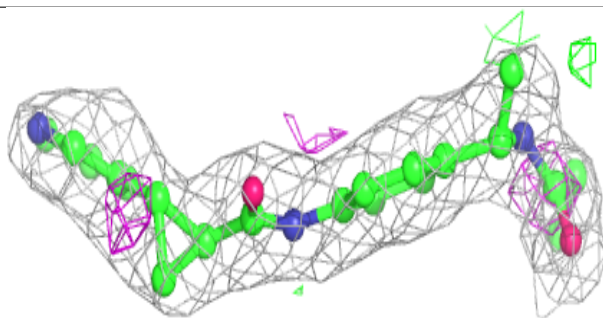
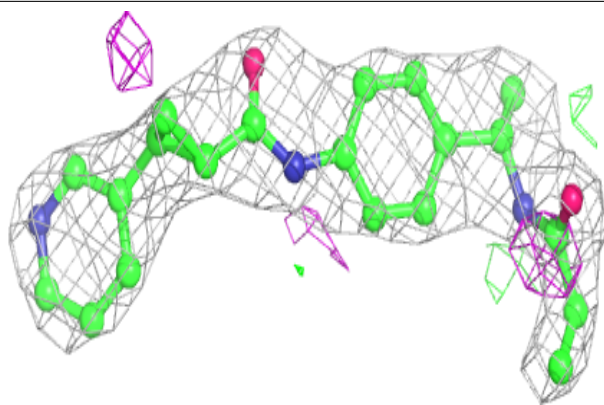
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	C	604	5/5	0.83	0.18	85,93,94,94	0
3	PO4	A	603	5/5	0.84	0.37	98,99,104,104	0
3	PO4	D	603	5/5	0.88	0.17	110,111,112,113	0
3	PO4	B	602	5/5	0.88	0.32	97,100,101,103	0
2	CVJ	D	601	25/25	0.90	0.20	57,63,67,69	0
3	PO4	C	602	5/5	0.91	0.31	64,72,75,77	0
3	PO4	C	603	5/5	0.93	0.16	85,88,89,89	0
3	PO4	A	604	5/5	0.93	0.15	105,105,106,108	0
2	CVJ	A	601	25/25	0.96	0.16	39,44,52,53	0
3	PO4	B	603	5/5	0.96	0.13	79,83,84,84	0
3	PO4	B	604	5/5	0.96	0.16	71,74,75,79	0
2	CVJ	C	601	25/25	0.97	0.15	33,36,42,46	0
3	PO4	D	602	5/5	0.97	0.16	64,65,69,70	0
2	CVJ	B	601	25/25	0.98	0.13	27,38,45,47	0
3	PO4	A	602	5/5	0.98	0.16	55,56,60,60	0

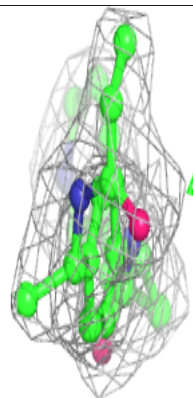
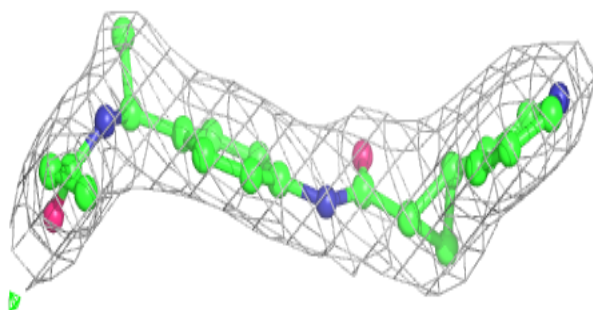
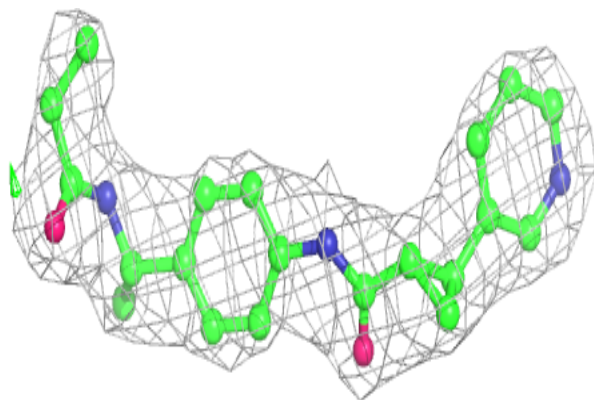
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CVJ D 601:

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

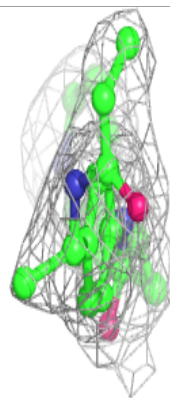
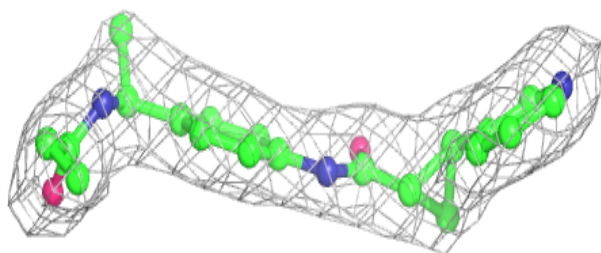
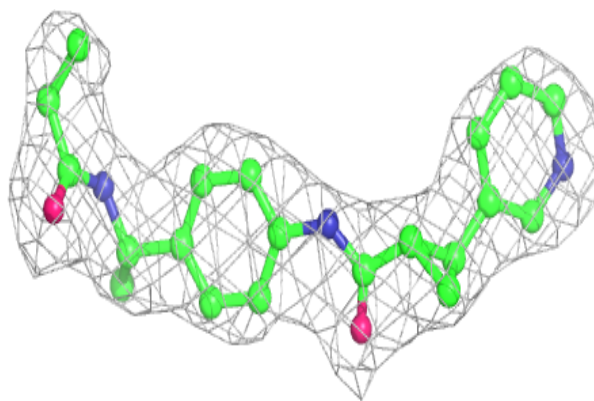
**Electron density around CVJ A 601:**

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

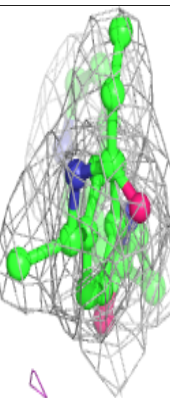
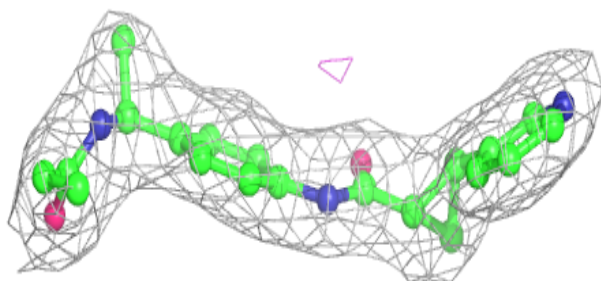
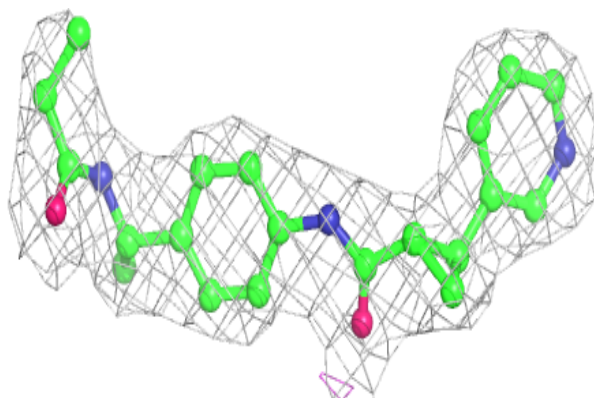


Electron density around CVJ C 601:

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

**Electron density around CVJ B 601:**

$2mF_o-DF_c$ (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.