Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:33 PM EDT

PDB ID	:	2XYN
Title	:	HUMAN ABL2 IN COMPLEX WITH AURORA KINASE INHIBITOR VX-680
Authors	:	Salah, E.; Ugochukwu, E.; Elkins, J.M.; Barr, A.J.; Shrestha, B.; Savitsky, P.; Mahajan, P.; Muniz, J.R.C.; Yue, W.W.; Chaikuad, A.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-11-18
Resolution	:	2.81 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 (i) 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 (i)) were used in the production of this report:

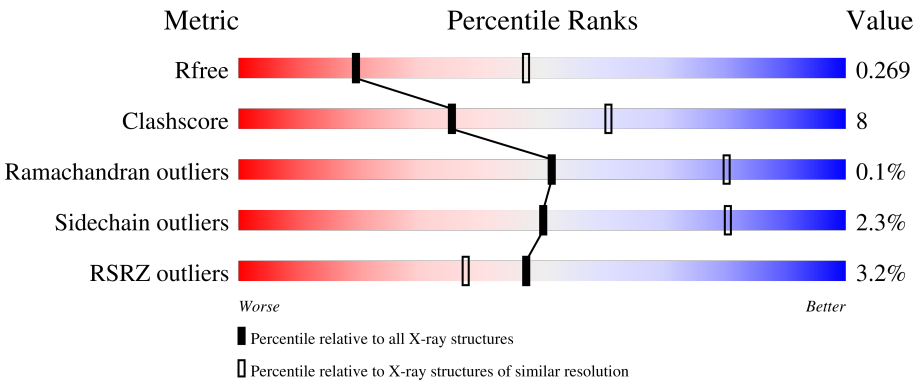
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	292	% 77% 13% 10%
1	B	292	3% 76% 14% • 10%
1	C	292	4% 82% 8% 10%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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	VX6	B	548	-	-	-	X
3	VX6	C	549	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6093 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 TYROSINE-PROTEIN KINASE ABL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2026	1311	328	372	15	0	1	0
1	B	264	2025	1314	326	369	16	0	0	0
1	C	262	1795	1147	306	330	12	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	MET	-	expression tag	UNP P42684
A	256	GLY	-	expression tag	UNP P42684
A	257	HIS	-	expression tag	UNP P42684
A	258	HIS	-	expression tag	UNP P42684
A	259	HIS	-	expression tag	UNP P42684
A	260	HIS	-	expression tag	UNP P42684
A	261	HIS	-	expression tag	UNP P42684
A	262	HIS	-	expression tag	UNP P42684
A	263	SER	-	expression tag	UNP P42684
A	264	SER	-	expression tag	UNP P42684
A	265	GLY	-	expression tag	UNP P42684
A	266	VAL	-	expression tag	UNP P42684
A	267	ASP	-	expression tag	UNP P42684
A	268	LEU	-	expression tag	UNP P42684
A	269	GLY	-	expression tag	UNP P42684
A	270	THR	-	expression tag	UNP P42684
A	271	GLU	-	expression tag	UNP P42684
A	272	ASN	-	expression tag	UNP P42684
A	273	LEU	-	expression tag	UNP P42684
A	274	TYR	-	expression tag	UNP P42684
A	275	PHE	-	expression tag	UNP P42684
A	276	GLN	-	expression tag	UNP P42684
A	277	SER	-	expression tag	UNP P42684

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Chain	Residue	Modelled	Actual	Comment	Reference
A	278	MET	-	expression tag	UNP P42684
B	255	MET	-	expression tag	UNP P42684
B	256	GLY	-	expression tag	UNP P42684
B	257	HIS	-	expression tag	UNP P42684
B	258	HIS	-	expression tag	UNP P42684
B	259	HIS	-	expression tag	UNP P42684
B	260	HIS	-	expression tag	UNP P42684
B	261	HIS	-	expression tag	UNP P42684
B	262	HIS	-	expression tag	UNP P42684
B	263	SER	-	expression tag	UNP P42684
B	264	SER	-	expression tag	UNP P42684
B	265	GLY	-	expression tag	UNP P42684
B	266	VAL	-	expression tag	UNP P42684
B	267	ASP	-	expression tag	UNP P42684
B	268	LEU	-	expression tag	UNP P42684
B	269	GLY	-	expression tag	UNP P42684
B	270	THR	-	expression tag	UNP P42684
B	271	GLU	-	expression tag	UNP P42684
B	272	ASN	-	expression tag	UNP P42684
B	273	LEU	-	expression tag	UNP P42684
B	274	TYR	-	expression tag	UNP P42684
B	275	PHE	-	expression tag	UNP P42684
B	276	GLN	-	expression tag	UNP P42684
B	277	SER	-	expression tag	UNP P42684
B	278	MET	-	expression tag	UNP P42684
C	255	MET	-	expression tag	UNP P42684
C	256	GLY	-	expression tag	UNP P42684
C	257	HIS	-	expression tag	UNP P42684
C	258	HIS	-	expression tag	UNP P42684
C	259	HIS	-	expression tag	UNP P42684
C	260	HIS	-	expression tag	UNP P42684
C	261	HIS	-	expression tag	UNP P42684
C	262	HIS	-	expression tag	UNP P42684
C	263	SER	-	expression tag	UNP P42684
C	264	SER	-	expression tag	UNP P42684
C	265	GLY	-	expression tag	UNP P42684
C	266	VAL	-	expression tag	UNP P42684
C	267	ASP	-	expression tag	UNP P42684
C	268	LEU	-	expression tag	UNP P42684
C	269	GLY	-	expression tag	UNP P42684
C	270	THR	-	expression tag	UNP P42684
C	271	GLU	-	expression tag	UNP P42684

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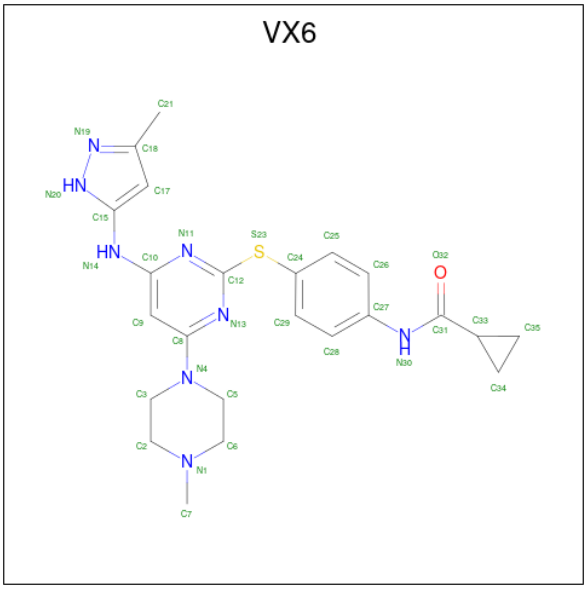
Chain	Residue	Modelled	Actual	Comment	Reference
C	272	ASN	-	expression tag	UNP P42684
C	273	LEU	-	expression tag	UNP P42684
C	274	TYR	-	expression tag	UNP P42684
C	275	PHE	-	expression tag	UNP P42684
C	276	GLN	-	expression tag	UNP P42684
C	277	SER	-	expression tag	UNP P42684
C	278	MET	-	expression tag	UNP P42684

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	2	2	2	0	0

- Molecule 3 is CYCLOPROPANECARBOXYLIC ACID {4-[4-(4-METHYL-PIPERAZIN-1-YL)-6-(5-METHYL-2H-PYRAZOL-3-YLAMINO)-PYRIMIDIN-2-YLSULFANYL]-PHENYL}-AMIDE (three-letter code: VX6) (formula: $C_{23}H_{28}N_8OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	33	23	8	1	1	0	0
			Total	C	N	O	S		
3	B	1	33	23	8	1	1	0	0
			Total	C	N	O	S		
3	B	1	33	23	8	1	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	33	23	8	1	1	0	0
3	C	1	33	23	8	1	1	0	0
3	C	1	33	23	8	1	1	0	0
3	C	1	33	23	8	1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is water.

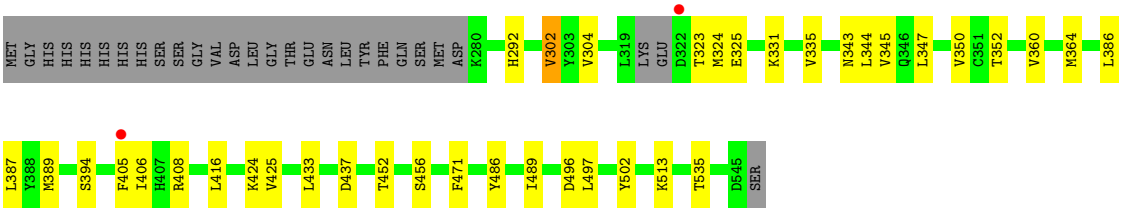
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	6	6	6	0	0
			Total	O		
5	B	7	7	7	0	0

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.

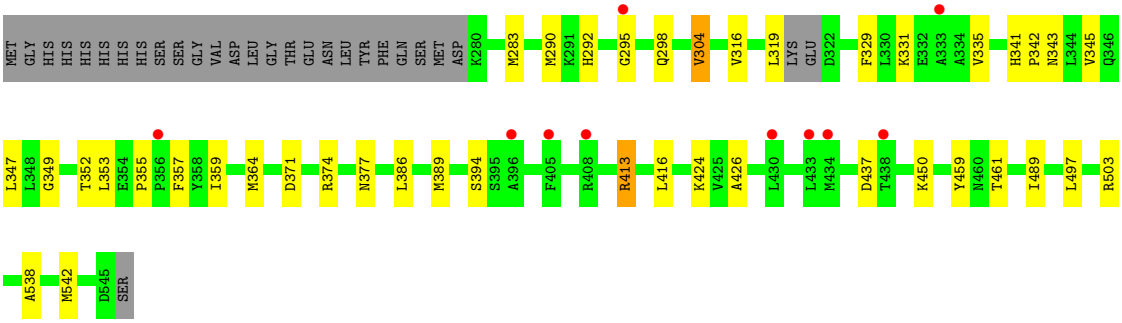
• Molecule 1: TYROSINE-PROTEIN KINASE ABL2

Chain A:



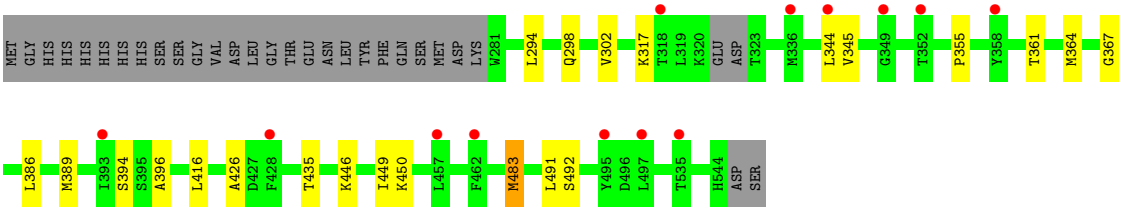
• Molecule 1: TYROSINE-PROTEIN KINASE ABL2

Chain B:



• Molecule 1: TYROSINE-PROTEIN KINASE ABL2

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.50Å 170.50Å 100.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	147.66 – 2.81 83.17 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.66-2.81) 99.9 (83.17-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.246 , 0.284 0.240 , 0.269	Depositor DCC
R_{free} test set	2086 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 97.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6093	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: VX6, NA, CL

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	0.61	0/2081	0.65	0/2838
1	B	0.57	0/2080	0.64	2/2839 (0.1%)
1	C	0.42	0/1839	0.55	0/2525
All	All	0.54	0/6000	0.62	2/8202 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	503	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	413	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	2026	0	1858	21	0
1	B	2025	0	1882	34	0
1	C	1795	0	1457	27	0
2	A	2	0	0	0	0
3	A	33	0	28	8	0
3	B	99	0	84	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	99	0	84	22	0
4	A	1	0	0	0	0
5	A	6	0	0	0	0
5	B	7	0	0	0	0
All	All	6093	0	5393	94	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 8.

All (94) 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)
3:B:547:VX6:H26	3:B:547:VX6:O32	1.68	0.94
1:A:364:MET:H	3:A:547:VX6:H20	1.10	0.91
1:B:450:LYS:NZ	1:C:492:SER:OG	2.06	0.87
1:B:295:GLY:HA2	1:C:483:MET:SD	2.14	0.87
1:B:290:MET:HE1	1:B:316:VAL:HG11	1.54	0.87
1:A:302:VAL:HG11	3:A:547:VX6:H26	1.58	0.84
1:B:364:MET:H	3:B:547:VX6:H20	1.24	0.82
1:B:319:LEU:HD21	1:B:329:PHE:HB2	1.71	0.73
1:B:353:LEU:HA	3:B:548:VX6:H52	1.72	0.71
3:B:547:VX6:O32	3:B:547:VX6:C26	2.37	0.71
1:C:449:ILE:HD11	3:C:549:VX6:H17	1.73	0.71
3:C:549:VX6:O32	3:C:549:VX6:H26	1.93	0.67
3:C:549:VX6:C28	3:C:549:VX6:H212	2.25	0.66
1:B:374:ARG:NH2	1:C:491:LEU:HG	2.11	0.66
1:C:364:MET:H	3:C:547:VX6:H20	1.44	0.66
1:A:302:VAL:HG11	3:A:547:VX6:C26	2.25	0.66
1:C:302:VAL:HG11	3:C:547:VX6:H26	1.77	0.66
1:B:283:MET:CE	1:B:349:GLY:HA3	2.27	0.65
3:C:549:VX6:H212	3:C:549:VX6:H28	1.81	0.63
1:B:355:PRO:HD3	3:B:548:VX6:C15	2.28	0.63
1:B:283:MET:HE3	1:B:349:GLY:HA3	1.81	0.63
1:B:292:HIS:CG	1:B:304:VAL:CG1	2.82	0.62
1:B:345:VAL:HG21	1:B:416:LEU:HD12	1.80	0.62
1:A:323:THR:O	1:A:325:GLU:N	2.30	0.61
3:B:548:VX6:O32	3:B:548:VX6:H26	2.00	0.61
1:C:294:LEU:HD22	3:C:547:VX6:C8	2.32	0.59
1:A:331:LYS:O	1:A:335:VAL:HG23	2.03	0.59
1:B:461:THR:HG21	3:B:549:VX6:C12	2.33	0.58
1:A:350:VAL:HB	1:A:352:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HG23	1:A:408:ARG:HG3	1.85	0.57
1:B:352:THR:HG22	1:B:357:PHE:CD2	2.40	0.56
1:C:345:VAL:HG21	1:C:416:LEU:HD12	1.87	0.56
1:B:459:TYR:HB3	3:B:549:VX6:C2	2.37	0.55
1:C:302:VAL:HG11	3:C:547:VX6:C26	2.36	0.55
1:C:367:GLY:N	3:C:547:VX6:H51	2.22	0.55
1:B:459:TYR:HB3	3:B:549:VX6:H21	1.88	0.55
1:C:344:LEU:CD2	1:C:396:ALA:HB1	2.37	0.55
3:A:547:VX6:H26	3:A:547:VX6:O32	2.05	0.55
1:A:347:LEU:HD12	1:A:360:VAL:O	2.08	0.54
1:C:345:VAL:HG21	1:C:426:ALA:HB2	1.89	0.54
1:C:344:LEU:HD21	1:C:396:ALA:HB1	1.91	0.53
1:C:446:LYS:HA	3:C:549:VX6:H211	1.91	0.53
1:A:343:ASN:HA	1:A:424:LYS:HG2	1.92	0.52
3:B:549:VX6:N11	3:B:549:VX6:H17	2.25	0.52
1:C:302:VAL:HG21	3:C:547:VX6:C26	2.40	0.52
1:A:471:PHE:CE2	1:A:535:THR:HG21	2.46	0.51
1:A:364:MET:N	3:A:547:VX6:H20	1.94	0.51
1:A:386:LEU:HD23	1:A:389:MET:CE	2.40	0.51
3:A:547:VX6:H17	3:A:547:VX6:N11	2.26	0.51
1:B:319:LEU:HD21	1:B:329:PHE:CB	2.38	0.51
1:B:386:LEU:HA	1:B:389:MET:HE2	1.93	0.51
1:A:292:HIS:CE1	1:A:304:VAL:HG11	2.45	0.51
1:B:386:LEU:HD23	1:B:389:MET:CE	2.42	0.49
3:B:549:VX6:N11	3:B:549:VX6:C17	2.74	0.49
1:A:345:VAL:HG21	1:A:416:LEU:HD12	1.93	0.49
1:B:347:LEU:CD1	1:B:359:ILE:HG23	2.43	0.48
3:C:549:VX6:N11	3:C:549:VX6:C17	2.76	0.47
3:A:547:VX6:N11	3:A:547:VX6:C17	2.73	0.47
3:B:547:VX6:H17	3:B:547:VX6:N11	2.30	0.47
1:C:416:LEU:HD13	3:C:547:VX6:N19	2.30	0.47
1:C:386:LEU:HD23	1:C:389:MET:CE	2.44	0.46
1:B:290:MET:CE	1:B:316:VAL:HG11	2.35	0.46
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.50	0.46
1:A:486:TYR:HB3	1:A:489:ILE:HD12	1.98	0.46
1:C:361:THR:HG21	3:C:547:VX6:H352	1.99	0.45
1:C:317:LYS:HD2	3:C:547:VX6:H33	1.98	0.45
1:A:502:TYR:HB2	1:B:497:LEU:HD21	1.99	0.44
3:C:549:VX6:H17	3:C:549:VX6:N11	2.33	0.44
1:A:405:PHE:CE1	1:A:433:LEU:HD13	2.53	0.44
1:B:377:ASN:HB2	1:C:298:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:CG2	1:C:426:ALA:HB2	2.48	0.43
3:B:548:VX6:O32	3:B:548:VX6:C26	2.67	0.43
3:C:549:VX6:H9	3:C:549:VX6:H51	1.85	0.43
1:A:302:VAL:HG11	3:A:547:VX6:C25	2.50	0.42
3:B:547:VX6:N11	3:B:547:VX6:C17	2.79	0.42
1:C:367:GLY:CA	3:C:547:VX6:H51	2.49	0.42
1:B:343:ASN:HA	1:B:424:LYS:HG2	2.02	0.42
1:B:345:VAL:HG21	1:B:426:ALA:HB2	2.02	0.42
3:B:549:VX6:H9	3:B:549:VX6:H51	1.82	0.42
1:B:295:GLY:CA	1:C:483:MET:SD	2.97	0.41
1:B:298:GLN:OE1	1:B:413:ARG:HD2	2.20	0.41
1:B:331:LYS:O	1:B:335:VAL:HG23	2.21	0.41
1:A:452:THR:CG2	1:A:456:SER:HB2	2.50	0.41
1:B:371:ASP:OD1	1:C:450:LYS:NZ	2.54	0.41
1:B:292:HIS:CG	1:B:304:VAL:HG13	2.55	0.41
3:C:548:VX6:H17	3:C:548:VX6:N11	2.36	0.41
1:A:344:LEU:HD23	1:A:425:VAL:HB	2.03	0.41
1:A:497:LEU:HD21	1:B:489:ILE:HD11	2.03	0.40
1:B:292:HIS:CG	1:B:304:VAL:HG11	2.54	0.40
1:C:483:MET:HB3	1:C:483:MET:HE3	1.49	0.40
1:B:538:ALA:O	1:B:542:MET:HG3	2.21	0.40
3:C:548:VX6:H17	3:C:548:VX6:C25	2.50	0.40
1:C:302:VAL:HG21	3:C:547:VX6:H26	2.02	0.40
1:C:355:PRO:HG3	3:C:548:VX6:H26	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	261/292 (89%)	254 (97%)	6 (2%)	1 (0%)	34 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/292 (89%)	252 (97%)	8 (3%)	0	100	100
1	C	258/292 (88%)	250 (97%)	8 (3%)	0	100	100
All	All	779/876 (89%)	756 (97%)	22 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	MET

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	191/253 (76%)	184 (96%)	7 (4%)	34	66
1	B	194/253 (77%)	191 (98%)	3 (2%)	65	88
1	C	128/253 (51%)	125 (98%)	3 (2%)	50	80
All	All	513/759 (68%)	500 (98%)	13 (2%)	50	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	VAL
1	A	387	LEU
1	A	394	SER
1	A	437	ASP
1	A	496[A]	ASP
1	A	496[B]	ASP
1	A	513	LYS
1	B	304	VAL
1	B	394	SER
1	B	437	ASP
1	C	394	SER
1	C	435	THR
1	C	483	MET

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

Mol	Chain	Res	Type
1	A	292	HIS
1	B	343	ASN
1	C	298	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	VX6	B	548	-	35,37,37	2.02	8 (22%)	49,52,52	2.09	11 (22%)
3	VX6	C	549	-	35,37,37	1.87	8 (22%)	49,52,52	2.09	13 (26%)
3	VX6	B	547	-	35,37,37	1.65	5 (14%)	49,52,52	2.21	16 (32%)
3	VX6	C	548	-	35,37,37	1.77	6 (17%)	49,52,52	2.09	10 (20%)
3	VX6	B	549	-	35,37,37	1.73	5 (14%)	49,52,52	1.93	14 (28%)
3	VX6	A	547	-	35,37,37	1.72	5 (14%)	49,52,52	2.24	16 (32%)
3	VX6	C	547	-	35,37,37	1.73	5 (14%)	49,52,52	2.17	14 (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	VX6	B	548	-	-	0/19/32/32	0/5/5/5
3	VX6	C	549	-	-	6/19/32/32	0/5/5/5
3	VX6	B	547	-	-	4/19/32/32	0/5/5/5
3	VX6	C	548	-	-	4/19/32/32	0/5/5/5
3	VX6	B	549	-	-	4/19/32/32	0/5/5/5
3	VX6	A	547	-	-	4/19/32/32	0/5/5/5
3	VX6	C	547	-	-	6/19/32/32	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	547	VX6	N20-N19	-7.20	1.23	1.37
3	C	549	VX6	N20-N19	-7.10	1.23	1.37
3	C	548	VX6	N20-N19	-7.09	1.23	1.37
3	B	548	VX6	N20-N19	-7.06	1.24	1.37
3	A	547	VX6	N20-N19	-7.04	1.24	1.37
3	B	549	VX6	N20-N19	-6.97	1.24	1.37
3	C	547	VX6	N20-N19	-6.60	1.24	1.37
3	B	548	VX6	C12-S23	4.41	1.82	1.76
3	A	547	VX6	C10-N14	-3.42	1.32	1.38
3	B	548	VX6	C8-N4	3.42	1.45	1.37
3	C	548	VX6	C27-N30	-3.28	1.35	1.41
3	B	549	VX6	C27-N30	-3.26	1.35	1.41
3	C	549	VX6	C17-C18	-3.12	1.33	1.39
3	B	548	VX6	C27-N30	-3.10	1.35	1.41
3	C	549	VX6	C33-C31	2.98	1.56	1.51
3	C	549	VX6	C27-N30	-2.96	1.35	1.41
3	B	547	VX6	C17-C18	-2.92	1.33	1.39
3	A	547	VX6	C17-C18	-2.80	1.33	1.39
3	B	549	VX6	C17-C18	-2.76	1.33	1.39
3	C	547	VX6	C24-S23	2.68	1.82	1.77
3	C	547	VX6	C15-N14	-2.64	1.34	1.38
3	B	548	VX6	C17-C18	-2.60	1.34	1.39
3	B	549	VX6	C10-N14	-2.55	1.34	1.38
3	B	547	VX6	C10-N14	-2.52	1.34	1.38
3	C	547	VX6	C17-C18	-2.50	1.34	1.39
3	A	547	VX6	C15-N14	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	549	VX6	C10-N14	-2.48	1.34	1.38
3	C	548	VX6	C17-C18	-2.47	1.34	1.39
3	C	548	VX6	C24-S23	-2.47	1.73	1.77
3	B	548	VX6	C5-N4	2.40	1.50	1.46
3	B	548	VX6	C3-N4	2.37	1.50	1.46
3	C	547	VX6	C12-S23	2.31	1.79	1.76
3	C	549	VX6	C3-N4	2.27	1.50	1.46
3	B	548	VX6	C33-C31	2.26	1.55	1.51
3	C	549	VX6	C15-N14	-2.25	1.34	1.38
3	B	547	VX6	C27-N30	-2.24	1.37	1.41
3	C	549	VX6	C8-N4	2.20	1.42	1.37
3	C	548	VX6	C10-N14	-2.19	1.34	1.38
3	C	548	VX6	C3-N4	2.18	1.50	1.46
3	A	547	VX6	C8-N4	2.16	1.42	1.37
3	B	549	VX6	C12-S23	-2.07	1.73	1.76
3	B	547	VX6	C15-N14	-2.07	1.35	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	548	VX6	C12-N13-C8	7.50	123.47	115.50
3	B	548	VX6	C12-N11-C10	7.09	121.75	115.15
3	A	547	VX6	C12-N11-C10	6.91	121.59	115.15
3	B	547	VX6	C12-N11-C10	6.80	121.49	115.15
3	B	548	VX6	C12-N13-C8	6.77	122.70	115.50
3	C	547	VX6	C12-N13-C8	6.32	122.22	115.50
3	C	549	VX6	C12-N11-C10	6.20	120.92	115.15
3	A	547	VX6	C12-S23-C24	5.79	113.24	102.76
3	C	549	VX6	C12-N13-C8	5.42	121.26	115.50
3	B	549	VX6	C12-N11-C10	5.22	120.01	115.15
3	A	547	VX6	N13-C8-N4	5.08	122.98	116.56
3	B	549	VX6	C10-C9-C8	5.07	120.69	116.64
3	C	548	VX6	C12-N11-C10	5.05	119.86	115.15
3	B	548	VX6	C10-C9-C8	4.93	120.58	116.64
3	C	548	VX6	C5-N4-C3	4.91	122.61	111.57
3	B	547	VX6	C12-N13-C8	4.79	120.59	115.50
3	B	547	VX6	C10-C9-C8	4.64	120.35	116.64
3	B	549	VX6	C12-N13-C8	4.48	120.25	115.50
3	C	548	VX6	C34-C33-C31	-4.47	112.87	117.24
3	C	547	VX6	C12-N11-C10	4.44	119.29	115.15
3	C	547	VX6	C10-C9-C8	4.40	120.16	116.64
3	C	547	VX6	N13-C8-N4	4.39	122.10	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	549	VX6	C10-C9-C8	4.20	120.00	116.64
3	B	548	VX6	N13-C12-N11	-4.19	119.34	127.00
3	C	549	VX6	C5-N4-C3	4.15	120.90	111.57
3	A	547	VX6	C12-N13-C8	4.14	119.89	115.50
3	B	549	VX6	N13-C8-N4	4.10	121.74	116.56
3	A	547	VX6	C10-C9-C8	4.07	119.89	116.64
3	B	547	VX6	C27-N30-C31	-3.97	118.30	127.37
3	C	547	VX6	C17-C15-N14	-3.95	125.66	131.11
3	B	547	VX6	C5-N4-C3	3.94	120.43	111.57
3	C	549	VX6	N13-C8-N4	3.92	121.51	116.56
3	C	547	VX6	C5-N4-C3	3.83	120.19	111.57
3	C	548	VX6	N13-C12-N11	-3.72	120.20	127.00
3	C	549	VX6	C12-S23-C24	3.59	109.26	102.76
3	B	547	VX6	N13-C8-N4	3.58	121.09	116.56
3	C	549	VX6	N13-C12-N11	-3.40	120.80	127.00
3	B	547	VX6	C35-C33-C31	-3.29	114.03	117.24
3	A	547	VX6	N13-C12-N11	-3.29	121.00	127.00
3	C	547	VX6	C21-C18-N19	3.28	126.56	120.08
3	A	547	VX6	C9-C8-N4	-3.23	118.45	122.35
3	C	547	VX6	N13-C12-N11	-3.22	121.11	127.00
3	C	549	VX6	C17-C15-N14	-3.20	126.70	131.11
3	A	547	VX6	C5-N4-C3	3.13	118.61	111.57
3	A	547	VX6	O32-C31-C33	-3.08	117.44	122.19
3	B	548	VX6	N13-C8-N4	3.08	120.45	116.56
3	B	548	VX6	C9-C8-N13	-3.08	117.41	123.34
3	B	547	VX6	N13-C12-N11	-3.03	121.47	127.00
3	C	547	VX6	C18-C17-C15	-2.98	103.31	106.77
3	B	547	VX6	C33-C31-N30	2.95	120.86	115.16
3	C	548	VX6	C18-C17-C15	-2.93	103.36	106.77
3	B	548	VX6	C5-N4-C3	2.92	118.13	111.57
3	C	547	VX6	C9-C8-N13	-2.91	117.73	123.34
3	C	549	VX6	C18-C17-C15	-2.86	103.44	106.77
3	B	547	VX6	C12-S23-C24	2.84	107.90	102.76
3	B	549	VX6	C9-C8-N13	-2.82	117.92	123.34
3	C	547	VX6	C35-C33-C31	-2.79	114.51	117.24
3	C	548	VX6	C12-S23-C24	2.79	107.81	102.76
3	B	547	VX6	O32-C31-C33	-2.78	117.90	122.19
3	B	549	VX6	C34-C33-C31	-2.74	114.56	117.24
3	C	548	VX6	C9-C8-N13	-2.72	118.11	123.34
3	C	549	VX6	C9-C8-N13	-2.71	118.13	123.34
3	C	547	VX6	C5-C6-N1	-2.69	106.54	110.86
3	C	547	VX6	O32-C31-C33	-2.69	118.04	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	547	VX6	C9-C10-N11	-2.68	117.79	123.35
3	B	547	VX6	C9-C8-N13	-2.63	118.27	123.34
3	A	547	VX6	C35-C33-C31	-2.62	114.67	117.24
3	B	549	VX6	C12-S23-C24	2.62	107.51	102.76
3	B	549	VX6	C5-N4-C3	2.57	117.36	111.57
3	C	547	VX6	N14-C10-N11	2.57	124.33	116.83
3	C	549	VX6	C21-C18-N19	2.54	125.10	120.08
3	A	547	VX6	C18-C17-C15	-2.52	103.83	106.77
3	B	548	VX6	C18-C17-C15	-2.49	103.87	106.77
3	A	547	VX6	C9-C8-N13	-2.48	118.56	123.34
3	B	548	VX6	C9-C10-N11	-2.48	118.21	123.35
3	B	549	VX6	C18-C17-C15	-2.47	103.90	106.77
3	B	549	VX6	N13-C12-N11	-2.45	122.53	127.00
3	B	548	VX6	N14-C10-N11	2.39	123.82	116.83
3	C	548	VX6	C9-C8-N4	2.36	125.21	122.35
3	B	547	VX6	C18-C17-C15	-2.35	104.03	106.77
3	A	547	VX6	C28-C27-C26	-2.33	115.95	119.04
3	B	549	VX6	C9-C10-N11	-2.30	118.59	123.35
3	A	547	VX6	C29-C28-C27	2.26	122.90	120.30
3	B	549	VX6	C21-C18-N19	2.24	124.50	120.08
3	B	547	VX6	C34-C33-C31	2.23	119.42	117.24
3	C	549	VX6	O32-C31-C33	-2.23	118.75	122.19
3	A	547	VX6	C34-C33-C31	2.18	119.37	117.24
3	C	549	VX6	C9-C10-N11	-2.15	118.89	123.35
3	B	549	VX6	C3-C2-N1	2.13	114.28	110.86
3	A	547	VX6	C9-C10-N11	-2.07	119.05	123.35
3	B	548	VX6	C21-C18-N19	2.06	124.14	120.08
3	C	548	VX6	S23-C12-N11	2.06	124.77	116.52
3	B	547	VX6	C6-N1-C2	-2.04	106.29	109.54
3	B	549	VX6	C35-C33-C31	-2.00	115.28	117.24

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	547	VX6	N30-C31-C33-C34
3	A	547	VX6	O32-C31-C33-C34
3	A	547	VX6	O32-C31-C33-C35
3	B	547	VX6	N30-C31-C33-C34
3	B	547	VX6	N30-C31-C33-C35
3	B	547	VX6	O32-C31-C33-C34
3	B	547	VX6	O32-C31-C33-C35

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Mol	Chain	Res	Type	Atoms
3	B	549	VX6	N30-C31-C33-C34
3	B	549	VX6	N30-C31-C33-C35
3	B	549	VX6	O32-C31-C33-C34
3	B	549	VX6	O32-C31-C33-C35
3	C	547	VX6	N30-C31-C33-C34
3	C	547	VX6	O32-C31-C33-C34
3	C	548	VX6	N30-C31-C33-C34
3	C	548	VX6	O32-C31-C33-C34
3	C	549	VX6	N30-C31-C33-C34
3	C	549	VX6	N30-C31-C33-C35
3	C	549	VX6	O32-C31-C33-C34
3	C	549	VX6	O32-C31-C33-C35
3	C	547	VX6	C9-C8-N4-C3
3	C	547	VX6	N13-C8-N4-C3
3	C	547	VX6	N13-C8-N4-C5
3	A	547	VX6	N30-C31-C33-C35
3	C	548	VX6	C25-C24-S23-C12
3	C	547	VX6	C9-C8-N4-C5
3	C	549	VX6	C29-C24-S23-C12
3	C	548	VX6	C29-C24-S23-C12
3	C	549	VX6	C25-C24-S23-C12

There are no ring outliers.

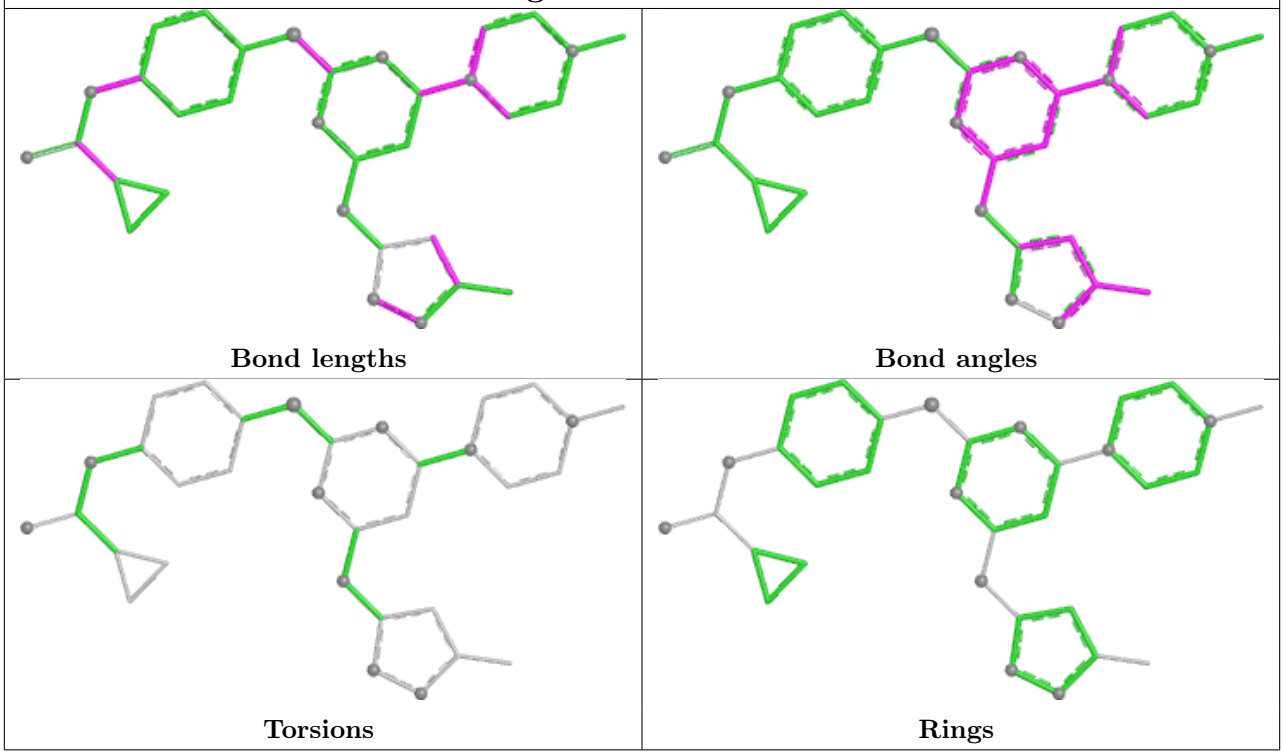
7 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	548	VX6	4	0
3	C	549	VX6	8	0
3	B	547	VX6	5	0
3	C	548	VX6	3	0
3	B	549	VX6	6	0
3	A	547	VX6	8	0
3	C	547	VX6	11	0

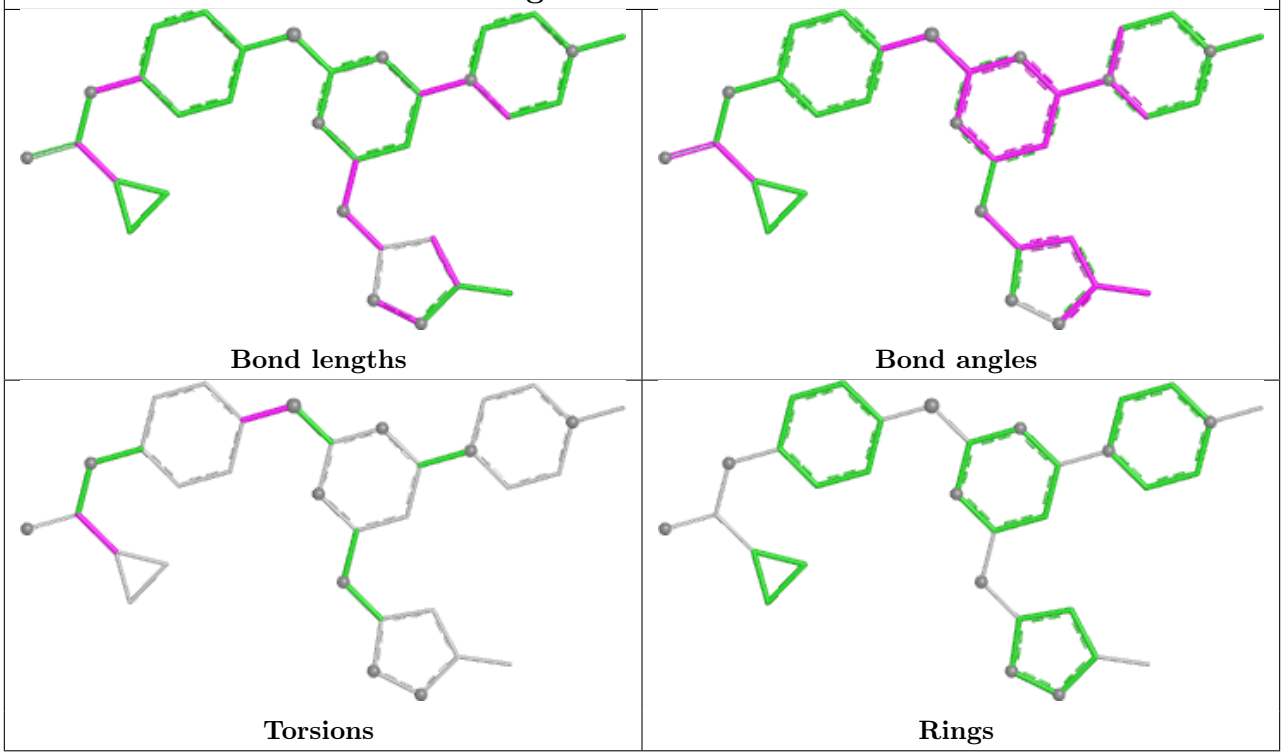
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

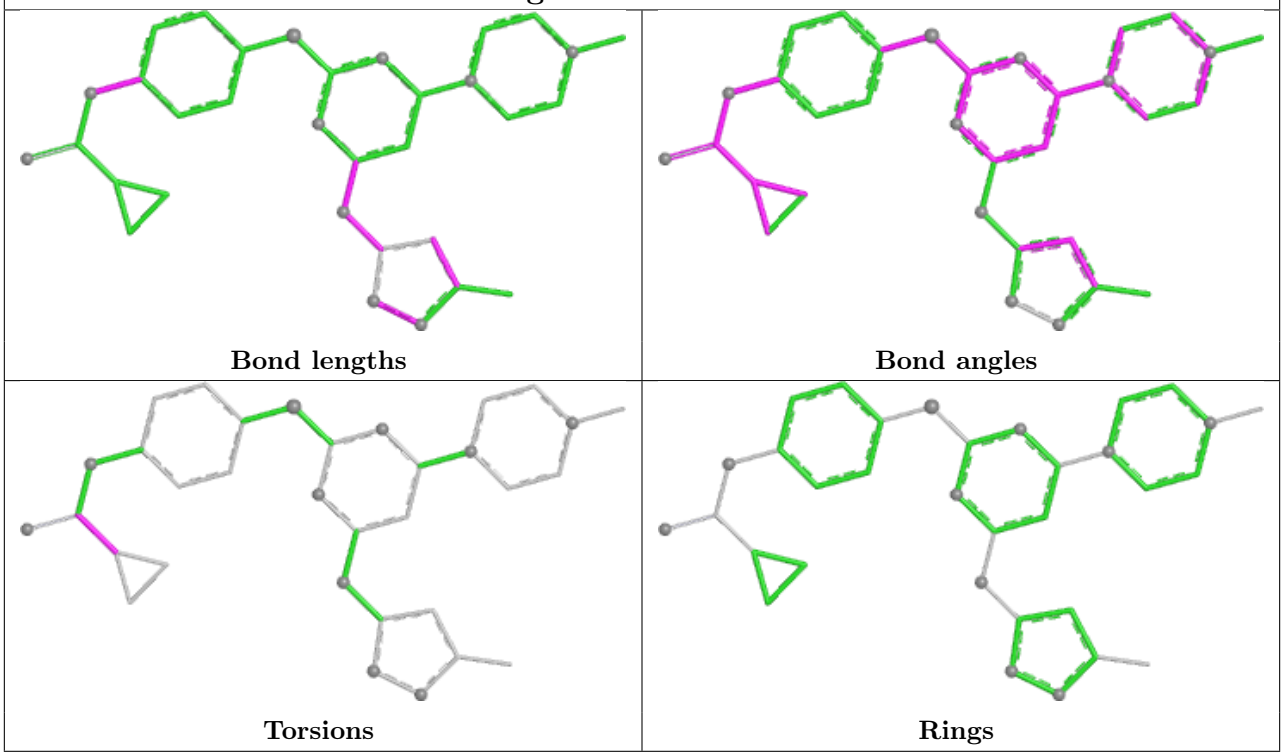
Ligand VX6 B 548



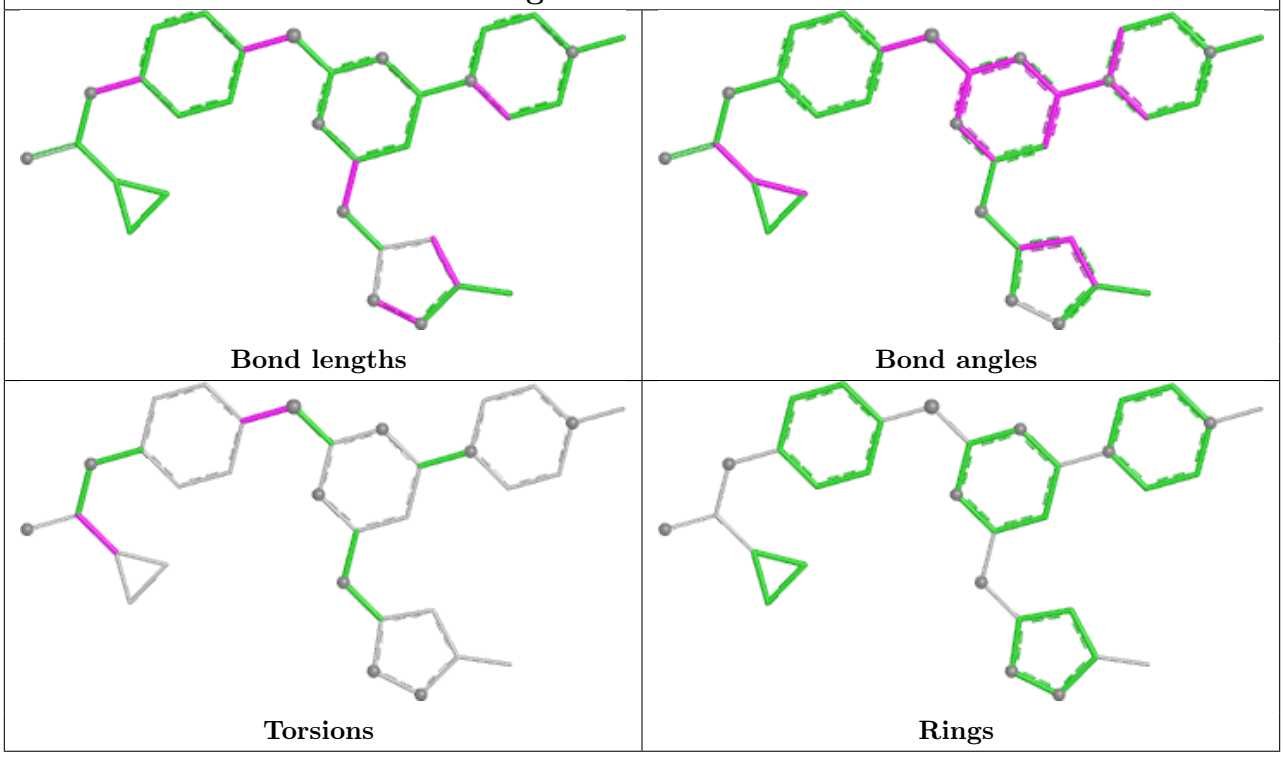
Ligand VX6 C 549



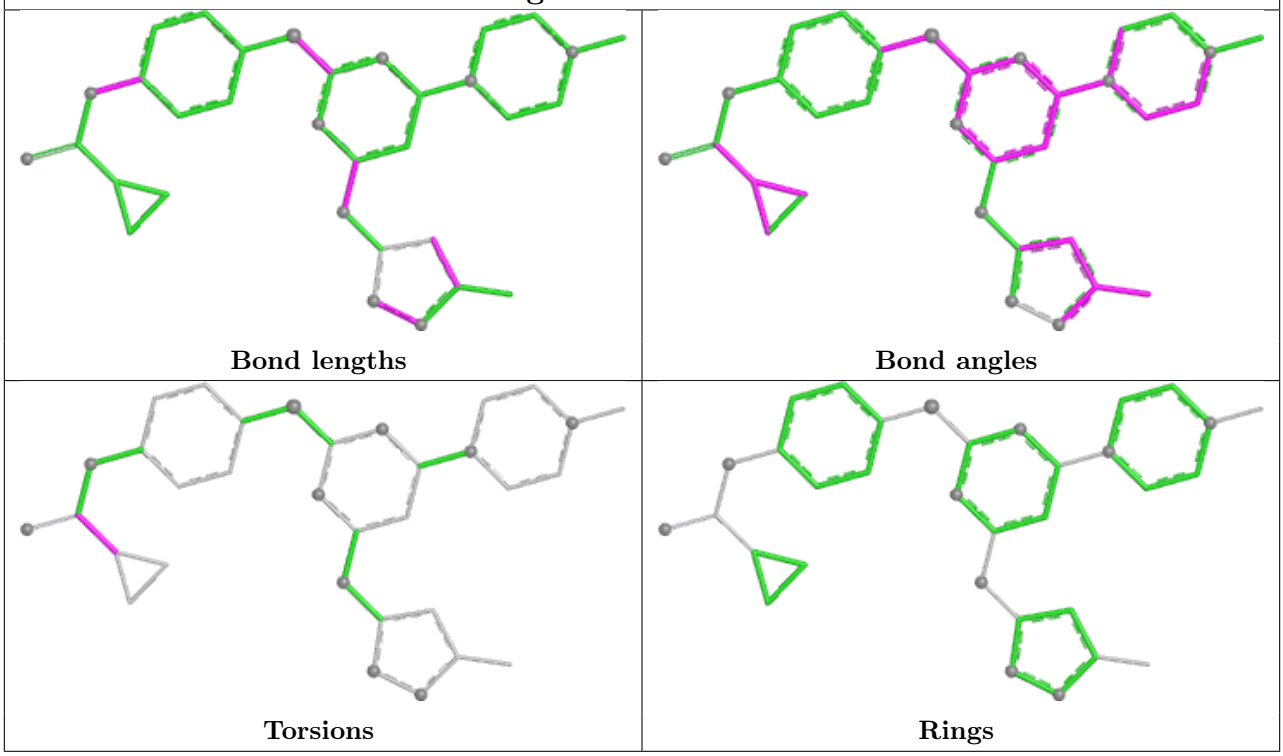
Ligand VX6 B 547



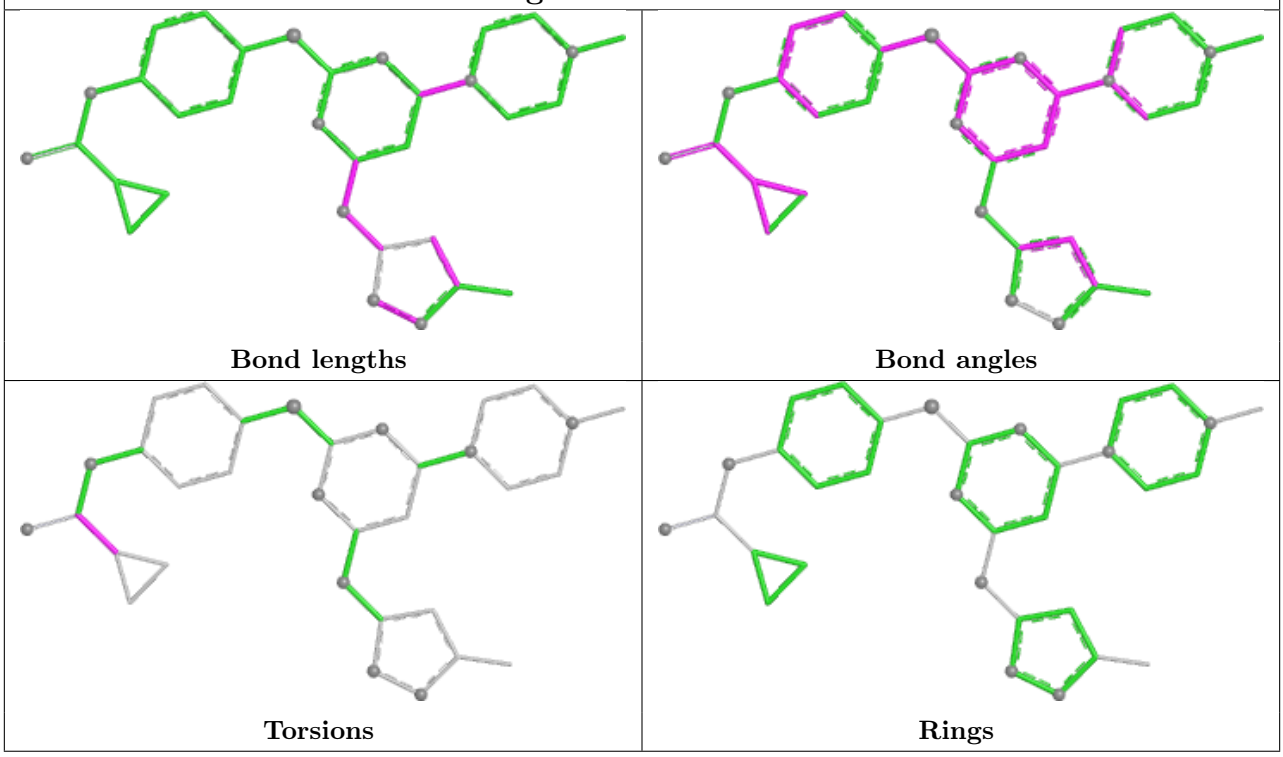
Ligand VX6 C 548

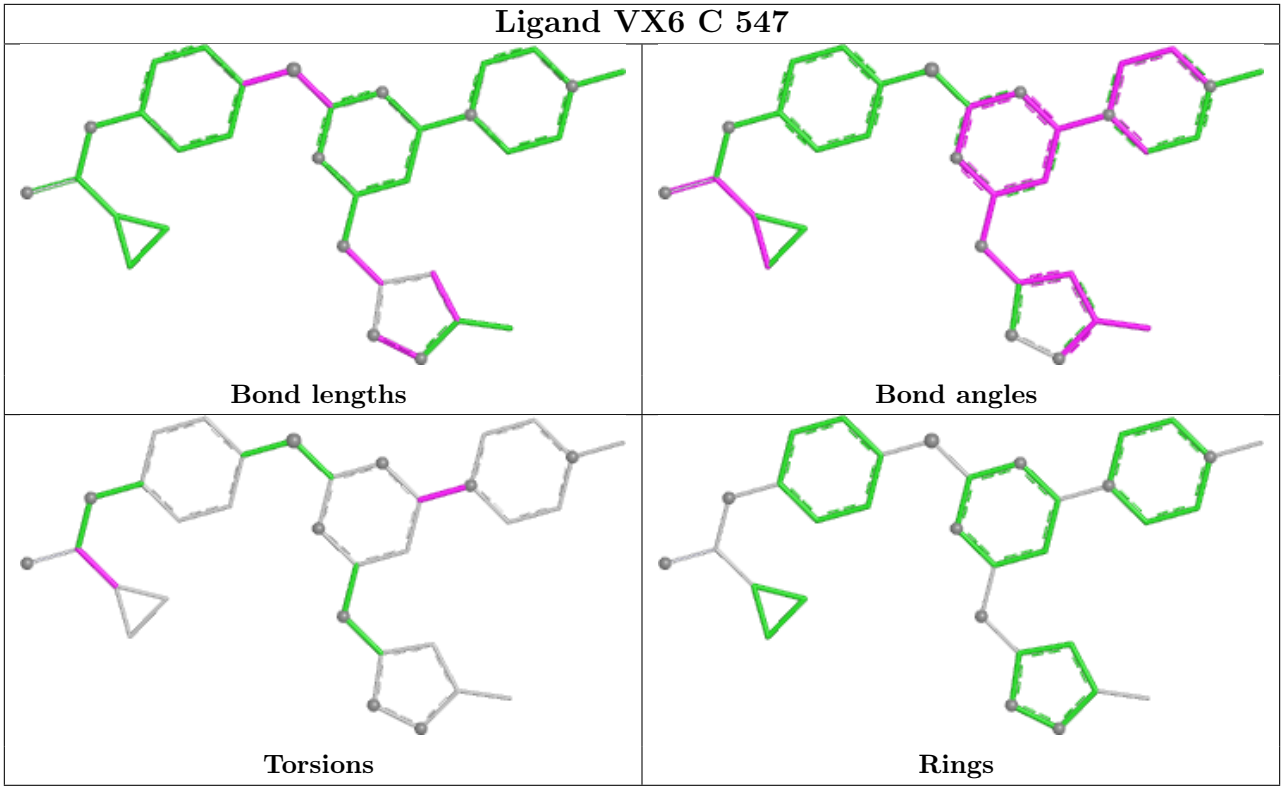


Ligand VX6 B 549



Ligand VX6 A 547





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	264/292 (90%)	0.34	2 (0%)	86	82	51, 77, 133, 171	0
1	B	264/292 (90%)	0.38	10 (3%)	40	30	55, 81, 132, 172	0
1	C	262/292 (89%)	0.28	13 (4%)	28	20	75, 113, 155, 174	0
All	All	790/876 (90%)	0.33	25 (3%)	47	37	51, 92, 146, 174	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	535	THR	6.2
1	C	462	PHE	3.5
1	B	433	LEU	3.5
1	B	396	ALA	3.3
1	C	318	THR	3.2
1	C	393	ILE	3.1
1	B	405	PHE	3.0
1	A	322	ASP	2.8
1	B	434	MET	2.6
1	B	408	ARG	2.5
1	C	358	TYR	2.4
1	B	356	PRO	2.4
1	B	438	THR	2.3
1	C	344	LEU	2.3
1	C	457	LEU	2.2
1	B	295	GLY	2.2
1	C	497	LEU	2.1
1	C	352	THR	2.1
1	C	428	PHE	2.1
1	C	336	MET	2.1
1	B	430	LEU	2.1
1	B	333	ALA	2.1
1	C	495	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	349	GLY	2.0
1	A	405	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

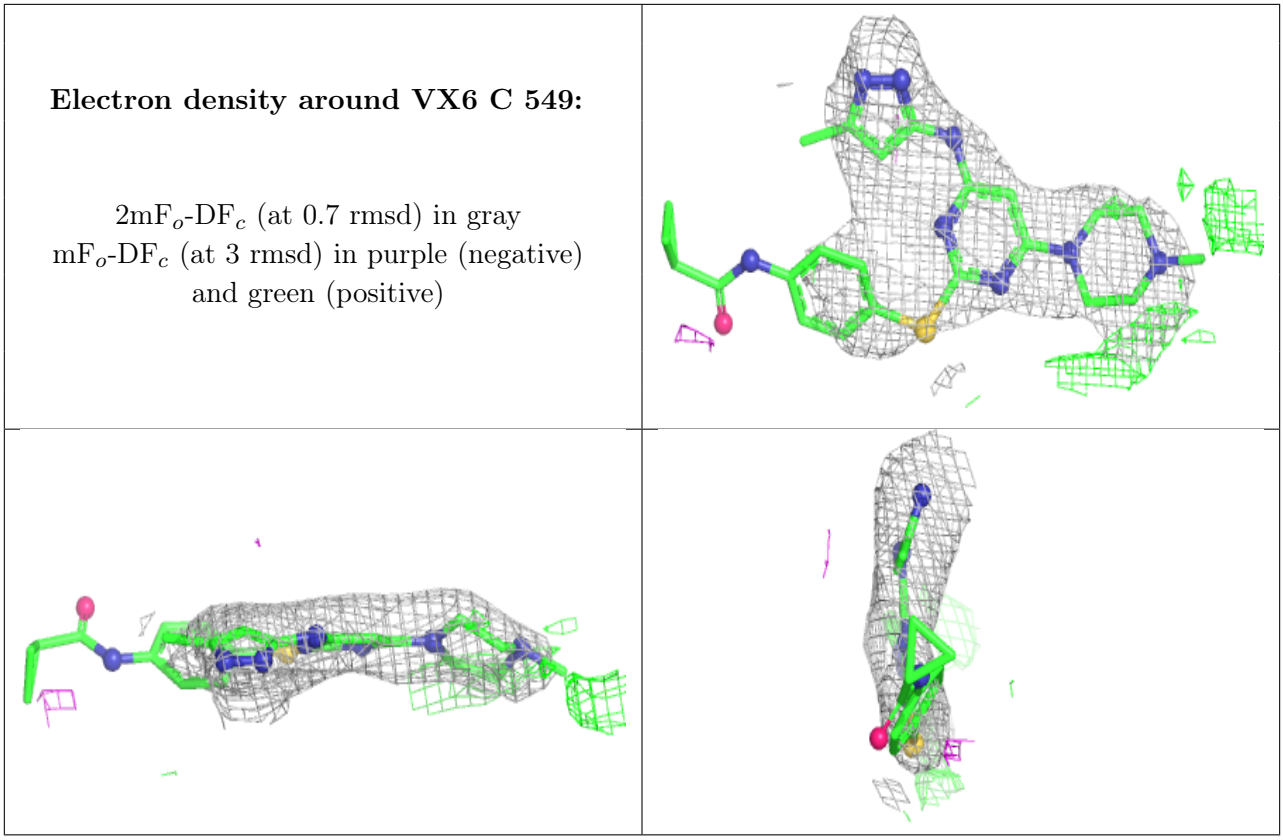
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	VX6	C	549	33/33	0.75	0.46	184,188,193,195	0
3	VX6	B	548	33/33	0.76	0.53	99,104,106,106	0
3	VX6	C	548	33/33	0.80	0.29	245,253,262,269	0
4	CL	A	548	1/1	0.85	0.14	126,126,126,126	0
3	VX6	C	547	33/33	0.89	0.30	132,137,156,159	0
3	VX6	B	549	33/33	0.90	0.40	94,97,103,104	0
3	VX6	B	547	33/33	0.95	0.28	65,72,77,78	0
2	NA	A	549	1/1	0.96	0.44	73,73,73,73	0
3	VX6	A	547	33/33	0.96	0.27	66,74,79,80	0
2	NA	A	1	1/1	0.96	0.71	65,65,65,65	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.

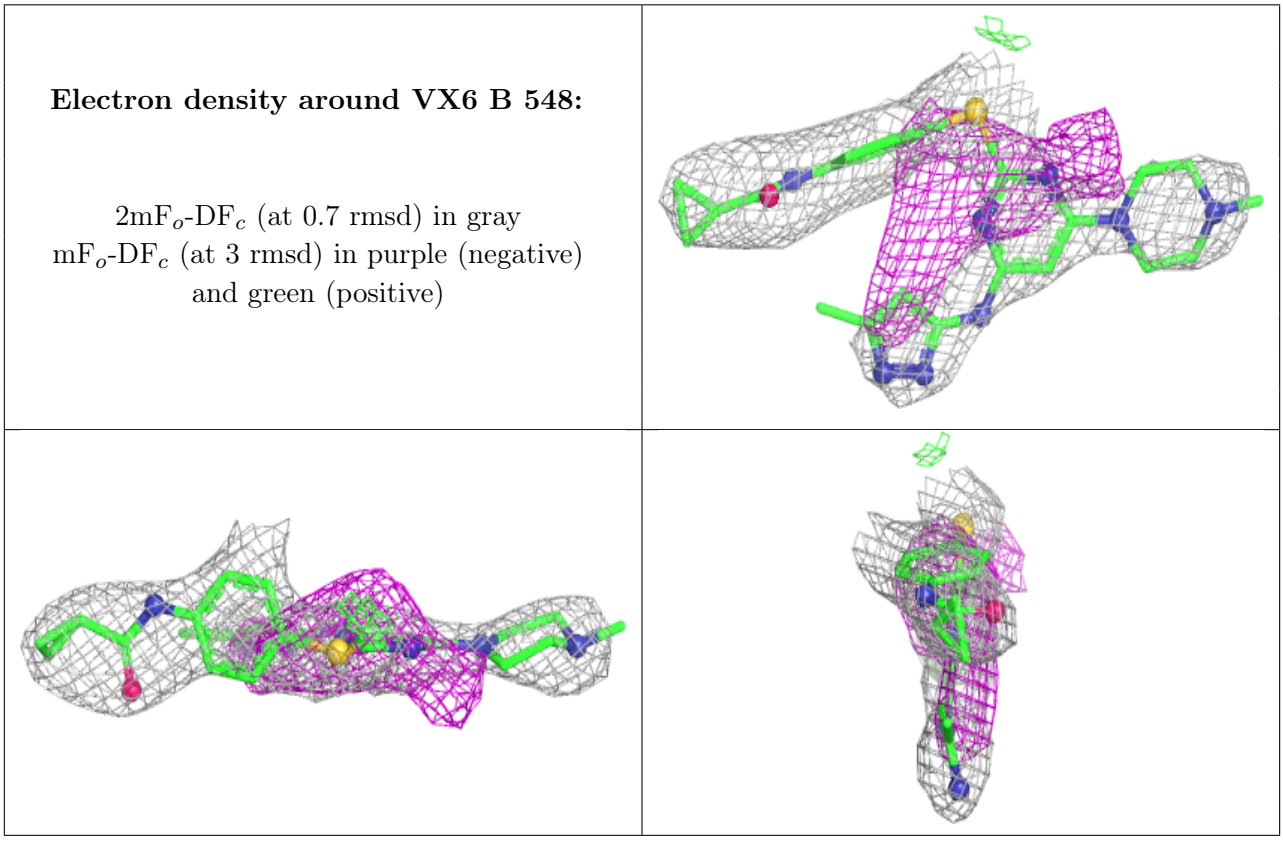
Electron density around VX6 C 549:

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



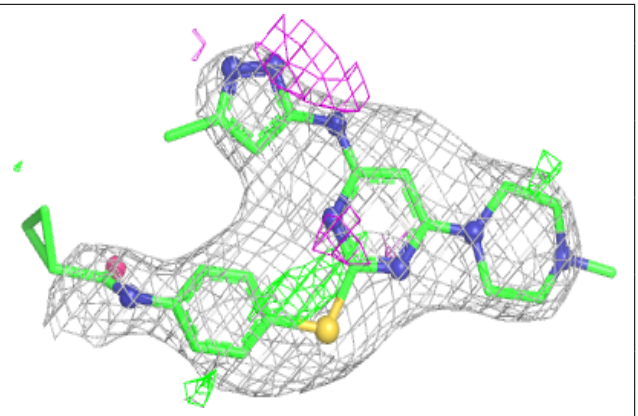
Electron density around VX6 B 548:

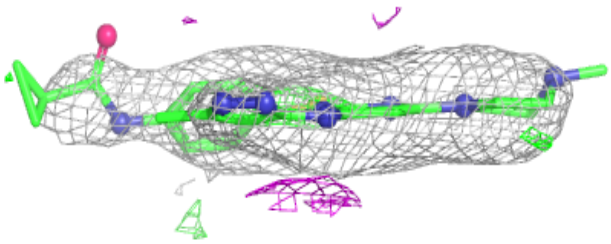
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

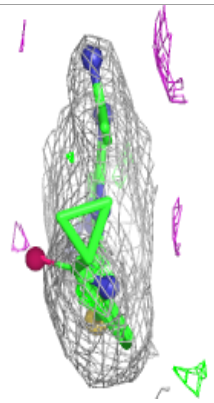


Electron density around VX6 C 548:

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

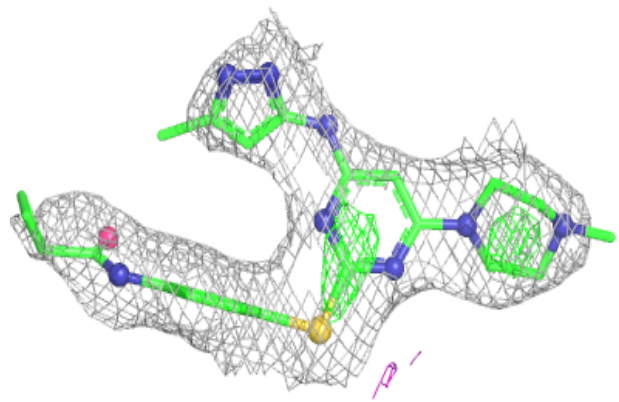


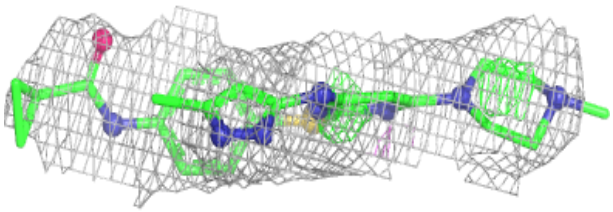


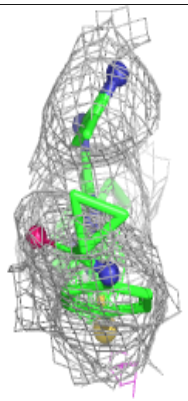


Electron density around VX6 C 547:

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

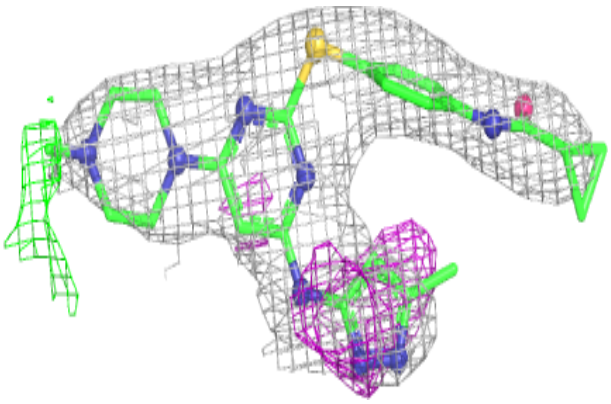


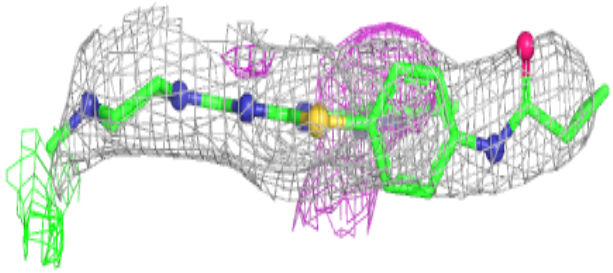


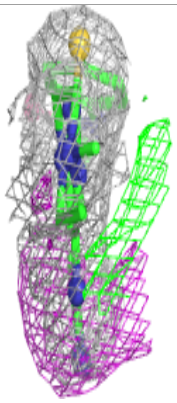


Electron density around VX6 B 549:

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

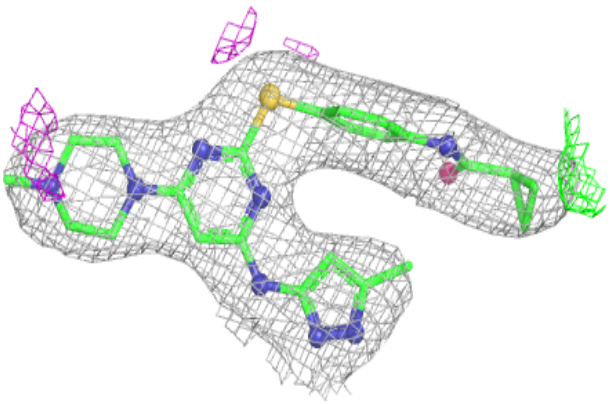


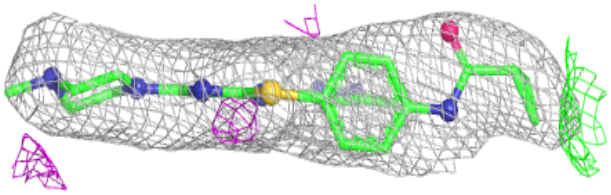


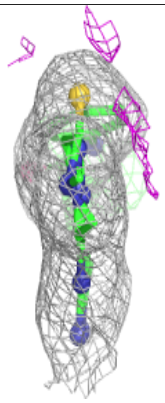


Electron density around VX6 B 547:

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

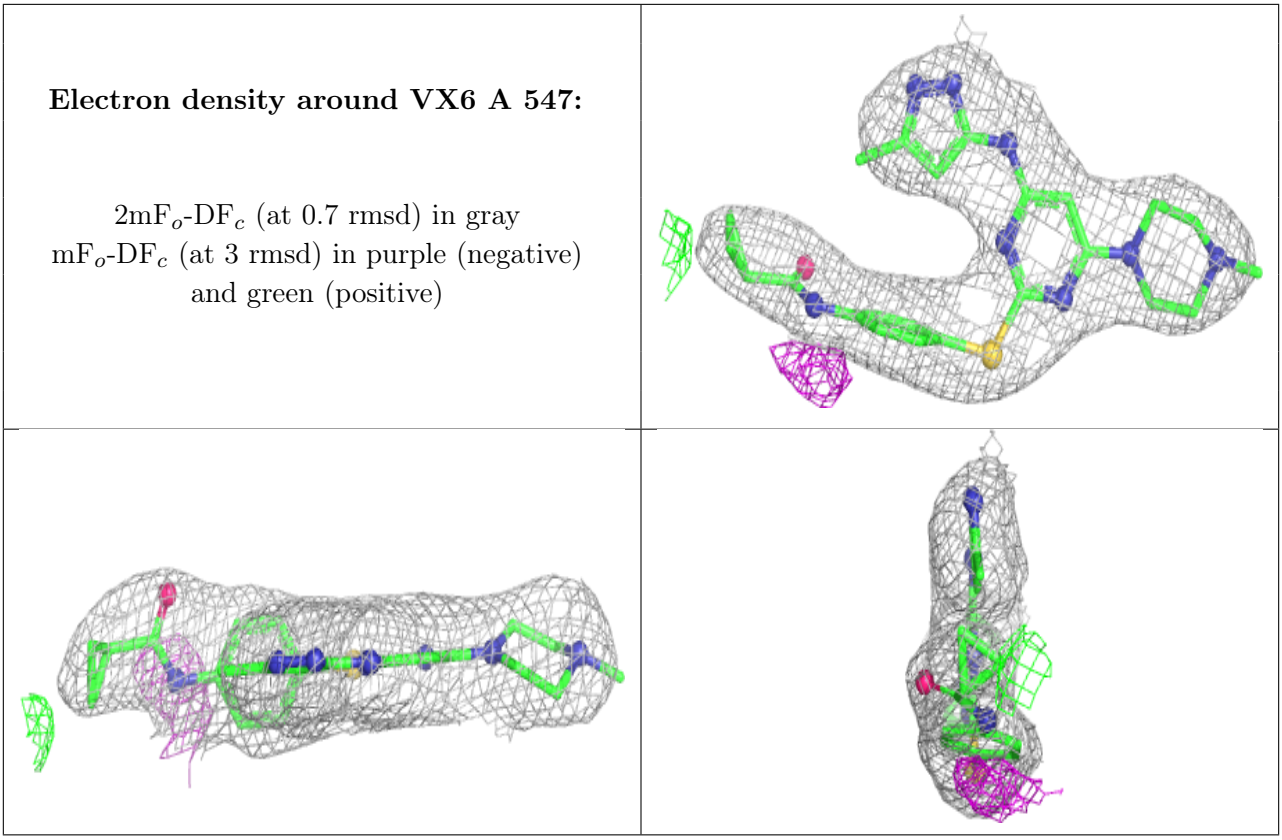






Electron density around VX6 A 547:

$2mF_o$-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.