



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:33 AM UTC

PDB ID : 6T8N / pdb_00006t8n
Title : Crystal structure of the ACVR1 (ALK2) kinase in complex with the compound M4K3007
Authors : Adamson, R.J.; Williams, E.P.; Bonomo, S.; Rankin, S.; Bacos, D.; Rae, A.; Cramp, S.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.N.
Deposited on : 2019-10-24
Resolution : 1.77 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

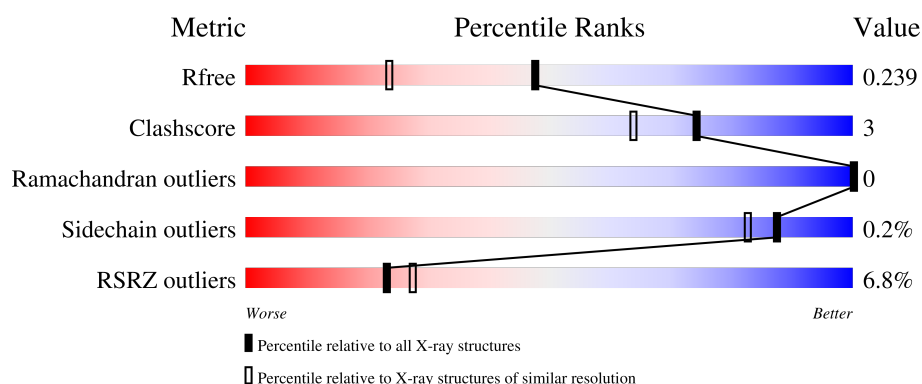
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	301	7% 89% 9% .
1	B	301	7% 92% 5% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9527 atoms, of which 4534 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.

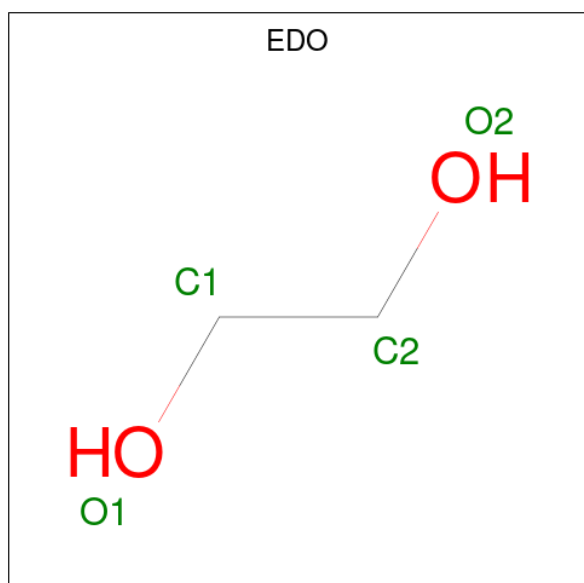
- Molecule 1 is a protein called Activin receptor type I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	H	N	O	S	0	4	0
			4534	1487	2198	403	430	16			
1	B	293	Total	C	H	N	O	S	0	4	0
			4538	1491	2194	405	432	16			

There are 6 discrepancies between the modelled and reference sequences:

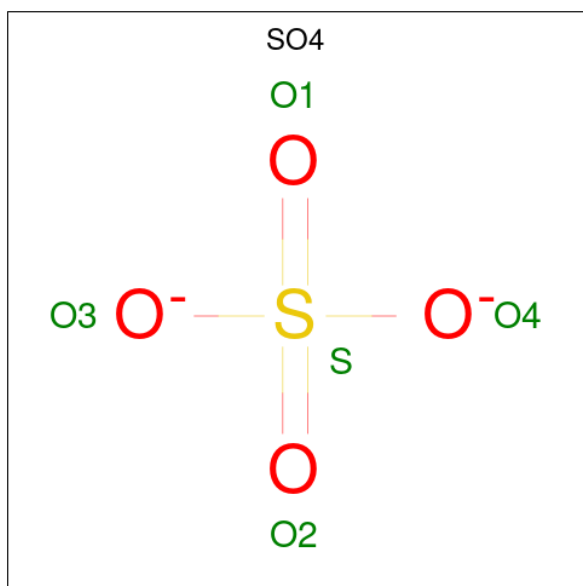
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



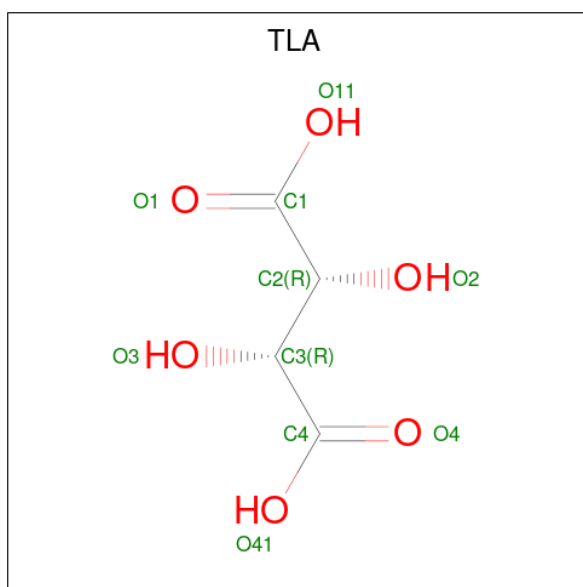
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



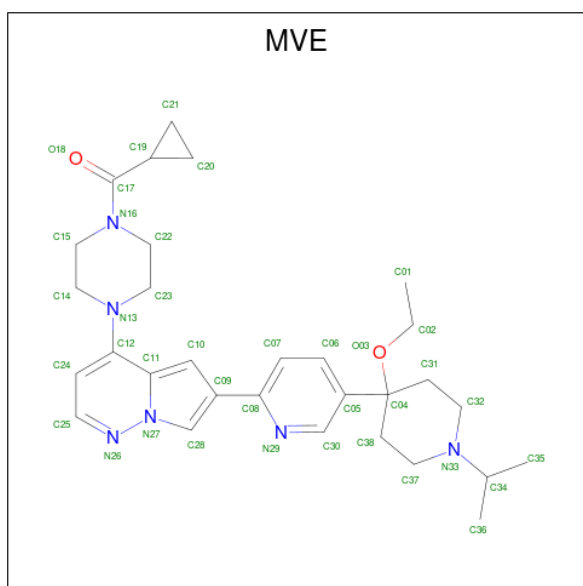
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



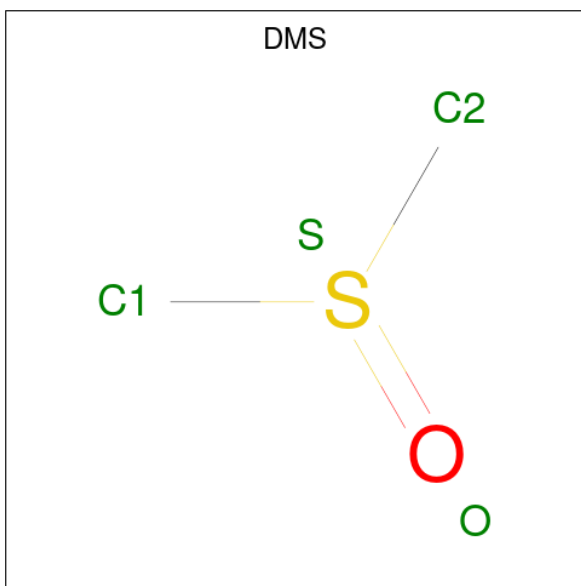
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	4	6		

- Molecule 5 is cyclopropyl-[4-[6-[5-(4-ethoxy-1-propan-2-yl-piperidin-4-yl)pyridin-2-yl]pyrrolo[1,2-b]pyridazin-4-yl]piperazin-1-yl]methanone (CCD ID: MVE) (formula: $C_{30}H_{40}N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			78	30	40	6	2		
5	B	1	Total	C	H	N	O	0	1
			156	60	80	12	4		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

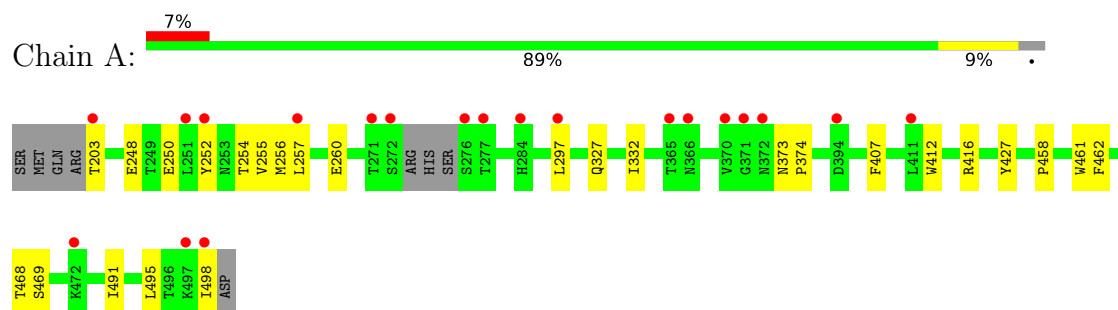
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total	O	0	0
			87	87		
7	B	70	Total	O	0	0
			70	70		

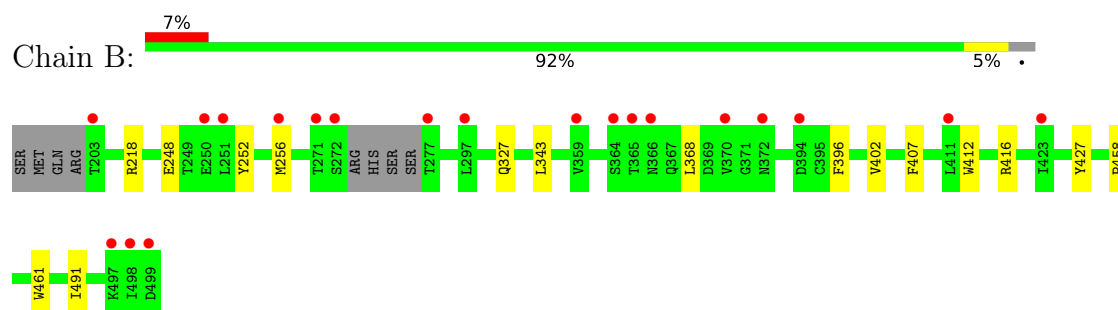
3 Residue-property plots [i](#)

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: Activin receptor type I



• Molecule 1: Activin receptor type I



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.27Å 69.23Å 164.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.34 – 1.77 82.34 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.34-1.77) 99.6 (82.34-1.77)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.203 , 0.237 0.206 , 0.239	Depositor DCC
R_{free} test set	2884 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9527	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3163e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, MVE, TLA, SO4, EDO

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	0.49	0/2407	0.63	0/3268
1	B	0.48	0/2415	0.64	1/3279 (0.0%)
All	All	0.49	0/4822	0.64	1/6547 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	LEU	CA-CB-CG	-6.25	94.44	116.30

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	2336	2198	2292	17	0
1	B	2344	2194	2294	12	0
2	A	4	6	6	0	0
3	A	5	0	0	0	0
3	B	15	0	0	1	0
4	A	10	4	4	1	0
5	A	38	40	0	0	0
5	B	76	80	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	12	12	2	0
7	A	87	0	0	0	0
7	B	70	0	0	2	0
All	All	4993	4534	4608	29	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 (29) 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:250:GLU:O	1:A:254:THR:HG22	1.89	0.71
3:B:604:SO4:O3	7:B:701:HOH:O	2.09	0.68
1:A:254:THR:HG23	1:A:255:VAL:HG23	1.76	0.67
1:B:218:ARG:HE	6:B:603:DMS:H23	1.64	0.61
1:A:256:MET:HE1	1:A:327:GLN:HA	1.83	0.60
1:B:407:PHE:HE2	1:B:491:ILE:HG21	1.68	0.58
1:A:257:LEU:HD21	1:A:332:ILE:CD1	2.33	0.57
1:B:218:ARG:H	6:B:603:DMS:H22	1.70	0.56
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.44	0.52
1:A:256:MET:SD	1:B:256:MET:HG3	2.50	0.52
1:A:469:SER:OG	1:A:498:ILE:HD11	2.10	0.51
1:B:368:LEU:HD13	1:B:396:PHE:HB2	1.94	0.48
1:B:256:MET:HE1	1:B:327:GLN:OE1	2.14	0.48
1:B:402:VAL:HG13	7:B:742:HOH:O	2.14	0.47
1:B:248:GLU:HG2	1:B:252:TYR:CE2	2.50	0.47
1:A:495:LEU:HD23	1:A:498:ILE:HD12	1.96	0.46
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.49	0.46
1:A:248:GLU:HG2	1:A:252:TYR:CE2	2.51	0.46
1:A:407:PHE:CE2	1:A:491:ILE:HG21	2.51	0.45
1:A:462:PHE:HA	1:A:468:THR:OG1	2.17	0.45
1:B:458:PRO:HD2	1:B:461:TRP:CE2	2.52	0.45
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.52	0.44
1:A:427:TYR:CD2	1:A:427:TYR:C	2.96	0.44
1:A:458:PRO:HD2	1:A:461:TRP:CE2	2.54	0.42
1:B:427:TYR:CD2	1:B:427:TYR:C	2.96	0.42
1:A:373:ASN:OD1	1:A:374:PRO:HD2	2.20	0.41
1:A:256:MET:HE3	1:A:327:GLN:O	2.20	0.41
1:A:297:LEU:HD12	1:A:297:LEU:C	2.47	0.40
1:A:260:GLU:O	4:A:603:TLA:O11	2.39	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	293/301 (97%)	288 (98%)	5 (2%)	0	100	100
1	B	293/301 (97%)	288 (98%)	5 (2%)	0	100	100
All	All	586/602 (97%)	576 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	260/270 (96%)	259 (100%)	1 (0%)	84	78
1	B	260/270 (96%)	260 (100%)	0	100	100
All	All	520/540 (96%)	519 (100%)	1 (0%)	87	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	296	GLN
1	A	318	HIS
1	A	349	GLN
1	B	296	GLN
1	B	453	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
6	DMS	B	602	-	3,3,3	0.66	0	3,3,3	1.03	0
6	DMS	B	603	-	3,3,3	0.64	0	3,3,3	0.72	0
3	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	B	601	-	4,4,4	0.17	0	6,6,6	0.52	0
2	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.96	0
3	SO4	B	605	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	A	602	-	4,4,4	0.35	0	6,6,6	0.39	0
5	MVE	B	606[A]	-	42,43,43	3.38	13 (30%)	54,63,63	2.14	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MVE	B	606[B]	-	42,43,43	3.34	13 (30%)	54,63,63	2.30	18 (33%)
5	MVE	A	604	-	42,43,43	3.32	13 (30%)	54,63,63	2.18	20 (37%)
4	TLA	A	603	-	9,9,9	1.13	0	12,12,12	1.51	1 (8%)

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	EDO	A	601	-	-	0/1/1/1	-
5	MVE	B	606[A]	-	-	3/30/54/54	0/6/6/6
5	MVE	B	606[B]	-	-	4/30/54/54	0/6/6/6
5	MVE	A	604	-	-	2/30/54/54	0/6/6/6
4	TLA	A	603	-	-	9/12/12/12	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606[A]	MVE	C34-N33	-12.85	1.23	1.48
5	B	606[B]	MVE	C34-N33	-12.81	1.23	1.48
5	A	604	MVE	C34-N33	-12.43	1.24	1.48
5	A	604	MVE	C04-C05	10.15	1.63	1.52
5	B	606[A]	MVE	C04-C05	9.52	1.63	1.52
5	B	606[B]	MVE	C04-C05	9.28	1.63	1.52
5	B	606[A]	MVE	C17-N16	7.72	1.46	1.35
5	B	606[B]	MVE	C17-N16	7.69	1.46	1.35
5	A	604	MVE	C17-N16	7.32	1.45	1.35
5	A	604	MVE	C31-C04	-6.23	1.47	1.53
5	B	606[A]	MVE	C31-C04	-6.01	1.47	1.53
5	B	606[B]	MVE	C31-C04	-5.47	1.48	1.53
5	B	606[B]	MVE	C38-C04	-5.14	1.48	1.53
5	B	606[A]	MVE	C38-C04	-5.00	1.48	1.53
5	A	604	MVE	C38-C04	-4.41	1.49	1.53
5	B	606[B]	MVE	C15-N16	-3.69	1.40	1.47
5	B	606[A]	MVE	C15-N16	-3.67	1.40	1.47
5	B	606[B]	MVE	C22-N16	-3.25	1.41	1.47
5	B	606[A]	MVE	C22-N16	-3.24	1.41	1.47
5	A	604	MVE	C37-N33	-3.09	1.41	1.47
5	A	604	MVE	C23-N13	2.92	1.52	1.47
5	B	606[B]	MVE	C32-N33	-2.81	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606[A]	MVE	C32-N33	-2.78	1.42	1.47
5	B	606[A]	MVE	C23-N13	2.76	1.52	1.47
5	A	604	MVE	C32-N33	-2.72	1.42	1.47
5	B	606[B]	MVE	C23-N13	2.72	1.51	1.47
5	B	606[B]	MVE	C37-N33	-2.67	1.42	1.47
5	A	604	MVE	C11-N27	-2.64	1.31	1.37
5	B	606[A]	MVE	C37-N33	-2.64	1.42	1.47
5	B	606[B]	MVE	C14-N13	2.64	1.51	1.47
5	B	606[A]	MVE	C14-N13	2.61	1.51	1.47
5	B	606[B]	MVE	C11-N27	-2.58	1.31	1.37
5	B	606[A]	MVE	C11-N27	-2.57	1.31	1.37
5	A	604	MVE	C12-N13	2.56	1.47	1.38
5	B	606[B]	MVE	C12-N13	2.47	1.47	1.38
5	B	606[A]	MVE	C12-N13	2.45	1.47	1.38
5	A	604	MVE	C15-N16	-2.44	1.42	1.47
5	A	604	MVE	C36-C34	2.06	1.57	1.52
5	A	604	MVE	C22-N16	-2.01	1.43	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606[A]	MVE	C38-C37-N33	6.29	119.99	111.00
5	B	606[B]	MVE	C38-C37-N33	6.26	119.95	111.00
5	B	606[B]	MVE	C31-C32-N33	6.18	119.84	111.00
5	B	606[A]	MVE	C25-N26-N27	4.68	120.74	113.68
5	B	606[B]	MVE	C25-N26-N27	4.66	120.71	113.68
5	A	604	MVE	C38-C04-C31	4.60	115.40	108.70
5	A	604	MVE	C25-N26-N27	4.57	120.59	113.68
5	A	604	MVE	C38-C04-C05	-4.41	102.42	111.99
5	B	606[B]	MVE	C37-N33-C32	4.34	117.41	109.13
5	A	604	MVE	C24-C12-N13	-4.04	120.46	123.45
5	B	606[A]	MVE	C31-C32-N33	3.90	116.58	111.00
5	A	604	MVE	C24-C25-N26	-3.82	120.44	124.99
5	B	606[A]	MVE	C24-C25-N26	-3.79	120.49	124.99
5	B	606[B]	MVE	C24-C25-N26	-3.77	120.51	124.99
5	A	604	MVE	C10-C11-N27	3.76	109.15	105.86
5	B	606[B]	MVE	C38-C04-C05	-3.64	104.08	111.99
5	B	606[A]	MVE	C10-C11-N27	3.63	109.04	105.86
5	B	606[B]	MVE	C10-C11-N27	3.61	109.02	105.86
5	A	604	MVE	C20-C19-C17	-3.59	112.30	116.91
5	B	606[A]	MVE	C37-N33-C32	3.39	115.59	109.13
5	A	604	MVE	C31-C32-N33	3.38	115.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	MVE	C09-C10-C11	-3.25	105.13	108.18
5	A	604	MVE	C38-C37-N33	3.23	115.61	111.00
4	A	603	TLA	O2-C2-C3	-3.22	103.61	110.17
5	B	606[A]	MVE	C38-C04-C05	-3.20	105.04	111.99
5	A	604	MVE	O18-C17-N16	-3.08	117.93	121.61
5	B	606[B]	MVE	C14-C15-N16	-3.04	104.38	110.42
5	B	606[B]	MVE	C09-C10-C11	-3.04	105.33	108.18
5	B	606[A]	MVE	C07-C06-C05	-3.02	117.00	121.17
5	B	606[B]	MVE	C07-C06-C05	-2.98	117.05	121.17
5	A	604	MVE	C14-C15-N16	-2.98	104.49	110.42
5	B	606[A]	MVE	C24-C12-N13	-2.97	121.25	123.45
5	B	606[A]	MVE	C09-C10-C11	-2.97	105.39	108.18
5	B	606[B]	MVE	C24-C12-N13	-2.95	121.27	123.45
5	B	606[A]	MVE	C14-C15-N16	-2.93	104.58	110.42
5	B	606[B]	MVE	C32-C31-C04	2.91	114.35	111.79
5	A	604	MVE	C32-N33-C34	-2.83	108.50	113.01
5	B	606[B]	MVE	C05-C30-N29	-2.81	120.74	123.38
5	A	604	MVE	C07-C06-C05	-2.74	117.39	121.17
5	B	606[A]	MVE	C05-C30-N29	-2.72	120.83	123.38
5	B	606[A]	MVE	C32-C31-C04	-2.72	109.41	111.79
5	A	604	MVE	C35-C34-N33	2.70	118.37	112.26
5	B	606[A]	MVE	C20-C19-C17	-2.56	113.63	116.91
5	B	606[B]	MVE	C20-C19-C17	-2.54	113.65	116.91
5	B	606[B]	MVE	O18-C17-N16	-2.51	118.61	121.61
5	A	604	MVE	C36-C34-N33	-2.49	106.62	112.26
5	B	606[A]	MVE	O18-C17-N16	-2.46	118.67	121.61
5	B	606[B]	MVE	C06-C05-C30	2.39	120.32	117.73
5	B	606[A]	MVE	C06-C05-C30	2.35	120.28	117.73
5	A	604	MVE	C37-C38-C04	2.33	113.84	111.79
5	B	606[B]	MVE	C23-C22-N16	-2.33	105.79	110.42
5	B	606[B]	MVE	C08-C09-C10	2.32	128.08	123.32
5	B	606[A]	MVE	C08-C09-C10	2.30	128.04	123.32
5	A	604	MVE	C08-C09-C10	2.25	127.94	123.32
5	B	606[A]	MVE	C23-C22-N16	-2.24	105.96	110.42
5	A	604	MVE	C23-C22-N16	-2.21	106.03	110.42
5	B	606[A]	MVE	O03-C04-C05	2.17	114.25	109.50
5	A	604	MVE	C36-C34-C35	-2.06	106.88	112.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

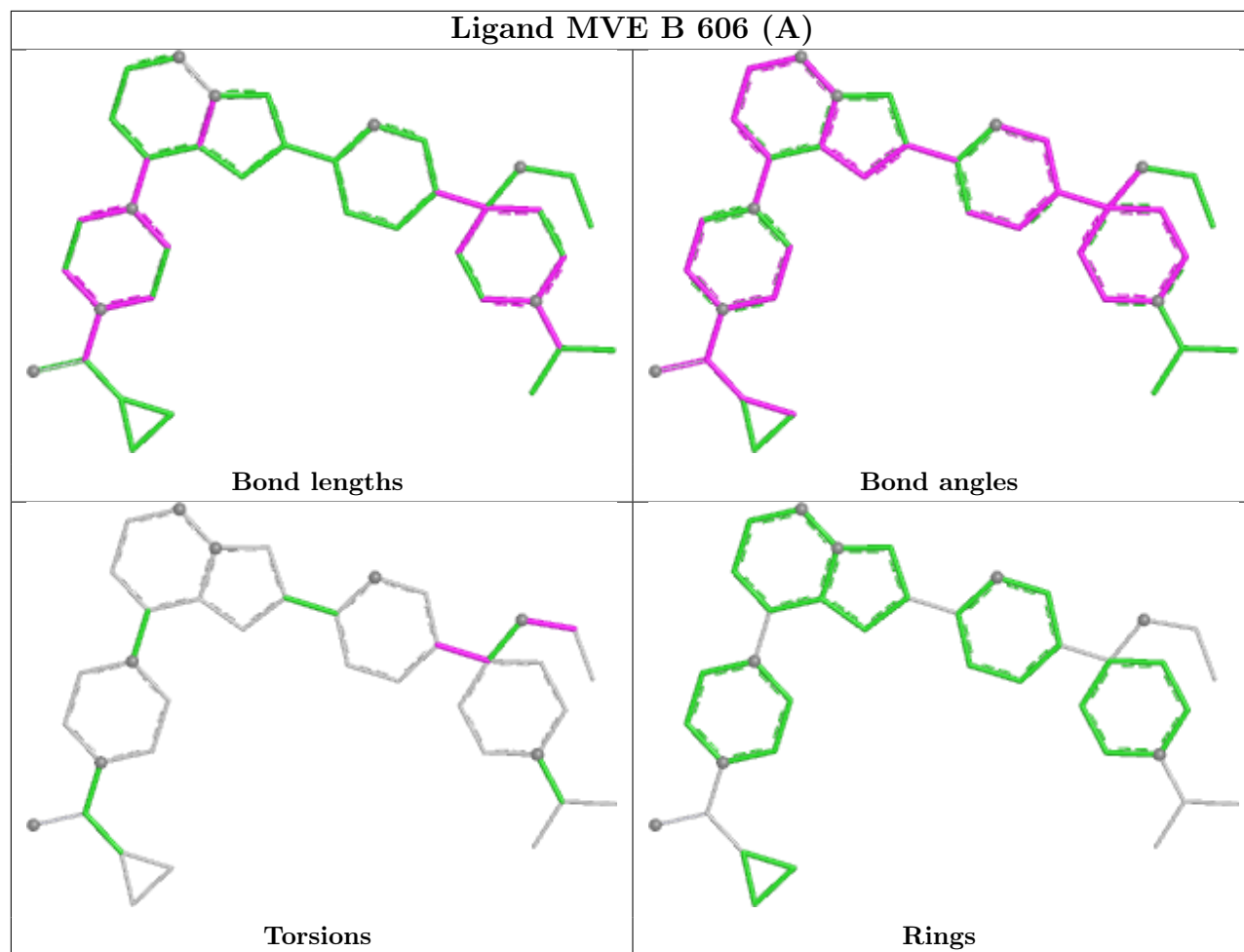
Mol	Chain	Res	Type	Atoms
5	B	606[A]	MVE	C01-C02-O03-C04
5	B	606[B]	MVE	C01-C02-O03-C04
5	B	606[B]	MVE	C05-C04-O03-C02
5	B	606[B]	MVE	C31-C04-O03-C02
5	B	606[B]	MVE	C38-C04-O03-C02
4	A	603	TLA	C2-C3-C4-O4
4	A	603	TLA	C2-C3-C4-O41
4	A	603	TLA	O1-C1-C2-O2
4	A	603	TLA	O11-C1-C2-O2
4	A	603	TLA	O3-C3-C4-O4
4	A	603	TLA	O3-C3-C4-O41
4	A	603	TLA	O2-C2-C3-C4
4	A	603	TLA	C1-C2-C3-O3
4	A	603	TLA	C1-C2-C3-C4
5	A	604	MVE	C35-C34-N33-C37
5	B	606[A]	MVE	O03-C04-C05-C30
5	A	604	MVE	O18-C17-C19-C20
5	B	606[A]	MVE	O03-C04-C05-C06

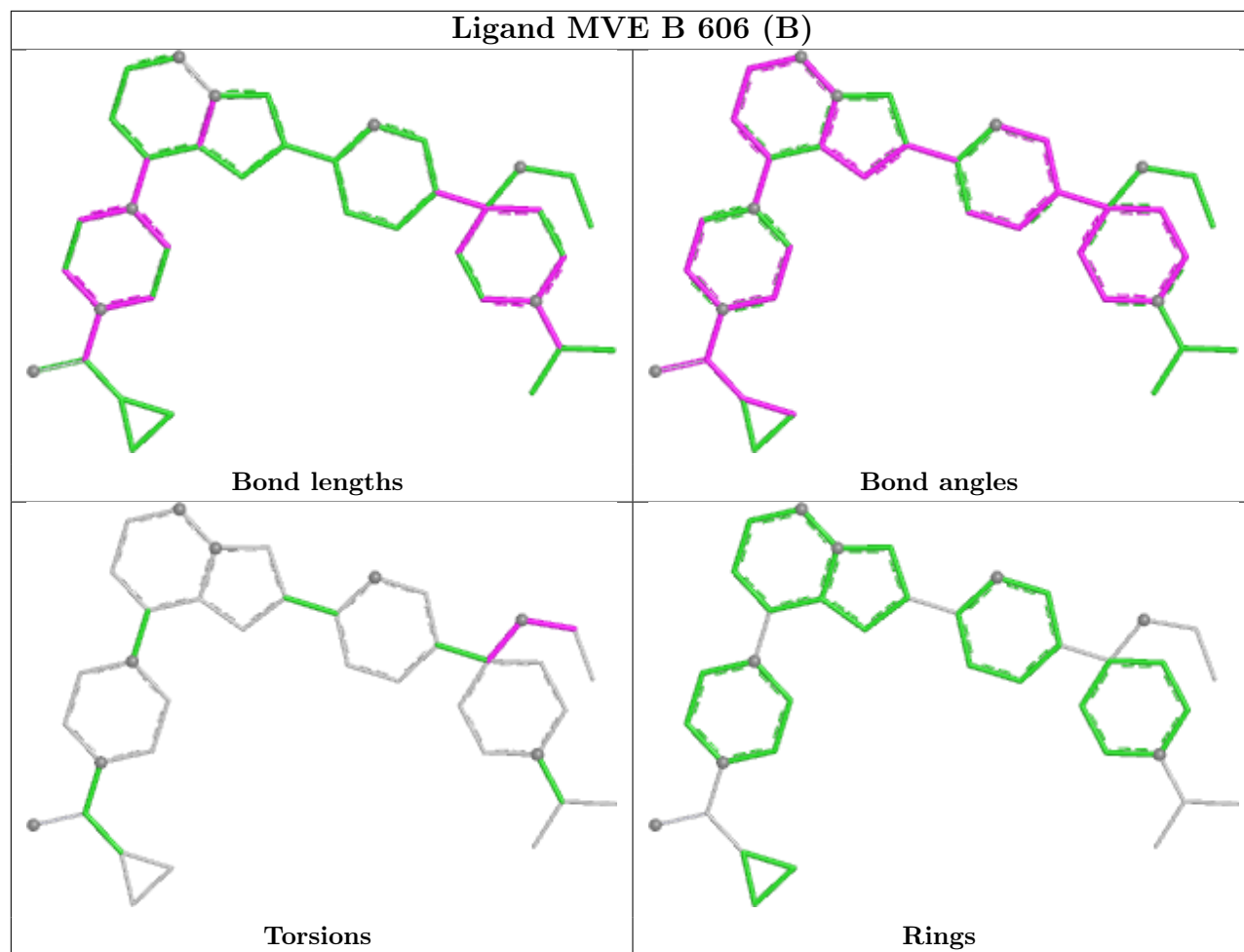
There are no ring outliers.

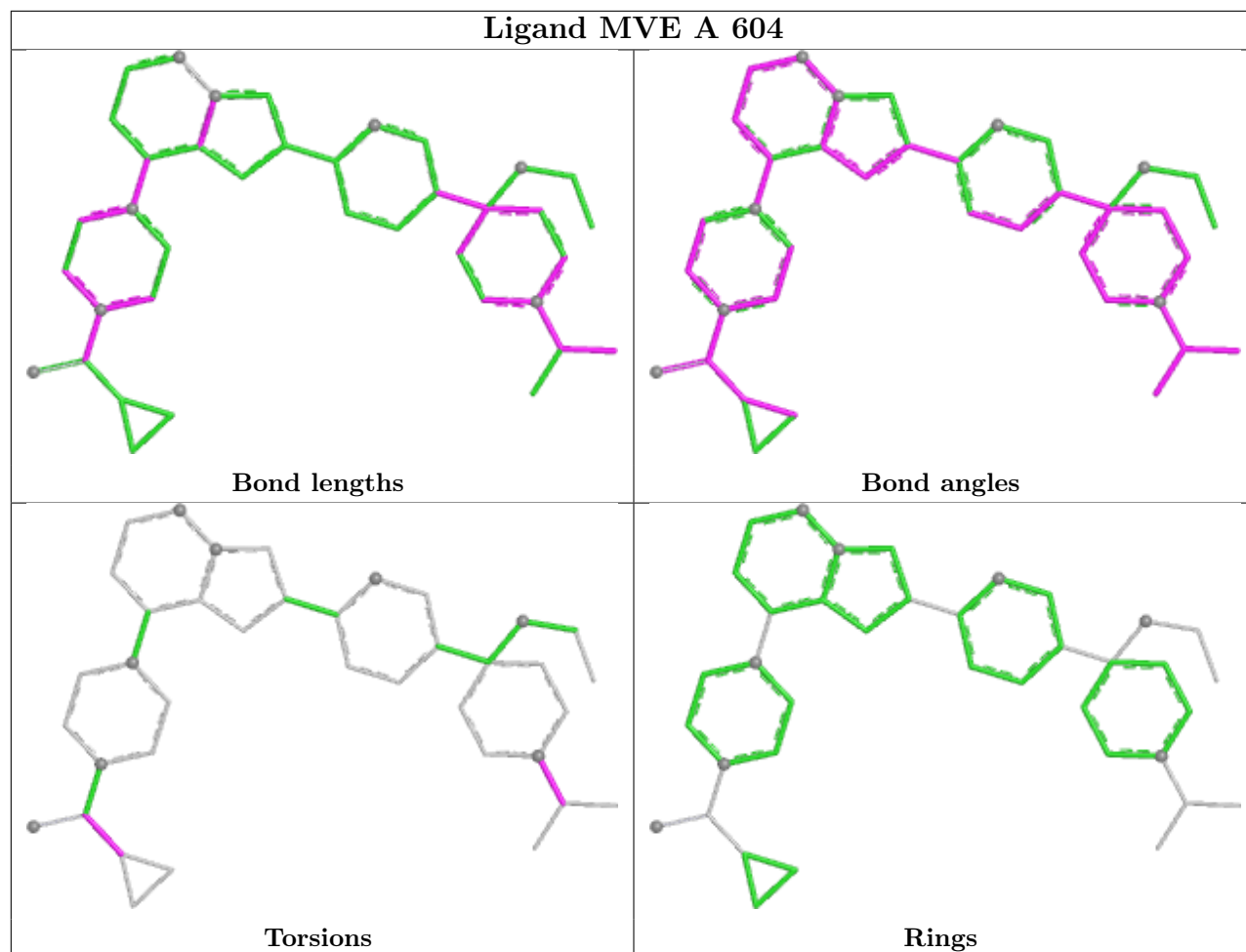
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	603	DMS	2	0
3	B	604	SO4	1	0
4	A	603	TLA	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	293/301 (97%)	0.56	20 (6%)	23 27	18, 32, 51, 98	1 (0%)
1	B	293/301 (97%)	0.57	20 (6%)	23 27	18, 33, 50, 91	1 (0%)
All	All	586/602 (97%)	0.56	40 (6%)	23 27	18, 32, 50, 98	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	SER	5.6
1	B	499	ASP	5.5
1	B	498	ILE	4.7
1	A	498	ILE	4.5
1	A	203	THR	4.3
1	A	297	LEU	4.0
1	A	371	GLY	4.0
1	B	277	THR	3.8
1	B	272	SER	3.7
1	A	277	THR	3.6
1	A	497	LYS	3.5
1	A	272	SER	3.3
1	A	271	THR	3.0
1	B	394	ASP	3.0
1	B	271	THR	2.9
1	A	370	VAL	2.8
1	B	370	VAL	2.8
1	B	297	LEU	2.8
1	A	365	THR	2.8
1	A	251	LEU	2.7
1	A	284	HIS	2.7
1	B	256	MET	2.6
1	B	365	THR	2.6
1	A	472	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	372	ASN	2.5
1	B	497	LYS	2.5
1	B	366	ASN	2.5
1	B	372	ASN	2.5
1	A	366	ASN	2.4
1	B	364	SER	2.4
1	B	251	LEU	2.4
1	A	252	TYR	2.4
1	B	411	LEU	2.3
1	B	203	THR	2.3
1	B	423	ILE	2.2
1	A	411	LEU	2.2
1	A	394	ASP	2.1
1	B	250	GLU	2.1
1	B	359	VAL	2.0
1	A	257	LEU	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(Å ²)	Q<0.9
3	SO4	B	605	5/5	0.66	0.19	82,92,99,166	0
2	EDO	A	601	4/4	0.71	0.17	31,38,45,54	0
4	TLA	A	603	10/10	0.80	0.28	58,133,204,236	0
3	SO4	B	604	5/5	0.85	0.10	32,50,60,66	0
6	DMS	B	603	4/4	0.86	0.18	51,61,88,88	0
6	DMS	B	602	4/4	0.87	0.21	43,81,102,102	0
5	MVE	B	606[A]	38/38	0.88	0.11	24,32,48,48	78

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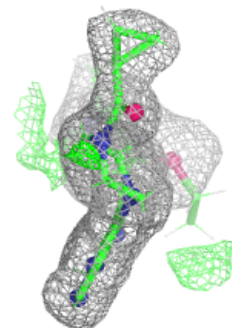
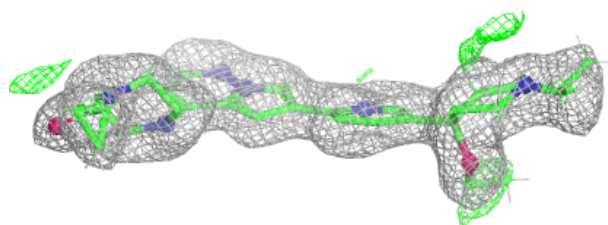
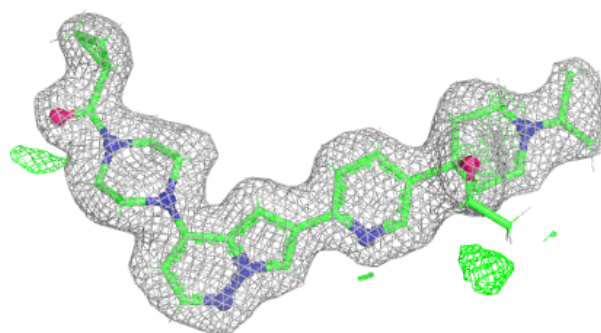
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MVE	B	606[B]	38/38	0.88	0.11	23,32,48,48	78
5	MVE	A	604	38/38	0.93	0.10	22,31,56,66	0
3	SO4	B	601	5/5	0.95	0.07	32,32,33,38	0
3	SO4	A	602	5/5	0.96	0.06	32,32,35,38	0

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.

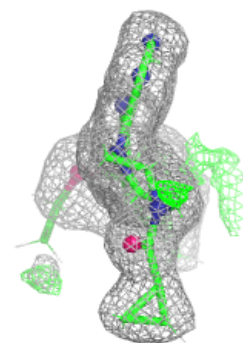
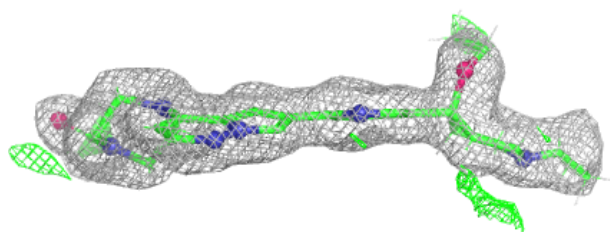
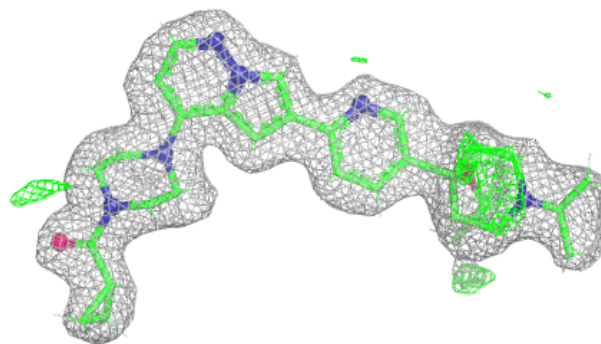
Electron density around MVE B 606 (A):

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

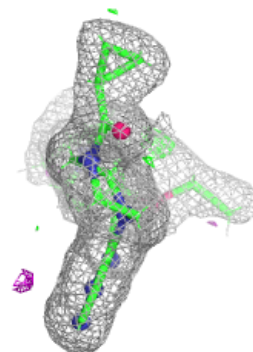
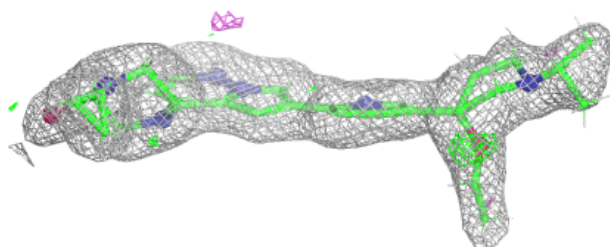
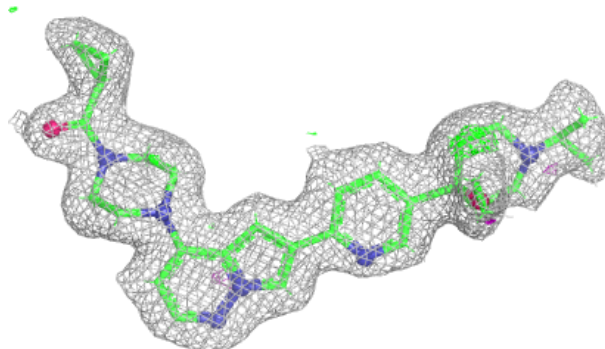


Electron density around MVE B 606 (B):

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

**Electron density around MVE A 604:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.