



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:33 AM UTC

PDB ID : 8R7G / pdb_00008r7g
Title : Crystal structure of the kinase domain of ACVR1 (ALK2) with M4K2234
Authors : Williams, E.P.; Cros, J.; Ensan, D.; Smil, D.; Edwards, A.M.; O'Meara, J.A.;
Fernandez-Cid, A.; Isaac, M.B.; Al-awar, R.; Bullock, A.N.
Deposited on : 2023-11-24
Resolution : 2.09 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

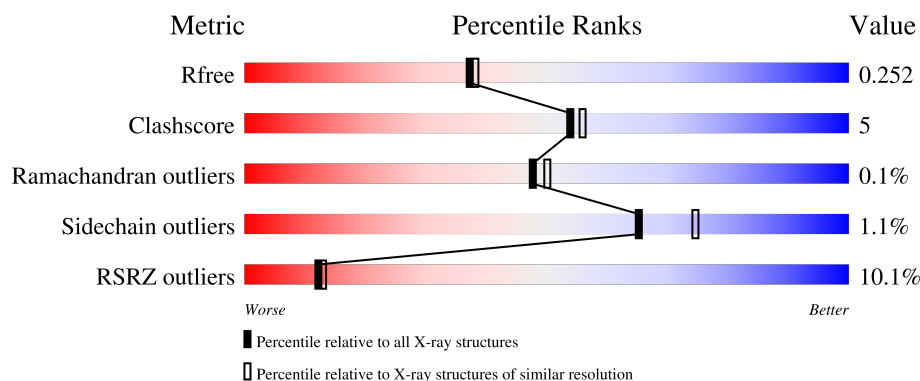
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	8% 88% 10% .
1	B	301	7% 87% 10% .
1	C	301	6% 77% 16% 7%
1	D	301	17% 84% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9015 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.

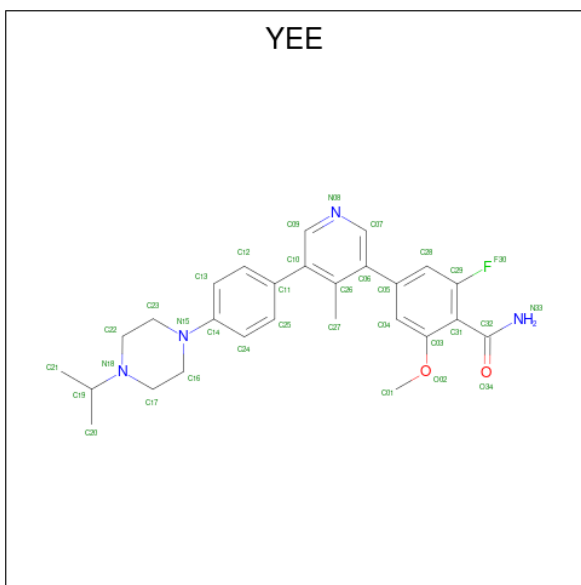
- Molecule 1 is a protein called Activin receptor type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2253	1434	392	413	14			
1	B	293	Total	C	N	O	S	0	0	0
			2243	1431	386	412	14			
1	C	280	Total	C	N	O	S	0	1	0
			2167	1392	370	390	15			
1	D	291	Total	C	N	O	S	0	0	0
			2119	1348	365	393	13			

There are 12 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
C	199	SER	-	expression tag	UNP Q04771
C	200	MET	-	expression tag	UNP Q04771
C	207	ASP	GLN	engineered mutation	UNP Q04771
D	199	SER	-	expression tag	UNP Q04771
D	200	MET	-	expression tag	UNP Q04771
D	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 2-fluoranyl-6-methoxy-4-[4-methyl-5-[4-(4-propan-2-ylpiperazin-1-yl)phenyl]pyridin-3-yl]benzamide (CCD ID: YEE) (formula: C₂₇H₃₁FN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	27	1	4	2		
2	B	1	Total	C	F	N	O	0	0
			34	27	1	4	2		
2	C	1	Total	C	F	N	O	0	0
			34	27	1	4	2		
2	D	1	Total	C	F	N	O	0	0
			34	27	1	4	2		

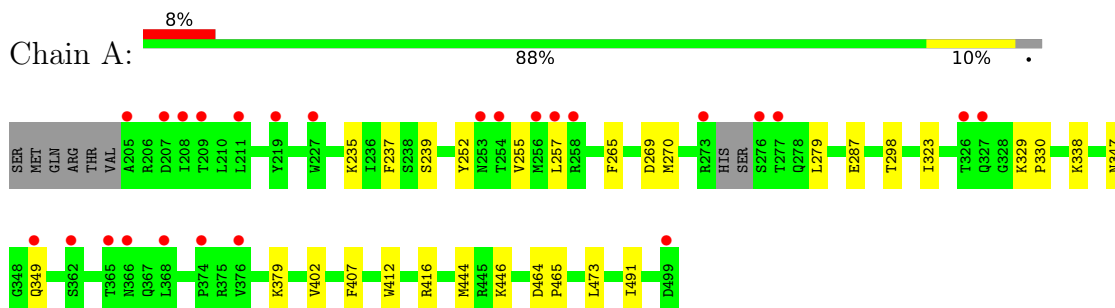
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	28	Total	O	0	0
			28	28		
3	C	16	Total	O	0	0
			16	16		
3	D	18	Total	O	0	0
			18	18		

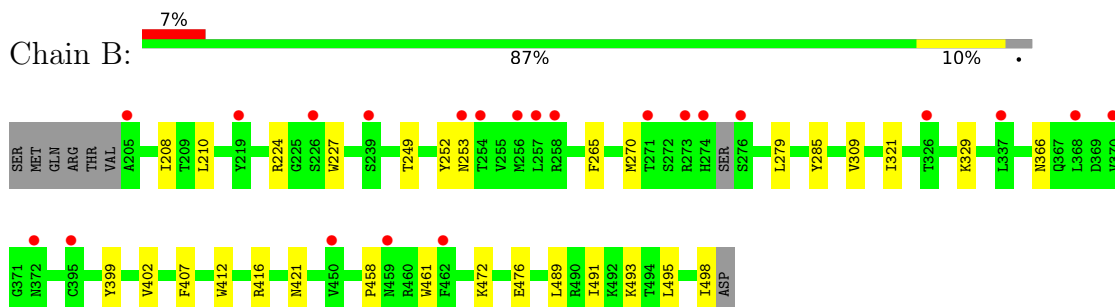
3 Residue-property plots

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

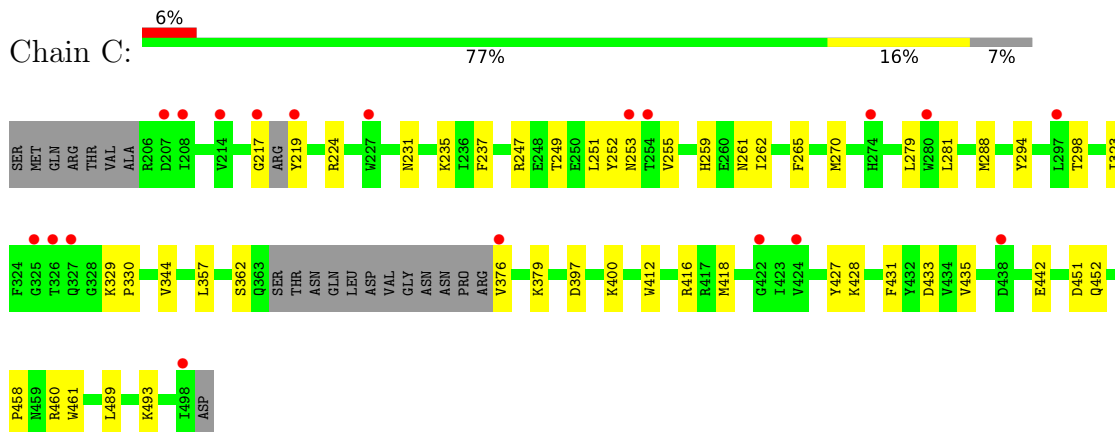
• Molecule 1: Activin receptor type I



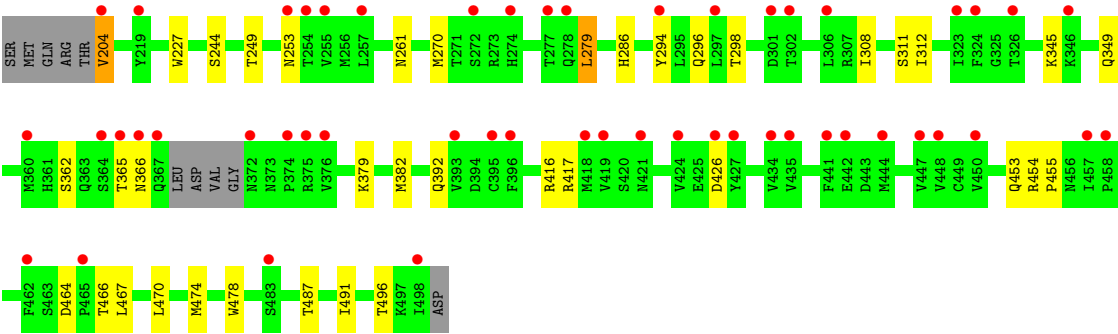
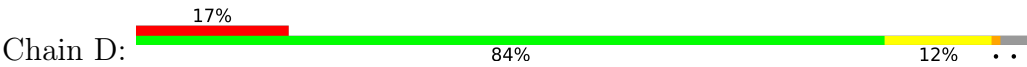
• Molecule 1: Activin receptor type I



• Molecule 1: Activin receptor type I



• Molecule 1: Activin receptor type I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.82Å 100.59Å 83.58Å 90.00° 118.13° 90.00°	Depositor
Resolution (Å)	73.71 – 2.09 73.71 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (73.71-2.09) 99.8 (73.71-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.253 0.226 , 0.252	Depositor DCC
R_{free} test set	3674 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.017 for h,-k,-h-l 0.007 for -h-l,-k,l 0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9015	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: YEE

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	0.23	0/2304	0.40	0/3133
1	B	0.23	0/2294	0.42	0/3126
1	C	0.25	0/2218	0.46	0/3019
1	D	0.17	0/2170	0.39	0/2975
All	All	0.22	0/8986	0.42	0/12253

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	2253	0	2131	16	0
1	B	2243	0	2129	19	0
1	C	2167	0	2067	28	0
1	D	2119	0	1843	23	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
3	C	16	0	0	1	0
3	D	18	0	0	1	0
All	All	9015	0	8170	83	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 5.

All (83) 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:B:407:PHE:HE2	1:B:491:ILE:HG21	1.49	0.77
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.55	0.69
1:B:489:LEU:HG	1:B:493:LYS:HE3	1.75	0.68
1:D:470:LEU:O	1:D:474:MET:HG3	1.95	0.66
1:C:427:TYR:O	1:C:428:LYS:HD3	1.98	0.62
1:B:224:ARG:HB2	1:B:285:TYR:CE1	2.35	0.61
1:C:451:ASP:O	1:C:452:GLN:HB2	1.99	0.61
1:D:455:PRO:HG2	1:D:478:TRP:CH2	2.37	0.60
1:A:287:GLU:H	1:A:287:GLU:CD	2.07	0.60
1:C:330:PRO:HB3	1:C:362:SER:HB3	1.85	0.59
1:C:224:ARG:NH1	1:C:231:ASN:OD1	2.36	0.58
1:D:464:ASP:HB3	1:D:467:LEU:HB2	1.86	0.58
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.40	0.57
1:A:270:MET:HG3	1:A:279:LEU:HD23	1.88	0.55
1:A:446:LYS:NZ	3:A:601:HOH:O	2.41	0.53
1:D:416:ARG:NH2	1:D:426:ASP:O	2.41	0.53
1:D:362:SER:H	1:D:366:ASN:CB	2.22	0.52
1:C:489:LEU:HG	1:C:493:LYS:HE3	1.91	0.52
1:A:252:TYR:CD1	1:A:265:PHE:HB2	2.45	0.52
1:C:217:GLY:HA3	1:C:219:TYR:CE1	2.45	0.52
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.38	0.51
1:D:466:THR:O	1:D:470:LEU:HD23	2.10	0.51
1:D:270:MET:HG3	1:D:279:LEU:HD23	1.93	0.50
1:C:418:MET:O	3:C:601:HOH:O	2.19	0.50
1:B:270:MET:HG3	1:B:279:LEU:HD23	1.94	0.50
1:D:379:LYS:HA	1:D:382:MET:HG3	1.94	0.50
1:A:407:PHE:CE2	1:A:491:ILE:HG21	2.47	0.49
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.48	0.49
1:C:235:LYS:HD3	1:C:237:PHE:CE2	2.48	0.48
1:D:487:THR:O	1:D:491:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:HIS:HB3	1:C:262:ILE:HG12	1.96	0.47
1:A:323:ILE:HB	1:A:329:LYS:HG2	1.96	0.47
1:B:366:ASN:HD21	1:D:392:GLN:HA	1.79	0.47
1:C:442:GLU:HG2	1:D:349:GLN:NE2	2.29	0.47
1:D:261:ASN:ND2	1:D:311:SER:HB2	2.30	0.47
1:B:224:ARG:HD3	1:B:285:TYR:CZ	2.50	0.47
1:C:412:TRP:CZ2	1:C:416:ARG:HD2	2.50	0.47
1:C:288:MET:HB2	1:C:344:VAL:O	2.15	0.46
1:B:321:ILE:O	1:B:329:LYS:NZ	2.48	0.46
1:A:255:VAL:HG13	1:A:330:PRO:HD2	1.98	0.46
1:C:261:ASN:O	1:C:262:ILE:HD13	2.16	0.45
1:C:460:ARG:HH12	1:C:461:TRP:HE1	1.64	0.45
1:D:286:HIS:CE1	1:D:345:LYS:HG2	2.51	0.45
1:D:204:VAL:HB	1:D:227:TRP:HZ2	1.81	0.45
1:B:249:THR:O	1:B:253:ASN:HB2	2.16	0.45
1:C:458:PRO:HG2	1:C:461:TRP:NE1	2.32	0.45
1:C:270:MET:HG3	1:C:279:LEU:HD23	1.98	0.45
1:B:224:ARG:HD3	1:B:285:TYR:OH	2.17	0.44
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.79	0.44
1:D:453:GLN:O	1:D:454:ARG:HD3	2.16	0.44
1:B:458:PRO:HD2	1:B:461:TRP:CD2	2.53	0.44
1:D:296:GLN:NE2	3:D:603:HOH:O	2.45	0.44
1:C:397:ASP:OD1	1:C:400:LYS:HE3	2.18	0.44
1:C:431:PHE:O	1:C:435:VAL:HG22	2.18	0.44
1:B:472:LYS:O	1:B:476:GLU:HG3	2.18	0.43
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.87	0.43
1:C:252:TYR:CG	1:C:265:PHE:HB2	2.53	0.43
1:D:294:TYR:O	1:D:298:THR:HG22	2.17	0.43
1:C:379:LYS:HE2	1:D:496:THR:O	2.19	0.43
1:A:379:LYS:O	1:A:444:MET:HG3	2.19	0.43
1:B:399:TYR:O	1:B:402:VAL:HG22	2.18	0.43
1:A:237:PHE:HB2	1:A:279:LEU:HB2	2.02	0.42
1:D:474:MET:HE2	1:D:478:TRP:CH2	2.54	0.42
1:C:249:THR:O	1:C:253:ASN:HB2	2.18	0.42
1:D:474:MET:HG3	1:D:474:MET:H	1.60	0.42
1:C:433:ASP:OD1	1:C:433:ASP:N	2.50	0.41
1:C:357:LEU:HD13	1:C:376:VAL:HG12	2.00	0.41
1:B:495:LEU:HD23	1:B:498:ILE:HD11	2.02	0.41
1:D:308:ILE:O	1:D:312:ILE:HG13	2.21	0.41
1:B:208:ILE:HG12	1:B:227:TRP:HB2	2.02	0.41
1:D:249:THR:O	1:D:253:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:OE1	1:A:287:GLU:N	2.43	0.41
1:C:235:LYS:HD3	1:C:237:PHE:CZ	2.55	0.41
1:A:235:LYS:HG2	1:A:237:PHE:CE1	2.56	0.41
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.56	0.41
1:C:251:LEU:O	1:C:255:VAL:HB	2.22	0.40
1:C:323:ILE:HG12	1:C:329:LYS:HB3	2.03	0.40
1:A:347:ASN:OD1	1:A:349:GLN:HB2	2.22	0.40
1:B:421:ASN:OD1	1:B:421:ASN:N	2.54	0.40
1:B:309:VAL:HG23	1:B:495:LEU:HD13	2.03	0.40
1:A:464:ASP:HA	1:A:465:PRO:HD3	1.98	0.40
1:C:294:TYR:O	1:C:298:THR:HG22	2.22	0.40
1:D:417:ARG:HD3	1:D:417:ARG:HA	1.84	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	289/301 (96%)	282 (98%)	7 (2%)	0	100	100
1	B	289/301 (96%)	284 (98%)	5 (2%)	0	100	100
1	C	275/301 (91%)	265 (96%)	10 (4%)	0	100	100
1	D	287/301 (95%)	280 (98%)	6 (2%)	1 (0%)	36	36
All	All	1140/1204 (95%)	1111 (98%)	28 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	365	THR

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	229/270 (85%)	224 (98%)	5 (2%)	45	53
1	B	230/270 (85%)	229 (100%)	1 (0%)	84	89
1	C	222/270 (82%)	221 (100%)	1 (0%)	81	88
1	D	192/270 (71%)	189 (98%)	3 (2%)	55	64
All	All	873/1080 (81%)	863 (99%)	10 (1%)	65	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	SER
1	A	269	ASP
1	A	298	THR
1	A	338	LYS
1	A	402	VAL
1	B	210	LEU
1	C	281	LEU
1	D	204	VAL
1	D	244	SER
1	D	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	GLN
1	B	318	HIS
1	C	318	HIS
1	C	320	HIS
1	C	481	ASN
1	D	286	HIS
1	D	318	HIS
1	D	349	GLN
1	D	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	YEE	D	501	-	37,37,37	2.80	15 (40%)	50,53,53	1.85	11 (22%)
2	YEE	A	501	-	37,37,37	2.77	15 (40%)	50,53,53	1.79	11 (22%)
2	YEE	B	501	-	37,37,37	2.78	13 (35%)	50,53,53	2.06	15 (30%)
2	YEE	C	501	-	37,37,37	2.73	15 (40%)	50,53,53	2.00	16 (32%)

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	YEE	D	501	-	-	1/22/32/32	0/4/4/4
2	YEE	A	501	-	-	0/22/32/32	0/4/4/4
2	YEE	B	501	-	-	2/22/32/32	0/4/4/4
2	YEE	C	501	-	-	0/22/32/32	0/4/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	YEE	C19-N18	-8.94	1.31	1.48
2	A	501	YEE	C19-N18	-8.89	1.31	1.48
2	D	501	YEE	C19-N18	-8.73	1.31	1.48
2	C	501	YEE	C19-N18	-8.57	1.31	1.48
2	D	501	YEE	C32-N33	7.05	1.45	1.33
2	B	501	YEE	C32-N33	6.83	1.45	1.33
2	A	501	YEE	C32-N33	6.73	1.45	1.33
2	C	501	YEE	C32-N33	6.64	1.45	1.33
2	B	501	YEE	C17-N18	-5.18	1.37	1.47
2	D	501	YEE	C22-N18	-4.97	1.37	1.47
2	D	501	YEE	C17-N18	-4.86	1.38	1.47
2	A	501	YEE	C17-N18	-4.84	1.38	1.47
2	C	501	YEE	C17-N18	-4.83	1.38	1.47
2	B	501	YEE	C22-N18	-4.65	1.38	1.47
2	C	501	YEE	C22-N18	-4.59	1.38	1.47
2	A	501	YEE	C14-N15	4.23	1.50	1.38
2	D	501	YEE	C14-N15	4.22	1.50	1.38
2	B	501	YEE	C14-N15	4.22	1.50	1.38
2	B	501	YEE	C06-C05	-4.15	1.42	1.49
2	C	501	YEE	C14-N15	4.11	1.50	1.38
2	A	501	YEE	C22-N18	-4.02	1.39	1.47
2	A	501	YEE	C06-C05	-3.89	1.42	1.49
2	C	501	YEE	O02-C03	3.87	1.43	1.37
2	D	501	YEE	C06-C05	-3.85	1.42	1.49
2	C	501	YEE	C06-C05	-3.72	1.42	1.49
2	D	501	YEE	O02-C03	3.70	1.43	1.37
2	A	501	YEE	O02-C03	3.55	1.42	1.37
2	B	501	YEE	O02-C03	3.50	1.42	1.37
2	A	501	YEE	C31-C32	3.18	1.56	1.51
2	C	501	YEE	C31-C32	3.12	1.56	1.51
2	D	501	YEE	C31-C32	3.08	1.56	1.51
2	A	501	YEE	C25-C24	3.02	1.43	1.38
2	D	501	YEE	C25-C24	2.97	1.43	1.38
2	C	501	YEE	C25-C24	2.90	1.43	1.38
2	B	501	YEE	C31-C32	2.81	1.55	1.51
2	B	501	YEE	C25-C24	2.54	1.42	1.38
2	C	501	YEE	C10-C11	-2.50	1.44	1.49
2	B	501	YEE	C10-C11	-2.50	1.44	1.49
2	D	501	YEE	C10-C26	2.49	1.44	1.40
2	A	501	YEE	C10-C26	2.48	1.44	1.40
2	C	501	YEE	C27-C26	2.45	1.56	1.51
2	A	501	YEE	C10-C11	-2.40	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	YEE	O34-C32	-2.38	1.19	1.24
2	A	501	YEE	O34-C32	-2.38	1.19	1.24
2	A	501	YEE	C04-C03	2.37	1.42	1.38
2	C	501	YEE	C04-C03	2.37	1.42	1.38
2	B	501	YEE	C27-C26	2.37	1.56	1.51
2	D	501	YEE	C20-C19	2.35	1.58	1.52
2	A	501	YEE	C27-C26	2.35	1.56	1.51
2	D	501	YEE	C27-C26	2.34	1.56	1.51
2	D	501	YEE	O34-C32	-2.33	1.19	1.24
2	C	501	YEE	C10-C26	2.31	1.44	1.40
2	B	501	YEE	C20-C19	2.23	1.57	1.52
2	D	501	YEE	C10-C11	-2.19	1.45	1.49
2	C	501	YEE	O34-C32	-2.16	1.20	1.24
2	C	501	YEE	C20-C19	2.15	1.57	1.52
2	D	501	YEE	C04-C03	2.15	1.42	1.38
2	A	501	YEE	C20-C19	2.14	1.57	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	YEE	C28-C29-C31	-5.81	118.41	123.96
2	C	501	YEE	C16-C17-N18	5.70	120.64	110.61
2	A	501	YEE	C22-N18-C17	5.43	119.48	109.13
2	A	501	YEE	C28-C29-C31	-5.13	119.05	123.96
2	D	501	YEE	C28-C29-C31	-5.07	119.11	123.96
2	B	501	YEE	C22-N18-C17	4.99	118.64	109.13
2	D	501	YEE	C16-C17-N18	4.87	119.19	110.61
2	D	501	YEE	C22-N18-C17	4.80	118.27	109.13
2	C	501	YEE	C28-C29-C31	-4.76	119.40	123.96
2	B	501	YEE	C22-N18-C19	4.26	119.81	113.01
2	B	501	YEE	C17-C16-N15	3.94	119.08	110.78
2	C	501	YEE	C13-C14-N15	-3.85	116.04	121.39
2	B	501	YEE	C09-C10-C11	-3.82	114.04	119.56
2	D	501	YEE	C16-N15-C14	3.61	127.94	118.11
2	A	501	YEE	C16-C17-N18	3.54	116.83	110.61
2	D	501	YEE	C13-C14-N15	-3.40	116.67	121.39
2	B	501	YEE	C16-C17-N18	3.40	116.59	110.61
2	C	501	YEE	C22-N18-C17	3.34	115.49	109.13
2	C	501	YEE	C17-N18-C19	-3.22	107.87	113.01
2	C	501	YEE	C16-N15-C14	3.18	126.77	118.11
2	A	501	YEE	C23-C22-N18	3.15	116.16	110.61
2	C	501	YEE	C29-C31-C32	-3.11	117.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	YEE	C05-C28-C29	3.11	122.06	119.61
2	D	501	YEE	C17-C16-N15	3.08	117.27	110.78
2	C	501	YEE	O02-C03-C31	3.08	120.20	115.84
2	C	501	YEE	C05-C28-C29	3.02	122.00	119.61
2	C	501	YEE	C22-C23-N15	3.00	117.09	110.78
2	B	501	YEE	C05-C28-C29	2.94	121.93	119.61
2	A	501	YEE	C01-O02-C03	-2.85	113.34	117.51
2	B	501	YEE	C17-N18-C19	2.83	117.52	113.01
2	D	501	YEE	C22-C23-N15	2.80	116.69	110.78
2	B	501	YEE	C23-C22-N18	2.70	115.36	110.61
2	B	501	YEE	C01-O02-C03	-2.68	113.58	117.51
2	A	501	YEE	C23-N15-C16	-2.67	105.57	111.57
2	C	501	YEE	C17-C16-N15	2.65	116.36	110.78
2	C	501	YEE	O02-C03-C04	-2.62	119.56	124.08
2	A	501	YEE	C13-C14-N15	-2.51	117.91	121.39
2	D	501	YEE	C09-N08-C07	2.42	120.79	117.51
2	C	501	YEE	C10-C09-N08	-2.35	120.95	124.27
2	B	501	YEE	O02-C03-C31	2.35	119.16	115.84
2	A	501	YEE	O02-C03-C04	-2.34	120.05	124.08
2	C	501	YEE	C22-N18-C19	-2.34	109.28	113.01
2	B	501	YEE	C11-C10-C26	2.31	126.28	122.47
2	A	501	YEE	C29-C31-C32	-2.28	118.74	122.20
2	B	501	YEE	O02-C03-C04	-2.28	120.15	124.08
2	D	501	YEE	C29-C31-C32	-2.27	118.76	122.20
2	A	501	YEE	O02-C03-C31	2.25	119.03	115.84
2	D	501	YEE	C05-C28-C29	2.25	121.39	119.61
2	C	501	YEE	C01-O02-C03	-2.21	114.28	117.51
2	B	501	YEE	F30-C29-C31	2.19	121.98	118.15
2	D	501	YEE	C10-C09-N08	-2.15	121.24	124.27
2	B	501	YEE	C22-C23-N15	2.09	115.18	110.78
2	C	501	YEE	C09-N08-C07	2.07	120.33	117.51

There are no chirality outliers.

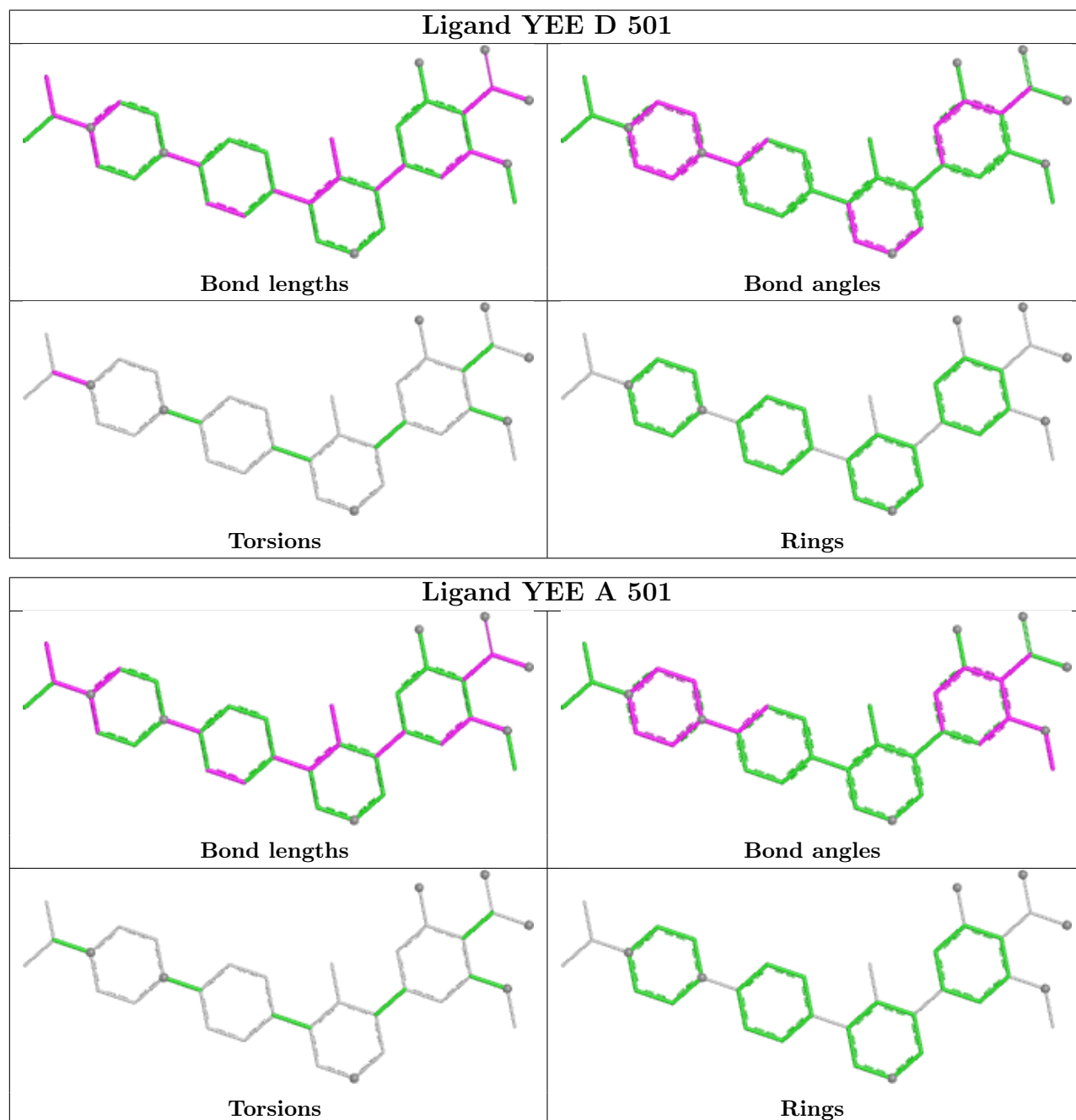
All (3) torsion outliers are listed below:

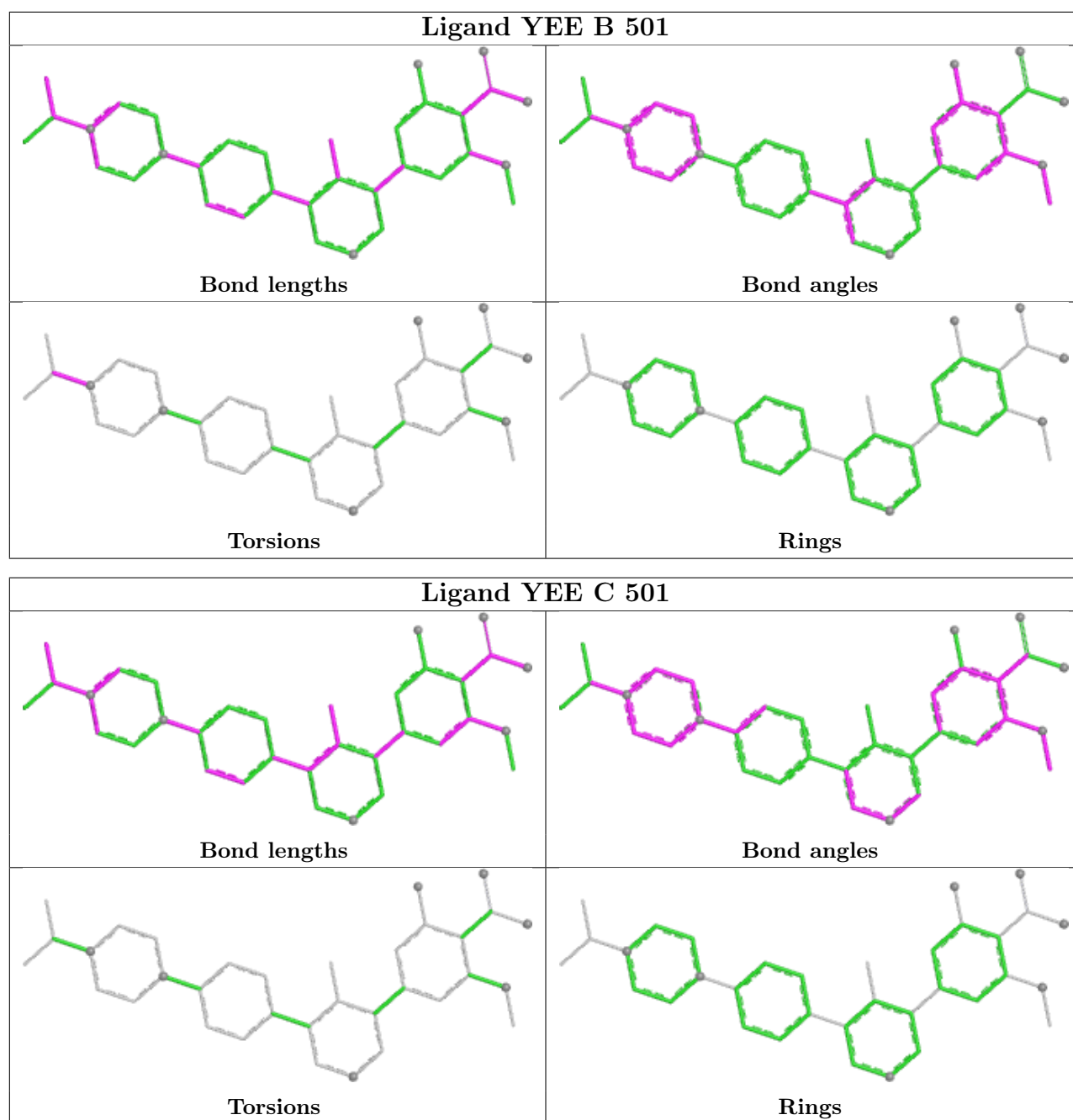
Mol	Chain	Res	Type	Atoms
2	B	501	YEE	C21-C19-N18-C22
2	D	501	YEE	C21-C19-N18-C22
2	B	501	YEE	C20-C19-N18-C22

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.





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%)	0.59	25 (8%)	16	17	37, 51, 83, 109	0
1	B	293/301 (97%)	0.68	22 (7%)	20	21	36, 52, 83, 107	0
1	C	280/301 (93%)	0.76	19 (6%)	23	25	30, 58, 89, 104	1 (0%)
1	D	291/301 (96%)	1.26	51 (17%)	4	4	48, 73, 104, 119	0
All	All	1157/1204 (96%)	0.83	117 (10%)	12	13	30, 58, 95, 119	1 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	THR	5.6
1	C	326	THR	5.5
1	D	374	PRO	5.4
1	D	257	LEU	5.0
1	B	205	ALA	4.7
1	B	274	HIS	4.3
1	C	208	ILE	4.3
1	D	365	THR	4.2
1	D	457	ILE	4.2
1	D	219	TYR	4.0
1	D	441	PHE	4.0
1	A	257	LEU	3.9
1	A	207	ASP	3.9
1	D	204	VAL	3.9
1	A	219	TYR	3.8
1	C	217	GLY	3.8
1	B	368	LEU	3.8
1	B	253	ASN	3.7
1	A	208	ILE	3.7
1	D	326	THR	3.7
1	D	323	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	273	ARG	3.7
1	D	367	GLN	3.7
1	C	219	TYR	3.7
1	B	276	SER	3.6
1	A	253	ASN	3.6
1	B	219	TYR	3.6
1	D	302	THR	3.6
1	B	326	THR	3.5
1	C	498	ILE	3.5
1	D	274	HIS	3.5
1	D	435	VAL	3.5
1	C	280[A]	TRP	3.4
1	D	324	PHE	3.4
1	A	256	MET	3.3
1	D	448	VAL	3.3
1	D	254	THR	3.3
1	B	257	LEU	3.2
1	A	326	THR	3.2
1	A	211	LEU	3.2
1	B	239	SER	3.2
1	C	438	ASP	3.1
1	D	255	VAL	3.1
1	D	376	VAL	3.1
1	A	254	THR	3.1
1	A	205	ALA	3.1
1	D	375	ARG	3.0
1	D	419	VAL	3.0
1	D	450	VAL	3.0
1	D	458	PRO	3.0
1	B	258	ARG	3.0
1	C	227	TRP	3.0
1	C	253	ASN	3.0
1	A	209	THR	3.0
1	B	273	ARG	2.9
1	D	421	ASN	2.9
1	B	450	VAL	2.9
1	D	346	LYS	2.8
1	C	207	ASP	2.8
1	A	365	THR	2.8
1	A	374	PRO	2.8
1	C	325	GLY	2.8
1	D	462	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	447	VAL	2.8
1	D	253	ASN	2.7
1	D	297	LEU	2.7
1	A	258	ARG	2.7
1	D	393	VAL	2.7
1	D	434	VAL	2.7
1	B	459	ASN	2.7
1	B	372	ASN	2.7
1	A	227	TRP	2.7
1	A	349	GLN	2.6
1	D	364	SER	2.6
1	D	498	ILE	2.6
1	D	483	SER	2.6
1	C	327	GLN	2.5
1	B	256	MET	2.5
1	A	277	THR	2.5
1	D	278	GLN	2.5
1	C	274	HIS	2.5
1	B	395	CYS	2.5
1	C	297	LEU	2.5
1	D	395	CYS	2.4
1	B	254	THR	2.4
1	D	306	LEU	2.4
1	D	426	ASP	2.4
1	C	214	VAL	2.4
1	C	376	VAL	2.4
1	D	424	VAL	2.4
1	A	366	ASN	2.3
1	D	372	ASN	2.3
1	A	376	VAL	2.3
1	A	499	ASP	2.3
1	D	418	MET	2.3
1	C	254	THR	2.3
1	D	360	MET	2.3
1	A	327	GLN	2.2
1	D	396	PHE	2.2
1	B	370	VAL	2.2
1	B	337	LEU	2.2
1	A	276	SER	2.2
1	B	226	SER	2.2
1	D	442	GLU	2.2
1	B	462	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	362	SER	2.1
1	D	294	TYR	2.1
1	D	366	ASN	2.1
1	D	444	MET	2.1
1	B	271	THR	2.1
1	C	422	GLY	2.1
1	A	368	LEU	2.0
1	D	301	ASP	2.0
1	D	465	PRO	2.0
1	C	424	VAL	2.0
1	D	272	SER	2.0
1	D	427	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

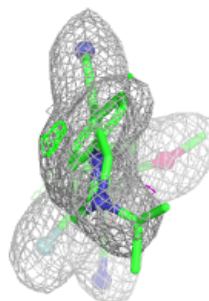
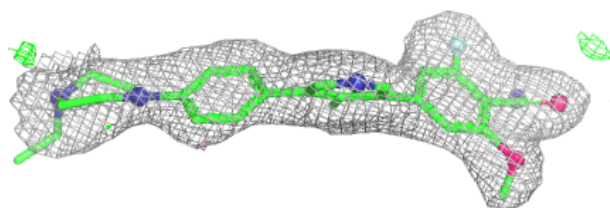
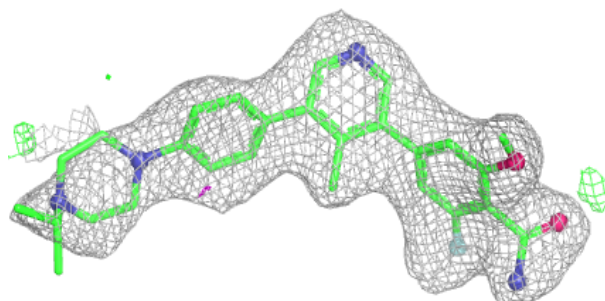
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	YEE	C	501	34/34	0.91	0.12	49,52,87,90	0
2	YEE	D	501	34/34	0.91	0.11	49,53,65,68	0
2	YEE	B	501	34/34	0.93	0.11	43,45,73,80	0
2	YEE	A	501	34/34	0.94	0.10	44,49,59,60	0

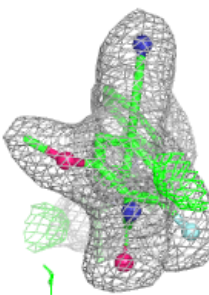
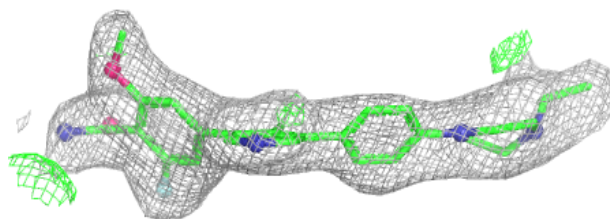
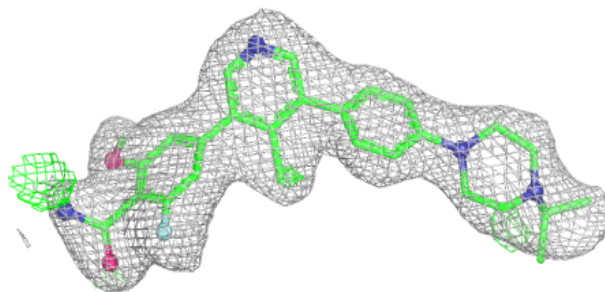
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YEE C 501:

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

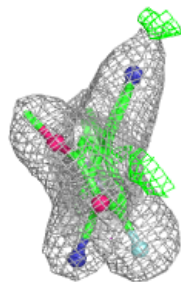
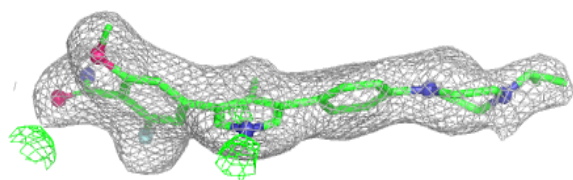
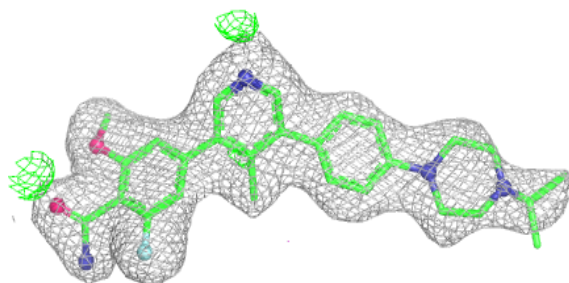
**Electron density around YEE D 501:**

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

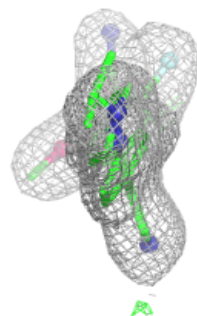
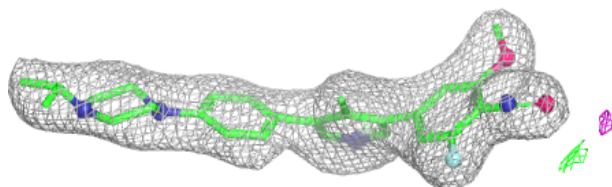
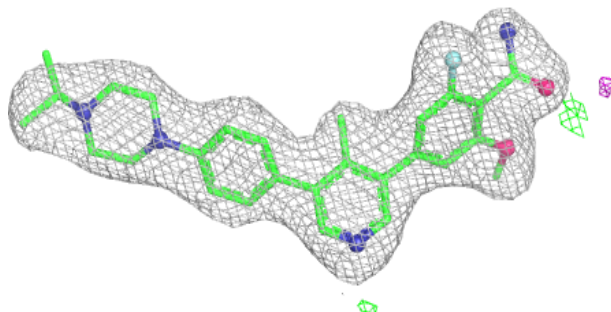


Electron density around YEE B 501:

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

**Electron density around YEE A 501:**

$2mF_o-DF_c$ (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.