



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:53 AM UTC

PDB ID : 6T6D / pdb_00006t6d
Title : Crystal structure of the ACVR1 (ALK2) kinase in complex with the compound M4K2149
Authors : Adamson, R.J.; Williams, E.P.; Smil, D.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.N.
Deposited on : 2019-10-18
Resolution : 2.56 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

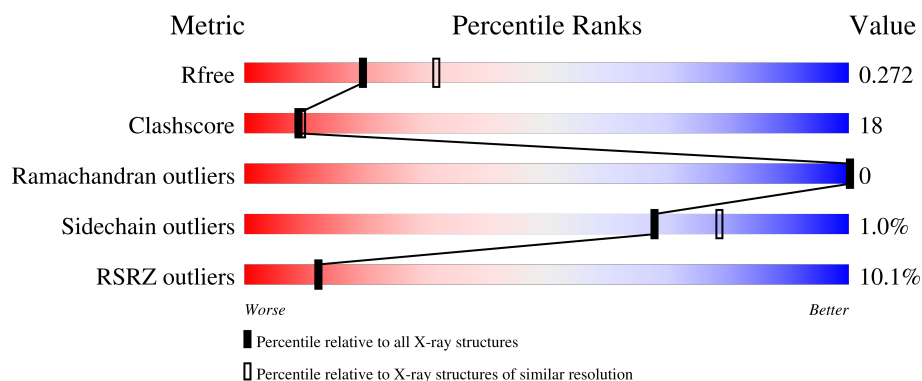
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	9% 67% 30% .
1	B	301	8% 68% 30% ..
1	C	301	11% 65% 27% 8%
1	D	301	10% 59% 35% 5%

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	SO4	A	504	-	-	X	-
3	SO4	B	503	-	-	X	-
3	SO4	D	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9250 atoms, of which 104 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.

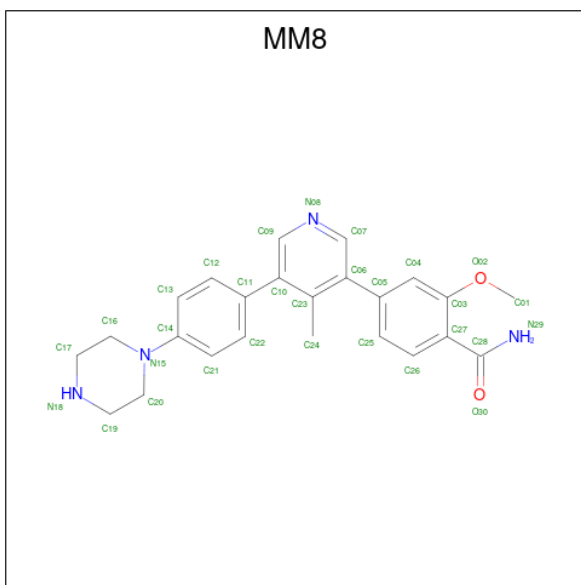
- Molecule 1 is a protein called Activin receptor type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	1	0
			2282	1460	386	421	15			
1	B	297	Total	C	N	O	S	0	1	0
			2288	1464	393	417	14			
1	C	278	Total	C	N	O	S	0	0	0
			2136	1371	365	386	14			
1	D	285	Total	C	N	O	S	0	2	0
			2235	1430	378	412	15			

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-methoxy-4-[4-methyl-5-(4-piperazin-1-ylphenyl)pyridin-3-yl]benzamide (CCD ID: MM8) (formula: C₂₄H₂₆N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			56	24	26	4	2		
2	B	1	Total	C	H	N	O	0	0
			56	24	26	4	2		
2	C	1	Total	C	H	N	O	0	0
			56	24	26	4	2		
2	D	1	Total	C	H	N	O	0	0
			56	24	26	4	2		

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



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

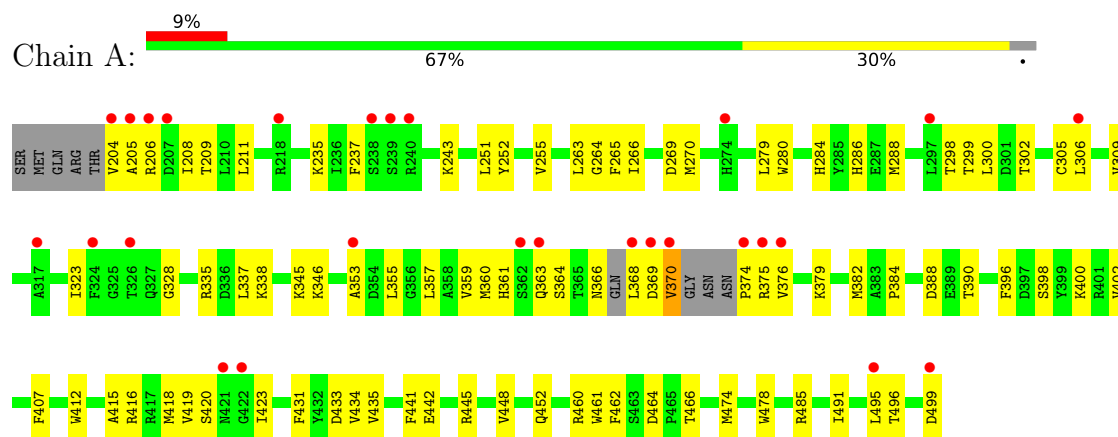
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	4	Total O 4 4	0	0
4	C	4	Total O 4 4	0	0
4	D	6	Total O 6 6	0	0

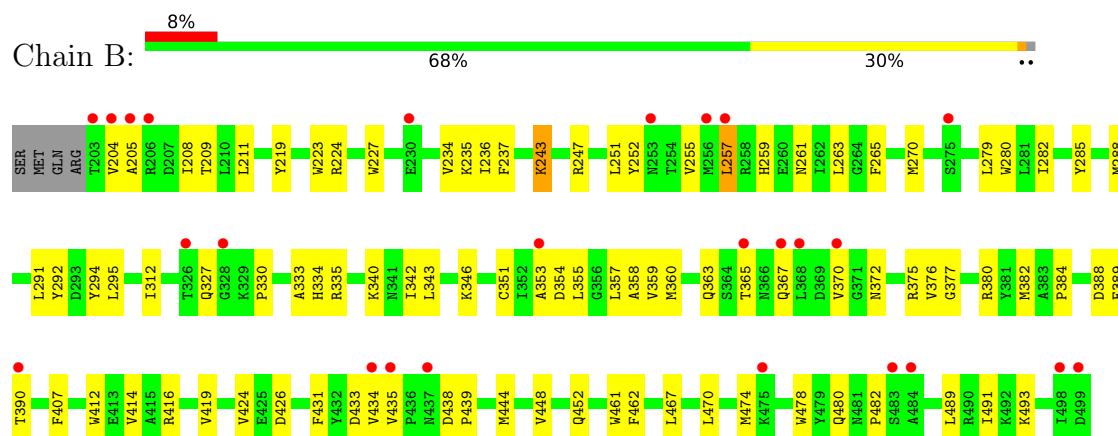
3 Residue-property plots [i](#)

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.

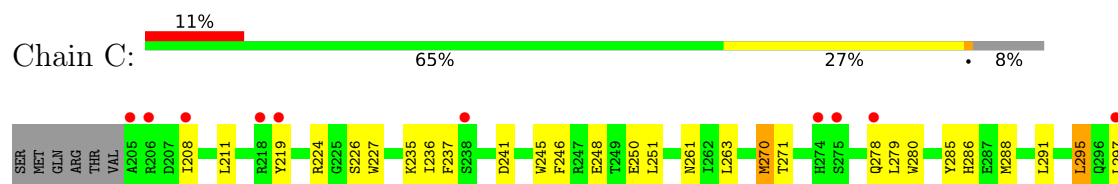
• Molecule 1: Activin receptor type I

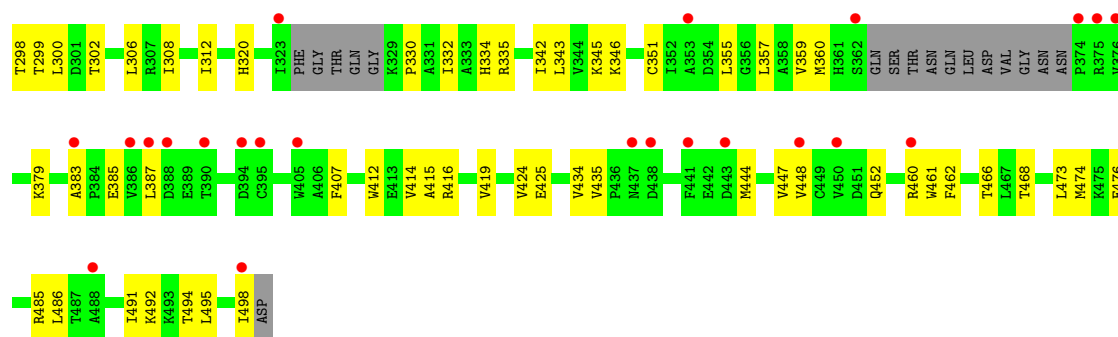


• Molecule 1: Activin receptor type I

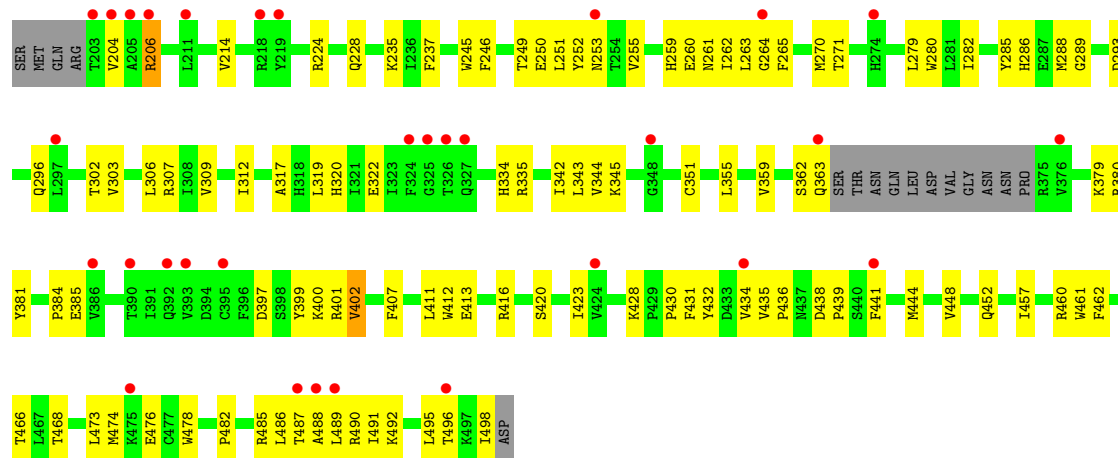


• Molecule 1: Activin receptor type I





• Molecule 1: Activin receptor type I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.09Å 101.88Å 84.27Å 90.00° 111.43° 90.00°	Depositor
Resolution (Å)	78.45 – 2.56 78.45 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (78.45-2.56) 99.8 (78.45-2.56)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.222 , 0.272 0.222 , 0.272	Depositor DCC
R_{free} test set	2494 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.941	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9250	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: SO4, MM8

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	0.09	0/2332	0.29	0/3171
1	B	0.09	0/2340	0.28	0/3191
1	C	0.09	0/2185	0.28	0/2977
1	D	0.09	0/2288	0.28	0/3113
All	All	0.09	0/9145	0.28	0/12452

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	206	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2222	86	0
1	B	2288	0	2196	84	0
1	C	2136	0	2053	69	0
1	D	2235	0	2167	96	0
2	A	30	26	0	0	0
2	B	30	26	0	0	0
2	C	30	26	0	0	0
2	D	30	26	0	4	0
3	A	15	0	0	3	0
3	B	15	0	0	2	0
3	C	15	0	0	0	0
3	D	10	0	0	3	0
4	A	16	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	6	0	0	0	0
All	All	9146	104	8638	328	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 18.

All (328) 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:204:VAL:HG23	1:A:206:ARG:H	1.26	0.99
1:B:288:MET:HE3	1:B:346:LYS:HA	1.46	0.96
1:D:270:MET:HG3	1:D:279:LEU:HD23	1.48	0.96
1:B:270:MET:HG3	1:B:279:LEU:HD23	1.51	0.91
1:D:286:HIS:NE2	3:D:503:SO4:O1	2.06	0.88
1:A:360:MET:H	1:A:368:LEU:HD23	1.40	0.87
1:A:286:HIS:NE2	3:A:504:SO4:O3	2.08	0.86
1:C:419:VAL:HA	1:C:424:VAL:HG12	1.54	0.86
1:D:288:MET:HE2	1:D:288:MET:HA	1.57	0.85
1:A:264:GLY:N	3:A:504:SO4:O1	2.08	0.85
1:A:302:THR:HA	1:A:418:MET:HE2	1.60	0.83
1:A:270:MET:HG3	1:A:279:LEU:HD23	1.57	0.83
1:D:270:MET:HG3	1:D:279:LEU:CD2	2.07	0.83
1:B:234:VAL:HG12	1:B:282:ILE:HD12	1.61	0.81
1:D:264:GLY:N	3:D:503:SO4:O4	2.13	0.81
1:A:305:CYS:HB3	1:A:418:MET:HE3	1.63	0.81
1:A:407:PHE:HE2	1:A:491:ILE:HG21	1.46	0.81
1:D:462:PHE:HA	1:D:468:THR:CG2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:VAL:HG21	1:B:444:MET:HE1	1.62	0.80
1:D:312:ILE:HD13	1:D:342:ILE:HD13	1.64	0.79
1:B:412:TRP:HB2	1:B:474:MET:HE3	1.64	0.78
1:C:412:TRP:HB2	1:C:474:MET:HE3	1.65	0.78
1:B:489:LEU:HG	1:B:493:LYS:HE3	1.63	0.78
1:D:259:HIS:HD2	1:D:261:ASN:H	1.30	0.78
1:A:270:MET:HG3	1:A:279:LEU:CD2	2.13	0.78
1:B:270:MET:HG3	1:B:279:LEU:CD2	2.15	0.77
1:D:204:VAL:HG23	1:D:206:ARG:H	1.50	0.76
1:D:462:PHE:HA	1:D:468:THR:HG23	1.69	0.74
1:D:487:THR:HG23	1:D:490:ARG:H	1.53	0.74
1:B:416:ARG:NH1	1:B:426:ASP:O	2.20	0.73
1:A:208:ILE:HG21	1:A:280:TRP:HZ3	1.52	0.73
1:A:286:HIS:CE1	1:A:345:LYS:HG2	2.22	0.73
1:A:305:CYS:CB	1:A:418:MET:HE3	2.19	0.73
1:D:206:ARG:HH12	1:D:271:THR:HG22	1.54	0.72
1:D:462:PHE:HD1	1:D:468:THR:HG22	1.54	0.71
1:C:444:MET:O	1:C:448:VAL:HG12	1.91	0.71
1:D:420:SER:O	1:D:423:ILE:HG22	1.90	0.71
1:A:288:MET:HE3	1:A:346:LYS:HA	1.73	0.71
1:C:476:GLU:HB3	1:C:486:LEU:CD1	2.21	0.71
1:A:412:TRP:HB2	1:A:474:MET:HE3	1.71	0.71
1:C:211:LEU:HD11	1:C:226:SER:OG	1.91	0.70
1:A:302:THR:O	1:A:306:LEU:HD13	1.90	0.70
1:A:375:ARG:HD2	1:A:441:PHE:CE1	2.26	0.70
1:D:476:GLU:HB3	1:D:486:LEU:CD1	2.22	0.70
1:A:496:THR:O	1:D:307:ARG:NH1	2.26	0.69
1:C:412:TRP:CZ2	1:C:416:ARG:HD2	2.28	0.68
1:D:259:HIS:CD2	1:D:261:ASN:H	2.11	0.68
1:B:412:TRP:O	1:B:416:ARG:HG3	1.94	0.68
1:C:219:TYR:HA	1:C:241:ASP:OD2	1.94	0.67
1:B:431:PHE:O	1:B:435:VAL:HG22	1.95	0.67
1:C:330:PRO:HG3	1:C:360:MET:HE3	1.77	0.66
1:C:419:VAL:CA	1:C:424:VAL:HG12	2.26	0.66
1:D:309:VAL:HG13	1:D:411:LEU:HD11	1.78	0.66
1:C:224:ARG:HD3	1:C:285:TYR:CZ	2.31	0.66
1:A:300:LEU:O	1:A:419:VAL:HG12	1.96	0.65
1:C:270:MET:HB2	1:C:279:LEU:HD23	1.78	0.65
1:D:206:ARG:HH12	1:D:271:THR:CG2	2.10	0.65
1:B:439:PRO:HG3	1:B:444:MET:HE3	1.80	0.64
1:C:288:MET:HE3	1:C:346:LYS:HA	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CG	1:A:265:PHE:HB2	2.32	0.64
1:D:492:LYS:O	1:D:496:THR:HG23	1.97	0.64
1:D:462:PHE:CD1	1:D:468:THR:HG22	2.33	0.63
1:D:431:PHE:O	1:D:435:VAL:HG12	1.98	0.63
1:B:288:MET:CE	1:B:346:LYS:HA	2.27	0.63
1:A:306:LEU:HD11	1:A:466:THR:CG2	2.29	0.63
1:C:476:GLU:HB3	1:C:486:LEU:HD13	1.78	0.63
1:B:439:PRO:CG	1:B:444:MET:HE3	2.29	0.62
1:A:390:THR:HG21	1:B:363:GLN:NE2	2.15	0.62
1:B:334:HIS:NE2	1:B:354:ASP:O	2.32	0.62
1:A:363:GLN:OE1	1:B:390:THR:HG21	2.00	0.62
1:D:435:VAL:HG22	1:D:436:PRO:HD2	1.82	0.61
1:A:418:MET:O	1:A:460:ARG:NH2	2.29	0.61
1:B:419:VAL:HG22	1:B:424:VAL:HB	1.81	0.61
1:A:357:LEU:HD13	1:A:376:VAL:HG13	1.83	0.61
1:D:385:GLU:OE2	1:D:485:ARG:NH2	2.34	0.61
1:B:412:TRP:HD1	1:B:474:MET:HE1	1.66	0.61
1:A:448:VAL:O	1:A:452:GLN:HA	2.01	0.60
1:D:476:GLU:HB3	1:D:486:LEU:HD11	1.83	0.60
1:C:237:PHE:HB2	1:C:279:LEU:HB2	1.83	0.60
1:A:209:THR:O	1:A:211:LEU:HD12	2.02	0.60
1:D:420:SER:HB3	1:D:460:ARG:HH11	1.67	0.60
1:D:252:TYR:CD1	1:D:265:PHE:HB2	2.38	0.59
1:D:466:THR:HG22	1:D:498:ILE:HG22	1.84	0.59
1:B:353:ALA:O	1:B:355:LEU:HD12	2.02	0.59
1:D:235:LYS:HD3	1:D:237:PHE:CZ	2.37	0.59
1:D:473:LEU:HD21	1:D:491:ILE:HG23	1.83	0.59
1:A:370:VAL:HG11	1:A:374:PRO:HD3	1.85	0.59
1:C:300:LEU:O	1:C:419:VAL:HG12	2.03	0.58
1:C:434:VAL:HG23	1:C:435:VAL:HG13	1.84	0.58
1:B:243:LYS:HD2	1:B:372:ASN:O	2.04	0.58
1:A:286:HIS:ND1	3:A:502:SO4:O2	2.36	0.58
1:B:236:ILE:HD12	1:B:280:TRP:NE1	2.19	0.58
1:B:461:TRP:CD1	1:B:467:LEU:HD13	2.39	0.58
1:D:435:VAL:CG2	1:D:439:PRO:HB3	2.33	0.58
1:A:302:THR:HA	1:A:418:MET:CE	2.32	0.58
1:A:418:MET:HE1	1:A:466:THR:HG21	1.86	0.58
1:D:397:ASP:O	1:D:401:ARG:HG3	2.04	0.57
1:D:288:MET:HB2	1:D:344:VAL:O	2.04	0.57
1:D:206:ARG:HD3	1:D:280:TRP:CE3	2.39	0.57
1:D:286:HIS:ND1	3:D:502:SO4:O4	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:VAL:HG12	1:D:495:LEU:HD13	1.87	0.57
1:A:364:SER:O	1:A:366:ASN:ND2	2.38	0.56
1:D:214:VAL:HG11	2:D:501:MM8:C22	2.35	0.56
1:B:435:VAL:HG21	1:B:444:MET:CE	2.32	0.56
1:D:302:THR:O	1:D:306:LEU:HD23	2.05	0.56
1:D:363:GLN:OE1	1:D:363:GLN:HA	2.06	0.56
1:D:380:ARG:HA	1:D:444:MET:HE2	1.87	0.56
1:C:308:ILE:O	1:C:312:ILE:HG13	2.05	0.56
1:D:309:VAL:CG1	1:D:411:LEU:HD11	2.35	0.56
1:B:434:VAL:HG23	1:B:435:VAL:HG13	1.88	0.56
1:C:379:LYS:O	1:C:444:MET:HG3	2.05	0.56
1:C:476:GLU:HB3	1:C:486:LEU:HD11	1.88	0.56
1:D:435:VAL:HG22	1:D:439:PRO:HB3	1.86	0.56
1:D:448:VAL:O	1:D:452:GLN:HA	2.06	0.56
1:A:412:TRP:HD1	1:A:474:MET:HE1	1.70	0.56
1:D:286:HIS:CE1	1:D:345:LYS:HG2	2.41	0.55
1:A:309:VAL:HG12	1:A:495:LEU:HD13	1.87	0.55
1:D:312:ILE:CD1	1:D:342:ILE:HD13	2.35	0.55
1:A:298:THR:HG22	1:A:299:THR:O	2.06	0.55
1:B:312:ILE:HD13	1:B:342:ILE:HD13	1.88	0.55
1:C:302:THR:O	1:C:306:LEU:HD23	2.06	0.55
1:C:235:LYS:HD3	1:C:237:PHE:CZ	2.41	0.55
1:A:376:VAL:O	1:A:376:VAL:HG22	2.07	0.55
1:B:295:LEU:HD21	1:B:414:VAL:HG22	1.89	0.55
1:B:330:PRO:HG3	1:B:360:MET:HE3	1.89	0.55
1:C:473:LEU:HD21	1:C:494:THR:HG21	1.89	0.55
1:A:208:ILE:CG2	1:A:280:TRP:HZ3	2.18	0.54
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.43	0.54
1:B:335:ARG:HD3	1:B:357:LEU:O	2.07	0.54
1:A:442:GLU:HG3	1:A:445:ARG:NH2	2.23	0.54
1:C:208:ILE:CG2	1:C:227:TRP:HB2	2.38	0.54
1:C:335:ARG:HD3	1:C:357:LEU:O	2.08	0.54
1:D:379:LYS:HE2	1:D:441:PHE:CZ	2.42	0.54
1:A:204:VAL:HG23	1:A:206:ARG:N	2.10	0.54
1:D:263:LEU:HD13	1:D:343:LEU:HD12	1.90	0.54
1:D:309:VAL:HG13	1:D:411:LEU:CD1	2.38	0.54
1:A:407:PHE:CE2	1:A:491:ILE:HG21	2.34	0.54
1:B:251:LEU:HB3	1:B:257:LEU:HD12	1.88	0.54
1:A:305:CYS:HB3	1:A:418:MET:CE	2.37	0.53
1:C:278:GLN:O	1:C:278:GLN:HG3	2.08	0.53
1:A:431:PHE:O	1:A:435:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TRP:HB2	1:B:234:VAL:HG22	1.91	0.53
1:A:251:LEU:HD13	1:A:355:LEU:HD23	1.91	0.53
1:B:247:ARG:NH2	1:B:360:MET:SD	2.81	0.53
1:B:377:GLY:O	1:B:382:MET:HE3	2.09	0.53
1:B:330:PRO:CG	1:B:360:MET:HE3	2.38	0.53
1:B:474:MET:HE2	1:B:478:TRP:CH2	2.44	0.53
1:D:322:GLU:OE2	1:D:362:SER:HB2	2.08	0.53
1:D:476:GLU:HB3	1:D:486:LEU:HD13	1.91	0.53
1:A:306:LEU:HD11	1:A:466:THR:HG21	1.89	0.53
1:A:370:VAL:CG1	1:A:374:PRO:HD3	2.39	0.52
1:C:306:LEU:HD21	1:C:466:THR:HG23	1.91	0.52
1:D:249:THR:O	1:D:253:ASN:N	2.41	0.52
1:B:208:ILE:CD1	1:B:227:TRP:HB2	2.39	0.52
1:C:298:THR:HG22	1:C:299:THR:O	2.09	0.52
1:D:251:LEU:HD23	1:D:355:LEU:HD13	1.91	0.52
1:D:251:LEU:O	1:D:255:VAL:HB	2.10	0.52
1:C:495:LEU:HD23	1:C:498:ILE:HD12	1.92	0.52
1:B:259:HIS:HE1	1:B:261:ASN:HD22	1.58	0.52
1:C:245:TRP:CZ2	1:C:270:MET:HB3	2.45	0.52
1:D:412:TRP:CZ2	1:D:416:ARG:HD2	2.45	0.52
1:B:235:LYS:HD3	1:B:237:PHE:CZ	2.45	0.51
1:B:435:VAL:HG11	1:B:444:MET:HE2	1.91	0.51
1:A:306:LEU:HD11	1:A:466:THR:HG23	1.91	0.51
1:C:271:THR:OG1	1:C:278:GLN:HG2	2.10	0.51
1:A:442:GLU:HG3	1:A:445:ARG:HH21	1.76	0.51
1:D:288:MET:HA	1:D:288:MET:CE	2.36	0.51
1:D:399:TYR:O	1:D:402:VAL:HG13	2.10	0.51
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.46	0.51
1:B:480:GLN:O	1:B:482:PRO:HD3	2.11	0.51
1:C:462:PHE:HA	1:C:468:THR:OG1	2.10	0.51
1:D:401:ARG:HD3	1:D:482:PRO:O	2.10	0.51
1:B:263:LEU:HD13	1:B:343:LEU:HD12	1.93	0.51
1:A:323:ILE:HG22	1:A:328:GLY:HA2	1.92	0.51
1:C:383:ALA:O	1:C:387:LEU:HD22	2.10	0.51
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.46	0.50
1:C:237:PHE:CG	1:C:245:TRP:HB2	2.46	0.50
1:D:206:ARG:HD3	1:D:280:TRP:CZ3	2.46	0.50
1:C:270:MET:HE2	1:C:279:LEU:HD21	1.92	0.50
1:C:208:ILE:HB	1:C:226:SER:O	2.11	0.50
1:C:385:GLU:OE2	1:C:485:ARG:NH1	2.37	0.50
1:D:457:ILE:HG23	1:D:461:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD11	1:B:358:ALA:HB3	1.93	0.49
1:D:359:VAL:HG21	1:D:399:TYR:CD2	2.48	0.49
1:B:470:LEU:O	1:B:474:MET:HG3	2.13	0.49
1:A:335:ARG:HD3	1:A:357:LEU:O	2.12	0.49
1:A:379:LYS:HA	1:A:382:MET:HG3	1.94	0.49
1:B:448:VAL:O	1:B:452:GLN:HA	2.13	0.49
1:C:407:PHE:HE2	1:C:491:ILE:HG21	1.78	0.49
1:C:492:LYS:NZ	4:C:601:HOH:O	2.42	0.49
1:B:255:VAL:HG13	1:B:330:PRO:HD2	1.95	0.48
1:B:261:ASN:O	1:B:351:CYS:HA	2.12	0.48
1:D:401:ARG:HD3	1:D:482:PRO:C	2.38	0.48
1:C:286:HIS:CE1	1:C:345:LYS:HG2	2.48	0.48
1:D:260:GLU:O	1:D:345:LYS:NZ	2.35	0.48
1:B:223:TRP:HB2	1:B:234:VAL:CG2	2.43	0.48
1:D:214:VAL:HG11	2:D:501:MM8:C11	2.44	0.48
1:A:396:PHE:CE2	1:A:400:LYS:HE3	2.49	0.48
1:B:224:ARG:HD3	1:B:285:TYR:CZ	2.49	0.48
1:C:263:LEU:HD13	1:C:343:LEU:HD12	1.95	0.48
1:A:398:SER:O	1:A:402:VAL:HG23	2.12	0.48
1:B:251:LEU:HD13	1:B:355:LEU:HD23	1.94	0.48
1:B:412:TRP:CB	1:B:474:MET:HE3	2.39	0.48
1:A:266:ILE:HD11	1:A:284:HIS:CD2	2.48	0.48
1:B:292:TYR:CE2	1:B:340:LYS:HE2	2.49	0.48
1:C:448:VAL:O	1:C:452:GLN:HA	2.13	0.48
1:C:425:GLU:OE1	1:C:460:ARG:NH2	2.40	0.48
1:A:474:MET:HE2	1:A:478:TRP:CH2	2.49	0.47
1:C:407:PHE:CE2	1:C:491:ILE:HG21	2.49	0.47
1:D:428:LYS:HB3	1:D:432:TYR:CD1	2.49	0.47
1:B:489:LEU:O	1:B:493:LYS:HG3	2.14	0.47
1:D:317:ALA:HA	1:D:488:ALA:HB1	1.96	0.47
1:D:412:TRP:O	1:D:416:ARG:HG3	2.14	0.47
1:D:407:PHE:CE2	1:D:411:LEU:HD13	2.49	0.47
1:A:375:ARG:HD2	1:A:441:PHE:CZ	2.49	0.47
1:A:462:PHE:CE2	1:C:297:LEU:HD21	2.49	0.47
1:B:209:THR:O	1:B:211:LEU:HD12	2.15	0.47
1:B:365:THR:O	1:B:367:GLN:N	2.48	0.47
1:C:330:PRO:CG	1:C:360:MET:HE3	2.44	0.47
1:A:337:LEU:HD23	1:A:338:LYS:N	2.30	0.47
1:B:294:TYR:HD2	1:B:295:LEU:HD12	1.79	0.47
1:A:353:ALA:O	1:A:355:LEU:HD12	2.15	0.47
1:A:288:MET:CE	1:A:346:LYS:HA	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:SER:O	1:A:423:ILE:HG22	2.16	0.46
1:A:384:PRO:HD2	1:A:485:ARG:NH2	2.31	0.46
1:C:236:ILE:HG12	1:C:280:TRP:NE1	2.29	0.46
1:D:435:VAL:CG2	1:D:436:PRO:HD2	2.42	0.46
1:A:252:TYR:OH	1:A:263:LEU:O	2.31	0.46
1:A:305:CYS:SG	1:A:418:MET:HE3	2.56	0.46
1:A:433:ASP:OD1	1:A:434:VAL:HG13	2.16	0.46
1:C:412:TRP:CB	1:C:474:MET:HE3	2.42	0.46
1:B:390:THR:O	1:B:390:THR:HG22	2.15	0.46
1:D:289:GLY:HA2	2:D:501:MM8:C13	2.45	0.46
1:A:335:ARG:NH2	1:A:369:ASP:OD2	2.49	0.46
1:B:291:LEU:HD12	1:B:295:LEU:HD13	1.98	0.46
1:A:384:PRO:HG3	1:A:448:VAL:CG1	2.45	0.46
1:B:204:VAL:HG12	1:B:205:ALA:N	2.31	0.46
1:B:388:ASP:O	1:B:389:GLU:HB2	2.16	0.46
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.51	0.46
1:A:374:PRO:HG2	1:A:375:ARG:H	1.80	0.46
1:D:435:VAL:HG21	1:D:444:MET:SD	2.55	0.46
1:B:370:VAL:HG13	1:B:370:VAL:O	2.16	0.45
1:B:435:VAL:HG11	1:B:444:MET:CE	2.47	0.45
1:A:396:PHE:CD2	1:A:400:LYS:HE3	2.51	0.45
1:A:499:ASP:CB	1:D:303:VAL:HG21	2.47	0.45
1:D:224:ARG:HB2	1:D:285:TYR:CE2	2.52	0.45
1:B:204:VAL:HG12	1:B:205:ALA:H	1.81	0.45
1:D:245:TRP:CZ2	1:D:270:MET:HB2	2.52	0.45
1:C:208:ILE:HG22	1:C:227:TRP:CD1	2.52	0.45
1:C:270:MET:HE2	1:C:279:LEU:CD2	2.47	0.45
1:D:407:PHE:CZ	1:D:411:LEU:HD13	2.51	0.45
1:A:252:TYR:CD1	1:A:265:PHE:HB2	2.51	0.45
1:B:334:HIS:O	1:B:335:ARG:HB2	2.17	0.44
1:A:205:ALA:HB3	1:A:269:ASP:OD2	2.18	0.44
1:D:282:ILE:N	1:D:282:ILE:HD12	2.32	0.44
1:D:380:ARG:HD3	1:D:430:PRO:O	2.17	0.44
1:A:335:ARG:HD2	1:A:359:VAL:HG13	1.99	0.44
1:C:291:LEU:O	1:C:295:LEU:HB2	2.18	0.44
1:D:259:HIS:HB3	1:D:262[A]:ILE:HG12	1.99	0.44
1:C:320:HIS:HD2	1:C:332:ILE:O	2.02	0.43
1:B:327:GLN:H	1:B:327:GLN:CD	2.24	0.43
1:C:208:ILE:HG22	1:C:227:TRP:HB2	2.00	0.43
1:B:252:TYR:CG	1:B:265:PHE:HB2	2.53	0.43
1:A:235:LYS:HD3	1:A:237:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:CE2	1:D:228:GLN:HA	2.54	0.43
1:C:246:PHE:O	1:C:250:GLU:HB2	2.18	0.43
1:A:370:VAL:HG22	1:A:374:PRO:N	2.34	0.43
1:A:415:ALA:HB3	1:A:461:TRP:CH2	2.53	0.43
1:B:219:TYR:H	1:B:219:TYR:HD1	1.67	0.43
1:C:248:GLU:HG3	1:C:355:LEU:HB2	1.99	0.43
1:C:224:ARG:HB2	1:C:285:TYR:CE1	2.53	0.43
1:A:300:LEU:HB2	1:A:418:MET:HA	2.00	0.43
1:B:234:VAL:CG1	1:B:282:ILE:HD12	2.40	0.43
2:D:501:MM8:C24	2:D:501:MM8:C12	2.97	0.43
1:D:309:VAL:HG12	1:D:495:LEU:CD1	2.48	0.42
1:D:334:HIS:O	1:D:335:ARG:HB2	2.19	0.42
1:C:312:ILE:HD13	1:C:342:ILE:HD13	2.01	0.42
1:D:438:ASP:N	1:D:439:PRO:HD3	2.34	0.42
1:C:335:ARG:HD2	1:C:359:VAL:HG22	2.01	0.42
1:D:489:LEU:C	1:D:489:LEU:HD23	2.45	0.42
1:A:464:ASP:OD1	1:A:466:THR:N	2.52	0.42
1:B:292:TYR:CD2	1:B:340:LYS:HE2	2.55	0.42
1:B:365:THR:C	1:B:367:GLN:N	2.77	0.42
1:C:295:LEU:HD21	1:C:414:VAL:HA	2.02	0.42
1:C:419:VAL:HB	1:C:424:VAL:CG1	2.50	0.42
1:D:381:TYR:OH	1:D:413:GLU:OE1	2.37	0.42
1:A:364:SER:CA	1:B:390:THR:HG23	2.50	0.42
1:B:438:ASP:N	3:B:503:SO4:O3	2.48	0.42
1:C:270:MET:HA	1:C:278:GLN:O	2.20	0.42
1:C:236:ILE:HG12	1:C:280:TRP:CD1	2.55	0.41
1:C:412:TRP:HD1	1:C:474:MET:HE1	1.84	0.41
1:D:261:ASN:O	1:D:351:CYS:HA	2.20	0.41
1:C:415:ALA:HB3	1:C:461:TRP:CH2	2.55	0.41
1:D:246:PHE:O	1:D:250:GLU:HB2	2.20	0.41
1:A:270:MET:HG3	1:A:279:LEU:HD21	1.98	0.41
1:A:364:SER:N	1:B:390:THR:HG23	2.35	0.41
1:D:335:ARG:HH11	1:D:359:VAL:HG13	1.85	0.41
1:B:333:ALA:HB3	1:B:359:VAL:HG22	2.02	0.41
1:B:376:VAL:HG22	1:B:382:MET:HE2	2.03	0.41
1:D:420:SER:HB3	1:D:460:ARG:NH1	2.34	0.41
1:A:255:VAL:O	1:A:255:VAL:HG12	2.19	0.41
1:C:219:TYR:CD2	1:C:235:LYS:HE3	2.56	0.41
1:B:330:PRO:HG3	1:B:360:MET:CE	2.50	0.41
1:C:208:ILE:C	1:C:208:ILE:HD12	2.46	0.41
1:C:261:ASN:O	1:C:351:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:LEU:HD12	1:D:319:LEU:HA	1.90	0.41
1:A:302:THR:CA	1:A:418:MET:HE2	2.41	0.41
1:A:388:ASP:HB3	1:A:390:THR:OG1	2.20	0.41
1:B:384:PRO:HG3	1:B:448:VAL:HG12	2.01	0.41
1:D:474:MET:HE3	1:D:478:TRP:HH2	1.86	0.41
1:B:461:TRP:HB3	1:B:467:LEU:HB3	2.02	0.41
1:C:270:MET:O	1:C:270:MET:HG3	2.21	0.41
1:D:293:ASP:O	1:D:296:GLN:HB2	2.21	0.41
1:D:320:HIS:HB3	1:D:400:LYS:HE3	2.02	0.41
1:D:434:VAL:O	1:D:434:VAL:HG12	2.21	0.41
1:C:334:HIS:O	1:C:335:ARG:HB2	2.21	0.41
1:B:365:THR:C	1:B:367:GLN:H	2.29	0.40
1:D:436:PRO:O	1:D:439:PRO:HG3	2.21	0.40
1:C:434:VAL:HG21	1:C:447:VAL:HG11	2.03	0.40
1:D:380:ARG:HA	1:D:444:MET:CE	2.50	0.40
1:D:384:PRO:HG3	1:D:448:VAL:CG1	2.51	0.40
1:B:251:LEU:HD21	1:B:360:MET:SD	2.61	0.40
1:B:489:LEU:CG	1:B:493:LYS:HE3	2.45	0.40
1:A:252:TYR:HB3	1:A:265:PHE:CG	2.56	0.40
1:B:357:LEU:HD11	1:B:375:ARG:HD3	2.03	0.40
1:B:380:ARG:NE	3:B:503:SO4:O4	2.48	0.40
1:A:205:ALA:O	1:A:208:ILE:HG22	2.22	0.40
1:D:474:MET:HE3	1:D:478:TRP:CH2	2.56	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	287/301 (95%)	279 (97%)	8 (3%)	0	100	100
1	B	296/301 (98%)	282 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	272/301 (90%)	261 (96%)	11 (4%)	0	100	100
1	D	283/301 (94%)	273 (96%)	10 (4%)	0	100	100
All	All	1138/1204 (94%)	1095 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	245/270 (91%)	243 (99%)	2 (1%)	73	82
1	B	237/270 (88%)	234 (99%)	3 (1%)	61	74
1	C	221/270 (82%)	218 (99%)	3 (1%)	59	73
1	D	238/270 (88%)	237 (100%)	1 (0%)	84	89
All	All	941/1080 (87%)	932 (99%)	9 (1%)	68	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	LYS
1	A	370	VAL
1	B	243	LYS
1	B	257	LEU
1	B	433	ASP
1	C	251	LEU
1	C	270	MET
1	C	295	LEU
1	D	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	261	ASN
1	B	318	HIS
1	B	347	ASN
1	B	349	GLN
1	B	361	HIS
1	C	361	HIS
1	D	259	HIS
1	D	261	ASN

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 ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.12	0
2	MM8	C	501	-	33,33,33	2.15	8 (24%)	44,46,46	1.24	7 (15%)
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	502	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.07	0
2	MM8	A	501	-	33,33,33	2.16	8 (24%)	44,46,46	1.25	3 (6%)
3	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.19	0
2	MM8	B	501	-	33,33,33	2.16	8 (24%)	44,46,46	1.27	7 (15%)
3	SO4	D	503	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.08	0
2	MM8	D	501	-	33,33,33	2.16	9 (27%)	44,46,46	1.19	2 (4%)

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	MM8	A	501	-	-	2/18/26/26	0/4/4/4
2	MM8	B	501	-	-	6/18/26/26	0/4/4/4
2	MM8	C	501	-	-	2/18/26/26	0/4/4/4
2	MM8	D	501	-	-	2/18/26/26	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	MM8	C28-N29	6.53	1.45	1.33
2	B	501	MM8	C28-N29	6.49	1.44	1.33
2	A	501	MM8	C28-N29	6.48	1.44	1.33
2	C	501	MM8	C28-N29	6.43	1.44	1.33
2	D	501	MM8	O02-C03	4.93	1.45	1.37
2	A	501	MM8	O02-C03	4.93	1.45	1.37
2	C	501	MM8	O02-C03	4.89	1.45	1.37
2	B	501	MM8	O02-C03	4.85	1.45	1.37
2	D	501	MM8	C14-N15	3.99	1.49	1.38
2	C	501	MM8	C14-N15	3.94	1.49	1.38
2	B	501	MM8	C14-N15	3.92	1.49	1.38
2	A	501	MM8	C14-N15	3.81	1.49	1.38
2	C	501	MM8	C06-C05	-3.78	1.42	1.49
2	B	501	MM8	C06-C05	-3.60	1.43	1.49
2	D	501	MM8	C06-C05	-3.55	1.43	1.49
2	A	501	MM8	C06-C05	-3.53	1.43	1.49
2	B	501	MM8	C10-C11	-3.42	1.43	1.49
2	A	501	MM8	C10-C11	-3.37	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	MM8	C10-C11	-3.33	1.43	1.49
2	C	501	MM8	O30-C28	-3.27	1.18	1.24
2	A	501	MM8	O30-C28	-3.25	1.18	1.24
2	D	501	MM8	O30-C28	-3.25	1.18	1.24
2	B	501	MM8	O30-C28	-3.23	1.18	1.24
2	D	501	MM8	C10-C11	-3.11	1.43	1.49
2	B	501	MM8	C27-C28	2.74	1.53	1.50
2	C	501	MM8	C27-C28	2.68	1.53	1.50
2	A	501	MM8	C27-C28	2.60	1.53	1.50
2	D	501	MM8	C27-C28	2.44	1.53	1.50
2	D	501	MM8	C16-N15	2.22	1.50	1.46
2	B	501	MM8	C16-N15	2.17	1.50	1.46
2	A	501	MM8	C16-N15	2.17	1.50	1.46
2	C	501	MM8	C16-N15	2.06	1.50	1.46
2	D	501	MM8	C22-C21	2.05	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MM8	C03-C27-C28	-4.67	119.97	125.06
2	D	501	MM8	C03-C27-C28	-4.29	120.38	125.06
2	B	501	MM8	C03-C27-C28	-3.58	121.16	125.06
2	C	501	MM8	C03-C27-C28	-2.84	121.96	125.06
2	B	501	MM8	C01-O02-C03	-2.55	113.77	117.51
2	B	501	MM8	O02-C03-C04	-2.46	119.83	124.08
2	C	501	MM8	O02-C03-C04	-2.46	119.84	124.08
2	A	501	MM8	C09-N08-C07	2.43	120.81	117.51
2	C	501	MM8	O02-C03-C27	2.41	120.05	116.55
2	C	501	MM8	C09-N08-C07	2.37	120.74	117.51
2	D	501	MM8	C09-N08-C07	2.31	120.65	117.51
2	B	501	MM8	O02-C03-C27	2.30	119.89	116.55
2	B	501	MM8	C09-N08-C07	2.28	120.61	117.51
2	C	501	MM8	O30-C28-N29	-2.20	119.44	122.62
2	C	501	MM8	C27-C28-N29	2.19	121.68	118.29
2	B	501	MM8	O30-C28-N29	-2.15	119.51	122.62
2	A	501	MM8	C10-C09-N08	-2.14	121.26	124.27
2	B	501	MM8	C10-C09-N08	-2.07	121.35	124.27
2	C	501	MM8	C20-N15-C16	-2.01	107.05	111.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

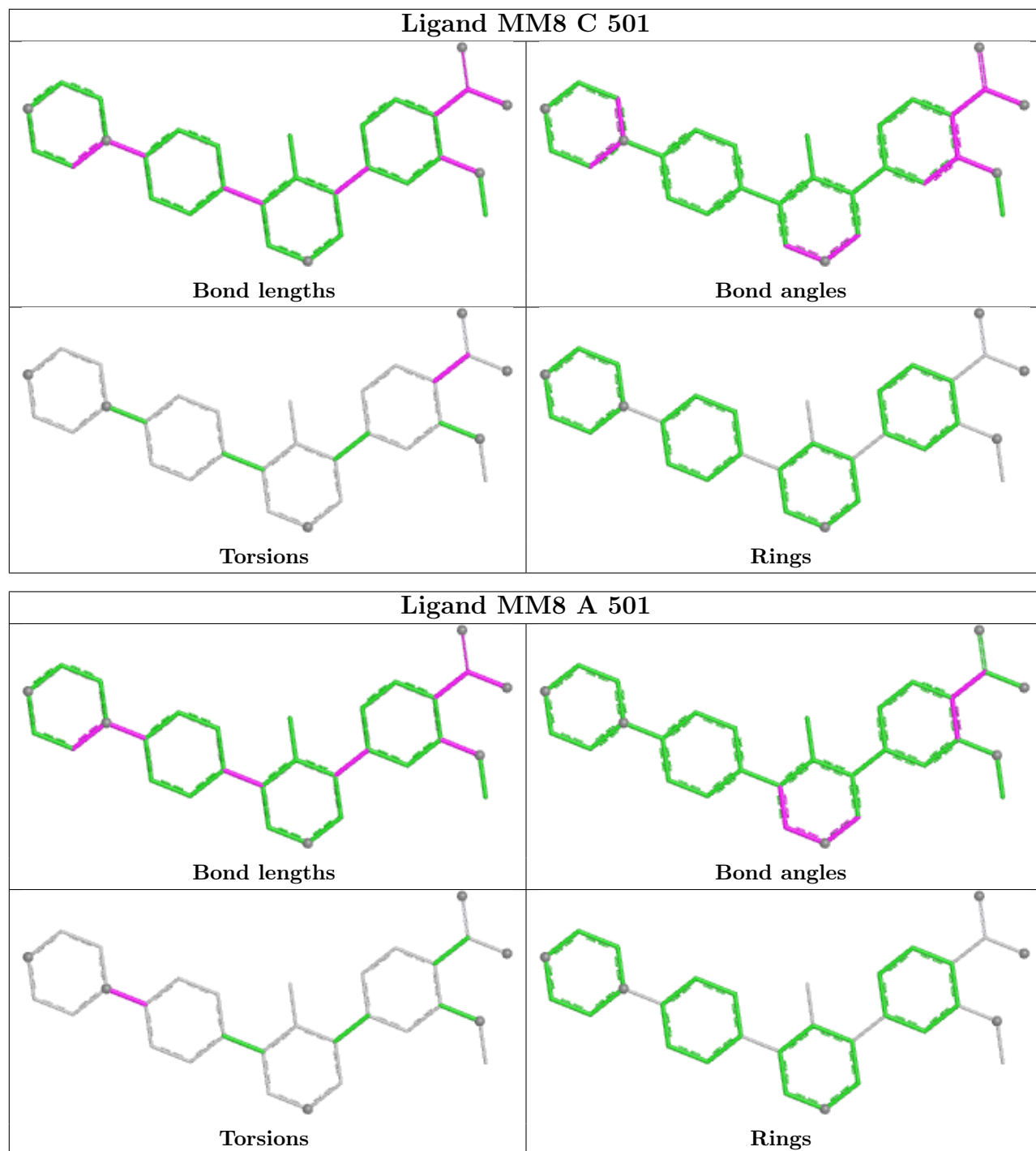
Mol	Chain	Res	Type	Atoms
2	B	501	MM8	C21-C14-N15-C16
2	B	501	MM8	C13-C14-N15-C16
2	D	501	MM8	C03-C27-C28-N29
2	B	501	MM8	C04-C03-O02-C01
2	B	501	MM8	C27-C03-O02-C01
2	D	501	MM8	C03-C27-C28-O30
2	A	501	MM8	C21-C14-N15-C16
2	A	501	MM8	C13-C14-N15-C16
2	B	501	MM8	C03-C27-C28-N29
2	B	501	MM8	C03-C27-C28-O30
2	C	501	MM8	C03-C27-C28-N29
2	C	501	MM8	C03-C27-C28-O30

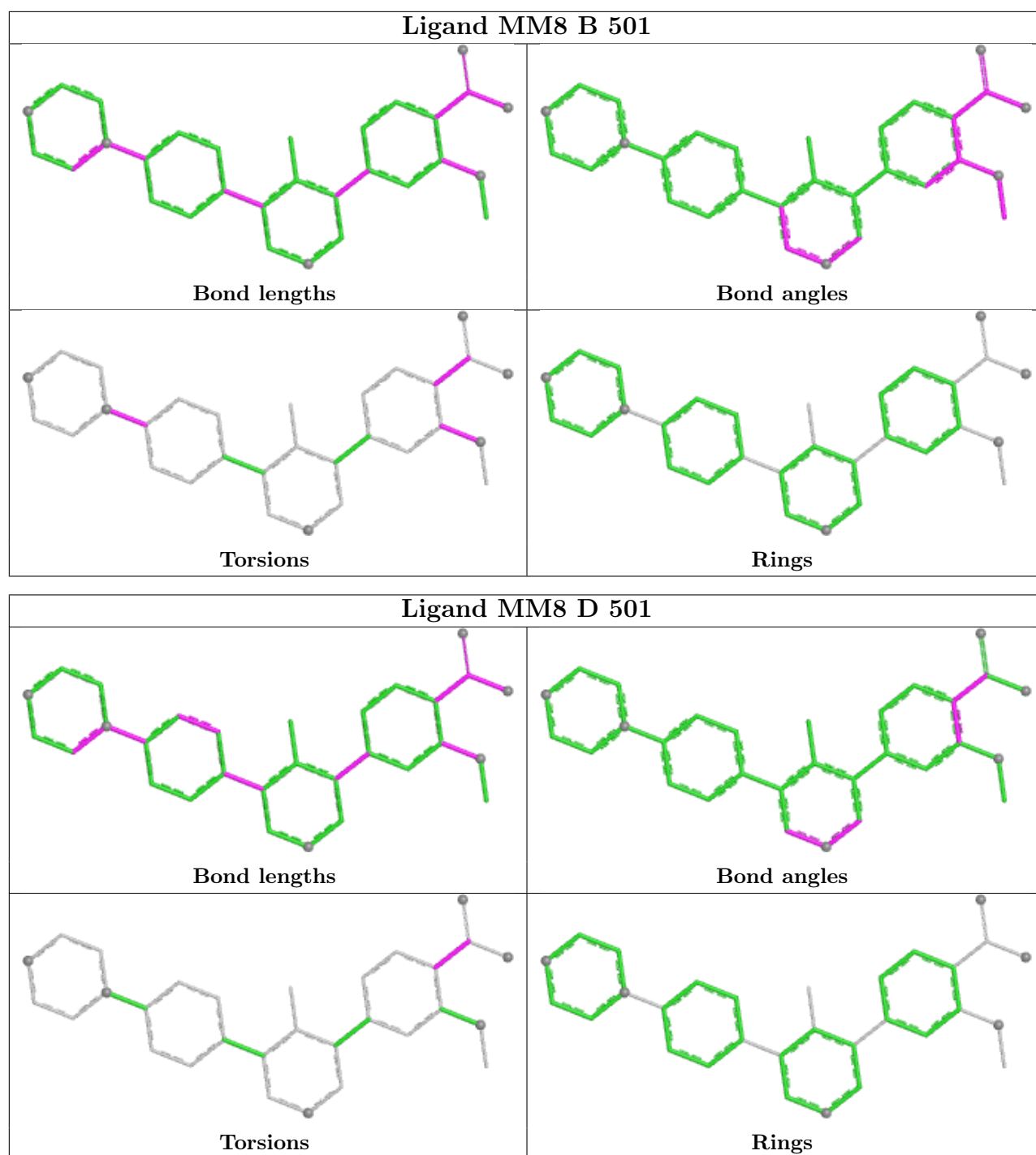
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	SO4	2	0
3	D	502	SO4	1	0
3	B	503	SO4	2	0
3	D	503	SO4	2	0
3	A	502	SO4	1	0
2	D	501	MM8	4	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 [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	292/301 (97%)	0.75	27 (9%)	14 14	39, 66, 96, 111	1 (0%)
1	B	297/301 (98%)	0.82	25 (8%)	17 17	32, 69, 98, 121	1 (0%)
1	C	278/301 (92%)	1.02	33 (11%)	9 8	56, 75, 99, 112	0
1	D	285/301 (94%)	0.99	31 (10%)	10 10	32, 76, 99, 116	2 (0%)
All	All	1152/1204 (95%)	0.89	116 (10%)	12 12	32, 72, 99, 121	4 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	4.7
1	B	206	ARG	4.5
1	C	374	PRO	4.4
1	A	205	ALA	4.4
1	D	205	ALA	4.3
1	A	374	PRO	4.2
1	B	205	ALA	4.2
1	A	499	ASP	4.1
1	C	275	SER	4.1
1	B	499	ASP	4.0
1	C	323	ILE	3.9
1	C	219	TYR	3.9
1	C	388	ASP	3.9
1	B	204	VAL	3.8
1	A	207[A]	ASP	3.7
1	D	376	VAL	3.7
1	B	253	ASN	3.6
1	B	230	GLU	3.6
1	A	368	LEU	3.6
1	D	441	PHE	3.5
1	D	390	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	205	ALA	3.4
1	D	203	THR	3.3
1	C	395	CYS	3.2
1	D	324	PHE	3.2
1	C	376	VAL	3.1
1	D	488	ALA	3.1
1	B	368	LEU	3.1
1	A	239	SER	3.0
1	A	204	VAL	3.0
1	D	219	TYR	3.0
1	C	218	ARG	3.0
1	D	211	LEU	3.0
1	C	437	ASN	3.0
1	C	353	ALA	2.9
1	C	383	ALA	2.9
1	A	363	GLN	2.9
1	D	206	ARG	2.9
1	C	450	VAL	2.9
1	A	422	GLY	2.8
1	D	264	GLY	2.8
1	B	275	SER	2.8
1	D	326	THR	2.8
1	D	204	VAL	2.8
1	D	424	VAL	2.8
1	C	375	ARG	2.8
1	C	362	SER	2.8
1	B	367	GLN	2.8
1	D	327	GLN	2.7
1	D	363	GLN	2.7
1	D	386	VAL	2.7
1	A	326	THR	2.7
1	C	460	ARG	2.7
1	D	489	LEU	2.6
1	B	353	ALA	2.6
1	D	496	THR	2.6
1	B	256	MET	2.6
1	B	365	THR	2.6
1	B	328	GLY	2.5
1	D	475	LYS	2.5
1	B	203	THR	2.5
1	B	437	ASN	2.5
1	A	376	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	326	THR	2.5
1	B	390	THR	2.5
1	B	257	LEU	2.4
1	D	392	GLN	2.4
1	C	448	VAL	2.4
1	C	498	ILE	2.4
1	A	240	ARG	2.4
1	D	218	ARG	2.4
1	D	395	CYS	2.4
1	C	441	PHE	2.4
1	A	218	ARG	2.3
1	C	387	LEU	2.3
1	B	498	ILE	2.3
1	D	297	LEU	2.3
1	C	386	VAL	2.3
1	C	405	TRP	2.3
1	D	325	GLY	2.3
1	A	375	ARG	2.3
1	D	348	GLY	2.3
1	B	475	LYS	2.3
1	B	434	VAL	2.3
1	D	393	VAL	2.3
1	C	390	THR	2.2
1	C	238	SER	2.2
1	B	435	VAL	2.2
1	C	206	ARG	2.2
1	C	208	ILE	2.2
1	A	317	ALA	2.2
1	A	306	LEU	2.2
1	A	206	ARG	2.2
1	D	434	VAL	2.2
1	A	297	LEU	2.2
1	C	394	ASP	2.2
1	C	274	HIS	2.1
1	A	421	ASN	2.1
1	B	484	ALA	2.1
1	C	488	ALA	2.1
1	D	253	ASN	2.1
1	A	324	PHE	2.1
1	B	370	VAL	2.1
1	D	274	HIS	2.1
1	C	297	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	443	ASP	2.1
1	B	483	SER	2.1
1	C	278	GLN	2.1
1	A	353	ALA	2.0
1	A	495	LEU	2.0
1	C	438	ASP	2.0
1	A	238	SER	2.0
1	D	487	THR	2.0
1	A	369	ASP	2.0
1	A	274	HIS	2.0
1	A	362	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

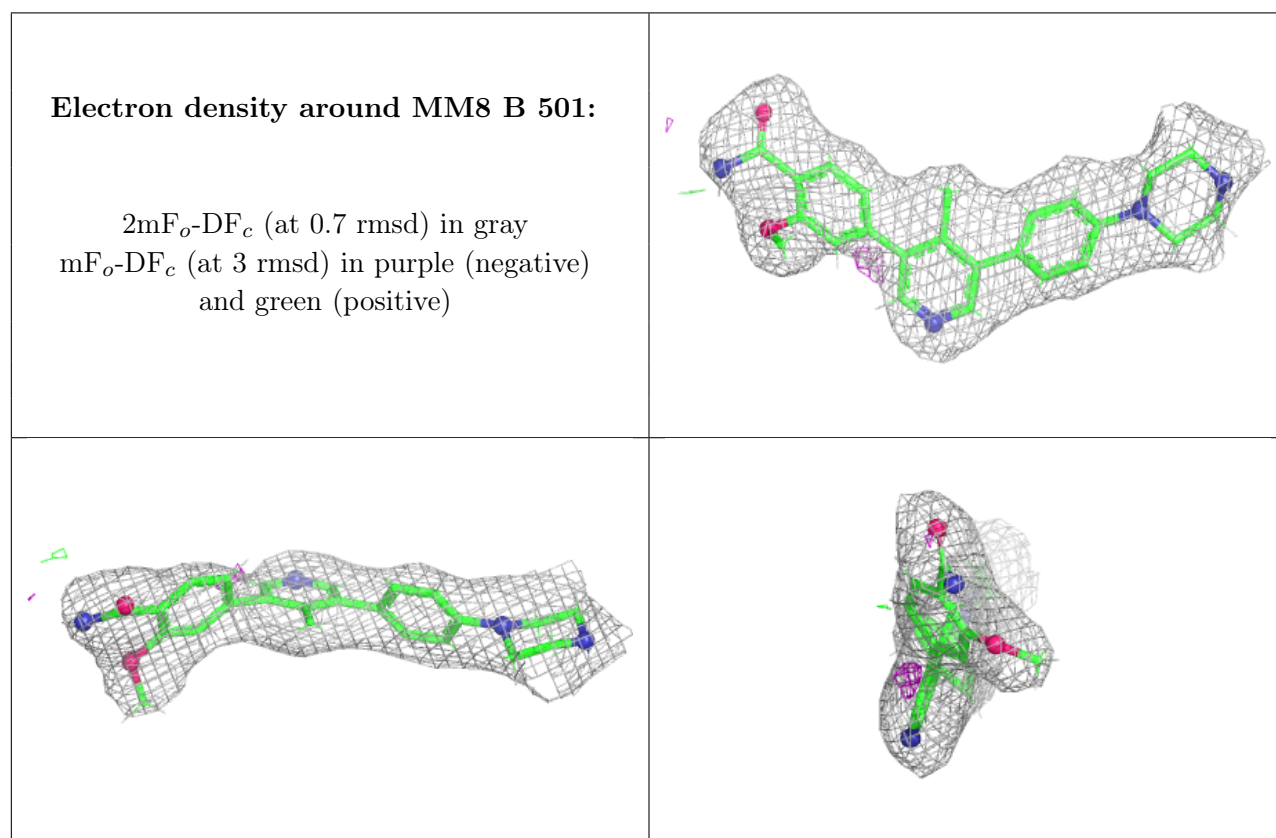
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	504	5/5	0.72	0.15	81,87,99,115	0
3	SO4	C	504	5/5	0.73	0.16	78,85,105,107	0
3	SO4	D	503	5/5	0.77	0.13	78,87,94,109	0
3	SO4	C	503	5/5	0.82	0.10	103,113,122,126	0
3	SO4	B	503	5/5	0.86	0.08	105,106,113,120	0
3	SO4	A	503	5/5	0.87	0.12	75,82,94,99	0
2	MM8	B	501	30/30	0.87	0.14	64,80,119,124	0
3	SO4	B	502	5/5	0.89	0.20	73,78,93,98	0
3	SO4	C	502	5/5	0.90	0.08	71,73,82,87	0
3	SO4	B	504	5/5	0.91	0.09	70,73,82,85	0
2	MM8	A	501	30/30	0.92	0.10	48,68,103,105	0
2	MM8	D	501	30/30	0.92	0.11	55,73,98,103	0

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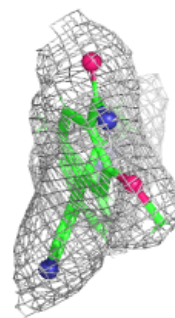
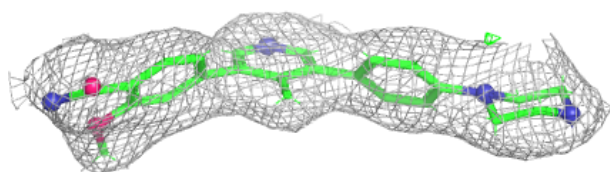
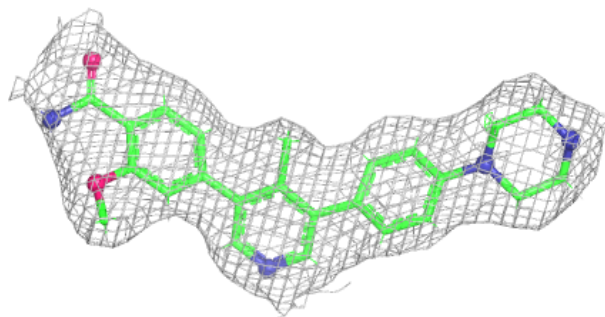
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	502	5/5	0.92	0.14	67,78,84,97	0
3	SO4	A	502	5/5	0.92	0.10	73,73,80,87	0
2	MM8	C	501	30/30	0.93	0.11	49,68,91,93	0

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.

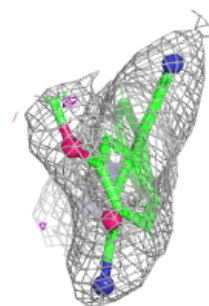
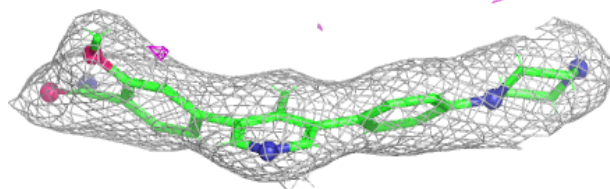
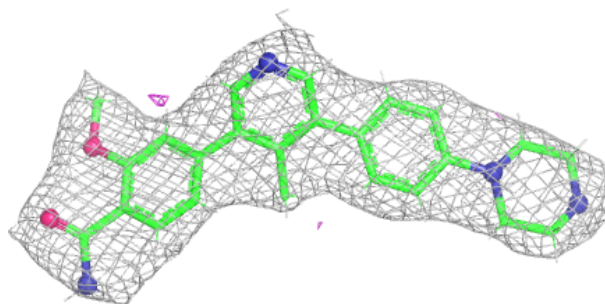


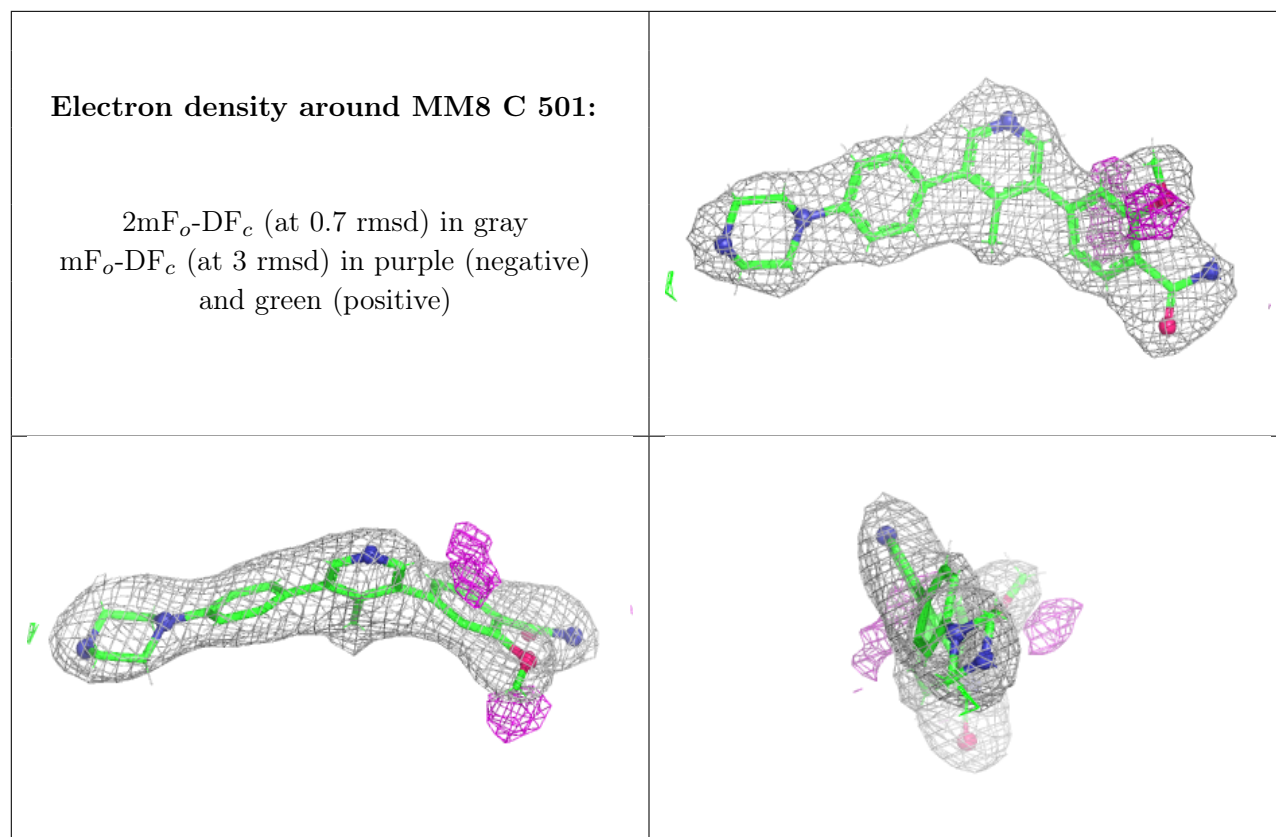
Electron density around MM8 A 501:

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

**Electron density around MM8 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.