



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 10:59 PM UTC

PDB ID : 4U42 / pdb_00004u42
Title : MAP4K4 T181E Mutant Bound to inhibitor compound 1
Authors : Harris, S.F.; Wu, P.; Coons, M.
Deposited on : 2014-07-23
Resolution : 2.50 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

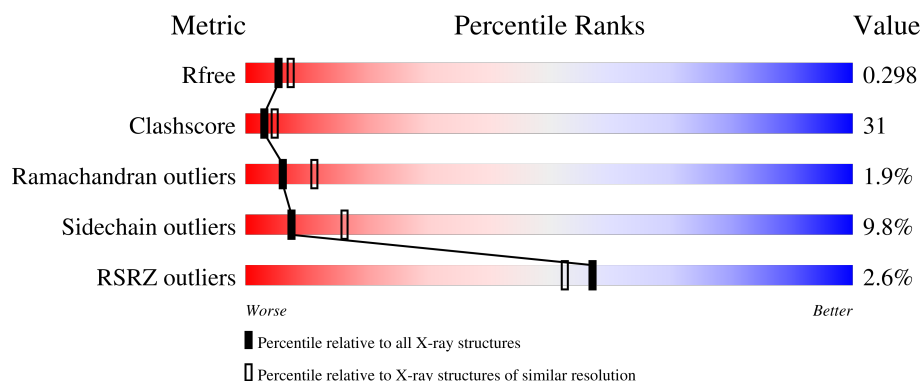
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	332	
1	B	332	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4530 atoms, of which 2 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.

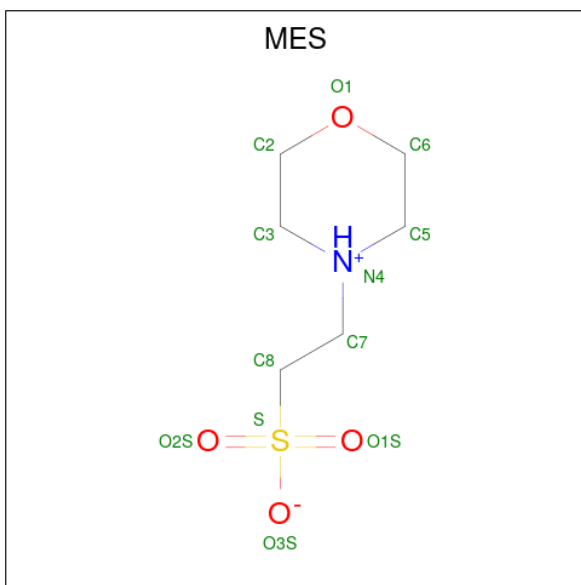
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2278	1453	400	412	13			
1	B	265	Total	C	N	O	S	0	1	0
			2143	1371	380	379	13			

There are 12 discrepancies between the modelled and reference sequences:

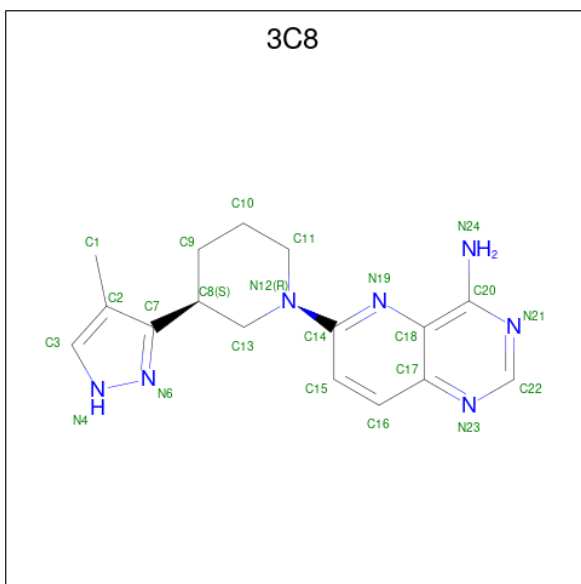
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O95819
A	1	SER	-	expression tag	UNP O95819
A	181	GLU	THR	engineered mutation	UNP O95819
A	329	GLY	-	expression tag	UNP O95819
A	330	ASN	-	expression tag	UNP O95819
A	331	SER	-	expression tag	UNP O95819
B	0	GLY	-	expression tag	UNP O95819
B	1	SER	-	expression tag	UNP O95819
B	181	GLU	THR	engineered mutation	UNP O95819
B	329	GLY	-	expression tag	UNP O95819
B	330	ASN	-	expression tag	UNP O95819
B	331	SER	-	expression tag	UNP O95819

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is 6-[(3S)-3-(4-methyl-1H-pyrazol-3-yl)piperidin-1-yl]pyrido[3,2-d]pyrimidin-4-amine (CCD ID: 3C8) (formula: C₁₆H₁₉N₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			24	16	1	7		
3	B	1	Total	C	H	N	0	0
			24	16	1	7		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	B	22	Total 22	O 22	0	0

SER
GLU
GLU
GLY
ASN
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.45Å 83.67Å 95.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.50 39.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.72-2.50) 99.5 (39.72-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.227 , 0.303 0.223 , 0.298	Depositor DCC
R_{free} test set	1146 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4530	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MG, MES, 3C8

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	0.54	1/2334 (0.0%)	0.92	4/3156 (0.1%)
1	B	0.51	0/2196	0.85	0/2970
All	All	0.53	1/4530 (0.0%)	0.89	4/6126 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ILE	CA-CB	5.46	1.56	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	N-CA-C	-5.54	107.52	114.56
1	A	94	PRO	CA-C-N	5.33	126.50	119.84
1	A	94	PRO	C-N-CA	5.33	126.50	119.84
1	A	30	VAL	N-CA-C	5.10	119.95	109.34

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	2278	0	2270	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2143	0	2143	121	0
2	A	12	0	12	0	0
3	A	23	1	19	7	0
3	B	23	1	19	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	0	1	0
5	B	22	0	0	2	0
All	All	4528	2	4463	281	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 31.

All (281) 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:236:MET:HE1	1:A:244:LEU:HD12	1.12	1.08
1:A:56:MET:HE3	1:A:101:LEU:HD23	1.34	1.06
1:B:260:LYS:HE2	1:B:260:LYS:HA	1.12	1.04
1:B:92:LYS:HB3	1:B:93:SER:HB3	1.34	1.03
1:B:260:LYS:HA	1:B:260:LYS:CE	1.94	0.96
1:B:236:MET:HG3	1:B:240:ARG:HG2	1.48	0.93
1:B:260:LYS:HE2	1:B:260:LYS:CA	1.99	0.92
1:A:21:PRO:HG2	1:A:91:LYS:HD3	1.51	0.91
1:A:90:ILE:HD12	1:A:90:ILE:O	1.71	0.90
1:A:46:LYS:HA	1:A:46:LYS:HE3	1.52	0.90
1:B:18:LEU:HB2	1:B:90:ILE:HD12	1.55	0.87
1:A:79:HIS:O	1:A:80:ARG:HB3	1.73	0.86
1:A:308:ARG:HH21	1:A:308:ARG:HB2	1.41	0.86
1:A:64:GLU:HG2	1:A:67:LYS:NZ	1.91	0.86
1:A:297:GLN:O	1:A:301:GLN:HG3	1.76	0.85
1:B:93:SER:HB2	1:B:94:PRO:CD	2.07	0.85
1:A:29:GLU:O	1:A:30:VAL:HG22	1.78	0.83
1:A:211:ASP:OD1	1:A:213:ARG:HD3	1.77	0.83
1:B:90:ILE:HG21	1:B:92:LYS:HE2	1.61	0.82
1:B:56:MET:HE3	1:B:101:LEU:HD23	1.64	0.79
1:B:113:ILE:O	1:B:117:VAL:HG23	1.82	0.79
1:A:21:PRO:CG	1:A:91:LYS:HD3	2.12	0.79
1:A:69:GLU:O	1:A:73:LEU:HD12	1.83	0.78
1:B:79:HIS:HD2	1:B:81:ASN:H	1.28	0.78
1:B:116:LEU:HD23	1:B:125:LEU:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:HG22	1:A:62:GLU:HG3	1.66	0.78
1:A:64:GLU:HG2	1:A:67:LYS:HZ3	1.47	0.77
1:B:310:ARG:NH1	1:B:310:ARG:HB2	1.98	0.77
1:A:94:PRO:O	1:A:97:HIS:HB2	1.83	0.77
1:A:117:VAL:HG11	1:A:229:GLY:HA2	1.67	0.76
1:B:305:HIS:O	1:B:309:THR:HG22	1.86	0.76
1:A:70:ILE:O	1:A:74:LYS:HG2	1.86	0.76
1:B:236:MET:CG	1:B:240:ARG:HG2	2.15	0.76
1:A:46:LYS:HE2	1:A:46:LYS:O	1.86	0.75
1:A:236:MET:HE1	1:A:244:LEU:CD1	2.06	0.75
1:A:296:ARG:HG3	1:A:297:GLN:H	1.52	0.75
1:B:85:TYR:CZ	1:B:87:GLY:HA2	2.22	0.74
1:A:21:PRO:HD2	1:A:91:LYS:HD2	1.69	0.74
1:A:105:MET:HE3	3:A:402:3C8:C2	2.18	0.73
1:A:305:HIS:HA	1:A:308:ARG:HD3	1.70	0.73
1:B:305:HIS:NE2	1:B:309:THR:HG21	2.02	0.73
1:B:243:PHE:O	1:B:247:ARG:HD2	1.89	0.73
1:B:204:GLU:N	1:B:204:GLU:CD	2.47	0.73
1:A:308:ARG:HB2	1:A:308:ARG:NH2	2.04	0.72
1:B:56:MET:CE	1:B:101:LEU:HD23	2.19	0.72
1:B:92:LYS:CB	1:B:93:SER:HB3	2.16	0.71
1:B:36:TYR:HB2	1:B:39:VAL:CG1	2.20	0.71
1:B:36:TYR:HB2	1:B:39:VAL:HG11	1.71	0.71
1:A:296:ARG:HG3	1:A:297:GLN:N	2.05	0.71
1:B:25:PHE:CE2	1:B:44:HIS:HD2	2.09	0.70
1:A:79:HIS:O	1:A:80:ARG:CB	2.38	0.70
1:B:151:HIS:O	1:B:152:ARG:HB2	1.92	0.70
1:A:38:GLN:HE21	1:A:55:VAL:HG12	1.57	0.69
1:A:59:THR:CG2	1:A:62:GLU:HG3	2.23	0.69
1:A:202:CYS:SG	1:A:204:GLU:HG2	2.33	0.68
1:A:202:CYS:SG	1:A:204:GLU:CG	2.81	0.68
1:A:236:MET:CE	1:A:244:LEU:HD12	2.07	0.68
1:B:120:THR:HG21	1:B:124:THR:O	1.93	0.68
1:A:212:TYR:CE2	1:A:213:ARG:HD2	2.28	0.68
1:B:28:VAL:O	1:B:29:GLU:HB3	1.93	0.67
1:A:209:THR:O	1:A:209:THR:HG22	1.95	0.67
1:A:66:ILE:CG2	1:A:101:LEU:HD22	2.26	0.66
1:A:239:MET:HE2	1:B:201:ALA:H	1.59	0.66
1:B:75:LYS:O	1:B:75:LYS:HG2	1.96	0.66
1:A:71:ASN:HA	1:A:74:LYS:CG	2.27	0.65
1:B:307:ASP:O	1:B:310:ARG:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD12	1:B:90:ILE:CD1	2.27	0.65
1:B:79:HIS:HB3	1:B:82:ILE:HD12	1.79	0.65
1:B:94:PRO:HD3	1:B:99:ASP:OD2	1.96	0.65
1:A:85:TYR:CE2	1:A:87:GLY:HA2	2.32	0.64
1:B:79:HIS:CD2	1:B:81:ASN:H	2.14	0.64
1:A:19:ARG:H	1:A:90:ILE:HG13	1.61	0.64
1:A:56:MET:CE	1:A:101:LEU:HD23	2.20	0.64
1:A:281:GLU:O	1:A:285:LYS:HG3	1.98	0.64
1:A:28:VAL:C	1:A:29:GLU:HG3	2.23	0.64
1:A:59:THR:CG2	1:A:62:GLU:CG	2.75	0.64
1:A:204:GLU:HA	5:A:504:HOH:O	1.98	0.64
1:A:296:ARG:HB3	1:A:296:ARG:NH1	2.13	0.64
1:B:93:SER:HB2	1:B:94:PRO:HD3	1.80	0.64
1:A:114:THR:HG21	1:A:157:GLN:HE21	1.63	0.64
1:B:29:GLU:C	1:B:40:TYR:HD1	2.06	0.63
3:A:402:3C8:C1	3:A:402:3C8:H10	2.30	0.62
1:A:151:HIS:O	1:A:152:ARG:HB2	1.99	0.62
1:A:188:PHE:HD1	1:B:190:GLY:HA2	1.64	0.62
1:B:24:ILE:HD12	1:B:89:PHE:HE1	1.64	0.62
1:A:18:LEU:HB2	1:A:90:ILE:HG23	1.82	0.61
1:A:28:VAL:H	1:A:29:GLU:HA	1.64	0.61
1:B:204:GLU:CD	1:B:204:GLU:H	2.05	0.61
1:A:228:GLU:CD	1:A:254:LYS:HD2	2.25	0.61
1:A:81:ASN:O	1:A:168:LYS:HA	2.00	0.61
3:B:401:3C8:C1	3:B:401:3C8:H10	2.31	0.61
1:A:46:LYS:HA	1:A:46:LYS:CE	2.29	0.60
1:B:80:ARG:NH2	5:B:511:HOH:O	2.34	0.60
3:A:402:3C8:H10	3:A:402:3C8:H12	1.83	0.60
1:A:79:HIS:HE1	1:A:81:ASN:HD22	1.49	0.60
1:A:237:HIS:HD2	1:A:239:MET:H	1.49	0.60
1:A:105:MET:HE3	3:A:402:3C8:C7	2.32	0.60
1:A:28:VAL:C	1:A:29:GLU:CG	2.75	0.60
1:A:296:ARG:CB	1:A:296:ARG:CZ	2.80	0.60
1:B:90:ILE:CG2	1:B:92:LYS:HE2	2.32	0.59
1:A:27:LEU:HB3	1:A:29:GLU:HB3	1.84	0.59
1:A:296:ARG:HB3	1:A:296:ARG:CZ	2.33	0.59
1:A:62:GLU:HB2	1:A:66:ILE:HD11	1.84	0.59
1:B:296:ARG:O	1:B:300:ILE:HG13	2.03	0.59
1:B:31:VAL:HG22	1:B:39:VAL:O	2.02	0.59
1:A:59:THR:OG1	1:A:60:GLU:N	2.35	0.59
1:A:237:HIS:CD2	1:A:239:MET:H	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:O	1:B:35:THR:HB	2.03	0.58
1:B:117:VAL:HG11	1:B:229:GLY:HA2	1.85	0.58
1:A:117:VAL:CG1	1:A:229:GLY:HA2	2.32	0.58
1:A:147:HIS:O	1:A:148:HIS:HB2	2.02	0.58
1:B:93:SER:HB2	1:B:94:PRO:HD2	1.84	0.58
1:A:29:GLU:C	1:A:30:VAL:HG22	2.28	0.58
1:A:106:GLU:OE2	1:A:168:LYS:HE3	2.04	0.58
1:B:36:TYR:CB	1:B:39:VAL:HG11	2.33	0.58
1:A:30:VAL:HG12	1:A:40:TYR:CE1	2.39	0.57
1:A:31:VAL:CG2	1:A:39:VAL:HG12	2.33	0.57
1:A:38:GLN:HG2	1:A:55:VAL:HB	1.85	0.57
1:A:21:PRO:HD2	1:A:91:LYS:CD	2.33	0.57
1:A:212:TYR:CZ	1:A:213:ARG:HD2	2.40	0.57
1:A:18:LEU:HD12	1:A:90:ILE:HG23	1.86	0.57
1:A:143:HIS:O	1:A:146:ILE:HG22	2.05	0.57
1:A:29:GLU:O	1:A:30:VAL:CG2	2.51	0.56
1:A:71:ASN:HA	1:A:74:LYS:HG3	1.87	0.56
1:B:260:LYS:CE	1:B:260:LYS:CA	2.64	0.56
1:A:20:ASP:CG	1:A:91:LYS:HD2	2.30	0.56
1:A:28:VAL:HG21	1:A:41:LYS:HD3	1.87	0.56
1:A:86:TYR:HB2	1:A:104:VAL:HG12	1.87	0.55
1:B:194:TRP:CZ2	1:B:231:PRO:HG3	2.42	0.55
1:A:239:MET:HE2	1:B:201:ALA:N	2.21	0.55
1:A:46:LYS:HE3	1:A:46:LYS:CA	2.32	0.55
1:A:237:HIS:CD2	1:A:238:PRO:HD2	2.42	0.55
1:B:233:LEU:O	1:B:236:MET:HB2	2.07	0.54
1:A:20:ASP:OD1	1:A:91:LYS:HD2	2.07	0.54
1:B:85:TYR:CE2	1:B:87:GLY:HA2	2.42	0.54
1:B:126:LYS:O	1:B:129:TRP:HB2	2.08	0.54
1:A:60:GLU:HG2	1:A:61:ASP:N	2.23	0.54
1:A:51:ALA:HA	1:A:107:PHE:HB2	1.89	0.53
1:B:18:LEU:HD12	1:B:90:ILE:HD11	1.89	0.53
1:B:35:THR:HG22	1:B:36:TYR:CD2	2.43	0.53
1:A:85:TYR:CZ	1:A:87:GLY:HA2	2.43	0.53
1:A:51:ALA:CA	1:A:107:PHE:HB2	2.39	0.53
1:B:57:ASP:HA	1:B:99:ASP:O	2.08	0.53
1:B:279:SER:OG	1:B:282:GLN:HG3	2.10	0.52
1:A:67:LYS:O	1:A:71:ASN:ND2	2.42	0.52
1:B:86:TYR:CE1	1:B:106:GLU:HA	2.45	0.52
1:A:62:GLU:O	1:A:64:GLU:N	2.42	0.52
1:A:188:PHE:CD1	1:B:190:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:A:67:LYS:CE	2.38	0.52
1:B:310:ARG:HB2	1:B:310:ARG:CZ	2.39	0.52
1:A:20:ASP:CG	1:A:21:PRO:HD2	2.34	0.52
1:B:56:MET:O	1:B:58:VAL:HG13	2.10	0.51
1:A:19:ARG:O	1:A:90:ILE:N	2.41	0.51
1:B:245:ILE:HB	1:B:246:PRO:HD3	1.92	0.51
1:A:57:ASP:OD1	1:A:100:GLN:HG2	2.10	0.51
1:B:110:ALA:HB2	1:B:306:ILE:HD13	1.92	0.51
1:B:132:TYR:O	1:B:136:GLU:HG2	2.11	0.51
1:B:305:HIS:CD2	1:B:309:THR:HG21	2.45	0.51
1:A:73:LEU:O	1:A:77:SER:OG	2.25	0.51
1:B:90:ILE:CG2	1:B:92:LYS:CE	2.89	0.51
3:B:401:3C8:H10	3:B:401:3C8:H12	1.90	0.51
1:A:308:ARG:NH2	1:A:308:ARG:CB	2.74	0.51
1:A:59:THR:CG2	1:A:62:GLU:HG2	2.41	0.50
1:A:79:HIS:CE1	1:A:81:ASN:HD22	2.29	0.50
1:A:245:ILE:HB	1:A:246:PRO:HD3	1.92	0.50
1:A:24:ILE:HG22	1:A:25:PHE:CD2	2.46	0.50
1:A:82:ILE:N	1:A:82:ILE:HD12	2.27	0.50
1:B:225:GLU:O	1:B:229:GLY:N	2.44	0.50
1:A:202:CYS:SG	1:A:204:GLU:OE1	2.64	0.50
1:A:296:ARG:CG	1:A:297:GLN:H	2.23	0.50
1:A:164:ASN:O	1:A:165:ALA:HB3	2.12	0.49
1:A:118:LYS:HD2	1:A:119:ASN:OD1	2.13	0.49
1:A:154:ILE:O	1:A:218:SER:HB3	2.12	0.49
1:A:228:GLU:OE1	1:A:254:LYS:HD2	2.12	0.49
1:A:71:ASN:HB3	1:A:75:LYS:HE3	1.95	0.49
1:B:251:PRO:HD2	1:B:270:LEU:HD13	1.94	0.49
1:A:30:VAL:O	1:A:30:VAL:HG23	2.13	0.49
1:B:30:VAL:N	1:B:40:TYR:HD1	2.10	0.49
1:A:28:VAL:HG22	1:A:41:LYS:HB3	1.94	0.48
1:B:85:TYR:CZ	1:B:87:GLY:CA	2.95	0.48
1:A:296:ARG:CG	1:A:297:GLN:N	2.76	0.48
1:A:77:SER:HB3	1:A:84:THR:HA	1.96	0.48
1:B:303:LYS:O	1:B:306:ILE:HB	2.12	0.48
1:A:28:VAL:H	1:A:29:GLU:CA	2.26	0.48
1:A:46:LYS:CE	1:A:46:LYS:CA	2.89	0.48
1:A:117:VAL:HG21	1:A:226:MET:HA	1.96	0.48
1:B:310:ARG:HB2	1:B:310:ARG:HH11	1.73	0.48
1:B:217:TRP:CD1	1:B:217:TRP:C	2.92	0.48
1:B:82:ILE:CD1	1:B:143:HIS:HD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:O	1:B:219[B]:CYS:HB2	2.14	0.47
1:B:44:HIS:HB3	1:B:47:THR:OG1	2.15	0.47
1:A:202:CYS:O	1:A:205:ASN:N	2.44	0.47
1:A:39:VAL:HG21	3:A:402:3C8:H4	1.95	0.47
1:B:211:ASP:HA	5:B:509:HOH:O	2.14	0.47
1:A:105:MET:HE3	3:A:402:3C8:C3	2.44	0.47
1:A:136:GLU:HB3	1:A:167:VAL:HB	1.97	0.47
1:A:59:THR:HG23	1:A:62:GLU:CG	2.44	0.47
1:A:71:ASN:HA	1:A:74:LYS:CD	2.44	0.46
1:B:89:PHE:HE2	1:B:104:VAL:HG21	1.80	0.46
1:B:116:LEU:HD23	1:B:125:LEU:CD1	2.39	0.46
1:A:90:ILE:HD12	1:A:90:ILE:C	2.39	0.46
1:A:151:HIS:O	1:A:152:ARG:CB	2.64	0.46
1:B:30:VAL:HA	1:B:40:TYR:CD1	2.51	0.46
1:B:59:THR:HG22	1:B:59:THR:O	2.16	0.45
1:B:248:ASN:O	1:B:272:LYS:NZ	2.49	0.45
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.70	0.45
1:A:154:ILE:HB	1:A:218:SER:HB2	1.99	0.45
1:B:310:ARG:CZ	1:B:310:ARG:CB	2.95	0.45
1:B:309:THR:O	1:B:310:ARG:C	2.59	0.45
1:A:150:ILE:HG22	1:A:152:ARG:HG3	1.98	0.45
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.75	0.45
1:A:122:GLY:O	1:A:123:ASN:C	2.60	0.45
1:B:141:LEU:CD1	1:B:219[B]:CYS:SG	3.05	0.45
1:B:154:ILE:HB	1:B:218:SER:HB2	2.00	0.44
1:B:24:ILE:HD12	1:B:89:PHE:CE1	2.48	0.44
1:A:59:THR:HG23	1:A:62:GLU:HG2	2.00	0.44
1:A:64:GLU:CG	1:A:67:LYS:NZ	2.73	0.44
1:A:135:ARG:HB2	1:A:289:ILE:HG23	1.99	0.44
1:A:121:LYS:O	1:A:121:LYS:HG3	2.16	0.44
1:B:113:ILE:HG23	1:B:159:VAL:O	2.17	0.44
1:B:57:ASP:OD1	1:B:100:GLN:HG2	2.17	0.44
1:B:77:SER:HA	1:B:82:ILE:HG21	1.99	0.44
1:A:64:GLU:HA	1:A:67:LYS:HB2	1.99	0.44
1:B:77:SER:HA	1:B:82:ILE:CG2	2.48	0.44
1:B:245:ILE:N	1:B:246:PRO:CD	2.81	0.44
1:A:28:VAL:N	1:A:29:GLU:CA	2.80	0.43
1:B:35:THR:CG2	1:B:36:TYR:CD2	3.00	0.43
1:B:90:ILE:HG21	1:B:92:LYS:CE	2.38	0.43
1:B:86:TYR:CZ	1:B:106:GLU:HA	2.53	0.43
1:A:238:PRO:HB2	1:B:189:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PRO:HB2	1:B:102:TRP:CZ3	2.53	0.43
1:B:35:THR:CG2	1:B:36:TYR:N	2.81	0.43
1:A:55:VAL:HA	1:A:101:LEU:O	2.18	0.43
1:A:66:ILE:HG23	1:A:101:LEU:HD22	2.00	0.43
1:A:237:HIS:CD2	1:A:239:MET:HB3	2.53	0.43
1:B:19:ARG:HD2	1:B:24:ILE:CD1	2.49	0.43
1:B:79:HIS:HD2	1:B:81:ASN:N	2.06	0.43
1:B:89:PHE:CE2	1:B:104:VAL:HG21	2.53	0.43
1:A:304:ASP:O	1:A:308:ARG:HG3	2.18	0.43
1:A:230:ALA:HB1	1:A:231:PRO:HD2	2.01	0.43
1:B:202:CYS:HB2	1:B:247:ARG:HH12	1.83	0.43
1:B:237:HIS:CE1	1:B:239:MET:HB3	2.53	0.43
1:A:82:ILE:HG22	1:A:83:ALA:O	2.19	0.42
1:A:90:ILE:HD13	1:A:92:LYS:HE2	2.01	0.42
1:A:202:CYS:O	1:A:205:ASN:C	2.62	0.42
1:A:71:ASN:HA	1:A:74:LYS:HD3	2.01	0.42
1:B:248:ASN:O	1:B:272:LYS:HE3	2.20	0.42
1:A:240:ARG:NH1	1:B:206:PRO:O	2.53	0.42
1:A:55:VAL:HG22	1:A:102:TRP:CD1	2.54	0.42
1:A:279:SER:OG	1:A:282:GLN:HB2	2.19	0.42
1:B:113:ILE:HD13	1:B:159:VAL:CG1	2.49	0.42
1:B:122:GLY:O	1:B:123:ASN:C	2.63	0.42
1:B:237:HIS:ND1	1:B:239:MET:HB3	2.35	0.42
1:A:172:PHE:CD1	1:A:172:PHE:C	2.98	0.42
1:A:237:HIS:HD2	1:A:239:MET:N	2.17	0.42
1:A:248:ASN:O	1:A:272:LYS:NZ	2.47	0.42
1:B:241:ALA:O	1:B:245:ILE:HG13	2.20	0.42
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.84	0.42
1:A:38:GLN:HG2	1:A:55:VAL:O	2.20	0.41
1:A:54:LYS:HB2	3:A:402:3C8:C3	2.50	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.50	0.41
1:A:150:ILE:HG22	1:A:152:ARG:CG	2.51	0.41
1:B:77:SER:HB2	1:B:84:THR:HA	2.02	0.41
1:B:81:ASN:ND2	1:B:139:ARG:HB3	2.35	0.41
1:B:85:TYR:OH	1:B:87:GLY:HA2	2.19	0.41
1:B:155:LYS:HB3	1:B:194:TRP:CG	2.56	0.41
1:A:88:ALA:HA	1:A:102:TRP:O	2.20	0.41
1:A:232:PRO:O	1:A:233:LEU:HB2	2.21	0.41
1:A:245:ILE:N	1:A:246:PRO:CD	2.83	0.41
1:A:69:GLU:O	1:A:72:MET:HB3	2.21	0.41
1:A:248:ASN:HB3	1:A:249:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD13	1:A:92:LYS:CE	2.50	0.41
1:B:30:VAL:N	1:B:40:TYR:CD1	2.89	0.41
1:A:135:ARG:HD3	1:A:292:GLN:NE2	2.36	0.40
1:B:302:LEU:O	1:B:306:ILE:HG13	2.22	0.40
1:A:38:GLN:HE21	1:A:55:VAL:CG1	2.31	0.40
1:B:81:ASN:HD22	1:B:139:ARG:HB3	1.87	0.40
1:A:269:CYS:O	1:A:277:ARG:HD3	2.22	0.40
1:B:31:VAL:CG2	1:B:39:VAL:O	2.66	0.40
1:B:132:TYR:HA	1:B:292:GLN:HE22	1.87	0.40
1:B:146:ILE:HD12	1:B:146:ILE:HA	1.74	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	278/332 (84%)	250 (90%)	21 (8%)	7 (2%)	4	7
1	B	258/332 (78%)	235 (91%)	20 (8%)	3 (1%)	10	20
All	All	536/664 (81%)	485 (90%)	41 (8%)	10 (2%)	6	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	63	GLU
1	A	80	ARG
1	A	97	HIS
1	B	173	GLY
1	B	308	ARG
1	A	95	PRO
1	A	208	ALA

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Mol	Chain	Res	Type
1	A	30	VAL
1	B	29	GLU

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	248/290 (86%)	221 (89%)	27 (11%)	6	13
1	B	233/290 (80%)	213 (91%)	20 (9%)	10	21
All	All	481/580 (83%)	434 (90%)	47 (10%)	7	16

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	29	GLU
1	A	33	ASN
1	A	35	THR
1	A	46	LYS
1	A	49	GLN
1	A	59	THR
1	A	60	GLU
1	A	62	GLU
1	A	68	LEU
1	A	72	MET
1	A	74	LYS
1	A	97	HIS
1	A	103	LEU
1	A	118	LYS
1	A	124	THR
1	A	126	LYS
1	A	157	GLN
1	A	191	THR
1	A	199	VAL
1	A	204	GLU

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Mol	Chain	Res	Type
1	A	213	ARG
1	A	281	GLU
1	A	282	GLN
1	A	291	ASP
1	A	296	ARG
1	A	310	ARG
1	B	24	ILE
1	B	31	VAL
1	B	35	THR
1	B	49	GLN
1	B	58	VAL
1	B	90	ILE
1	B	103	LEU
1	B	146	ILE
1	B	163	GLU
1	B	174	VAL
1	B	203	ASP
1	B	204	GLU
1	B	209	THR
1	B	240	ARG
1	B	260	LYS
1	B	280	THR
1	B	302	LEU
1	B	304	ASP
1	B	308	ARG
1	B	310	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	71	ASN
1	A	81	ASN
1	A	123	ASN
1	A	143	HIS
1	A	157	GLN
1	A	237	HIS
1	A	276	GLN
1	A	294	ASN
1	B	33	ASN
1	B	44	HIS
1	B	79	HIS

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Mol	Chain	Res	Type
1	B	81	ASN
1	B	143	HIS
1	B	292	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MES	A	401	-	12,12,12	1.35	2 (16%)	15,16,16	1.53	3 (20%)
3	3C8	B	401	-	26,26,26	0.89	1 (3%)	31,37,37	2.56	13 (41%)
3	3C8	A	402	-	26,26,26	0.85	1 (3%)	31,37,37	2.62	12 (38%)

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	MES	A	401	-	-	4/6/14/14	0/1/1/1
3	3C8	B	401	-	-	4/8/18/18	0/4/4/4
3	3C8	A	402	-	-	4/8/18/18	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	MES	C8-S	-2.51	1.74	1.77
3	A	402	3C8	N4-N6	2.18	1.40	1.36
2	A	401	MES	O2S-S	2.07	1.51	1.45
3	B	401	3C8	N4-N6	2.01	1.40	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	3C8	C3-C2-C7	5.25	107.75	104.92
3	B	401	3C8	C3-C2-C7	5.16	107.70	104.92
3	B	401	3C8	C22-N23-C17	5.16	121.30	115.43
3	A	402	3C8	C13-N12-C14	-5.00	107.08	120.41
3	A	402	3C8	C11-N12-C14	-4.89	107.39	120.41
3	B	401	3C8	N23-C22-N21	-4.70	122.29	128.67
3	B	401	3C8	C14-N19-C18	4.51	121.49	117.89
3	A	402	3C8	C22-N23-C17	4.32	120.34	115.43
3	A	402	3C8	C14-N19-C18	4.29	121.31	117.89
3	A	402	3C8	N23-C22-N21	-4.20	122.98	128.67
3	B	401	3C8	C10-C9-C8	-3.92	104.08	111.24
3	A	402	3C8	C10-C9-C8	-3.90	104.12	111.24
3	B	401	3C8	C11-N12-C14	-3.89	110.06	120.41
2	A	401	MES	C5-N4-C3	3.77	116.96	108.84
3	A	402	3C8	C9-C10-C11	-3.52	106.13	110.75
3	B	401	3C8	C13-N12-C14	-3.41	111.33	120.41
3	A	402	3C8	C3-N4-N6	-3.23	107.64	112.59
3	B	401	3C8	N19-C14-N12	2.96	120.08	117.49
3	B	401	3C8	C3-N4-N6	-2.93	108.10	112.59
3	B	401	3C8	C20-C18-N19	2.83	122.50	120.33
3	A	402	3C8	C16-C17-N23	2.56	122.67	118.55
3	A	402	3C8	N19-C14-N12	2.46	119.64	117.49
3	B	401	3C8	C16-C17-N23	2.41	122.44	118.55
2	A	401	MES	C6-C5-N4	2.32	113.64	110.12
3	B	401	3C8	C10-C11-N12	2.21	115.24	111.06
3	A	402	3C8	C20-C18-N19	2.11	121.95	120.33
2	A	401	MES	C7-N4-C3	2.10	116.83	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	3C8	C15-C16-C17	-2.09	118.30	120.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

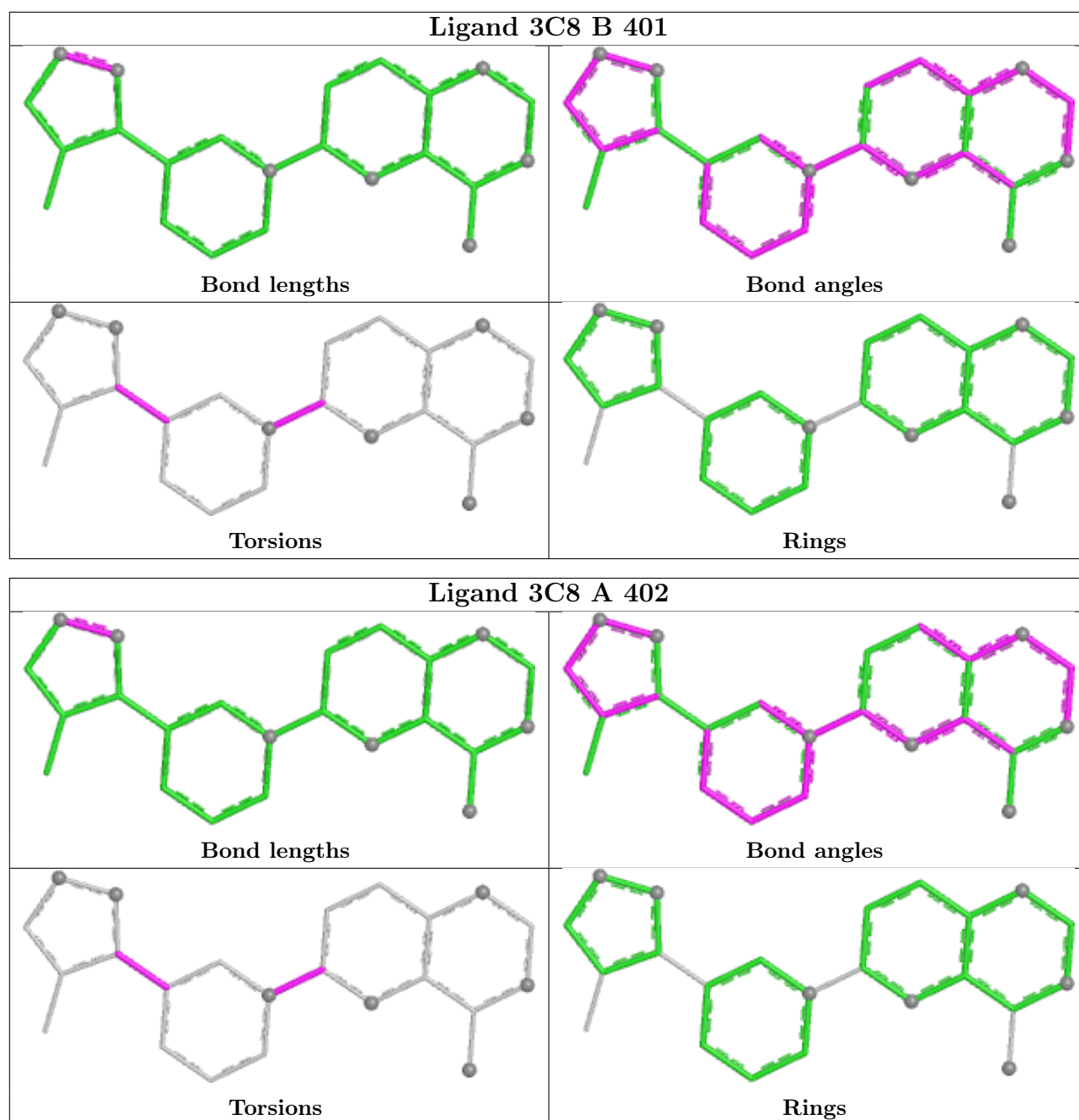
Mol	Chain	Res	Type	Atoms
3	A	402	3C8	C15-C14-N12-C13
3	A	402	3C8	N6-C7-C8-C13
3	B	401	3C8	N6-C7-C8-C13
2	A	401	MES	C8-C7-N4-C3
3	A	402	3C8	N19-C14-N12-C13
2	A	401	MES	C7-C8-S-O3S
2	A	401	MES	C7-C8-S-O1S
2	A	401	MES	C7-C8-S-O2S
3	A	402	3C8	C2-C7-C8-C13
3	B	401	3C8	C2-C7-C8-C13
3	B	401	3C8	C15-C14-N12-C13
3	B	401	3C8	N19-C14-N12-C13

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	3C8	2	0
3	A	402	3C8	7	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	282/332 (84%)	0.27	5 (1%) 67 64	39, 63, 98, 130	0
1	B	265/332 (79%)	0.29	9 (3%) 48 43	23, 63, 102, 132	1 (0%)
All	All	547/664 (82%)	0.28	14 (2%) 57 52	23, 63, 101, 132	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	PRO	4.0
1	B	188	PHE	3.0
1	B	174	VAL	3.0
1	B	209	THR	2.5
1	A	17	SER	2.3
1	B	23	GLY	2.3
1	B	24	ILE	2.2
1	B	26	GLU	2.2
1	A	68	LEU	2.2
1	A	235	ASP	2.2
1	A	167	VAL	2.1
1	A	16	SER	2.1
1	B	210	TYR	2.0
1	B	75	LYS	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](#)

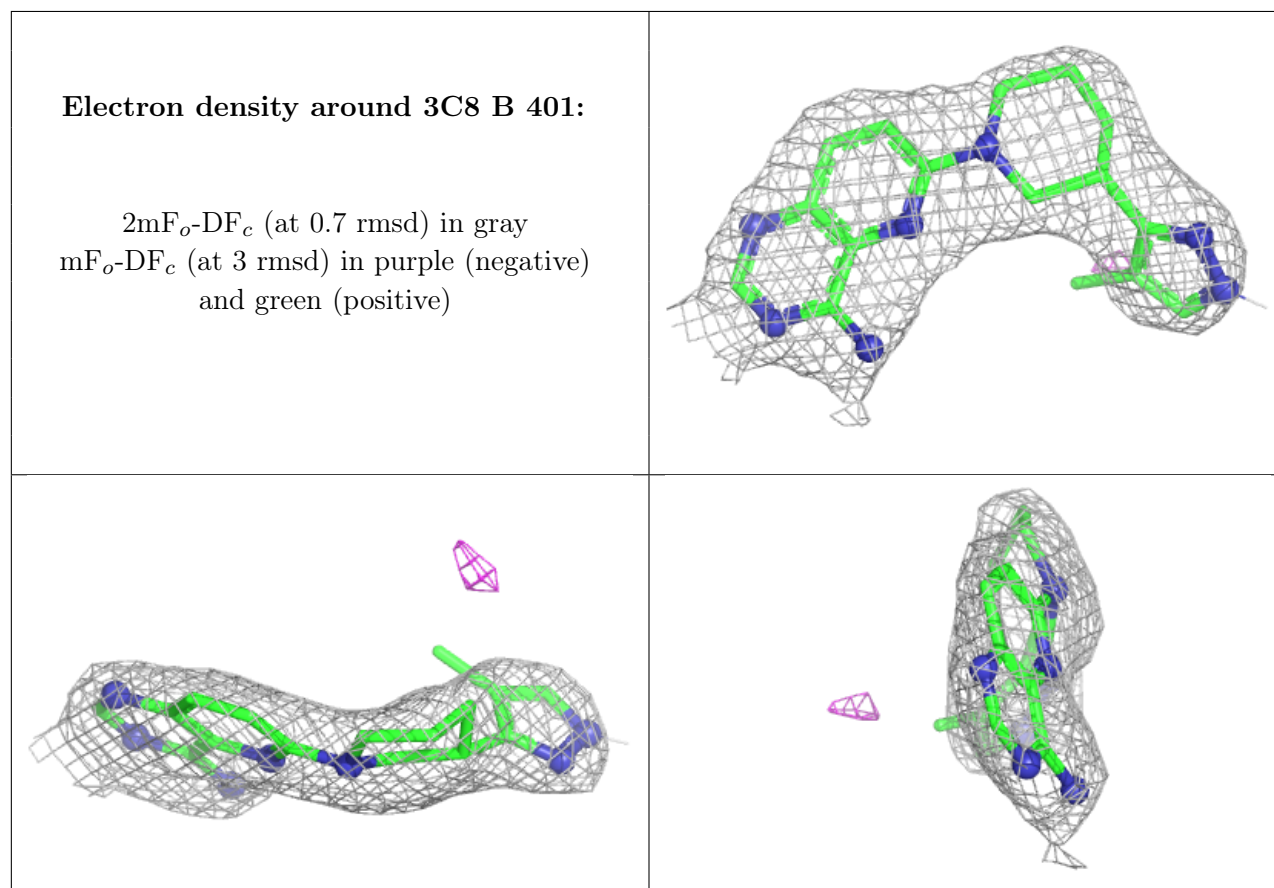
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

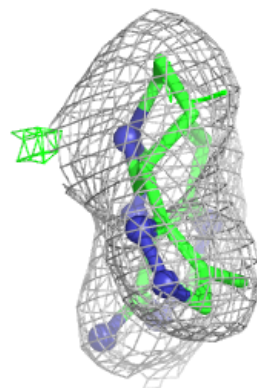
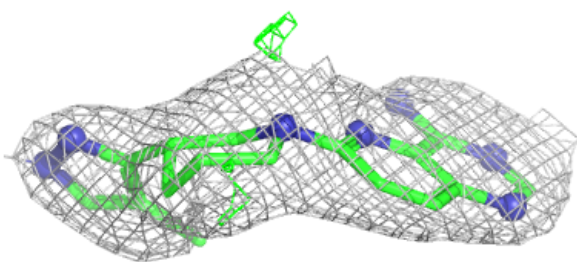
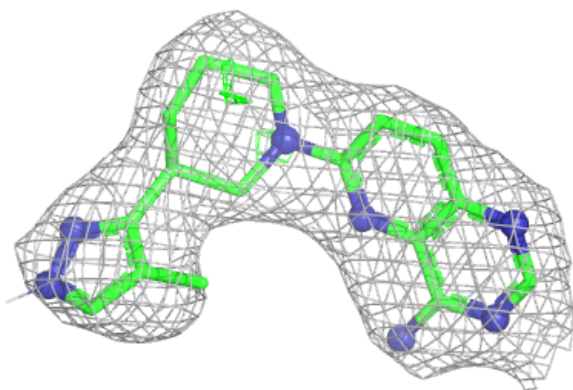
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	403	1/1	0.86	0.12	79,79,79,79	0
3	3C8	B	401	23/23	0.89	0.11	63,69,76,92	0
3	3C8	A	402	23/23	0.92	0.12	58,67,78,93	0
4	MG	B	402	1/1	0.93	0.13	65,65,65,65	0
2	MES	A	401	12/12	0.95	0.08	58,61,70,71	0

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 3C8 A 402:

$2mF_o-DF_c$ (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.