WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 01:59 PM EDT

PDB ID	:	3HV4
Title	:	Human p38 MAP Kinase in Complex with RL51
Authors	:	Gruetter, C.; Simard, J.R.; Getlik, M.; Rauh, D.
Deposited on	:	2009-06-15
Resolution	:	2.60 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
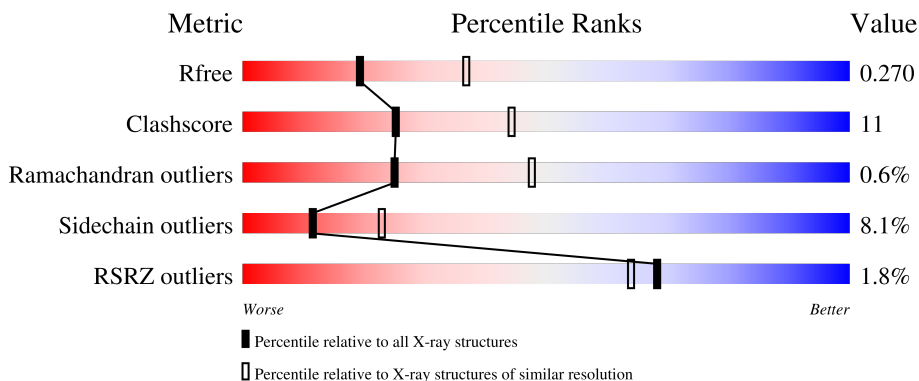
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	2% 74% 17% · 6%
1	B	360	.% 70% 20% · 6%

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5737 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.
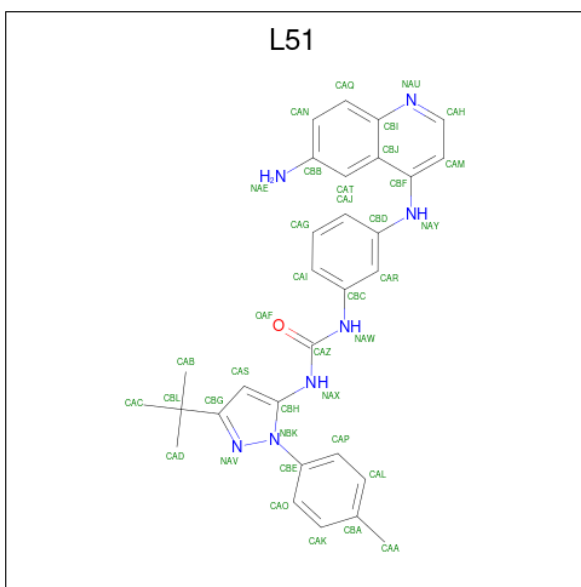
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2721	1746	464	499	12			
1	B	338	Total	C	N	O	S	0	0	0
			2711	1740	461	498	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q16539
B	1	GLY	-	expression tag	UNP Q16539

- Molecule 2 is 1-{3-[(6-aminoquinolin-4-yl)amino]phenyl}-3-[3-tert-butyl-1-(4-methylphenyl)-1H-pyrazol-5-yl]urea (three-letter code: L51) (formula: $C_{30}H_{31}N_7O$).
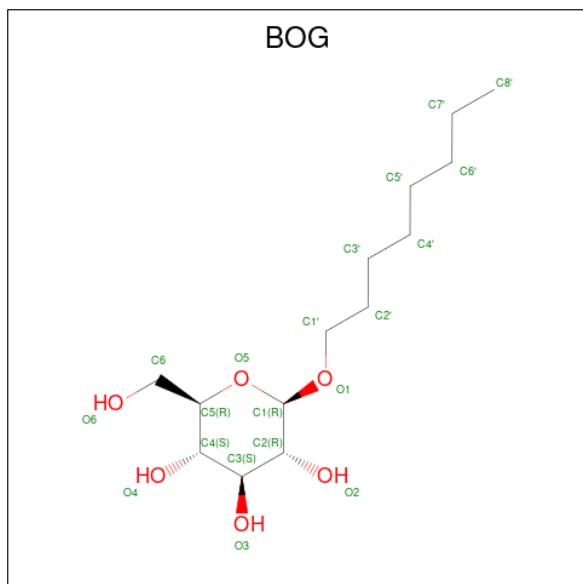

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	30	7	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total C N O				0	0
			38	30	7	1		

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C O			0	0
			20	14	6		
3	A	1	Total C O			0	0
			20	14	6		
3	B	1	Total C O			0	0
			20	14	6		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	70	Total 70	O 70	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: Mitogen-activated protein kinase 14

Chain A:

• Molecule 1: Mitogen-activated protein kinase 14

Chain B:
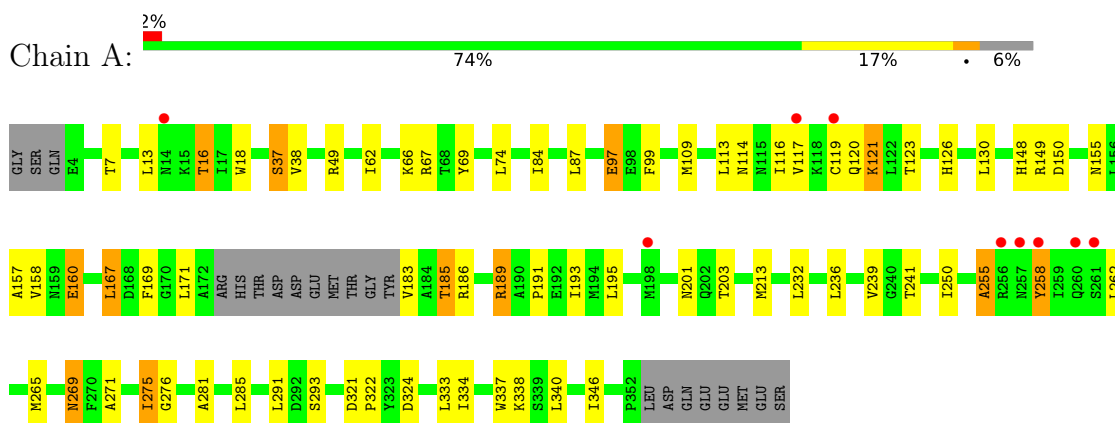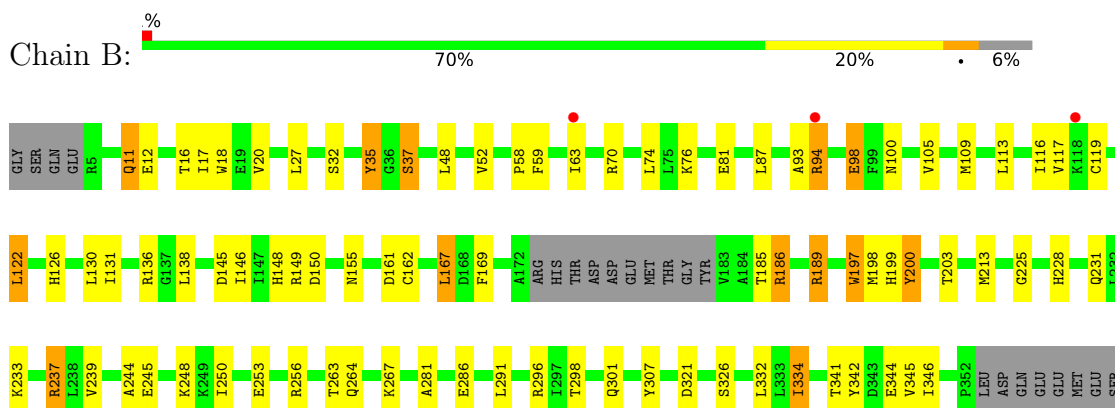
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.64Å 74.06Å 72.00Å 90.00° 93.90° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 42.62 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.60) 99.5 (42.62-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.271 0.200 , 0.270	Depositor DCC
R_{free} test set	915 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5737	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: L51, BOG, MES

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	0.68	0/2784	0.76	2/3783 (0.1%)
1	B	0.68	0/2773	0.76	0/3768
All	All	0.68	0/5557	0.76	2/7551 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	324	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2721	0	2710	63	0
1	B	2711	0	2703	57	0
2	A	38	0	31	3	0
2	B	38	0	31	0	0
3	A	40	0	56	3	0
3	B	20	0	28	1	0
4	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	87	0	0	6	0
5	B	70	0	0	1	0
All	All	5737	0	5571	119	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 11.

All (119) 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:84:ILE:HD13	1:A:109:MET:HE2	1.48	0.96
1:A:123:THR:HG23	1:A:126:HIS:HB2	1.55	0.88
1:A:84:ILE:HD13	1:A:109:MET:CE	2.03	0.87
1:A:148:HIS:HD2	1:A:150:ASP:H	1.23	0.86
1:A:275:ILE:HA	5:A:400:HOH:O	1.75	0.84
1:A:109:MET:HB3	1:A:157:ALA:HB1	1.57	0.84
1:A:123:THR:CG2	1:A:126:HIS:HB2	2.14	0.77
1:B:148:HIS:HD2	1:B:150:ASP:H	1.30	0.76
1:A:84:ILE:CD1	1:A:109:MET:CE	2.63	0.75
1:B:267:LYS:NZ	1:B:286:GLU:HG2	2.02	0.75
1:B:155:ASN:ND2	1:B:169:PHE:H	1.84	0.75
1:A:74:LEU:HD23	2:A:361:L51:HAO	1.67	0.74
1:A:155:ASN:ND2	1:A:169:PHE:H	1.86	0.73
1:B:239:VAL:HG21	1:B:291:LEU:HD13	1.74	0.68
1:A:84:ILE:CD1	1:A:109:MET:HE2	2.23	0.67
1:B:74:LEU:HD13	1:B:146:ILE:HD11	1.76	0.67
1:B:150:ASP:OD2	1:B:185:THR:HG23	1.93	0.67
1:A:67:ARG:HD3	5:A:436:HOH:O	1.95	0.65
1:B:239:VAL:CG2	1:B:291:LEU:HD13	2.27	0.64
1:A:123:THR:HG23	1:A:126:HIS:CB	2.26	0.64
1:B:161:ASP:O	1:B:162:CYS:HB2	1.99	0.63
1:B:122:LEU:HD22	1:B:122:LEU:H	1.64	0.62
1:A:239:VAL:HG21	1:A:291:LEU:HD13	1.81	0.61
1:B:186:ARG:NH1	1:B:225:GLY:O	2.32	0.61
1:A:113:LEU:O	1:A:117:VAL:HG23	2.01	0.61
1:A:269:ASN:ND2	1:A:271:ALA:HB3	2.18	0.59
1:B:20:VAL:HG21	1:B:27:LEU:HD21	1.85	0.58
1:A:195:LEU:HD11	1:A:232:LEU:HD11	1.86	0.58
1:A:148:HIS:HE1	1:A:167:LEU:O	1.86	0.58
1:A:113:LEU:HD11	1:A:130:LEU:HD13	1.85	0.58
1:B:52:VAL:HG22	1:B:105:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:HA	1:A:258:TYR:CE1	2.39	0.56
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.05	0.56
1:A:84:ILE:CD1	1:A:109:MET:HE1	2.35	0.56
1:B:341:THR:O	1:B:345:VAL:HG23	2.05	0.55
1:B:74:LEU:HD13	1:B:146:ILE:CD1	2.36	0.55
1:A:155:ASN:HD22	1:A:169:PHE:H	1.52	0.55
1:A:109:MET:HG2	2:A:361:L51:HAH	1.88	0.54
1:A:232:LEU:HD22	3:A:1000:BOG:H8'2	1.89	0.54
1:A:13:LEU:O	1:A:16:THR:HG23	2.08	0.54
1:B:155:ASN:ND2	1:B:169:PHE:N	2.55	0.54
1:B:267:LYS:HZ3	1:B:286:GLU:HG2	1.72	0.54
1:B:342:TYR:CE2	1:B:346:ILE:HD11	2.44	0.53
1:B:131:ILE:HG13	1:B:213:MET:HG3	1.89	0.53
1:B:245:GLU:O	1:B:248:LYS:HG2	2.09	0.53
1:B:267:LYS:HZ1	1:B:286:GLU:HG2	1.72	0.53
1:A:201:ASN:HB2	5:A:445:HOH:O	2.08	0.52
1:B:113:LEU:O	1:B:117:VAL:HG23	2.09	0.52
1:A:213:MET:HE2	1:A:281:ALA:HB1	1.91	0.52
1:B:11:GLN:HE21	1:B:12:GLU:H	1.58	0.51
1:B:228:HIS:O	1:B:231:GLN:HB3	2.10	0.51
1:B:281:ALA:HB2	1:B:307:TYR:CE1	2.46	0.51
1:A:185:THR:HG21	1:A:189:ARG:HH21	1.77	0.50
1:B:94:ARG:H	1:B:94:ARG:HH11	1.60	0.50
1:B:233:LYS:HE2	1:B:237:ARG:NH2	2.27	0.49
1:B:126:HIS:NE2	1:B:162:CYS:SG	2.81	0.49
1:A:99:PHE:O	1:A:338:LYS:HE3	2.12	0.49
1:B:93:ALA:HB2	1:B:98:GLU:O	2.12	0.49
1:A:18:TRP:HZ2	1:A:37:SER:HB2	1.78	0.49
1:A:148:HIS:O	1:A:149:ARG:HB2	2.13	0.49
1:A:49:ARG:HD2	5:A:434:HOH:O	2.13	0.48
1:B:155:ASN:HD21	1:B:169:PHE:N	2.10	0.48
1:A:123:THR:HG23	1:A:126:HIS:H	1.78	0.48
1:A:185:THR:CG2	1:A:189:ARG:HH21	2.27	0.48
1:A:62:ILE:HG13	1:A:334:ILE:HG13	1.95	0.48
1:A:189:ARG:HG2	1:A:193:ILE:HB	1.96	0.48
1:B:321:ASP:OD1	1:B:321:ASP:C	2.52	0.48
1:B:59:PHE:HB3	1:B:334:ILE:HD13	1.95	0.47
1:B:74:LEU:CD1	1:B:146:ILE:CD1	2.92	0.47
1:A:191:PRO:HB2	3:A:1000:BOG:H4'1	1.97	0.47
1:B:59:PHE:HB3	1:B:334:ILE:CD1	2.45	0.47
1:B:148:HIS:HD2	1:B:150:ASP:N	2.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:HIS:O	1:B:200:TYR:HB3	2.15	0.47
1:A:239:VAL:CG2	1:A:291:LEU:HD13	2.45	0.47
1:B:74:LEU:HD11	1:B:146:ILE:HD13	1.98	0.46
1:A:185:THR:CG2	1:A:189:ARG:HE	2.28	0.46
1:A:189:ARG:HH11	1:A:193:ILE:HG21	1.81	0.46
1:B:148:HIS:O	1:B:149:ARG:HB2	2.14	0.46
1:A:155:ASN:ND2	1:A:169:PHE:N	2.62	0.45
1:B:155:ASN:HD22	1:B:169:PHE:H	1.63	0.45
1:A:38:VAL:HG23	1:A:171:LEU:HD11	1.98	0.45
1:B:150:ASP:OD2	1:B:185:THR:CG2	2.64	0.45
1:A:160:GLU:HG2	1:B:63:ILE:HD12	1.97	0.45
1:A:121:LYS:HE2	1:A:121:LYS:HB2	1.83	0.45
1:A:157:ALA:HB2	1:A:167:LEU:HD21	1.99	0.44
1:B:18:TRP:HZ2	1:B:37:SER:HB2	1.82	0.44
1:B:74:LEU:CD1	1:B:146:ILE:HD13	2.48	0.44
1:B:326:SER:O	1:B:326:SER:OG	2.32	0.44
1:A:84:ILE:HD12	1:A:109:MET:HE1	2.00	0.44
1:A:195:LEU:CD1	1:A:232:LEU:HD11	2.46	0.44
1:A:232:LEU:O	1:A:236:LEU:HG	2.18	0.43
1:B:81:GLU:HB2	1:B:136:ARG:HH12	1.83	0.43
1:A:97:GLU:H	1:A:97:GLU:CD	2.21	0.43
1:A:148:HIS:CD2	1:A:150:ASP:H	2.15	0.43
1:B:149:ARG:O	1:B:189:ARG:NH2	2.46	0.43
1:B:197:TRP:CZ3	3:B:362:BOG:H3'2	2.53	0.43
1:B:70:ARG:HD2	5:B:400:HOH:O	2.18	0.43
1:B:76:LYS:NZ	1:B:344:GLU:OE1	2.43	0.43
1:A:148:HIS:HD2	1:A:150:ASP:N	2.03	0.43
1:A:276:GLY:N	5:A:400:HOH:O	2.48	0.43
1:A:321:ASP:O	1:A:322:PRO:C	2.57	0.43
1:B:148:HIS:HE1	1:B:167:LEU:O	2.02	0.43
1:A:69:TYR:CE2	1:A:340:LEU:HB3	2.54	0.42
1:B:148:HIS:CD2	1:B:150:ASP:H	2.21	0.42
1:A:291:LEU:HG	3:A:1000:BOG:H3'1	2.00	0.42
1:A:67:ARG:CD	5:A:436:HOH:O	2.59	0.42
1:B:342:TYR:CZ	1:B:346:ILE:HD11	2.54	0.42
1:B:58:PRO:HG2	1:B:100:ASN:O	2.20	0.42
1:A:109:MET:HG2	2:A:361:L51:CAH	2.49	0.42
1:A:183:VAL:HG12	1:A:183:VAL:O	2.20	0.41
1:B:59:PHE:O	1:B:334:ILE:HD13	2.21	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.95	0.41
1:B:250:ILE:HG22	1:B:256:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:HG23	1:A:265:MET:HB2	2.03	0.41
1:A:346:ILE:HD13	1:A:346:ILE:HA	1.79	0.41
1:A:203:THR:OG1	1:A:293:SER:HB2	2.20	0.40
1:B:203:THR:HB	1:B:296:ARG:HD2	2.02	0.40
1:A:66:LYS:HG3	1:A:337:TRP:CZ2	2.56	0.40
1:B:35:TYR:CD2	1:B:35:TYR:N	2.89	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	335/360 (93%)	316 (94%)	17 (5%)	2 (1%)	25	47
1	B	334/360 (93%)	309 (92%)	23 (7%)	2 (1%)	25	47
All	All	669/720 (93%)	625 (93%)	40 (6%)	4 (1%)	25	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ALA
1	B	244	ALA
1	B	186	ARG
1	A	116	ILE

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	297/319 (93%)	277 (93%)	20 (7%)	16	33
1	B	296/319 (93%)	268 (90%)	28 (10%)	8	16
All	All	593/638 (93%)	545 (92%)	48 (8%)	11	23

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	16	THR
1	A	37	SER
1	A	87	LEU
1	A	97	GLU
1	A	114	ASN
1	A	119	CYS
1	A	120	GLN
1	A	121	LYS
1	A	158	VAL
1	A	160	GLU
1	A	167	LEU
1	A	185	THR
1	A	186	ARG
1	A	189	ARG
1	A	250	ILE
1	A	258	TYR
1	A	269	ASN
1	A	275	ILE
1	A	333	LEU
1	B	11	GLN
1	B	16	THR
1	B	17	ILE
1	B	32	SER
1	B	35	TYR
1	B	37	SER
1	B	48	LEU
1	B	87	LEU
1	B	94	ARG
1	B	98	GLU
1	B	109	MET
1	B	116	ILE
1	B	119	CYS
1	B	122	LEU

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	138	LEU
1	B	145	ASP
1	B	167	LEU
1	B	189	ARG
1	B	197	TRP
1	B	198	MET
1	B	200	TYR
1	B	237	ARG
1	B	253	GLU
1	B	263	THR
1	B	264	GLN
1	B	332	LEU
1	B	334	ILE

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	14	ASN
1	A	100	ASN
1	A	107	HIS
1	A	114	ASN
1	A	148	HIS
1	A	155	ASN
1	A	196	ASN
1	A	257	ASN
1	A	269	ASN
1	B	11	GLN
1	B	100	ASN
1	B	148	HIS
1	B	155	ASN
1	B	257	ASN
1	B	269	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	#$|Z| > 2$
4	MES	A	362	-	12,12,12	2.10	1 (8%)	14,16,16	2.57	9 (64%)
3	BOG	A	363	-	20,20,20	1.38	2 (10%)	25,25,25	1.91	8 (32%)
2	L51	A	361	-	39,42,42	1.40	6 (15%)	51,61,61	1.35	9 (17%)
3	BOG	A	1000	-	20,20,20	1.05	1 (5%)	25,25,25	1.15	3 (12%)
2	L51	B	361	-	39,42,42	1.41	6 (15%)	51,61,61	1.39	6 (11%)
3	BOG	B	362	-	20,20,20	0.67	0	25,25,25	1.44	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	362	-	-	1/6/14/14	0/1/1/1
3	BOG	A	363	-	-	6/11/31/31	0/1/1/1
2	L51	A	361	-	-	3/16/22/22	0/5/5/5
3	BOG	A	1000	-	-	8/11/31/31	0/1/1/1
2	L51	B	361	-	-	2/16/22/22	0/5/5/5
3	BOG	B	362	-	-	3/11/31/31	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	362	MES	C8-S	-6.78	1.67	1.77
2	B	361	L51	CAS-CBG	-4.57	1.33	1.39
3	A	363	BOG	O1-C1	4.35	1.47	1.40
2	A	361	L51	CAS-CBG	-4.23	1.33	1.39
2	A	361	L51	CBC-NAW	-3.43	1.34	1.41
3	A	1000	BOG	O1-C1	3.36	1.45	1.40
2	B	361	L51	CBC-NAW	-2.84	1.35	1.41
2	B	361	L51	CBH-NAX	-2.68	1.34	1.39
2	B	361	L51	CAQ-CAN	2.53	1.41	1.36
2	B	361	L51	CAP-CAL	2.40	1.41	1.36
2	A	361	L51	CAR-CBD	2.25	1.43	1.39
2	A	361	L51	CAZ-NAW	-2.22	1.32	1.37
2	A	361	L51	CBD-NAY	-2.16	1.36	1.40
2	B	361	L51	CBD-NAY	-2.14	1.36	1.40
3	A	363	BOG	O5-C1	2.12	1.47	1.41
2	A	361	L51	CAO-CAK	2.05	1.40	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	362	MES	C5-N4-C3	5.89	122.09	108.83
3	A	363	BOG	O5-C5-C4	4.74	118.30	109.69
3	A	363	BOG	O1-C1-C2	4.67	115.59	108.30
3	B	362	BOG	C1'-O1-C1	-4.51	106.35	113.84
3	B	362	BOG	O1-C1-C2	3.83	114.29	108.30
2	A	361	L51	CAL-CAP-CBE	-3.36	118.98	121.79
4	A	362	MES	C6-C5-N4	-3.31	105.08	110.10
2	A	361	L51	CBL-CBG-NAV	3.16	123.99	120.59
4	A	362	MES	C7-N4-C3	3.12	119.21	111.23
2	B	361	L51	CAH-NAU-CBI	3.11	121.75	116.93
2	A	361	L51	CAH-NAU-CBI	3.05	121.64	116.93
3	A	363	BOG	C4-C3-C2	2.96	115.99	110.82
2	B	361	L51	CBD-NAY-CBF	2.92	133.96	126.71
4	A	362	MES	C7-N4-C5	2.92	118.69	111.23
3	A	363	BOG	C1-O5-C5	2.81	119.20	113.69
3	A	1000	BOG	C1'-O1-C1	-2.80	109.20	113.84
2	A	361	L51	CAS-CBG-CBL	-2.72	125.52	129.07
3	A	363	BOG	C1-C2-C3	2.72	115.67	110.00
2	B	361	L51	CAC-CBL-CBG	2.68	115.02	109.76
4	A	362	MES	O1S-S-C8	2.63	110.08	106.92
2	B	361	L51	CAM-CAH-NAU	-2.59	120.57	124.58
2	B	361	L51	CBJ-CBI-NAU	-2.54	120.13	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	361	L51	CAO-CBE-CAP	2.43	119.91	116.27
2	A	361	L51	CAO-CAK-CBA	-2.34	117.41	121.64
3	A	363	BOG	C3-C4-C5	2.29	114.32	110.24
4	A	362	MES	C6-O1-C2	2.28	117.52	109.89
2	A	361	L51	CAM-CAH-NAU	-2.24	121.11	124.58
4	A	362	MES	C2-C3-N4	-2.24	106.71	110.10
2	B	361	L51	CAB-CBL-CBG	-2.19	105.45	109.76
2	A	361	L51	CBJ-CBI-NAU	-2.19	120.50	122.83
3	A	1000	BOG	C3-C4-C5	2.18	114.13	110.24
3	A	1000	BOG	O1-C1-C2	2.17	111.69	108.30
2	A	361	L51	CAG-CAI-CBC	2.13	122.28	119.72
4	A	362	MES	O2S-S-C8	2.12	109.46	106.92
3	A	363	BOG	C6-C5-C4	-2.11	108.06	113.00
3	A	363	BOG	C1'-O1-C1	-2.05	110.45	113.84
4	A	362	MES	O2S-S-O1S	-2.01	107.01	113.95

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	363	BOG	C2'-C1'-O1-C1
3	B	362	BOG	C2'-C1'-O1-C1
3	A	1000	BOG	C4-C5-C6-O6
3	A	363	BOG	O5-C5-C6-O6
3	A	1000	BOG	O5-C5-C6-O6
3	A	1000	BOG	O1-C1'-C2'-C3'
3	A	1000	BOG	C1'-C2'-C3'-C4'
3	A	1000	BOG	C2'-C3'-C4'-C5'
3	A	1000	BOG	C3'-C4'-C5'-C6'
3	A	363	BOG	C4-C5-C6-O6
3	A	1000	BOG	C5'-C6'-C7'-C8'
3	A	1000	BOG	C2'-C1'-O1-C1
4	A	362	MES	C8-C7-N4-C3
3	B	362	BOG	C5'-C6'-C7'-C8'
3	B	362	BOG	C4'-C5'-C6'-C7'
3	A	363	BOG	C5'-C6'-C7'-C8'
3	A	363	BOG	C2'-C3'-C4'-C5'
3	A	363	BOG	C4'-C5'-C6'-C7'
2	A	361	L51	CAI-CBC-NAW-CAZ
2	A	361	L51	CAR-CBD-NAY-CBF
2	A	361	L51	CAR-CBC-NAW-CAZ
2	B	361	L51	CAR-CBC-NAW-CAZ

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Mol	Chain	Res	Type	Atoms
2	B	361	L51	CAI-CBC-NAW-CAZ

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	L51	3	0
3	A	1000	BOG	3	0
3	B	362	BOG	1	0

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

Ligand BOG A 363

Bond lengths

Bond angles

Torsions

Rings

Ligand L51 A 361

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG A 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand L51 B 361

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG B 362

Bond lengths

Bond angles

Torsions

Rings
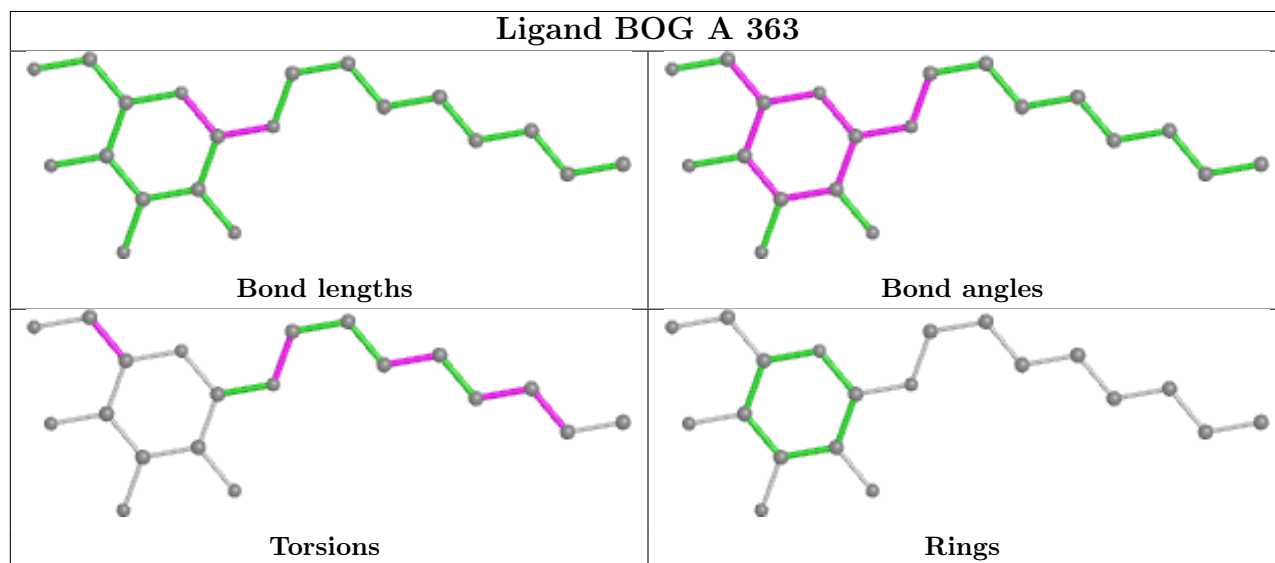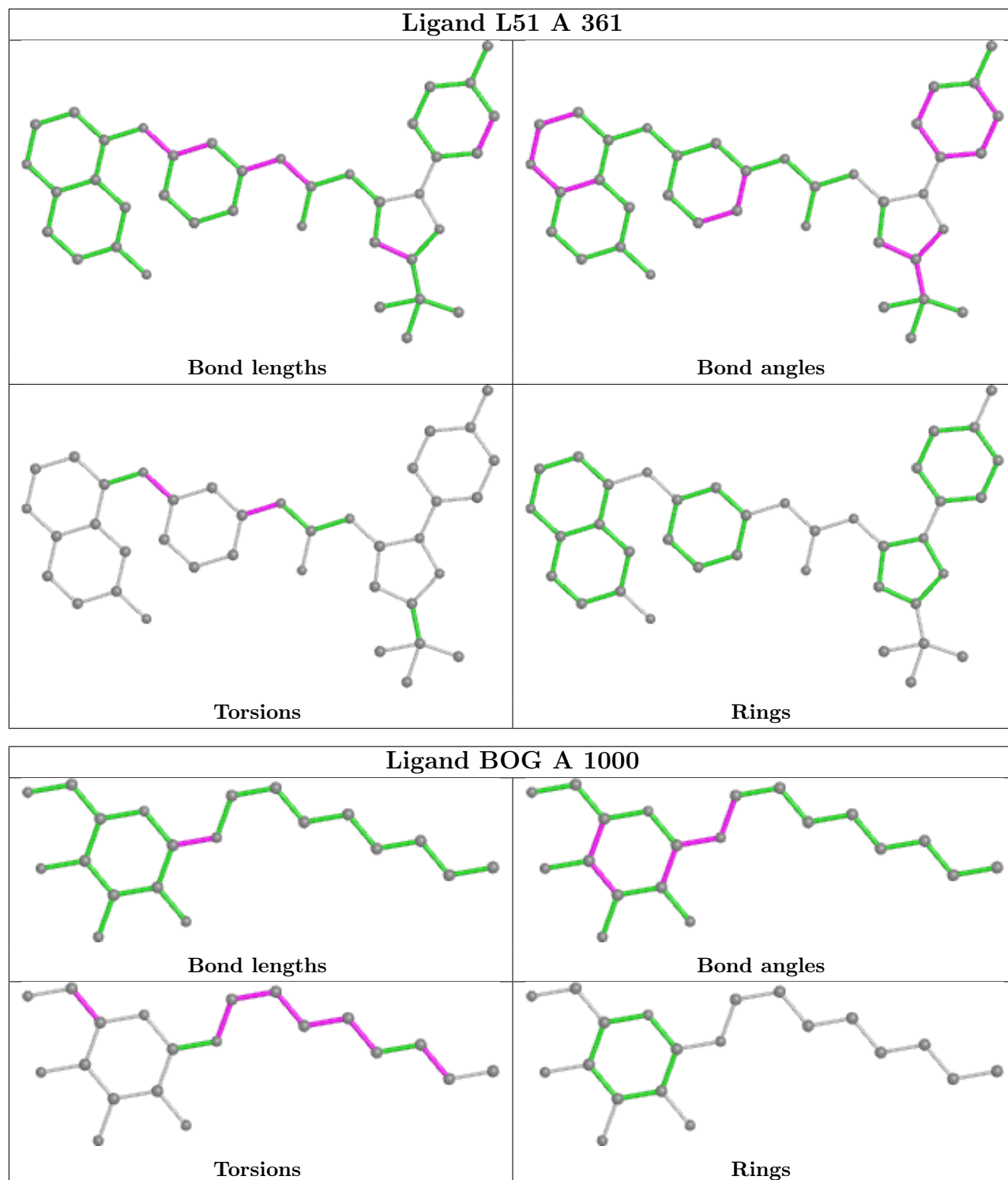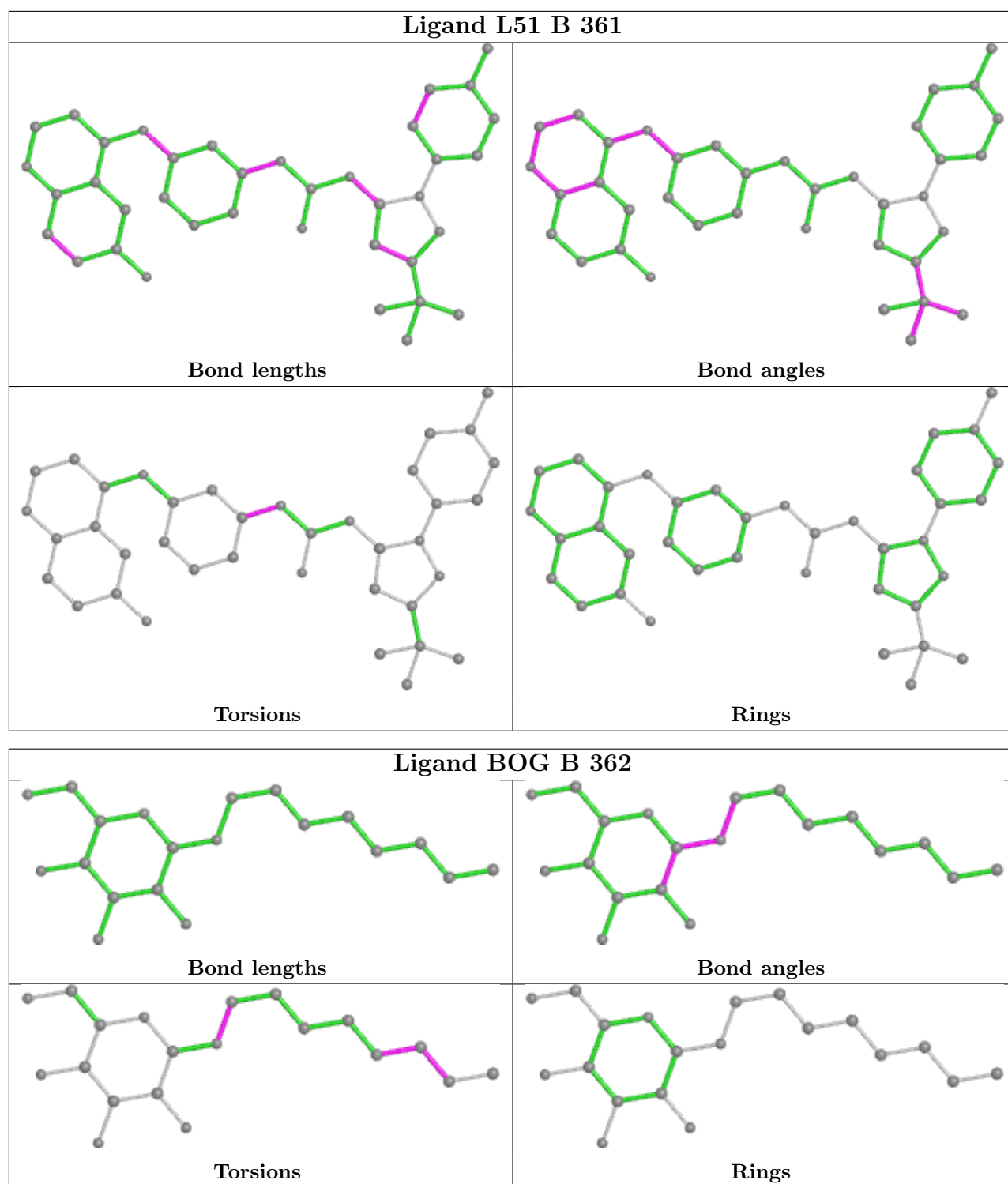
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	339/360 (94%)	-0.24	9 (2%) 54	48	2, 13, 52, 75	1 (0%)
1	B	338/360 (93%)	-0.19	3 (0%) 84	82	2, 15, 45, 56	1 (0%)
All	All	677/720 (94%)	-0.21	12 (1%) 68	64	2, 13, 48, 75	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ASN	4.0
1	A	119	CYS	3.7
1	A	260	GLN	3.0
1	B	118	LYS	2.9
1	A	198	MET	2.8
1	A	261	SER	2.7
1	A	258	TYR	2.5
1	B	94	ARG	2.4
1	A	256	ARG	2.3
1	A	14	ASN	2.1
1	A	117	VAL	2.1
1	B	63	ILE	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides 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
3	BOG	A	363	20/20	0.74	0.31	50,59,62,62	0
4	MES	A	362	12/12	0.84	0.27	48,50,51,51	0
3	BOG	A	1000	20/20	0.92	0.20	27,38,41,42	0
3	BOG	B	362	20/20	0.95	0.17	8,14,19,20	0
2	L51	B	361	38/38	0.95	0.16	2,6,21,21	0
2	L51	A	361	38/38	0.96	0.15	2,3,16,17	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 BOG A 363:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
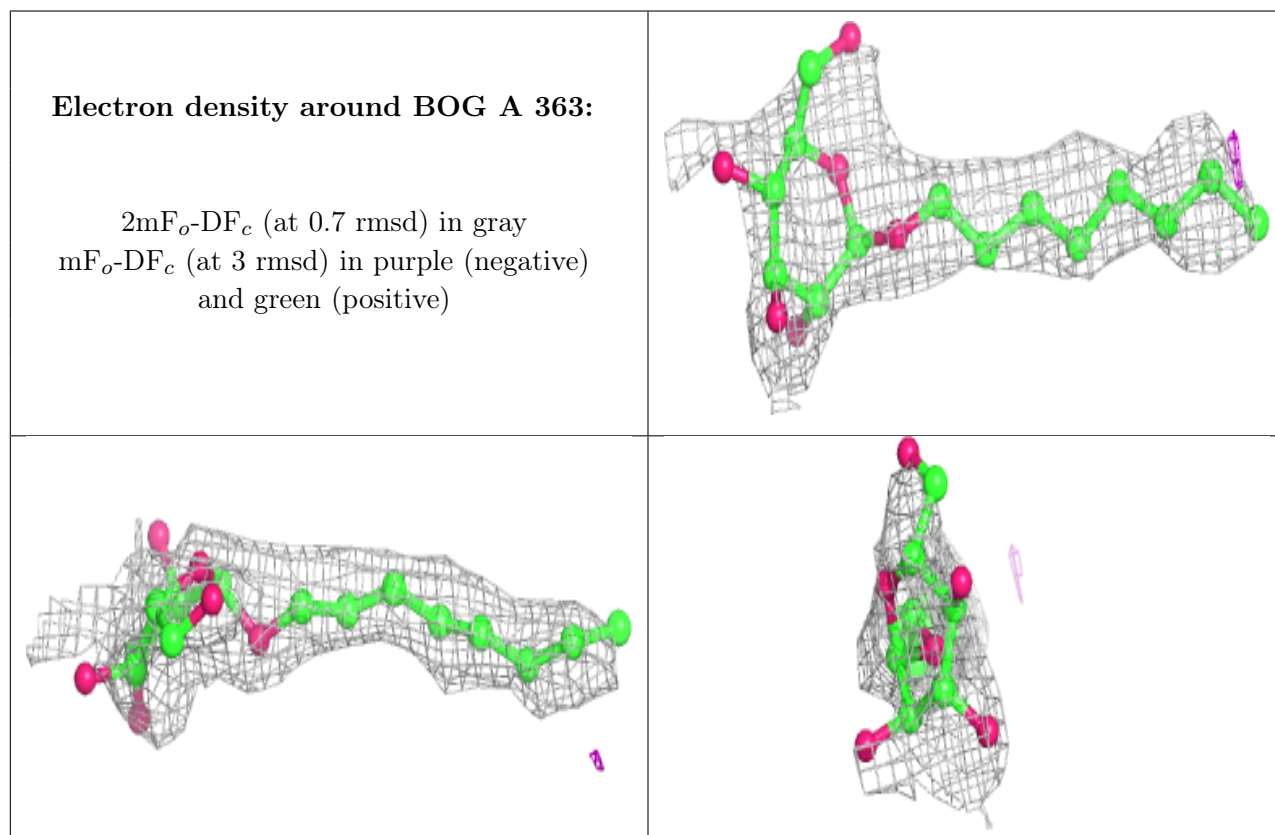
Electron density around BOG A 1000:

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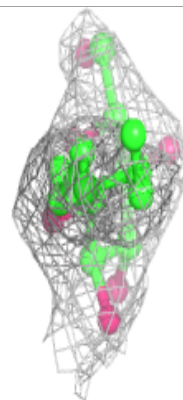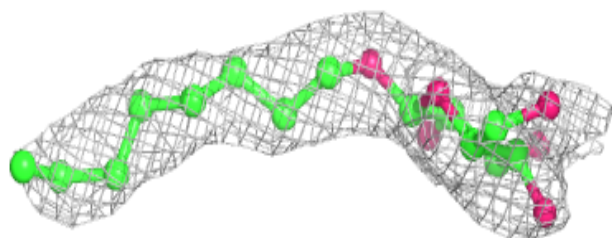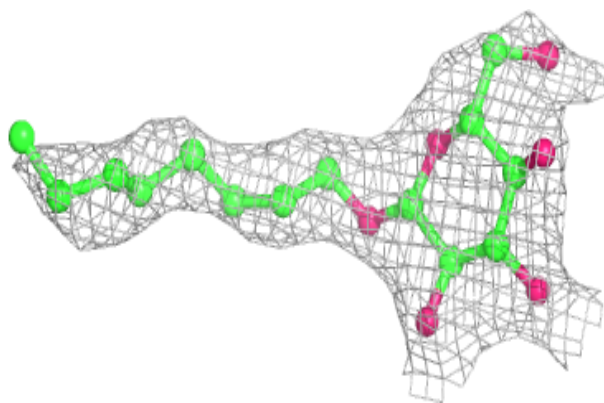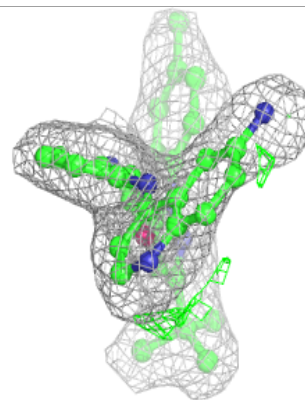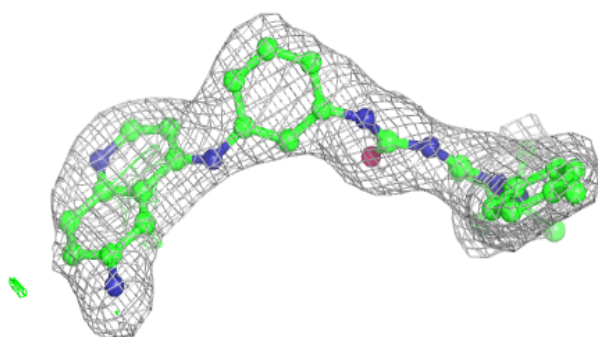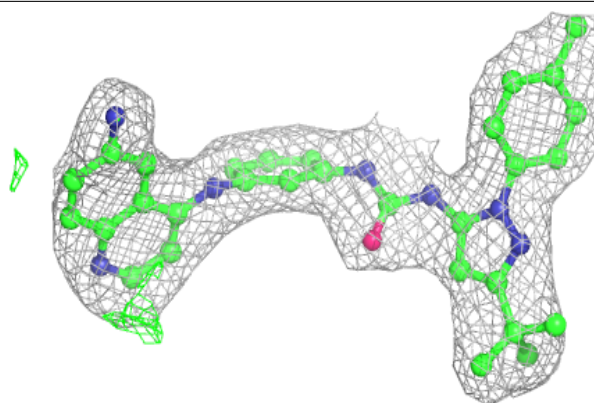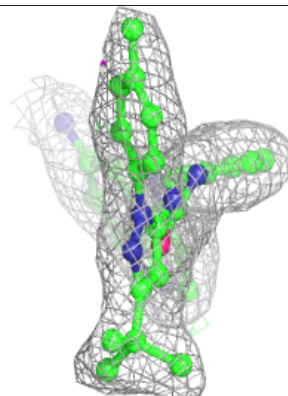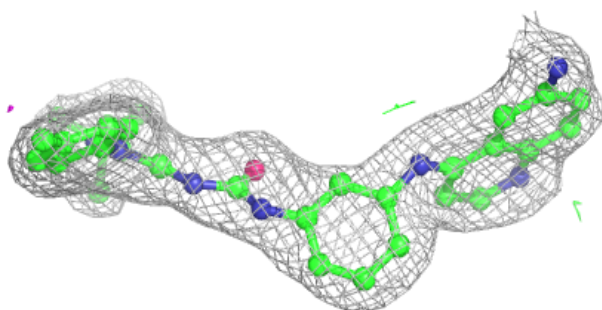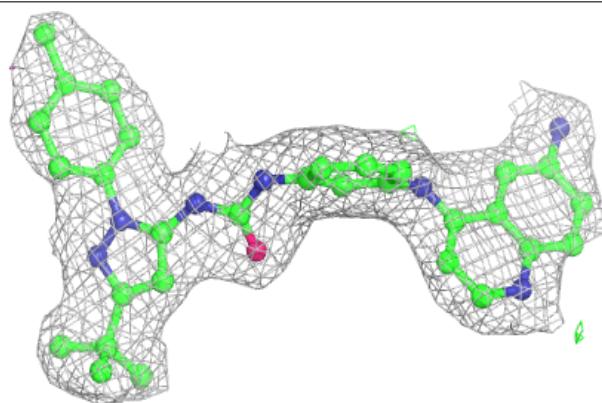

Electron density around BOG B 362:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
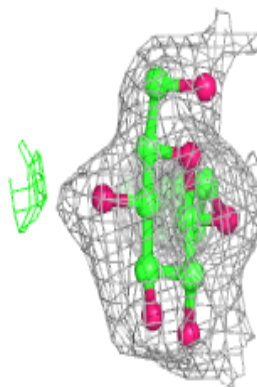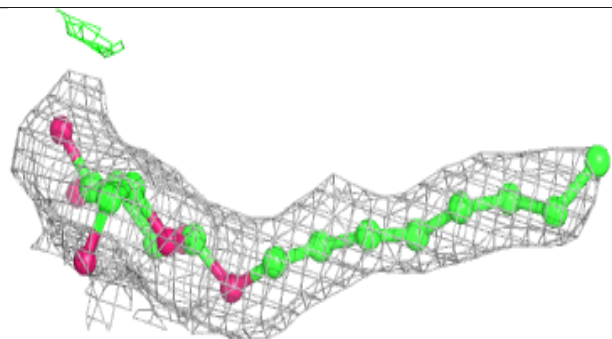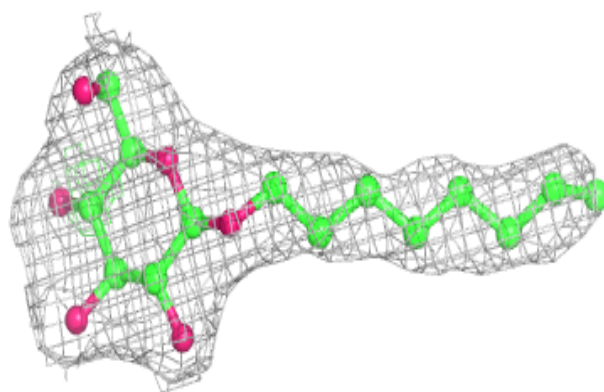
Electron density around L51 B 361:

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

Electron density around L51 A 361:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.