



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:03 PM UTC

PDB ID : 7BK4 / pdb_00007bk4
Title : Crystal structure of RXRalpha ligand binding domain in complex with a fragment of the TIF2 coactivator
Authors : le Maire, A.; Bourguet, W.
Deposited on : 2021-01-15
Resolution : 2.80 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

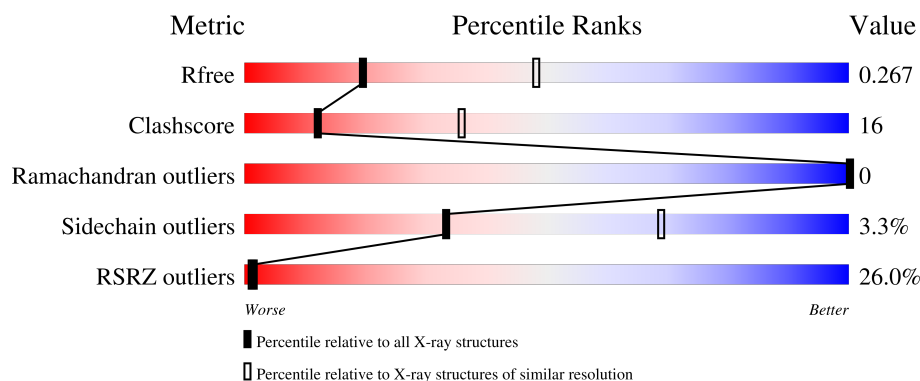
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	244	20% 69% 18% 5% 8%
1	C	244	25% 63% 21% • 14%
2	B	28	18% 43% 18% 11% 29%
2	D	28	18% 11% 18% 71%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3772 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1759	1127	301	320	11			
1	C	210	Total	C	N	O	S	0	1	0
			1662	1069	286	297	10			

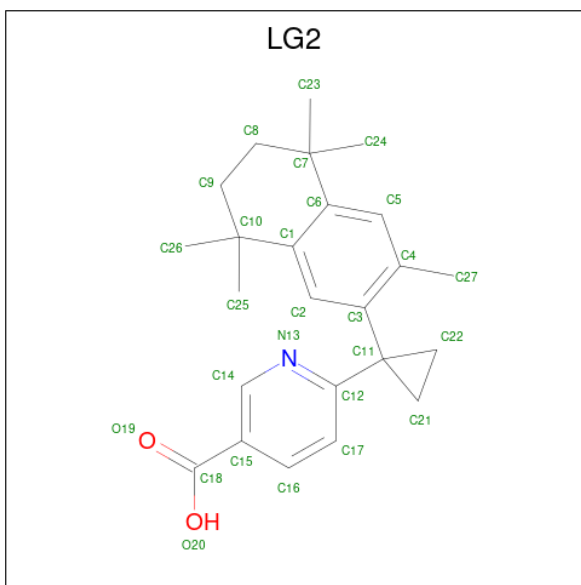
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP P19793
A	220	SER	-	expression tag	UNP P19793
A	221	HIS	-	expression tag	UNP P19793
A	222	MET	-	expression tag	UNP P19793
C	219	GLY	-	expression tag	UNP P19793
C	220	SER	-	expression tag	UNP P19793
C	221	HIS	-	expression tag	UNP P19793
C	222	MET	-	expression tag	UNP P19793

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	0	0	0
			156	98	30	28			
2	D	8	Total	C	N	O	0	0	0
			72	48	16	8			

- Molecule 3 is 6-[1-(3,5,5,8,8-PENTAMETHYL-5,6,7,8-TETRAHYDRONAPHTHALEN-2-YL)CYCLOPROPYL]PYRIDINE-3-CARBOXYLIC ACID (CCD ID: LG2) (formula: C₂₄H₂₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	24	1	2		
3	C	1	Total	C	N	O	0	0
			27	24	1	2		

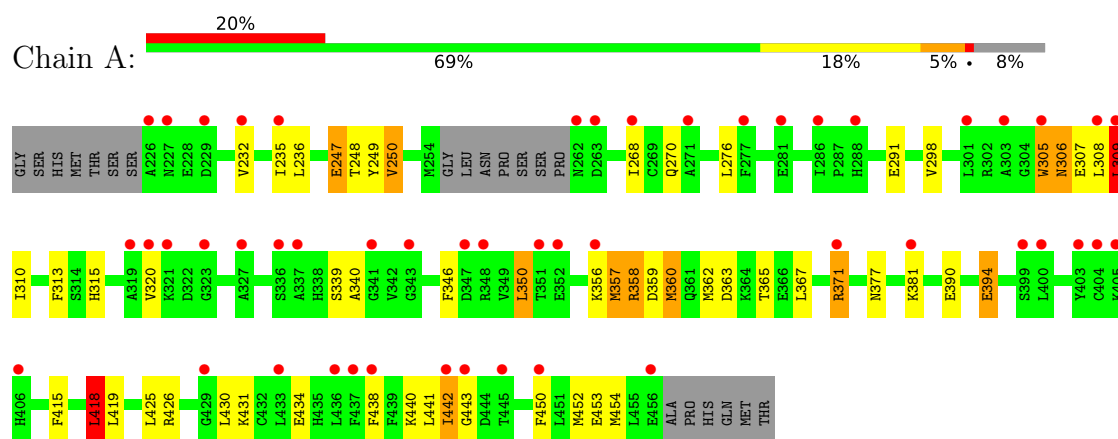
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	2	Total	O	0	0
			2	2		
4	C	18	Total	O	0	0
			18	18		
4	D	1	Total	O	0	0
			1	1		

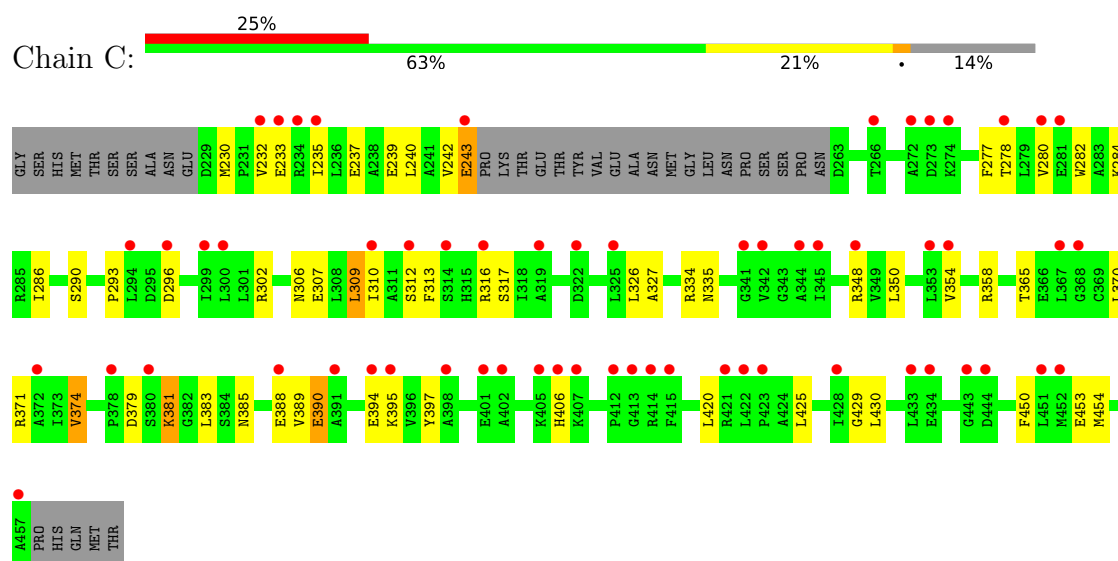
3 Residue-property plots [i](#)

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.

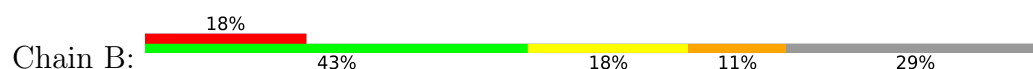
• Molecule 1: Retinoic acid receptor RXR-alpha

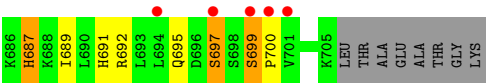


• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 2: Nuclear receptor coactivator 2





● Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.13Å 64.66Å 48.51Å 90.00° 95.28° 90.00°	Depositor
Resolution (Å)	48.31 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.31-2.80) 96.2 (48.31-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.50 (at 2.81Å)	Xtriage
Refinement program	REFMAC 7.1.005, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.246 , 0.265 0.257 , 0.267	Depositor DCC
R_{free} test set	1048 reflections (7.61%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	1.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3772	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LG2

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	1.10	14/1800 (0.8%)	0.90	7/2435 (0.3%)
1	C	0.83	7/1698 (0.4%)	0.77	2/2295 (0.1%)
2	B	1.01	1/158 (0.6%)	1.27	1/212 (0.5%)
2	D	0.62	0/73	0.69	0/96
All	All	0.97	22/3729 (0.6%)	0.86	10/5038 (0.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	SER	CA-C	-7.03	1.43	1.52
1	C	390	GLU	C-O	-6.81	1.16	1.24
1	A	358	ARG	C-O	-6.72	1.16	1.24
1	A	340	ALA	C-O	-6.42	1.15	1.24
1	C	309	LEU	C-O	-6.39	1.15	1.24
1	A	250	VAL	C-O	-6.35	1.17	1.24
1	A	249	TYR	C-O	-6.21	1.16	1.24
1	A	270	GLN	C-O	-6.11	1.16	1.24
1	A	360	MET	C-O	-5.98	1.16	1.24
1	A	359	ASP	C-O	-5.95	1.16	1.24
1	A	339	SER	C-O	-5.87	1.17	1.24
1	A	247	GLU	C-O	-5.70	1.17	1.24
1	A	394	GLU	C-O	-5.60	1.17	1.24
1	C	389	VAL	C-O	-5.49	1.17	1.24
2	B	697	SER	C-O	-5.38	1.17	1.24
1	C	334	ARG	C-O	-5.37	1.17	1.24
1	A	306	ASN	C-O	-5.36	1.18	1.24
1	C	335	ASN	C-O	-5.26	1.17	1.24
1	C	348	ARG	C-O	-5.16	1.18	1.24
1	C	374	VAL	N-CA	-5.11	1.40	1.46
1	A	350	LEU	C-O	-5.06	1.17	1.24
1	A	248	THR	C-O	-5.06	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	MET	N-CA-C	-6.82	103.91	111.82
1	C	406	HIS	N-CA-C	-6.47	104.08	112.23
1	C	277	PHE	N-CA-C	-6.27	104.52	111.36
1	A	249	TYR	N-CA-C	-6.09	104.72	111.36
1	A	305	TRP	N-CA-C	5.56	117.79	111.11
2	B	700	PRO	CA-C-O	-5.39	115.50	122.13
1	A	443	GLY	N-CA-C	5.37	121.33	112.30
1	A	418	LEU	N-CA-C	-5.36	105.52	111.36
1	A	309	LEU	CA-C-O	-5.14	115.10	120.55
1	A	441	LEU	N-CA-C	5.04	117.55	111.40

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	1759	0	1777	53	0
1	C	1662	0	1700	62	0
2	B	156	0	161	7	0
2	D	72	0	83	8	0
3	A	27	0	28	6	0
3	C	27	0	28	5	0
4	A	48	0	0	2	0
4	B	2	0	0	0	0
4	C	18	0	0	2	0
4	D	1	0	0	0	0
All	All	3772	0	3777	117	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 16.

All (117) 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:C:316:ARG:HH22	1:C:327:ALA:CA	1.65	1.09
1:C:242:VAL:O	1:C:243:GLU:HB2	1.48	1.07
1:C:316:ARG:NH2	1:C:327:ALA:N	2.03	1.05
1:C:316:ARG:NH2	1:C:327:ALA:CA	2.20	1.02
1:C:316:ARG:HH22	1:C:327:ALA:CB	1.71	1.02
1:C:381:LYS:HD2	1:C:381:LYS:H	1.23	1.01
1:A:305:TRP:CD1	1:A:454:MET:HE3	1.95	1.00
1:C:316:ARG:HH22	1:C:327:ALA:HB2	1.29	0.95
1:A:360:MET:HE1	1:A:418:LEU:CD2	1.98	0.92
1:A:346:PHE:O	1:A:350:LEU:HD13	1.71	0.89
1:A:357:MET:HE2	1:A:362:MET:HE1	1.54	0.88
1:C:316:ARG:HH21	1:C:327:ALA:N	1.69	0.87
1:A:360:MET:HE1	1:A:418:LEU:HD21	1.60	0.82
1:A:346:PHE:O	1:A:350:LEU:CD1	2.28	0.82
1:C:309:LEU:HD23	3:C:501:LG2:HC71	1.63	0.81
1:C:316:ARG:NH2	1:C:327:ALA:HA	1.95	0.81
1:A:367:LEU:O	1:A:371:ARG:HG3	1.83	0.79
1:C:280:VAL:O	1:C:284:LYS:HG3	1.87	0.74
1:C:230:MET:HE2	1:C:235:ILE:HD11	1.69	0.73
4:A:609:HOH:O	2:B:699:SER:HB2	1.87	0.73
1:C:309:LEU:HB3	3:C:501:LG2:H212	1.69	0.73
1:C:316:ARG:HH21	1:C:326:LEU:C	1.98	0.72
1:C:313:PHE:HA	1:C:316:ARG:HG2	1.72	0.71
1:C:370:LEU:O	1:C:374:VAL:HG23	1.92	0.70
1:A:305:TRP:HD1	1:A:454:MET:HE3	1.49	0.70
1:A:315:HIS:HD2	1:A:362:MET:HE2	1.61	0.65
1:C:313:PHE:HA	1:C:316:ARG:CD	2.27	0.65
1:C:293:PRO:HG2	1:C:296:ASP:HB2	1.78	0.65
1:C:296:ASP:OD1	1:C:383:LEU:HA	1.97	0.64
1:C:302:ARG:CD	2:D:687:HIS:CE1	2.80	0.64
1:C:313:PHE:HA	1:C:316:ARG:HD3	1.80	0.63
1:C:381:LYS:HD2	1:C:381:LYS:N	2.05	0.63
1:C:313:PHE:HA	1:C:316:ARG:CG	2.27	0.63
1:C:350:LEU:HA	1:C:354:VAL:HG12	1.81	0.63
1:C:450:PHE:HA	2:D:689:ILE:HD12	1.80	0.63
1:A:306:ASN:O	1:A:310:ILE:HG13	1.99	0.61
1:C:302:ARG:NE	2:D:687:HIS:CE1	2.68	0.61
1:C:242:VAL:O	1:C:243:GLU:CB	2.31	0.61
1:C:302:ARG:HD2	2:D:687:HIS:CE1	2.36	0.61
1:C:316:ARG:NH2	1:C:327:ALA:HB2	2.09	0.61
1:C:454:MET:HE1	2:D:690:LEU:HD22	1.81	0.60
1:A:453:GLU:OE2	2:B:689:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HB3	1:A:371:ARG:HH11	1.66	0.60
1:C:358:ARG:HD2	4:C:601:HOH:O	2.01	0.59
1:A:367:LEU:O	1:A:371:ARG:CG	2.51	0.59
1:C:309:LEU:HB3	3:C:501:LG2:HC71	1.85	0.58
1:A:298:VAL:HG21	2:B:691:HIS:CE1	2.39	0.57
1:C:316:ARG:HH22	1:C:327:ALA:N	1.84	0.57
1:A:360:MET:CE	1:A:418:LEU:CD2	2.81	0.56
1:A:431:LYS:NZ	1:A:434:GLU:OE1	2.28	0.56
1:C:358:ARG:HG2	4:C:609:HOH:O	2.06	0.55
1:A:305:TRP:CE3	1:A:306:ASN:N	2.75	0.55
1:C:381:LYS:H	1:C:381:LYS:CD	1.95	0.54
1:C:453:GLU:CD	2:D:687:HIS:HB3	2.33	0.54
1:C:242:VAL:HB	1:C:278:THR:HG22	1.90	0.53
1:A:438:PHE:CZ	1:A:442:ILE:HD11	2.43	0.52
1:A:440:LYS:HG3	1:A:452:MET:HE1	1.92	0.52
1:A:419:LEU:HD22	1:C:420:LEU:HD21	1.93	0.51
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.46	0.51
1:A:415:PHE:O	1:A:418:LEU:HB2	2.10	0.50
1:A:276:LEU:HB3	1:A:450:PHE:CE2	2.46	0.50
1:A:247:GLU:O	1:A:250:VAL:HB	2.11	0.50
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.47	0.50
1:C:313:PHE:O	1:C:317:SER:OG	2.22	0.50
1:C:394:GLU:HA	1:C:397:TYR:CE2	2.47	0.49
1:A:309:LEU:HB3	3:A:501:LG2:H212	1.94	0.49
1:C:232:VAL:HG22	1:C:365:THR:HG22	1.95	0.49
1:A:363:ASP:OD1	1:A:365:THR:OG1	2.21	0.49
1:A:232:VAL:O	1:A:235:ILE:HG13	2.13	0.49
2:B:687:HIS:N	2:B:687:HIS:ND1	2.59	0.49
1:A:315:HIS:CD2	1:A:362:MET:HE2	2.44	0.48
1:A:356:LYS:NZ	1:C:379:ASP:OD1	2.31	0.48
1:A:362:MET:HE3	1:A:367:LEU:HB2	1.95	0.48
1:A:268:ILE:HD13	3:A:501:LG2:H233	1.96	0.48
1:A:305:TRP:CD2	1:A:306:ASN:N	2.82	0.48
1:A:377:ASN:HD21	1:A:426:ARG:NH2	2.12	0.48
1:C:306:ASN:HD21	1:C:429:GLY:C	2.22	0.47
1:A:313:PHE:CZ	3:A:501:LG2:H263	2.50	0.47
1:A:360:MET:CE	1:A:418:LEU:HD21	2.38	0.47
1:C:385:ASN:ND2	1:C:388:GLU:HB2	2.31	0.46
1:A:309:LEU:HD13	3:A:501:LG2:HC71	1.98	0.46
1:A:346:PHE:CE2	1:A:350:LEU:HD11	2.51	0.46
1:A:390:GLU:O	1:A:394:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:VAL:HB	1:C:278:THR:CG2	2.46	0.45
1:C:280:VAL:HG12	1:C:284:LYS:HE2	1.97	0.45
1:A:430:LEU:HD13	1:C:430:LEU:HD12	1.98	0.45
1:A:346:PHE:O	1:A:350:LEU:HD12	2.14	0.45
4:A:609:HOH:O	2:B:699:SER:CB	2.56	0.44
1:A:305:TRP:CE3	1:A:306:ASN:HA	2.53	0.44
3:C:501:LG2:HC71	3:C:501:LG2:H212	1.54	0.44
1:C:282:TRP:CE2	1:C:286:ILE:HD11	2.53	0.44
1:C:296:ASP:CG	1:C:383:LEU:HD23	2.42	0.44
1:A:315:HIS:HB3	1:A:367:LEU:HD22	1.99	0.44
1:A:360:MET:HE2	1:A:362:MET:HB2	2.01	0.43
1:A:320:VAL:O	1:A:358:ARG:NH2	2.52	0.43
1:C:280:VAL:HG11	2:D:693:LEU:HB3	2.00	0.42
1:C:233:GLU:O	1:C:237:GLU:N	2.42	0.42
1:C:350:LEU:HA	1:C:354:VAL:CG1	2.48	0.42
1:C:239:GLU:OE2	1:C:371:ARG:HD3	2.19	0.42
1:A:313:PHE:HZ	3:A:501:LG2:H263	1.85	0.42
1:A:236:LEU:HB2	1:A:365:THR:HG22	2.02	0.41
1:C:230:MET:HG2	1:C:395:LYS:HB3	2.02	0.41
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.78	0.41
1:C:313:PHE:CD1	1:C:313:PHE:C	2.98	0.41
1:A:307:GLU:HG2	1:A:425:LEU:HG	2.02	0.41
1:A:346:PHE:CD2	1:A:350:LEU:HD11	2.56	0.41
1:C:302:ARG:CD	2:D:687:HIS:HE1	2.33	0.41
1:A:381:LYS:HA	1:A:381:LYS:HD2	1.71	0.41
1:A:276:LEU:HB3	1:A:450:PHE:CD2	2.56	0.41
1:C:313:PHE:CZ	3:C:501:LG2:H263	2.56	0.41
1:A:453:GLU:OE1	2:B:689:ILE:HB	2.21	0.40
1:C:312:SER:O	1:C:316:ARG:HD3	2.22	0.40
1:A:310:ILE:HG12	3:A:501:LG2:H211	2.04	0.40
2:B:692:ARG:O	2:B:695:GLN:HG2	2.22	0.40
1:A:305:TRP:CE3	1:A:306:ASN:CA	3.05	0.40
1:C:232:VAL:HG22	1:C:365:THR:CG2	2.51	0.40
1:C:307:GLU:HB3	1:C:425:LEU:HG	2.03	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	221/244 (91%)	218 (99%)	3 (1%)	0	100	100
1	C	207/244 (85%)	201 (97%)	6 (3%)	0	100	100
2	B	18/28 (64%)	17 (94%)	1 (6%)	0	100	100
2	D	6/28 (21%)	4 (67%)	2 (33%)	0	100	100
All	All	452/544 (83%)	440 (97%)	12 (3%)	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	190/210 (90%)	185 (97%)	5 (3%)	40	75
1	C	180/210 (86%)	176 (98%)	4 (2%)	45	78
2	B	18/24 (75%)	15 (83%)	3 (17%)	2	8
2	D	8/24 (33%)	7 (88%)	1 (12%)	4	15
All	All	396/468 (85%)	383 (97%)	13 (3%)	33	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	A	309	LEU

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Mol	Chain	Res	Type
1	A	371	ARG
1	A	418	LEU
1	A	442	ILE
2	B	687	HIS
2	B	697	SER
2	B	699	SER
1	C	243	GLU
1	C	290	SER
1	C	381	LYS
1	C	390	GLU
2	D	688	LYS

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

Mol	Chain	Res	Type
1	A	288	HIS
1	A	297	GLN
1	A	331	HIS
2	B	691	HIS
1	C	306	ASN
1	C	335	ASN
1	C	361	GLN
2	D	687	HIS

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](#)

2 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	LG2	A	501	-	29,30,30	1.19	4 (13%)	44,49,49	4.39	11 (25%)
3	LG2	C	501	-	29,30,30	1.16	3 (10%)	44,49,49	4.32	10 (22%)

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
3	LG2	A	501	-	-	6/15/39/39	0/4/4/4
3	LG2	C	501	-	-	5/15/39/39	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	LG2	C10-C1	3.10	1.57	1.53
3	C	501	LG2	C10-C1	3.09	1.57	1.53
3	A	501	LG2	C7-C6	2.30	1.56	1.53
3	A	501	LG2	C27-C4	2.26	1.55	1.51
3	C	501	LG2	C15-C18	2.25	1.54	1.49
3	C	501	LG2	C27-C4	2.24	1.55	1.51
3	A	501	LG2	C15-C18	2.15	1.54	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	LG2	C21-C11-C3	16.81	141.18	117.13
3	A	501	LG2	C21-C11-C12	-16.60	91.12	117.30
3	C	501	LG2	C21-C11-C3	16.41	140.61	117.13
3	C	501	LG2	C21-C11-C12	-15.44	92.95	117.30
3	C	501	LG2	C22-C11-C12	14.67	140.43	117.30
3	A	501	LG2	C22-C11-C12	13.89	139.21	117.30
3	A	501	LG2	C22-C11-C3	-5.02	109.95	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	LG2	C22-C11-C3	-4.21	111.10	117.13
3	C	501	LG2	C14-N13-C12	3.85	121.72	117.60
3	A	501	LG2	C14-N13-C12	3.30	121.13	117.60
3	C	501	LG2	C8-C7-C6	3.27	115.34	110.11
3	C	501	LG2	C9-C10-C1	3.03	114.96	110.11
3	C	501	LG2	C17-C12-N13	-2.91	118.82	122.33
3	A	501	LG2	C17-C16-C15	-2.89	117.72	120.80
3	A	501	LG2	C8-C7-C6	2.86	114.68	110.11
3	C	501	LG2	C17-C16-C15	-2.60	118.02	120.80
3	A	501	LG2	C17-C12-N13	-2.56	119.24	122.33
3	A	501	LG2	O20-C18-C15	2.31	120.78	114.84
3	A	501	LG2	C9-C10-C1	2.24	113.69	110.11
3	A	501	LG2	C16-C17-C12	2.17	121.36	119.11
3	C	501	LG2	C16-C17-C12	2.03	121.22	119.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	LG2	C14-C15-C18-O19
3	A	501	LG2	C14-C15-C18-O20
3	A	501	LG2	C16-C15-C18-O19
3	A	501	LG2	C16-C15-C18-O20
3	C	501	LG2	C16-C15-C18-O19
3	C	501	LG2	C16-C15-C18-O20
3	C	501	LG2	C14-C15-C18-O19
3	C	501	LG2	C14-C15-C18-O20
3	C	501	LG2	C22-C11-C12-C17
3	A	501	LG2	C22-C11-C12-C17
3	A	501	LG2	C3-C11-C12-C17

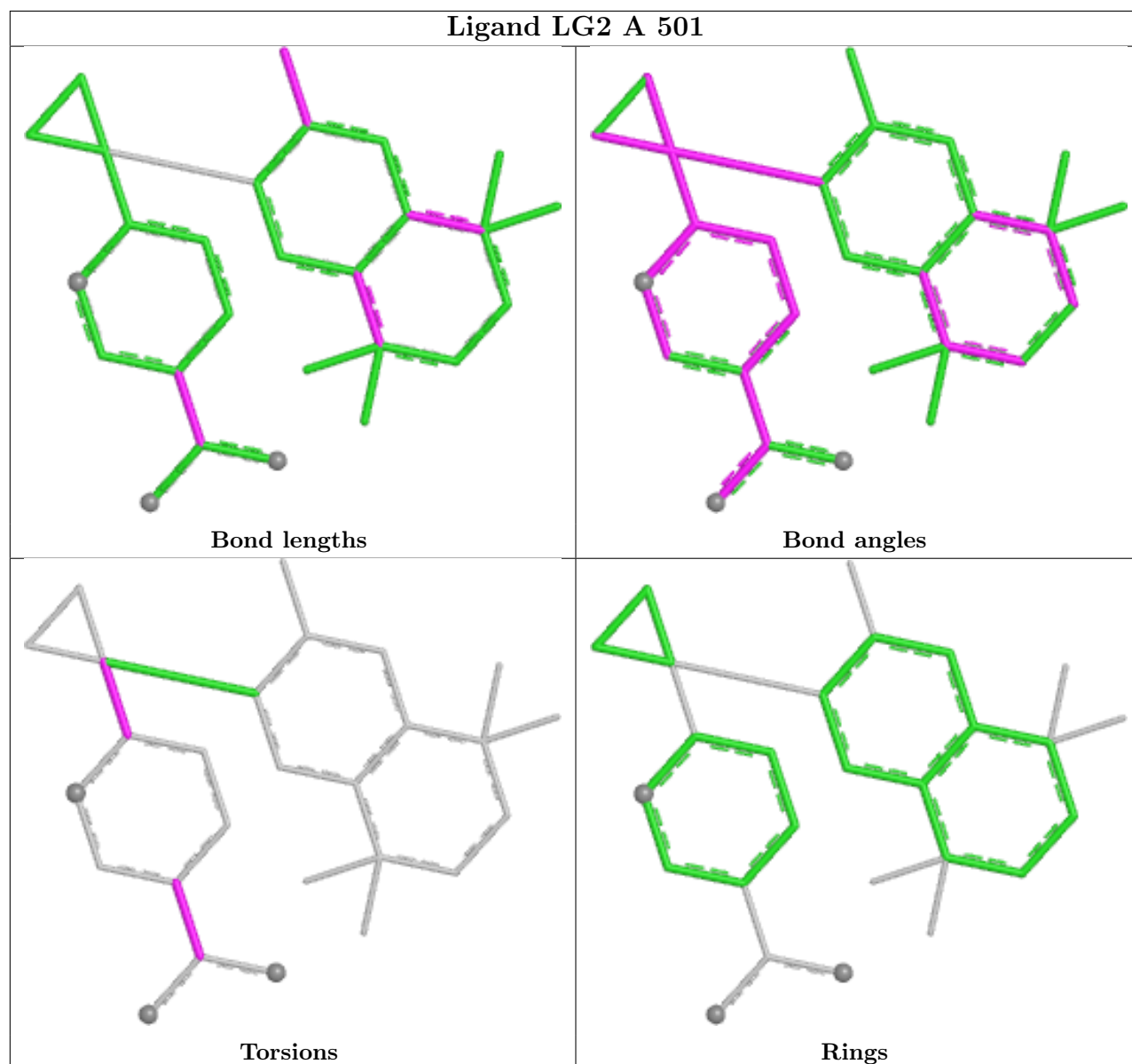
There are no ring outliers.

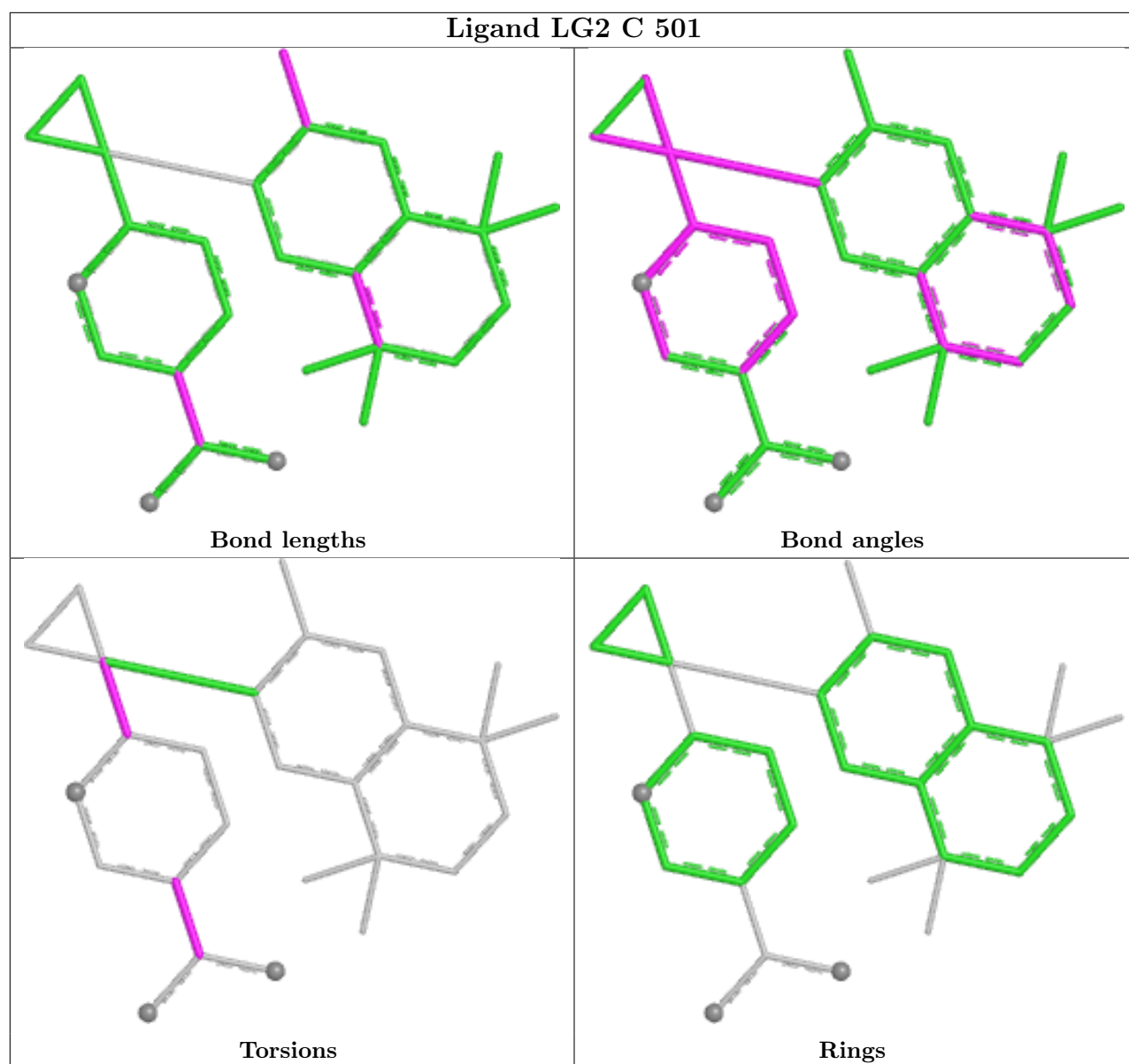
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	LG2	6	0
3	C	501	LG2	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/244 (91%)	1.43	50 (22%) 2 1	17, 25, 39, 63	1 (0%)
1	C	210/244 (86%)	1.58	60 (28%) 1 1	19, 33, 48, 61	1 (0%)
2	B	20/28 (71%)	1.46	5 (25%) 2 1	23, 33, 52, 54	0
2	D	8/28 (28%)	2.10	5 (62%) 0 0	48, 52, 60, 61	0
All	All	462/544 (84%)	1.51	120 (25%) 1 1	17, 29, 48, 63	2 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	406	HIS	4.2
1	C	273	ASP	4.2
1	A	262	ASN	4.0
1	C	354	VAL	3.9
1	C	401	GLU	3.8
1	A	405	LYS	3.7
2	B	701	VAL	3.5
1	A	337	ALA	3.5
1	A	327	ALA	3.5
1	A	232	VAL	3.5
1	C	345	ILE	3.4
1	C	415	PHE	3.4
1	A	456	GLU	3.3
1	C	235	ILE	3.3
1	C	278	THR	3.3
1	A	229	ASP	3.2
1	C	444	ASP	3.2
1	A	347	ASP	3.1
1	C	341	GLY	3.1
2	D	688	LYS	3.1
1	C	368	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	398	ALA	3.0
1	C	412	PRO	3.0
1	A	341	GLY	3.0
1	A	352	GLU	3.0
1	A	226	ALA	3.0
2	D	691	HIS	3.0
1	A	403	TYR	2.9
1	C	325	LEU	2.9
1	C	402	ALA	2.9
1	A	442	ILE	2.8
1	C	423	PRO	2.8
1	A	371	ARG	2.8
1	A	438	PHE	2.8
1	A	309	LEU	2.8
1	C	353	LEU	2.8
2	B	699	SER	2.8
1	A	227	ASN	2.8
1	A	263	ASP	2.8
1	C	296	ASP	2.8
1	C	299	ILE	2.7
1	C	428	ILE	2.7
1	C	407	LYS	2.7
1	A	381	LYS	2.7
1	A	429	GLY	2.7
1	C	281	GLU	2.7
1	C	391	ALA	2.7
1	A	235	ILE	2.6
1	A	399	SER	2.6
1	C	443	GLY	2.6
2	B	697	SER	2.5
1	A	343	GLY	2.5
1	A	348	ARG	2.5
1	C	234	ARG	2.5
1	A	406	HIS	2.5
1	C	314	SER	2.5
1	C	380	SER	2.5
1	C	422	LEU	2.5
1	C	388	GLU	2.5
1	C	405	LYS	2.5
1	A	404	CYS	2.5
1	C	413	GLY	2.4
1	A	288	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	336	SER	2.4
1	A	268	ILE	2.4
1	A	356	LYS	2.4
1	A	433	LEU	2.4
1	A	319	ALA	2.3
1	C	367	LEU	2.3
1	C	232	VAL	2.3
1	C	294	LEU	2.3
1	C	378	PRO	2.3
1	C	452	MET	2.3
1	A	400	LEU	2.3
2	D	693	LEU	2.3
1	A	320	VAL	2.3
1	A	303	ALA	2.3
1	C	451	LEU	2.3
1	C	414	ARG	2.3
1	C	434	GLU	2.2
1	C	457	ALA	2.2
2	B	700	PRO	2.2
1	C	421	ARG	2.2
1	A	305	TRP	2.2
1	C	348	ARG	2.2
1	A	323	GLY	2.2
1	C	310	ILE	2.2
1	C	316	ARG	2.2
1	C	274	LYS	2.2
1	C	243	GLU	2.2
1	C	322	ASP	2.1
1	A	301	LEU	2.1
1	A	436	LEU	2.1
1	A	437	PHE	2.1
2	B	694	LEU	2.1
1	C	312	SER	2.1
1	A	281	GLU	2.1
1	C	233	GLU	2.1
1	A	308	LEU	2.1
1	C	344	ALA	2.1
1	C	372	ALA	2.1
1	C	394	GLU	2.1
1	A	321	LYS	2.1
1	C	280	VAL	2.1
1	A	450	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	266	THR	2.1
1	A	286	ILE	2.1
1	C	395	LYS	2.1
1	C	300	LEU	2.1
1	C	433	LEU	2.1
2	D	694	LEU	2.1
1	C	342	VAL	2.0
1	A	443	GLY	2.0
2	D	692	ARG	2.0
1	A	445	THR	2.0
1	C	319	ALA	2.0
1	A	277	PHE	2.0
1	A	271	ALA	2.0
1	A	351	THR	2.0
1	C	272	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

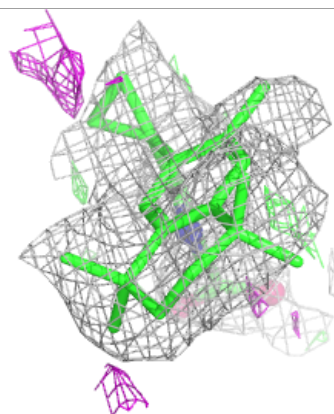
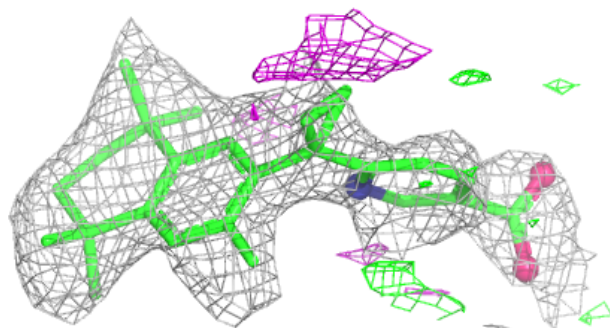
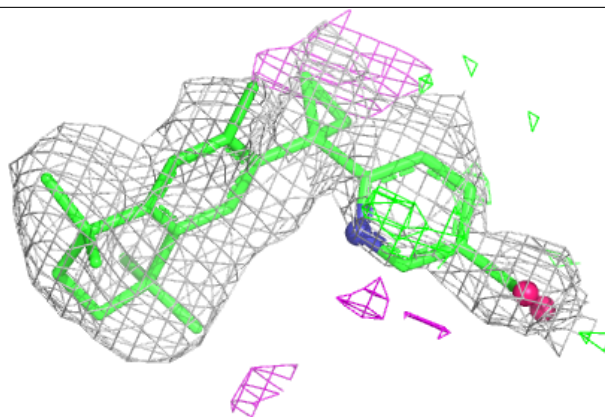
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LG2	A	501	27/27	0.73	0.22	21,25,32,34	0
3	LG2	C	501	27/27	0.77	0.20	23,28,31,34	0

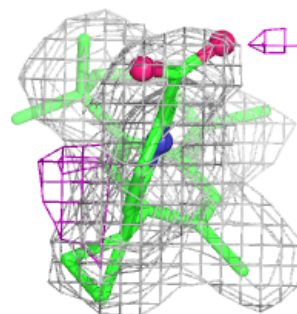
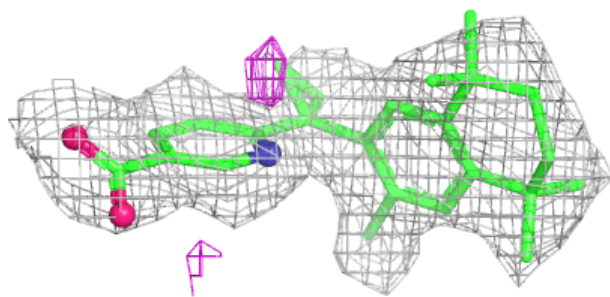
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LG2 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 LG2 C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.