



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:10 am BST

PDB ID : 1H9U  
Title : The structure of the human retinoid-X-receptor beta ligand binding domain  
in complex with the specific synthetic agonist LG100268  
Authors : Schwabe, J.W.R.; Love, J.D.; Gooch, J.T.  
Deposited on : 2001-03-21  
Resolution : 2.70 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

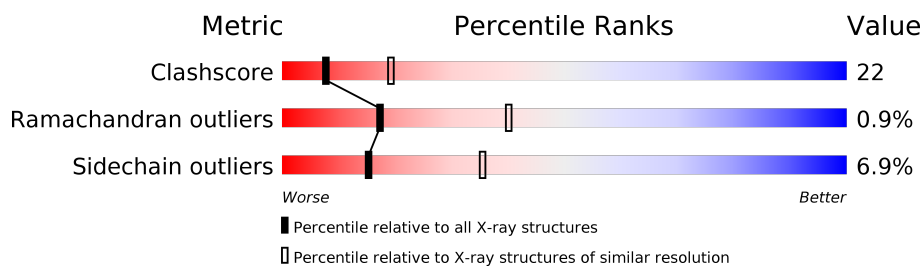
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	<div> <div>54%</div> <div>32%</div> <div>•</div> <div>10%</div> </div>
1	B	224	<div> <div>61%</div> <div>25%</div> <div>•</div> <div>10%</div> </div>
1	C	224	<div> <div>58%</div> <div>30%</div> <div>•</div> <div>10%</div> </div>
1	D	224	<div> <div>57%</div> <div>31%</div> <div>•</div> <div>10%</div> </div>

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
2	LG2	C	1	-	-	X	-

## 2 Entry composition [i](#)

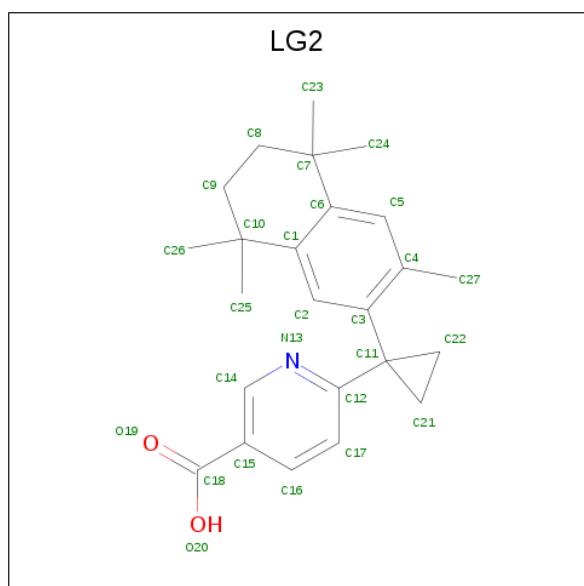
There are 5 unique types of molecules in this entry. The entry contains 6338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOID X RECEPTOR, BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1560	999	276	277	8			
1	B	201	Total	C	N	O	S	0	0	0
			1553	994	275	276	8			
1	C	201	Total	C	N	O	S	0	0	0
			1555	1001	271	275	8			
1	D	201	Total	C	N	O	S	0	0	0
			1552	996	272	276	8			

- Molecule 2 is 6-[1-(3,5,5,8,8-PENTAMETHYL-5,6,7,8-TETRAHYDRONAPHTHALE N-2-YL)CYCLOPROPYL]PYRIDINE-3-CARBOXYLIC ACID (three-letter code: LG2) (formula: C<sub>24</sub>H<sub>29</sub>NO<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	24	1	2		
2	C	1	Total	C	N	O	0	0
			27	24	1	2		
2	D	1	Total	C	N	O	0	0
			27	24	1	2		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

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

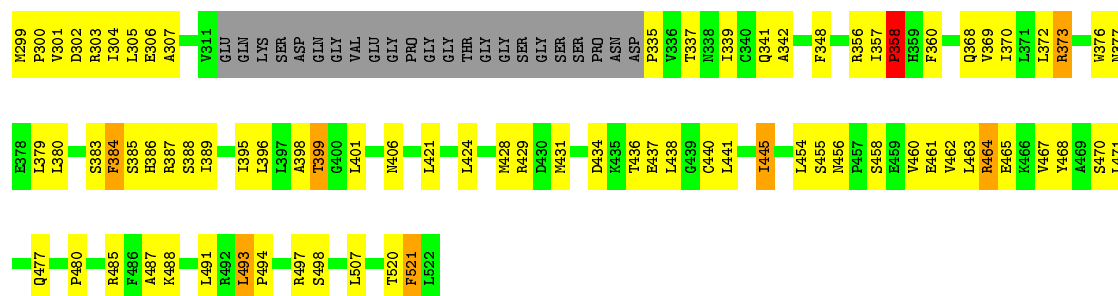
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

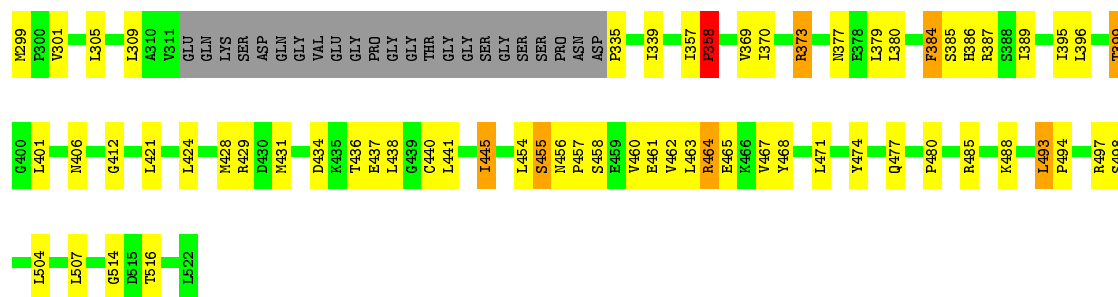
#### • Molecule 1: RETINOID X RECEPTOR, BETA

Chain A: 



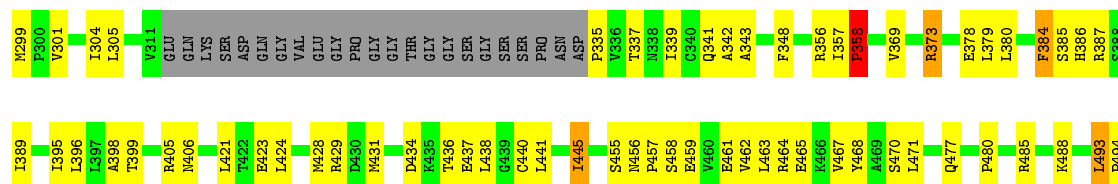
#### • Molecule 1: RETINOID X RECEPTOR, BETA

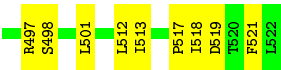
Chain B: 



#### • Molecule 1: RETINOID X RECEPTOR, BETA

Chain C: 





● Molecule 1: RETINOID X RECEPTOR, BETA



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.89Å 106.88Å 100.59Å 90.00° 122.56° 90.00°	Depositor
Resolution (Å)	38.14 – 2.70	Depositor
% Data completeness (in resolution range)	97.3 (38.14-2.70)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.273 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 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: LG2, NI, CL

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	0.46	0/1589	0.65	0/2149
1	B	0.44	0/1582	0.65	0/2139
1	C	0.43	0/1585	0.65	0/2143
1	D	0.41	0/1582	0.63	0/2138
All	All	0.44	0/6338	0.65	0/8569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1560	0	1581	81	0
1	B	1553	0	1571	64	0
1	C	1555	0	1580	74	0
1	D	1552	0	1567	66	0
2	A	27	0	28	6	0
2	B	27	0	28	2	0
2	C	27	0	28	9	0
2	D	27	0	28	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	2	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
All	All	6338	0	6411	278	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 22.

All (278) 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:379:LEU:HG	1:C:445:ILE:HD11	1.46	0.98
1:D:385:SER:HB3	1:D:428:MET:HE1	1.46	0.98
1:A:379:LEU:HG	1:A:445:ILE:HD11	1.46	0.97
1:C:385:SER:HB3	1:C:428:MET:HE1	1.44	0.97
1:B:389:ILE:HG23	1:B:429:ARG:HG3	1.47	0.96
1:D:379:LEU:HG	1:D:445:ILE:HD11	1.47	0.96
1:B:385:SER:HB3	1:B:428:MET:HE1	1.49	0.95
1:B:379:LEU:HG	1:B:445:ILE:HD11	1.50	0.93
1:C:389:ILE:HG23	1:C:429:ARG:HG3	1.50	0.93
1:A:385:SER:HB3	1:A:428:MET:HE1	1.51	0.92
1:D:389:ILE:HG23	1:D:429:ARG:HG3	1.52	0.92
1:A:389:ILE:HG23	1:A:429:ARG:HG3	1.55	0.86
1:B:514:GLY:O	1:B:516:THR:HG23	1.78	0.84
1:C:380:LEU:HB3	2:C:1:LG2:HC71	1.61	0.83
1:D:373:ARG:HG2	1:D:373:ARG:HH11	1.47	0.79
1:C:385:SER:CB	1:C:428:MET:HE1	2.16	0.76
1:C:373:ARG:HG2	1:C:373:ARG:HH11	1.50	0.75
1:D:385:SER:HB3	1:D:428:MET:CE	2.18	0.74
1:A:373:ARG:HH11	1:A:373:ARG:HG2	1.53	0.72
1:A:385:SER:CB	1:A:428:MET:HE1	2.19	0.71
1:D:385:SER:CB	1:D:428:MET:HE1	2.21	0.71
1:B:385:SER:CB	1:B:428:MET:HE1	2.20	0.70
1:B:301:VAL:CG1	1:B:436:THR:HG23	2.21	0.70
1:A:301:VAL:CG1	1:A:436:THR:HG23	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:MET:HE1	1:C:304:ILE:HD11	1.74	0.68
1:D:373:ARG:NH1	1:D:373:ARG:HG2	2.07	0.68
1:A:335:PRO:O	1:A:339:ILE:HG13	1.94	0.67
1:A:301:VAL:HG23	1:A:470:SER:HB3	1.75	0.67
1:A:380:LEU:HB3	2:A:1:LG2:HC71	1.77	0.66
1:D:451:ALA:HB3	1:D:454:LEU:HD11	1.76	0.66
2:C:1:LG2:HC61	5:C:2001:HOH:O	1.97	0.65
1:A:465:GLU:HA	1:A:468:TYR:CE2	2.31	0.65
1:D:440:CYS:CB	1:D:471:LEU:HD13	2.26	0.65
1:D:458:SER:O	1:D:462:VAL:HG23	1.95	0.65
1:A:454:LEU:HD13	1:A:460:VAL:HG21	1.77	0.65
1:C:389:ILE:O	1:C:429:ARG:NH1	2.28	0.65
1:D:299:MET:CE	1:D:467:VAL:HG22	2.27	0.65
1:C:387:ARG:HD2	1:C:396:LEU:O	1.96	0.65
1:C:518:ILE:O	1:C:521:PHE:HB2	1.97	0.64
1:D:389:ILE:O	1:D:429:ARG:NH1	2.29	0.64
1:B:454:LEU:HD13	1:B:460:VAL:HG21	1.79	0.64
1:C:373:ARG:HG2	1:C:373:ARG:NH1	2.11	0.64
1:C:384:PHE:C	1:C:384:PHE:CD1	2.71	0.64
1:C:389:ILE:CG2	1:C:429:ARG:HG3	2.26	0.63
1:B:387:ARG:HD2	1:B:396:LEU:O	1.98	0.63
1:D:301:VAL:HG12	1:D:436:THR:HG23	1.81	0.63
1:B:465:GLU:HA	1:B:468:TYR:CE2	2.33	0.63
1:B:384:PHE:C	1:B:384:PHE:CD1	2.72	0.63
1:A:373:ARG:NH1	1:A:373:ARG:HG2	2.11	0.63
1:B:373:ARG:HG2	1:B:373:ARG:HH11	1.64	0.62
1:B:389:ILE:O	1:B:429:ARG:NH1	2.29	0.62
1:C:465:GLU:HA	1:C:468:TYR:CE2	2.33	0.62
2:A:1:LG2:HC61	5:A:2001:HOH:O	1.99	0.62
1:A:373:ARG:O	1:A:373:ARG:HD3	1.99	0.62
1:B:440:CYS:CB	1:B:471:LEU:HD13	2.30	0.61
1:C:301:VAL:HG12	1:C:436:THR:HG23	1.82	0.61
1:B:335:PRO:O	1:B:339:ILE:HG13	2.01	0.61
1:A:384:PHE:CD1	1:A:384:PHE:C	2.73	0.61
1:B:458:SER:O	1:B:462:VAL:HG23	1.99	0.61
1:D:335:PRO:O	1:D:339:ILE:HG13	2.01	0.61
1:C:385:SER:HB3	1:C:428:MET:CE	2.26	0.61
1:B:385:SER:HB3	1:B:428:MET:CE	2.29	0.60
1:A:458:SER:O	1:A:462:VAL:HG23	1.99	0.60
1:D:385:SER:C	1:D:428:MET:HE1	2.22	0.60
1:B:380:LEU:HB3	2:B:1:LG2:HC71	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:CG2	1:B:429:ARG:HG3	2.27	0.60
1:C:440:CYS:CB	1:C:471:LEU:HD13	2.30	0.60
1:B:299:MET:CE	1:B:358:PRO:HG2	2.31	0.60
1:B:373:ARG:O	1:B:373:ARG:HD3	2.02	0.60
1:C:335:PRO:O	1:C:339:ILE:HG13	2.02	0.59
1:D:456:ASN:ND2	1:D:459:GLU:HB2	2.16	0.59
1:A:385:SER:HB3	1:A:428:MET:CE	2.29	0.59
1:D:384:PHE:C	1:D:384:PHE:CD1	2.76	0.59
1:B:301:VAL:HG11	1:B:436:THR:HG23	1.84	0.59
1:D:380:LEU:HB3	2:D:1:LG2:HC71	1.85	0.59
1:D:514:GLY:O	1:D:516:THR:HG23	2.03	0.59
1:D:299:MET:HE2	1:D:467:VAL:HG22	1.85	0.59
1:A:342:ALA:HB1	2:A:1:LG2:O20	2.02	0.58
1:A:299:MET:CE	1:A:304:ILE:HD11	2.33	0.58
1:C:357:ILE:HG23	1:C:358:PRO:HD2	1.86	0.58
1:D:465:GLU:HA	1:D:468:TYR:CE2	2.39	0.58
1:D:373:ARG:O	1:D:373:ARG:HD3	2.04	0.57
1:A:389:ILE:CG2	1:A:429:ARG:HG3	2.29	0.57
1:D:387:ARG:HD2	1:D:396:LEU:O	2.04	0.57
1:A:389:ILE:O	1:A:429:ARG:NH1	2.34	0.57
1:B:389:ILE:HG23	1:B:429:ARG:CG	2.30	0.57
1:A:385:SER:C	1:A:428:MET:HE1	2.25	0.56
1:A:463:LEU:O	1:A:467:VAL:HG23	2.03	0.56
1:C:389:ILE:HG23	1:C:429:ARG:CG	2.29	0.56
1:B:440:CYS:SG	1:B:471:LEU:HD13	2.46	0.56
1:A:440:CYS:CB	1:A:471:LEU:HD13	2.36	0.56
1:B:377:ASN:ND2	1:B:504:LEU:HD13	2.21	0.55
1:B:463:LEU:O	1:B:467:VAL:HG23	2.07	0.55
1:B:386:HIS:HD1	1:B:386:HIS:C	2.10	0.55
1:D:389:ILE:CG2	1:D:429:ARG:HG3	2.31	0.55
1:C:301:VAL:HG22	1:C:470:SER:HB3	1.89	0.54
1:B:301:VAL:HG12	1:B:436:THR:HG23	1.88	0.54
1:C:458:SER:O	1:C:462:VAL:HG23	2.08	0.54
1:C:301:VAL:CG2	1:C:470:SER:HB3	2.38	0.54
1:A:498:SER:HB3	1:B:497:ARG:HD2	1.90	0.54
1:B:434:ASP:OD1	1:B:437:GLU:HG3	2.07	0.54
1:C:386:HIS:CD2	1:C:438:LEU:HD22	2.43	0.54
1:C:455:SER:O	1:C:457:PRO:HD3	2.08	0.54
1:C:385:SER:C	1:C:428:MET:HE1	2.28	0.53
1:A:386:HIS:HD1	1:A:386:HIS:C	2.10	0.53
1:C:343:ALA:HB2	2:C:1:LG2:H273	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:LEU:O	1:C:467:VAL:HG23	2.08	0.53
1:C:373:ARG:HD3	1:C:373:ARG:O	2.09	0.53
1:D:301:VAL:CG1	1:D:436:THR:HG23	2.39	0.53
1:D:389:ILE:HG23	1:D:429:ARG:CG	2.32	0.53
1:A:387:ARG:HD2	1:A:396:LEU:O	2.08	0.52
1:D:301:VAL:HG13	1:D:440:CYS:SG	2.49	0.52
1:A:520:THR:O	1:A:521:PHE:O	2.26	0.52
1:A:389:ILE:HG23	1:A:429:ARG:CG	2.33	0.52
1:B:373:ARG:HG2	1:B:373:ARG:NH1	2.23	0.52
1:D:431:MET:SD	1:D:488:LYS:HD3	2.50	0.52
1:D:441:LEU:O	1:D:445:ILE:HG23	2.10	0.52
1:D:397:LEU:HA	2:D:1:LG2:O20	2.08	0.52
1:D:431:MET:O	1:D:485:ARG:NH2	2.42	0.52
1:D:301:VAL:CG2	1:D:470:SER:HB3	2.40	0.52
1:D:434:ASP:OD1	1:D:437:GLU:HG3	2.10	0.51
1:B:431:MET:O	1:B:485:ARG:NH2	2.41	0.51
1:C:440:CYS:SG	1:C:471:LEU:HD13	2.50	0.51
1:A:461:GLU:O	1:A:465:GLU:HG2	2.10	0.51
1:B:385:SER:C	1:B:428:MET:HE1	2.31	0.51
1:C:437:GLU:OE2	1:C:485:ARG:HD3	2.10	0.51
1:D:463:LEU:O	1:D:467:VAL:HG23	2.10	0.51
1:A:431:MET:O	1:A:485:ARG:NH2	2.42	0.51
1:D:357:ILE:HG23	1:D:358:PRO:HD2	1.93	0.51
1:A:305:LEU:HD22	1:A:436:THR:OG1	2.10	0.51
1:A:441:LEU:O	1:A:445:ILE:HG23	2.11	0.50
1:B:357:ILE:HG23	1:B:358:PRO:HD2	1.94	0.50
1:C:513:ILE:O	1:C:519:ASP:HB2	2.10	0.50
1:A:370:ILE:HG21	1:A:454:LEU:HD23	1.94	0.50
1:C:299:MET:CE	1:C:358:PRO:HG2	2.42	0.50
1:A:299:MET:HE3	1:A:358:PRO:HG2	1.92	0.50
1:D:386:HIS:HD1	1:D:386:HIS:C	2.15	0.50
1:D:451:ALA:HB3	1:D:454:LEU:CD1	2.42	0.50
1:B:299:MET:HE3	1:B:358:PRO:HG2	1.93	0.50
1:B:301:VAL:HG11	1:B:436:THR:CG2	2.42	0.50
1:D:440:CYS:HB2	1:D:471:LEU:HD13	1.93	0.50
1:C:461:GLU:O	1:C:465:GLU:HG2	2.11	0.50
1:D:440:CYS:SG	1:D:471:LEU:HD13	2.52	0.50
1:C:465:GLU:HA	1:C:468:TYR:CD2	2.47	0.49
1:B:424:LEU:O	1:B:428:MET:HG3	2.12	0.49
1:A:357:ILE:HG23	1:A:358:PRO:HD2	1.94	0.49
1:B:441:LEU:O	1:B:445:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:HIS:C	1:C:386:HIS:HD1	2.16	0.49
1:C:456:ASN:CG	1:C:459:GLU:HB2	2.33	0.49
1:A:380:LEU:HB3	2:A:1:LG2:C17	2.42	0.49
1:D:437:GLU:OE2	1:D:485:ARG:HD3	2.12	0.49
1:A:360:PHE:CZ	1:A:368:GLN:HG2	2.47	0.49
1:C:380:LEU:CB	2:C:1:LG2:HC71	2.38	0.49
1:B:386:HIS:CD2	1:B:438:LEU:HD22	2.47	0.48
1:B:461:GLU:O	1:B:465:GLU:HG2	2.14	0.48
1:C:441:LEU:O	1:C:445:ILE:HG23	2.12	0.48
1:C:431:MET:O	1:C:485:ARG:NH2	2.44	0.48
1:D:299:MET:SD	1:D:358:PRO:HB2	2.54	0.48
1:C:431:MET:SD	1:C:488:LYS:HD3	2.53	0.48
1:D:377:ASN:ND2	1:D:504:LEU:HD13	2.29	0.48
1:A:440:CYS:SG	1:A:471:LEU:HD13	2.54	0.48
1:A:431:MET:SD	1:A:488:LYS:HD3	2.54	0.48
1:A:388:SER:OG	1:A:396:LEU:N	2.35	0.47
1:A:455:SER:OG	1:A:456:ASN:N	2.46	0.47
1:C:468:TYR:CE1	1:D:487:ALA:HB3	2.49	0.47
1:A:380:LEU:CB	2:A:1:LG2:HC71	2.43	0.47
1:A:437:GLU:OE2	1:A:485:ARG:HD3	2.14	0.47
1:B:477:GLN:O	1:B:480:PRO:HD3	2.14	0.47
1:A:383:SER:HB3	5:A:2001:HOH:O	2.15	0.47
1:D:424:LEU:O	1:D:428:MET:HG3	2.15	0.47
1:B:437:GLU:OE2	1:B:485:ARG:HD3	2.14	0.47
1:D:301:VAL:HG22	1:D:470:SER:HB3	1.96	0.46
1:A:477:GLN:O	1:A:480:PRO:HD3	2.15	0.46
1:D:477:GLN:O	1:D:480:PRO:HD3	2.16	0.46
1:A:487:ALA:HB3	1:B:468:TYR:CE1	2.51	0.46
1:C:386:HIS:O	1:C:389:ILE:HG13	2.16	0.46
1:D:507:LEU:O	1:D:511:LYS:HB2	2.16	0.46
1:C:384:PHE:C	1:C:384:PHE:HD1	2.19	0.46
1:D:398:ALA:HB2	2:D:1:LG2:O19	2.15	0.46
1:C:498:SER:HB3	1:D:497:ARG:HD2	1.98	0.46
1:B:455:SER:OG	1:B:456:ASN:N	2.49	0.46
1:A:373:ARG:HH11	1:A:373:ARG:CG	2.25	0.46
1:C:301:VAL:CG1	1:C:436:THR:HG23	2.46	0.46
1:C:342:ALA:HB1	2:C:1:LG2:O20	2.15	0.45
1:C:378:GLU:HB2	1:C:445:ILE:HD12	1.98	0.45
1:B:384:PHE:CD1	1:B:385:SER:N	2.84	0.45
1:B:386:HIS:C	1:B:386:HIS:ND1	2.70	0.45
1:C:398:ALA:HB2	2:C:1:LG2:O19	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:HB3	2:C:1:LG2:C17	2.39	0.45
1:A:307:ALA:HB2	1:A:356:ARG:HB3	1.99	0.45
1:B:454:LEU:HB2	1:B:457:PRO:HG3	1.98	0.45
1:C:384:PHE:CD1	1:C:385:SER:N	2.85	0.45
1:B:387:ARG:HG2	1:B:396:LEU:HD23	1.99	0.45
2:A:1:LG2:H272	2:A:1:LG2:H212	1.98	0.45
1:D:386:HIS:HD2	1:D:438:LEU:HB2	1.82	0.44
1:A:299:MET:HE3	1:A:304:ILE:HD11	2.00	0.44
1:A:386:HIS:ND1	1:A:386:HIS:C	2.70	0.44
1:A:424:LEU:O	1:A:428:MET:HG3	2.17	0.44
1:A:300:PRO:HG2	1:A:303:ARG:HB2	2.00	0.44
1:A:370:ILE:CG2	1:A:454:LEU:HD23	2.47	0.44
1:D:377:ASN:O	1:D:381:ILE:HG13	2.18	0.44
1:B:305:LEU:HD23	1:B:436:THR:CA	2.48	0.44
1:D:379:LEU:HG	1:D:445:ILE:CD1	2.34	0.44
1:B:465:GLU:HA	1:B:468:TYR:CD2	2.52	0.44
1:B:436:THR:HG21	1:B:474:TYR:CE1	2.53	0.44
1:A:497:ARG:HD2	1:B:498:SER:HB3	2.00	0.44
1:D:337:THR:O	1:D:341:GLN:HG3	2.18	0.44
1:C:301:VAL:HG13	1:C:440:CYS:SG	2.58	0.44
1:A:299:MET:SD	1:A:358:PRO:HB2	2.58	0.44
1:B:299:MET:HE1	1:B:358:PRO:HG2	1.99	0.44
1:B:431:MET:SD	1:B:488:LYS:HD3	2.58	0.44
1:A:386:HIS:CD2	1:A:438:LEU:HD22	2.53	0.44
1:A:520:THR:O	1:A:521:PHE:C	2.54	0.44
1:B:412:GLY:O	1:C:517:PRO:HB3	2.17	0.44
1:A:386:HIS:O	1:A:389:ILE:HG13	2.18	0.43
1:B:370:ILE:HG21	1:B:454:LEU:HD23	2.00	0.43
1:D:386:HIS:CD2	1:D:438:LEU:HD22	2.52	0.43
1:D:456:ASN:CG	1:D:459:GLU:HB2	2.39	0.43
1:B:305:LEU:CD1	1:B:309:LEU:HD11	2.48	0.43
1:C:468:TYR:HA	1:C:471:LEU:HB3	2.01	0.43
1:C:423:GLU:HG2	1:D:450:ASP:OD1	2.18	0.43
1:A:384:PHE:CD1	1:A:385:SER:N	2.86	0.43
1:B:399:THR:HG22	1:B:401:LEU:H	1.83	0.43
1:C:343:ALA:CB	2:C:1:LG2:H273	2.49	0.43
2:B:1:LG2:H212	2:B:1:LG2:H272	2.00	0.43
1:B:399:THR:HG23	1:B:399:THR:O	2.19	0.43
1:C:434:ASP:OD1	1:C:437:GLU:HG3	2.18	0.43
1:D:302:ASP:O	1:D:306:GLU:OE1	2.37	0.43
1:A:387:ARG:NH1	1:A:398:ALA:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ARG:HG3	1:A:465:GLU:N	2.32	0.43
1:B:468:TYR:HA	1:B:471:LEU:HB3	2.00	0.42
1:A:465:GLU:HA	1:A:468:TYR:CD2	2.54	0.42
1:D:379:LEU:CD2	1:D:445:ILE:HG12	2.49	0.42
1:C:497:ARG:HD2	1:D:498:SER:HB3	2.01	0.42
1:A:493:LEU:N	1:A:494:PRO:HD2	2.34	0.42
1:C:424:LEU:O	1:C:428:MET:HG3	2.19	0.42
1:A:337:THR:O	1:A:341:GLN:HG3	2.19	0.42
1:C:379:LEU:HG	1:C:445:ILE:CD1	2.31	0.42
2:D:1:LG2:H272	2:D:1:LG2:H212	2.00	0.42
1:C:477:GLN:O	1:C:480:PRO:HD3	2.19	0.42
1:D:307:ALA:HA	1:D:356:ARG:CD	2.49	0.42
1:A:307:ALA:HA	1:A:356:ARG:HD2	2.00	0.42
1:A:373:ARG:HD3	1:A:373:ARG:C	2.39	0.42
1:A:384:PHE:C	1:A:384:PHE:HD1	2.20	0.42
1:B:384:PHE:C	1:B:384:PHE:HD1	2.20	0.42
1:C:337:THR:O	1:C:341:GLN:HG3	2.20	0.42
1:A:348:PHE:CD1	1:C:369:VAL:HG12	2.54	0.42
1:C:387:ARG:HG2	1:C:396:LEU:HD23	2.00	0.42
1:A:399:THR:O	1:A:399:THR:HG23	2.20	0.42
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.94	0.42
1:A:348:PHE:HB2	1:C:369:VAL:HG12	2.01	0.41
1:C:387:ARG:HG2	1:C:387:ARG:O	2.20	0.41
1:A:386:HIS:HD2	1:A:438:LEU:HB2	1.84	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.87	0.41
1:B:373:ARG:C	1:B:373:ARG:HD3	2.40	0.41
1:B:493:LEU:N	1:B:494:PRO:HD2	2.35	0.41
1:A:399:THR:HG22	1:A:401:LEU:H	1.85	0.41
1:A:301:VAL:HG13	1:A:436:THR:HG23	2.02	0.41
1:C:501:LEU:HD12	1:D:501:LEU:HD12	2.01	0.41
1:A:372:LEU:HD22	1:C:348:PHE:HE1	1.84	0.41
1:B:464:ARG:HG3	1:B:465:GLU:N	2.34	0.41
1:C:493:LEU:N	1:C:494:PRO:HD2	2.35	0.41
1:D:468:TYR:HA	1:D:471:LEU:HB3	2.02	0.41
1:A:369:VAL:HG12	1:C:348:PHE:CD1	2.56	0.41
1:A:301:VAL:HG11	1:A:436:THR:HG23	2.02	0.41
1:B:507:LEU:HA	1:B:507:LEU:HD23	1.95	0.41
1:D:492:ARG:HA	1:D:492:ARG:NE	2.36	0.41
1:A:434:ASP:OD1	1:A:437:GLU:HG3	2.21	0.41
1:D:300:PRO:HG2	1:D:303:ARG:HB2	2.02	0.41
1:D:454:LEU:HD22	1:D:460:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:LG2:H272	2:C:1:LG2:H212	2.02	0.40
1:A:299:MET:HE2	1:A:467:VAL:HG22	2.01	0.40
1:D:307:ALA:HA	1:D:356:ARG:HD3	2.03	0.40
1:C:356:ARG:HH11	1:C:356:ARG:HG3	1.86	0.40
1:C:299:MET:HE3	1:C:358:PRO:HG2	2.03	0.40
1:C:386:HIS:HD2	1:C:438:LEU:HB2	1.86	0.40
1:A:376:TRP:CG	1:A:377:ASN:N	2.89	0.40
1:C:455:SER:OG	1:C:456:ASN:N	2.55	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	197/224 (88%)	186 (94%)	9 (5%)	2 (1%)	15	37
1	B	197/224 (88%)	188 (95%)	8 (4%)	1 (0%)	29	54
1	C	197/224 (88%)	190 (96%)	5 (2%)	2 (1%)	15	37
1	D	197/224 (88%)	188 (95%)	7 (4%)	2 (1%)	15	37
All	All	788/896 (88%)	752 (95%)	29 (4%)	7 (1%)	17	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	PRO
1	A	521	PHE
1	B	358	PRO
1	C	358	PRO
1	D	358	PRO
1	D	405	ARG
1	C	405	ARG



### 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	166/191 (87%)	154 (93%)	12 (7%)	14	34
1	B	165/191 (86%)	153 (93%)	12 (7%)	14	33
1	C	166/191 (87%)	154 (93%)	12 (7%)	14	34
1	D	165/191 (86%)	155 (94%)	10 (6%)	18	41
All	All	662/764 (87%)	616 (93%)	46 (7%)	15	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	A	306	GLU
1	A	358	PRO
1	A	373	ARG
1	A	384	PHE
1	A	395	ILE
1	A	399	THR
1	A	406	ASN
1	A	421	LEU
1	A	445	ILE
1	A	464	ARG
1	A	493	LEU
1	B	358	PRO
1	B	369	VAL
1	B	373	ARG
1	B	384	PHE
1	B	395	ILE
1	B	399	THR
1	B	406	ASN
1	B	421	LEU
1	B	445	ILE
1	B	455	SER
1	B	464	ARG
1	B	493	LEU

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Mol	Chain	Res	Type
1	C	305	LEU
1	C	358	PRO
1	C	373	ARG
1	C	384	PHE
1	C	395	ILE
1	C	399	THR
1	C	406	ASN
1	C	421	LEU
1	C	445	ILE
1	C	464	ARG
1	C	493	LEU
1	C	512	LEU
1	D	358	PRO
1	D	373	ARG
1	D	384	PHE
1	D	395	ILE
1	D	399	THR
1	D	406	ASN
1	D	421	LEU
1	D	445	ILE
1	D	464	ARG
1	D	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	477	GLN
1	A	506	HIS
1	B	346	GLN
1	B	377	ASN
1	B	506	HIS
1	C	377	ASN
1	C	477	GLN
1	C	506	HIS
1	D	377	ASN
1	D	506	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	LG2	D	1	-	27,30,30	3.25	10 (37%)	41,49,49	1.19	2 (4%)
2	LG2	A	1	-	27,30,30	2.55	11 (40%)	41,49,49	1.20	3 (7%)
2	LG2	C	1	-	27,30,30	2.83	10 (37%)	41,49,49	1.12	2 (4%)
2	LG2	B	1	-	27,30,30	2.92	11 (40%)	41,49,49	1.16	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	LG2	D	1	-	-	5/11/39/39	0/4/4/4
2	LG2	A	1	-	-	5/11/39/39	0/4/4/4
2	LG2	C	1	-	-	3/11/39/39	0/4/4/4
2	LG2	B	1	-	-	3/11/39/39	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	LG2	C4-C3	11.80	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	LG2	C4-C3	10.19	1.49	1.41
2	C	1	LG2	C4-C3	8.59	1.48	1.41
2	A	1	LG2	C4-C3	7.38	1.47	1.41
2	D	1	LG2	C15-C18	7.05	1.54	1.47
2	B	1	LG2	C15-C18	5.85	1.53	1.47
2	C	1	LG2	C15-C18	5.72	1.53	1.47
2	A	1	LG2	C15-C18	5.10	1.52	1.47
2	C	1	LG2	C5-C6	4.38	1.46	1.39
2	B	1	LG2	C5-C4	4.25	1.45	1.39
2	A	1	LG2	C5-C4	3.95	1.45	1.39
2	C	1	LG2	C5-C4	3.89	1.45	1.39
2	D	1	LG2	C5-C6	3.86	1.45	1.39
2	B	1	LG2	C6-C1	3.74	1.47	1.40
2	A	1	LG2	C5-C6	3.69	1.45	1.39
2	B	1	LG2	C5-C6	3.63	1.45	1.39
2	D	1	LG2	C14-C15	3.58	1.45	1.39
2	C	1	LG2	C6-C1	3.54	1.46	1.40
2	C	1	LG2	C17-C12	3.52	1.45	1.39
2	D	1	LG2	C5-C4	3.34	1.44	1.39
2	D	1	LG2	C6-C1	3.32	1.46	1.40
2	A	1	LG2	C2-C3	3.32	1.44	1.39
2	A	1	LG2	C6-C1	3.27	1.46	1.40
2	C	1	LG2	C2-C1	3.25	1.44	1.39
2	D	1	LG2	C17-C12	3.21	1.45	1.39
2	C	1	LG2	C2-C3	3.17	1.44	1.39
2	A	1	LG2	C2-C1	3.14	1.44	1.39
2	D	1	LG2	C2-C1	3.03	1.44	1.39
2	B	1	LG2	C14-C15	2.88	1.44	1.39
2	C	1	LG2	C14-C15	2.74	1.44	1.39
2	C	1	LG2	C17-C16	2.69	1.43	1.38
2	D	1	LG2	C17-C16	2.65	1.43	1.38
2	A	1	LG2	C17-C12	2.63	1.44	1.39
2	A	1	LG2	C14-C15	2.55	1.43	1.39
2	B	1	LG2	C2-C1	2.54	1.43	1.39
2	B	1	LG2	C2-C3	2.51	1.43	1.39
2	B	1	LG2	C17-C16	2.50	1.43	1.38
2	D	1	LG2	C2-C3	2.20	1.42	1.39
2	B	1	LG2	C17-C12	2.19	1.43	1.39
2	B	1	LG2	C16-C15	2.15	1.43	1.39
2	A	1	LG2	C17-C16	2.07	1.42	1.38
2	A	1	LG2	C12-N13	2.02	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	LG2	C21-C11-C12	-3.24	111.89	117.28
2	A	1	LG2	C22-C11-C21	2.93	60.51	58.70
2	B	1	LG2	C21-C11-C12	-2.84	112.56	117.28
2	A	1	LG2	C21-C11-C12	-2.63	112.91	117.28
2	C	1	LG2	C21-C11-C12	-2.43	113.24	117.28
2	A	1	LG2	C26-C10-C1	2.33	114.11	110.10
2	B	1	LG2	C24-C7-C6	2.20	113.88	110.10
2	D	1	LG2	C26-C10-C1	2.13	113.76	110.10
2	C	1	LG2	C22-C11-C12	2.01	120.62	117.28

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	LG2	C22-C11-C3-C4
2	A	1	LG2	C22-C11-C3-C4
2	C	1	LG2	C22-C11-C3-C4
2	B	1	LG2	C22-C11-C3-C4
2	A	1	LG2	C22-C11-C12-C17
2	D	1	LG2	C21-C11-C3-C4
2	A	1	LG2	C21-C11-C3-C4
2	C	1	LG2	C21-C11-C3-C4
2	B	1	LG2	C21-C11-C3-C4
2	D	1	LG2	C22-C11-C3-C2
2	D	1	LG2	C22-C11-C12-N13
2	A	1	LG2	C21-C11-C12-N13
2	D	1	LG2	C3-C11-C12-C17
2	A	1	LG2	C3-C11-C12-C17
2	C	1	LG2	C3-C11-C12-C17
2	B	1	LG2	C3-C11-C12-C17

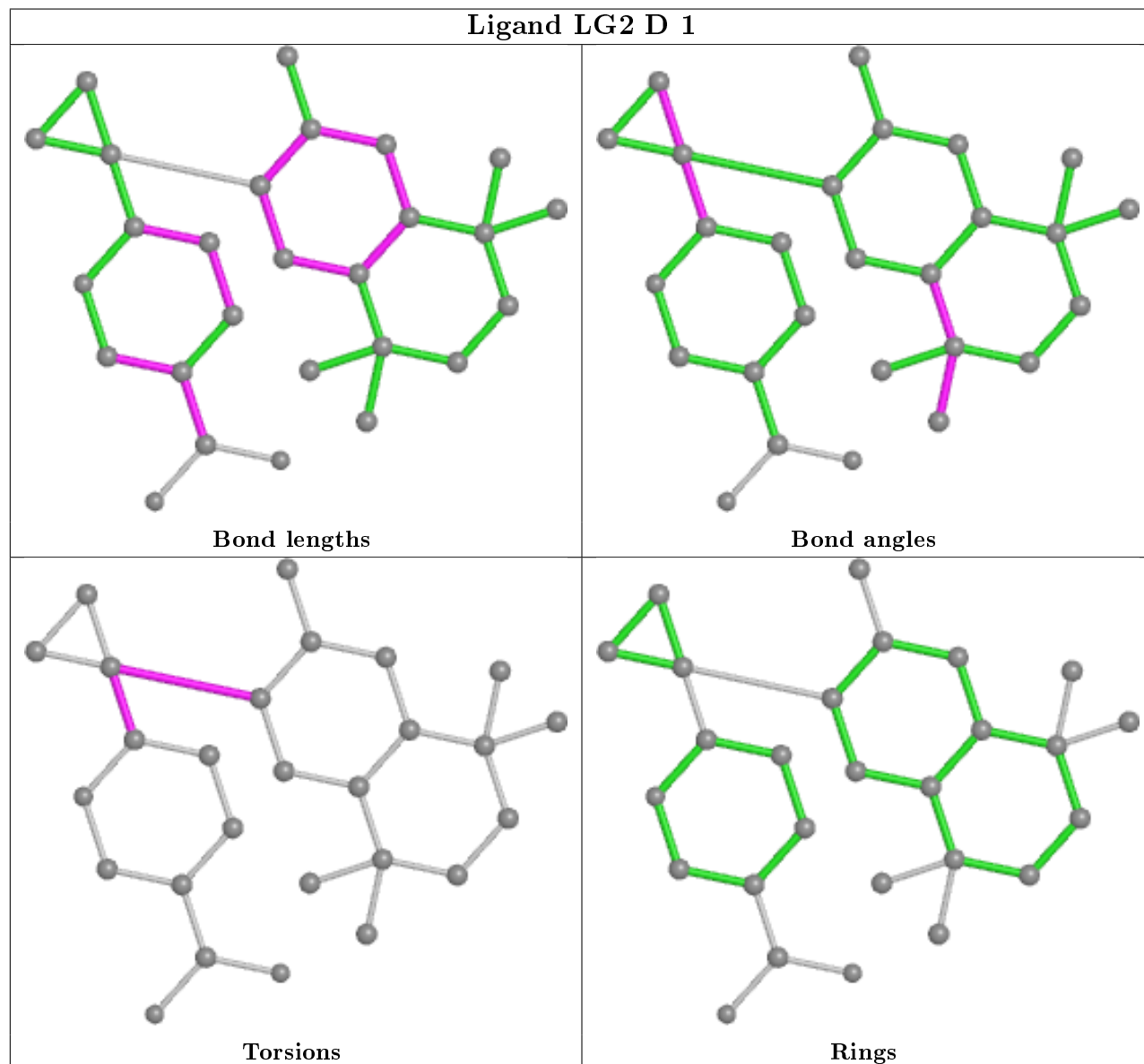
There are no ring outliers.

4 monomers are involved in 21 short contacts:

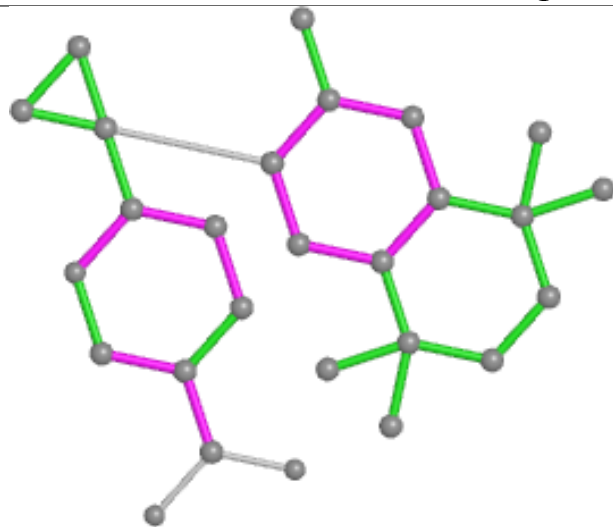
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	LG2	4	0
2	A	1	LG2	6	0
2	C	1	LG2	9	0
2	B	1	LG2	2	0

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

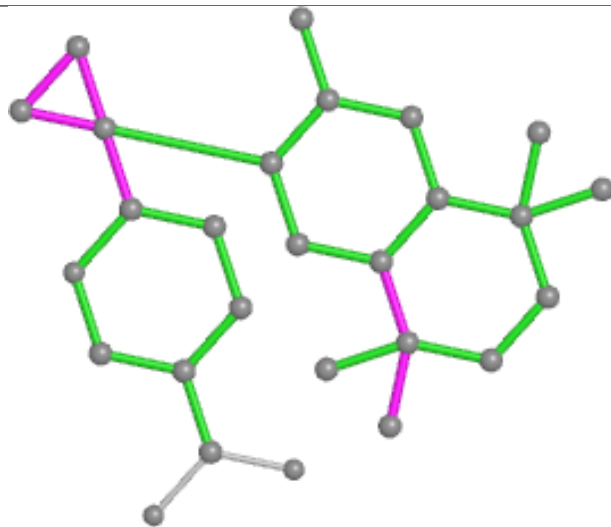
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



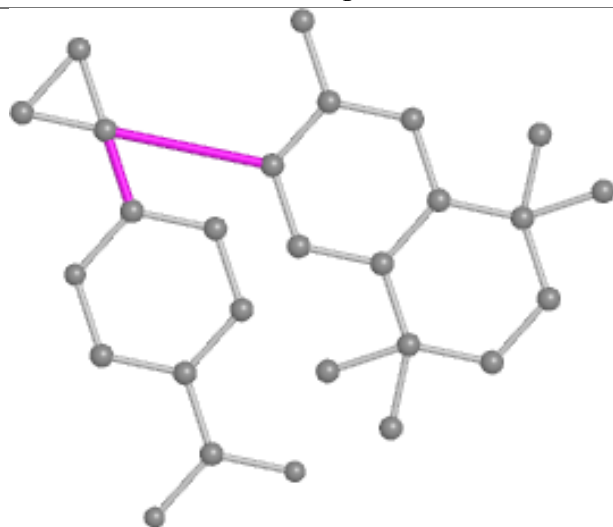
## Ligand LG2 A 1



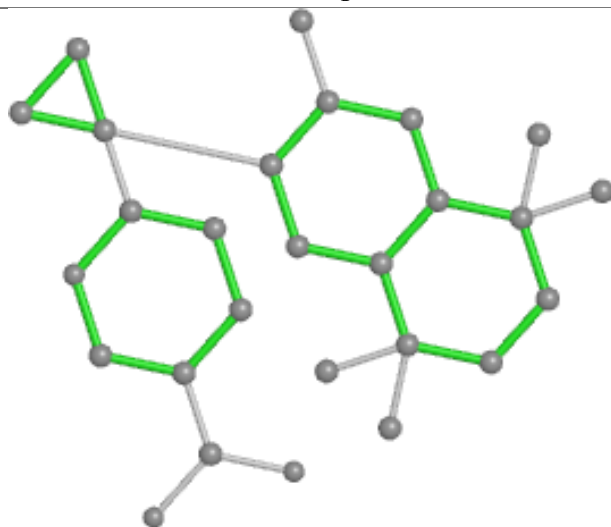
Bond lengths



Bond angles

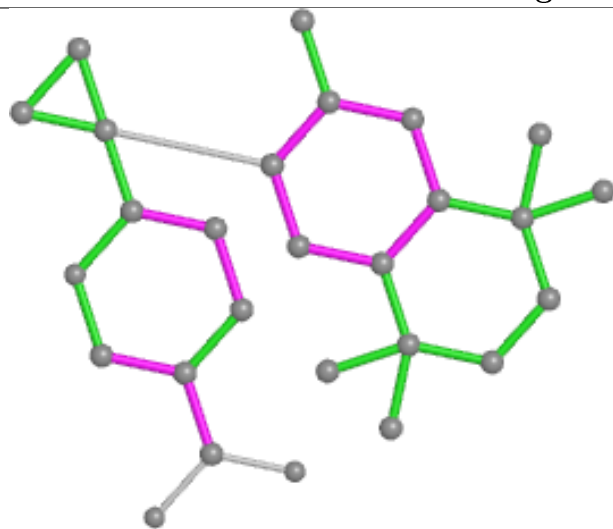


Torsions

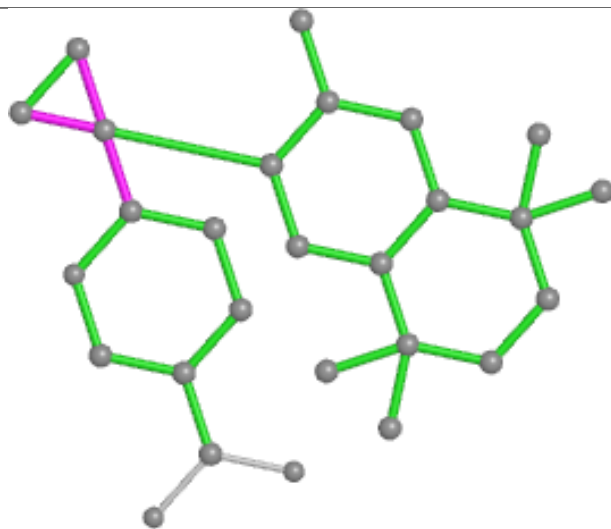


Rings

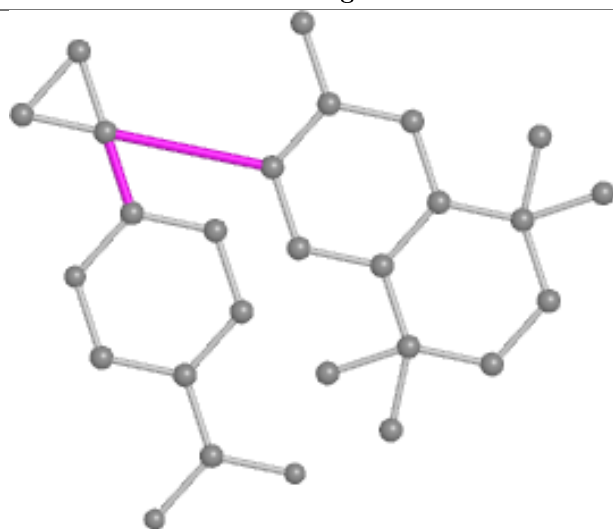
## Ligand LG2 C 1



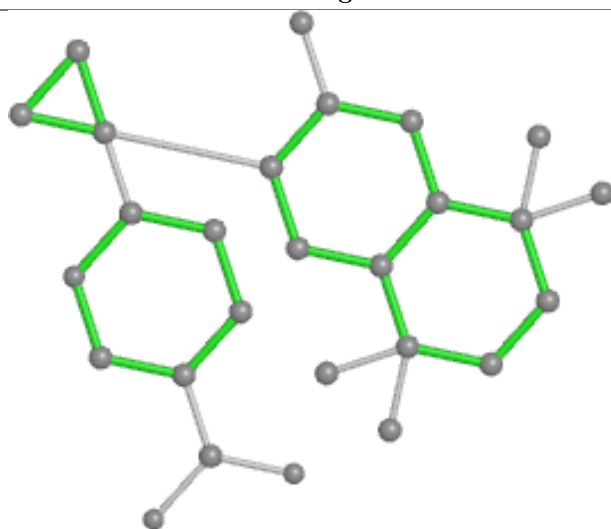
Bond lengths



Bond angles

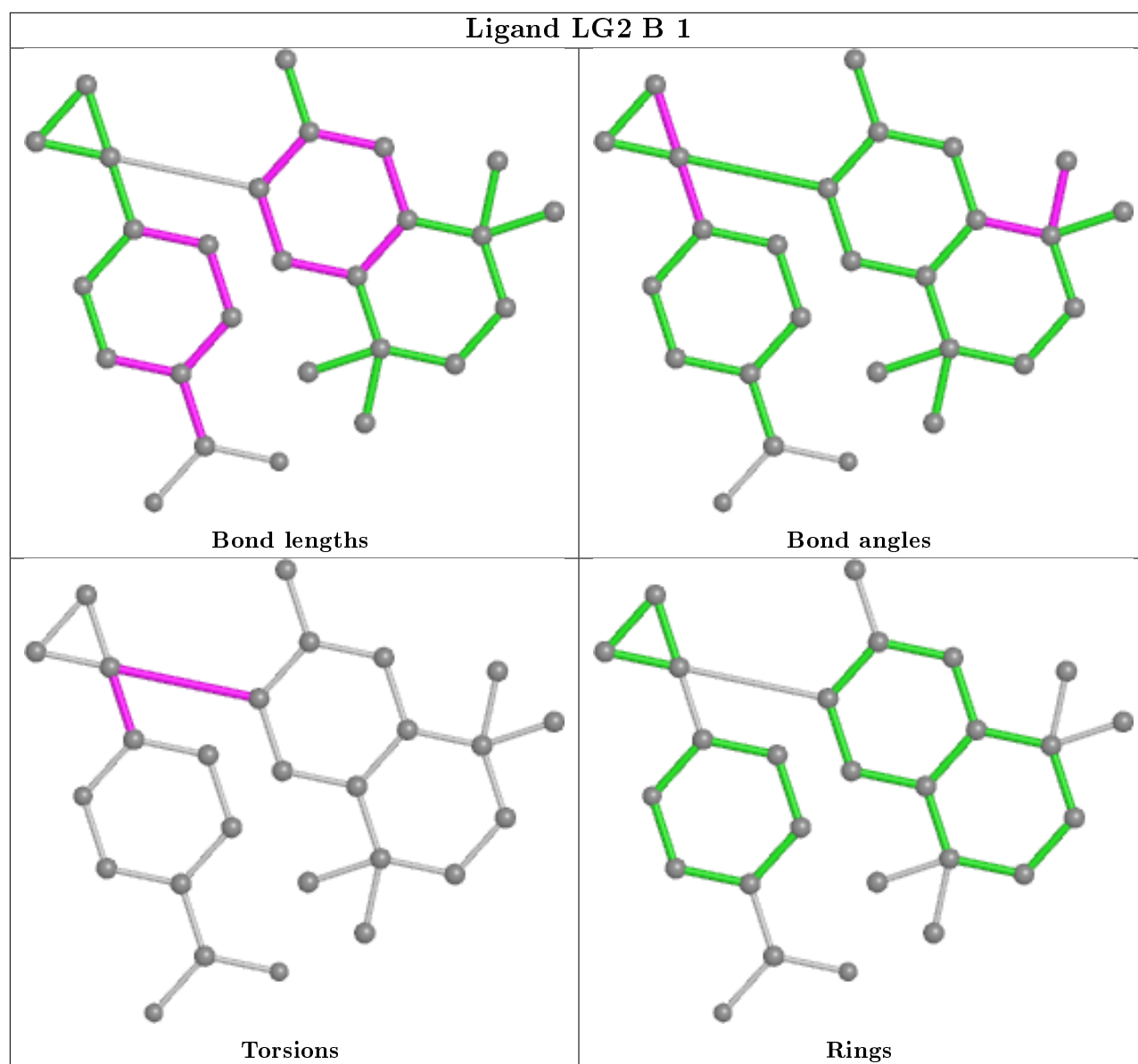


Torsions



Rings





## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.