



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 07:49 PM EDT

PDB ID : 3Q4U  
Title : Crystal structure of the ACVR1 kinase domain in complex with LDN-193189  
Authors : Chaikuad, A.; Sanvitale, C.; Cooper, C.D.O.; Mahajan, P.; Daga, N.; Petrie, K.; Alfano, I.; Gileadi, O.; Fedorov, O.; Allerston, C.K.; Krojer, T.; Vollmar, M.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-12-24  
Resolution : 1.82 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

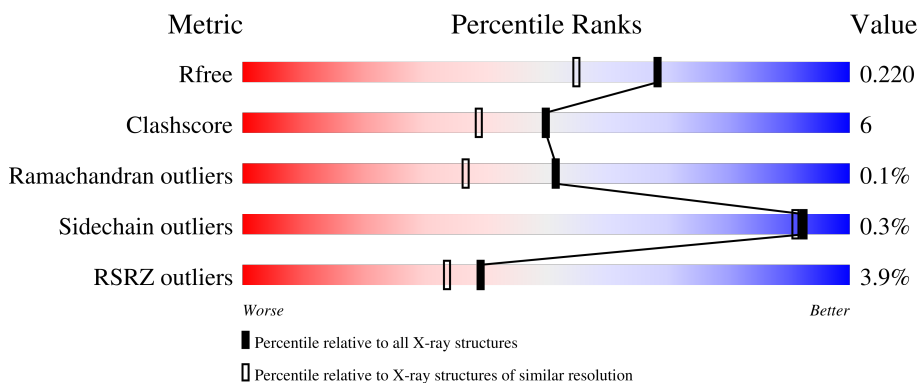
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">88% 10%</p>
1	B	301	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">8% 90% 10%</p>
1	C	301	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">3% 90% 7%</p>
1	D	301	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">3% 86% 14%</p>

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
4	FLC	B	5	-	X	-	-
4	FLC	B	501	-	X	-	-
4	FLC	C	12	-	X	-	-
4	FLC	C	3	-	X	-	-
4	FLC	D	10	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11134 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.

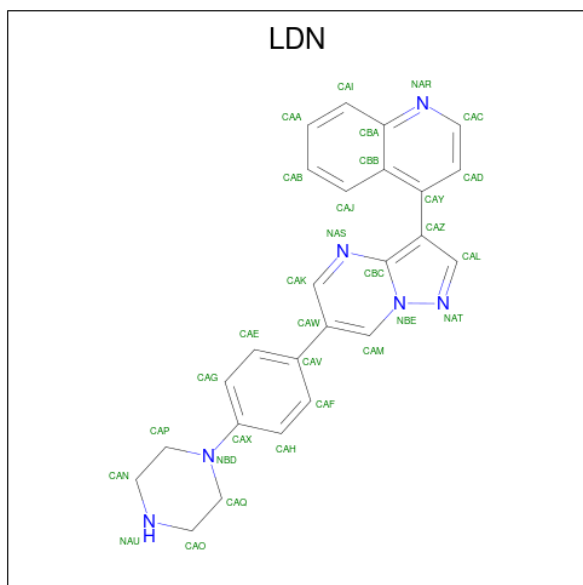
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2435	1550	421	446	18	0	10	0
1	B	300	2408	1533	420	438	17	0	6	0
1	C	296	2459	1570	421	451	17	0	17	0
1	D	299	2465	1568	426	454	17	0	12	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771
C	199	SER	-	expression tag	UNP Q04771
C	200	MET	-	expression tag	UNP Q04771
C	207	ASP	GLN	engineered mutation	UNP Q04771
D	199	SER	-	expression tag	UNP Q04771
D	200	MET	-	expression tag	UNP Q04771
D	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 4-[6-(4-piperazin-1-ylphenyl)pyrazolo[1,5-a]pyrimidin-3-yl]quinoline (three-letter code: LDN) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>).



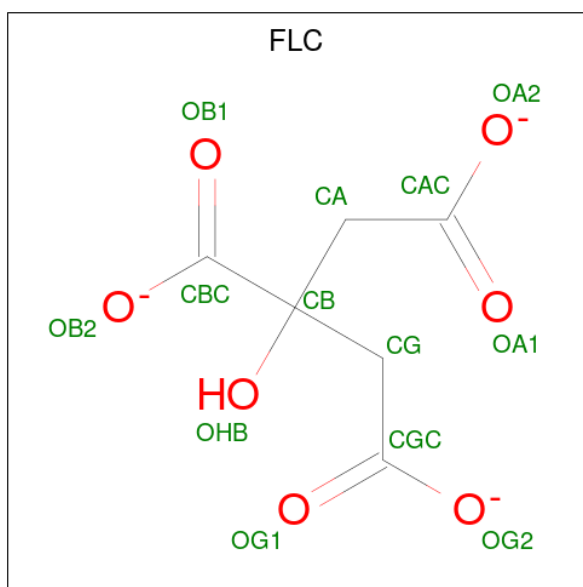
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C N	0	0
			31	25 6		
2	B	1	Total	C N	0	0
			31	25 6		
2	C	1	Total	C N	0	0
			31	25 6		
2	D	1	Total	C N	0	0
			31	25 6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 8 4 4	0	1
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 8 4 4	0	1
3	D	1	Total C O 8 4 4	0	1

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

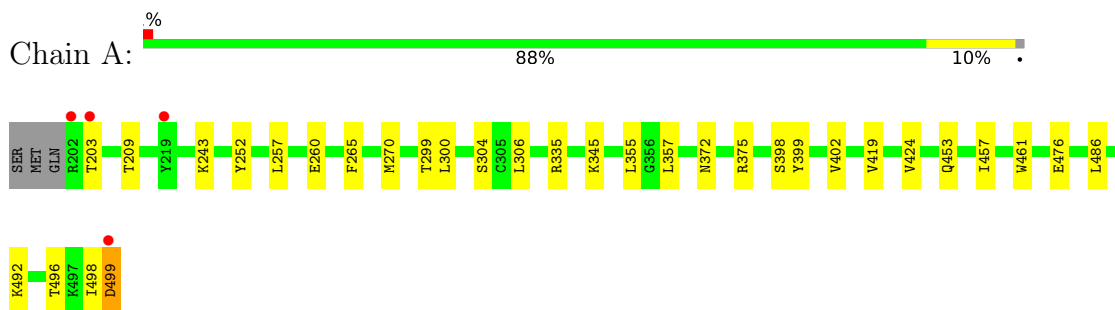


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	254	Total 254	O 254	0	0
5	B	218	Total 218	O 218	0	0
5	C	254	Total 254	O 254	0	0
5	D	293	Total 293	O 293	0	0

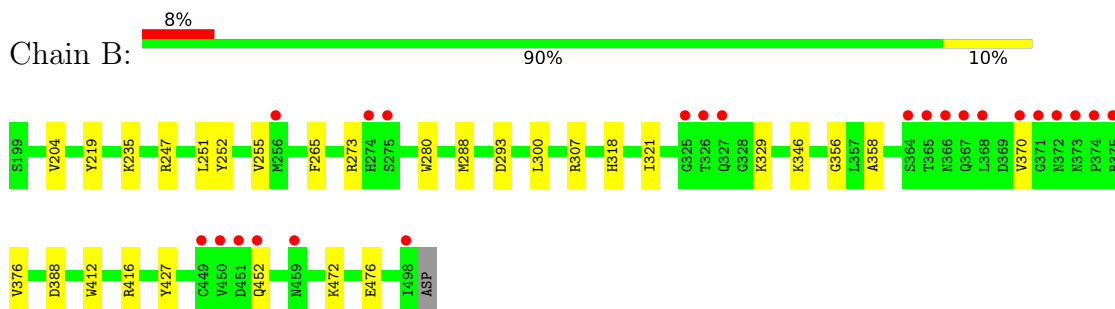
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

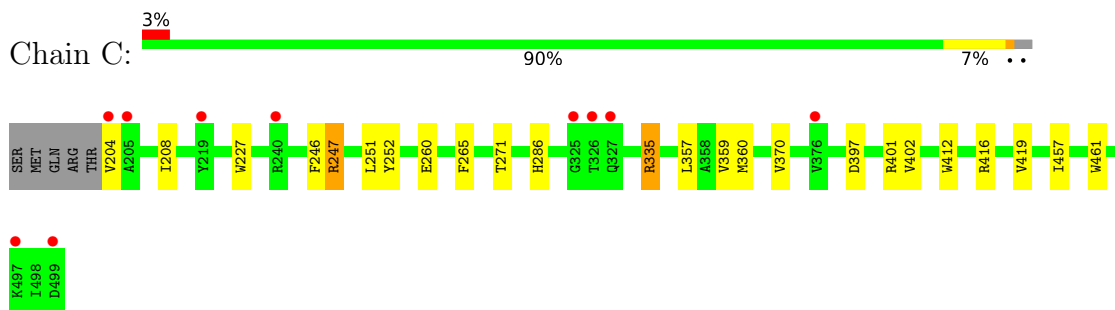
- Molecule 1: Activin receptor type-1



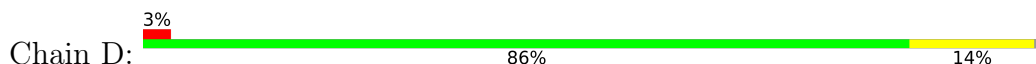
- Molecule 1: Activin receptor type-1

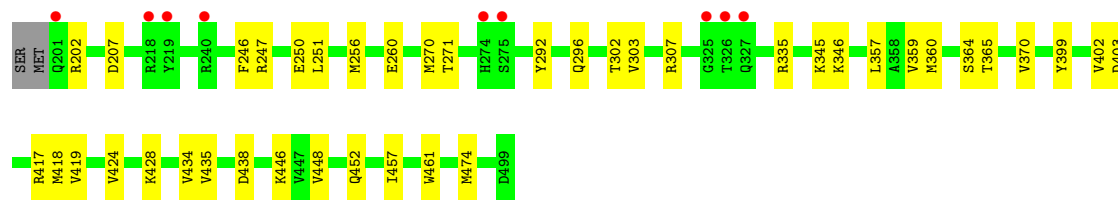


- Molecule 1: Activin receptor type-1



- Molecule 1: Activin receptor type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.60Å 98.70Å 83.85Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	37.22 – 1.82 37.21 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.22-1.82) 99.1 (37.21-1.82)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.163 , 0.219 0.166 , 0.220	Depositor DCC
$R_{free}$ test set	5385 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.018 for h,-k,-h-l 0.020 for -h-l,-k,l 0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDN, FLC, EDO

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	0.73	0/2519	0.69	0/3414
1	B	0.66	0/2480	0.67	0/3365
1	C	0.78	0/2565	0.75	3/3478 (0.1%)
1	D	0.79	0/2553	0.76	4/3460 (0.1%)
All	All	0.74	0/10117	0.72	7/13717 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	417	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	247	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	335	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	D	247	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	403	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	417	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	247	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2435	0	2449	23	0
1	B	2408	0	2399	26	0
1	C	2459	0	2482	25	0
1	D	2465	0	2471	30	0
2	A	31	0	22	0	0
2	B	31	0	22	2	0
2	C	31	0	22	1	0
2	D	31	0	22	0	0
3	A	20	0	30	4	0
3	B	8	0	12	2	0
3	C	16	0	24	5	0
3	D	24	0	36	2	0
4	A	26	0	10	3	0
4	B	52	0	20	5	0
4	C	39	0	15	4	0
4	D	39	0	15	5	0
5	A	254	0	0	2	0
5	B	218	0	0	7	0
5	C	254	0	0	6	0
5	D	293	0	0	9	0
All	All	11134	0	10051	116	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 6.

All (116) 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:247:ARG:HD3	3:C:9[B]:EDO:H21	1.68	0.76
4:D:11:FLC:OG2	5:D:1152:HOH:O	2.09	0.70
4:D:9:FLC:CBC	4:D:9:FLC:OA2	2.37	0.69
1:C:397[B]:ASP:OD2	1:C:401[B]:ARG:CZ	2.40	0.69
1:B:293:ASP:OD2	5:B:972:HOH:O	2.11	0.66
1:C:397[B]:ASP:OD2	1:C:401[B]:ARG:NH2	2.29	0.65
1:A:492:LYS:O	1:A:496[B]:THR:HG23	1.98	0.64
4:C:3:FLC:HA1	4:C:3:FLC:OG2	1.97	0.64
1:A:498:ILE:O	5:A:552:HOH:O	2.16	0.63
1:C:286:HIS:CE1	4:C:3:FLC:HG2	2.33	0.62
1:D:271[B]:THR:HG23	5:D:650:HOH:O	2.00	0.62
1:D:302[B]:THR:HG22	1:D:418:MET:CE	2.30	0.62
4:A:501:FLC:CBC	4:A:501:FLC:OA2	2.47	0.61
1:C:260:GLU:HG3	5:C:568:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD21	1:D:360[B]:MET:SD	2.41	0.60
1:D:345:LYS:NZ	4:D:10:FLC:HA1	2.17	0.60
4:C:3:FLC:OA2	4:C:3:FLC:OB2	2.21	0.58
1:D:303:VAL:HG21	5:D:672:HOH:O	2.03	0.58
4:B:501:FLC:HG1	5:B:984:HOH:O	2.04	0.57
1:B:247:ARG:HD3	1:B:358:ALA:O	2.04	0.57
1:A:243:LYS:HD3	1:A:372:ASN:O	2.05	0.57
1:D:335:ARG:HD3	1:D:357:LEU:O	2.06	0.56
1:C:260:GLU:CG	5:C:568:HOH:O	2.52	0.55
1:C:335:ARG:HD3	1:C:357:LEU:O	2.06	0.55
1:B:376:VAL:HG11	5:B:776:HOH:O	2.06	0.55
1:A:304:SER:OG	3:A:500:EDO:H22	2.07	0.55
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.40	0.55
4:C:500:FLC:HG1	5:C:624:HOH:O	2.07	0.55
1:A:306:LEU:HD13	1:A:499:ASP:HB3	1.89	0.54
1:C:370[B]:VAL:HG22	5:C:559:HOH:O	2.08	0.54
1:A:476:GLU:HB3	1:A:486:LEU:HG	1.88	0.54
1:A:299:THR:O	3:A:4:EDO:H22	2.08	0.54
1:C:359:VAL:HG22	1:C:370[B]:VAL:HA	1.90	0.54
1:A:419:VAL:HG22	1:A:424:VAL:HG13	1.90	0.53
1:A:345:LYS:NZ	4:A:502:FLC:OHB	2.42	0.53
1:B:300:LEU:HA	3:B:8:EDO:C1	2.39	0.53
1:D:370:VAL:HG12	1:D:370:VAL:O	2.09	0.52
3:D:13[B]:EDO:C2	5:D:1064:HOH:O	2.57	0.52
1:C:359:VAL:HG22	1:C:370[A]:VAL:HA	1.91	0.52
1:D:438:ASP:HA	3:D:13[B]:EDO:H11	1.92	0.51
1:C:401[B]:ARG:NH1	5:C:1041:HOH:O	2.35	0.51
1:C:402:VAL:HG13	5:C:1025:HOH:O	2.10	0.51
4:B:6:FLC:CGC	4:B:6:FLC:OB2	2.59	0.51
1:B:251:LEU:O	1:B:255:VAL:HB	2.12	0.50
1:B:346:LYS:HB2	4:B:5:FLC:OB1	2.11	0.50
1:A:399:TYR:O	1:A:402[B]:VAL:HG22	2.12	0.49
4:B:500:FLC:OG2	4:B:500:FLC:OHB	2.30	0.49
1:C:251:LEU:HD21	1:C:360[B]:MET:SD	2.52	0.49
1:B:300:LEU:HA	3:B:8:EDO:H12	1.95	0.49
1:D:307:ARG:NH1	5:D:726:HOH:O	2.44	0.48
1:D:202:ARG:HA	1:D:207:ASP:OD1	2.13	0.48
1:A:357:LEU:HD21	1:A:375:ARG:HB3	1.96	0.48
1:A:300:LEU:HA	3:A:500:EDO:C2	2.43	0.48
1:D:399:TYR:O	1:D:402:VAL:HG22	2.14	0.47
1:C:412:TRP:CZ2	1:C:416:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:MET:HB2	5:D:1055:HOH:O	2.13	0.47
1:C:246:PHE:HD2	3:C:9[B]:EDO:H22	1.79	0.47
1:B:288[B]:MET:HE1	5:B:630:HOH:O	2.13	0.47
1:B:307:ARG:NH1	5:B:674:HOH:O	2.48	0.47
1:A:402[A]:VAL:HG13	5:A:571:HOH:O	2.16	0.46
4:B:500:FLC:CBC	4:B:500:FLC:OA1	2.63	0.46
1:D:370:VAL:O	1:D:370:VAL:CG1	2.64	0.45
1:A:260:GLU:HA	4:A:502:FLC:HA1	1.98	0.45
1:A:300:LEU:HA	3:A:500:EDO:H22	1.97	0.45
1:B:376:VAL:HG21	5:B:990:HOH:O	2.16	0.45
1:C:246:PHE:HD2	3:C:9[A]:EDO:H22	1.81	0.45
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.51	0.45
1:B:472:LYS:O	1:B:476:GLU:HG3	2.16	0.45
1:D:345:LYS:HD3	4:D:10:FLC:OG2	2.17	0.45
1:D:335:ARG:CD	1:D:359:VAL:HG13	2.47	0.45
1:B:288[A]:MET:HB3	1:B:288[A]:MET:HE3	1.88	0.44
1:A:457:ILE:HG23	1:A:461:TRP:CE3	2.52	0.44
1:D:448:VAL:O	1:D:452:GLN:HA	2.18	0.44
1:B:318:HIS:O	1:B:329:LYS:HE3	2.18	0.44
1:C:457:ILE:HG23	1:C:461:TRP:CE3	2.53	0.44
1:D:335:ARG:HD2	1:D:359:VAL:HG13	2.00	0.44
1:D:428:LYS:NZ	5:D:1106:HOH:O	2.51	0.43
2:B:1:LDN:CBC	2:B:1:LDN:HAJ	2.49	0.43
1:C:251:LEU:HD21	1:C:360[B]:MET:CE	2.47	0.43
1:A:335:ARG:HD3	1:A:357:LEU:O	2.18	0.43
1:B:204:VAL:HG11	1:B:280:TRP:CE2	2.53	0.43
1:A:257:LEU:HD23	1:A:355:LEU:CD1	2.49	0.43
2:C:4:LDN:HAG	2:C:4:LDN:HAQ	1.80	0.43
1:B:219:TYR:HB2	1:B:235:LYS:NZ	2.33	0.43
1:C:271[B]:THR:HG23	3:C:11:EDO:H22	2.01	0.43
1:A:398:SER:O	1:A:402[B]:VAL:HG13	2.18	0.43
1:B:219:TYR:HD2	1:B:235:LYS:HZ1	1.62	0.43
1:B:247:ARG:HD2	1:B:356:GLY:O	2.19	0.42
1:D:246:PHE:CE2	1:D:250:GLU:HG3	2.54	0.42
1:A:203:THR:O	1:B:273:ARG:NH1	2.41	0.42
1:C:252:TYR:CD1	1:C:265:PHE:HB2	2.54	0.42
1:D:303:VAL:HG21	5:D:607:HOH:O	2.19	0.42
1:D:434:VAL:HG23	1:D:435:VAL:HG13	2.02	0.42
1:D:364:SER:OG	1:D:365:THR:HG23	2.19	0.42
1:B:427:TYR:CD2	1:B:427:TYR:C	2.92	0.42
1:A:209:THR:OG1	1:C:419:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453[A]:GLN:HA	1:A:453[A]:GLN:OE1	2.20	0.41
1:D:461:TRP:CZ3	1:D:474:MET:HE1	2.55	0.41
1:B:288[B]:MET:HB3	1:B:288[B]:MET:HE2	1.98	0.41
1:D:457:ILE:HG23	1:D:461:TRP:CE3	2.55	0.41
1:C:204:VAL:O	1:C:208:ILE:HG13	2.21	0.41
1:C:335:ARG:HD2	1:C:359:VAL:CG2	2.50	0.41
1:A:252:TYR:CD1	1:A:265:PHE:HB2	2.56	0.41
1:C:247:ARG:HD3	3:C:9[A]:EDO:H21	2.02	0.41
1:D:251:LEU:CD2	1:D:360[B]:MET:SD	3.08	0.41
1:B:452:GLN:HG2	5:B:771:HOH:O	2.21	0.41
2:B:1:LDN:HAH	2:B:1:LDN:HAPA	1.80	0.41
1:D:260[A]:GLU:OE1	1:D:345:LYS:NZ	2.53	0.41
1:C:204:VAL:HG13	1:C:227:TRP:CE2	2.56	0.40
1:D:446:LYS:NZ	5:D:595:HOH:O	2.21	0.40
1:B:388:ASP:OD1	1:B:388:ASP:C	2.59	0.40
1:D:346:LYS:HD2	4:D:9:FLC:HG1	2.04	0.40
1:D:292:TYR:O	1:D:296:GLN:HG2	2.21	0.40
1:D:419:VAL:HG22	1:D:424:VAL:HB	2.03	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	306/301 (102%)	301 (98%)	5 (2%)	0	100	100
1	B	304/301 (101%)	293 (96%)	10 (3%)	1 (0%)	41	27
1	C	311/301 (103%)	306 (98%)	5 (2%)	0	100	100
1	D	309/301 (103%)	304 (98%)	5 (2%)	0	100	100
All	All	1230/1204 (102%)	1204 (98%)	25 (2%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	VAL

### 5.3.2 Protein sidechains [i](#)

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	275/270 (102%)	273 (99%)	2 (1%)	84 80
1	B	266/270 (98%)	266 (100%)	0	100 100
1	C	280/270 (104%)	280 (100%)	0	100 100
1	D	278/270 (103%)	277 (100%)	1 (0%)	91 89
All	All	1099/1080 (102%)	1096 (100%)	3 (0%)	92 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	A	499	ASP
1	D	270	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

33 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	FLC	B	501	-	12,12,12	1.50	2 (16%)	17,17,17	6.84	12 (70%)
3	EDO	A	1	-	3,3,3	0.50	0	2,2,2	0.26	0
3	EDO	A	5	-	3,3,3	0.62	0	2,2,2	0.52	0
4	FLC	D	10	-	12,12,12	1.93	3 (25%)	17,17,17	7.19	9 (52%)
4	FLC	D	11	-	12,12,12	0.94	0	17,17,17	1.79	5 (29%)
3	EDO	C	9[B]	-	3,3,3	0.42	0	2,2,2	0.14	0
3	EDO	C	9[A]	-	3,3,3	0.49	0	2,2,2	0.08	0
4	FLC	A	501	-	12,12,12	0.97	0	17,17,17	1.77	4 (23%)
3	EDO	D	14[B]	-	3,3,3	0.62	0	2,2,2	0.15	0
3	EDO	B	8	-	3,3,3	0.63	0	2,2,2	0.32	0
3	EDO	D	14[A]	-	3,3,3	0.56	0	2,2,2	0.27	0
3	EDO	A	4	-	3,3,3	0.52	0	2,2,2	0.56	0
4	FLC	C	500	-	12,12,12	1.33	0	17,17,17	1.41	3 (17%)
3	EDO	B	7	-	3,3,3	0.56	0	2,2,2	0.50	0
4	FLC	D	9	-	12,12,12	1.09	0	17,17,17	1.66	4 (23%)
2	LDN	A	3	-	30,36,36	1.77	4 (13%)	35,51,51	1.96	8 (22%)
3	EDO	D	12	-	3,3,3	0.48	0	2,2,2	0.45	0
2	LDN	C	4	-	30,36,36	1.34	5 (16%)	35,51,51	1.93	5 (14%)
4	FLC	C	3	-	12,12,12	1.61	1 (8%)	17,17,17	8.08	10 (58%)
4	FLC	B	500	-	12,12,12	1.23	1 (8%)	17,17,17	1.72	3 (17%)
4	FLC	C	12	-	12,12,12	1.81	4 (33%)	17,17,17	1.57	5 (29%)
4	FLC	B	6	-	12,12,12	1.20	1 (8%)	17,17,17	1.04	0
3	EDO	A	500	-	3,3,3	0.46	0	2,2,2	0.50	0
4	FLC	A	502	-	12,12,12	1.34	2 (16%)	17,17,17	2.28	5 (29%)
3	EDO	C	10	-	3,3,3	0.48	0	2,2,2	0.57	0
4	FLC	B	5	-	12,12,12	1.64	1 (8%)	17,17,17	6.77	11 (64%)
3	EDO	C	11	-	3,3,3	0.43	0	2,2,2	0.96	0
3	EDO	A	2	-	3,3,3	0.17	0	2,2,2	0.28	0
2	LDN	B	1	-	30,36,36	1.58	7 (23%)	35,51,51	1.75	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	6	-	3,3,3	0.72	0	2,2,2	0.43	0
2	LDN	D	2	-	30,36,36	1.50	5 (16%)	35,51,51	1.91	8 (22%)
3	EDO	D	13[A]	-	3,3,3	0.56	0	2,2,2	0.22	0
3	EDO	D	13[B]	-	3,3,3	0.36	0	2,2,2	0.49	0

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	FLC	B	501	-	-	7/16/16/16	-
3	EDO	A	1	-	-	1/1/1/1	-
3	EDO	A	5	-	-	0/1/1/1	-
4	FLC	D	10	-	-	6/16/16/16	-
4	FLC	D	11	-	-	8/16/16/16	-
3	EDO	C	9[B]	-	-	0/1/1/1	-
3	EDO	C	9[A]	-	-	0/1/1/1	-
4	FLC	A	501	-	-	4/16/16/16	-
3	EDO	D	14[B]	-	-	1/1/1/1	-
3	EDO	B	8	-	-	0/1/1/1	-
3	EDO	D	14[A]	-	-	1/1/1/1	-
3	EDO	A	4	-	-	1/1/1/1	-
4	FLC	C	500	-	-	2/16/16/16	-
3	EDO	B	7	-	-	1/1/1/1	-
4	FLC	D	9	-	-	9/16/16/16	-
2	LDN	A	3	-	-	0/4/20/20	0/6/6/6
3	EDO	D	12	-	-	0/1/1/1	-
2	LDN	C	4	-	-	0/4/20/20	0/6/6/6
4	FLC	C	3	-	-	15/16/16/16	-
4	FLC	B	500	-	-	2/16/16/16	-
4	FLC	C	12	-	-	9/16/16/16	-
4	FLC	B	6	-	-	5/16/16/16	-
3	EDO	A	500	-	-	0/1/1/1	-
4	FLC	A	502	-	-	4/16/16/16	-
3	EDO	C	10	-	-	1/1/1/1	-
4	FLC	B	5	-	-	8/16/16/16	-
3	EDO	C	11	-	-	0/1/1/1	-
3	EDO	A	2	-	-	0/1/1/1	-
2	LDN	B	1	-	-	0/4/20/20	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	6	-	-	1/1/1/1	-
2	LDN	D	2	-	-	0/4/20/20	0/6/6/6
3	EDO	D	13[A]	-	-	0/1/1/1	-
3	EDO	D	13[B]	-	-	1/1/1/1	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	LDN	CAK-NAS	5.66	1.37	1.30
4	D	10	FLC	CG-CB	4.50	1.59	1.53
4	C	3	FLC	OHB-CB	4.48	1.52	1.43
4	B	5	FLC	OHB-CB	4.44	1.51	1.43
2	D	2	LDN	CAK-NAS	4.26	1.35	1.30
2	A	3	LDN	CAL-CAZ	-3.95	1.32	1.40
2	B	1	LDN	CAD-CAC	3.90	1.42	1.36
4	C	12	FLC	CB-CBC	-3.69	1.49	1.53
2	A	3	LDN	CAD-CAC	3.46	1.41	1.36
4	B	501	FLC	CB-CBC	-3.43	1.49	1.53
2	D	2	LDN	CAL-CAZ	-3.28	1.33	1.40
2	B	1	LDN	CBC-NAS	3.08	1.37	1.33
2	B	1	LDN	CAK-NAS	3.07	1.34	1.30
2	C	4	LDN	CAK-NAS	2.96	1.34	1.30
2	C	4	LDN	CAF-CAH	2.84	1.42	1.36
4	A	502	FLC	CG-CB	2.72	1.57	1.53
2	D	2	LDN	CAD-CAC	2.72	1.40	1.36
4	C	12	FLC	CG-CB	-2.69	1.50	1.53
4	D	10	FLC	CA-CB	2.69	1.57	1.53
4	B	500	FLC	CB-CBC	-2.63	1.50	1.53
2	C	4	LDN	CBC-NAS	2.61	1.37	1.33
2	C	4	LDN	CAD-CAC	2.52	1.40	1.36
2	B	1	LDN	CAZ-CBC	-2.49	1.37	1.43
4	B	6	FLC	CB-CBC	-2.49	1.50	1.53
4	B	501	FLC	OHB-CB	2.45	1.48	1.43
2	C	4	LDN	CAL-CAZ	-2.40	1.35	1.40
2	B	1	LDN	CAL-CAZ	-2.37	1.35	1.40
2	B	1	LDN	CBA-NAR	-2.32	1.33	1.37
4	A	502	FLC	CB-CBC	-2.27	1.51	1.53
4	D	10	FLC	CB-CBC	-2.23	1.51	1.53
4	C	12	FLC	OA2-CAC	-2.19	1.23	1.30
2	B	1	LDN	CAF-CAH	2.15	1.41	1.36
2	D	2	LDN	CAB-CAJ	2.15	1.41	1.36
4	C	12	FLC	OG2-CGC	-2.14	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	LDN	CAF-CAH	2.14	1.41	1.36
2	D	2	LDN	CAE-CAG	2.01	1.40	1.36

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	FLC	OHB-CB-CBC	-23.31	76.14	108.86
4	D	10	FLC	OHB-CB-CBC	-18.31	83.16	108.86
4	B	501	FLC	OHB-CB-CBC	-16.41	85.82	108.86
4	B	5	FLC	OHB-CB-CBC	-14.66	88.28	108.86
4	C	3	FLC	OB1-CBC-CB	-13.32	103.40	122.25
4	D	10	FLC	OHB-CB-CA	-12.76	79.54	109.40
4	B	5	FLC	OHB-CB-CA	-12.00	81.32	109.40
4	B	501	FLC	OHB-CB-CA	-11.97	81.39	109.40
4	C	3	FLC	OHB-CB-CA	-11.38	82.78	109.40
4	B	5	FLC	OB1-CBC-CB	-11.02	106.65	122.25
4	B	501	FLC	OHB-CB-CG	-10.91	83.86	109.40
4	B	5	FLC	OB2-CBC-CB	10.62	131.49	113.05
4	D	10	FLC	OB1-CBC-CB	-10.04	108.04	122.25
4	B	5	FLC	OHB-CB-CG	-9.46	87.27	109.40
4	B	501	FLC	OB1-CBC-CB	-9.21	109.21	122.25
4	C	3	FLC	OB2-CBC-CB	9.17	128.97	113.05
4	D	10	FLC	CA-CB-CBC	8.92	129.27	110.11
4	B	501	FLC	CB-CA-CAC	-8.39	93.49	113.81
4	C	3	FLC	OHB-CB-CG	-8.27	90.05	109.40
4	D	10	FLC	OHB-CB-CG	-7.99	90.70	109.40
2	C	4	LDN	CAL-NAT-NBE	7.74	109.33	103.70
2	D	2	LDN	CAL-NAT-NBE	7.43	109.10	103.70
2	A	3	LDN	CAL-NAT-NBE	7.35	109.05	103.70
4	C	3	FLC	CA-CB-CBC	7.12	125.41	110.11
4	D	10	FLC	OB2-CBC-CB	6.96	125.14	113.05
2	B	1	LDN	CAL-NAT-NBE	6.95	108.76	103.70
4	B	5	FLC	CA-CB-CBC	5.87	122.72	110.11
4	B	501	FLC	OB2-CBC-CB	5.83	123.17	113.05
4	B	501	FLC	CG-CB-CA	5.76	124.18	109.16
4	D	10	FLC	CB-CG-CGC	-5.75	99.90	113.81
4	A	502	FLC	OB1-CBC-CB	-5.02	115.14	122.25
4	D	10	FLC	CB-CA-CAC	5.01	125.95	113.81
4	A	502	FLC	OHB-CB-CA	-4.82	98.12	109.40
4	C	3	FLC	CG-CB-CA	4.82	121.72	109.16
4	B	5	FLC	CG-CB-CBC	4.49	119.76	110.11
4	D	10	FLC	CG-CB-CA	4.47	120.81	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	11	FLC	OB2-CBC-CB	4.20	120.35	113.05
2	A	3	LDN	CAD-CAC-NAR	-4.17	120.52	125.10
4	B	500	FLC	OB1-CBC-CB	-4.16	116.36	122.25
4	B	5	FLC	CB-CG-CGC	4.04	123.60	113.81
4	A	501	FLC	OB2-CBC-CB	3.87	119.76	113.05
2	C	4	LDN	CAW-CAK-NAS	-3.56	120.21	125.05
4	D	9	FLC	OB2-CBC-CB	3.53	119.18	113.05
4	B	500	FLC	OB2-CBC-CB	3.41	118.97	113.05
4	B	501	FLC	CA-CB-CBC	3.39	117.39	110.11
4	A	502	FLC	OB2-CBC-CB	3.33	118.84	113.05
4	A	501	FLC	OHB-CB-CBC	3.31	113.50	108.86
4	A	502	FLC	CG-CB-CA	3.29	117.75	109.16
2	C	4	LDN	CAK-NAS-CBC	3.29	120.93	116.73
2	D	2	LDN	CAC-NAR-CBA	3.28	122.01	116.93
4	C	500	FLC	OB2-CBC-CB	3.20	118.61	113.05
4	B	500	FLC	CB-CG-CGC	-3.17	106.14	113.81
2	D	2	LDN	CAD-CAC-NAR	-3.15	121.64	125.10
4	C	3	FLC	OA1-CAC-CA	-3.13	113.79	122.94
2	B	1	LDN	CAQ-NBD-CAP	3.10	118.36	111.52
2	C	4	LDN	CAD-CAC-NAR	-3.06	121.74	125.10
4	D	9	FLC	CB-CA-CAC	-3.01	106.52	113.81
2	D	2	LDN	CAK-NAS-CBC	3.00	120.57	116.73
2	A	3	LDN	CAG-CAX-NBD	-3.00	117.24	121.38
4	B	501	FLC	OG1-CGC-CG	-2.94	114.34	122.94
4	C	12	FLC	CB-CA-CAC	-2.91	106.77	113.81
2	D	2	LDN	CAQ-NBD-CAP	2.90	117.92	111.52
2	B	1	LDN	CAW-CAK-NAS	-2.83	121.21	125.05
4	C	3	FLC	CB-CG-CGC	2.76	120.49	113.81
4	D	11	FLC	CG-CB-CA	2.74	116.32	109.16
2	B	1	LDN	CAD-CAC-NAR	-2.74	122.09	125.10
4	C	12	FLC	CG-CB-CBC	-2.73	104.24	110.11
4	D	11	FLC	OG1-CGC-CG	-2.67	115.13	122.94
2	A	3	LDN	CAQ-NBD-CAP	2.66	117.38	111.52
4	A	501	FLC	OHB-CB-CA	-2.65	103.21	109.40
4	D	11	FLC	OB1-CBC-CB	-2.64	118.52	122.25
4	B	5	FLC	OG2-CGC-CG	2.64	122.81	114.35
2	B	1	LDN	CAL-CAZ-CBC	2.59	107.59	105.20
4	D	9	FLC	OB1-CBC-CB	-2.57	118.62	122.25
4	B	5	FLC	CG-CB-CA	2.55	115.80	109.16
2	B	1	LDN	CAK-NAS-CBC	2.54	119.97	116.73
2	A	3	LDN	CAC-NAR-CBA	2.51	120.82	116.93
2	C	4	LDN	CAN-CAP-NBD	-2.49	105.10	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	LDN	CAW-CAK-NAS	-2.40	121.79	125.05
4	A	501	FLC	OG2-CGC-CG	2.40	122.06	114.35
4	C	12	FLC	OB1-CBC-CB	-2.37	118.89	122.25
2	D	2	LDN	CAH-CAX-NBD	-2.32	118.18	121.38
4	B	5	FLC	OG1-CGC-CG	-2.31	116.19	122.94
4	B	501	FLC	OA1-CAC-CA	-2.31	116.19	122.94
4	A	502	FLC	OA1-CAC-CA	-2.30	116.22	122.94
2	A	3	LDN	CAC-CAD-CAY	2.24	121.69	119.77
4	C	12	FLC	OB2-CBC-CB	2.22	116.90	113.05
4	C	12	FLC	OA1-CAC-CA	-2.18	116.56	122.94
4	B	501	FLC	OG2-CGC-CG	2.17	121.33	114.35
4	B	501	FLC	CG-CB-CBC	2.16	114.75	110.11
4	C	3	FLC	OG2-CGC-CG	2.16	121.29	114.35
4	C	500	FLC	OA1-CAC-CA	-2.14	116.70	122.94
2	A	3	LDN	CAW-CAK-NAS	-2.11	122.18	125.05
4	D	11	FLC	OG2-CGC-CG	2.06	120.98	114.35
2	D	2	LDN	CAQ-NBD-CAX	2.06	123.67	118.09
4	D	9	FLC	CB-CG-CGC	-2.03	108.91	113.81
2	A	3	LDN	CAN-CAP-NBD	-2.02	106.12	110.48
4	C	500	FLC	OA2-CAC-CA	2.00	120.79	114.35

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5	FLC	CAC-CA-CB-CBC
4	B	6	FLC	OHB-CB-CBC-OB2
4	B	501	FLC	CAC-CA-CB-CG
4	B	501	FLC	CA-CB-CG-CGC
4	C	3	FLC	CAC-CA-CB-CG
4	C	3	FLC	CA-CB-CBC-OB1
4	C	3	FLC	CA-CB-CBC-OB2
4	C	3	FLC	OHB-CB-CBC-OB1
4	C	3	FLC	OHB-CB-CBC-OB2
4	C	3	FLC	CA-CB-CG-CGC
4	C	12	FLC	CA-CB-CBC-OB1
4	C	12	FLC	CA-CB-CBC-OB2
4	C	12	FLC	OHB-CB-CBC-OB2
4	D	9	FLC	CA-CB-CBC-OB2
4	D	9	FLC	OHB-CB-CBC-OB1
4	D	9	FLC	OHB-CB-CBC-OB2
4	D	10	FLC	CBC-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
4	D	11	FLC	CA-CB-CG-CGC
4	D	11	FLC	CBC-CB-CG-CGC
4	B	5	FLC	CBC-CB-CG-CGC
4	B	501	FLC	CBC-CB-CG-CGC
4	C	12	FLC	CA-CB-CG-CGC
4	C	12	FLC	CBC-CB-CG-CGC
4	D	10	FLC	CAC-CA-CB-CBC
4	D	10	FLC	CA-CB-CG-CGC
4	D	11	FLC	OHB-CB-CG-CGC
4	B	5	FLC	CAC-CA-CB-OHB
4	C	3	FLC	CAC-CA-CB-CBC
4	D	10	FLC	CAC-CA-CB-CG
4	B	6	FLC	CA-CB-CBC-OB2
4	B	6	FLC	CG-CB-CBC-OB2
4	C	12	FLC	CG-CB-CBC-OB2
3	A	4	EDO	O1-C1-C2-O2
3	C	10	EDO	O1-C1-C2-O2
4	D	11	FLC	CAC-CA-CB-CBC
4	B	5	FLC	CA-CB-CG-CGC
4	B	501	FLC	CAC-CA-CB-CBC
4	D	11	FLC	CAC-CA-CB-CG
4	D	11	FLC	CAC-CA-CB-OHB
3	D	6	EDO	O1-C1-C2-O2
4	A	502	FLC	CA-CB-CBC-OB2
4	B	5	FLC	CG-CB-CBC-OB2
4	C	3	FLC	CG-CB-CBC-OB1
4	C	3	FLC	CG-CB-CBC-OB2
4	C	12	FLC	CG-CB-CBC-OB1
4	D	9	FLC	CA-CB-CBC-OB1
4	D	9	FLC	CG-CB-CBC-OB1
4	D	9	FLC	CG-CB-CBC-OB2
4	A	501	FLC	CB-CG-CGC-OG1
4	B	500	FLC	CA-CB-CG-CGC
4	B	500	FLC	CBC-CB-CG-CGC
3	A	1	EDO	O1-C1-C2-O2
4	C	500	FLC	CAC-CA-CB-OHB
4	A	501	FLC	CB-CG-CGC-OG2
4	B	5	FLC	CB-CG-CGC-OG2
4	B	5	FLC	CB-CG-CGC-OG1
4	A	502	FLC	CAC-CA-CB-OHB
4	A	502	FLC	CA-CB-CBC-OB1
4	B	5	FLC	CG-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
4	B	501	FLC	CG-CB-CBC-OB2
4	C	3	FLC	CB-CG-CGC-OG2
4	C	3	FLC	CB-CG-CGC-OG1
4	C	3	FLC	OHB-CB-CG-CGC
4	C	12	FLC	OHB-CB-CG-CGC
4	D	10	FLC	OHB-CB-CG-CGC
4	B	501	FLC	CAC-CA-CB-OHB
4	C	12	FLC	OHB-CB-CBC-OB1
4	B	6	FLC	CA-CB-CBC-OB1
4	B	6	FLC	CG-CB-CBC-OB1
4	D	10	FLC	CG-CB-CBC-OB1
4	D	11	FLC	CG-CB-CBC-OB2
4	D	9	FLC	CB-CA-CAC-OA2
4	D	9	FLC	CB-CA-CAC-OA1
4	A	501	FLC	CB-CA-CAC-OA2
4	C	3	FLC	CBC-CB-CG-CGC
4	B	501	FLC	CG-CB-CBC-OB1
3	B	7	EDO	O1-C1-C2-O2
3	D	14[B]	EDO	O1-C1-C2-O2
4	A	501	FLC	CB-CA-CAC-OA1
4	C	3	FLC	CB-CA-CAC-OA1
4	C	3	FLC	CB-CA-CAC-OA2
4	D	9	FLC	OHB-CB-CG-CGC
3	D	13[B]	EDO	O1-C1-C2-O2
3	D	14[A]	EDO	O1-C1-C2-O2
4	A	502	FLC	CB-CG-CGC-OG2
4	D	11	FLC	CB-CG-CGC-OG2
4	C	500	FLC	OHB-CB-CG-CGC

There are no ring outliers.

20 monomers are involved in 33 short contacts:

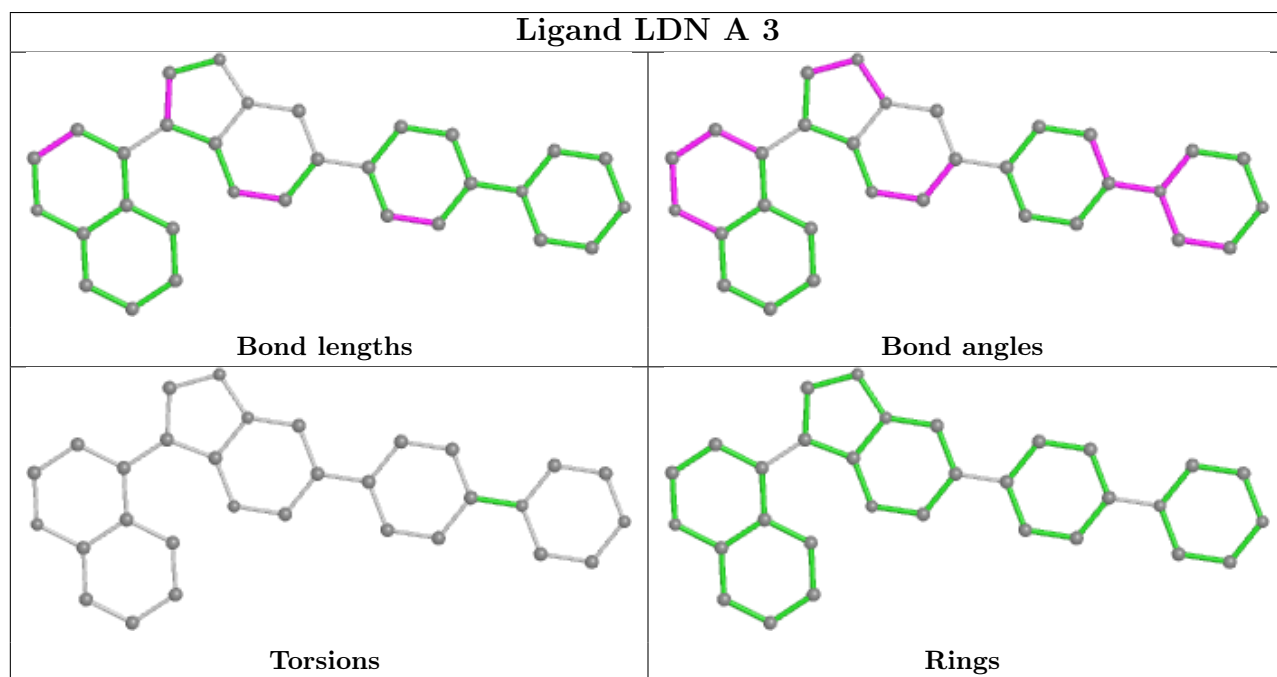
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	FLC	1	0
4	D	10	FLC	2	0
4	D	11	FLC	1	0
3	C	9[B]	EDO	2	0
3	C	9[A]	EDO	2	0
4	A	501	FLC	1	0
3	B	8	EDO	2	0
3	A	4	EDO	1	0
4	C	500	FLC	1	0

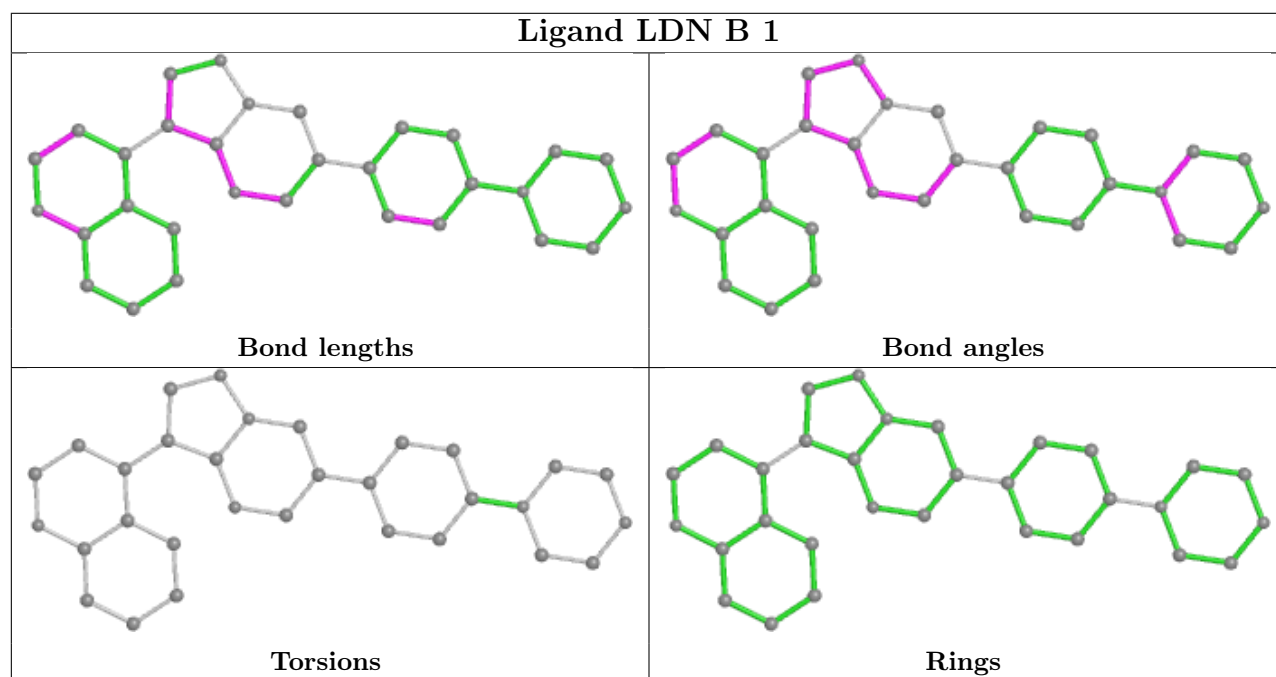
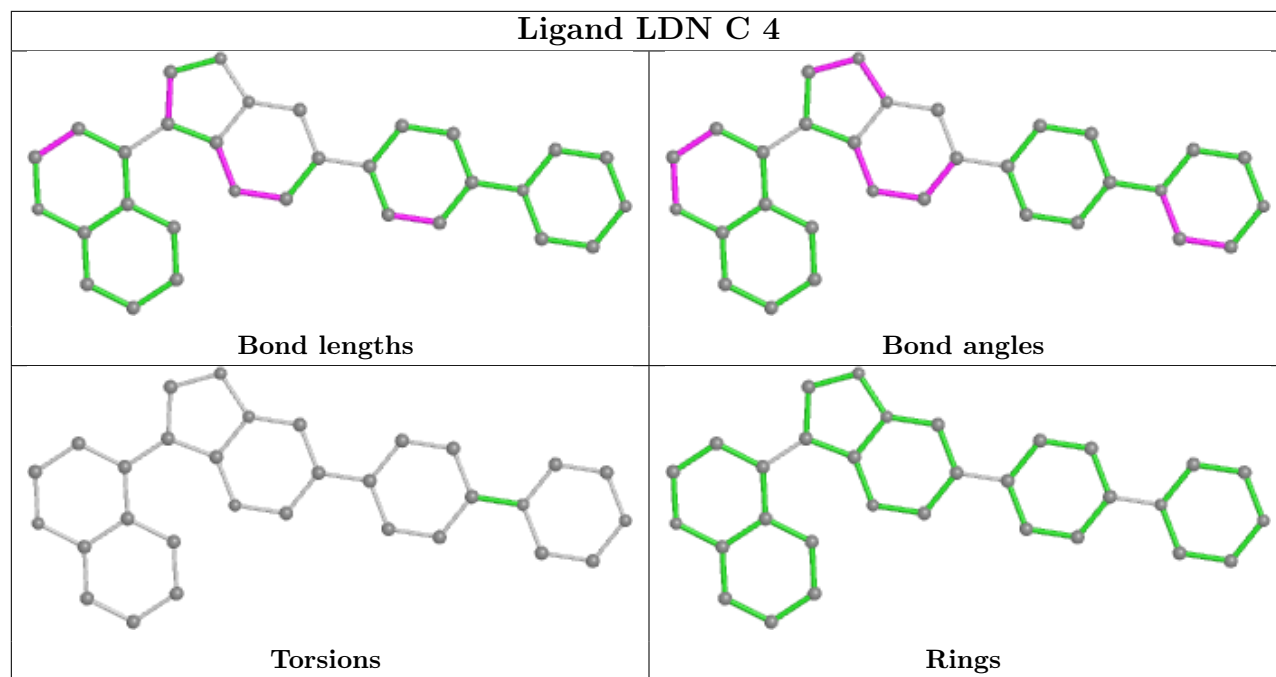
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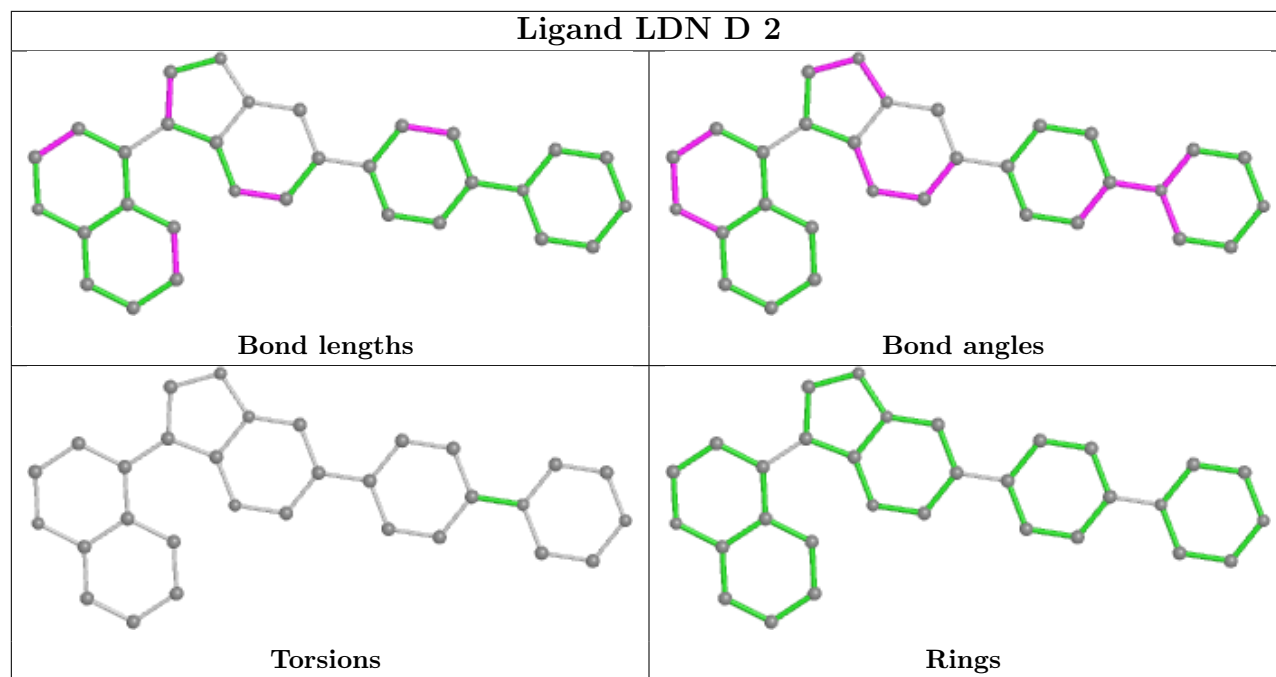
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	9	FLC	2	0
2	C	4	LDN	1	0
4	C	3	FLC	3	0
4	B	500	FLC	2	0
4	B	6	FLC	1	0
3	A	500	EDO	3	0
4	A	502	FLC	2	0
4	B	5	FLC	1	0
3	C	11	EDO	1	0
2	B	1	LDN	2	0
3	D	13[B]	EDO	2	0

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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/301 (99%)	-0.34	4 (1%) 77 74	13, 24, 47, 69	0
1	B	300/301 (99%)	0.14	23 (7%) 13 10	14, 32, 71, 108	0
1	C	296/301 (98%)	-0.22	10 (3%) 45 39	10, 22, 47, 69	0
1	D	299/301 (99%)	-0.21	9 (3%) 50 44	10, 21, 49, 94	0
All	All	1193/1204 (99%)	-0.16	46 (3%) 39 34	10, 24, 56, 108	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	GLN	7.3
1	B	372	ASN	7.2
1	B	371	GLY	5.8
1	B	450	VAL	5.6
1	B	375	ARG	5.6
1	D	326	THR	5.3
1	B	370	VAL	5.2
1	B	374	PRO	4.8
1	B	366	ASN	4.8
1	C	204	VAL	4.5
1	B	256	MET	4.4
1	D	275	SER	4.4
1	D	274	HIS	4.1
1	D	325	GLY	4.0
1	D	219[A]	TYR	4.0
1	B	326	THR	3.8
1	B	373	ASN	3.7
1	C	326	THR	3.7
1	B	274	HIS	3.4
1	B	327	GLN	3.4
1	B	498	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	368	LEU	3.2
1	A	202	ARG	3.1
1	C	219[A]	TYR	3.1
1	C	376	VAL	3.0
1	A	219	TYR	3.0
1	C	325	GLY	3.0
1	B	364	SER	3.0
1	B	325	GLY	2.9
1	C	499	ASP	2.9
1	D	327	GLN	2.9
1	A	499	ASP	2.6
1	B	449	CYS	2.6
1	B	459	ASN	2.6
1	D	240	ARG	2.5
1	C	327	GLN	2.5
1	C	240	ARG	2.5
1	B	275	SER	2.4
1	B	365	THR	2.3
1	D	218	ARG	2.3
1	A	203	THR	2.2
1	B	367	GLN	2.2
1	B	452	GLN	2.2
1	B	451	ASP	2.1
1	C	205	ALA	2.0
1	C	497	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

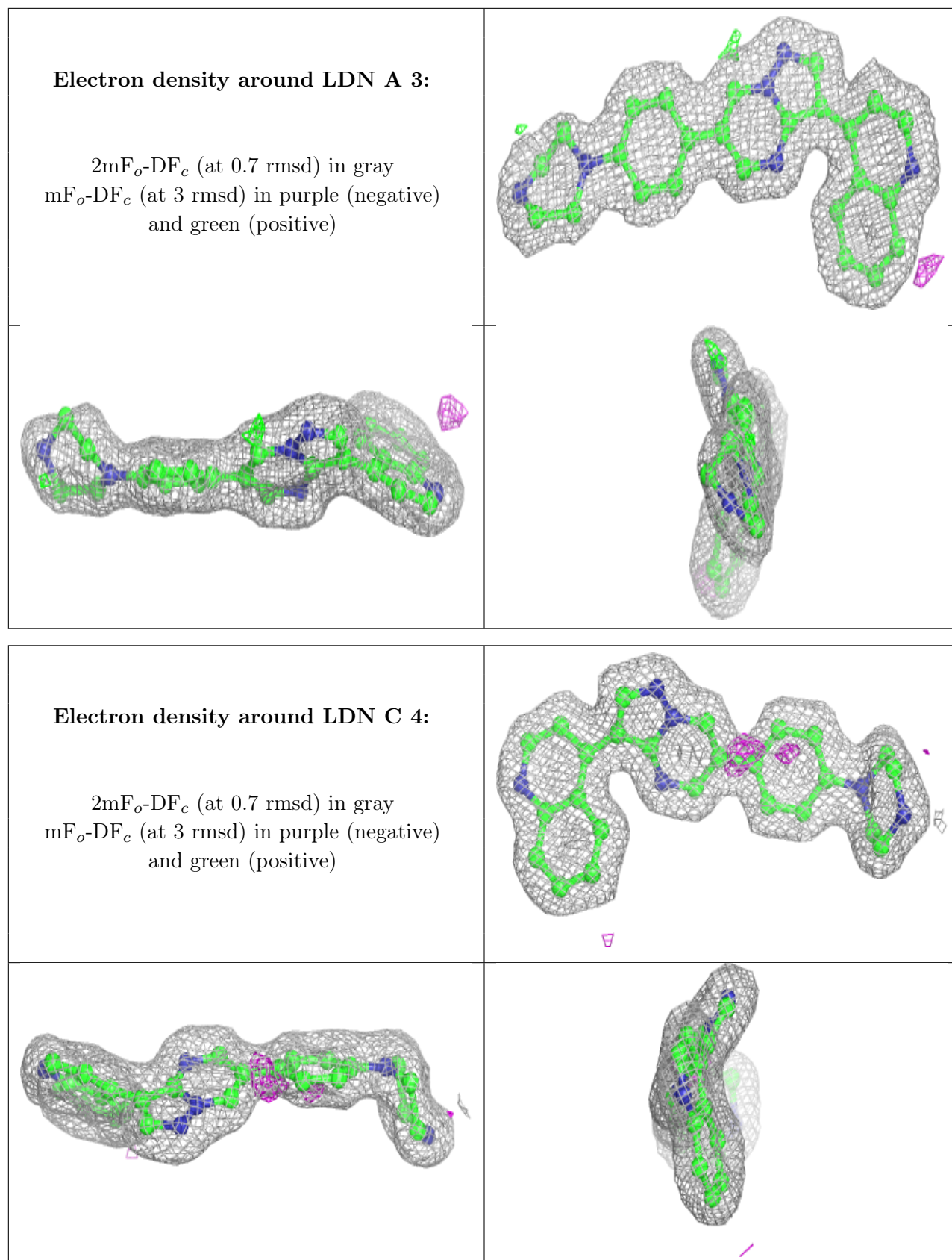
## 6.4 Ligands [i](#)

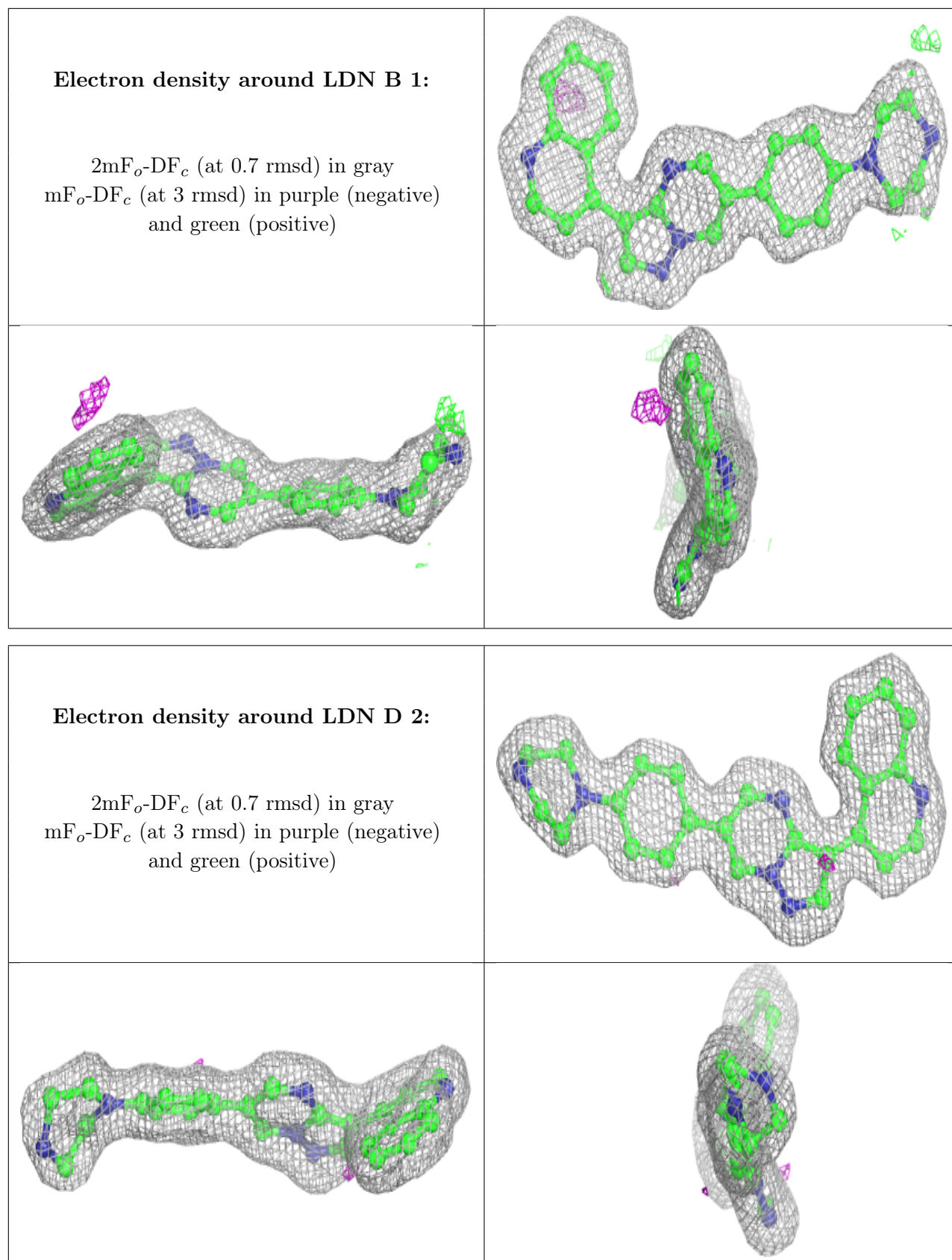
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	EDO	D	6	4/4	0.67	0.22	31,38,40,48	0
4	FLC	C	3	13/13	0.72	0.27	30,42,50,52	0
4	FLC	B	501	13/13	0.77	0.18	33,41,48,49	13
3	EDO	D	14[A]	4/4	0.78	0.23	27,44,44,46	4
3	EDO	D	14[B]	4/4	0.78	0.23	36,45,47,49	4
4	FLC	D	10	13/13	0.80	0.27	19,44,53,62	0
3	EDO	A	5	4/4	0.81	0.15	32,35,37,49	0
3	EDO	C	9[A]	4/4	0.81	0.20	27,29,31,35	4
3	EDO	C	9[B]	4/4	0.81	0.20	20,27,34,36	4
3	EDO	A	4	4/4	0.82	0.30	32,34,35,42	0
4	FLC	A	502	13/13	0.84	0.19	19,41,49,61	0
3	EDO	A	1	4/4	0.84	0.19	33,34,39,40	0
4	FLC	C	12	13/13	0.85	0.21	9,30,41,56	13
3	EDO	C	10	4/4	0.85	0.22	35,37,42,51	0
4	FLC	B	6	13/13	0.86	0.28	36,44,51,53	0
4	FLC	D	11	13/13	0.86	0.23	23,47,52,53	0
4	FLC	B	500	13/13	0.87	0.19	29,42,45,49	0
4	FLC	C	500	13/13	0.89	0.17	20,40,57,60	0
4	FLC	B	5	13/13	0.89	0.23	26,34,49,50	0
4	FLC	D	9	13/13	0.90	0.25	28,39,47,62	0
3	EDO	B	8	4/4	0.90	0.12	29,32,39,41	0
4	FLC	A	501	13/13	0.90	0.15	30,42,47,49	0
3	EDO	D	13[B]	4/4	0.91	0.12	21,27,33,42	4
3	EDO	C	11	4/4	0.91	0.11	29,35,41,44	0
3	EDO	D	13[A]	4/4	0.91	0.12	13,24,31,32	4
3	EDO	A	500	4/4	0.92	0.14	29,31,42,44	0
3	EDO	B	7	4/4	0.94	0.09	19,29,36,41	0
3	EDO	D	12	4/4	0.94	0.10	24,30,31,34	0
2	LDN	A	3	31/31	0.95	0.11	11,19,37,58	0
2	LDN	C	4	31/31	0.95	0.09	9,15,21,25	0
2	LDN	B	1	31/31	0.96	0.08	14,19,65,70	0
2	LDN	D	2	31/31	0.96	0.09	12,18,49,55	0
3	EDO	A	2	4/4	0.97	0.08	22,25,27,30	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.