Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 05:26 pm BST

PDB ID	:	8BYJ
Title	:	The structures of Ace2 in complex with bicyclic peptide inhibitor
Authors	:	Brear, P.; Lulla, A.; Harman, M.; Dods, R.; Chen, L.; Bezerra, G.; Demydchuk, Y.; Stanway, S.; Hyvonen, M.
Deposited on	:	2022-12-13
Resolution	:	2.07 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:

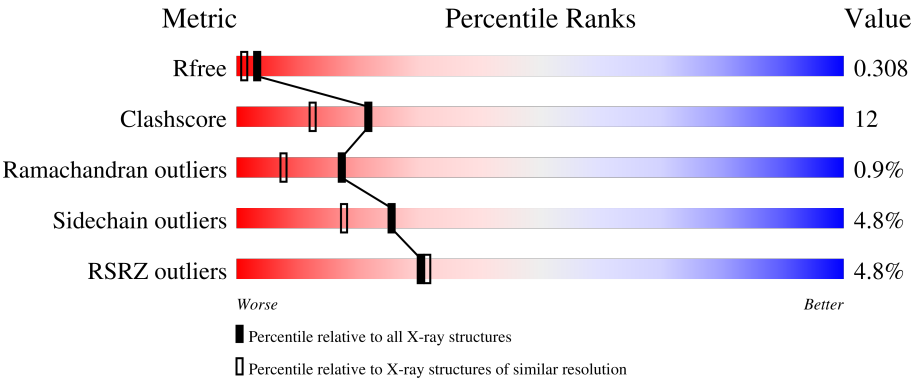
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	609	2% 77% 19%
1	B	609	7% 62% 33%
2	C	18	11% 56% 33% 11%
2	D	18	6% 56% 33% 6% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10139 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	B	595	Total	C	N	O	S	0	0	0
			4856	3108	804	915	29			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	PRO	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
B	18	GLY	-	expression tag	UNP Q9BYF1
B	616	SER	-	expression tag	UNP Q9BYF1
B	617	SER	-	expression tag	UNP Q9BYF1
B	618	PRO	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1
B	622	HIS	-	expression tag	UNP Q9BYF1
B	623	HIS	-	expression tag	UNP Q9BYF1
B	624	HIS	-	expression tag	UNP Q9BYF1
B	625	HIS	-	expression tag	UNP Q9BYF1
B	626	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called ALA-CYS-VAL-ARG-SER-HIS-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	S	0	0	1
			127	76	28	20	3			
2	D	18	Total	C	N	O	S	0	0	1
			127	76	28	20	3			

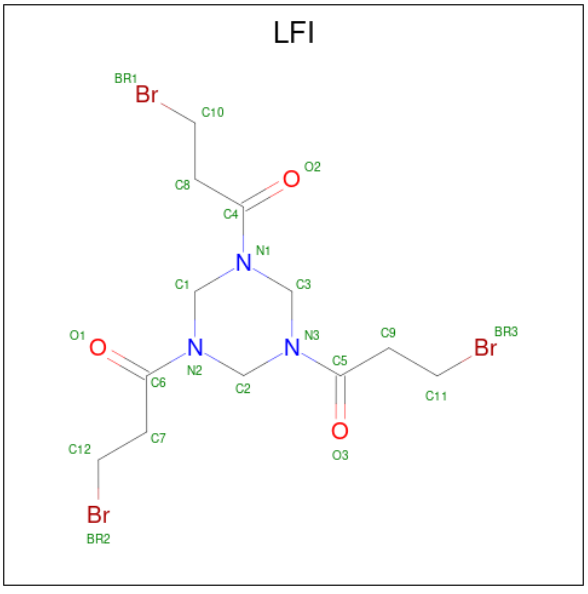
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is 1-[3,5-bis(3-bromanylpropanoyl)-1,3,5-triazinan-1-yl]-3-bromanyl-propan-1-one (three-letter code: LFI) (formula: $C_{12}H_{18}Br_3N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			18	12	3	3		
5	D	1	Total	C	N	O	0	0
			18	12	3	3		

- Molecule 6 is water.

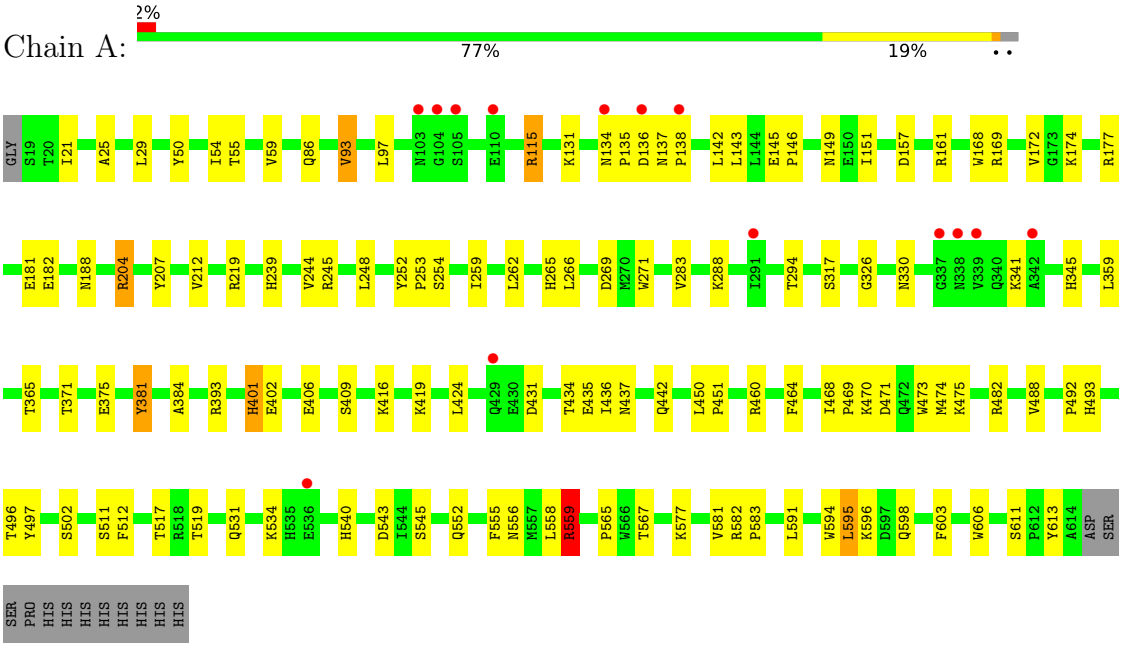
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	47	Total	O	0	0
			47	47		
6	C	1	Total	O	0	0
			1	1		
6	D	4	Total	O	0	0
			4	4		

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.

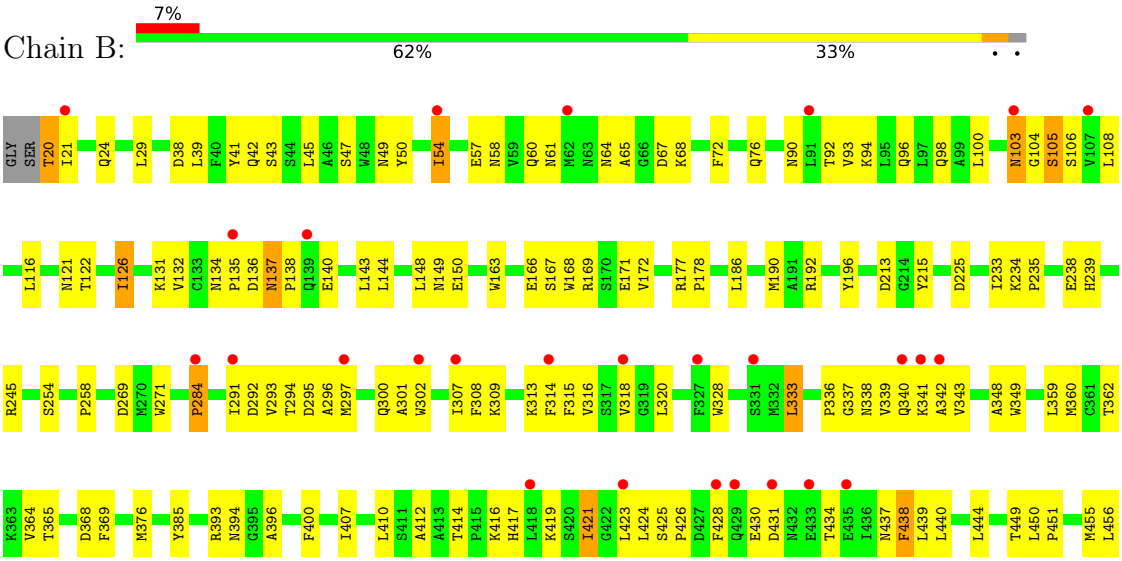
• Molecule 1: Processed angiotensin-converting enzyme 2

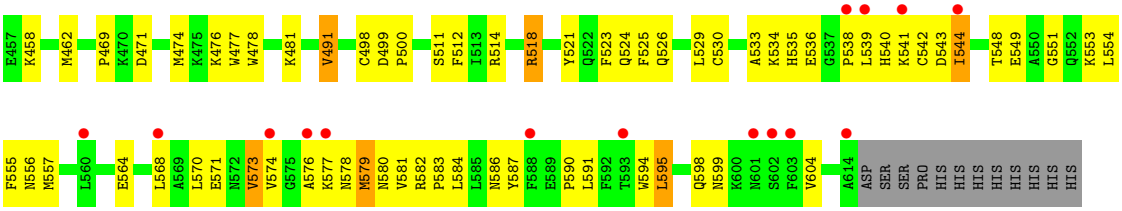
Chain A:



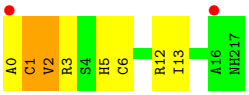
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain B:

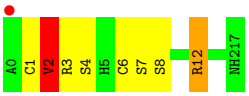




• Molecule 2: ALA-CYS-VAL-ARG-SER-HIS-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA



• Molecule 2: ALA-CYS-VAL-ARG-SER-HIS-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.78Å 75.96Å 114.91Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	77.02 – 2.07 77.02 – 2.07	Depositor EDS
% Data completeness (in resolution range)	84.8 (77.02-2.07) 84.8 (77.02-2.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.224 , 0.304 0.233 , 0.308	Depositor DCC
R_{free} test set	3336 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LFI, ZN, NA, NH2

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	0.43	0/4999	0.68	0/6792
1	B	0.42	0/4993	0.68	0/6784
2	C	0.43	0/128	0.77	0/172
2	D	0.57	0/128	1.02	0/172
All	All	0.43	0/10248	0.69	0/13920

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
2	D	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	559	ARG	Sidechain
1	B	518	ARG	Sidechain
2	D	3	ARG	Sidechain

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	4862	0	4639	74	0
1	B	4856	0	4633	153	0
2	C	127	0	128	6	0
2	D	127	0	128	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	C	18	0	0	1	0
5	D	18	0	0	2	0
6	A	76	0	0	3	0
6	B	47	0	0	3	0
6	C	1	0	0	0	0
6	D	4	0	0	0	0
All	All	10139	0	9528	233	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 12.

All (233) 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:B:535:HIS:NE2	1:B:538:PRO:O	2.22	0.72
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.25	0.72
1:B:524:GLN:HB3	1:B:574:VAL:HG11	1.69	0.72
1:B:542:CYS:SG	1:B:544:ILE:HG23	2.29	0.72
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.25	0.72
1:B:428:PHE:CE2	1:B:430:GLU:HB3	2.25	0.71
1:B:29:LEU:HD12	1:B:93:VAL:HG23	1.72	0.70
2:D:4:SER:HA	5:D:101:LFI:O2	1.91	0.70
2:D:6:CYS:O	2:D:8:SER:N	2.25	0.68
1:B:39:LEU:HD22	1:B:68:LYS:HB3	1.75	0.67
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.77	0.66
1:B:294:THR:HG23	1:B:365:THR:HA	1.77	0.65
1:B:564:GLU:HB3	1:B:568:LEU:HD23	1.80	0.64
1:B:336:PRO:HG3	1:B:342:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HD3	1:A:613:TYR:CD2	2.35	0.61
1:B:337:GLY:HA2	6:B:838:HOH:O	2.00	0.61
1:A:174:LYS:HD3	1:A:496:THR:HG22	1.83	0.61
2:D:1:CYS:O	2:D:2:VAL:HB	1.99	0.60
1:B:336:PRO:HB2	1:B:340:GLN:HB3	1.84	0.59
1:B:571:GLU:HA	1:B:576:ALA:H	1.68	0.59
1:B:307:ILE:HG23	1:B:369:PHE:HD1	1.67	0.59
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.38	0.59
1:A:591:LEU:HG	1:A:595:LEU:CD2	2.33	0.58
1:B:43:SER:HA	1:B:65:ALA:HB1	1.84	0.58
1:A:259:ILE:HG22	1:A:603:PHE:CG	2.38	0.58
1:B:92:THR:HG22	1:B:96:GLN:HE21	1.67	0.58
2:C:1:CYS:SG	2:C:1:CYS:O	2.62	0.57
1:B:594:TRP:CH2	1:B:598:GLN:HG3	2.40	0.57
1:A:474:MET:HE3	1:A:474:MET:HA	1.86	0.57
1:A:245:ARG:HB2	1:A:262:LEU:HD21	1.85	0.57
1:B:41:TYR:HE1	1:B:45:LEU:HD22	1.68	0.57
1:A:55:THR:O	1:A:59:VAL:HG23	2.03	0.57
1:A:552:GLN:HE21	1:A:556:ASN:HD21	1.53	0.57
1:B:417:HIS:O	1:B:421:ILE:HD13	2.04	0.57
1:A:207:TYR:CE2	1:A:517:THR:HG21	2.40	0.56
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.70	0.56
1:B:393:ARG:HB2	2:C:3:ARG:HD2	1.86	0.56
1:A:212:VAL:HG11	1:A:565:PRO:HG2	1.88	0.56
1:B:225:ASP:OD2	1:B:578:ASN:ND2	2.31	0.56
1:B:245:ARG:HD3	1:B:258:PRO:HA	1.88	0.55
1:A:359:LEU:C	1:A:359:LEU:HD23	2.27	0.55
1:B:41:TYR:CE1	1:B:45:LEU:HD22	2.42	0.55
1:B:192:ARG:HA	1:B:196:TYR:O	2.07	0.55
1:B:121:ASN:HD22	2:C:13:ILE:HG22	1.71	0.54
1:B:300:GLN:HB2	1:B:302:TRP:CD1	2.43	0.54
1:B:543:ASP:O	1:B:544:ILE:C	2.45	0.54
1:A:181:GLU:CD	1:A:470:LYS:HE3	2.28	0.54
2:C:1:CYS:O	2:C:2:VAL:HG22	2.07	0.54
1:A:259:ILE:HG22	1:A:603:PHE:CD2	2.43	0.53
1:A:149:ASN:ND2	6:A:806:HOH:O	2.41	0.53
1:B:137:ASN:HB2	1:B:140:GLU:HB2	1.91	0.53
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.90	0.52
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.45	0.52
1:B:76:GLN:HB3	1:B:100:LEU:HD21	1.92	0.52
1:A:419:LYS:HG2	1:A:424:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:LYS:HD3	1:B:573:VAL:O	2.09	0.52
1:B:318:VAL:O	1:B:548:THR:HA	2.10	0.52
1:B:336:PRO:HG3	1:B:342:ALA:CB	2.39	0.52
1:A:134:ASN:HB2	1:A:137:ASN:HB2	1.91	0.51
1:A:345:HIS:HE1	6:A:863:HOH:O	1.91	0.51
1:B:166:GLU:CD	1:B:491:VAL:HG21	2.31	0.51
1:B:49:ASN:C	1:B:58:ASN:HD22	2.14	0.51
1:B:94:LYS:O	1:B:98:GLN:HG3	2.11	0.51
1:A:450:LEU:HD21	1:A:519:THR:HG21	1.91	0.51
1:B:20:THR:O	1:B:24:GLN:NE2	2.38	0.51
1:A:555:PHE:O	1:A:559:ARG:HB2	2.11	0.51
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.92	0.51
1:A:341:LYS:HA	1:A:341:LYS:CE	2.41	0.51
1:B:591:LEU:CD1	1:B:595:LEU:HD13	2.40	0.51
1:B:134:ASN:HB3	1:B:137:ASN:H	1.76	0.51
1:B:54:ILE:HD11	1:B:343:VAL:HG23	1.92	0.51
1:A:591:LEU:HG	1:A:595:LEU:HD22	1.93	0.51
1:B:438:PHE:CD1	1:B:438:PHE:C	2.84	0.51
1:B:29:LEU:CD1	1:B:93:VAL:HG23	2.39	0.50
1:B:595:LEU:O	1:B:599:ASN:ND2	2.44	0.50
1:B:65:ALA:HA	1:B:68:LYS:HE2	1.93	0.50
1:B:439:LEU:HD12	1:B:590:PRO:HB2	1.94	0.50
1:A:157:ASP:O	1:A:161:ARG:HG3	2.12	0.50
1:A:594:TRP:CH2	1:A:598:GLN:HG3	2.47	0.50
1:B:456:LEU:HD12	1:B:477:TRP:CH2	2.47	0.50
1:B:478:TRP:CZ3	1:B:481:LYS:HG3	2.46	0.50
1:B:456:LEU:HD12	1:B:477:TRP:HH2	1.76	0.50
1:B:72:PHE:O	1:B:76:GLN:HG2	2.12	0.50
1:B:318:VAL:O	1:B:551:GLY:HA3	2.12	0.50
1:A:482:ARG:O	1:A:606:TRP:NE1	2.45	0.49
1:B:284:PRO:HD2	1:B:437:ASN:OD1	2.12	0.49
1:B:424:LEU:HD21	1:B:428:PHE:CD2	2.47	0.49
1:A:252:TYR:N	1:A:253:PRO:HD3	2.27	0.49
1:A:283:VAL:HG23	1:A:437:ASN:ND2	2.28	0.49
1:B:499:ASP:N	1:B:500:PRO:CD	2.74	0.49
1:A:402:GLU:O	1:A:406:GLU:HG2	2.13	0.49
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.12	0.49
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.94	0.49
1:B:308:PHE:CG	1:B:333:LEU:HD23	2.48	0.49
1:B:348:ALA:O	2:C:6:CYS:HA	2.13	0.48
1:B:412:ALA:HA	1:B:417:HIS:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:TYR:HE1	1:B:579:MET:HB3	1.78	0.48
1:B:540:HIS:ND1	1:B:540:HIS:C	2.66	0.48
1:B:574:VAL:HG23	1:B:576:ALA:HB3	1.96	0.48
2:D:12:ARG:NH1	5:D:101:LFI:C7	2.77	0.48
1:B:300:GLN:O	1:B:301:ALA:HB3	2.14	0.48
1:B:318:VAL:HG23	1:B:320:LEU:HG	1.95	0.48
1:B:456:LEU:CD2	1:B:512:PHE:CD2	2.96	0.48
1:A:381:TYR:HB3	1:A:401:HIS:CE1	2.49	0.48
1:A:531:GLN:O	1:A:534:LYS:N	2.45	0.48
1:B:341:LYS:N	1:B:341:LYS:HD3	2.28	0.48
1:B:360:MET:O	1:B:362:THR:N	2.46	0.48
1:B:57:GLU:O	1:B:60:GLN:HB3	2.13	0.47
1:A:239:HIS:NE2	1:A:596:LYS:HG2	2.28	0.47
1:B:419:LYS:NZ	1:B:428:PHE:HB3	2.28	0.47
1:B:50:TYR:HB2	1:B:58:ASN:HB3	1.96	0.47
1:B:419:LYS:HZ2	1:B:428:PHE:HB3	1.79	0.47
1:A:25:ALA:HB1	1:A:97:LEU:HD11	1.97	0.47
1:B:92:THR:HG22	1:B:96:GLN:NE2	2.30	0.47
1:B:122:THR:O	1:B:126:ILE:HG23	2.15	0.47
1:B:215:TYR:CE1	1:B:577:LYS:HE2	2.50	0.47
1:B:499:ASP:N	1:B:500:PRO:HD2	2.30	0.47
1:B:529:LEU:HD11	1:B:554:LEU:HD13	1.97	0.47
1:B:116:LEU:HD13	1:B:186:LEU:HB2	1.96	0.47
1:B:530:CYS:O	1:B:534:LYS:N	2.47	0.47
1:B:90:ASN:ND2	1:B:93:VAL:H	2.12	0.46
1:A:431:ASP:N	1:A:434:THR:OG1	2.44	0.46
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.79	0.46
1:B:456:LEU:HD23	1:B:512:PHE:CG	2.51	0.46
1:B:132:VAL:HG22	1:B:148:LEU:HD11	1.98	0.46
1:B:338:ASN:O	1:B:341:LYS:HD2	2.16	0.46
1:B:416:LYS:HD3	1:B:543:ASP:OD1	2.15	0.46
1:B:167:SER:O	1:B:171:GLU:HB2	2.15	0.46
1:B:431:ASP:OD1	1:B:434:THR:HG23	2.15	0.46
1:A:188:ASN:ND2	1:A:464:PHE:O	2.44	0.46
1:B:38:ASP:O	1:B:42:GLN:NE2	2.49	0.46
1:A:86:GLN:NE2	1:B:108:LEU:O	2.47	0.46
1:A:168:TRP:CE3	1:A:172:VAL:HG21	2.51	0.46
1:B:136:ASP:O	1:B:138:PRO:HD3	2.16	0.46
1:B:407:ILE:HB	1:B:526:GLN:OE1	2.16	0.46
1:B:591:LEU:HD11	1:B:595:LEU:HD13	1.97	0.46
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HE2	1:A:288:LYS:HA	1.97	0.45
1:B:239:HIS:CE1	1:B:604:VAL:HG11	2.52	0.45
1:B:149:ASN:ND2	6:B:802:HOH:O	2.49	0.45
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.52	0.45
1:B:511:SER:O	1:B:514:ARG:HD2	2.16	0.45
1:A:442:GLN:HA	1:A:442:GLN:NE2	2.32	0.45
1:B:103:ASN:O	1:B:105:SER:N	2.40	0.45
1:B:574:VAL:CG2	1:B:576:ALA:HB3	2.47	0.45
1:A:283:VAL:CG2	1:A:437:ASN:ND2	2.80	0.45
1:B:166:GLU:OE1	1:B:166:GLU:HA	2.17	0.45
1:B:474:MET:HE1	1:B:499:ASP:HB2	1.99	0.45
1:B:555:PHE:O	1:B:556:ASN:C	2.55	0.45
1:B:309:LYS:HG2	1:B:328:TRP:CZ2	2.52	0.45
1:B:64:ASN:O	1:B:68:LYS:HG3	2.17	0.44
1:A:212:VAL:HG21	1:A:565:PRO:HG3	1.99	0.44
1:B:239:HIS:CE1	1:B:604:VAL:HG21	2.52	0.44
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.81	0.44
1:B:291:ILE:O	1:B:291:ILE:HG22	2.17	0.44
1:A:326:GLY:O	1:A:330:ASN:ND2	2.51	0.44
1:A:567:THR:HG22	1:A:577:LYS:O	2.17	0.44
1:B:428:PHE:HE2	1:B:430:GLU:HB3	1.78	0.44
1:A:134:ASN:O	1:A:135:PRO:C	2.56	0.44
1:B:234:LYS:N	1:B:235:PRO:CD	2.81	0.44
1:B:410:LEU:O	1:B:414:THR:HG23	2.18	0.44
1:A:371:THR:O	1:A:375:GLU:HG2	2.18	0.44
1:B:307:ILE:HG23	1:B:369:PHE:CD1	2.50	0.44
1:A:435:GLU:HG3	1:A:540:HIS:CE1	2.53	0.44
1:B:234:LYS:O	1:B:238:GLU:HB2	2.17	0.44
1:B:308:PHE:CD2	1:B:333:LEU:HD23	2.52	0.44
1:A:204:ARG:NH1	6:A:801:HOH:O	2.21	0.43
1:B:126:ILE:O	1:B:126:ILE:HG13	2.17	0.43
1:B:333:LEU:N	1:B:333:LEU:HD12	2.34	0.43
1:B:417:HIS:CE1	1:B:421:ILE:HD11	2.53	0.43
1:B:440:LEU:O	1:B:444:LEU:HG	2.19	0.43
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.18	0.43
1:A:29:LEU:HD12	1:A:93:VAL:HG22	2.01	0.43
1:B:529:LEU:O	1:B:533:ALA:N	2.51	0.43
1:A:145:GLU:HA	1:A:146:PRO:HA	1.87	0.43
1:B:414:THR:HG21	1:B:542:CYS:O	2.19	0.43
1:A:384:ALA:CB	1:A:558:LEU:HB3	2.48	0.43
1:B:523:PHE:CE2	1:B:584:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:HD23	1:B:587:TYR:N	2.34	0.43
1:A:177:ARG:HD3	1:A:497:TYR:O	2.18	0.43
1:B:393:ARG:O	1:B:394:ASN:ND2	2.52	0.43
1:B:177:ARG:HB3	1:B:178:PRO:HD3	2.01	0.42
1:B:521:TYR:CE1	1:B:579:MET:HB3	2.55	0.42
1:B:524:GLN:CD	1:B:580:ASN:H	2.22	0.42
1:B:296:ALA:O	1:B:300:GLN:HG3	2.19	0.42
1:A:86:GLN:OE1	1:B:106:SER:HB2	2.18	0.42
1:B:425:SER:O	1:B:426:PRO:C	2.56	0.42
1:B:458:LYS:O	1:B:462:MET:HG3	2.19	0.42
1:B:333:LEU:HD12	1:B:333:LEU:H	1.84	0.42
1:B:396:ALA:HB3	1:B:400:PHE:CD2	2.54	0.42
1:B:135:PRO:HD3	1:B:163:TRP:NE1	2.35	0.42
2:C:0:ALA:O	5:C:101:LFI:C11	2.68	0.42
1:A:265:HIS:CD2	1:A:266:LEU:CD2	3.03	0.42
1:B:294:THR:O	1:B:297:MET:HB2	2.19	0.42
1:B:313:LYS:O	1:B:316:VAL:N	2.53	0.42
1:B:478:TRP:CE3	1:B:481:LYS:HG3	2.55	0.42
1:B:540:HIS:CE1	1:B:541:LYS:HG2	2.55	0.42
1:A:431:ASP:CG	1:A:434:THR:HG23	2.40	0.42
1:A:582:ARG:N	1:A:583:PRO:CD	2.83	0.42
1:B:292:ASP:OD1	1:B:293:VAL:N	2.52	0.41
1:A:341:LYS:HA	1:A:341:LYS:HE2	2.02	0.41
1:A:493:HIS:CD2	1:A:497:TYR:CZ	3.08	0.41
1:B:291:ILE:HD11	1:B:434:THR:HB	2.02	0.41
1:A:317:SER:HB2	1:A:545:SER:O	2.20	0.41
1:B:169:ARG:NH1	1:B:271:TRP:CD1	2.88	0.41
1:A:294:THR:HG23	1:A:365:THR:HA	2.01	0.41
1:B:131:LYS:HG3	1:B:143:LEU:HD23	2.02	0.41
1:B:132:VAL:HB	1:B:167:SER:HB3	2.02	0.41
1:B:225:ASP:CG	1:B:578:ASN:HD21	2.18	0.41
1:B:476:LYS:HE2	6:B:832:HOH:O	2.21	0.41
1:B:582:ARG:N	1:B:583:PRO:CD	2.84	0.41
1:A:294:THR:O	1:A:294:THR:HG22	2.20	0.41
1:B:302:TRP:CE2	1:B:423:LEU:HD21	2.56	0.41
1:A:244:VAL:O	1:A:248:LEU:HG	2.21	0.41
1:B:47:SER:HB3	1:B:349:TRP:CH2	2.56	0.41
1:A:142:LEU:CD1	1:A:151:ILE:HD11	2.51	0.41
1:A:253:PRO:O	1:A:254:SER:CB	2.69	0.40
1:A:460:ARG:HH11	1:A:512:PHE:HB2	1.85	0.40
1:A:488:VAL:HG21	1:A:611:SER:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:HB2	1:B:140:GLU:CB	2.50	0.40
1:B:419:LYS:CG	1:B:424:LEU:HD23	2.51	0.40
1:B:539:LEU:HD23	1:B:587:TYR:CA	2.51	0.40
1:B:570:LEU:HG	1:B:574:VAL:HG22	2.03	0.40
2:D:1:CYS:O	2:D:2:VAL:CB	2.66	0.40
1:A:115:ARG:NH1	1:A:182:GLU:HG2	2.35	0.40
1:B:41:TYR:CD1	1:B:41:TYR:C	2.94	0.40
1:B:315:PHE:CE2	1:B:376:MET:HG2	2.55	0.40
1:B:525:PHE:HE1	1:B:570:LEU:HD12	1.86	0.40
1:A:169:ARG:HH21	1:A:169:ARG:HG3	1.87	0.40
1:B:47:SER:HB3	1:B:349:TRP:HH2	1.87	0.40
1:B:177:ARG:HD3	1:B:498:CYS:HB2	2.03	0.40
1:B:213:ASP:OD1	1:B:213:ASP:N	2.54	0.40
1:B:233:ILE:HG13	1:B:581:VAL:HG21	2.02	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	594/609 (98%)	569 (96%)	24 (4%)	1 (0%)	47 39
1	B	593/609 (97%)	548 (92%)	38 (6%)	7 (1%)	13 4
2	C	16/18 (89%)	13 (81%)	2 (12%)	1 (6%)	1 0
2	D	16/18 (89%)	9 (56%)	5 (31%)	2 (12%)	0 0
All	All	1219/1254 (97%)	1139 (93%)	69 (6%)	11 (1%)	17 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	2	VAL

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Mol	Chain	Res	Type
2	D	2	VAL
2	D	7	SER
1	B	103	ASN
1	B	364	VAL
1	B	104	GLY
1	B	536	GLU
1	B	54	ILE
1	B	544	ILE
1	B	284	PRO
1	A	138	PRO

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	526/538 (98%)	510 (97%)	16 (3%)	41 35
1	B	525/538 (98%)	494 (94%)	31 (6%)	19 11
2	C	15/15 (100%)	12 (80%)	3 (20%)	1 0
2	D	15/15 (100%)	13 (87%)	2 (13%)	4 1
All	All	1081/1106 (98%)	1029 (95%)	52 (5%)	25 18

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	93	VAL
1	A	115	ARG
1	A	136	ASP
1	A	269	ASP
1	A	271	TRP
1	A	381	TYR
1	A	401	HIS
1	A	409	SER
1	A	436	ILE
1	A	475	LYS

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Mol	Chain	Res	Type
1	A	502	SER
1	A	511	SER
1	A	559	ARG
1	A	581	VAL
1	A	595	LEU
1	B	20	THR
1	B	21	ILE
1	B	61	ASN
1	B	67	ASP
1	B	105	SER
1	B	126	ILE
1	B	137	ASN
1	B	150	GLU
1	B	172	VAL
1	B	190	MET
1	B	254	SER
1	B	269	ASP
1	B	295	ASP
1	B	314	PHE
1	B	333	LEU
1	B	339	VAL
1	B	359	LEU
1	B	368	ASP
1	B	385	TYR
1	B	421	ILE
1	B	438	PHE
1	B	449	THR
1	B	455	MET
1	B	491	VAL
1	B	518	ARG
1	B	549	GLU
1	B	557	MET
1	B	573	VAL
1	B	579	MET
1	B	586	ASN
1	B	595	LEU
2	C	1	CYS
2	C	5	HIS
2	C	12	ARG
2	D	2	VAL
2	D	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	96	GLN
1	A	102	GLN
1	A	121	ASN
1	A	149	ASN
1	A	437	ASN
1	A	442	GLN
1	A	552	GLN
1	A	556	ASN
1	B	42	GLN
1	B	58	ASN
1	B	61	ASN
1	B	90	ASN
1	B	96	GLN
1	B	121	ASN
1	B	149	ASN
1	B	239	HIS
1	B	345	HIS
1	B	432	ASN
1	B	546	ASN
1	B	599	ASN
2	D	5	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	LFI	C	101	2	18,18,21	0.65	0	24,24,27	1.24	3 (12%)
5	LFI	D	101	2	18,18,21	0.48	0	24,24,27	1.31	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LFI	C	101	2	-	11/18/30/33	0/0/1/1
5	LFI	D	101	2	-	13/18/30/33	0/0/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	101	LFI	N3-C2-N2	-4.17	104.30	110.77
5	D	101	LFI	N3-C3-N1	-4.12	104.37	110.77
5	C	101	LFI	N3-C2-N2	-3.23	105.76	110.77
5	C	101	LFI	C3-N3-C2	2.60	117.83	111.73
5	C	101	LFI	C2-N2-C6	2.43	130.37	122.49

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	101	LFI	C8-C4-N1-C3
5	C	101	LFI	O2-C4-N1-C3
5	C	101	LFI	C9-C5-N3-C2
5	C	101	LFI	C9-C5-N3-C3
5	C	101	LFI	O3-C5-N3-C2
5	C	101	LFI	O3-C5-N3-C3

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Mol	Chain	Res	Type	Atoms
5	D	101	LFI	C8-C4-N1-C1
5	D	101	LFI	C8-C4-N1-C3
5	D	101	LFI	O2-C4-N1-C1
5	D	101	LFI	O2-C4-N1-C3
5	D	101	LFI	C7-C6-N2-C1
5	D	101	LFI	C7-C6-N2-C2
5	D	101	LFI	O1-C6-N2-C1
5	D	101	LFI	O1-C6-N2-C2
5	C	101	LFI	O2-C4-N1-C1
5	C	101	LFI	C8-C4-N1-C1
5	C	101	LFI	C7-C6-N2-C1
5	C	101	LFI	O1-C6-N2-C1
5	D	101	LFI	C9-C5-N3-C2
5	D	101	LFI	N1-C4-C8-C10
5	C	101	LFI	O1-C6-N2-C2
5	D	101	LFI	O2-C4-C8-C10
5	D	101	LFI	N2-C6-C7-C12
5	D	101	LFI	O3-C5-N3-C2

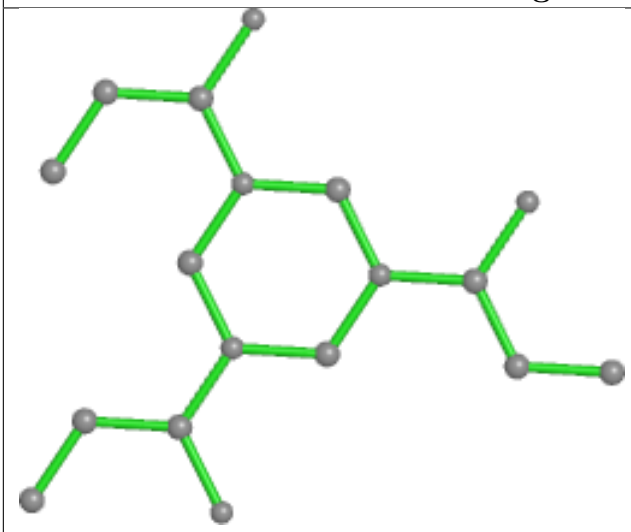
There are no ring outliers.

2 monomers are involved in 3 short contacts:

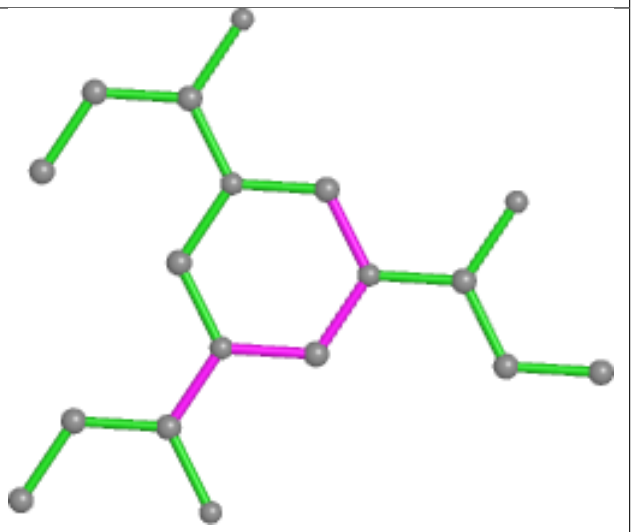
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	101	LFI	1	0
5	D	101	LFI	2	0

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

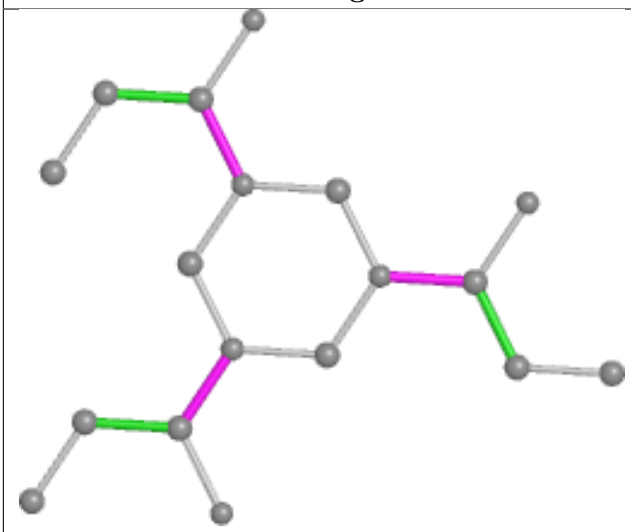
Ligand LFI C 101



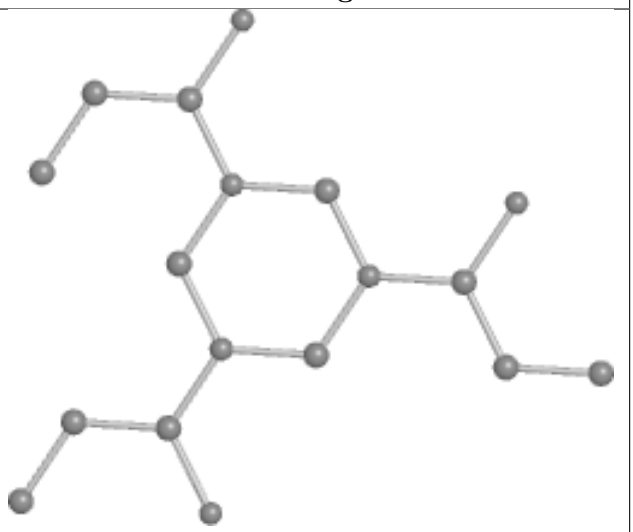
Bond lengths



Bond angles

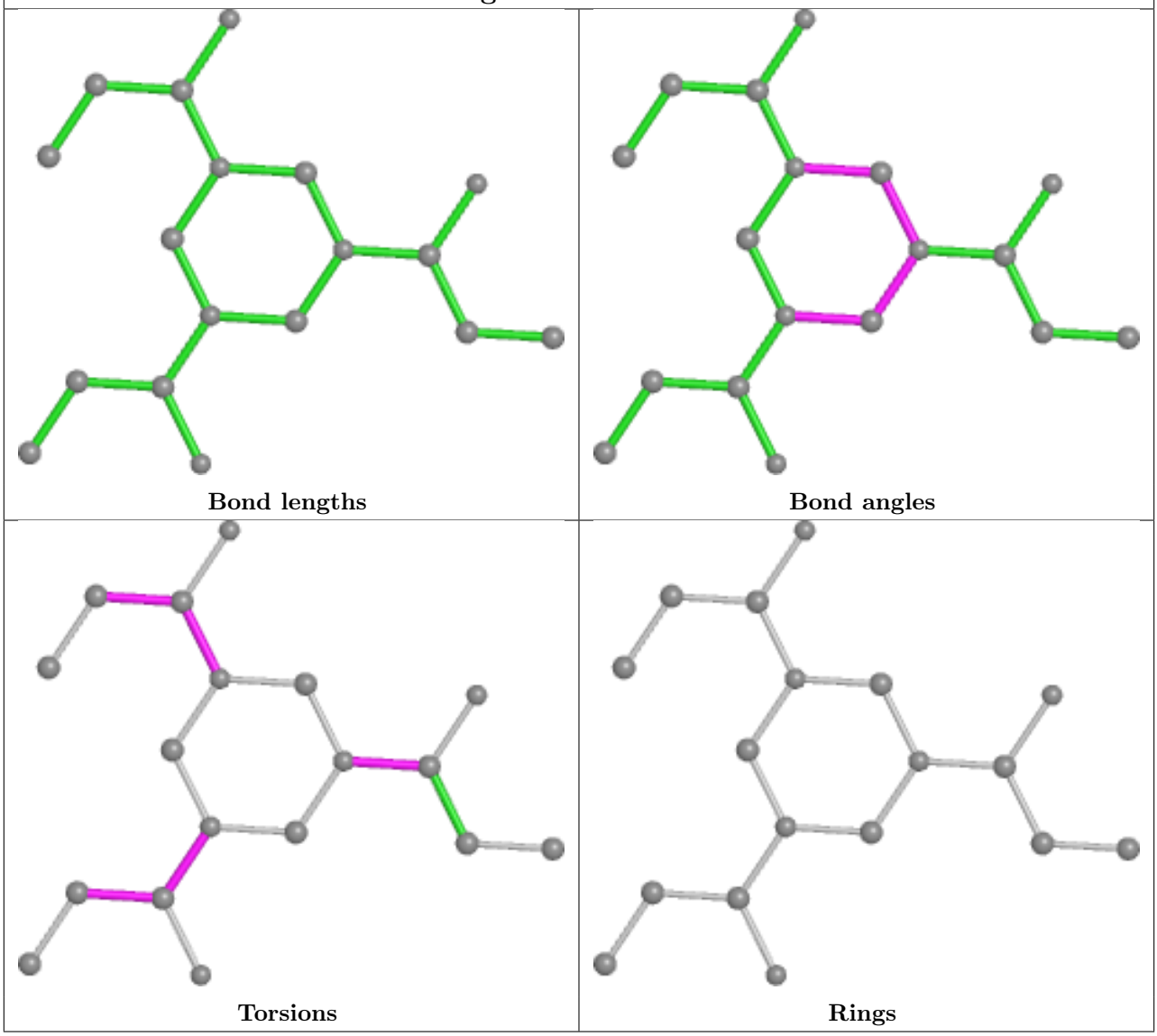


Torsions



Rings

Ligand LFI D 101



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, 95^{th} 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	596/609 (97%)	0.18	14 (2%) 60 63	40, 64, 103, 158	0
1	B	595/609 (97%)	0.53	42 (7%) 16 16	45, 91, 136, 161	0
2	C	17/18 (94%)	1.41	2 (11%) 4 4	72, 90, 141, 144	0
2	D	17/18 (94%)	0.85	1 (5%) 22 23	56, 67, 109, 124	0
All	All	1225/1254 (97%)	0.38	59 (4%) 30 31	40, 72, 131, 161	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	16	ALA	12.3
1	B	342	ALA	6.3
1	B	103	ASN	5.7
1	A	338	ASN	5.7
1	B	574	VAL	5.6
1	B	603	PHE	5.4
1	B	341	LYS	5.3
1	B	428	PHE	5.1
2	D	0	ALA	4.8
1	B	423	LEU	4.8
1	B	601	ASN	4.7
1	B	302	TRP	4.6
1	B	139	GLN	4.6
1	B	539	LEU	4.3
1	A	339	VAL	4.3
1	B	107	VAL	4.3
1	A	136	ASP	4.2
1	B	318	VAL	4.1
1	B	435	GLU	4.0
1	A	337	GLY	3.7
1	B	291	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	577	LYS	3.6
1	A	104	GLY	3.6
1	A	536	GLU	3.5
1	B	429	GLN	3.5
2	C	0	ALA	3.5
1	B	614	ALA	3.4
1	B	576	ALA	3.3
1	B	135	PRO	3.2
1	B	91	LEU	3.1
1	B	314	PHE	3.1
1	B	544	ILE	2.9
1	A	429	GLN	2.9
1	A	105	SER	2.8
1	B	588	PHE	2.8
1	B	331	SER	2.8
1	A	134	ASN	2.7
1	B	284	PRO	2.7
1	B	327	PHE	2.6
1	B	54	ILE	2.6
1	B	593	THR	2.5
1	A	103	ASN	2.5
1	B	62	MET	2.5
1	B	602	SER	2.5
1	A	291	ILE	2.4
1	B	433	GLU	2.4
1	B	340	GLN	2.3
1	B	560	LEU	2.3
1	B	307	ILE	2.3
1	B	431	ASP	2.2
1	B	541	LYS	2.2
1	A	110	GLU	2.2
1	B	297	MET	2.2
1	A	342	ALA	2.2
1	B	21	ILE	2.1
1	B	418	LEU	2.1
1	B	538	PRO	2.1
1	B	568	LEU	2.0
1	A	138	PRO	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)

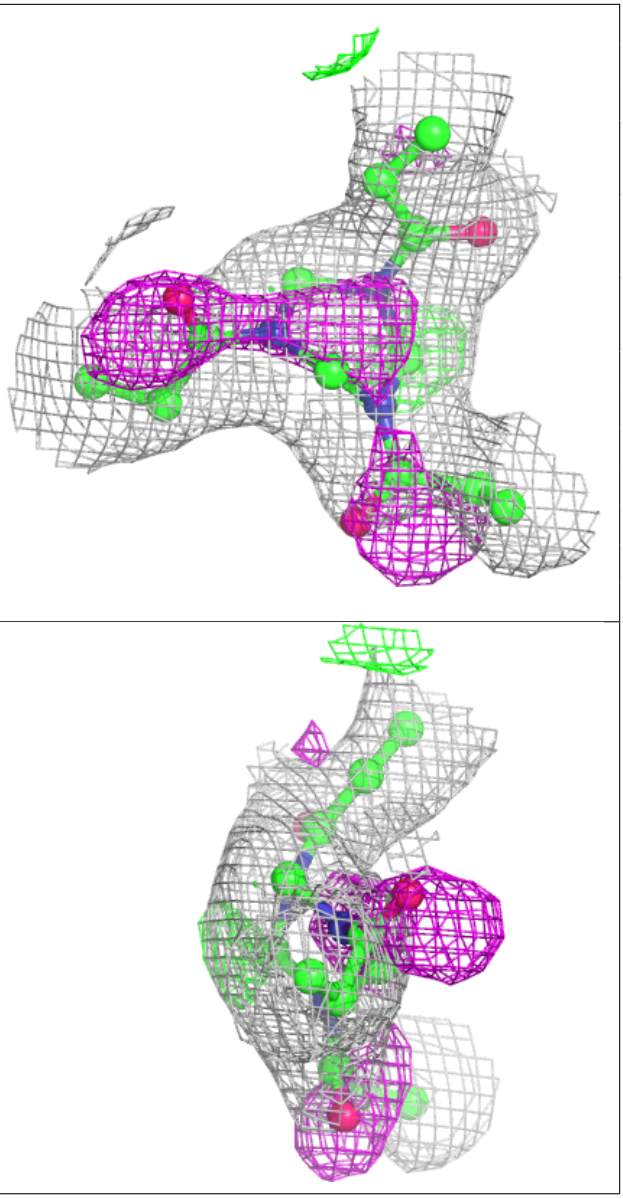
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LFI	D	101	18/21	0.73	0.20	46,56,72,75	0
4	NA	B	702	1/1	0.78	0.15	75,75,75,75	0
5	LFI	C	101	18/21	0.89	0.10	56,64,77,80	0
3	ZN	B	701	1/1	0.96	0.15	82,82,82,82	0
3	ZN	A	701	1/1	0.99	0.17	48,48,48,48	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.

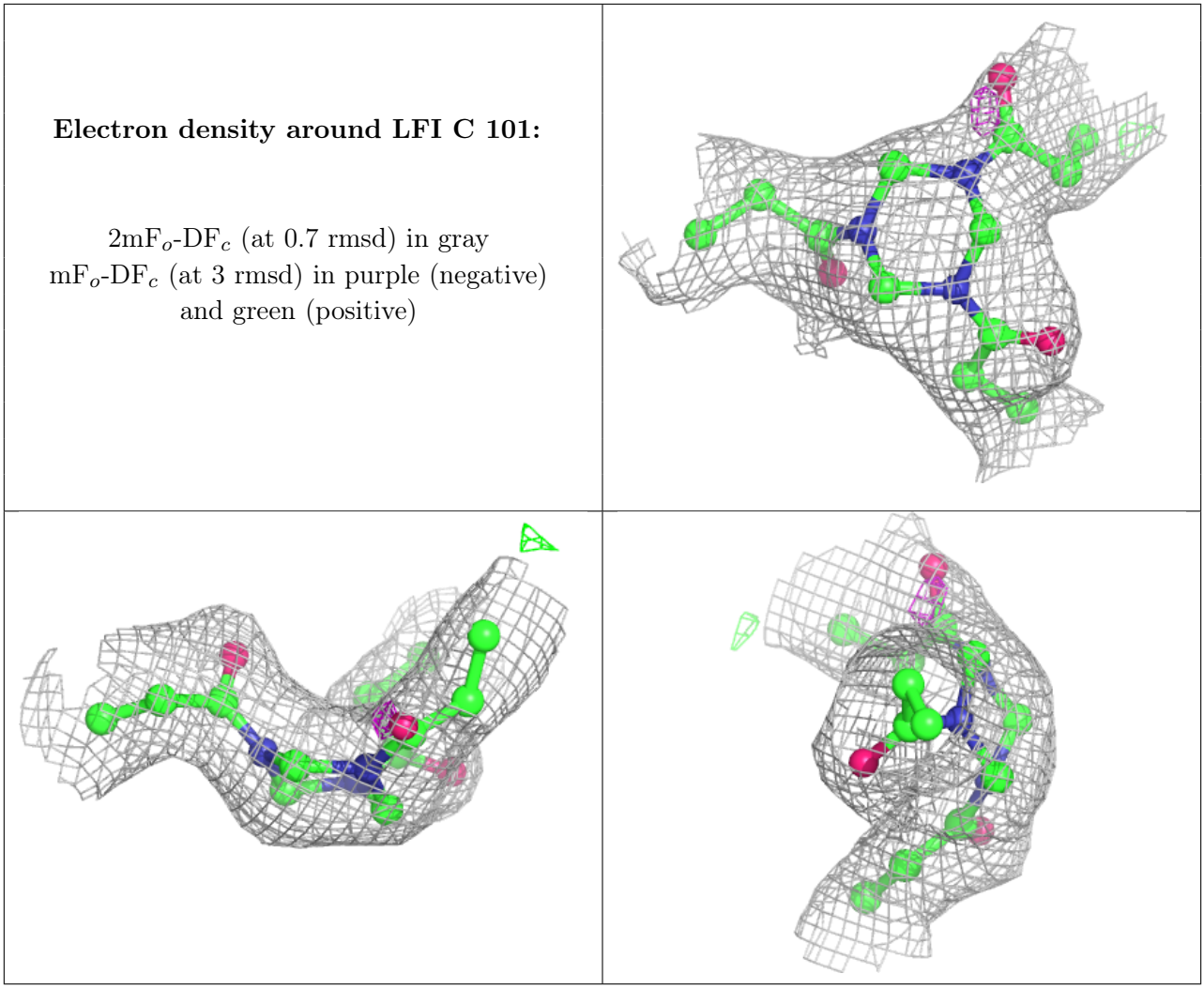
Electron density around LFI D 101:

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



Electron density around LFI C 101:

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



6.5 Other polymers

There are no such residues in this entry.