Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 08:17 pm BST

PDB ID	:	8BFW
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	:	2022-10-27
Resolution	:	2.33 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:

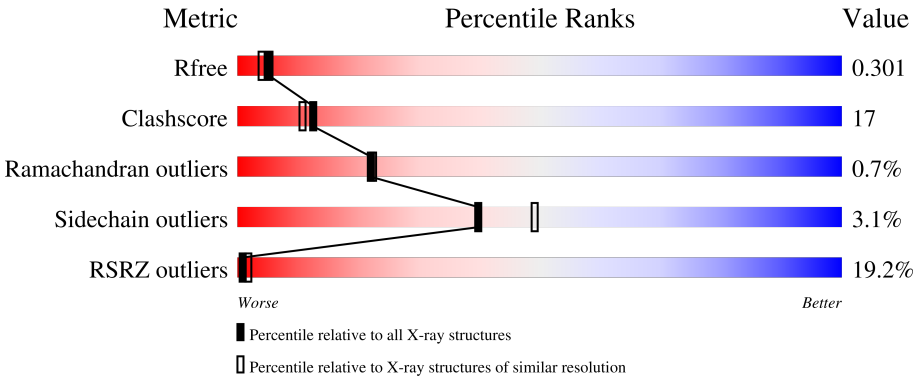
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	14% 64% 33%
1	C	609	23% 61% 35%
2	B	18	22% 56% 39% 6%
2	D	18	44% 56% 33% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10013 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	2	0
			4879	3120	808	922	29			
1	C	591	Total	C	N	O	S	0	0	0
			4823	3088	800	906	29			

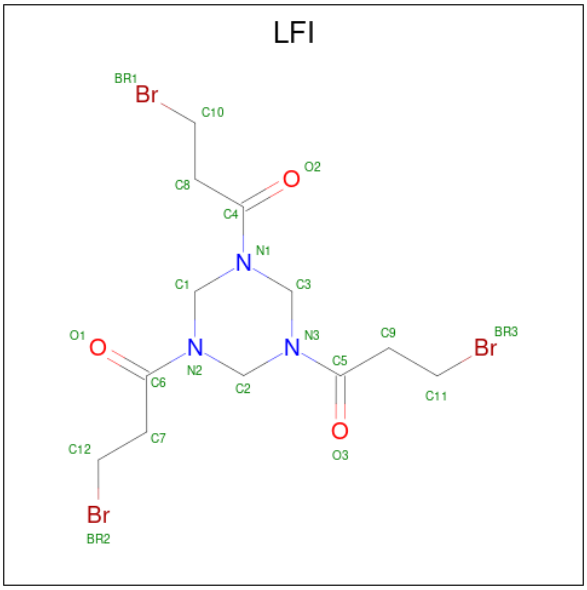
There are 24 discrepancies between the modelled and reference sequences:

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
C	18	GLY	-	expression tag	UNP Q9BYF1
C	616	SER	-	expression tag	UNP Q9BYF1
C	617	SER	-	expression tag	UNP Q9BYF1
C	618	PRO	-	expression tag	UNP Q9BYF1
C	619	HIS	-	expression tag	UNP Q9BYF1
C	620	HIS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1
C	624	HIS	-	expression tag	UNP Q9BYF1
C	625	HIS	-	expression tag	UNP Q9BYF1
C	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-NH2.

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

- Molecule 4 is water.

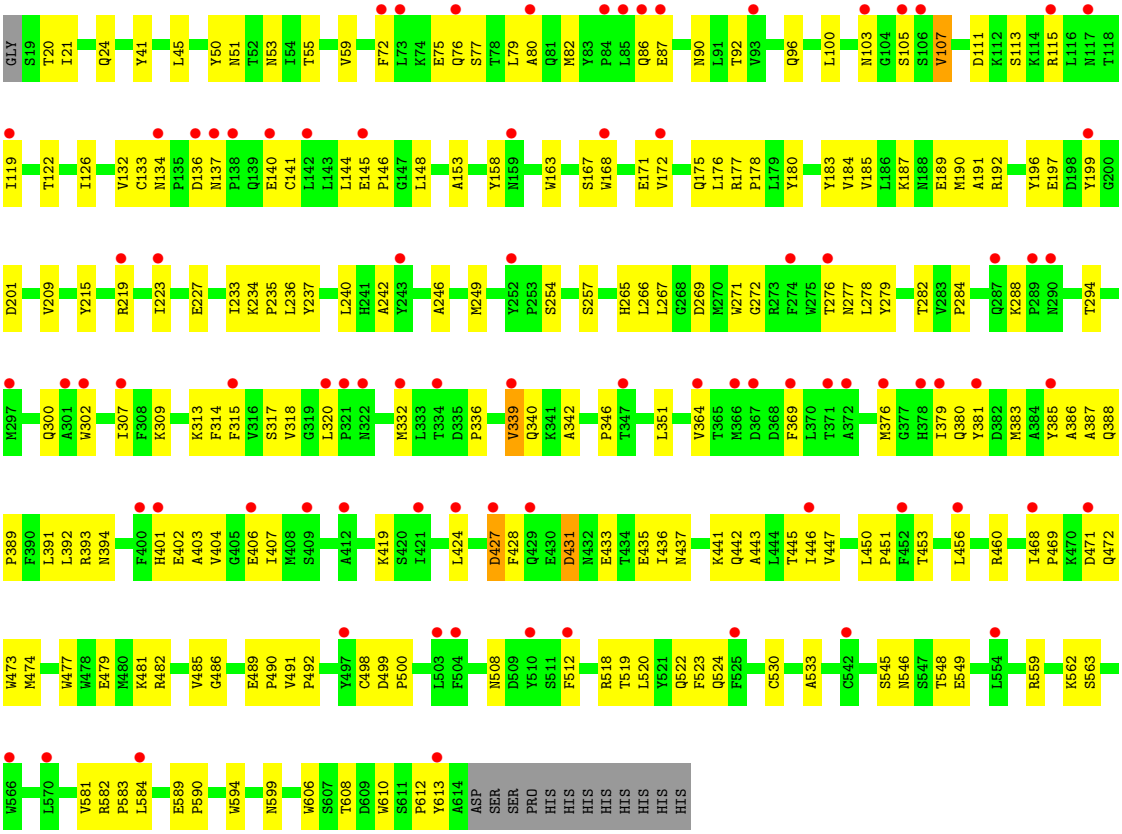
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	1	Total	O	0	0
			1	1		
4	C	7	Total	O	0	0
			7	7		

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.

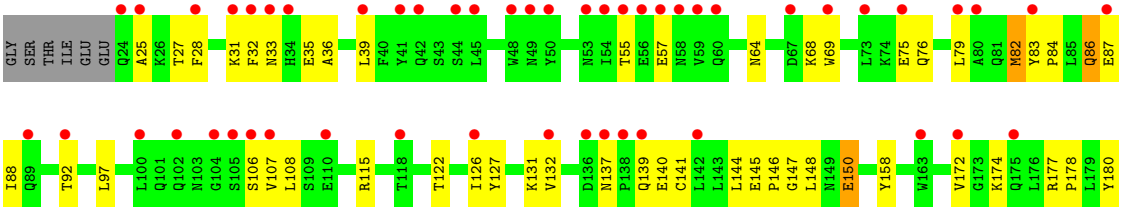
• Molecule 1: Processed angiotensin-converting enzyme 2

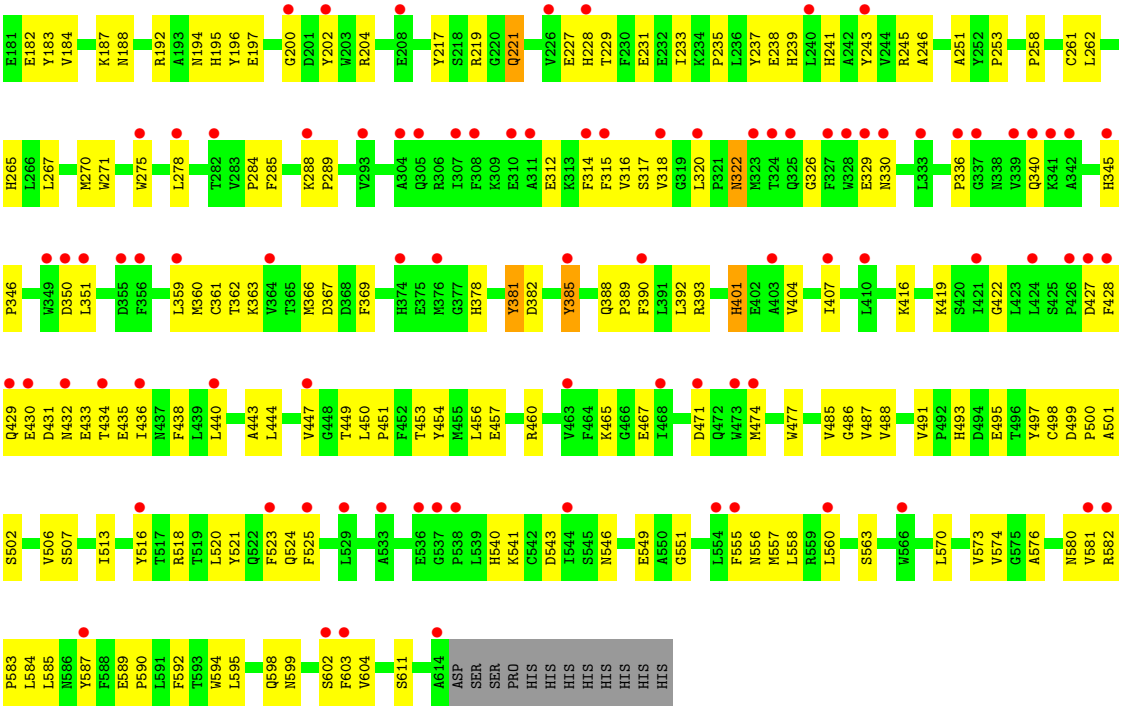
Chain A:



• Molecule 1: Processed angiotensin-converting enzyme 2

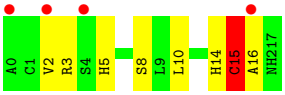
Chain C:





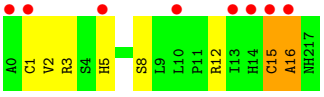
• Molecule 2: ALA-CYS-VAL-ARG-SER-HIS-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA-NH2

Chain B:



• Molecule 2: ALA-CYS-VAL-ARG-SER-HIS-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA-NH2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.94Å 76.97Å 124.23Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	58.75 – 2.33 58.75 – 2.33	Depositor EDS
% Data completeness (in resolution range)	79.3 (58.75-2.33) 79.3 (58.75-2.33)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.323 0.265 , 0.301	Depositor DCC
R_{free} test set	2355 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10013	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 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	0.60	0/5016	0.67	0/6815
1	C	0.61	0/4960	0.68	0/6739
2	B	0.69	0/128	0.80	0/172
2	D	0.70	0/128	0.81	0/172
All	All	0.61	0/10232	0.68	0/13898

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	219	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4879	0	4649	159	0
1	C	4823	0	4604	159	0
2	B	127	0	128	12	0
2	D	127	0	128	6	0
3	B	18	0	0	4	0
3	D	18	0	0	0	0
4	A	13	0	0	1	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
All	All	10013	0	9509	327	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 17.

All (327) 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:140:GLU:HA	1:C:140:GLU:OE1	1.75	0.87
1:C:237:TYR:CE1	1:C:451:PRO:HG2	2.15	0.81
1:A:137:ASN:HB3	1:A:140:GLU:HB3	1.62	0.81
1:A:336:PRO:HB2	1:A:340:GLN:HB3	1.62	0.80
1:A:288:LYS:HE3	1:A:433:GLU:HB2	1.66	0.78
2:B:15:CYS:O	2:B:15:CYS:SG	2.42	0.77
1:A:86:GLN:HG3	1:C:108:LEU:O	1.86	0.75
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.68	0.74
1:A:477:TRP:CD2	1:A:500:PRO:HG3	2.24	0.72
1:A:307:ILE:HG21	1:A:369:PHE:HA	1.72	0.71
1:A:404:VAL:O	1:A:407:ILE:HG12	1.90	0.71
1:C:431:ASP:HB3	1:C:434:THR:HG23	1.71	0.70
1:C:428:PHE:CE2	1:C:430:GLU:HA	2.27	0.70
1:C:25:ALA:O	1:C:28:PHE:HB3	1.93	0.68
1:A:267:LEU:HA	1:A:278:LEU:HD11	1.76	0.68
1:C:237:TYR:CD1	1:C:451:PRO:HG2	2.29	0.67
1:A:132:VAL:HG22	1:A:148:LEU:HD21	1.75	0.67
1:C:382:ASP:HA	1:C:385:TYR:CZ	2.31	0.66
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.78	0.66
1:C:457:GLU:HA	1:C:457:GLU:OE1	1.95	0.66
1:A:339:VAL:HG23	1:A:340:GLN:H	1.62	0.65
1:C:144:LEU:HA	1:C:148:LEU:HB2	1.78	0.65
1:C:351:LEU:H	1:C:351:LEU:HD12	1.61	0.65
1:A:126:ILE:HD11	1:A:176:LEU:CD2	2.27	0.64
1:A:307:ILE:HG23	1:A:369:PHE:HD1	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:O	1:C:82:MET:HG3	1.97	0.64
1:C:580:ASN:HD21	1:C:582:ARG:HD2	1.63	0.64
1:C:126:ILE:HG22	1:C:172:VAL:HG13	1.81	0.63
1:A:520:LEU:HD11	1:A:581:VAL:HG23	1.80	0.62
1:A:107:VAL:HG11	1:A:190:MET:HG3	1.82	0.62
1:C:582:ARG:HB2	1:C:583:PRO:HD3	1.82	0.62
1:C:581:VAL:HG12	1:C:585:LEU:HG	1.83	0.61
1:C:453:THR:HG21	1:C:516:TYR:HB2	1.82	0.61
1:A:122:THR:O	1:A:126:ILE:HG23	2.00	0.60
1:C:31:LYS:O	1:C:35:GLU:HG2	2.02	0.60
1:A:158:TYR:CD2	1:A:266:LEU:HD11	2.37	0.60
1:C:284:PRO:HG2	1:C:436:ILE:HG22	1.83	0.60
1:C:491:VAL:O	1:C:493:HIS:HD2	1.84	0.60
1:A:240:LEU:HD22	1:A:447:VAL:CG2	2.33	0.59
2:B:8:SER:O	3:B:101:LFI:O1	2.20	0.59
1:C:312:GLU:O	1:C:316:VAL:HG23	2.02	0.59
2:B:15:CYS:SG	3:B:101:LFI:O3	2.60	0.59
1:C:416:LYS:HD3	1:C:543:ASP:HB3	1.85	0.59
1:A:134:ASN:HA	1:A:163:TRP:CZ2	2.37	0.59
1:A:469:PRO:HD2	1:A:472:GLN:HE21	1.68	0.59
1:A:269:ASP:HB3	1:A:272:GLY:H	1.68	0.58
1:C:385:TYR:HE2	1:C:401:HIS:HE1	1.50	0.58
1:A:153:ALA:HB1	1:A:277:ASN:ND2	2.18	0.58
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.84	0.58
1:A:191:ALA:O	1:A:196:TYR:HB2	2.03	0.58
1:C:485:VAL:O	1:C:487:VAL:HG23	2.02	0.58
1:C:501:ALA:HA	1:C:506:VAL:CG1	2.34	0.58
1:C:180:TYR:O	1:C:183:TYR:HB3	2.04	0.58
1:C:523:PHE:CE2	1:C:584:LEU:HD13	2.39	0.58
1:A:520:LEU:O	1:A:524:GLN:HG3	2.04	0.58
1:C:378:HIS:ND1	1:C:401:HIS:HD2	2.01	0.58
1:C:456:LEU:CD2	1:C:460:ARG:HD2	2.34	0.57
1:C:140:GLU:OE1	1:C:140:GLU:CA	2.48	0.57
1:A:427:ASP:OD1	1:A:427:ASP:N	2.37	0.57
1:A:72:PHE:O	1:A:76:GLN:HG2	2.05	0.57
1:A:168:TRP:O	1:A:172:VAL:HG13	2.05	0.57
1:C:36:ALA:HB1	1:C:69:TRP:HH2	1.69	0.57
1:C:75:GLU:O	1:C:79:LEU:HG	2.04	0.57
1:C:499:ASP:N	1:C:500:PRO:HD2	2.20	0.56
1:A:55:THR:O	1:A:59:VAL:HG23	2.05	0.56
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:HIS:HB3	1:C:599:ASN:ND2	2.21	0.56
1:C:471:ASP:O	1:C:495:GLU:HG3	2.06	0.56
1:C:456:LEU:HD23	1:C:460:ARG:HD2	1.88	0.56
1:A:519:THR:O	1:A:522:GLN:HG2	2.06	0.55
1:C:326:GLY:HA2	1:C:329:GLU:HG2	1.87	0.55
1:A:419:LYS:HG3	1:A:424:LEU:HD23	1.87	0.55
1:C:228:HIS:O	1:C:231:GLU:HB2	2.06	0.55
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.42	0.55
1:A:111:ASP:O	1:A:115:ARG:HG3	2.06	0.55
1:A:75:GLU:O	1:A:79:LEU:HG	2.06	0.55
1:C:275:TRP:HB3	1:C:278:LEU:HD12	1.89	0.54
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.88	0.54
2:B:15:CYS:O	2:B:16:ALA:HB3	2.07	0.54
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.43	0.54
1:C:315:PHE:O	1:C:320:LEU:HB2	2.08	0.54
1:A:20:THR:O	1:A:24:GLN:HG3	2.08	0.54
1:C:336:PRO:HG2	1:C:340:GLN:O	2.08	0.54
1:A:315:PHE:CE2	1:A:376:MET:HG2	2.42	0.54
1:A:132:VAL:CG2	1:A:148:LEU:HD21	2.38	0.54
1:A:294:THR:HG23	1:A:364:VAL:O	2.07	0.54
1:A:307:ILE:HG23	1:A:369:PHE:CD1	2.43	0.53
1:A:482:ARG:O	1:A:606:TRP:NE1	2.39	0.53
1:C:429:GLN:O	1:C:430:GLU:C	2.47	0.53
1:A:403:ALA:O	1:A:407:ILE:HG23	2.08	0.53
1:C:76:GLN:HA	1:C:79:LEU:HD12	1.90	0.53
1:A:469:PRO:CD	1:A:472:GLN:HE21	2.21	0.53
1:A:242:ALA:HB3	1:A:599:ASN:ND2	2.24	0.53
1:A:240:LEU:HD22	1:A:447:VAL:HG23	1.91	0.52
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.43	0.52
1:A:77:SER:HA	1:A:100:LEU:HG	1.91	0.52
1:C:432:ASN:HA	1:C:435:GLU:HG2	1.91	0.52
1:A:489:GLU:OE2	1:A:489:GLU:N	2.29	0.52
1:C:229:THR:HB	1:C:581:VAL:CG2	2.40	0.52
1:C:122:THR:O	1:C:126:ILE:HG13	2.10	0.52
1:C:267:LEU:HA	1:C:278:LEU:HD11	1.92	0.52
1:C:361:CYS:O	1:C:363:LYS:HE2	2.10	0.52
1:C:465:LYS:HD3	1:C:467:GLU:OE1	2.10	0.52
1:C:549:GLU:CD	1:C:549:GLU:H	2.11	0.51
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.44	0.51
1:A:257:SER:HB2	1:A:610:TRP:CE2	2.45	0.51
1:A:317:SER:CB	1:A:546:ASN:H	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:LEU:HB2	1:C:451:PRO:HD3	1.92	0.51
1:C:457:GLU:HG2	1:C:513:ILE:HB	1.91	0.51
1:A:72:PHE:O	1:A:75:GLU:HG2	2.09	0.51
1:C:288:LYS:HA	1:C:288:LYS:HE2	1.93	0.51
1:C:524:GLN:HG2	1:C:583:PRO:HG2	1.93	0.51
1:A:41:TYR:HE1	1:A:45:LEU:HD22	1.75	0.51
1:A:115:ARG:O	1:A:119:ILE:HG13	2.11	0.51
1:A:469:PRO:HD2	1:A:472:GLN:HG3	1.93	0.51
1:C:594:TRP:CE2	1:C:598:GLN:HG3	2.45	0.51
1:A:391:LEU:HD22	2:B:2:VAL:HG11	1.93	0.50
1:A:392:LEU:HD13	1:A:563:SER:HA	1.94	0.50
1:C:589:GLU:HB3	1:C:590:PRO:HD3	1.92	0.50
1:A:300:GLN:HB2	1:A:302:TRP:CD1	2.45	0.50
1:A:402:GLU:O	1:A:406:GLU:HG2	2.11	0.50
1:C:390:PHE:CZ	2:D:3:ARG:HD3	2.47	0.50
1:A:177:ARG:N	1:A:178:PRO:HD2	2.26	0.50
1:C:84:PRO:HG2	1:C:87:GLU:HB3	1.93	0.50
1:C:390:PHE:O	2:D:3:ARG:HD2	2.12	0.50
1:A:134:ASN:ND2	1:A:136:ASP:HB2	2.27	0.50
1:A:144:LEU:HD21	1:A:271:TRP:HH2	1.76	0.50
1:A:386:ALA:HA	1:A:393:ARG:HD3	1.93	0.50
1:C:314:PHE:O	1:C:318:VAL:HG23	2.11	0.50
1:C:435:GLU:CD	1:C:541:LYS:HE2	2.32	0.50
1:A:589:GLU:N	1:A:590:PRO:CD	2.75	0.50
1:C:392:LEU:HD13	1:C:563:SER:HA	1.92	0.50
1:A:389:PRO:HG2	1:A:392:LEU:HG	1.94	0.50
1:C:556:ASN:O	1:C:560:LEU:HD13	2.11	0.50
1:A:284:PRO:HG2	1:A:436:ILE:HG22	1.94	0.50
1:A:318:VAL:HG23	1:A:320:LEU:HG	1.93	0.49
1:A:332:MET:SD	1:A:336:PRO:HD3	2.52	0.49
1:C:174:LYS:HE3	1:C:497:TYR:CZ	2.46	0.49
1:C:217:TYR:CZ	1:C:221:GLN:HB3	2.47	0.49
1:A:315:PHE:O	1:A:318:VAL:HG22	2.12	0.49
1:C:32:PHE:HD1	1:C:33:ASN:HD22	1.58	0.49
1:C:227:GLU:HG2	1:C:454:TYR:OH	2.12	0.49
1:C:188:ASN:HB3	1:C:192:ARG:HE	1.78	0.49
1:A:318:VAL:O	1:A:548:THR:HA	2.13	0.49
1:C:243:TYR:O	1:C:246:ALA:HB3	2.13	0.49
1:A:424:LEU:HD21	1:A:428:PHE:CD2	2.48	0.49
1:A:380:GLN:HA	1:A:383:MET:HE2	1.95	0.49
2:D:15:CYS:O	2:D:16:ALA:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:CE2	1:A:266:LEU:HD11	2.48	0.48
1:C:318:VAL:HG12	1:C:551:GLY:HA3	1.96	0.48
1:C:64:ASN:O	1:C:68:LYS:HG3	2.13	0.48
1:C:194:ASN:O	1:C:195:HIS:HB2	2.13	0.48
1:A:482:ARG:NE	1:A:608:THR:O	2.38	0.48
1:C:419:LYS:O	1:C:422:GLY:N	2.46	0.48
1:A:469:PRO:HD2	1:A:472:GLN:CG	2.43	0.48
1:C:350:ASP:N	2:D:5:HIS:O	2.44	0.48
1:C:360:MET:O	1:C:362:THR:N	2.47	0.48
1:C:499:ASP:N	1:C:500:PRO:CD	2.76	0.48
1:C:603:PHE:CE1	1:C:604:VAL:O	2.66	0.48
1:A:314:PHE:HD1	1:A:545:SER:OG	1.97	0.48
1:A:185:VAL:O	1:A:189:GLU:HG3	2.12	0.48
1:A:133:CYS:HA	1:A:141:CYS:HA	1.96	0.48
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.95	0.48
1:A:486:GLY:HA2	1:A:606:TRP:NE1	2.29	0.48
1:A:192:ARG:HA	1:A:196:TYR:O	2.14	0.48
1:C:86:GLN:CD	1:C:86:GLN:H	2.18	0.48
1:C:500:PRO:O	1:C:506:VAL:HG21	2.13	0.48
1:C:329:GLU:HG3	1:C:330:ASN:OD1	2.14	0.48
1:A:192:ARG:NH2	1:A:197:GLU:O	2.47	0.47
1:A:389:PRO:O	1:A:393:ARG:HG3	2.14	0.47
1:C:521:TYR:HB3	1:C:525:PHE:CE2	2.48	0.47
2:B:8:SER:O	3:B:101:LFI:C6	2.62	0.47
1:C:127:TYR:HE1	1:C:502:SER:O	1.96	0.47
1:A:474:MET:HE1	1:A:499:ASP:CB	2.44	0.47
1:A:508:ASN:HA	4:A:701:HOH:O	2.14	0.47
1:C:35:GLU:O	1:C:39:LEU:HG	2.15	0.47
1:C:362:THR:O	1:C:363:LYS:HD3	2.14	0.47
1:C:366:MET:O	1:C:369:PHE:HB3	2.14	0.47
1:A:279:TYR:HA	1:A:282:THR:OG1	2.15	0.47
1:C:145:GLU:HA	1:C:146:PRO:HA	1.67	0.47
1:C:158:TYR:CE1	1:C:265:HIS:CE1	3.02	0.47
1:A:549:GLU:H	1:A:549:GLU:CD	2.17	0.47
1:C:540:HIS:NE2	1:C:541:LYS:HE3	2.30	0.47
1:A:265:HIS:CE1	1:A:266:LEU:HD21	2.49	0.47
1:A:307:ILE:CG2	1:A:369:PHE:HA	2.44	0.47
1:C:520:LEU:O	1:C:524:GLN:HG3	2.15	0.46
1:A:317:SER:O	1:A:546:ASN:HA	2.16	0.46
1:C:147:GLY:O	1:C:150:GLU:HG3	2.15	0.46
1:C:174:LYS:HE3	1:C:497:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HB3	1:C:178:PRO:HD3	1.97	0.46
1:C:106:SER:O	1:C:107:VAL:C	2.53	0.46
2:D:1:CYS:O	2:D:1:CYS:SG	2.73	0.46
1:A:134:ASN:HD22	1:A:136:ASP:HB2	1.81	0.46
1:A:379:ILE:O	1:A:383:MET:HG3	2.15	0.46
1:C:453:THR:CG2	1:C:516:TYR:HB2	2.45	0.46
1:A:86:GLN:O	1:A:86:GLN:HG2	2.14	0.46
1:A:431:ASP:O	1:A:435[A]:GLU:HG2	2.15	0.46
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.16	0.46
1:C:431:ASP:HB3	1:C:434:THR:CG2	2.42	0.46
1:C:540:HIS:HA	1:C:587:TYR:CE2	2.51	0.46
1:A:137:ASN:CB	1:A:140:GLU:HB3	2.40	0.46
1:A:51:ASN:OD1	2:B:10:LEU:HD21	2.15	0.46
1:A:450:LEU:CB	1:A:451:PRO:HD3	2.40	0.46
1:A:481:LYS:O	1:A:485:VAL:HB	2.16	0.46
1:C:381:TYR:CE1	1:C:558:LEU:HA	2.50	0.46
1:C:438:PHE:CD1	1:C:438:PHE:C	2.89	0.46
1:A:21:ILE:HD12	1:A:87:GLU:OE1	2.16	0.45
1:C:359:LEU:HD23	1:C:359:LEU:C	2.37	0.45
1:C:431:ASP:CG	1:C:432:ASN:H	2.19	0.45
1:A:50:TYR:CD1	1:A:59:VAL:HG22	2.51	0.45
1:A:53:ASN:HB2	1:A:340:GLN:HE21	1.81	0.45
1:C:345:HIS:O	1:C:346:PRO:C	2.54	0.45
1:C:574:VAL:HG23	1:C:576:ALA:HB3	1.98	0.45
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.81	0.45
1:C:284:PRO:CG	1:C:436:ILE:HG22	2.44	0.45
1:A:523:PHE:CE2	1:A:584:LEU:HD13	2.52	0.45
1:C:570:LEU:O	1:C:574:VAL:HG22	2.17	0.45
1:A:41:TYR:CE1	1:A:45:LEU:HD22	2.51	0.45
1:A:72:PHE:HA	1:A:75:GLU:OE1	2.17	0.45
1:C:580:ASN:HD21	1:C:582:ARG:CD	2.30	0.45
1:A:176:LEU:O	1:A:177:ARG:C	2.55	0.45
1:C:27:THR:O	1:C:31:LYS:HG3	2.17	0.45
1:C:115:ARG:NH2	1:C:182:GLU:HG3	2.32	0.45
1:A:126:ILE:HD11	1:A:176:LEU:HD23	1.99	0.44
1:A:126:ILE:HD11	1:A:176:LEU:HG	2.00	0.44
1:C:285:PHE:CE2	1:C:433:GLU:HG2	2.52	0.44
1:C:326:GLY:HA2	1:C:329:GLU:CG	2.47	0.44
1:C:177:ARG:NH1	1:C:495:GLU:O	2.50	0.44
1:A:336:PRO:HG3	1:A:342:ALA:HB2	1.99	0.44
1:A:441:LYS:O	1:A:445:THR:HG23	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:HB2	1:C:262:LEU:HD21	2.00	0.44
1:C:317:SER:HB2	1:C:546:ASN:OD1	2.17	0.44
1:C:440:LEU:O	1:C:444:LEU:HG	2.17	0.44
1:C:137:ASN:O	1:C:139:GLN:N	2.51	0.44
1:A:76:GLN:HB3	1:A:100:LEU:HD21	2.00	0.44
2:D:12:ARG:O	2:D:15:CYS:HB2	2.17	0.44
1:A:41:TYR:HA	1:A:351:LEU:O	2.18	0.44
1:A:92:THR:O	1:A:96:GLN:HG3	2.18	0.44
1:A:394:ASN:OD1	2:B:3:ARG:HA	2.18	0.44
1:C:389:PRO:HG2	1:C:392:LEU:HD12	2.00	0.44
1:A:90:ASN:C	1:A:90:ASN:OD1	2.56	0.43
1:C:144:LEU:HD21	1:C:271:TRP:CZ2	2.53	0.43
1:A:276:THR:OG1	1:A:445:THR:HG22	2.19	0.43
1:C:88:ILE:HG13	1:C:97:LEU:CD1	2.48	0.43
1:A:309:LYS:O	1:A:313:LYS:HG3	2.18	0.43
1:C:192:ARG:NH2	1:C:197:GLU:O	2.51	0.43
1:C:132:VAL:CG2	1:C:148:LEU:HD21	2.48	0.43
1:C:158:TYR:CE1	1:C:265:HIS:NE2	2.86	0.43
1:C:456:LEU:HD12	1:C:477:TRP:HH2	1.84	0.43
1:C:488:VAL:HG21	1:C:611:SER:HA	2.01	0.43
1:A:180:TYR:O	1:A:184:VAL:HG23	2.18	0.43
2:B:15:CYS:O	3:B:101:LFI:C11	2.66	0.43
1:C:592:PHE:O	1:C:595:LEU:HB2	2.18	0.43
1:A:246:ALA:O	1:A:249:MET:HB2	2.18	0.43
1:A:279:TYR:OH	1:A:437:ASN:HB3	2.19	0.43
1:C:180:TYR:O	1:C:184:VAL:HG23	2.19	0.43
1:C:270:MET:HB3	1:C:271:TRP:CD2	2.53	0.43
1:C:241:HIS:HE1	1:C:245:ARG:NH1	2.16	0.43
1:C:430:GLU:O	1:C:434:THR:OG1	2.24	0.43
1:A:53:ASN:HB2	1:A:340:GLN:NE2	2.33	0.42
1:A:443:ALA:HB1	1:A:447:VAL:HG22	2.01	0.42
1:C:137:ASN:O	1:C:140:GLU:N	2.52	0.42
1:C:388:GLN:OE1	1:C:389:PRO:HD2	2.19	0.42
1:C:555:PHE:O	1:C:556:ASN:C	2.56	0.42
1:C:79:LEU:O	1:C:82:MET:HB3	2.19	0.42
1:A:392:LEU:HD22	1:A:562:LYS:O	2.19	0.42
1:C:270:MET:HB3	1:C:271:TRP:CE2	2.54	0.42
1:A:167:SER:O	1:A:171:GLU:HB2	2.18	0.42
1:A:453:THR:HG23	1:A:512:PHE:CD2	2.55	0.42
1:C:432:ASN:O	1:C:435:GLU:N	2.53	0.42
1:A:132:VAL:HG13	1:A:148:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG11	1:A:215:TYR:O	2.20	0.42
1:A:582:ARG:HB2	1:A:583:PRO:HD3	2.01	0.42
1:C:557:MET:HB2	1:C:573:VAL:CG2	2.50	0.42
1:A:385:TYR:C	1:A:387:ALA:N	2.72	0.42
1:C:233:ILE:C	1:C:235:PRO:HD2	2.39	0.42
1:C:318:VAL:HG12	1:C:551:GLY:CA	2.49	0.42
1:A:145:GLU:HA	1:A:146:PRO:HA	1.76	0.42
1:C:267:LEU:HB3	1:C:275:TRP:CD1	2.55	0.42
1:C:390:PHE:HA	1:C:393:ARG:HD2	2.02	0.42
1:C:498:CYS:C	1:C:500:PRO:HD2	2.39	0.42
1:A:171:GLU:O	1:A:175:GLN:NE2	2.51	0.41
1:A:201:ASP:CG	1:A:219:ARG:HE	2.24	0.41
1:A:388:GLN:HB3	1:A:389:PRO:HD2	2.02	0.41
1:A:477:TRP:CE2	1:A:500:PRO:HG3	2.55	0.41
1:C:183:TYR:CD1	1:C:187:LYS:HG3	2.55	0.41
1:A:103:ASN:N	1:A:103:ASN:HD22	2.17	0.41
1:C:245:ARG:NH2	1:C:258:PRO:O	2.52	0.41
1:C:261:CYS:SG	1:C:486:GLY:HA2	2.60	0.41
1:C:381:TYR:HA	1:C:558:LEU:HD23	2.02	0.41
1:A:237:TYR:CE1	1:A:451:PRO:HG2	2.55	0.41
1:A:562:LYS:NZ	2:B:2:VAL:HG13	2.35	0.41
1:C:200:GLY:O	1:C:204:ARG:HG3	2.20	0.41
1:C:382:ASP:HA	1:C:385:TYR:CE1	2.55	0.41
1:A:107:VAL:CG1	1:A:190:MET:HG3	2.48	0.41
1:A:236:LEU:HD21	1:A:447:VAL:HG11	2.02	0.41
1:C:83:TYR:HE1	1:C:88:ILE:HD11	1.86	0.41
1:C:404:VAL:O	1:C:407:ILE:HG12	2.20	0.41
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.85	0.41
1:A:559:ARG:NH1	1:A:559:ARG:HB2	2.36	0.41
1:C:196:TYR:CD2	1:C:202:TYR:HA	2.55	0.41
1:C:251:ALA:C	1:C:253:PRO:HD3	2.41	0.41
1:C:316:VAL:HG21	1:C:322:ASN:HD22	1.86	0.41
1:C:389:PRO:HG2	1:C:392:LEU:CG	2.50	0.41
1:C:443:ALA:O	1:C:447:VAL:HG22	2.21	0.41
1:A:223:ILE:O	1:A:227:GLU:HG3	2.21	0.41
1:A:269:ASP:HB3	1:A:272:GLY:N	2.35	0.41
1:A:385:TYR:O	1:A:393:ARG:HG2	2.20	0.41
1:C:131:LYS:HG2	1:C:141:CYS:HB3	2.03	0.41
1:C:474:MET:HE1	1:C:499:ASP:HB2	2.03	0.41
1:A:187:LYS:HD2	1:A:199:TYR:CZ	2.56	0.41
1:A:456:LEU:O	1:A:460:ARG:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HG3	1:A:76:GLN:HE21	1.86	0.40
1:A:393:ARG:HB2	2:B:3:ARG:HD2	2.04	0.40
1:A:80:ALA:HB2	1:A:100:LEU:HD23	2.02	0.40
1:A:453:THR:HG23	1:A:512:PHE:HD2	1.85	0.40
1:A:492:PRO:HB3	1:A:613:TYR:CE2	2.56	0.40
1:A:524:GLN:HG2	1:A:583:PRO:HG2	2.03	0.40
1:C:435:GLU:OE1	1:C:540:HIS:HE1	2.03	0.40
1:A:530:CYS:O	1:A:533:ALA:N	2.54	0.40
2:B:15:CYS:O	2:B:16:ALA:CB	2.69	0.40
1:C:235:PRO:O	1:C:238:GLU:HB2	2.21	0.40
1:A:50:TYR:HD2	1:A:51:ASN:ND2	2.20	0.40
1:C:367:ASP:OD1	1:C:367:ASP:N	2.54	0.40
1:C:431:ASP:OD1	1:C:432:ASN:N	2.47	0.40
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.87	0.40
1:C:594:TRP:CZ2	1:C:598:GLN:HG3	2.57	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	596/609 (98%)	551 (92%)	42 (7%)	3 (0%)	29 31
1	C	589/609 (97%)	537 (91%)	51 (9%)	1 (0%)	47 55
2	B	16/18 (89%)	10 (62%)	4 (25%)	2 (12%)	0 0
2	D	16/18 (89%)	12 (75%)	2 (12%)	2 (12%)	0 0
All	All	1217/1254 (97%)	1110 (91%)	99 (8%)	8 (1%)	22 22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	VAL
2	D	16	ALA
2	B	14	HIS
2	B	15	CYS
1	A	105	SER
1	A	346	PRO
1	C	289	PRO
1	A	339	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	528/538 (98%)	515 (98%)	13 (2%)	47 58
1	C	521/538 (97%)	505 (97%)	16 (3%)	40 49
2	B	15/15 (100%)	13 (87%)	2 (13%)	4 3
2	D	15/15 (100%)	13 (87%)	2 (13%)	4 3
All	All	1079/1106 (98%)	1046 (97%)	33 (3%)	40 49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	MET
1	A	107	VAL
1	A	113	SER
1	A	183	TYR
1	A	254	SER
1	A	381	TYR
1	A	401	HIS
1	A	427	ASP
1	A	431	ASP
1	A	479	GLU
1	A	491	VAL
1	A	498	CYS
1	A	518	ARG
2	B	5	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	15	CYS
1	C	55	THR
1	C	57	GLU
1	C	82	MET
1	C	86	GLN
1	C	92	THR
1	C	150	GLU
1	C	221	GLN
1	C	322	ASN
1	C	381	TYR
1	C	385	TYR
1	C	401	HIS
1	C	427	ASP
1	C	449	THR
1	C	507	SER
1	C	518	ARG
1	C	602	SER
2	D	8	SER
2	D	15	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	64	ASN
1	A	76	GLN
1	A	98	GLN
1	A	103	ASN
1	A	134	ASN
1	A	149	ASN
1	A	159	ASN
1	A	194	ASN
1	A	277	ASN
1	A	305	GLN
1	A	325	GLN
1	A	442	GLN
1	A	472	GLN
1	A	531	GLN
1	A	535	HIS
1	A	599	ASN
1	C	33	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	34	HIS
1	C	61	ASN
1	C	89	GLN
1	C	102	GLN
1	C	149	ASN
1	C	159	ASN
1	C	175	GLN
1	C	194	ASN
1	C	277	ASN
1	C	290	ASN
1	C	300	GLN
1	C	322	ASN
1	C	401	HIS
1	C	531	GLN
2	D	5	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFI	B	101	2	18,18,21	0.25	0	24,24,27	0.80	0
3	LFI	D	101	2	18,18,21	0.57	0	24,24,27	1.67	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFI	B	101	2	-	4/18/30/33	0/0/1/1
3	LFI	D	101	2	-	2/18/30/33	0/0/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	101	LFI	N2-C1-N1	-5.00	103.00	110.77
3	D	101	LFI	N3-C3-N1	-4.14	104.34	110.77
3	D	101	LFI	N3-C2-N2	-3.92	104.69	110.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	101	LFI	C7-C6-N2-C2
3	B	101	LFI	O1-C6-N2-C2
3	D	101	LFI	C8-C4-N1-C1
3	D	101	LFI	O2-C4-N1-C1
3	B	101	LFI	O1-C6-N2-C1
3	B	101	LFI	O2-C4-N1-C1

There are no ring outliers.

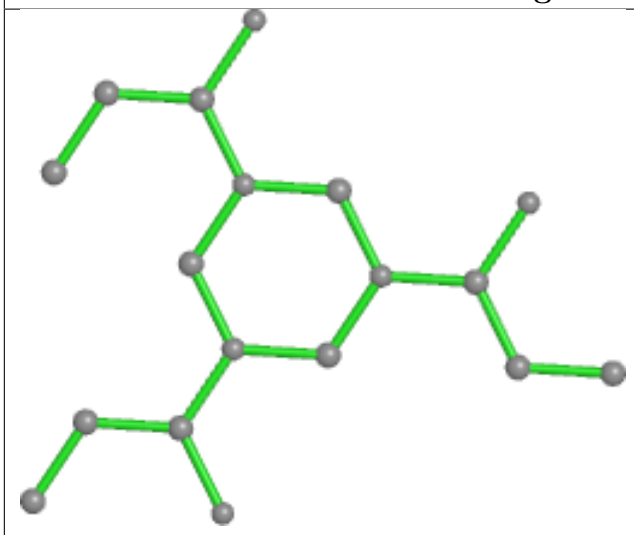
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	101	LFI	4	0

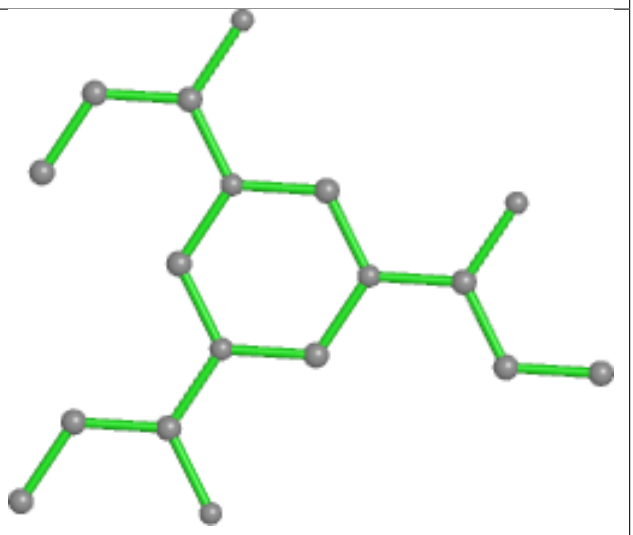
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

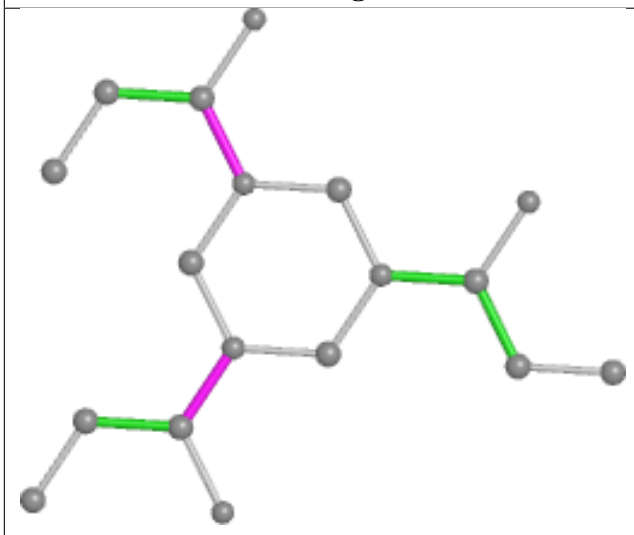
Ligand LFI B 101



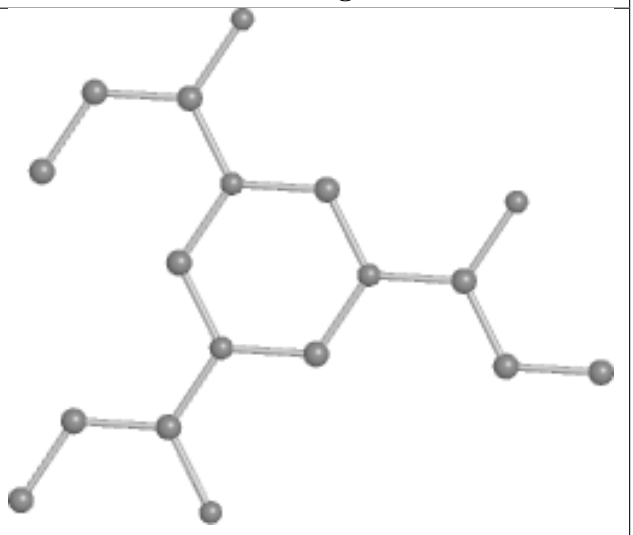
Bond lengths



Bond angles

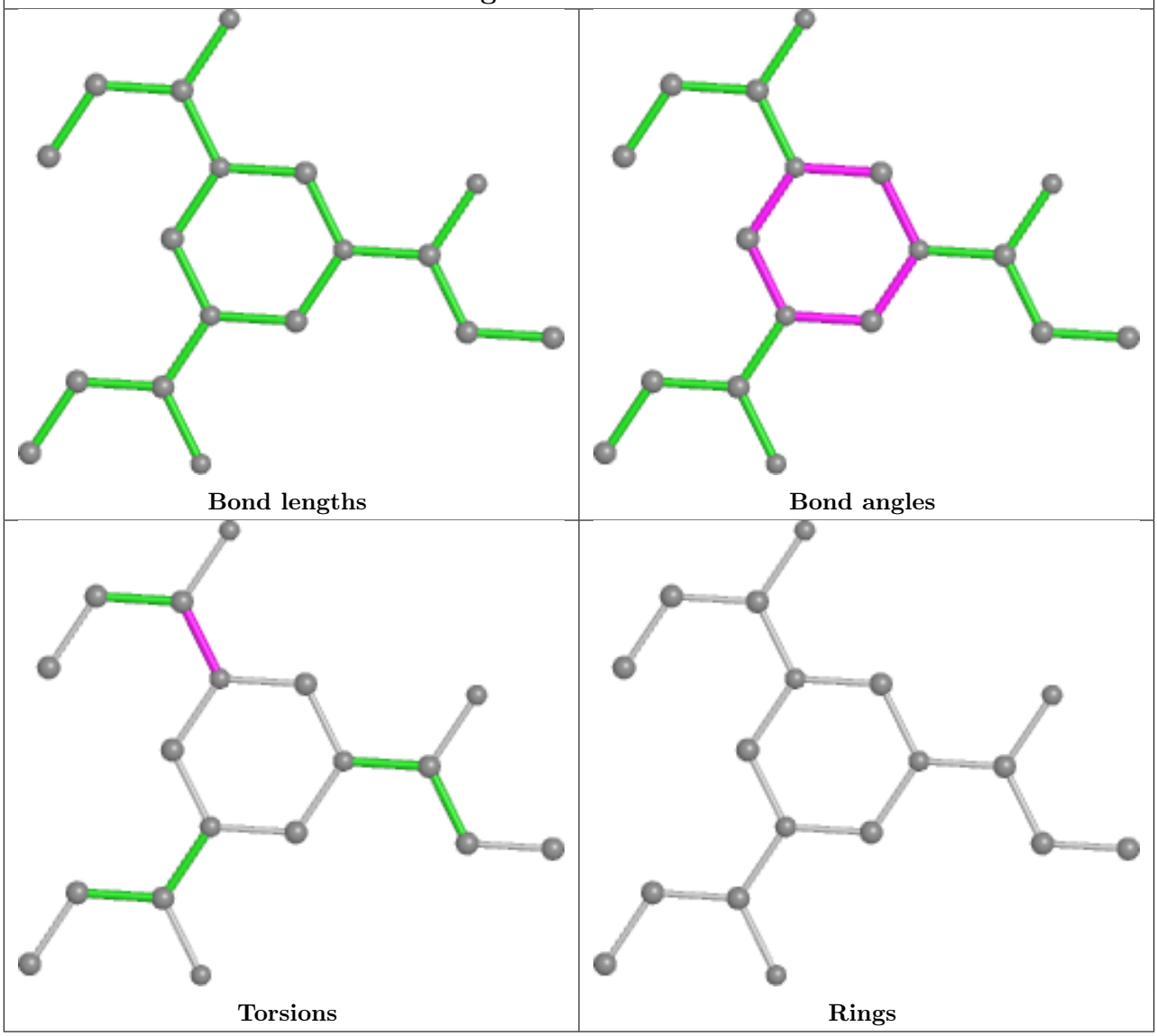


Torsions



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%)	1.12	84 (14%) 2 4	37, 62, 100, 141	0
1	C	591/609 (97%)	1.45	138 (23%) 0 1	39, 72, 114, 172	0
2	B	17/18 (94%)	1.39	4 (23%) 0 1	30, 61, 101, 106	0
2	D	17/18 (94%)	2.87	8 (47%) 0 0	30, 84, 115, 117	0
All	All	1221/1254 (97%)	1.31	234 (19%) 1 2	30, 66, 109, 172	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	428	PHE	12.7
1	C	73	LEU	12.0
2	D	0	ALA	11.1
1	C	339	VAL	9.6
1	C	106	SER	8.8
1	A	136	ASP	8.3
2	D	16	ALA	8.2
2	B	0	ALA	7.7
1	C	327	PHE	7.6
1	A	105	SER	6.6
2	D	14	HIS	6.6
1	C	555	PHE	6.5
1	C	351	LEU	6.0
1	A	87	GLU	6.0
1	C	83	TYR	5.9
1	C	100	LEU	5.8
1	C	390	PHE	5.7
1	C	340	GLN	5.6
1	C	107	VAL	5.6
1	A	400	PHE	5.5
1	A	115	ARG	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	72	PHE	5.1
1	C	104	GLY	5.0
1	C	48	TRP	5.0
1	C	421	ILE	5.0
1	C	471	ASP	4.9
1	C	427	ASP	4.9
1	C	308	PHE	4.8
1	C	328	TRP	4.8
1	C	325	GLN	4.8
1	C	356	PHE	4.7
1	C	80	ALA	4.7
1	A	103	ASN	4.7
1	C	45	LEU	4.6
1	C	92	THR	4.6
1	C	529	LEU	4.4
1	C	60	GLN	4.4
1	C	105	SER	4.4
1	C	69	TRP	4.3
1	C	67	ASP	4.3
1	C	403	ALA	4.2
1	C	311	ALA	4.1
1	C	342	ALA	4.1
2	B	16	ALA	4.1
2	B	2	VAL	4.0
1	C	434	THR	4.0
1	C	429	GLN	4.0
1	C	54	ILE	4.0
1	C	323	MET	4.0
1	C	163	TRP	4.0
1	C	587	TYR	3.9
1	A	134	ASN	3.8
1	C	172	VAL	3.8
1	C	138	PRO	3.8
1	C	537	GLY	3.7
1	C	341	LYS	3.7
1	C	430	GLU	3.6
1	C	57	GLU	3.6
1	A	86	GLN	3.6
1	C	447	VAL	3.5
1	C	536	GLU	3.5
1	A	289	PRO	3.5
2	D	10	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	3.4
2	D	15	CYS	3.4
1	C	330	ASN	3.4
1	C	432	ASN	3.4
1	C	525	PHE	3.3
1	C	324	THR	3.3
1	C	79	LEU	3.3
1	C	75	GLU	3.3
2	D	1	CYS	3.2
1	A	503	LEU	3.2
1	A	140	GLU	3.2
1	C	320	LEU	3.2
1	C	349	TRP	3.2
1	C	560	LEU	3.2
1	C	42	GLN	3.2
1	C	582	ARG	3.2
1	C	337	GLY	3.2
1	A	497	TYR	3.1
1	A	168	TRP	3.1
1	A	80	ALA	3.1
1	C	538	PRO	3.1
1	C	436	ILE	3.1
1	C	310	GLU	3.1
1	A	554	LEU	3.1
1	C	424	LEU	3.1
1	C	58	ASN	3.0
1	A	378	HIS	3.0
2	D	13	ILE	3.0
1	C	314	PHE	3.0
1	A	274	PHE	3.0
1	C	318	VAL	3.0
1	C	137	ASN	2.9
1	C	56	GLU	2.9
2	D	5	HIS	2.9
1	A	142	LEU	2.9
1	C	50	TYR	2.9
1	C	226	VAL	2.8
1	A	456	LEU	2.8
1	C	410	LEU	2.8
1	A	137	ASN	2.8
1	A	427	ASP	2.8
1	A	315	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	55	THR	2.8
1	A	613	TYR	2.8
1	C	523	PHE	2.8
1	C	333	LEU	2.7
1	A	409	SER	2.7
1	A	287	GLN	2.7
1	A	339	VAL	2.7
1	A	566	TRP	2.7
1	C	293	VAL	2.7
1	A	401	HIS	2.7
1	A	372	ALA	2.7
1	C	41	TYR	2.7
1	C	32	PHE	2.7
1	C	139	GLN	2.7
1	A	138	PRO	2.6
1	C	602	SER	2.6
1	C	175	GLN	2.6
1	C	544	ILE	2.6
1	A	512	PHE	2.6
1	C	53	ASN	2.6
1	C	329	GLU	2.6
1	A	172	VAL	2.6
1	A	369	PHE	2.6
1	A	406	GLU	2.6
1	C	463	VAL	2.6
1	C	345	HIS	2.6
1	C	110	GLU	2.5
1	C	359	LEU	2.5
1	C	554	LEU	2.5
1	A	542	CYS	2.5
1	C	473	TRP	2.5
1	C	374	HIS	2.5
1	C	474	MET	2.5
1	C	28	PHE	2.5
1	A	106	SER	2.5
1	C	516	TYR	2.5
1	A	421	ILE	2.5
1	C	228	HIS	2.5
1	A	376	MET	2.5
1	A	424	LEU	2.5
1	C	136	ASP	2.5
1	C	25	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	336	PRO	2.4
1	C	87	GLU	2.4
1	A	290	ASN	2.4
1	A	276	THR	2.4
1	C	282	THR	2.4
1	C	126	ILE	2.4
1	C	566	TRP	2.4
1	A	468	ILE	2.4
1	C	307	ILE	2.4
2	B	4	SER	2.4
1	C	208	GLU	2.4
1	A	73	LEU	2.4
1	A	332	MET	2.4
1	C	350	ASP	2.4
1	A	117	ASN	2.4
1	A	145	GLU	2.4
1	A	322	ASN	2.4
1	C	288	LYS	2.3
1	A	367	ASP	2.3
1	A	302	TRP	2.3
1	A	446	ILE	2.3
1	C	407	ILE	2.3
1	C	385	TYR	2.3
1	C	275	TRP	2.3
1	A	199	TYR	2.3
1	C	142	LEU	2.3
1	C	533	ALA	2.3
1	A	347	THR	2.3
1	A	364	VAL	2.3
1	A	504	PHE	2.3
1	C	315	PHE	2.3
1	A	301	ALA	2.3
1	A	320	LEU	2.3
1	A	219	ARG	2.3
1	A	243	TYR	2.3
1	C	24	GLN	2.3
1	C	31	LYS	2.3
1	A	85	LEU	2.2
1	A	334	THR	2.2
1	A	252	TYR	2.2
1	C	243	TYR	2.2
1	A	371	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	118	THR	2.2
1	A	510	TYR	2.2
1	C	59	VAL	2.2
1	C	102	GLN	2.2
1	C	305	GLN	2.2
1	C	44	SER	2.2
1	A	76	GLN	2.2
1	A	429	GLN	2.2
1	C	89	GLN	2.2
1	C	39	LEU	2.2
1	A	84	PRO	2.2
1	A	381	TYR	2.2
1	C	49	ASN	2.2
1	A	307	ILE	2.2
1	C	202	TYR	2.2
1	A	93	VAL	2.2
1	C	355	ASP	2.2
1	A	119	ILE	2.1
1	C	468	ILE	2.1
1	A	321	PRO	2.1
1	A	452	PHE	2.1
1	C	603	PHE	2.1
1	A	223	ILE	2.1
1	C	278	LEU	2.1
1	A	366	MET	2.1
1	C	376	MET	2.1
1	C	581	VAL	2.1
1	A	570	LEU	2.1
1	C	34	HIS	2.1
1	C	33	ASN	2.1
1	A	412	ALA	2.1
1	C	614	ALA	2.1
1	C	364	VAL	2.1
1	A	584	LEU	2.0
1	C	304	ALA	2.0
1	C	440	LEU	2.0
1	C	426	PRO	2.0
1	A	525	PHE	2.0
1	A	159	ASN	2.0
1	A	385	TYR	2.0
1	A	379	ILE	2.0
1	C	240	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	297	MET	2.0
1	C	200	GLY	2.0
1	A	471	ASP	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)

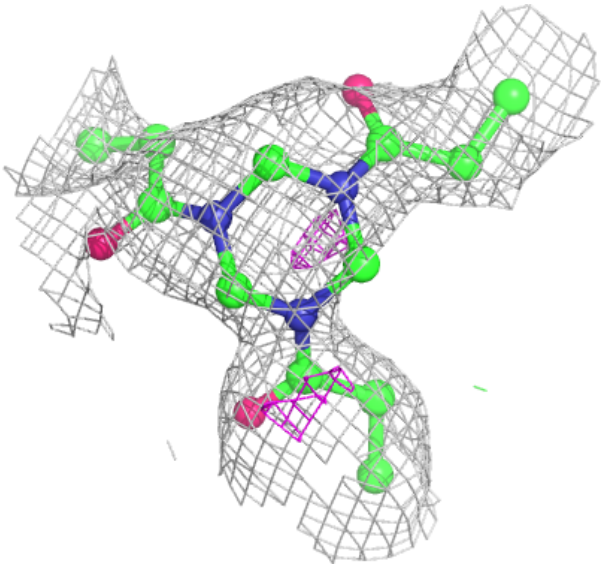
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

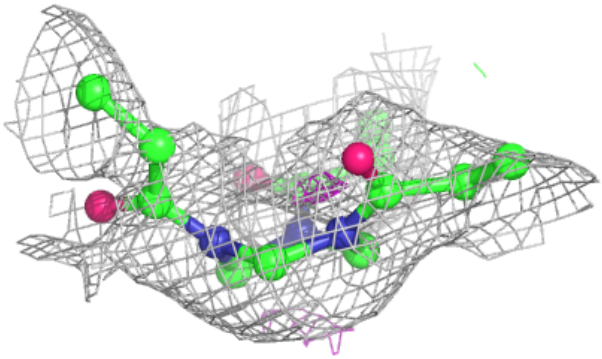
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFI	B	101	18/21	0.71	0.24	87,105,112,116	0
3	LFI	D	101	18/21	0.86	0.27	71,83,95,96	0

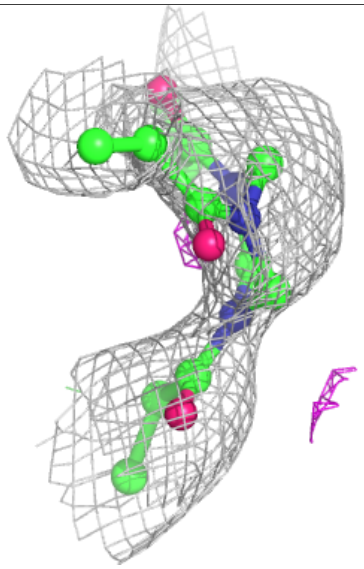
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFI B 101:

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

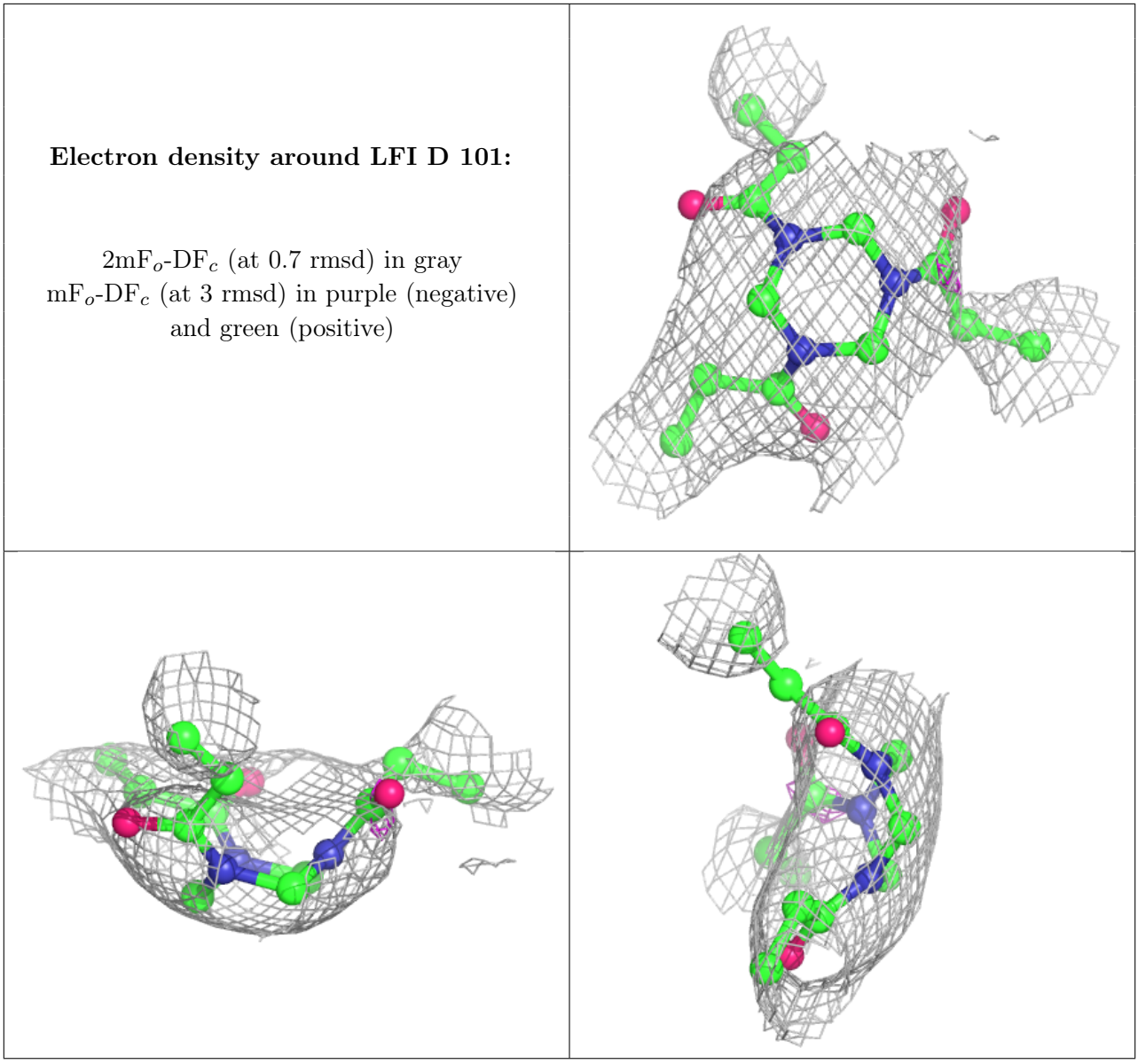






Electron density around LFI D 101:

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



6.5 Other polymers

There are no such residues in this entry.