Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 05:25 pm BST

PDB ID	:	8BN1
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	:	2022-11-11
Resolution	:	2.61 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:

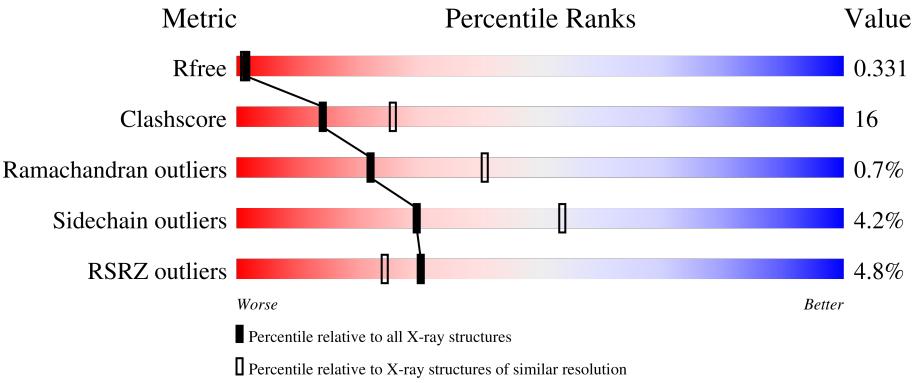
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	5% 61% 34%
1	B	609	4% 65% 31%
2	C	18	6% 67% 22% 11%
2	D	18	6% 44% 44% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10092 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	595	Total	C	N	O	S	0	0	0
			4856	3108	804	915	29			
1	B	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	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

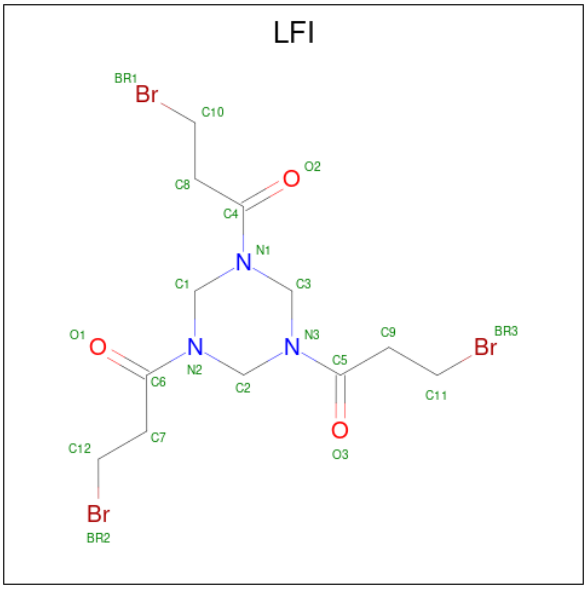
- Molecule 2 is a protein called ALA-CYS-VAL-ARG-SER-4PH-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	S	0	0	1
			129	80	26	20	3			
2	D	18	Total	C	N	O	S	0	0	1
			129	80	26	20	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 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
4	C	1	Total	C	N	O	0	0
			18	12	3	3		
4	D	1	Total	C	N	O	0	0
			18	12	3	3		

- Molecule 5 is water.

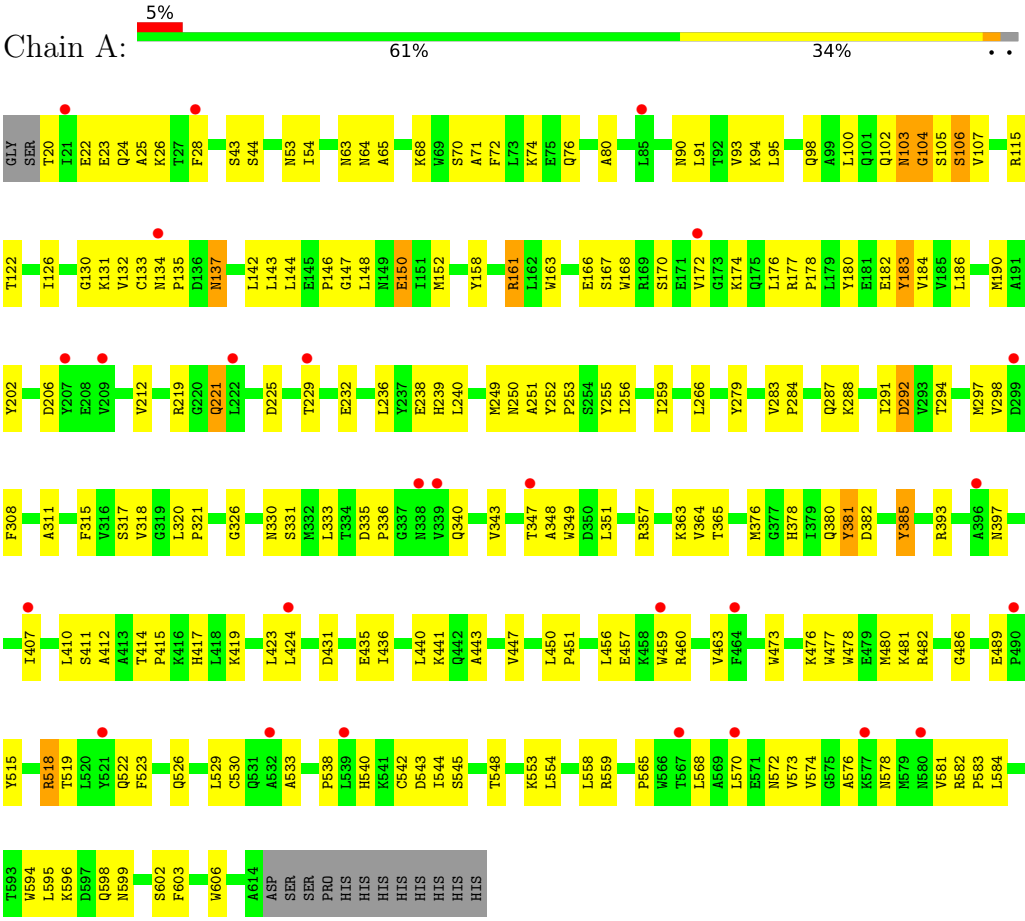
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	39	Total O 39 39	0	0
5	C	3	Total O 3 3	0	0
5	D	3	Total O 3 3	0	0

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.

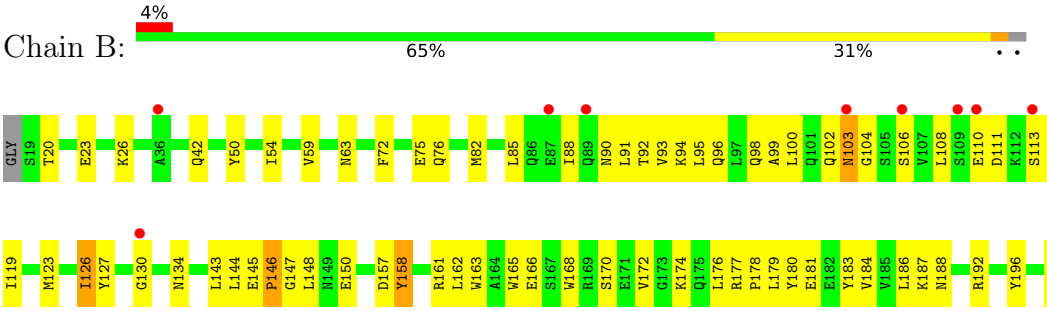
• Molecule 1: Processed angiotensin-converting enzyme 2

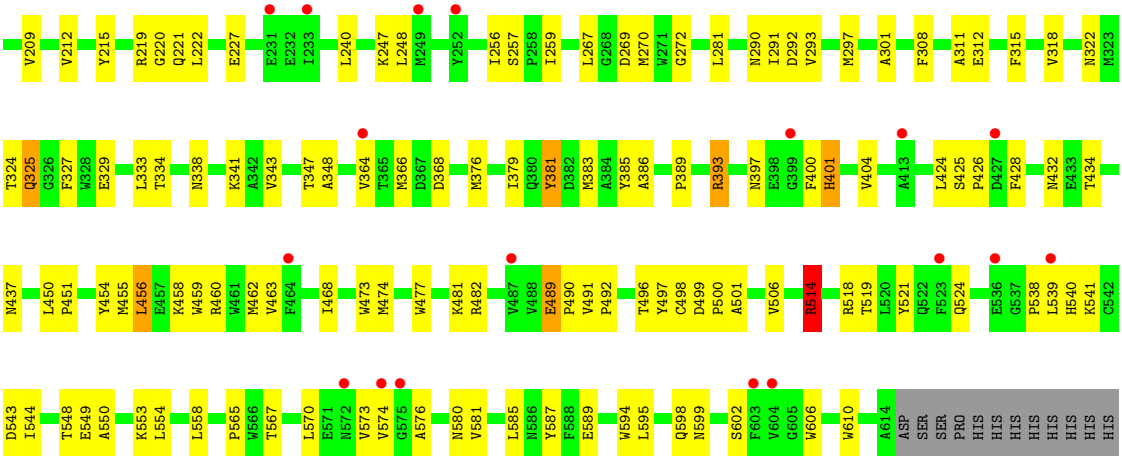
Chain A:



• Molecule 1: Processed angiotensin-converting enzyme 2

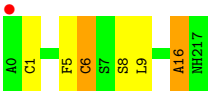
Chain B:





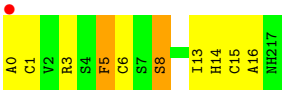
• Molecule 2: ALA-CYS-VAL-ARG-SER-4PH-CYS-SER-SER-LEU-LEU-PRO-ARG-ILE-HIS-CYS-ALA-NH2

Chain C:



• Molecule 2: ALA-CYS-VAL-ARG-SER-4PH-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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	193.25Å 55.79Å 122.84Å 90.00° 114.09° 90.00°	Depositor
Resolution (Å)	58.75 – 2.61 112.14 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (58.75-2.61) 99.3 (112.14-2.61)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.255 , 0.325 0.269 , 0.331	Depositor DCC
R_{free} test set	1827 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10092	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.45% 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: NH2, ZN, LFI, 4PH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/4993	0.67	0/6784
1	B	0.46	0/4999	0.66	0/6792
2	C	0.65	0/116	0.90	0/154
2	D	0.53	0/116	0.74	0/154
All	All	0.46	0/10224	0.67	0/13884

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	3
1	B	0	2
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	161	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	306	ARG	Sidechain
1	B	393	ARG	Sidechain
1	B	514	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	4856	0	4634	165	0
1	B	4862	0	4639	134	0
2	C	129	0	132	8	0
2	D	129	0	132	12	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	C	18	0	0	2	0
4	D	18	0	0	1	0
5	A	32	0	0	2	0
5	B	39	0	0	1	0
5	C	3	0	0	1	0
5	D	3	0	0	0	0
All	All	10092	0	9537	305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (305) 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:A:450:LEU:HB2	1:A:451:PRO:HD3	1.60	0.83
1:A:91:LEU:O	1:A:94:LYS:HG2	1.83	0.79
1:A:538:PRO:HB2	1:A:540:HIS:HD2	1.46	0.79
1:A:103:ASN:HB3	2:D:0:ALA:HA	1.63	0.78
1:B:126:ILE:HD12	1:B:127:TYR:N	1.99	0.78
1:A:131:LYS:HG2	1:A:143:LEU:HG	1.66	0.78
1:B:76:GLN:HB3	1:B:100:LEU:HD21	1.67	0.77
1:A:482:ARG:HH11	1:A:489:GLU:CD	1.91	0.74
1:B:85:LEU:HB3	1:B:94:LYS:HE3	1.69	0.74
1:A:71:ALA:HA	1:A:74:LYS:HD2	1.71	0.73
1:A:519:THR:O	1:A:522:GLN:HG2	1.88	0.73
1:B:126:ILE:HD12	1:B:126:ILE:C	2.12	0.69
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.75	0.69
1:A:115:ARG:NH1	1:A:186:LEU:HD11	2.06	0.68
2:C:6:CYS:H	4:C:101:LFI:C11	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ALA:O	2:C:6:CYS:HA	1.93	0.68
1:A:348:ALA:O	2:D:6:CYS:HA	1.95	0.67
1:A:385:TYR:HD1	1:A:385:TYR:O	1.78	0.66
1:A:376:MET:O	1:A:376:MET:HG2	1.95	0.66
1:B:123:MET:HG2	1:B:176:LEU:HD22	1.77	0.66
1:B:397:ASN:HD21	1:B:521:TYR:HE2	1.44	0.66
1:A:411:SER:HA	1:A:414:THR:HG23	1.76	0.66
1:A:95:LEU:HA	1:A:98:GLN:HE21	1.61	0.65
1:A:180:TYR:O	1:A:184:VAL:HG23	1.95	0.65
1:B:292:ASP:HA	1:B:366:MET:SD	2.37	0.65
1:B:460:ARG:HH21	1:B:506:VAL:HA	1.62	0.64
1:B:85:LEU:HD22	1:B:94:LYS:HG3	1.80	0.63
1:A:404:VAL:O	1:A:407:ILE:HG12	1.99	0.63
1:A:168:TRP:O	1:A:172:VAL:HG22	1.98	0.63
1:B:434:THR:HA	1:B:437:ASN:HD22	1.64	0.63
1:B:381:TYR:CD1	1:B:558:LEU:HG	2.35	0.62
1:B:308:PHE:CD2	1:B:333:LEU:HD13	2.34	0.62
1:A:326:GLY:O	1:A:330:ASN:ND2	2.33	0.62
1:A:287:GLN:HG3	1:A:288:LYS:H	1.64	0.62
1:A:294:THR:HG23	1:A:365:THR:HA	1.80	0.62
1:B:90:ASN:HB3	1:B:93:VAL:HG22	1.80	0.62
1:A:239:HIS:CE1	1:A:596:LYS:HG2	2.35	0.62
1:B:549:GLU:O	1:B:553:LYS:HD3	1.99	0.61
1:A:287:GLN:HG3	1:A:288:LYS:N	2.14	0.61
1:B:54:ILE:HD11	1:B:343:VAL:HG23	1.82	0.61
1:A:103:ASN:HA	1:A:202:TYR:OH	2.01	0.61
2:D:5:4PH:CD2	2:D:5:4PH:H	2.12	0.61
1:B:168:TRP:O	1:B:172:VAL:HG22	2.00	0.61
1:A:249:MET:CG	1:A:256:ILE:HB	2.31	0.60
1:B:215:TYR:HB3	1:B:567:THR:OG1	2.02	0.60
1:A:318:VAL:O	1:A:548:THR:HA	2.02	0.60
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.84	0.60
1:A:206:ASP:OD2	1:A:397:ASN:HB2	2.02	0.59
1:A:412:ALA:HA	1:A:417:HIS:CD2	2.37	0.59
1:A:236:LEU:HD13	1:A:592:PHE:HB2	1.83	0.59
1:B:474:MET:HE1	1:B:499:ASP:HB2	1.82	0.59
1:A:20:THR:O	1:A:24:GLN:HG3	2.02	0.59
1:A:80:ALA:HB2	1:A:100:LEU:HD23	1.83	0.59
1:A:134:ASN:HB2	1:A:137:ASN:C	2.23	0.59
1:A:249:MET:HG3	1:A:256:ILE:HB	1.84	0.58
1:A:166:GLU:O	1:A:170:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:CYS:SG	1:A:544:ILE:HG23	2.43	0.58
1:B:162:LEU:HD11	1:B:491:VAL:HG13	1.84	0.58
1:B:259:ILE:O	1:B:606:TRP:HA	2.04	0.58
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.84	0.58
1:A:347:THR:CG2	2:D:6:CYS:HB2	2.34	0.58
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.85	0.57
1:A:291:ILE:O	1:A:292:ASP:C	2.41	0.57
2:C:6:CYS:N	4:C:101:LFI:C11	2.67	0.57
1:A:91:LEU:HD12	1:A:94:LYS:HE3	1.87	0.56
1:A:385:TYR:O	1:A:385:TYR:CD1	2.58	0.56
1:A:591:LEU:O	1:A:595:LEU:HB2	2.05	0.56
1:B:110:GLU:HA	1:B:113:SER:HB2	1.86	0.56
1:B:98:GLN:O	1:B:102:GLN:HG2	2.06	0.56
1:A:70:SER:O	1:A:74:LYS:HG3	2.05	0.56
1:A:349:TRP:HA	2:D:5:4PH:O	2.06	0.56
1:B:401:HIS:HB2	5:B:808:HOH:O	2.06	0.55
1:B:594:TRP:O	1:B:598:GLN:HG2	2.06	0.55
1:A:315:PHE:CD1	1:A:380:GLN:HG3	2.41	0.55
1:A:107:VAL:HG21	1:A:193:ALA:HB1	1.88	0.55
1:A:533:ALA:HB2	1:A:544:ILE:HG22	1.88	0.55
1:A:376:MET:O	1:A:376:MET:CG	2.54	0.55
1:A:172:VAL:O	1:A:176:LEU:HG	2.06	0.55
1:A:308:PHE:CG	1:A:333:LEU:HD13	2.42	0.55
1:B:425:SER:HB2	1:B:426:PRO:HD2	1.89	0.55
1:A:526:GLN:HG3	1:A:530:CYS:SG	2.47	0.54
1:A:134:ASN:HB2	1:A:137:ASN:O	2.07	0.54
1:A:64:ASN:O	1:A:68:LYS:HG3	2.07	0.54
1:A:419:LYS:HA	1:A:424:LEU:O	2.08	0.54
1:B:499:ASP:N	1:B:500:PRO:CD	2.70	0.53
1:B:389:PRO:O	1:B:393:ARG:HG3	2.07	0.53
1:B:240:LEU:HA	1:B:595:LEU:HD21	1.91	0.53
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.89	0.53
1:B:50:TYR:CE1	1:B:59:VAL:HG23	2.43	0.53
1:B:174:LYS:HG2	1:B:496:THR:O	2.08	0.53
1:B:538:PRO:HB3	1:B:540:HIS:NE2	2.24	0.53
1:A:378:HIS:O	1:A:382:ASP:N	2.39	0.53
1:B:92:THR:HG22	1:B:96:GLN:NE2	2.23	0.53
1:A:343:VAL:HG21	2:D:14:HIS:CD2	2.45	0.53
1:A:72:PHE:O	1:A:76:GLN:HG2	2.09	0.52
1:A:459:TRP:O	1:A:463:VAL:HG23	2.08	0.52
1:B:92:THR:HG22	1:B:96:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:CE2	1:B:376:MET:HG2	2.45	0.52
1:B:325:GLN:O	1:B:329:GLU:HG3	2.09	0.52
1:B:347:THR:HG22	2:C:8:SER:CB	2.40	0.52
1:A:142:LEU:HD11	1:A:147:GLY:HA3	1.92	0.52
1:A:142:LEU:HD21	1:A:147:GLY:HA3	1.92	0.52
1:A:300:GLN:NE2	1:A:423:LEU:HD23	2.24	0.52
1:B:63:ASN:HA	2:C:16:ALA:HB2	1.92	0.52
1:A:284:PRO:HG2	1:A:436:ILE:HG22	1.91	0.52
1:A:212:VAL:HG21	1:A:565:PRO:HG3	1.92	0.51
1:A:335:ASP:OD1	1:A:336:PRO:HD2	2.10	0.51
1:A:297:MET:O	1:A:301:ALA:N	2.44	0.51
1:A:63:ASN:HA	2:D:16:ALA:HB2	1.91	0.51
1:A:76:GLN:HB3	1:A:100:LEU:HD21	1.91	0.51
1:B:524:GLN:NE2	1:B:580:ASN:HB2	2.26	0.51
1:B:544:ILE:HD11	1:B:550:ALA:HB1	1.91	0.51
1:B:544:ILE:HD11	1:B:550:ALA:CB	2.41	0.51
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.46	0.51
1:B:82:MET:O	1:B:82:MET:HG2	2.11	0.51
1:B:424:LEU:HD21	1:B:428:PHE:HD2	1.76	0.51
1:B:581:VAL:O	1:B:585:LEU:HG	2.11	0.51
1:A:443:ALA:HA	1:A:447:VAL:HG23	1.93	0.51
1:A:538:PRO:HB2	1:A:540:HIS:CD2	2.37	0.50
1:A:20:THR:HG22	1:A:22:GLU:H	1.75	0.50
1:A:457:GLU:HA	1:A:457:GLU:OE1	2.11	0.50
1:B:176:LEU:HD13	1:B:501:ALA:HB1	1.92	0.50
1:A:132:VAL:HG22	1:A:148:LEU:HD11	1.93	0.50
1:B:248:LEU:HB3	1:B:256:ILE:CD1	2.41	0.50
1:A:142:LEU:HD23	1:A:148:LEU:HD23	1.93	0.50
1:A:515:TYR:O	1:A:518:ARG:HG3	2.12	0.50
1:B:168:TRP:CE2	1:B:172:VAL:HG21	2.47	0.50
1:B:192:ARG:HA	1:B:196:TYR:O	2.12	0.50
1:B:99:ALA:O	1:B:103:ASN:ND2	2.45	0.50
1:B:291:ILE:O	1:B:293:VAL:HG13	2.12	0.49
1:A:410:LEU:HD12	5:A:820:HOH:O	2.11	0.49
1:B:165:TRP:CZ2	1:B:490:PRO:HD2	2.46	0.49
1:A:192:ARG:HA	1:A:196:TYR:O	2.12	0.49
1:B:85:LEU:O	1:B:88:ILE:N	2.45	0.49
1:B:570:LEU:O	1:B:574:VAL:HG22	2.13	0.49
1:B:174:LYS:HE3	1:B:497:TYR:CE1	2.48	0.49
1:A:582:ARG:N	1:A:583:PRO:CD	2.75	0.49
1:B:269:ASP:OD1	1:B:272:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PHE:CE2	1:A:584:LEU:HD13	2.48	0.49
1:B:270:MET:HG3	1:B:270:MET:O	2.10	0.49
1:A:385:TYR:O	1:A:393:ARG:HG2	2.13	0.48
1:A:595:LEU:O	1:A:599:ASN:ND2	2.45	0.48
1:A:482:ARG:NH1	1:A:489:GLU:OE2	2.46	0.48
1:B:247:LYS:HB3	1:B:281:LEU:O	2.13	0.48
1:B:491:VAL:HB	1:B:492:PRO:HD2	1.95	0.48
1:A:221:GLN:HG3	1:A:225:ASP:OD2	2.13	0.48
1:A:148:LEU:O	1:A:152:MET:HG2	2.13	0.48
1:B:386:ALA:HA	1:B:393:ARG:CD	2.44	0.48
1:B:538:PRO:HB2	1:B:541:LYS:HE2	1.95	0.48
1:A:347:THR:HG23	2:D:6:CYS:HB2	1.95	0.48
1:A:239:HIS:ND1	1:A:596:LYS:HA	2.29	0.48
1:B:539:LEU:HD23	1:B:587:TYR:HD1	1.78	0.48
1:B:267:LEU:HD12	1:B:272:GLY:HA3	1.96	0.48
1:B:538:PRO:HB3	1:B:540:HIS:CD2	2.49	0.47
1:A:415:PRO:O	1:A:419:LYS:HG3	2.14	0.47
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.97	0.47
1:A:23:GLU:OE2	1:A:26:LYS:HD2	2.13	0.47
1:A:225:ASP:CG	1:A:578:ASN:HD21	2.18	0.47
1:A:249:MET:HG2	1:A:256:ILE:HB	1.97	0.47
1:B:147:GLY:O	1:B:150:GLU:N	2.47	0.47
1:B:201:ASP:O	1:B:219:ARG:HD2	2.15	0.47
1:B:318:VAL:O	1:B:548:THR:HA	2.15	0.47
1:B:400:PHE:O	1:B:404:VAL:HG23	2.15	0.47
2:C:1:CYS:HB3	5:C:201:HOH:O	2.14	0.47
1:A:419:LYS:HG2	1:A:424:LEU:HD23	1.96	0.47
1:B:85:LEU:CD2	1:B:94:LYS:HG3	2.44	0.47
1:A:105:SER:O	1:A:106:SER:C	2.53	0.46
1:A:158:TYR:CE2	1:A:255:TYR:CG	3.03	0.46
1:A:251:ALA:O	1:A:253:PRO:HD3	2.15	0.46
1:A:294:THR:O	1:A:298:VAL:HG23	2.15	0.46
1:B:215:TYR:HD1	1:B:567:THR:HG1	1.61	0.46
1:A:259:ILE:O	1:A:606:TRP:HA	2.15	0.46
1:B:257:SER:HB2	1:B:610:TRP:NE1	2.30	0.46
1:B:450:LEU:HB2	1:B:451:PRO:CD	2.44	0.46
1:B:455:MET:HE1	1:B:481:LYS:HE3	1.98	0.46
1:A:456:LEU:HD12	1:A:477:TRP:HH2	1.81	0.46
1:A:477:TRP:CZ2	1:A:481:LYS:HE2	2.50	0.46
1:B:514:ARG:NH1	2:C:9:LEU:HD11	2.30	0.46
1:A:102:GLN:O	1:A:103:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:CG	1:B:219:ARG:HE	2.19	0.46
1:A:403:ALA:O	1:A:407:ILE:HG23	2.15	0.46
1:B:166:GLU:O	1:B:170:SER:N	2.48	0.46
1:B:177:ARG:N	1:B:178:PRO:HD2	2.30	0.46
2:D:8:SER:O	4:D:101:LFI:C6	2.63	0.46
1:A:279:TYR:CZ	1:A:283:VAL:HG23	2.51	0.46
1:A:174:LYS:O	1:A:178:PRO:HD3	2.16	0.45
1:A:134:ASN:H	1:A:134:ASN:HD22	1.64	0.45
1:B:308:PHE:O	1:B:311:ALA:HB3	2.16	0.45
1:A:308:PHE:O	1:A:311:ALA:HB3	2.16	0.45
1:B:116:LEU:HD13	1:B:186:LEU:HB2	1.98	0.45
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.81	0.45
1:A:240:LEU:CA	1:A:595:LEU:HD21	2.46	0.45
1:B:458:LYS:HE3	1:B:462:MET:CE	2.47	0.45
1:A:43:SER:HA	1:A:65:ALA:HB1	1.98	0.45
1:B:72:PHE:O	1:B:76:GLN:HG2	2.17	0.45
1:A:104:GLY:O	1:A:105:SER:HB3	2.16	0.45
1:A:135:PRO:HD3	1:A:163:TRP:CD1	2.52	0.45
1:A:553:LYS:HE3	1:A:573:VAL:HA	1.99	0.45
1:B:381:TYR:CE1	1:B:558:LEU:HA	2.52	0.45
1:A:363:LYS:O	1:A:365:THR:N	2.50	0.44
1:B:126:ILE:O	1:B:130:GLY:N	2.50	0.44
1:B:489:GLU:OE1	1:B:492:PRO:HA	2.18	0.44
1:A:158:TYR:CD2	1:A:255:TYR:CD2	3.05	0.44
1:A:168:TRP:CZ3	1:A:172:VAL:HG11	2.52	0.44
1:B:188:ASN:HB3	1:B:192:ARG:CZ	2.48	0.44
1:B:312:GLU:HG2	1:B:322:ASN:HD22	1.83	0.44
1:A:570:LEU:O	1:A:574:VAL:HG22	2.18	0.44
1:B:134:ASN:HA	1:B:163:TRP:CZ2	2.53	0.44
1:B:72:PHE:O	1:B:75:GLU:HG2	2.18	0.44
1:A:104:GLY:HA2	1:A:190:MET:HE2	1.98	0.44
1:A:554:LEU:HG	1:A:558:LEU:HG	1.98	0.44
1:B:26:LYS:HG2	1:B:93:VAL:HG11	1.99	0.44
1:A:239:HIS:CE1	1:A:596:LYS:HA	2.52	0.44
1:A:308:PHE:CE1	1:A:333:LEU:HD22	2.53	0.44
1:B:212:VAL:HG21	1:B:565:PRO:CG	2.48	0.44
1:B:544:ILE:HG23	1:B:544:ILE:O	2.18	0.44
1:B:554:LEU:HG	1:B:558:LEU:HD13	1.99	0.44
1:A:22:GLU:O	1:A:26:LYS:HG3	2.18	0.44
1:A:576:ALA:HA	5:A:819:HOH:O	2.16	0.44
1:B:386:ALA:HA	1:B:393:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HA	1:A:170:SER:OG	2.18	0.44
1:A:331:SER:OG	1:A:357:ARG:HA	2.18	0.44
1:B:188:ASN:O	1:B:192:ARG:HG3	2.17	0.44
1:B:456:LEU:HD12	1:B:477:TRP:HH2	1.81	0.44
1:A:232:GLU:OE2	1:A:581:VAL:HG11	2.17	0.43
1:B:110:GLU:O	1:B:114:LYS:N	2.42	0.43
1:A:95:LEU:HD23	1:A:98:GLN:NE2	2.33	0.43
1:A:240:LEU:HA	1:A:595:LEU:HD21	1.99	0.43
1:B:595:LEU:O	1:B:599:ASN:ND2	2.51	0.43
1:A:25:ALA:O	1:A:28:PHE:N	2.46	0.43
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.01	0.43
1:A:533:ALA:CB	1:A:544:ILE:HG22	2.49	0.43
1:B:347:THR:HG22	2:C:8:SER:HB2	2.00	0.43
1:A:594:TRP:O	1:A:598:GLN:HG2	2.18	0.43
1:B:157:ASP:O	1:B:161:ARG:HG3	2.18	0.43
2:D:5:4PH:CD2	2:D:5:4PH:N	2.79	0.43
1:B:126:ILE:CG1	1:B:176:LEU:HD21	2.48	0.43
1:B:143:LEU:O	1:B:144:LEU:C	2.57	0.43
1:A:431:ASP:O	1:A:435:GLU:HG2	2.18	0.43
1:A:529:LEU:N	1:A:529:LEU:HD23	2.33	0.43
1:B:54:ILE:O	1:B:54:ILE:HG22	2.19	0.43
1:B:324:THR:O	1:B:327:PHE:HB3	2.19	0.43
1:A:107:VAL:CG2	1:A:193:ALA:HB1	2.49	0.43
1:B:168:TRP:CZ3	1:B:172:VAL:HG11	2.54	0.43
1:B:180:TYR:O	1:B:184:VAL:HG23	2.19	0.43
1:A:252:TYR:CE2	1:A:266:LEU:HD22	2.54	0.42
1:A:489:GLU:O	1:A:489:GLU:HG2	2.19	0.42
1:B:450:LEU:HD21	1:B:519:THR:HG21	2.00	0.42
1:A:543:ASP:O	1:A:544:ILE:C	2.57	0.42
1:A:119:ILE:HG21	1:A:183:TYR:HB2	2.01	0.42
1:A:121:ASN:HD22	2:D:13:ILE:HG22	1.85	0.42
1:A:146:PRO:O	1:A:150:GLU:HB3	2.18	0.42
1:A:347:THR:CG2	2:D:6:CYS:CB	2.97	0.42
1:A:476:LYS:O	1:A:480:MET:HG3	2.18	0.42
1:A:486:GLY:HA2	1:A:606:TRP:CD1	2.55	0.42
1:A:589:GLU:N	1:A:590:PRO:CD	2.83	0.42
1:B:23:GLU:OE2	1:B:26:LYS:HD2	2.19	0.42
1:B:187:LYS:HD2	1:B:199:TYR:CZ	2.54	0.42
1:A:91:LEU:HA	1:A:94:LYS:HE3	2.02	0.42
1:B:385:TYR:HD1	1:B:385:TYR:O	2.03	0.42
1:A:238:GLU:HG2	1:A:606:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HG22	1:A:603:PHE:CG	2.55	0.42
1:B:126:ILE:C	1:B:126:ILE:CD1	2.84	0.42
1:B:459:TRP:O	1:B:463:VAL:HG23	2.20	0.42
1:A:385:TYR:CD1	1:A:385:TYR:C	2.93	0.42
1:A:457:GLU:O	1:A:460:ARG:N	2.52	0.42
1:B:106:SER:C	1:B:108:LEU:N	2.74	0.41
1:B:220:GLY:C	1:B:222:LEU:N	2.74	0.41
1:A:397:ASN:OD1	1:A:400:PHE:HD1	2.02	0.41
1:B:297:MET:O	1:B:301:ALA:N	2.54	0.41
1:A:53:ASN:HB2	1:A:340:GLN:NE2	2.34	0.41
1:A:317:SER:OG	1:A:545:SER:O	2.38	0.41
1:A:440:LEU:O	1:A:441:LYS:C	2.59	0.41
1:A:476:LYS:O	1:A:480:MET:CG	2.68	0.41
1:A:90:ASN:ND2	1:A:93:VAL:HG12	2.36	0.41
1:B:119:ILE:HG23	1:B:179:LEU:HB3	2.01	0.41
1:B:158:TYR:CD1	1:B:158:TYR:C	2.94	0.41
1:A:119:ILE:HD11	1:A:182:GLU:HB3	2.01	0.41
1:B:482:ARG:NH2	1:B:489:GLU:OE2	2.51	0.41
1:B:181:GLU:HG2	1:B:473:TRP:CZ3	2.55	0.41
1:A:250:ASN:N	1:A:250:ASN:HD22	2.17	0.41
1:B:91:LEU:O	1:B:95:LEU:HG	2.20	0.41
1:B:227:GLU:HG2	1:B:454:TYR:OH	2.20	0.41
1:B:379:ILE:CG2	1:B:383:MET:HE3	2.51	0.41
1:B:386:ALA:HA	1:B:393:ARG:HD3	2.03	0.41
1:B:574:VAL:HG23	1:B:576:ALA:H	1.86	0.41
1:B:589:GLU:OE2	1:B:589:GLU:HA	2.20	0.41
1:A:126:ILE:O	1:A:130:GLY:N	2.54	0.41
1:A:135:PRO:HD3	1:A:163:TRP:NE1	2.36	0.41
1:B:209:VAL:HG11	1:B:215:TYR:O	2.21	0.41
1:A:118:THR:O	1:A:122:THR:HG23	2.20	0.40
1:A:315:PHE:O	1:A:318:VAL:HG22	2.21	0.40
1:B:106:SER:C	1:B:108:LEU:H	2.23	0.40
1:A:568:LEU:O	1:A:572:ASN:OD1	2.40	0.40
1:B:201:ASP:OD2	1:B:219:ARG:NH2	2.54	0.40
1:A:54:ILE:HD11	1:A:343:VAL:HG23	2.03	0.40
1:A:225:ASP:O	1:A:229:THR:OG1	2.36	0.40
1:B:172:VAL:O	1:B:176:LEU:HG	2.22	0.40
1:B:543:ASP:O	1:B:544:ILE:C	2.59	0.40
1:A:44:SER:CB	1:A:351:LEU:HD22	2.52	0.40
1:A:478:TRP:O	1:A:482:ARG:HG3	2.21	0.40
1:B:104:GLY:O	1:B:106:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HG23	1:B:383:MET:HE1	2.03	0.40
1:A:142:LEU:HD21	1:A:147:GLY:CA	2.51	0.40
1:B:145:GLU:HA	1:B:146:PRO:HA	1.84	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	593/609 (97%)	551 (93%)	37 (6%)	5 (1%)	19 36
1	B	594/609 (98%)	553 (93%)	39 (7%)	2 (0%)	41 62
2	C	15/18 (83%)	11 (73%)	3 (20%)	1 (7%)	1 1
2	D	15/18 (83%)	14 (93%)	0	1 (7%)	1 1
All	All	1217/1254 (97%)	1129 (93%)	79 (6%)	9 (1%)	22 41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	VAL
1	A	104	GLY
1	A	292	ASP
1	B	364	VAL
2	D	1	CYS
1	B	103	ASN
2	C	16	ALA
1	A	103	ASN
1	A	106	SER

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	525/538 (98%)	508 (97%)	17 (3%)	39 63
1	B	526/538 (98%)	501 (95%)	25 (5%)	25 47
2	C	14/14 (100%)	13 (93%)	1 (7%)	14 28
2	D	14/14 (100%)	12 (86%)	2 (14%)	3 5
All	All	1079/1104 (98%)	1034 (96%)	45 (4%)	30 53

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	133	CYS
1	A	137	ASN
1	A	150	GLU
1	A	161	ARG
1	A	183	TYR
1	A	221	GLN
1	A	306	ARG
1	A	381	TYR
1	A	385	TYR
1	A	401	HIS
1	A	473	TRP
1	A	496	THR
1	A	511	SER
1	A	518	ARG
1	A	559	ARG
1	A	602	SER
1	B	20	THR
1	B	42	GLN
1	B	111	ASP
1	B	126	ILE
1	B	146	PRO
1	B	158	TYR
1	B	183	TYR

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Mol	Chain	Res	Type
1	B	202	TYR
1	B	221	GLN
1	B	290	ASN
1	B	325	GLN
1	B	334	THR
1	B	338	ASN
1	B	341	LYS
1	B	368	ASP
1	B	381	TYR
1	B	401	HIS
1	B	432	ASN
1	B	456	LEU
1	B	489	GLU
1	B	498	CYS
1	B	514	ARG
1	B	518	ARG
1	B	573	VAL
1	B	602	SER
2	C	6	CYS
2	D	8	SER
2	D	15	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	51	ASN
1	A	60	GLN
1	A	96	GLN
1	A	98	GLN
1	A	121	ASN
1	A	134	ASN
1	A	194	ASN
1	A	221	GLN
1	A	250	ASN
1	A	287	GLN
1	A	290	ASN
1	A	300	GLN
1	A	330	ASN
1	A	417	HIS
1	A	531	GLN
1	A	540	HIS

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Mol	Chain	Res	Type
1	A	546	ASN
1	A	578	ASN
1	B	24	GLN
1	B	42	GLN
1	B	53	ASN
1	B	60	GLN
1	B	76	GLN
1	B	96	GLN
1	B	121	ASN
1	B	322	ASN
1	B	437	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	4PH	D	5	2	11,12,13	0.32	0	12,15,17	0.86	1 (8%)
2	4PH	C	5	2	11,12,13	0.29	0	12,15,17	0.78	1 (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
2	4PH	D	5	2	-	2/5/6/8	0/1/1/1
2	4PH	C	5	2	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	4PH	CB-CA-C	-2.56	106.68	111.47
2	C	5	4PH	CB-CA-C	-2.41	106.95	111.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	4PH	N-CA-CB-CG
2	D	5	4PH	C-CA-CB-CG
2	D	5	4PH	N-CA-CB-CG
2	C	5	4PH	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	4PH	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	LFI	D	101	2	18,18,21	0.72	0	24,24,27	1.69	3 (12%)
4	LFI	C	101	2	18,18,21	0.77	0	24,24,27	1.82	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
4	LFI	D	101	2	-	14/18/30/33	0/0/1/1
4	LFI	C	101	2	-	8/18/30/33	0/0/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	LFI	N2-C1-N1	-5.52	102.19	110.77
4	D	101	LFI	N3-C2-N2	-5.01	103.00	110.77
4	D	101	LFI	N3-C3-N1	-4.76	103.37	110.77
4	C	101	LFI	N3-C2-N2	-4.75	103.39	110.77
4	C	101	LFI	N3-C3-N1	-4.53	103.74	110.77
4	D	101	LFI	N2-C1-N1	-3.61	105.17	110.77

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	LFI	C7-C6-N2-C1
4	C	101	LFI	C7-C6-N2-C2
4	C	101	LFI	O1-C6-N2-C1
4	C	101	LFI	O1-C6-N2-C2
4	D	101	LFI	C8-C4-N1-C1
4	D	101	LFI	C8-C4-N1-C3
4	D	101	LFI	O2-C4-N1-C1
4	D	101	LFI	O2-C4-N1-C3
4	D	101	LFI	O3-C5-N3-C3
4	D	101	LFI	O3-C5-N3-C2
4	D	101	LFI	C9-C5-N3-C2
4	D	101	LFI	C7-C6-N2-C2
4	C	101	LFI	N1-C4-C8-C10
4	C	101	LFI	N3-C5-C9-C11
4	D	101	LFI	N3-C5-C9-C11
4	D	101	LFI	O1-C6-N2-C2
4	D	101	LFI	N2-C6-C7-C12
4	C	101	LFI	O2-C4-C8-C10
4	C	101	LFI	O3-C5-C9-C11

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Mol	Chain	Res	Type	Atoms
4	D	101	LFI	O1-C6-C7-C12
4	D	101	LFI	O3-C5-C9-C11
4	D	101	LFI	C9-C5-N3-C3

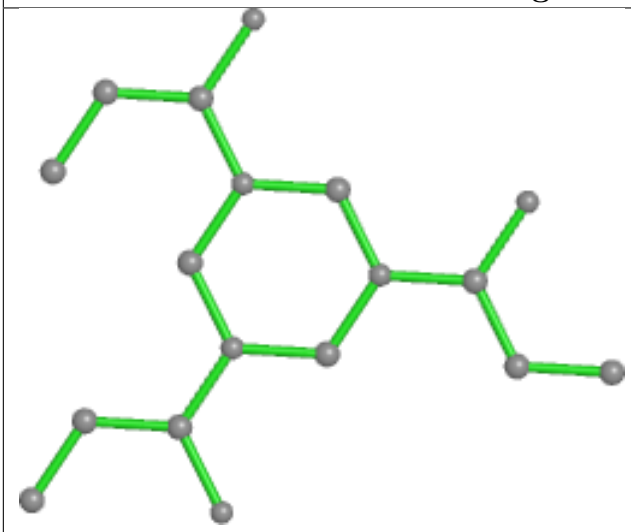
There are no ring outliers.

2 monomers are involved in 3 short contacts:

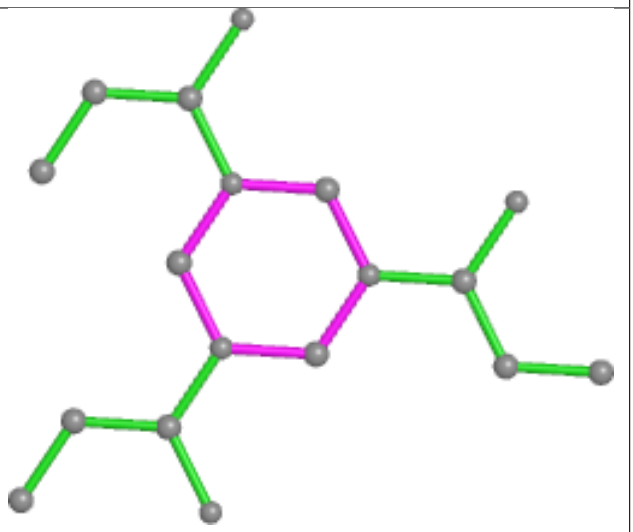
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	101	LFI	1	0
4	C	101	LFI	2	0

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.

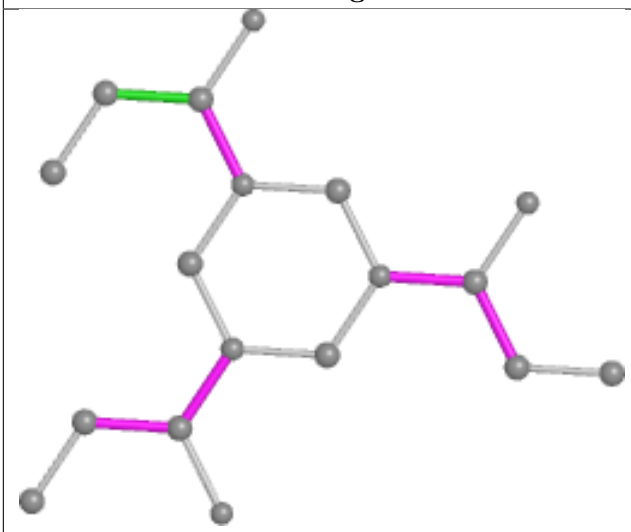
Ligand LFI D 101



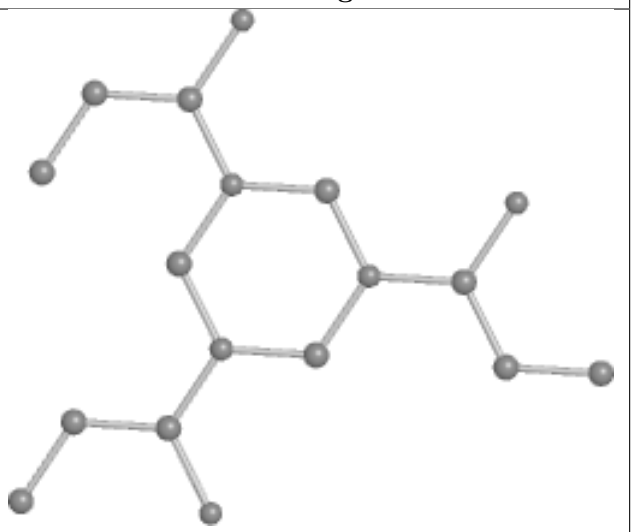
Bond lengths



Bond angles

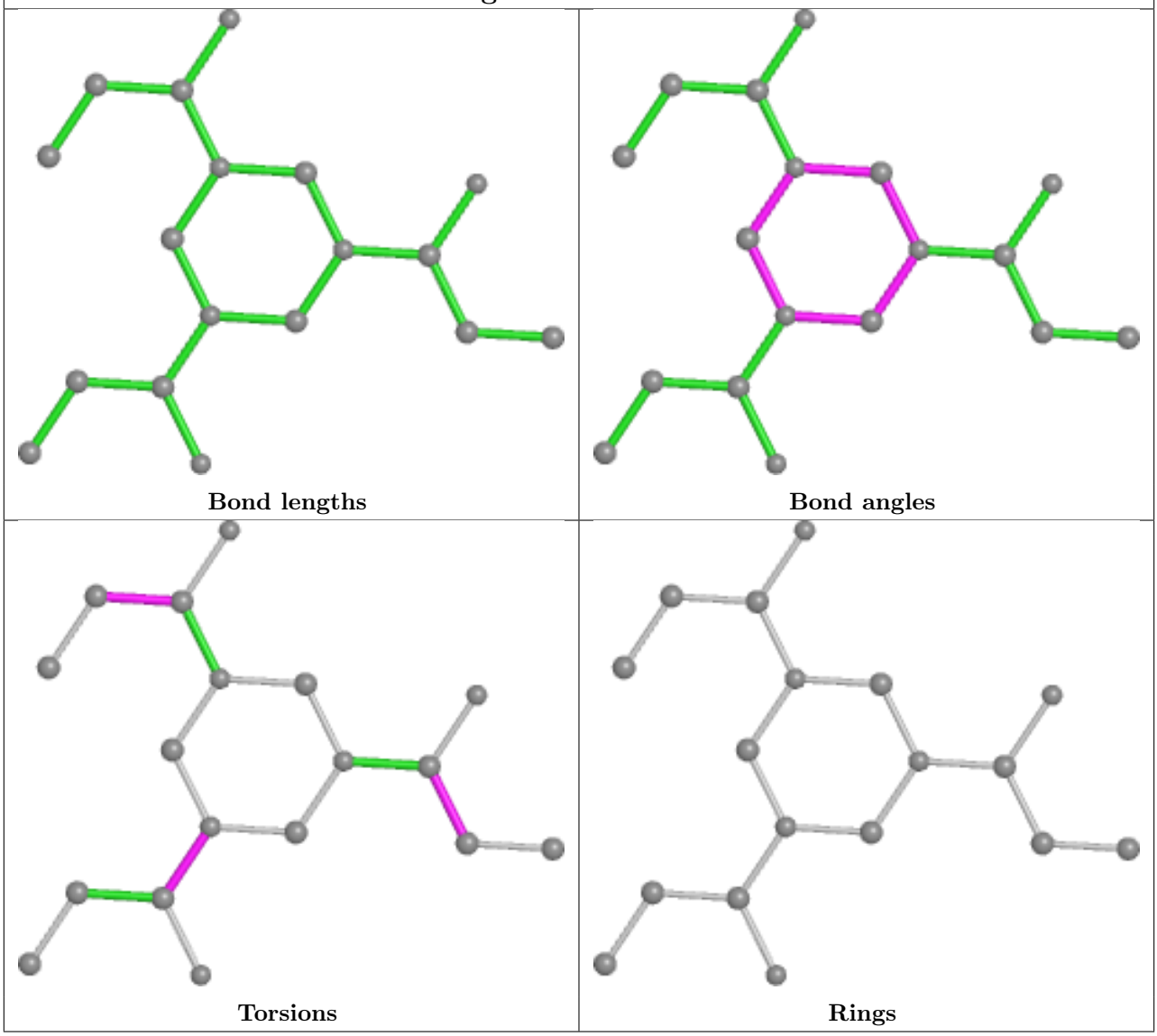


Torsions



Rings

Ligand LFI C 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	595/609 (97%)	0.43	30 (5%)	28	23	44, 77, 118, 156	0
1	B	596/609 (97%)	0.33	27 (4%)	33	27	38, 69, 102, 139	0
2	C	16/18 (88%)	0.52	1 (6%)	20	15	51, 65, 95, 96	0
2	D	16/18 (88%)	0.27	1 (6%)	20	15	60, 77, 100, 111	0
All	All	1223/1254 (97%)	0.38	59 (4%)	30	24	38, 73, 111, 156	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ASP	6.7
2	C	0	ALA	4.9
1	A	407	ILE	4.6
1	B	427	ASP	4.5
1	A	464	PHE	4.2
1	A	396	ALA	3.6
1	B	106	SER	3.6
1	A	134	ASN	3.5
1	A	539	LEU	3.3
1	A	338	ASN	3.2
1	B	574	VAL	3.2
1	B	464	PHE	3.1
1	B	36	ALA	3.1
1	B	89	GLN	3.1
1	A	300	GLN	3.0
1	A	222	LEU	3.0
1	A	339	VAL	3.0
1	A	229	THR	3.0
1	B	103	ASN	2.9
1	B	109	SER	2.9
1	A	521	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	572	ASN	2.9
1	B	233	ILE	2.8
1	B	110	GLU	2.7
1	B	364	VAL	2.7
1	B	413	ALA	2.7
1	A	577	LYS	2.7
1	A	424	LEU	2.7
1	A	588	PHE	2.7
1	B	252	TYR	2.6
1	A	532	ALA	2.5
1	A	347	THR	2.5
1	A	567	THR	2.5
1	B	249	MET	2.4
1	B	539	LEU	2.4
1	B	523	PHE	2.3
1	B	536	GLU	2.3
1	B	604	VAL	2.3
1	A	459	TRP	2.3
1	B	575	GLY	2.3
1	A	28	PHE	2.3
1	A	580	ASN	2.3
1	A	301	ALA	2.2
1	A	21	ILE	2.2
1	B	603	PHE	2.2
1	A	570	LEU	2.2
2	D	0	ALA	2.2
1	A	172	VAL	2.2
1	B	130	GLY	2.2
1	B	399	GLY	2.2
1	A	85	LEU	2.1
1	A	209	VAL	2.1
1	A	192	ARG	2.1
1	B	231	GLU	2.1
1	A	490	PRO	2.0
1	B	487	VAL	2.0
1	B	87	GLU	2.0
1	B	113	SER	2.0
1	A	207	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	4PH	C	5	12/13	0.82	0.28	66,79,87,90	0
2	4PH	D	5	12/13	0.90	0.25	75,83,88,98	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

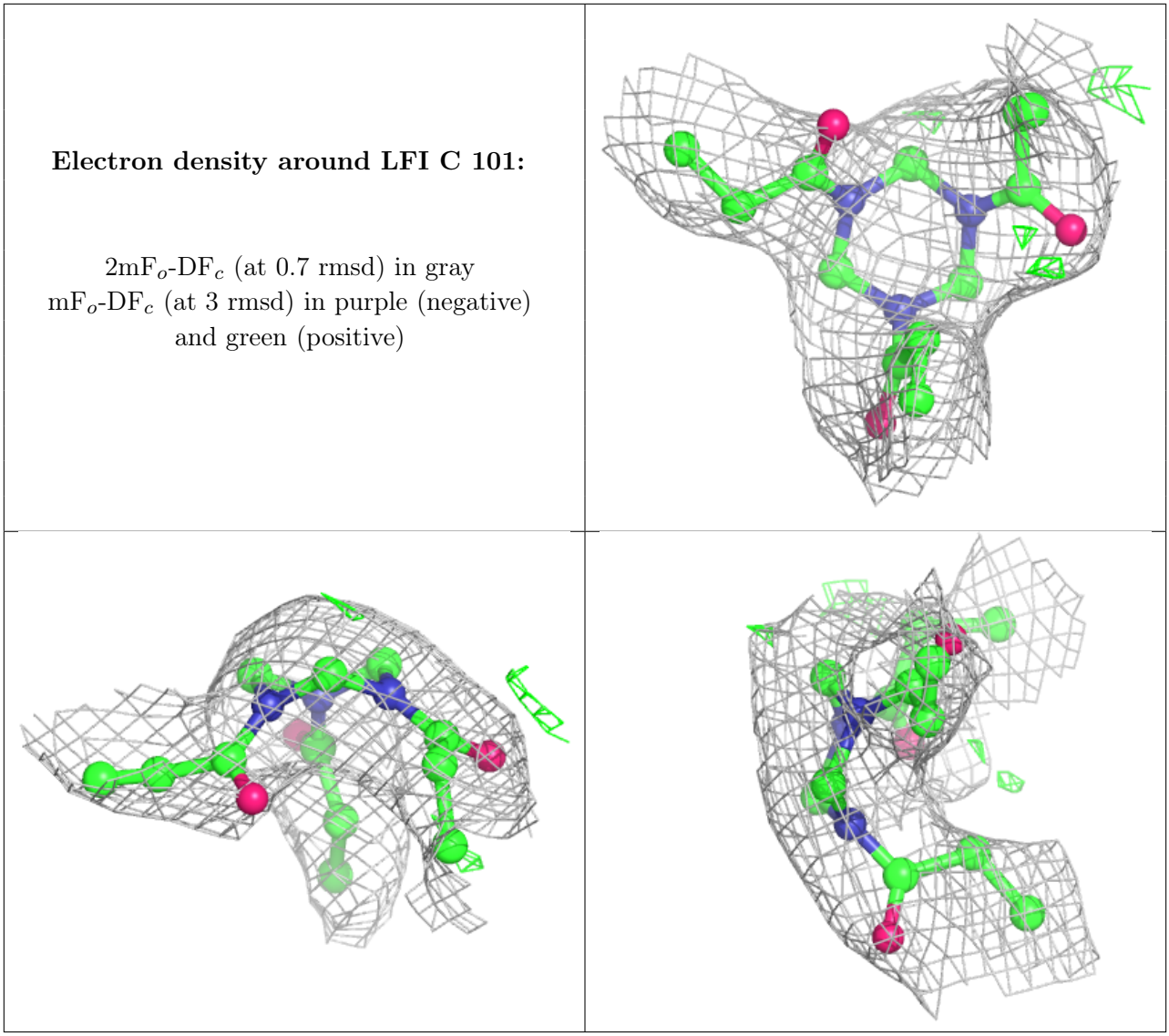
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ZN	A	702	1/1	0.52	0.14	121,121,121,121	0
4	LFI	C	101	18/21	0.88	0.21	44,58,63,69	0
4	LFI	D	101	18/21	0.89	0.15	54,67,75,86	0
3	ZN	A	701	1/1	0.94	0.10	86,86,86,86	0
3	ZN	B	701	1/1	0.98	0.13	85,85,85,85	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.

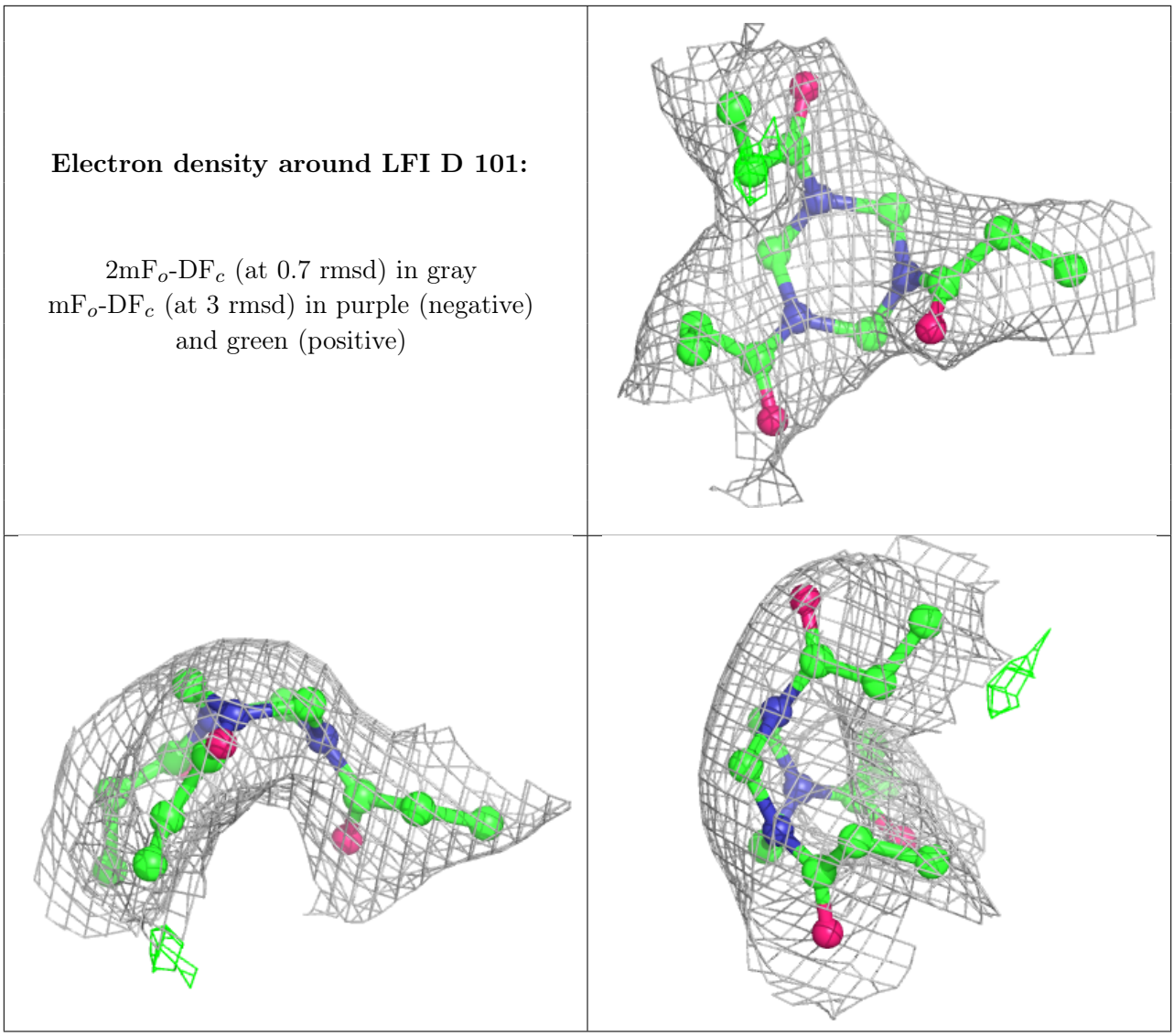
Electron density around LFI C 101:

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



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.