



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:52 AM EDT

PDB ID : 8FJ4
Title : LSD1-CoREST in complex with T108, short soaking
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-12-19
Resolution : 2.76 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

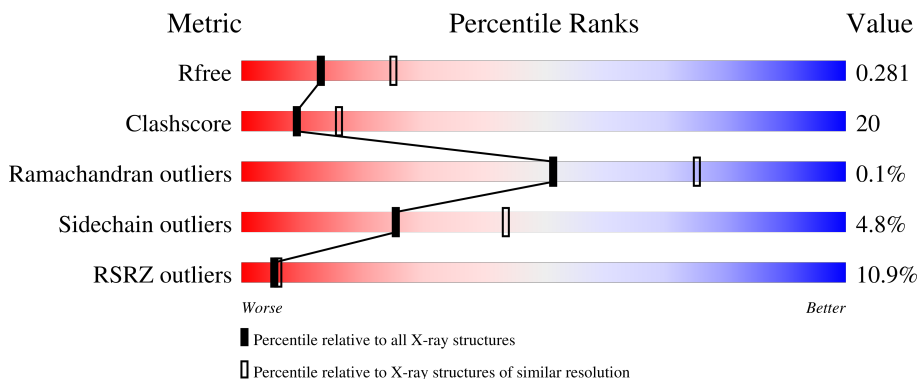
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	871	
2	B	144	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6434 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	20	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

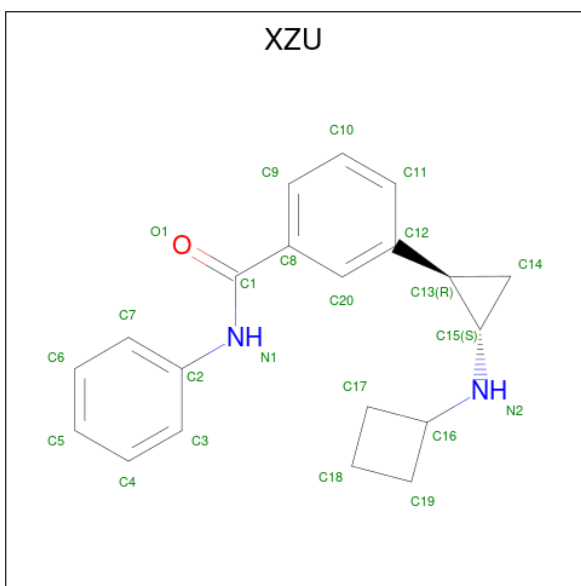
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

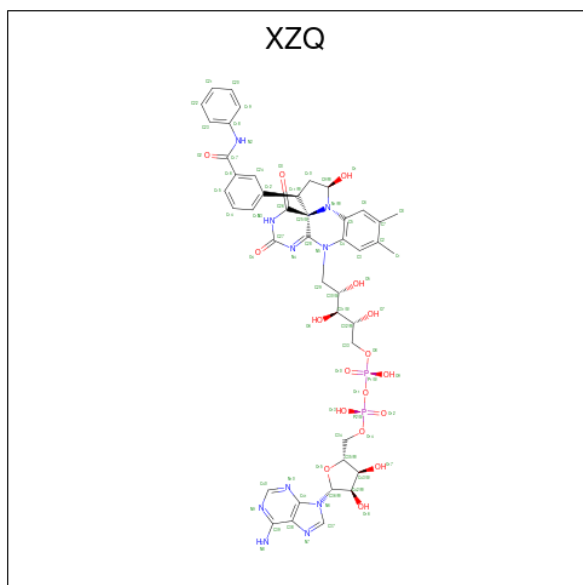
Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is 3-[(1R,2S)-2-(cyclobutylamino)cyclopropyl]-N-phenylbenzamide (three-letter code: XZU) (formula: C₂₀H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



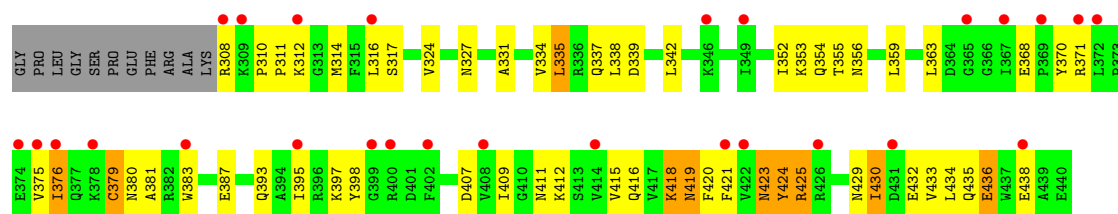
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			23	20	2	1		
3	A	1	Total	C	N	O	0	0
			23	20	2	1		
3	A	1	Total	C	N	O	0	0
			23	20	2	1		

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-2,3,4-trihydroxy-5-[(1R,3R,3aS,13R)-1-hydroxy-10,11-dimethyl-4,6-dioxo-3-[3-(phenylcarbamoyl)phenyl]-2,3,5,6-tetrahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-8(4H)-yl]pentyl dihydrogen diphosphate (three-letter code: XZQ) (formula: C₄₃H₄₈N₁₀O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	72	43	10	17	2	0	0

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.35Å 179.74Å 232.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.76 48.78 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.78-2.76) 97.9 (48.78-2.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.224 , 0.248 0.258 , 0.281	Depositor DCC
R_{free} test set	1983 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å ²)	80.6	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6434	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XZU, XZQ

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	0.59	0/5331	0.74	0/7232
2	B	0.58	0/1091	0.76	0/1471
All	All	0.59	0/6422	0.74	0/8703

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	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	A	214	ARG	Mainchain

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	5217	0	5252	206	0
2	B	1076	0	1091	89	0
3	A	69	0	0	2	0
4	A	72	0	0	5	0
All	All	6434	0	6343	256	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 20.

All (256) 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)
2:B:419:ASN:C	2:B:423:ASN:HD21	1.33	1.32
2:B:419:ASN:O	2:B:423:ASN:ND2	1.72	1.20
1:A:441:LEU:O	1:A:445:LEU:HD12	1.48	1.13
1:A:448:MET:CE	1:A:497:LEU:HB3	1.85	1.05
1:A:188:MET:CE	1:A:200:ILE:HG13	1.87	1.04
1:A:449:VAL:HG23	2:B:363:LEU:CD1	1.86	1.04
1:A:448:MET:HE2	1:A:497:LEU:HB3	1.05	1.03
1:A:441:LEU:O	1:A:445:LEU:CD1	2.07	1.01
1:A:188:MET:HE3	1:A:200:ILE:HG13	1.40	0.99
1:A:449:VAL:HG23	2:B:363:LEU:HD11	1.46	0.97
1:A:209:VAL:O	1:A:213:ILE:HG13	1.65	0.97
1:A:374:LYS:NZ	1:A:525:ASP:OD1	1.98	0.96
1:A:392:LEU:HD11	2:B:316:LEU:CD2	1.99	0.93
2:B:419:ASN:C	2:B:423:ASN:ND2	2.16	0.93
1:A:445:LEU:HD12	1:A:445:LEU:H	1.30	0.92
1:A:449:VAL:CG2	2:B:363:LEU:CD1	2.49	0.90
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.55	0.89
2:B:420:PHE:CA	2:B:423:ASN:ND2	2.37	0.87
2:B:387:GLU:OE1	2:B:411:ASN:ND2	2.07	0.87
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.58	0.86
1:A:449:VAL:CG2	2:B:363:LEU:HD11	2.05	0.85
2:B:420:PHE:C	2:B:423:ASN:HD22	1.81	0.84
1:A:188:MET:CE	1:A:200:ILE:CG1	2.56	0.83
1:A:188:MET:HE3	1:A:200:ILE:CG1	2.08	0.82
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.63	0.80
2:B:324:VAL:HG13	2:B:331:ALA:HB2	1.63	0.80
1:A:437:THR:OG1	1:A:508:LEU:HD21	1.81	0.80
2:B:387:GLU:CD	2:B:411:ASN:HD21	1.84	0.80
1:A:441:LEU:HG	1:A:445:LEU:HD11	1.65	0.79
2:B:423:ASN:ND2	2:B:423:ASN:H	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:OD2	2:B:398:TYR:OH	2.01	0.77
1:A:197:PRO:O	1:A:201:SER:HB3	1.86	0.75
1:A:188:MET:CE	1:A:200:ILE:CB	2.64	0.75
1:A:461:GLN:OE1	1:A:483:LYS:NZ	2.13	0.75
4:A:1404:XZQ:O3	4:A:1404:XZQ:O1	2.05	0.74
1:A:793:ILE:HD12	1:A:793:ILE:H	1.52	0.73
1:A:188:MET:HE1	1:A:200:ILE:CA	2.19	0.72
1:A:437:THR:OG1	1:A:508:LEU:CD2	2.37	0.72
1:A:446:ASN:OD1	2:B:359:LEU:HD21	1.89	0.72
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.71	0.72
1:A:230:THR:OG1	1:A:232:GLU:OE1	2.06	0.72
1:A:392:LEU:HD11	2:B:316:LEU:HD22	1.70	0.72
1:A:449:VAL:HG23	2:B:363:LEU:HD13	1.69	0.72
1:A:439:GLU:HG2	2:B:352:ILE:CD1	2.20	0.72
1:A:384:ARG:NH2	2:B:312:LYS:O	2.23	0.71
1:A:821:GLU:HA	1:A:821:GLU:OE1	1.91	0.71
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.89	0.71
1:A:503:LYS:HG2	1:A:504:LEU:HD23	1.72	0.71
1:A:392:LEU:CD1	2:B:316:LEU:HD22	2.21	0.70
1:A:439:GLU:CG	2:B:352:ILE:CD1	2.70	0.70
1:A:188:MET:CE	1:A:200:ILE:HB	2.22	0.70
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.24	0.70
1:A:441:LEU:C	1:A:445:LEU:CD1	2.61	0.69
1:A:445:LEU:HD12	1:A:445:LEU:N	2.06	0.69
1:A:188:MET:HE3	1:A:200:ILE:HB	1.74	0.69
1:A:230:THR:HG23	1:A:233:ALA:H	1.56	0.69
2:B:420:PHE:N	2:B:423:ASN:HD21	1.88	0.69
1:A:564:HIS:ND1	4:A:1404:XZQ:C19	2.55	0.69
1:A:425:ASP:OD2	2:B:338:LEU:CD1	2.41	0.69
2:B:420:PHE:HA	2:B:423:ASN:ND2	2.07	0.68
1:A:188:MET:HE3	1:A:200:ILE:CB	2.24	0.67
2:B:420:PHE:C	2:B:423:ASN:ND2	2.48	0.67
1:A:458:LEU:HB3	1:A:487:LEU:HD12	1.78	0.66
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.26	0.66
2:B:376:ILE:HG12	2:B:376:ILE:O	1.96	0.65
1:A:337:LEU:HD23	1:A:337:LEU:N	2.10	0.65
2:B:436:GLU:OE1	2:B:436:GLU:HA	1.96	0.64
1:A:188:MET:HE1	1:A:200:ILE:CB	2.27	0.64
2:B:420:PHE:N	2:B:423:ASN:ND2	2.45	0.64
1:A:448:MET:CE	1:A:497:LEU:C	2.65	0.64
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ASN:HD21	1:A:608:ARG:HE	1.44	0.63
1:A:395:GLN:HE21	2:B:308:ARG:N	1.96	0.63
1:A:499:GLU:HA	1:A:499:GLU:OE1	1.98	0.62
1:A:209:VAL:O	1:A:213:ILE:CG1	2.42	0.62
1:A:188:MET:HE1	1:A:200:ILE:HA	1.82	0.62
1:A:330:GLY:O	1:A:661:LYS:NZ	2.33	0.62
1:A:439:GLU:HG2	2:B:352:ILE:HD13	1.81	0.62
1:A:206:THR:O	1:A:209:VAL:HB	2.00	0.62
2:B:335:LEU:N	2:B:335:LEU:HD23	2.15	0.61
1:A:188:MET:HE2	1:A:200:ILE:HG13	1.77	0.61
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.35	0.61
1:A:438:GLN:CD	1:A:508:LEU:HD11	2.21	0.61
1:A:198:ASP:OD1	1:A:198:ASP:N	2.22	0.61
1:A:331:ALA:HA	4:A:1404:XZQ:N1	2.16	0.61
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.83	0.60
1:A:425:ASP:OD2	2:B:338:LEU:HD13	2.01	0.60
1:A:448:MET:HE3	1:A:497:LEU:O	2.00	0.60
2:B:375:VAL:HG12	2:B:375:VAL:O	2.00	0.60
2:B:338:LEU:N	2:B:338:LEU:HD23	2.16	0.60
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.84	0.60
1:A:804:ILE:HG23	1:A:804:ILE:O	2.02	0.59
1:A:448:MET:HE3	1:A:497:LEU:C	2.22	0.59
1:A:432:LYS:HA	1:A:435:VAL:HG22	1.85	0.59
2:B:420:PHE:CA	2:B:423:ASN:HD22	2.11	0.58
1:A:467:GLU:OE2	1:A:467:GLU:HA	2.04	0.58
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.85	0.58
1:A:445:LEU:CD1	1:A:445:LEU:H	2.08	0.58
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.85	0.58
1:A:755:PRO:HA	1:A:758:ARG:NE	2.19	0.58
1:A:439:GLU:HG3	2:B:352:ILE:CD1	2.34	0.57
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.85	0.57
1:A:449:VAL:HG22	2:B:363:LEU:CD1	2.34	0.57
1:A:209:VAL:C	1:A:213:ILE:HG13	2.25	0.57
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.69	0.57
1:A:308:GLU:OE1	4:A:1404:XZQ:O17	2.23	0.57
1:A:333:VAL:HG21	4:A:1404:XZQ:C17	2.35	0.56
1:A:448:MET:CE	1:A:497:LEU:CB	2.74	0.56
2:B:434:LEU:O	2:B:438:GLU:HG3	2.05	0.56
1:A:535:ASN:OD1	1:A:692:PHE:HE1	1.88	0.56
1:A:755:PRO:HA	1:A:758:ARG:HE	1.69	0.56
1:A:671:TRP:HA	1:A:735:PHE:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PHE:CD1	2:B:393:GLN:HB3	2.41	0.55
1:A:666:PHE:O	1:A:701:PRO:HG2	2.05	0.55
1:A:448:MET:HB3	2:B:363:LEU:HD21	1.89	0.55
1:A:475:THR:HA	2:B:393:GLN:HE22	1.72	0.55
1:A:442:LYS:HD2	2:B:355:THR:HG21	1.89	0.54
1:A:438:GLN:CD	1:A:508:LEU:CD1	2.76	0.54
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.88	0.54
1:A:441:LEU:CG	1:A:445:LEU:HD11	2.35	0.54
1:A:671:TRP:O	1:A:673:PRO:HD3	2.08	0.53
1:A:340:ASN:HB2	1:A:560:PHE:CD1	2.44	0.53
1:A:541:ALA:O	1:A:657:GLY:HA3	2.09	0.53
1:A:438:GLN:HE22	2:B:353:LYS:HG3	1.73	0.53
2:B:416:GLN:OE1	2:B:416:GLN:N	2.30	0.53
1:A:438:GLN:CG	1:A:508:LEU:HD11	2.39	0.53
1:A:205:GLN:O	1:A:209:VAL:HG23	2.09	0.53
1:A:343:ALA:O	1:A:346:SER:OG	2.25	0.53
1:A:391:TYR:CZ	2:B:310:PRO:HD3	2.44	0.52
1:A:229:LEU:N	1:A:263:ASN:OD1	2.37	0.52
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.90	0.52
2:B:424:TYR:N	2:B:424:TYR:CD2	2.78	0.52
2:B:383:TRP:CD2	2:B:412:LYS:HE2	2.45	0.52
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.75	0.51
1:A:395:GLN:NE2	2:B:308:ARG:N	2.57	0.51
2:B:423:ASN:HB2	2:B:424:TYR:CD2	2.45	0.51
1:A:439:GLU:HG3	2:B:352:ILE:HD12	1.92	0.51
2:B:379:CYS:SG	2:B:380:ASN:N	2.84	0.51
2:B:415:VAL:O	2:B:418:LYS:HB2	2.11	0.51
1:A:609:SER:O	1:A:609:SER:OG	2.21	0.51
2:B:383:TRP:CH2	2:B:412:LYS:HG3	2.45	0.50
2:B:423:ASN:HB2	2:B:424:TYR:HD2	1.77	0.50
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.46	0.50
1:A:366:ASN:OD1	1:A:367:GLY:N	2.44	0.50
1:A:773:TYR:HB2	1:A:805:ARG:HB2	1.93	0.50
2:B:334:VAL:HG12	2:B:335:LEU:HD23	1.94	0.49
1:A:354:ALA:HB2	1:A:568:ARG:HD2	1.93	0.49
1:A:216:ARG:HG3	1:A:220:LEU:CD1	2.43	0.49
1:A:716:GLU:OE2	1:A:750:ARG:HB3	2.11	0.49
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.94	0.49
1:A:504:LEU:HD23	1:A:504:LEU:N	2.28	0.49
3:A:1403:XZU:C9	3:A:1403:XZU:C3	2.91	0.49
2:B:409:ILE:HG22	2:B:411:ASN:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLY:HA3	1:A:733:GLY:O	2.14	0.48
1:A:181:SER:OG	1:A:218:LEU:HD23	2.14	0.48
1:A:216:ARG:O	1:A:220:LEU:HD12	2.14	0.48
1:A:670:PHE:HZ	1:A:731:LEU:HD13	1.78	0.48
1:A:525:ASP:O	1:A:528:ILE:N	2.47	0.47
1:A:582:LEU:HB2	1:A:584:ILE:HD11	1.96	0.47
1:A:216:ARG:HG3	1:A:220:LEU:HD11	1.96	0.47
1:A:319:THR:HB	1:A:572:SER:HB3	1.96	0.47
1:A:366:ASN:OD1	1:A:368:GLN:N	2.45	0.47
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.49	0.47
1:A:539:ALA:HA	3:A:1401:XZU:C10	2.45	0.47
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.45	0.47
1:A:214:ARG:HG3	1:A:218:LEU:CD1	2.45	0.47
1:A:793:ILE:HG22	1:A:794:PRO:HD2	1.97	0.47
1:A:353:LEU:HD13	1:A:565:LEU:HD22	1.96	0.46
1:A:392:LEU:HD12	2:B:316:LEU:HD22	1.96	0.46
1:A:632:GLN:OE1	1:A:636:ALA:HB2	2.16	0.46
1:A:646:TRP:CZ3	1:A:647:LYS:HE3	2.51	0.46
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.96	0.46
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.81	0.46
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.97	0.46
1:A:540:ASN:HB3	1:A:547:LEU:HD21	1.98	0.46
1:A:624:THR:HG22	1:A:799:ALA:HB3	1.98	0.46
1:A:416:ILE:O	1:A:420:GLU:HG3	2.16	0.46
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.98	0.46
1:A:216:ARG:HA	1:A:216:ARG:HD2	1.80	0.46
1:A:338:GLY:O	1:A:560:PHE:HB3	2.16	0.46
1:A:664:LEU:HD11	1:A:727:CYS:SG	2.55	0.45
1:A:565:LEU:HD12	1:A:565:LEU:N	2.32	0.45
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.81	0.45
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.67	0.45
1:A:660:ASN:ND2	1:A:716:GLU:OE1	2.49	0.45
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.96	0.45
1:A:428:ILE:HG12	2:B:342:LEU:CD1	2.46	0.45
1:A:485:ARG:HG3	2:B:407:ASP:HB2	1.99	0.45
1:A:419:GLN:NE2	2:B:314:MET:HA	2.32	0.44
1:A:594:ARG:CZ	1:A:640:VAL:HG11	2.47	0.44
1:A:710:GLU:O	1:A:714:ILE:HG12	2.18	0.44
1:A:758:ARG:HA	1:A:758:ARG:HD3	1.80	0.44
1:A:425:ASP:OD2	2:B:338:LEU:HD11	2.15	0.44
1:A:600:CYS:HB2	1:A:618:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ILE:HG21	1:A:617:LYS:HE3	1.99	0.44
2:B:354:GLN:HE21	2:B:354:GLN:HB2	1.57	0.44
1:A:445:LEU:HB2	2:B:359:LEU:HD23	1.99	0.44
1:A:306:LEU:HD13	1:A:584:ILE:HG13	1.98	0.44
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.46	0.44
1:A:392:LEU:HD23	1:A:398:PHE:CD1	2.53	0.44
1:A:193:ALA:HB2	1:A:200:ILE:HD12	2.00	0.44
1:A:534:ALA:HB2	1:A:688:ARG:HG3	1.99	0.44
1:A:263:ASN:O	1:A:267:TYR:CE1	2.71	0.43
1:A:188:MET:HE1	1:A:200:ILE:HB	1.94	0.43
1:A:632:GLN:HG2	1:A:634:PRO:O	2.17	0.43
2:B:429:ASN:HB3	2:B:432:GLU:HB2	1.99	0.43
1:A:355:LYS:HD3	1:A:563:SER:CB	2.49	0.43
1:A:392:LEU:CD1	2:B:316:LEU:CD2	2.78	0.43
1:A:485:ARG:HD3	1:A:485:ARG:C	2.38	0.43
2:B:395:ILE:CG2	2:B:433:VAL:CG1	2.94	0.43
1:A:332:MET:SD	1:A:661:LYS:HE2	2.59	0.43
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.54	0.43
1:A:572:SER:O	1:A:575:PRO:HD2	2.18	0.43
1:A:340:ASN:CG	1:A:560:PHE:CE1	2.93	0.43
1:A:438:GLN:NE2	2:B:353:LYS:HG3	2.34	0.43
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.51	0.43
1:A:647:LYS:O	1:A:651:VAL:HG23	2.19	0.43
1:A:478:PHE:CE1	2:B:393:GLN:HB3	2.53	0.42
1:A:469:LYS:HE2	1:A:469:LYS:HA	2.01	0.42
1:A:214:ARG:HG3	1:A:218:LEU:HD11	2.01	0.42
1:A:684:THR:HG22	1:A:685:THR:N	2.35	0.42
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.79	0.42
2:B:368:GLU:OE1	2:B:371:ARG:NE	2.49	0.42
1:A:428:ILE:HG12	2:B:342:LEU:HD12	2.02	0.42
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.55	0.42
1:A:183:LEU:HD23	1:A:189:THR:HG21	2.01	0.42
1:A:374:LYS:HE3	1:A:374:LYS:HB3	1.84	0.42
1:A:392:LEU:HD11	2:B:316:LEU:HD23	1.95	0.42
1:A:601:GLU:HA	1:A:616:TYR:O	2.20	0.42
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.49	0.42
1:A:691:LEU:N	1:A:691:LEU:HD12	2.35	0.42
1:A:191:GLN:HE22	1:A:259:HIS:CD2	2.38	0.41
2:B:424:TYR:N	2:B:424:TYR:HD2	2.17	0.41
1:A:782:PRO:O	1:A:792:PRO:HG2	2.20	0.41
1:A:441:LEU:O	1:A:445:LEU:HD13	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:CYS:HA	2:B:411:ASN:O	2.20	0.41
2:B:423:ASN:ND2	2:B:423:ASN:N	2.60	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.94	0.41
1:A:333:VAL:HA	1:A:565:LEU:O	2.21	0.41
2:B:395:ILE:CG2	2:B:433:VAL:HG11	2.50	0.41
1:A:367:GLY:HA2	1:A:734:ILE:HG12	2.02	0.41
2:B:415:VAL:O	2:B:418:LYS:N	2.53	0.41
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.93	0.40
1:A:715:MET:CE	1:A:723:ILE:HG12	2.52	0.40
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.04	0.40
1:A:374:LYS:O	1:A:377:MET:N	2.54	0.40
1:A:761:TYR:CD2	1:A:809:ALA:HB1	2.56	0.40
1:A:340:ASN:ND2	1:A:560:PHE:CE1	2.90	0.40
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.95	0.40
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.80	0.40
1:A:691:LEU:HA	1:A:706:LEU:O	2.21	0.40
1:A:739:ALA:O	1:A:741:PRO:HD3	2.21	0.40
1:A:418:LEU:HD12	2:B:324:VAL:HG21	2.03	0.40
2:B:380:ASN:OD1	2:B:381:ALA:N	2.55	0.40
2:B:419:ASN:HD22	2:B:419:ASN:HA	1.59	0.40
1:A:540:ASN:O	1:A:542:THR:HG22	2.21	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	664/871 (76%)	630 (95%)	33 (5%)	1 (0%)	47	69
2	B	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
All	All	795/1015 (78%)	754 (95%)	40 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	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	566/715 (79%)	549 (97%)	17 (3%)	41 61
2	B	117/125 (94%)	101 (86%)	16 (14%)	3 5
All	All	683/840 (81%)	650 (95%)	33 (5%)	25 44

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

Mol	Chain	Res	Type
1	A	198	ASP
1	A	200	ILE
1	A	204	GLN
1	A	205	GLN
1	A	214	ARG
1	A	447	LYS
1	A	448	MET
1	A	449	VAL
1	A	453	GLU
1	A	458	LEU
1	A	472	ARG
1	A	503	LYS
1	A	508	LEU
1	A	510	GLU
1	A	571	TYR
1	A	610	THR
1	A	805	ARG
2	B	317	SER
2	B	327	ASN
2	B	335	LEU
2	B	337	GLN
2	B	339	ASP

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Mol	Chain	Res	Type
2	B	376	ILE
2	B	379	CYS
2	B	397	LYS
2	B	418	LYS
2	B	419	ASN
2	B	423	ASN
2	B	424	TYR
2	B	425	ARG
2	B	430	ILE
2	B	435	GLN
2	B	436	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	204	GLN
1	A	399	ASN
2	B	351	ASN
2	B	354	GLN
2	B	393	GLN
2	B	419	ASN
2	B	423	ASN

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	XZQ	A	1404	-	71,80,80	1.32	9 (12%)	84,123,123	0.94	6 (7%)
3	XZU	A	1403	-	25,26,26	0.57	0	29,36,36	0.98	1 (3%)
3	XZU	A	1401	-	25,26,26	0.70	0	29,36,36	1.68	6 (20%)
3	XZU	A	1402	-	25,26,26	0.76	1 (4%)	29,36,36	0.92	2 (6%)

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	XZQ	A	1404	-	-	15/42/114/114	0/8/9/9
3	XZU	A	1403	-	-	4/12/27/27	0/4/4/4
3	XZU	A	1401	-	-	5/12/27/27	0/4/4/4
3	XZU	A	1402	-	-	0/12/27/27	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1404	XZQ	C25-C26	-3.75	1.50	1.54
4	A	1404	XZQ	C27-N4	-3.05	1.29	1.36
4	A	1404	XZQ	C26-N3	-2.86	1.32	1.37
4	A	1404	XZQ	O5-C30	-2.83	1.37	1.43
4	A	1404	XZQ	C37-N7	-2.50	1.30	1.34
4	A	1404	XZQ	C5-C4	-2.24	1.37	1.40
4	A	1404	XZQ	O4-C27	-2.19	1.20	1.24
4	A	1404	XZQ	O6-C31	-2.16	1.37	1.43
3	A	1402	XZU	C15-N2	-2.11	1.43	1.47
4	A	1404	XZQ	C9-N1	-2.06	1.43	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	XZU	C18-C17-C16	-4.26	84.67	88.37
3	A	1401	XZU	C18-C19-C16	-4.14	84.77	88.37
3	A	1401	XZU	C11-C12-C13	-3.44	114.56	121.08
3	A	1401	XZU	C20-C12-C13	3.16	126.11	120.01
4	A	1404	XZQ	C26-N3-C27	-2.81	121.19	125.42
3	A	1402	XZU	C18-C19-C16	-2.77	85.96	88.37
3	A	1402	XZU	C18-C17-C16	-2.75	85.97	88.37
4	A	1404	XZQ	O15-C36-C42	-2.52	103.24	106.93
4	A	1404	XZQ	C25-N1-C9	-2.44	107.09	109.54
4	A	1404	XZQ	C38-C39-N8	2.35	123.93	120.35
3	A	1401	XZU	C17-C16-N2	-2.31	112.92	117.94
4	A	1404	XZQ	O13-P2-O12	2.13	122.78	112.24
3	A	1401	XZU	C14-C15-C13	-2.07	59.06	60.53
3	A	1403	XZU	C2-N1-C1	2.05	131.91	126.58
4	A	1404	XZQ	O5-C30-C29	-2.00	104.95	109.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	XZU	C8-C1-N1-C2
3	A	1403	XZU	C8-C1-N1-C2
3	A	1403	XZU	O1-C1-N1-C2
4	A	1404	XZQ	O5-C30-C31-C32
4	A	1404	XZQ	O7-C32-C33-O8
4	A	1404	XZQ	C33-O8-P1-O10
4	A	1404	XZQ	C34-O14-P2-O12
3	A	1401	XZU	O1-C1-N1-C2
4	A	1404	XZQ	O5-C30-C31-O6
3	A	1403	XZU	C3-C2-N1-C1
3	A	1403	XZU	C7-C2-N1-C1
3	A	1401	XZU	C11-C12-C13-C14
3	A	1401	XZU	C20-C12-C13-C14
4	A	1404	XZQ	P2-O11-P1-O8
4	A	1404	XZQ	C33-O8-P1-O11
4	A	1404	XZQ	P1-O11-P2-O12
4	A	1404	XZQ	C29-C30-C31-C32
4	A	1404	XZQ	P1-O11-P2-O13
4	A	1404	XZQ	O14-C34-C35-O15
4	A	1404	XZQ	C34-O14-P2-O11
4	A	1404	XZQ	C31-C32-C33-O8
4	A	1404	XZQ	C33-O8-P1-O9
3	A	1401	XZU	N1-C1-C8-C9

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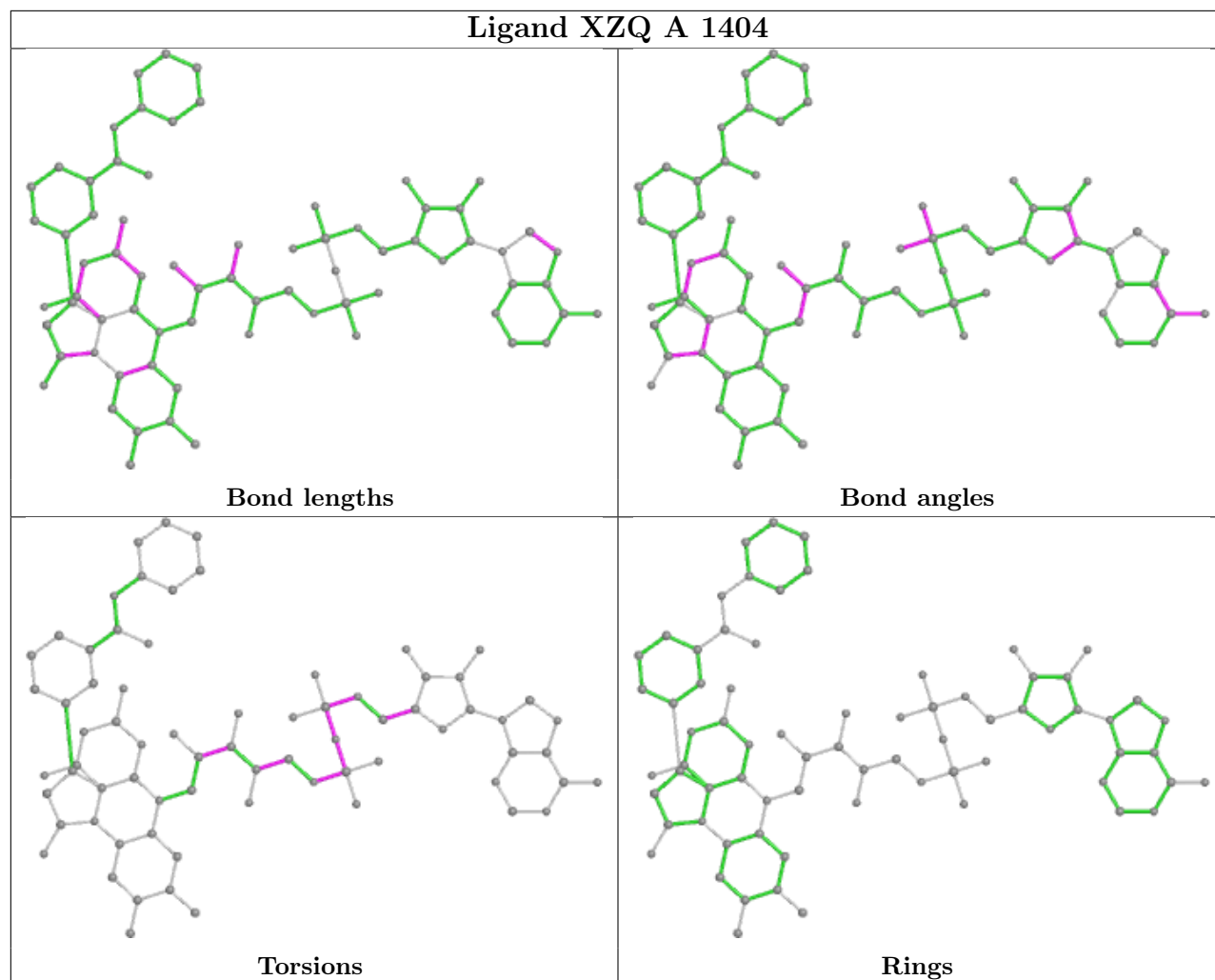
Mol	Chain	Res	Type	Atoms
4	A	1404	XZQ	C29-C30-C31-O6

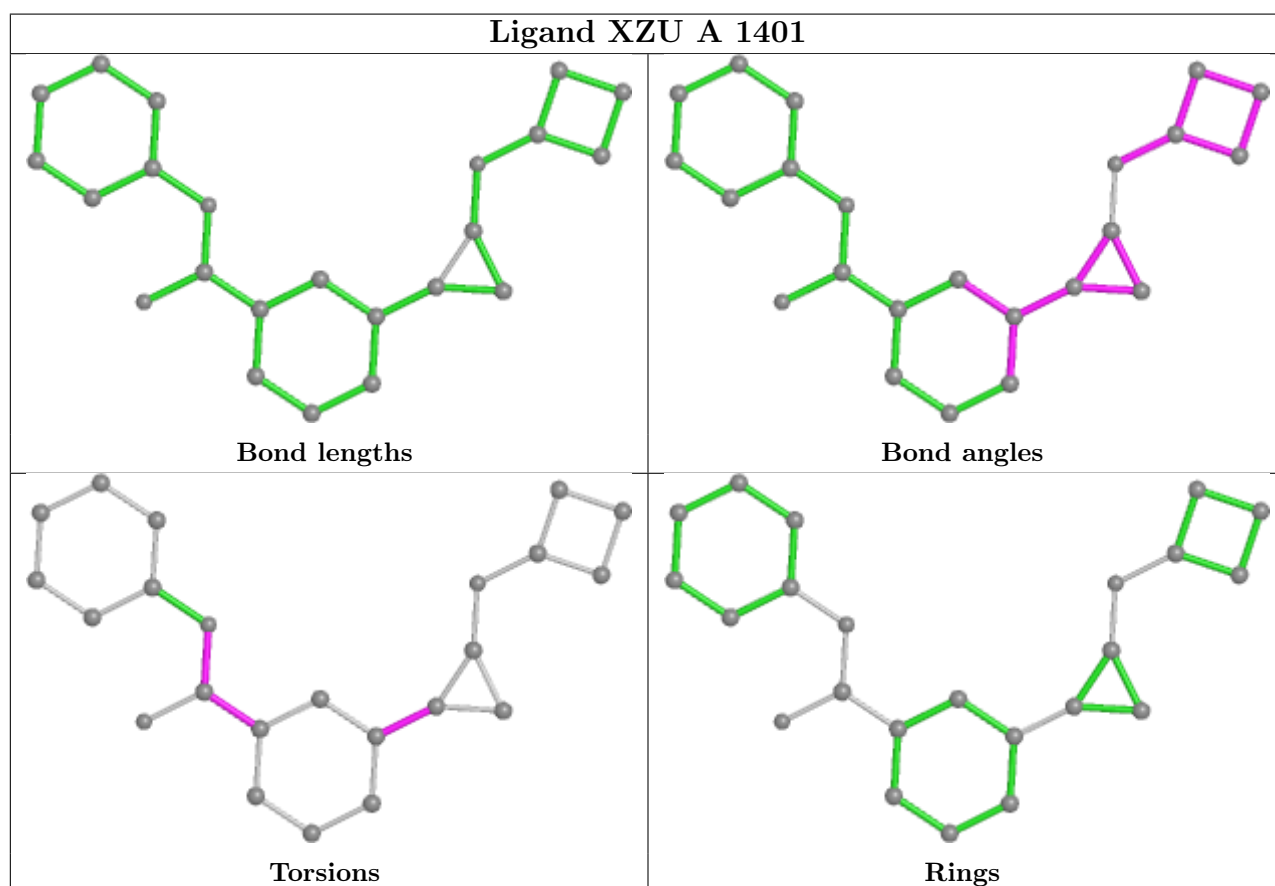
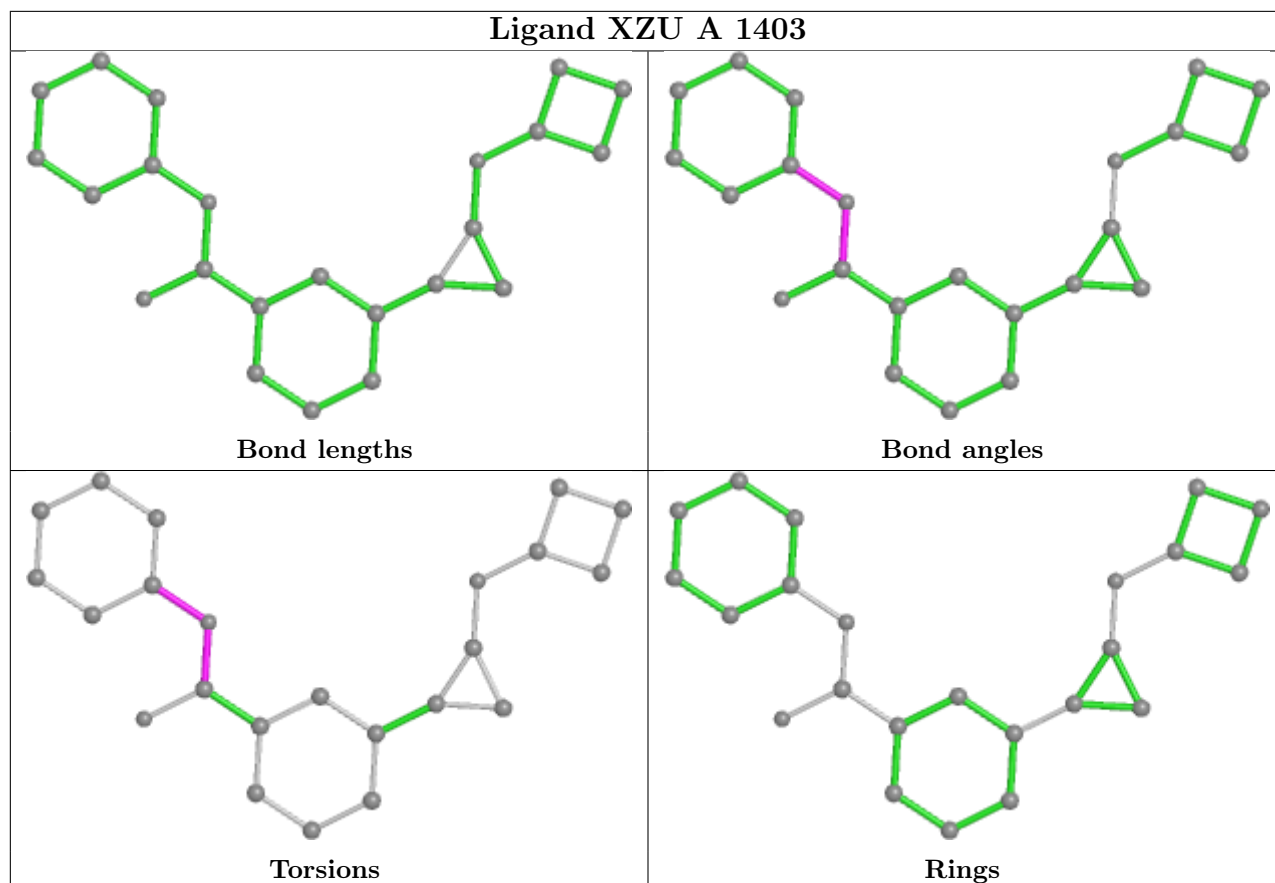
There are no ring outliers.

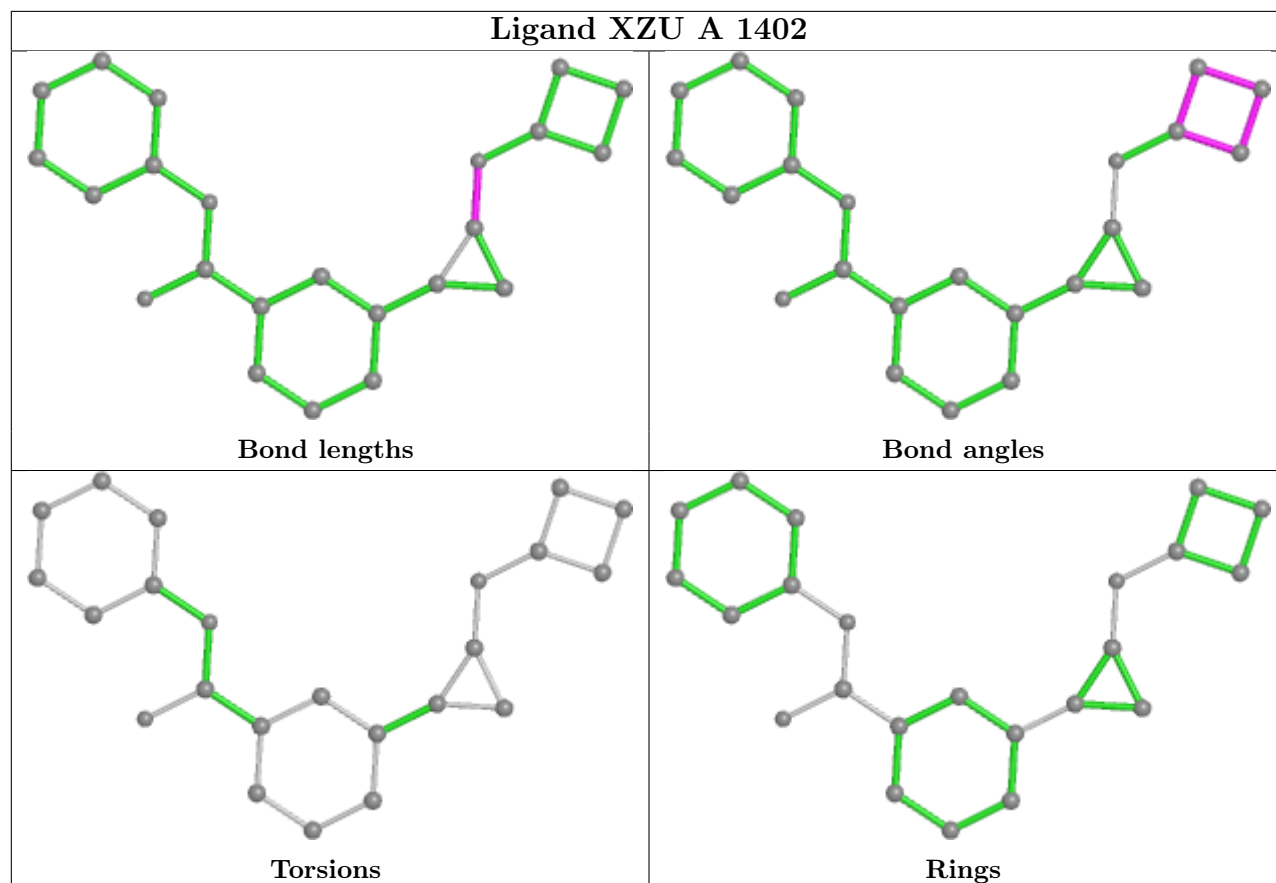
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1404	XZQ	5	0
3	A	1403	XZU	1	0
3	A	1401	XZU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th 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	666/871 (76%)	0.85	60 (9%) 9 11	58, 84, 117, 135	0
2	B	133/144 (92%)	1.08	27 (20%) 1 1	83, 116, 138, 148	0
All	All	799/1015 (78%)	0.88	87 (10%) 5 6	58, 90, 128, 148	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	5.5
1	A	508	LEU	5.4
1	A	174	VAL	4.9
2	B	402	PHE	4.6
2	B	400	ARG	4.5
1	A	836	LEU	4.3
1	A	273	LEU	4.3
2	B	308	ARG	4.3
1	A	171	PRO	4.3
2	B	376	ILE	4.0
2	B	365	GLY	4.0
2	B	312	LYS	3.9
2	B	422	VAL	3.8
2	B	367	ILE	3.6
1	A	275	THR	3.5
2	B	374	GLU	3.5
1	A	235	LEU	3.4
1	A	239	GLU	3.3
2	B	414	VAL	3.2
2	B	375	VAL	3.2
1	A	241	PRO	3.2
2	B	378	LYS	3.1
1	A	398	PHE	3.1
1	A	238	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	PRO	3.0
2	B	421	PHE	3.0
1	A	444	LEU	3.0
1	A	506	GLU	3.0
1	A	212	PHE	2.9
2	B	371	ARG	2.9
2	B	383	TRP	2.9
2	B	309	LYS	2.9
1	A	271	LYS	2.9
1	A	490	LEU	2.9
1	A	539	ALA	2.8
1	A	808	PRO	2.8
2	B	349	ILE	2.8
2	B	369	PRO	2.8
2	B	399	GLY	2.8
1	A	811	VAL	2.7
1	A	668	ARG	2.7
1	A	504	LEU	2.7
2	B	395	ILE	2.7
2	B	426	ARG	2.6
1	A	307	LEU	2.6
1	A	815	LEU	2.6
2	B	438	GLU	2.5
2	B	316	LEU	2.5
1	A	538	PHE	2.5
1	A	809	ALA	2.5
1	A	256	LEU	2.5
1	A	691	LEU	2.4
1	A	761	TYR	2.4
2	B	346	LYS	2.4
1	A	331	ALA	2.4
1	A	494	TYR	2.4
1	A	234	THR	2.4
1	A	709	GLY	2.4
1	A	455	ILE	2.3
1	A	544	LEU	2.3
1	A	762	SER	2.3
1	A	514	ASN	2.2
1	A	810	THR	2.2
1	A	703	LEU	2.2
1	A	396	LEU	2.2
1	A	440	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	2.2
1	A	657	GLY	2.2
1	A	487	LEU	2.2
1	A	542	THR	2.2
1	A	773	TYR	2.2
2	B	431	ASP	2.2
1	A	656	PHE	2.2
1	A	624	THR	2.1
1	A	447	LYS	2.1
1	A	326	VAL	2.1
1	A	777	ALA	2.1
2	B	372	LEU	2.1
1	A	428	ILE	2.1
1	A	492	LYS	2.1
1	A	765	ALA	2.1
1	A	240	ALA	2.0
1	A	814	ALA	2.0
1	A	540	ASN	2.0
2	B	408	VAL	2.0
1	A	282	ILE	2.0
1	A	373	GLU	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, 95th 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.

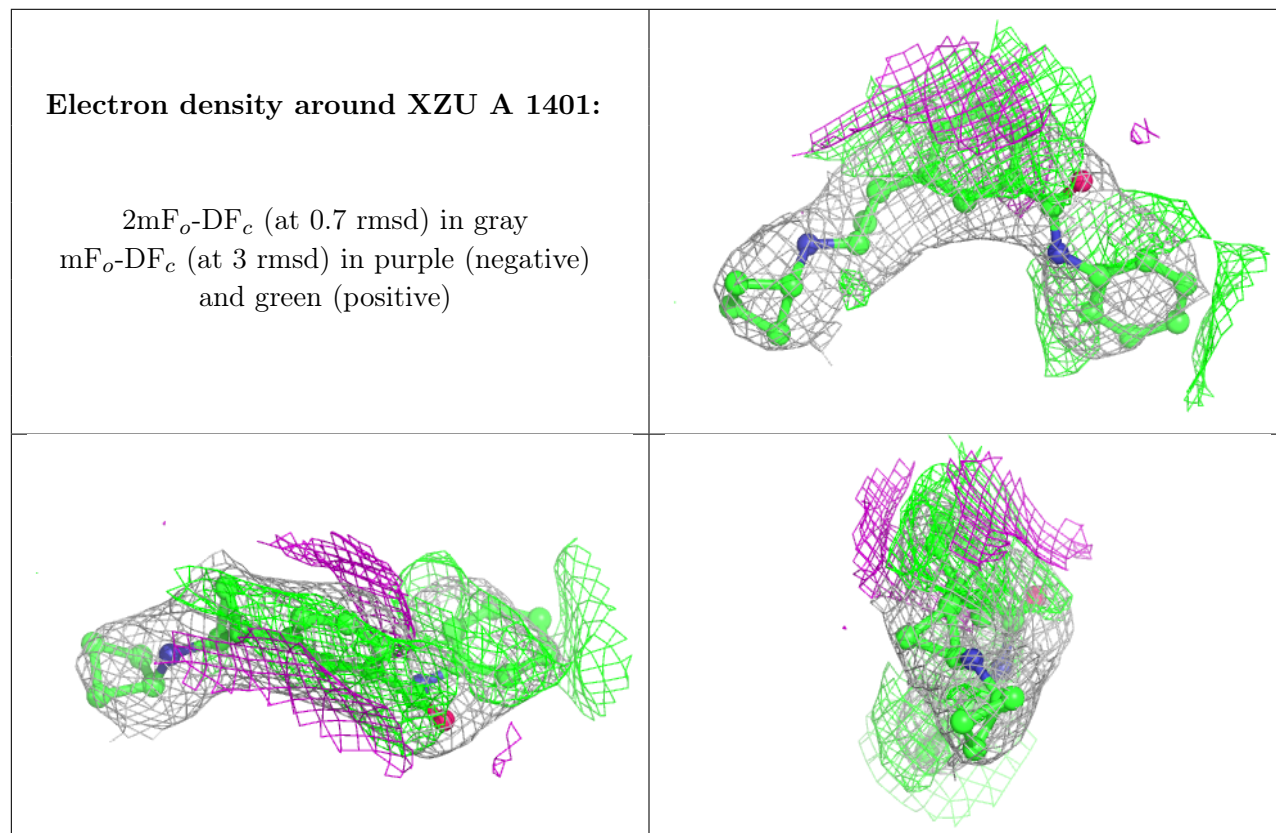
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	XZU	A	1401	23/23	0.88	0.35	70,83,91,98	0
3	XZU	A	1403	23/23	0.91	0.29	88,95,101,108	0

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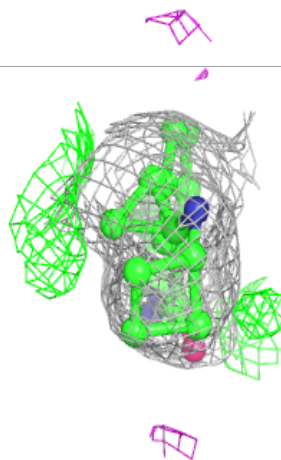
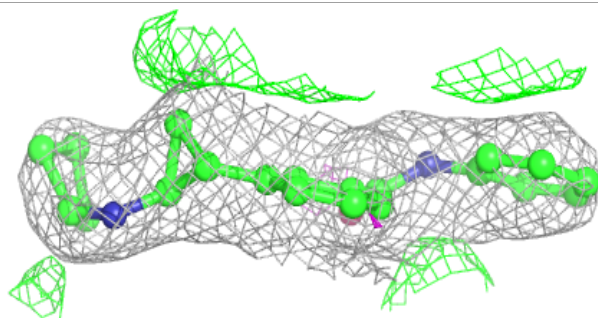
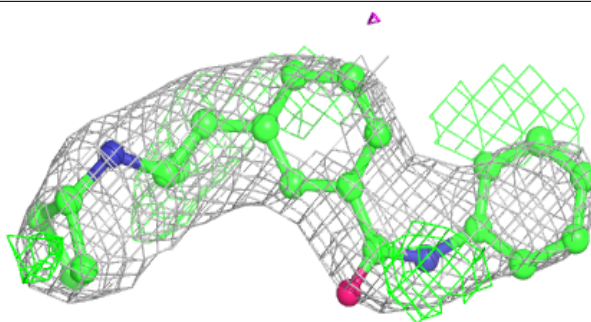
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	XZQ	A	1404	72/72	0.94	0.15	0,0,0,0	0
3	XZU	A	1402	23/23	0.96	0.23	77,83,92,97	0

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.

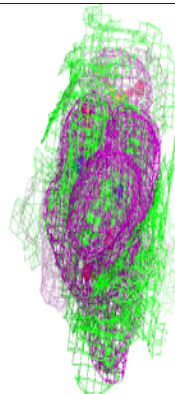
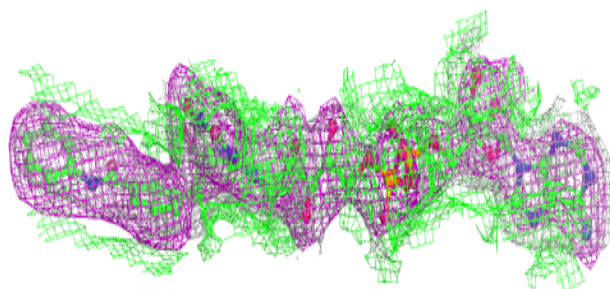
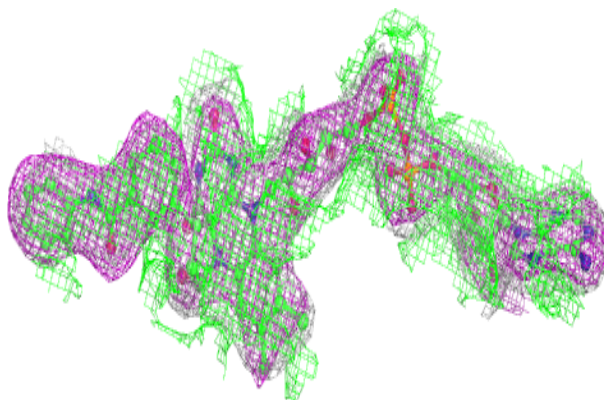


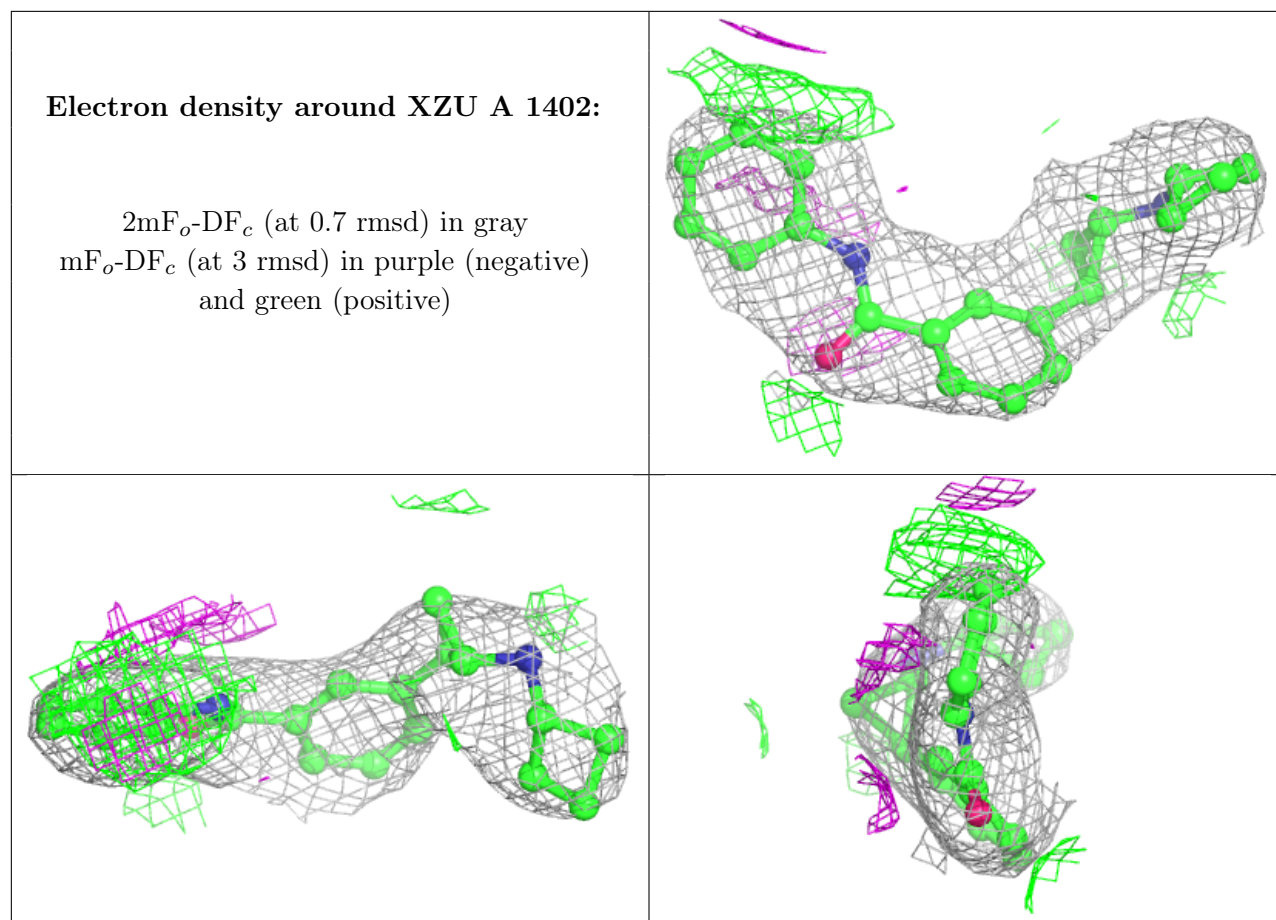
Electron density around XZU A 1403:

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

**Electron density around XZQ A 1404:**

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.