Full wwPDB X-ray Structure Validation Report ⓘ

Dec 26, 2022 – 12:10 PM JST

PDB ID	:	7F97
Title	:	Plasmodium falciparum Prolyl-tRNA Synthetase (PfPRS) in Complex with L-proline and compound L97
Authors	:	Mishra, S.; Malhotra, N.; Manickam, Y.; Sharma, A.
Deposited on	:	2021-07-04
Resolution	:	2.39 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:

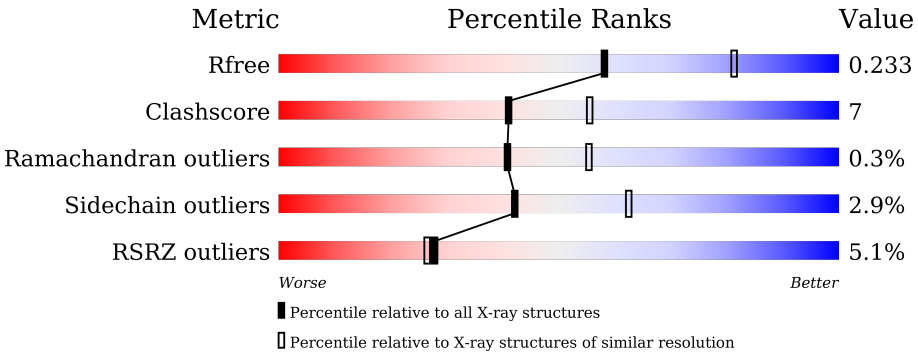
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	497	4% 82% 15%
1	B	497	2% 82% 14%
1	C	497	3% 75% 20%
1	D	497	10% 74% 20%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16025 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.

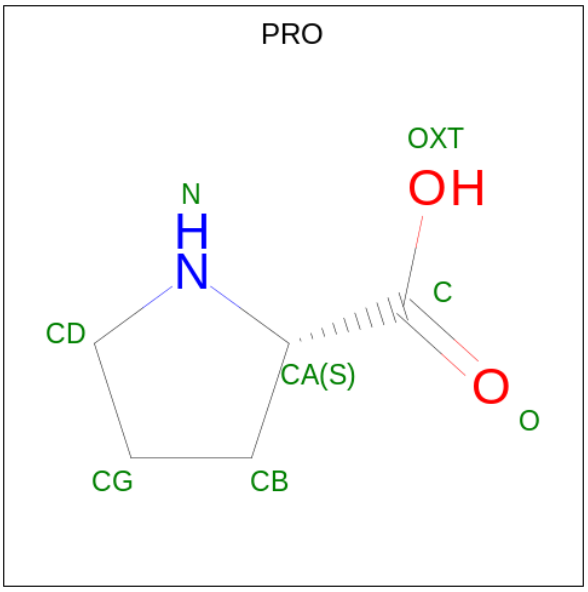
- Molecule 1 is a protein called Proline–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	2	0	0
			3998	2580	666	730	22			
1	B	481	Total	C	N	O	S	0	0	0
			3945	2544	657	722	22			
1	C	478	Total	C	N	O	S	2	0	0
			3925	2534	653	716	22			
1	D	475	Total	C	N	O	S	3	0	0
			3904	2521	652	709	22			

There are 16 discrepancies between the modelled and reference sequences:

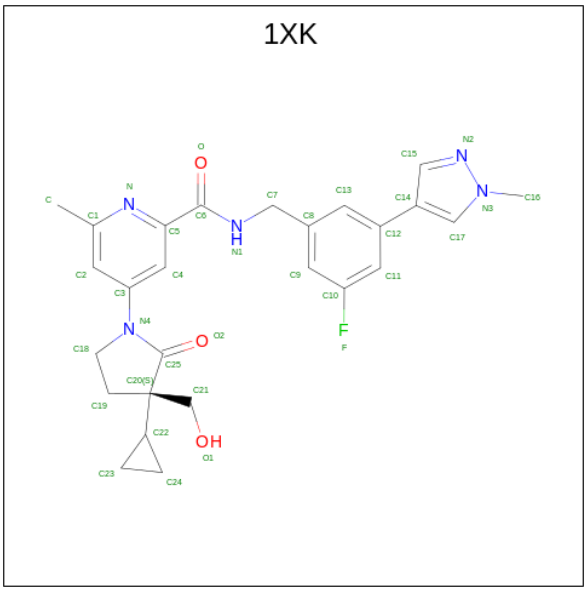
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP Q8I5R7
A	251	ALA	-	expression tag	UNP Q8I5R7
A	252	MET	-	expression tag	UNP Q8I5R7
A	253	ALA	-	expression tag	UNP Q8I5R7
B	250	GLY	-	expression tag	UNP Q8I5R7
B	251	ALA	-	expression tag	UNP Q8I5R7
B	252	MET	-	expression tag	UNP Q8I5R7
B	253	ALA	-	expression tag	UNP Q8I5R7
C	250	GLY	-	expression tag	UNP Q8I5R7
C	251	ALA	-	expression tag	UNP Q8I5R7
C	252	MET	-	expression tag	UNP Q8I5R7
C	253	ALA	-	expression tag	UNP Q8I5R7
D	250	GLY	-	expression tag	UNP Q8I5R7
D	251	ALA	-	expression tag	UNP Q8I5R7
D	252	MET	-	expression tag	UNP Q8I5R7
D	253	ALA	-	expression tag	UNP Q8I5R7

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



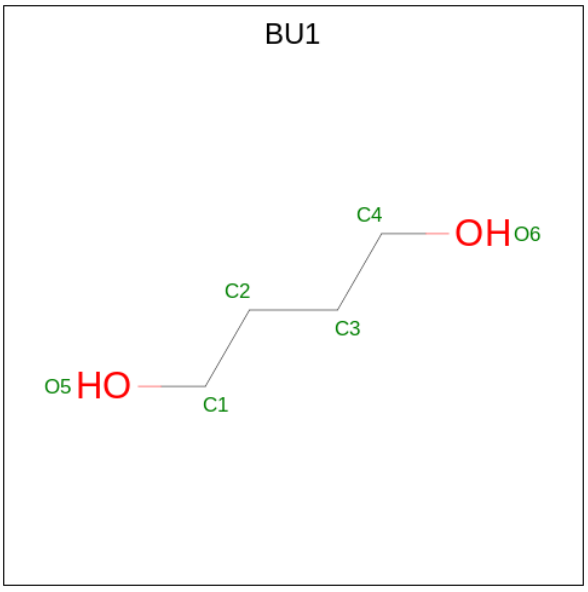
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 8 5 1 2	0	0
2	B	1	Total C N O 8 5 1 2	0	0
2	C	1	Total C N O 8 5 1 2	0	0
2	D	1	Total C N O 8 5 1 2	0	0

- Molecule 3 is 4-[(3S)-3-cyclopropyl-3-(hydroxymethyl)-2-oxidanylidene-pyrrolidin-1-yl]-N-[[3-fluoranyl-5-(1-methylpyrazol-4-yl)phenyl]methyl]-6-methyl-pyridine-2-carboxamide (three-letter code: 1XK) (formula: $C_{26}H_{28}FN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			35	26	1	5	3		
3	B	1	Total	C	F	N	O	0	0
			35	26	1	5	3		
3	C	1	Total	C	F	N	O	0	0
			35	26	1	5	3		
3	D	1	Total	C	F	N	O	0	0
			35	26	1	5	3		

- Molecule 4 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).

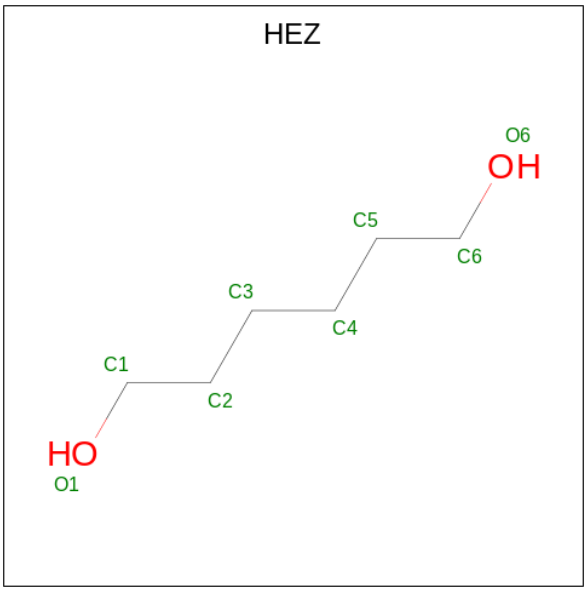


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 4 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0

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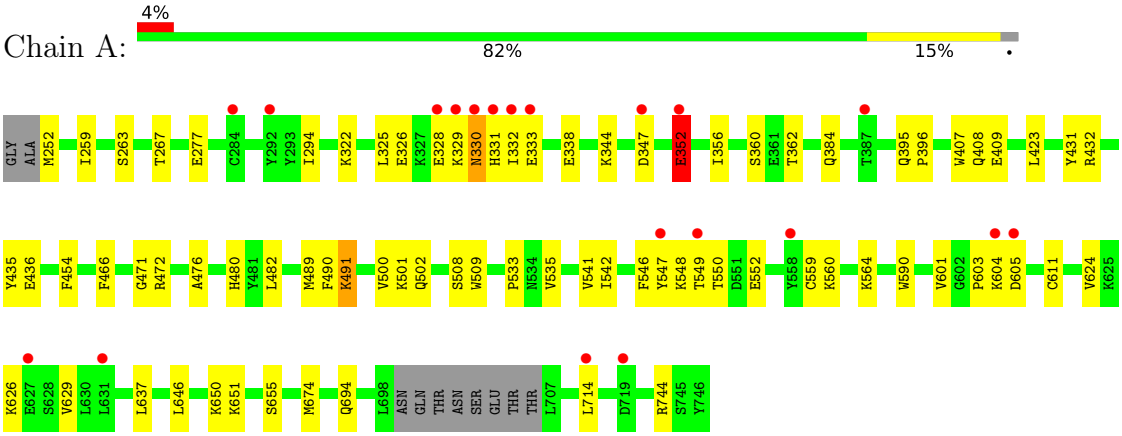
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	16	Total O 16 16	0	0
7	C	14	Total O 14 14	0	0
7	D	9	Total O 9 9	0	0

3 Residue-property plots

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.

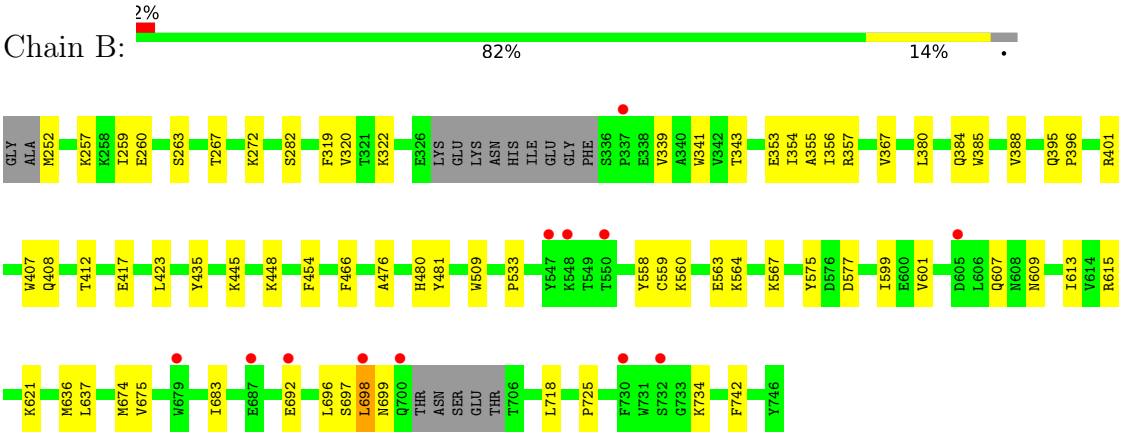
• Molecule 1: Proline–tRNA ligase

Chain A:



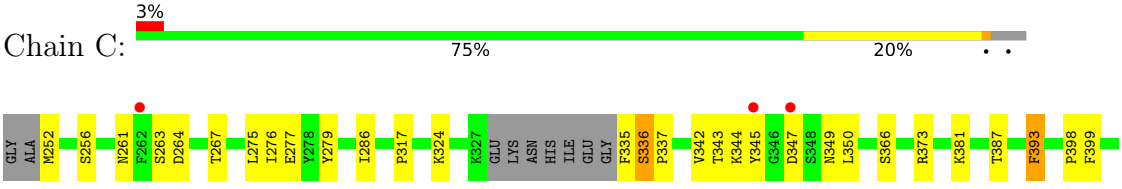
• Molecule 1: Proline–tRNA ligase

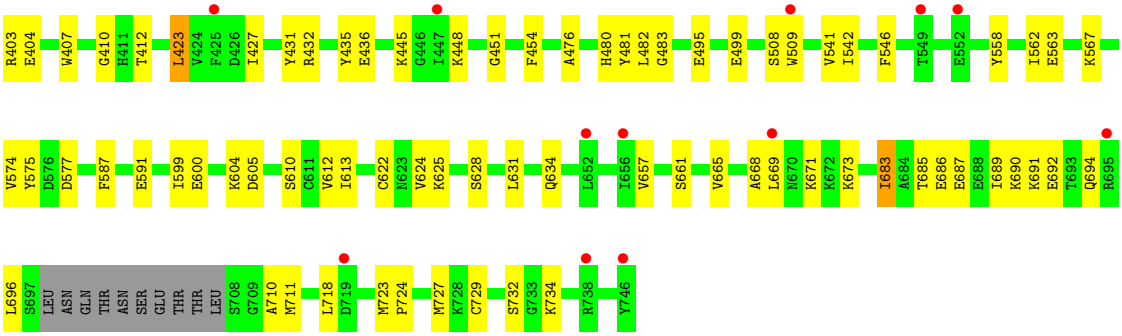
Chain B:



• Molecule 1: Proline–tRNA ligase

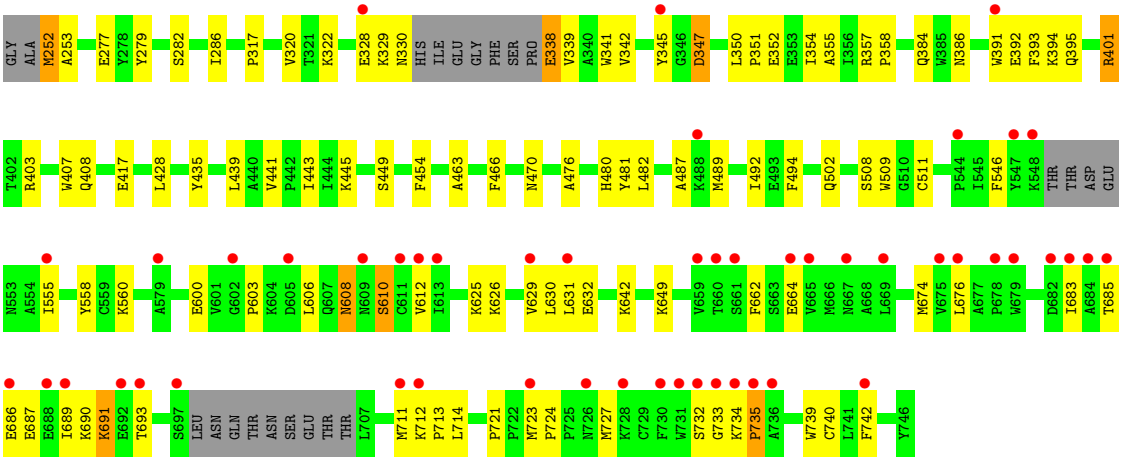
Chain C:





• Molecule 1: Proline–tRNA ligase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.02Å 140.60Å 187.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.39 46.81 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.90-2.39) 99.9 (46.81-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15rc2_3428	Depositor
R, R_{free}	0.175 , 0.232 0.180 , 0.233	Depositor DCC
R_{free} test set	4298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16025	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: 1XK, BU1, CL, HEZ

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	0.39	0/4100	0.54	0/5544
1	B	0.39	0/4044	0.54	0/5470
1	C	0.35	0/4025	0.53	0/5442
1	D	0.41	0/4001	0.56	0/5405
All	All	0.39	0/16170	0.54	0/21861

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3998	0	3989	52	0
1	B	3945	0	3935	43	0
1	C	3925	0	3914	73	0
1	D	3904	0	3904	71	0
2	A	8	0	7	0	0
2	B	8	0	7	0	0
2	C	8	0	7	0	0
2	D	8	0	7	0	0
3	A	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	0	2	0
3	C	35	0	0	0	0
3	D	35	0	0	1	0
4	A	6	0	10	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	C	8	0	14	0	0
7	A	17	0	0	0	0
7	B	16	0	0	0	0
7	C	14	0	0	0	0
7	D	9	0	0	0	0
All	All	16025	0	15794	225	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 7.

All (225) 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:328:GLU:HB3	1:A:331:HIS:HB3	1.63	0.81
1:C:345:TYR:HB2	1:C:350:LEU:HD21	1.65	0.78
1:D:691:LYS:HB2	1:D:691:LYS:HZ2	1.49	0.77
1:A:328:GLU:HB2	1:A:332:ILE:HG23	1.64	0.77
1:C:324:LYS:HE2	1:C:366:SER:HB2	1.66	0.75
1:D:693:THR:HG21	1:D:711:MET:HB3	1.70	0.73
1:A:328:GLU:CD	1:A:362:THR:HG22	2.09	0.72
1:D:608:ASN:N	1:D:608:ASN:HD22	1.86	0.71
1:A:322:LYS:O	1:A:326:GLU:HG2	1.90	0.71
1:B:357:ARG:HG3	1:B:388:VAL:HG12	1.73	0.69
1:C:344:LYS:HE2	1:C:349:ASN:HD21	1.58	0.68
1:D:691:LYS:HB2	1:D:691:LYS:NZ	2.09	0.67
1:C:723:MET:HE3	1:C:724:PRO:HD2	1.77	0.67
1:B:435:TYR:CZ	1:B:476:ALA:HB1	2.31	0.66
1:C:665:VAL:HG13	1:C:669:LEU:HD13	1.77	0.65
1:D:687:GLU:HA	1:D:690:LYS:HB2	1.78	0.65
1:C:345:TYR:HB2	1:C:350:LEU:CD2	2.26	0.65
1:C:345:TYR:CE2	1:D:393:PHE:HD2	2.15	0.65
1:D:435:TYR:CZ	1:D:476:ALA:HB1	2.32	0.65
1:A:332:ILE:HG13	1:A:333:GLU:OE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:GLU:HG3	1:D:489:MET:HE1	1.80	0.64
1:D:610:SER:HA	1:D:625:LYS:HA	1.80	0.62
1:C:431:TYR:HH	1:C:509:TRP:HD1	1.45	0.62
1:D:487:ALA:HA	1:D:492:ILE:HD12	1.81	0.61
1:D:350:LEU:HD22	1:D:352:GLU:O	2.00	0.61
1:C:587:PHE:O	1:C:591:GLU:HG3	2.01	0.60
1:C:451:GLY:HA3	1:C:686:GLU:OE2	2.01	0.60
1:A:435:TYR:CZ	1:A:476:ALA:HB1	2.37	0.60
1:C:669:LEU:HD21	1:C:711:MET:HB3	1.84	0.59
1:D:408:GLN:HE21	1:D:511:CYS:N	1.99	0.59
1:B:533:PRO:HB3	1:B:637:LEU:HD22	1.85	0.59
1:D:401:ARG:HG2	3:D:802:1XK:C12	2.33	0.59
1:C:345:TYR:CE1	1:D:338:GLU:HA	2.38	0.59
1:C:732:SER:OG	1:C:734:LYS:CD	2.51	0.58
1:C:683:ILE:O	1:C:683:ILE:HG13	2.02	0.58
1:B:698:LEU:O	1:B:699:ASN:ND2	2.37	0.58
1:A:263:SER:O	1:A:267:THR:HG23	2.04	0.58
1:C:687:GLU:O	1:C:691:LYS:HG3	2.05	0.57
1:C:263:SER:O	1:C:267:THR:HG23	2.05	0.57
1:B:259:ILE:HD12	1:B:259:ILE:H	1.69	0.56
1:C:431:TYR:OH	1:C:509:TRP:HD1	1.88	0.56
1:C:410:GLY:HA3	1:C:509:TRP:CE2	2.40	0.56
1:B:401:ARG:HG2	3:B:802:1XK:C12	2.35	0.56
1:C:393:PHE:HA	1:C:403:ARG:HH21	1.71	0.56
1:A:344:LYS:NZ	1:A:347:ASP:HA	2.21	0.56
1:C:345:TYR:HE1	1:D:338:GLU:HA	1.70	0.56
1:C:613:ILE:HD12	1:C:624:VAL:HG21	1.87	0.56
1:A:325:LEU:O	1:A:328:GLU:HG2	2.06	0.56
1:D:408:GLN:HE21	1:D:511:CYS:H	1.52	0.56
1:C:435:TYR:CZ	1:C:476:ALA:HB1	2.41	0.55
1:C:541:VAL:HG23	1:C:574:VAL:HG13	1.88	0.55
1:A:259:ILE:HD12	1:A:259:ILE:H	1.72	0.55
1:A:546:PHE:CD1	1:A:552:GLU:HG2	2.41	0.55
1:C:732:SER:OG	1:C:734:LYS:HD3	2.07	0.55
1:D:322:LYS:HD2	1:D:341:TRP:CH2	2.42	0.55
1:B:615:ARG:HG2	1:B:636:MET:HE3	1.90	0.54
1:C:495:GLU:HG2	1:C:499:GLU:HA	1.90	0.54
1:A:328:GLU:CD	1:A:362:THR:CG2	2.74	0.54
1:C:686:GLU:O	1:C:690:LYS:HG3	2.08	0.54
1:B:559:CYS:SG	1:B:601:VAL:HG11	2.47	0.54
1:C:445:LYS:HB3	1:C:718:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HD11	1:A:508:SER:HB2	1.87	0.54
1:A:329:LYS:HE2	1:A:330:ASN:HB2	1.90	0.54
1:C:275:LEU:O	1:C:276:ILE:HD13	2.08	0.54
1:B:343:THR:HG22	1:B:353:GLU:HG2	1.90	0.54
1:A:490:PHE:O	1:A:491:LYS:HG2	2.08	0.53
1:A:432:ARG:O	1:A:436:GLU:HG3	2.08	0.53
1:B:692:GLU:O	1:B:696:LEU:HG	2.07	0.53
1:D:417:GLU:HG3	1:D:481:TYR:OH	2.09	0.53
1:C:344:LYS:HE2	1:C:349:ASN:ND2	2.23	0.53
1:A:626:LYS:HA	1:A:629:VAL:HG23	1.90	0.52
1:D:734:LYS:HG2	1:D:735:PRO:HD2	1.90	0.52
1:B:683:ILE:HD12	1:B:683:ILE:H	1.75	0.52
1:D:393:PHE:HA	1:D:403:ARG:HH21	1.75	0.52
1:C:342:VAL:HG22	1:D:342:VAL:HG12	1.91	0.52
1:B:599:ILE:HG12	1:B:613:ILE:HD13	1.90	0.51
1:D:357:ARG:NH2	1:D:386:ASN:HB2	2.25	0.51
1:B:395:GLN:HG2	1:B:396:PRO:HD2	1.91	0.51
1:D:454:PHE:HB2	1:D:480:HIS:CE1	2.45	0.51
1:D:676:LEU:HD21	1:D:721:PRO:HG2	1.91	0.51
1:C:427:ILE:HG21	1:C:509:TRP:CG	2.46	0.51
1:D:608:ASN:N	1:D:608:ASN:ND2	2.58	0.51
1:D:342:VAL:HG22	1:D:354:ILE:HG12	1.92	0.51
1:A:347:ASP:HB3	1:C:261:ASN:ND2	2.26	0.51
1:B:322:LYS:HG2	1:B:341:TRP:CH2	2.45	0.50
1:C:685:THR:O	1:C:689:ILE:HG13	2.11	0.50
1:D:662:PHE:C	1:D:662:PHE:CD2	2.84	0.50
1:A:356:ILE:HD11	1:B:356:ILE:HD11	1.94	0.50
1:B:560:LYS:O	1:B:564:LYS:HG3	2.11	0.50
1:D:466:PHE:CE1	1:D:674:MET:HG3	2.47	0.49
1:A:344:LYS:HB3	1:B:341:TRP:HB2	1.94	0.49
1:A:533:PRO:HB3	1:A:637:LEU:HD22	1.94	0.49
1:D:347:ASP:OD2	1:D:347:ASP:N	2.44	0.49
1:A:454:PHE:HB2	1:A:480:HIS:CE1	2.48	0.49
1:B:417:GLU:HG3	1:B:481:TYR:OH	2.11	0.49
1:D:676:LEU:HD11	1:D:739:TRP:HB3	1.94	0.49
1:A:344:LYS:HZ1	1:A:347:ASP:HA	1.77	0.49
1:C:454:PHE:HB2	1:C:480:HIS:CE1	2.47	0.49
1:A:674:MET:HE1	1:A:714:LEU:HD13	1.94	0.49
1:A:329:LYS:HG3	1:A:330:ASN:N	2.27	0.48
1:C:276:ILE:HD11	1:C:399:PHE:CZ	2.48	0.48
1:A:277:GLU:HG2	1:B:367:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:MET:HE3	1:B:636:MET:HB3	1.62	0.48
1:C:575:TYR:CE2	1:C:577:ASP:HB3	2.47	0.48
1:C:423:LEU:HD21	1:C:509:TRP:CZ3	2.49	0.48
1:A:395:GLN:NE2	1:A:396:PRO:HD2	2.29	0.48
1:A:601:VAL:HA	1:A:605:ASP:OD2	2.14	0.48
1:B:319:PHE:CG	1:B:354:ILE:HD12	2.48	0.48
1:C:373:ARG:HH11	1:C:373:ARG:HG3	1.78	0.48
1:B:466:PHE:CE1	1:B:674:MET:HG3	2.49	0.48
1:B:675:VAL:HG22	1:B:742:PHE:HB2	1.94	0.47
1:C:277:GLU:HB3	1:C:286:ILE:HB	1.95	0.47
1:C:412:THR:HG23	1:C:509:TRP:CZ3	2.49	0.47
1:D:558:TYR:CD1	1:D:606:LEU:HD13	2.50	0.47
1:A:408:GLN:NE2	1:A:431:TYR:OH	2.31	0.47
1:C:724:PRO:HB2	1:C:727:MET:HG2	1.96	0.47
1:D:277:GLU:HB3	1:D:286:ILE:HB	1.97	0.47
1:D:428:LEU:HG	1:D:445:LYS:HD3	1.97	0.47
1:D:482:LEU:HD11	1:D:508:SER:HB2	1.97	0.47
1:C:279:TYR:CD2	1:D:317:PRO:HG2	2.50	0.47
1:D:732:SER:OG	1:D:733:GLY:N	2.48	0.47
1:A:550:THR:OG1	1:A:603:PRO:HB3	2.15	0.47
1:B:417:GLU:HG3	1:B:481:TYR:CZ	2.50	0.47
1:C:387:THR:HG21	1:C:404:GLU:OE2	2.14	0.46
1:B:252:MET:HG3	1:B:272:LYS:HD3	1.97	0.46
1:C:671:LYS:HB2	1:C:673:LYS:HG3	1.97	0.46
1:C:683:ILE:O	1:C:686:GLU:HG3	2.15	0.46
1:C:723:MET:HE2	1:C:727:MET:HG3	1.96	0.46
1:A:472:ARG:NH1	1:A:744:ARG:HB3	2.30	0.46
1:C:345:TYR:CZ	1:D:391:TRP:O	2.69	0.46
1:D:384:GLN:O	1:D:408:GLN:HA	2.15	0.46
1:B:385:TRP:CE3	1:B:408:GLN:HB3	2.51	0.46
1:B:263:SER:O	1:B:267:THR:HG23	2.15	0.46
1:D:662:PHE:CD2	1:D:662:PHE:O	2.69	0.46
1:B:698:LEU:C	1:B:699:ASN:HD22	2.19	0.46
1:A:328:GLU:CB	1:A:331:HIS:HB3	2.42	0.46
1:A:466:PHE:CZ	1:A:471:GLY:HA2	2.50	0.46
1:C:691:LYS:HB3	1:C:691:LYS:HE2	1.80	0.46
1:A:501:LYS:HE2	1:A:501:LYS:HB2	1.68	0.45
1:A:605:ASP:OD2	1:A:611:CYS:HA	2.16	0.45
1:B:607:GLN:O	1:B:607:GLN:HG2	2.17	0.45
1:D:626:LYS:O	1:D:629:VAL:HG12	2.16	0.45
1:C:381:LYS:HG2	1:C:412:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:ILE:HA	1:D:686:GLU:HG3	1.99	0.45
1:D:686:GLU:OE2	1:D:713:PRO:HG2	2.16	0.45
1:C:605:ASP:HB3	1:C:610:SER:O	2.17	0.45
1:D:740:CYS:HB3	1:D:742:PHE:CE1	2.52	0.45
1:B:384:GLN:O	1:B:408:GLN:HA	2.17	0.44
1:A:604:LYS:HD3	1:A:604:LYS:HA	1.65	0.44
1:D:443:ILE:HD13	1:D:463:ALA:HB1	1.98	0.44
1:D:449:SER:HB2	1:D:686:GLU:OE1	2.17	0.44
1:C:600:GLU:HB2	1:C:612:VAL:CG1	2.47	0.44
1:A:547:TYR:C	1:A:549:THR:H	2.20	0.44
1:A:542:ILE:HG21	1:A:559:CYS:HB3	2.00	0.44
1:B:445:LYS:HB3	1:B:718:LEU:HD12	1.98	0.44
1:B:454:PHE:HB2	1:B:480:HIS:CE1	2.53	0.44
1:C:563:GLU:HG2	1:C:567:LYS:HD2	2.00	0.44
1:C:692:GLU:O	1:C:696:LEU:HB2	2.17	0.44
1:D:555:ILE:HG13	1:D:606:LEU:CD2	2.48	0.44
1:A:329:LYS:HG3	1:A:330:ASN:H	1.83	0.44
1:D:328:GLU:CG	1:D:489:MET:HE1	2.46	0.44
1:A:624:VAL:HG11	1:A:629:VAL:HA	2.00	0.43
1:C:345:TYR:CG	1:C:345:TYR:O	2.70	0.43
1:C:343:THR:C	1:C:350:LEU:HD12	2.38	0.43
1:D:329:LYS:O	1:D:330:ASN:ND2	2.51	0.43
1:C:336:SER:N	1:C:337:PRO:HD2	2.33	0.43
1:D:392:GLU:OE1	1:D:394:LYS:HE2	2.18	0.43
1:A:466:PHE:CE2	1:A:655:SER:HB3	2.54	0.43
1:D:649:LYS:HE3	1:D:649:LYS:HB3	1.75	0.43
1:B:320:VAL:HG13	1:B:355:ALA:HB3	2.00	0.43
1:C:256:SER:OG	1:C:264:ASP:OD2	2.30	0.43
1:C:393:PHE:CE1	1:D:345:TYR:CZ	3.06	0.43
1:A:352:GLU:O	1:A:352:GLU:HG2	2.17	0.43
1:A:294:ILE:HG12	1:A:535:VAL:HB	2.00	0.43
1:A:651:LYS:O	1:A:655:SER:OG	2.26	0.43
1:D:252:MET:HE2	1:D:253:ALA:H	1.84	0.43
1:D:600:GLU:HB2	1:D:612:VAL:CG1	2.49	0.43
1:C:482:LEU:HD11	1:C:508:SER:HB2	2.00	0.42
1:B:575:TYR:CE2	1:B:577:ASP:HB3	2.54	0.42
1:C:393:PHE:HE1	1:D:345:TYR:CE2	2.38	0.42
1:A:328:GLU:OE1	1:A:362:THR:HG22	2.19	0.42
1:B:563:GLU:O	1:B:567:LYS:HG2	2.20	0.42
1:D:320:VAL:HG13	1:D:355:ALA:HB3	2.01	0.42
1:A:541:VAL:HG21	1:A:590:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ARG:HG2	3:B:802:1XK:C13	2.50	0.42
1:C:432:ARG:O	1:C:436:GLU:HG3	2.18	0.42
1:D:724:PRO:HB2	1:D:727:MET:HG2	2.01	0.42
1:B:734:LYS:HD2	1:B:734:LYS:N	2.33	0.42
1:C:665:VAL:CG1	1:C:669:LEU:HD13	2.46	0.42
1:D:494:PHE:CE1	1:D:502:GLN:HB2	2.54	0.42
1:B:339:VAL:HG11	1:B:355:ALA:HB1	2.02	0.42
1:B:558:TYR:CD2	1:B:601:VAL:HG21	2.55	0.42
1:A:384:GLN:O	1:A:408:GLN:HA	2.20	0.42
1:C:558:TYR:CE2	1:C:562:ILE:HD11	2.54	0.42
1:B:380:LEU:O	1:B:412:THR:HA	2.20	0.42
1:C:481:TYR:CZ	1:C:483:GLY:HA2	2.54	0.42
1:D:712:LYS:HE3	1:D:714:LEU:HD23	2.02	0.42
1:A:500:VAL:HG13	1:A:502:GLN:HE21	1.84	0.42
1:C:600:GLU:HB2	1:C:612:VAL:HG13	2.01	0.42
1:D:687:GLU:O	1:D:690:LYS:HB3	2.20	0.42
1:C:694:GLN:HB2	1:C:710:ALA:HB2	2.01	0.42
1:D:339:VAL:HG22	1:D:358:PRO:HG3	2.02	0.42
1:D:642:LYS:HA	1:D:642:LYS:HD3	1.65	0.41
1:D:439:LEU:O	1:D:441:VAL:HG23	2.20	0.41
1:C:317:PRO:HG2	1:D:279:TYR:CD2	2.56	0.41
1:C:657:VAL:HG11	1:C:668:ALA:HB1	2.00	0.41
1:B:697:SER:O	1:B:699:ASN:N	2.50	0.41
1:C:624:VAL:HG12	1:C:625:LYS:O	2.20	0.41
1:D:691:LYS:HD3	1:D:691:LYS:HA	1.54	0.41
1:A:360:SER:HB2	1:A:409:GLU:OE1	2.20	0.41
1:C:398:PRO:O	1:C:399:PHE:HB2	2.21	0.41
1:B:675:VAL:CG2	1:B:742:PHE:HB2	2.51	0.41
1:D:629:VAL:HG13	1:D:630:LEU:N	2.35	0.41
1:A:330:ASN:HA	1:A:333:GLU:OE2	2.21	0.41
1:D:555:ILE:HD11	1:D:603:PRO:HA	2.02	0.41
1:D:685:THR:O	1:D:689:ILE:HG13	2.21	0.41
1:D:350:LEU:HG	1:D:351:PRO:HD2	2.02	0.41
1:D:606:LEU:O	1:D:606:LEU:HD12	2.21	0.41
1:C:345:TYR:OH	1:D:392:GLU:HA	2.21	0.40
1:D:560:LYS:HB2	1:D:560:LYS:HE2	1.82	0.40
1:A:560:LYS:O	1:A:564:LYS:HG2	2.22	0.40
1:C:542:ILE:HD13	1:C:599:ILE:HB	2.03	0.40
1:A:646:LEU:HD23	1:A:646:LEU:HA	1.90	0.40
1:B:257:LYS:HE3	1:B:260:GLU:OE2	2.22	0.40
1:C:631:LEU:HD12	1:C:634:GLN:OE1	2.22	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	483/497 (97%)	469 (97%)	12 (2%)	2 (0%)	34	48
1	B	475/497 (96%)	459 (97%)	14 (3%)	2 (0%)	34	48
1	C	472/497 (95%)	455 (96%)	17 (4%)	0	100	100
1	D	467/497 (94%)	445 (95%)	21 (4%)	1 (0%)	47	62
All	All	1897/1988 (95%)	1828 (96%)	64 (3%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	698	LEU
1	A	548	LYS
1	B	725	PRO
1	D	735	PRO
1	A	352	GLU

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	442/450 (98%)	431 (98%)	11 (2%)	47	67
1	B	437/450 (97%)	430 (98%)	7 (2%)	62	79
1	C	434/450 (96%)	419 (96%)	15 (4%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	431/450 (96%)	414 (96%)	17 (4%)	32 50
All	All	1744/1800 (97%)	1694 (97%)	50 (3%)	42 62

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	330	ASN
1	A	338	GLU
1	A	352	GLU
1	A	407	TRP
1	A	423	LEU
1	A	489	MET
1	A	491	LYS
1	A	509	TRP
1	A	650	LYS
1	A	694	GLN
1	B	282	SER
1	B	407	TRP
1	B	423	LEU
1	B	448	LYS
1	B	509	TRP
1	B	609	ASN
1	B	621	LYS
1	C	252	MET
1	C	335	PHE
1	C	336	SER
1	C	347	ASP
1	C	393	PHE
1	C	407	TRP
1	C	423	LEU
1	C	448	LYS
1	C	546	PHE
1	C	604	LYS
1	C	622	CYS
1	C	628	SER
1	C	661	SER
1	C	683	ILE
1	C	729	CYS
1	D	252	MET
1	D	282	SER
1	D	338	GLU

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Mol	Chain	Res	Type
1	D	347	ASP
1	D	395	GLN
1	D	401	ARG
1	D	407	TRP
1	D	470	ASN
1	D	509	TRP
1	D	546	PHE
1	D	608	ASN
1	D	610	SER
1	D	631	LEU
1	D	632	GLU
1	D	664	GLU
1	D	691	LYS
1	D	723	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	395	GLN
1	A	408	GLN
1	A	667	ASN
1	A	694	GLN
1	B	408	GLN
1	B	699	ASN
1	B	700	GLN
1	C	349	ASN
1	C	670	ASN
1	D	330	ASN
1	D	408	GLN
1	D	608	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)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
3	1XK	B	802	-	35,39,39	4.96	13 (37%)	46,58,58	3.87	17 (36%)
2	PRO	D	801	-	8,8,8	0.80	0	10,10,10	1.45	2 (20%)
3	1XK	C	802	-	35,39,39	4.87	14 (40%)	46,58,58	4.07	16 (34%)
3	1XK	A	802	-	35,39,39	4.94	12 (34%)	46,58,58	3.48	13 (28%)
2	PRO	C	801	-	8,8,8	0.89	1 (12%)	10,10,10	1.34	2 (20%)
4	BU1	A	803	-	5,5,5	0.34	0	4,4,4	0.53	0
2	PRO	B	801	-	8,8,8	0.86	0	10,10,10	1.54	2 (20%)
6	HEZ	C	803	-	7,7,7	0.35	0	6,6,6	0.66	0
2	PRO	A	801	-	8,8,8	0.95	1 (12%)	10,10,10	1.32	2 (20%)
3	1XK	D	802	-	35,39,39	5.00	13 (37%)	46,58,58	3.63	13 (28%)

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	1XK	B	802	-	-	4/24/44/44	0/5/5/5
2	PRO	D	801	-	-	0/4/11/11	0/1/1/1
3	1XK	C	802	-	-	2/24/44/44	0/5/5/5
3	1XK	A	802	-	-	0/24/44/44	0/5/5/5
2	PRO	C	801	-	-	0/4/11/11	0/1/1/1
4	BU1	A	803	-	-	0/3/3/3	-
2	PRO	B	801	-	-	2/4/11/11	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEZ	C	803	-	-	2/5/5/5	-
2	PRO	A	801	-	-	2/4/11/11	0/1/1/1
3	1XK	D	802	-	-	2/24/44/44	0/5/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	1XK	C25-N4	20.38	1.59	1.36
3	D	802	1XK	C25-N4	20.18	1.59	1.36
3	B	802	1XK	C25-N4	20.03	1.59	1.36
3	C	802	1XK	C25-N4	19.72	1.58	1.36
3	B	802	1XK	C19-C20	-13.43	1.33	1.54
3	D	802	1XK	C19-C20	-13.38	1.33	1.54
3	A	802	1XK	C19-C20	-12.88	1.34	1.54
3	C	802	1XK	C19-C20	-12.83	1.34	1.54
3	C	802	1XK	C18-N4	-9.18	1.35	1.47
3	D	802	1XK	C18-N4	-9.11	1.35	1.47
3	A	802	1XK	C18-N4	-9.04	1.35	1.47
3	B	802	1XK	C18-N4	-8.96	1.35	1.47
3	A	802	1XK	C19-C18	7.55	1.67	1.52
3	C	802	1XK	C19-C18	6.98	1.66	1.52
3	D	802	1XK	C19-C18	6.94	1.65	1.52
3	B	802	1XK	C19-C18	6.88	1.65	1.52
3	D	802	1XK	C6-N1	6.26	1.47	1.33
3	B	802	1XK	C6-N1	5.96	1.46	1.33
3	A	802	1XK	C6-N1	5.76	1.46	1.33
3	C	802	1XK	C6-N1	5.71	1.46	1.33
3	D	802	1XK	C23-C22	-5.24	1.38	1.50
3	D	802	1XK	C24-C22	-5.14	1.39	1.50
3	C	802	1XK	C23-C22	-5.13	1.39	1.50
3	C	802	1XK	C24-C22	-5.05	1.39	1.50
3	B	802	1XK	C24-C22	-4.94	1.39	1.50
3	A	802	1XK	C23-C22	-4.92	1.39	1.50
3	A	802	1XK	C24-C22	-4.90	1.39	1.50
3	B	802	1XK	C23-C22	-4.80	1.39	1.50
3	D	802	1XK	O2-C25	3.47	1.27	1.22
3	B	802	1XK	O2-C25	3.28	1.27	1.22
3	C	802	1XK	C17-N3	-3.21	1.32	1.35
3	A	802	1XK	O2-C25	3.05	1.27	1.22
3	B	802	1XK	C17-N3	-3.03	1.32	1.35
3	A	802	1XK	C17-N3	-2.96	1.32	1.35
3	D	802	1XK	C17-N3	-2.94	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	1XK	C20-C25	2.85	1.58	1.53
3	C	802	1XK	O2-C25	2.58	1.26	1.22
3	B	802	1XK	C14-C12	2.52	1.55	1.49
3	B	802	1XK	C24-C23	-2.44	1.39	1.48
3	C	802	1XK	C24-C23	-2.40	1.39	1.48
3	D	802	1XK	C24-C23	-2.40	1.39	1.48
3	D	802	1XK	C20-C25	2.38	1.57	1.53
3	A	802	1XK	C24-C23	-2.38	1.39	1.48
3	D	802	1XK	C14-C12	2.37	1.54	1.49
3	C	802	1XK	C14-C12	2.28	1.54	1.49
3	A	802	1XK	C14-C12	2.27	1.54	1.49
2	A	801	PRO	OXT-C	-2.21	1.23	1.30
3	C	802	1XK	C20-C25	2.17	1.56	1.53
3	B	802	1XK	C17-C14	2.15	1.42	1.38
2	C	801	PRO	OXT-C	-2.14	1.23	1.30
3	D	802	1XK	C17-C14	2.13	1.42	1.38
3	C	802	1XK	C3-N4	2.07	1.47	1.43
3	C	802	1XK	C17-C14	2.07	1.42	1.38
3	A	802	1XK	O-C6	-2.03	1.19	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	1XK	O2-C25-N4	-16.54	109.51	125.81
3	C	802	1XK	O2-C25-N4	-14.97	111.06	125.81
3	D	802	1XK	O2-C25-N4	-13.93	112.09	125.81
3	C	802	1XK	C18-N4-C25	-13.43	100.56	112.86
3	A	802	1XK	O2-C25-N4	-13.36	112.64	125.81
3	C	802	1XK	O2-C25-C20	-11.32	110.09	128.02
3	B	802	1XK	C20-C25-N4	-10.78	102.26	109.15
3	A	802	1XK	O2-C25-C20	-9.62	112.79	128.02
3	A	802	1XK	C20-C25-N4	-9.24	103.24	109.15
3	D	802	1XK	C20-C25-N4	-8.96	103.42	109.15
3	B	802	1XK	O2-C25-C20	-8.58	114.43	128.02
3	D	802	1XK	O2-C25-C20	-8.34	114.82	128.02
3	D	802	1XK	C18-N4-C25	-7.92	105.60	112.86
3	D	802	1XK	C3-N4-C25	-7.84	119.72	126.30
3	A	802	1XK	C18-N4-C25	-7.74	105.77	112.86
3	B	802	1XK	C18-N4-C25	-7.58	105.92	112.86
3	C	802	1XK	C20-C25-N4	-7.27	104.50	109.15
3	C	802	1XK	C15-N2-N3	6.33	110.82	104.23
3	D	802	1XK	C15-N2-N3	6.12	110.60	104.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	1XK	C15-N2-N3	6.11	110.59	104.23
3	A	802	1XK	C15-N2-N3	5.67	110.14	104.23
3	C	802	1XK	C3-N4-C25	-4.56	122.48	126.30
3	D	802	1XK	C5-N-C1	4.31	121.83	118.23
3	D	802	1XK	C16-N3-N2	4.27	125.52	120.50
3	C	802	1XK	C16-N3-N2	4.22	125.47	120.50
3	A	802	1XK	C16-N3-N2	3.94	125.14	120.50
3	A	802	1XK	C18-N4-C3	3.87	126.32	120.76
3	B	802	1XK	C16-N3-N2	3.85	125.03	120.50
3	C	802	1XK	C5-N-C1	3.84	121.44	118.23
3	B	802	1XK	C2-C3-N4	3.82	125.32	119.85
3	A	802	1XK	C3-N4-C25	-3.81	123.10	126.30
3	D	802	1XK	C19-C18-N4	3.49	107.03	103.36
3	B	802	1XK	C3-N4-C25	3.28	129.04	126.30
3	B	802	1XK	C4-C3-N4	-3.21	115.25	119.85
3	B	802	1XK	C8-C7-N1	-3.18	106.23	113.05
3	D	802	1XK	C5-C6-N1	3.09	119.91	115.59
3	C	802	1XK	C5-C6-N1	3.06	119.87	115.59
3	B	802	1XK	C5-N-C1	3.02	120.75	118.23
3	B	802	1XK	C6-C5-N	2.98	122.15	117.42
3	C	802	1XK	C9-C10-C11	-2.94	119.80	123.52
2	B	801	PRO	OXT-C-O	-2.93	117.44	124.09
3	C	802	1XK	C18-N4-C3	2.89	124.91	120.76
3	C	802	1XK	F-C10-C11	2.80	122.25	118.25
2	D	801	PRO	OXT-C-O	-2.74	117.88	124.09
3	B	802	1XK	C18-C19-C20	-2.71	101.16	104.52
3	A	802	1XK	C-C1-N	2.71	120.89	116.56
3	A	802	1XK	C19-C18-N4	2.69	106.19	103.36
2	C	801	PRO	OXT-C-O	-2.59	118.20	124.09
2	B	801	PRO	OXT-C-CA	2.59	122.00	113.40
3	B	802	1XK	O1-C21-C20	-2.56	106.26	111.86
3	B	802	1XK	C9-C10-C11	-2.55	120.30	123.52
3	C	802	1XK	C8-C7-N1	-2.52	107.64	113.05
3	D	802	1XK	C6-C5-N	2.50	121.39	117.42
2	D	801	PRO	OXT-C-CA	2.47	121.60	113.40
3	B	802	1XK	C18-N4-C3	2.44	124.27	120.76
2	A	801	PRO	OXT-C-O	-2.44	118.56	124.09
3	A	802	1XK	C6-C5-N	2.43	121.29	117.42
3	B	802	1XK	C19-C18-N4	2.42	105.91	103.36
3	A	802	1XK	C-C1-C2	-2.34	118.24	121.81
3	D	802	1XK	C-C1-N	2.33	120.27	116.56
3	A	802	1XK	C9-C10-C11	-2.29	120.62	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802	1XK	C-C1-N	2.24	120.14	116.56
3	C	802	1XK	C6-C5-N	2.19	120.90	117.42
2	A	801	PRO	OXT-C-CA	2.18	120.64	113.40
2	C	801	PRO	OXT-C-CA	2.10	120.36	113.40
3	C	802	1XK	C17-N3-N2	-2.04	109.78	111.56
3	D	802	1XK	C9-C10-C11	-2.03	120.95	123.52

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	1XK	C22-C20-C21-O1
3	B	802	1XK	C25-C20-C21-O1
3	B	802	1XK	C19-C20-C22-C24
3	C	802	1XK	C25-C20-C22-C23
3	D	802	1XK	C19-C20-C22-C23
3	D	802	1XK	C25-C20-C22-C23
6	C	803	HEZ	C1-C2-C3-C4
6	C	803	HEZ	C3-C4-C5-C6
3	C	802	1XK	C25-C20-C22-C24
3	B	802	1XK	C19-C20-C21-O1
2	A	801	PRO	O-C-CA-CB
2	B	801	PRO	O-C-CA-CB
2	A	801	PRO	OXT-C-CA-CB
2	B	801	PRO	OXT-C-CA-CB

There are no ring outliers.

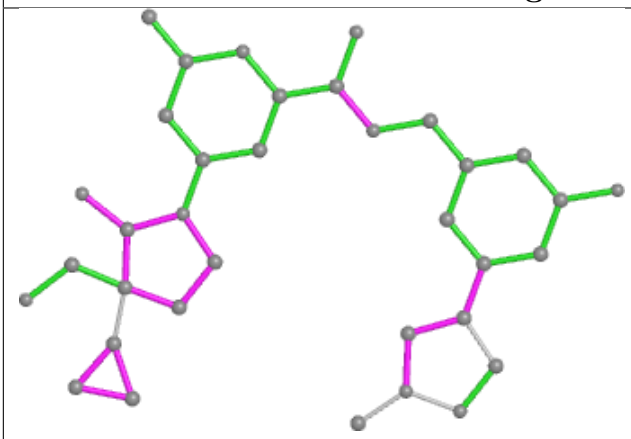
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	1XK	2	0
3	D	802	1XK	1	0

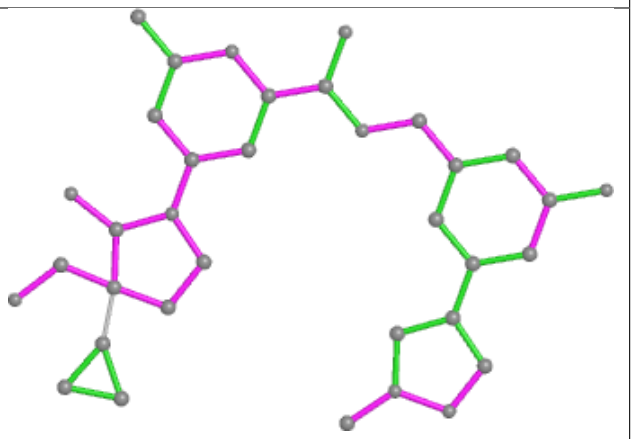
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

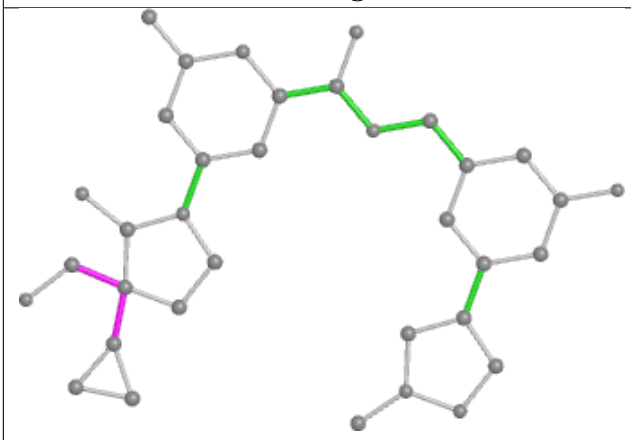
Ligand 1XK B 802



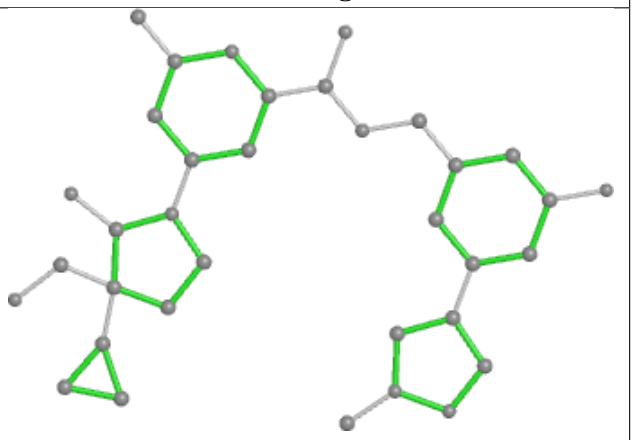
Bond lengths



Bond angles

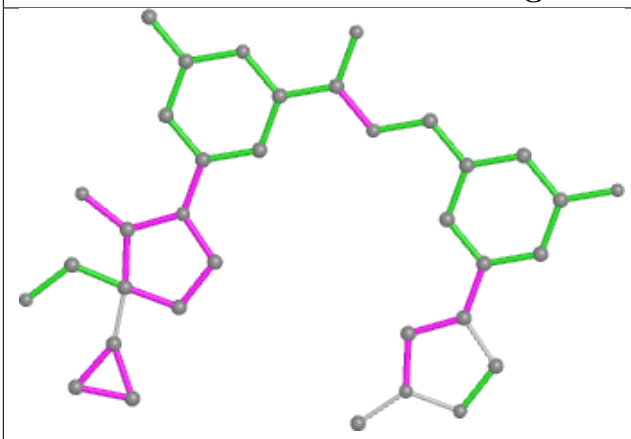


Torsions

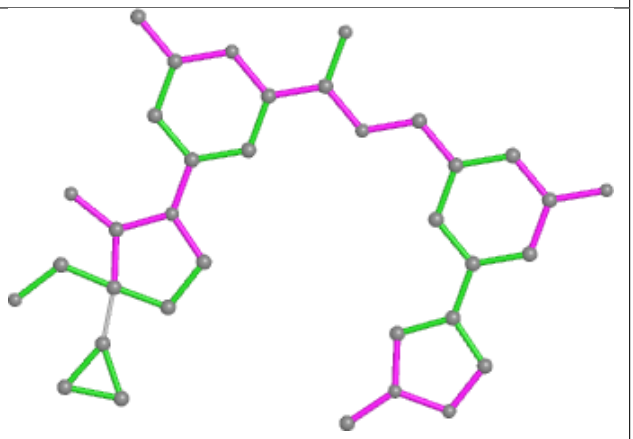


Rings

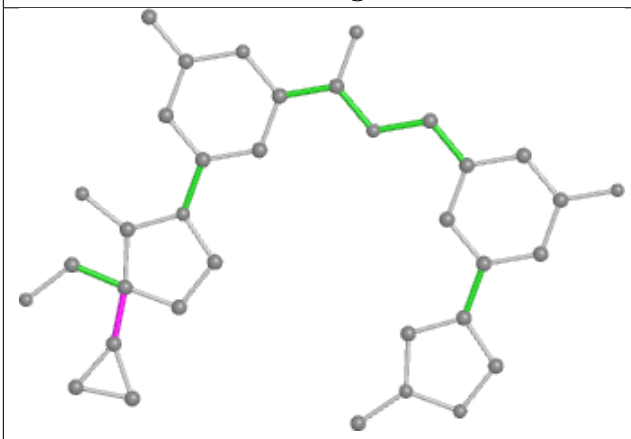
Ligand 1XK C 802



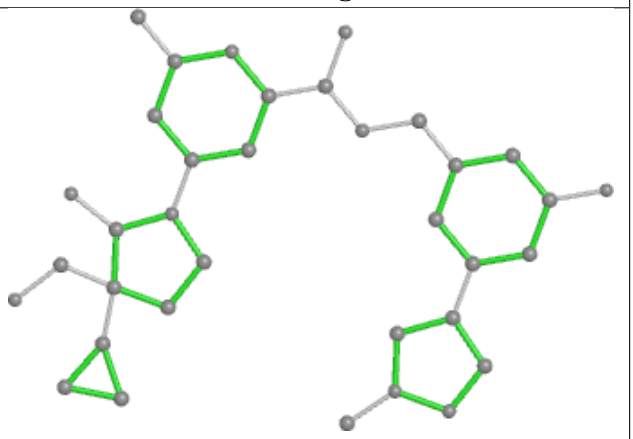
Bond lengths



Bond angles

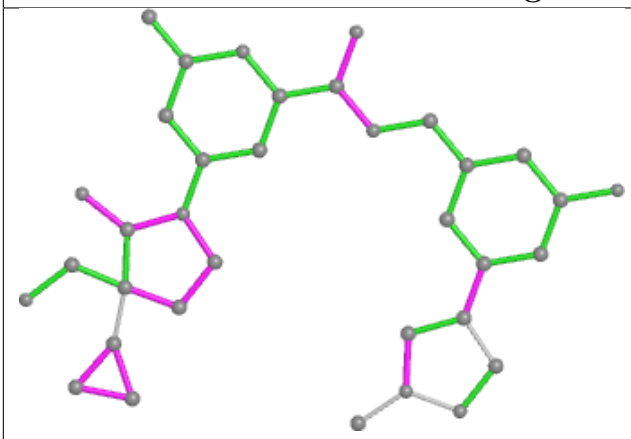


Torsions

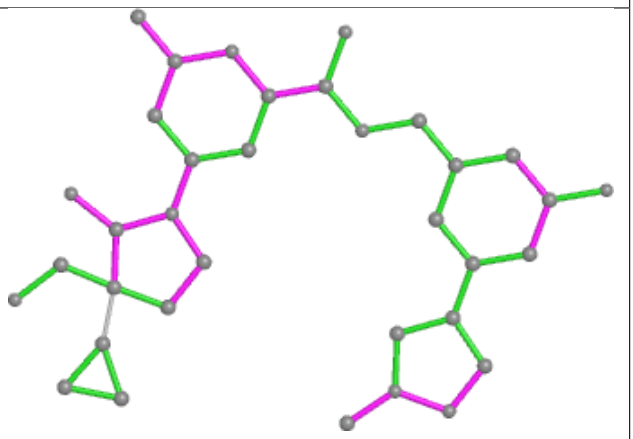


Rings

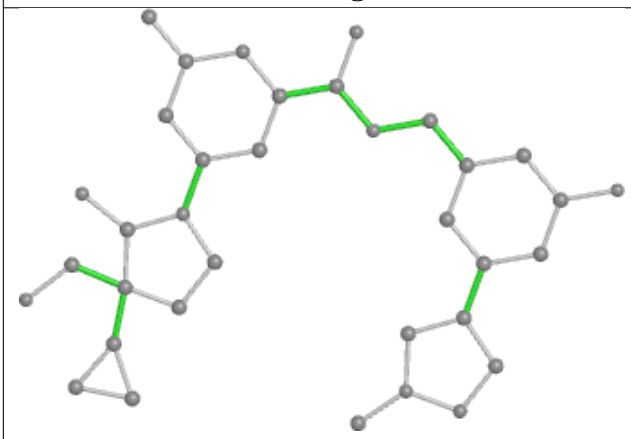
Ligand 1XK A 802



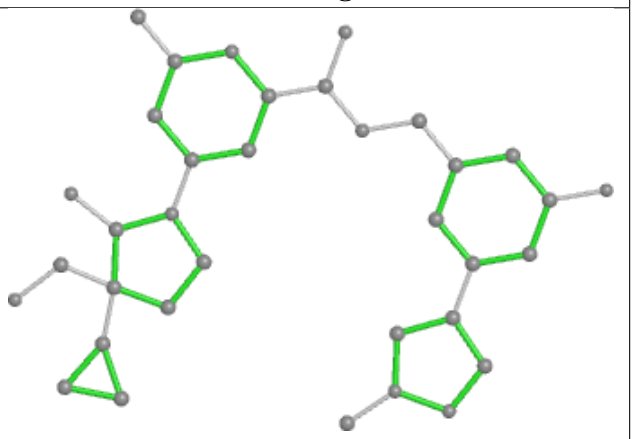
Bond lengths



Bond angles

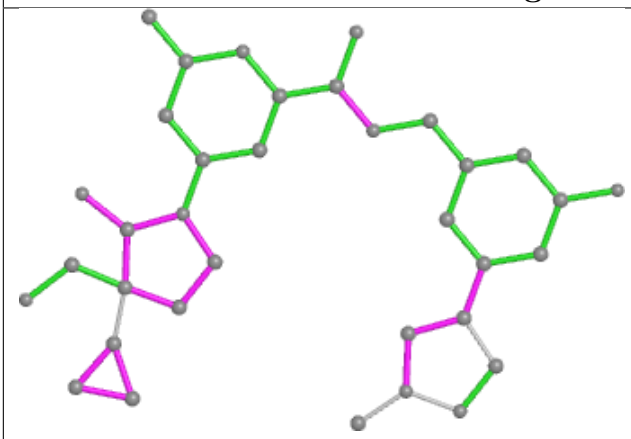


Torsions

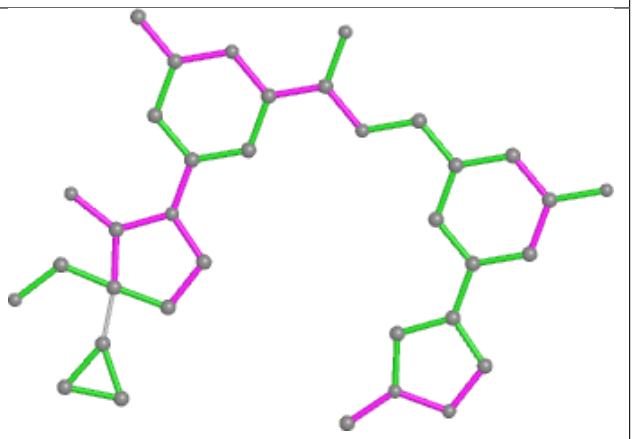


Rings

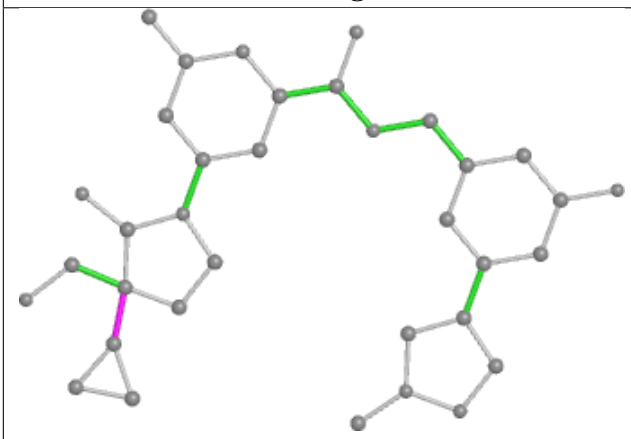
Ligand 1XK D 802



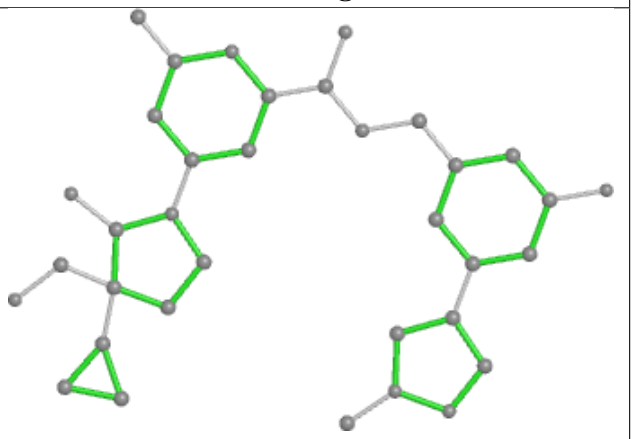
Bond lengths



Bond angles



Torsions



Rings

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	487/497 (97%)	0.43	20 (4%) 37 36	44, 66, 101, 134	2 (0%)
1	B	481/497 (96%)	0.37	12 (2%) 57 55	43, 68, 101, 125	2 (0%)
1	C	478/497 (96%)	0.43	15 (3%) 49 47	46, 76, 114, 137	3 (0%)
1	D	475/497 (95%)	0.68	51 (10%) 6 5	47, 75, 121, 143	5 (1%)
All	All	1921/1988 (96%)	0.48	98 (5%) 28 26	43, 71, 114, 143	12 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLU	9.5
1	D	730	PHE	5.7
1	A	332	ILE	5.3
1	D	547	TYR	5.2
1	D	685	THR	5.0
1	D	736	ALA	4.9
1	D	665	VAL	4.7
1	D	735	PRO	4.6
1	C	347	ASP	4.4
1	A	331	HIS	4.3
1	A	330	ASN	4.1
1	D	328	GLU	4.0
1	B	547	TYR	3.9
1	C	656	ILE	3.8
1	D	731	TRP	3.8
1	D	711	MET	3.6
1	D	675	VAL	3.6
1	C	695	ARG	3.5
1	A	547	TYR	3.5
1	A	605	ASP	3.5
1	D	684	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	692	GLU	3.4
1	B	548	LYS	3.4
1	D	664	GLU	3.4
1	D	728	LYS	3.2
1	A	719	ASP	3.2
1	D	679	TRP	3.2
1	D	629	VAL	3.2
1	D	726	ASN	3.2
1	A	329	LYS	3.2
1	C	447	ILE	3.2
1	C	719	ASP	3.2
1	D	686	GLU	3.2
1	A	333	GLU	3.1
1	C	652	LEU	3.1
1	D	723	MET	3.1
1	D	733	GLY	3.0
1	D	605	ASP	3.0
1	D	689	ILE	3.0
1	D	697	SER	2.9
1	B	550	THR	2.8
1	D	734	LYS	2.8
1	D	683	ILE	2.8
1	C	509	TRP	2.8
1	D	611	CYS	2.8
1	D	631	LEU	2.8
1	A	549	THR	2.7
1	D	602	GLY	2.7
1	C	669	LEU	2.7
1	C	549	THR	2.7
1	D	678	PRO	2.6
1	B	337	PRO	2.6
1	D	669	LEU	2.5
1	D	660	THR	2.5
1	D	693	THR	2.5
1	A	604	LYS	2.5
1	B	700	GLN	2.5
1	B	605	ASP	2.5
1	A	347	ASP	2.5
1	D	742	PHE	2.5
1	D	613	ILE	2.5
1	D	688	GLU	2.4
1	A	352	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	345	TYR	2.4
1	C	345	TYR	2.4
1	D	548	LYS	2.4
1	A	627	GLU	2.4
1	D	732	SER	2.4
1	A	714	LEU	2.3
1	D	609	ASN	2.3
1	D	488	LYS	2.3
1	D	555	ILE	2.3
1	B	730	PHE	2.3
1	C	262	PHE	2.2
1	B	679	TRP	2.2
1	A	292	TYR	2.2
1	D	692	GLU	2.2
1	D	667	ASN	2.2
1	D	579	ALA	2.2
1	D	391	TRP	2.2
1	C	552	GLU	2.2
1	D	659	VAL	2.1
1	A	284	CYS	2.1
1	B	698	LEU	2.1
1	D	676	LEU	2.1
1	D	682	ASP	2.1
1	A	631	LEU	2.1
1	D	544	PRO	2.1
1	B	687	GLU	2.1
1	C	738	ARG	2.1
1	B	732	SER	2.1
1	D	712	LYS	2.0
1	A	387	THR	2.0
1	D	612	VAL	2.0
1	A	558	TYR	2.0
1	C	746	TYR	2.0
1	C	425	PHE	2.0
1	D	661	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

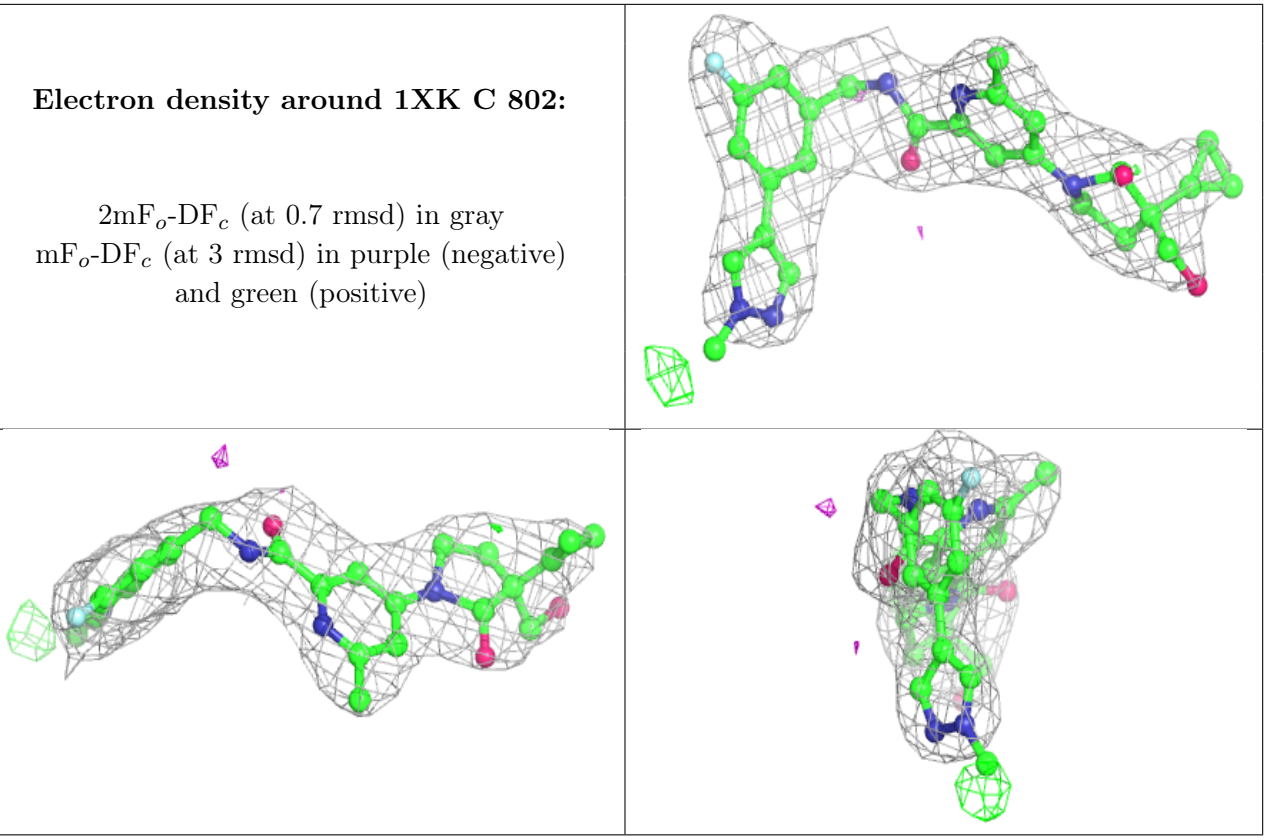
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	C	805	1/1	0.62	0.14	104,104,104,104	0
6	HEZ	C	803	8/8	0.72	0.25	88,92,101,101	0
4	BU1	A	803	6/6	0.74	0.19	81,85,86,90	0
5	CL	A	804	1/1	0.77	0.24	101,101,101,101	0
5	CL	A	805	1/1	0.82	0.14	98,98,98,98	0
5	CL	B	803[A]	1/1	0.83	0.41	76,76,76,76	1
5	CL	B	803[B]	1/1	0.83	0.41	57,57,57,57	1
5	CL	A	806	1/1	0.88	0.12	108,108,108,108	0
5	CL	B	805	1/1	0.93	0.20	102,102,102,102	0
5	CL	B	804	1/1	0.94	0.44	96,96,96,96	0
2	PRO	B	801	8/8	0.94	0.17	60,73,77,79	0
2	PRO	C	801	8/8	0.94	0.18	49,60,64,65	8
3	1XK	C	802	35/35	0.94	0.21	60,68,83,83	0
2	PRO	D	801	8/8	0.95	0.15	60,73,83,84	0
3	1XK	D	802	35/35	0.95	0.19	55,73,86,89	0
3	1XK	A	802	35/35	0.95	0.20	46,57,79,87	0
2	PRO	A	801	8/8	0.96	0.19	46,57,64,64	0
5	CL	D	803	1/1	0.96	0.34	97,97,97,97	0
5	CL	D	804	1/1	0.96	0.18	93,93,93,93	0
5	CL	C	804	1/1	0.96	0.39	94,94,94,94	0
3	1XK	B	802	35/35	0.97	0.19	45,58,74,81	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.

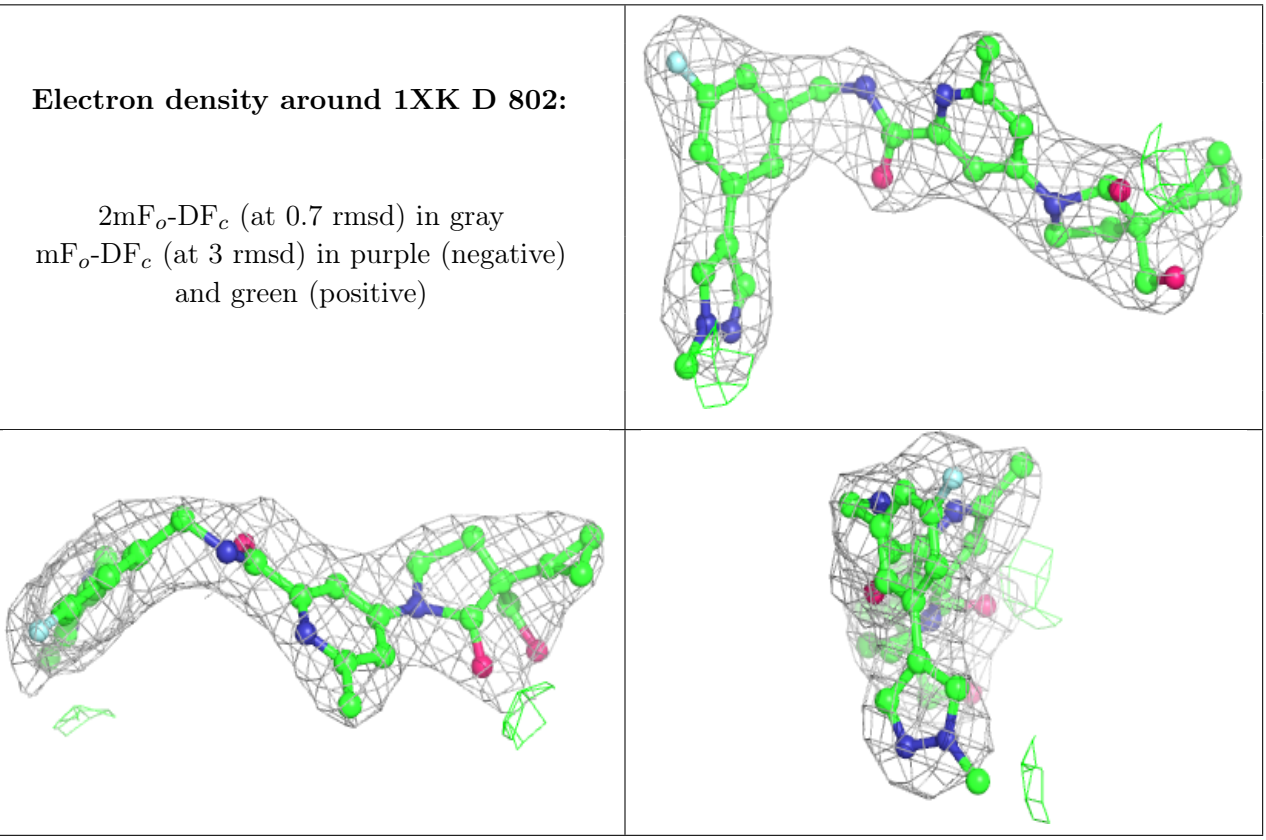
Electron density around 1XK C 802:

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



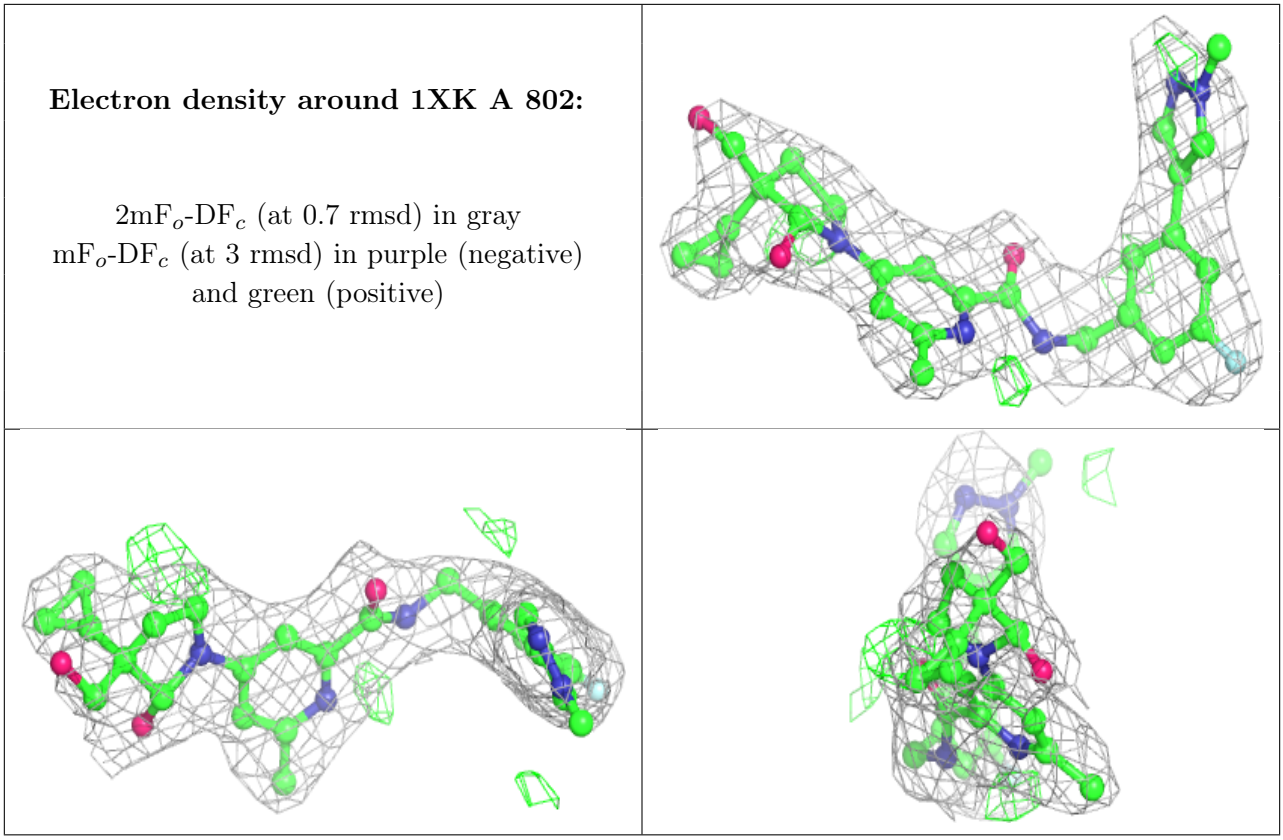
Electron density around 1XK D 802:

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



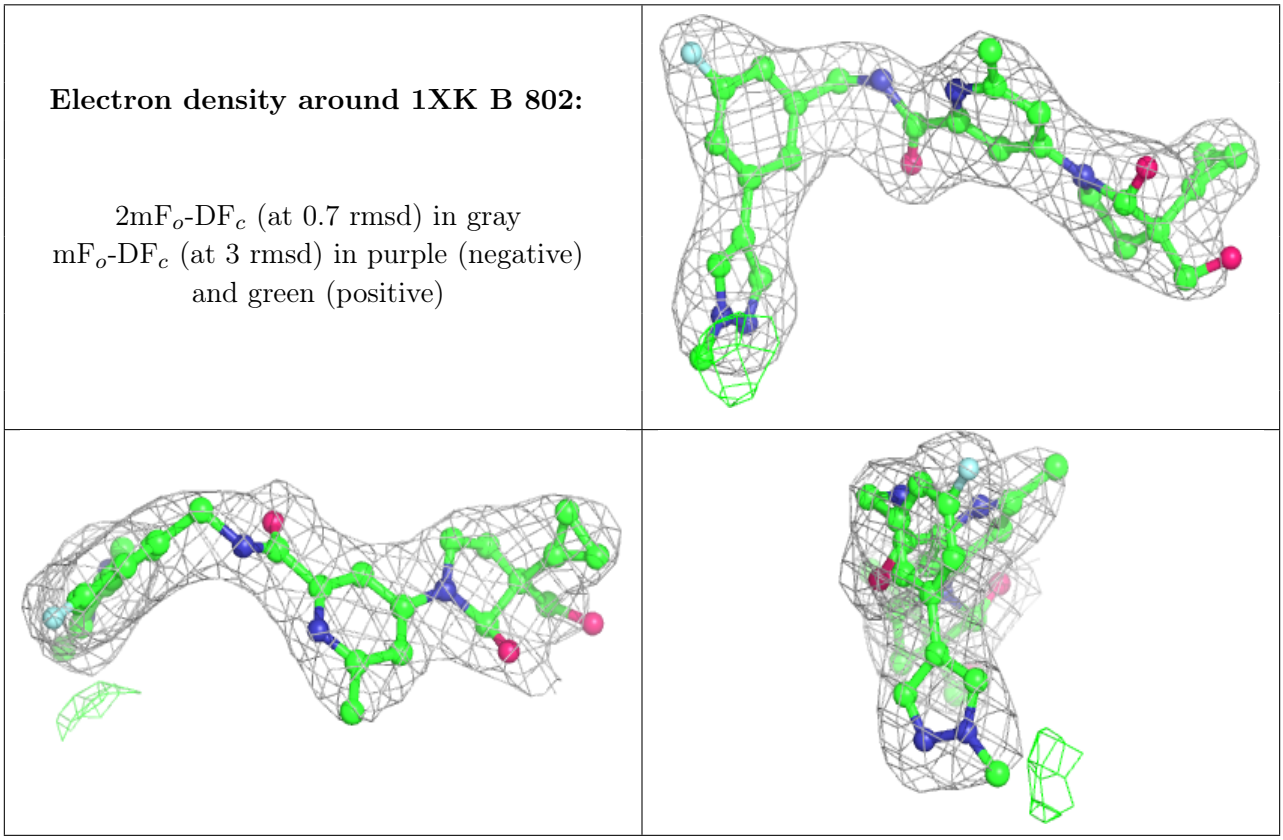
Electron density around 1XK A 802:

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



Electron density around 1XK B 802:

$2mF_o$-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.