



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:15 PM UTC

PDB ID : 7F97 / pdb_00007f97
Title : Plasmodium falciparum Prolyl-tRNA Synthetase (PfPRS) in Complex with L-proline and compound L97
Authors : Mishra, S.; Malhotra, N.; Yogavel, M.; 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

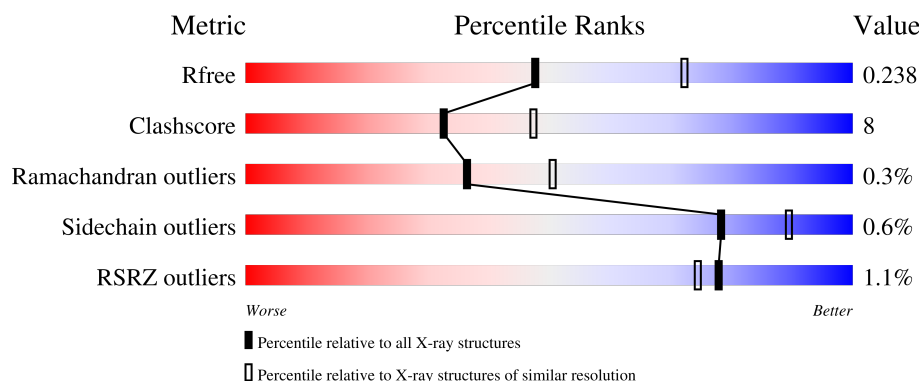
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	497	% 82% 15% .
1	B	497	82% 14% .
1	C	497	% 75% 21% .
1	D	497	% 74% 21% ..

2 Entry composition

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:

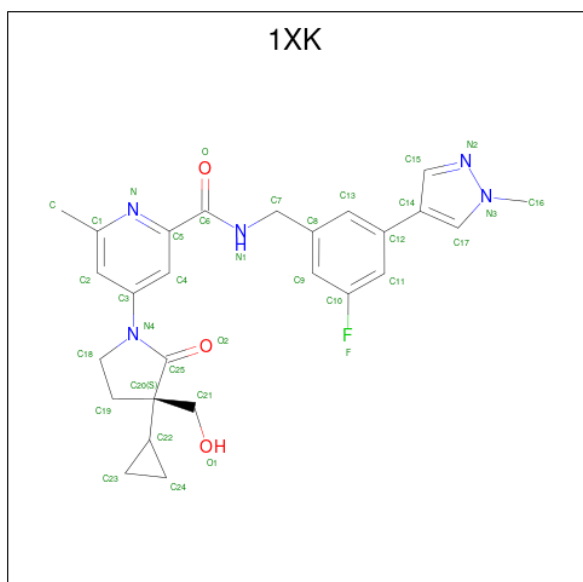
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP Q8I5R7
A	251	ALA	-	expression tag	UNP Q8I5R7
A	252	MET	-	expression tag	UNP Q8I5R7
A	253	ALA	-	expression tag	UNP Q8I5R7
B	250	GLY	-	expression tag	UNP Q8I5R7
B	251	ALA	-	expression tag	UNP Q8I5R7
B	252	MET	-	expression tag	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 (CCD ID: PRO) (formula: C₅H₉NO₂).



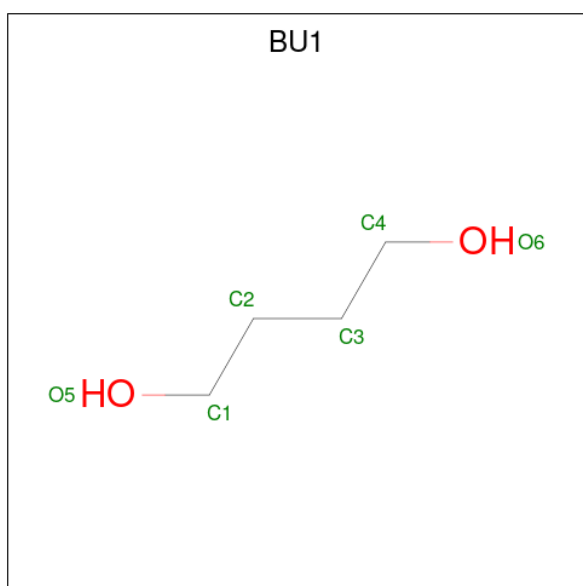
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		
2	C	1	Total	C	N	O	0	0
			8	5	1	2		
2	D	1	Total	C	N	O	0	0
			8	5	1	2		

- 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 (CCD ID: 1XK) (formula: C₂₆H₂₈FN₅O₃) (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 (CCD ID: BU1) (formula: $C_4H_{10}O_2$).

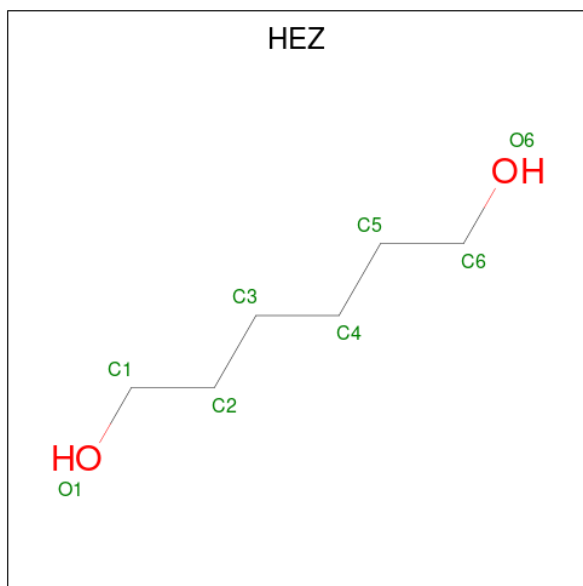


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

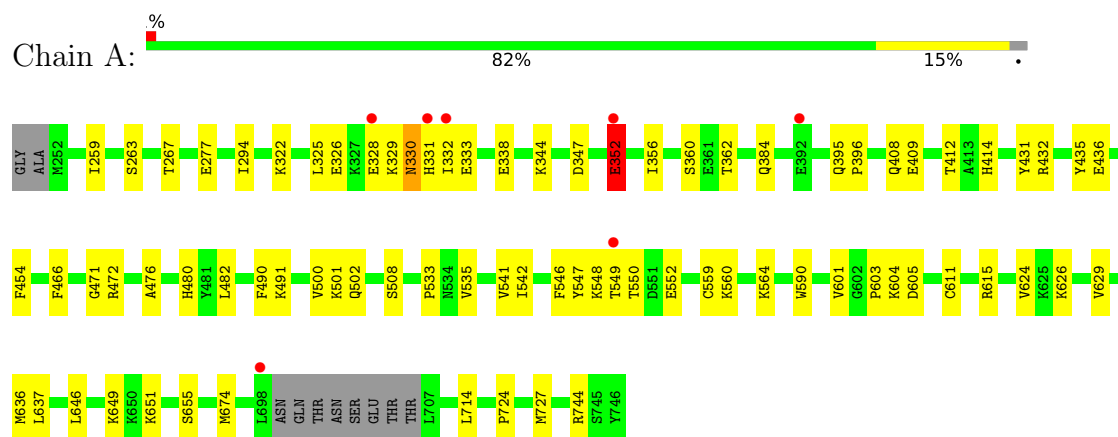
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	16	Total	O	0	0
			16	16		
7	C	14	Total	O	0	0
			14	14		
7	D	9	Total	O	0	0
			9	9		

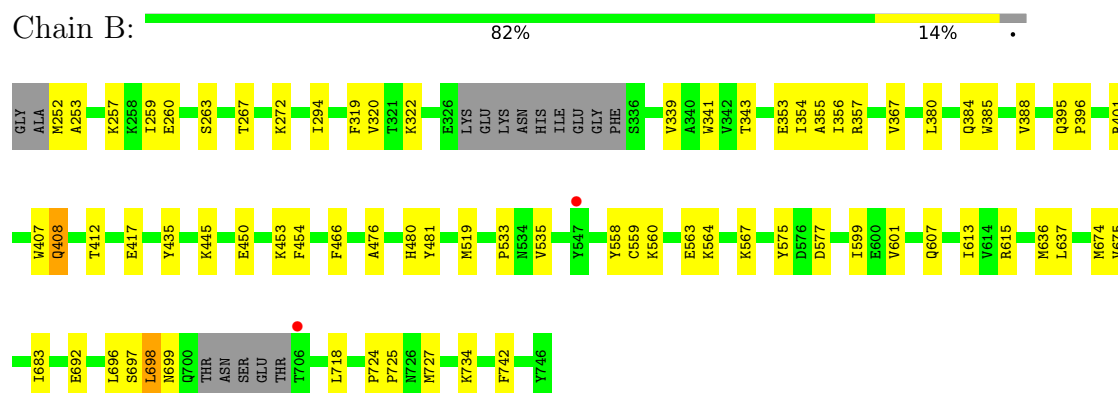
3 Residue-property plots [i](#)

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.

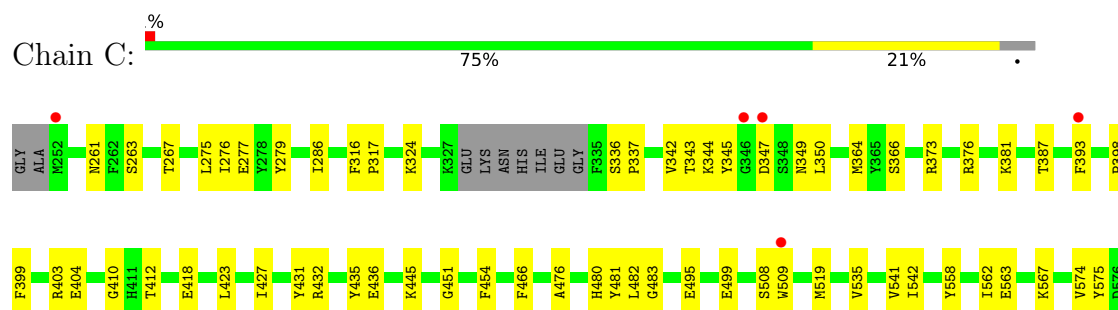
• Molecule 1: Proline-tRNA ligase

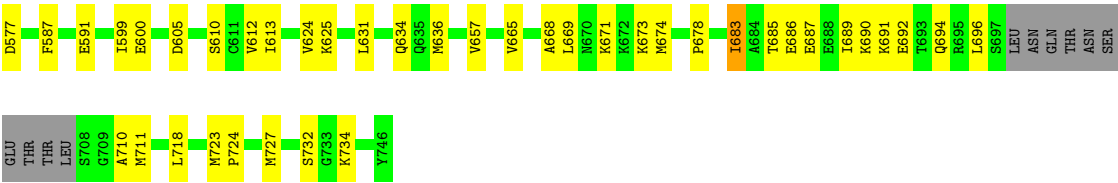


• Molecule 1: Proline-tRNA ligase

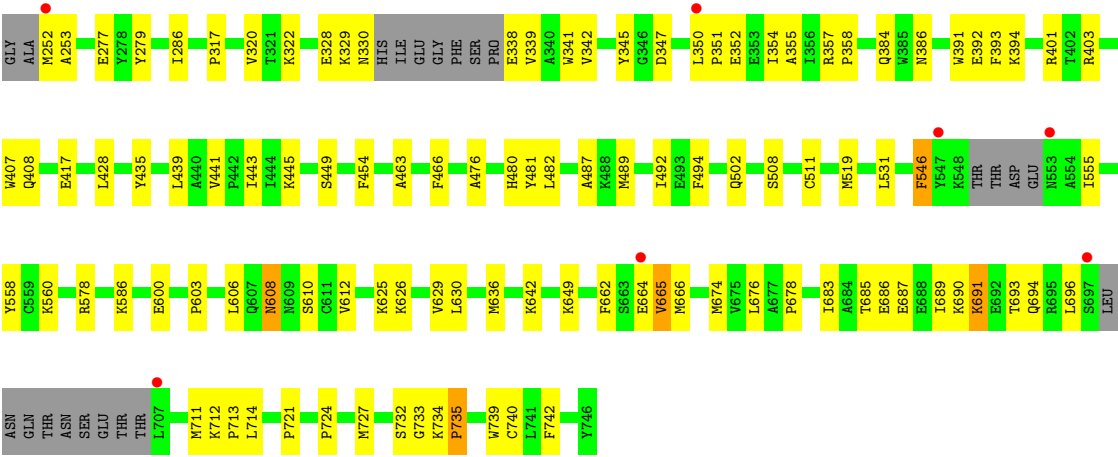


• Molecule 1: Proline-tRNA ligase





• Molecule 1: Proline–tRNA ligase



4 Data and refinement statistics

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 41.90 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.90-2.39) 99.9 (41.90-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15rc2_3428	Depositor
R, R_{free}	0.175 , 0.232 0.185 , 0.238	Depositor DCC
R_{free} test set	4305 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)	0.33 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: BU1, HEZ, CL, 1XK

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	0.33	0/4100	0.54	0/5544
1	B	0.34	1/4044 (0.0%)	0.53	0/5470
1	C	0.30	1/4025 (0.0%)	0.52	0/5442
1	D	0.38	0/4001	0.58	2/5405 (0.0%)
All	All	0.34	2/16170 (0.0%)	0.55	2/21861 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLN	C-O	-7.67	1.14	1.23
1	C	376	ARG	C-O	-5.32	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	665	VAL	N-CA-C	7.76	117.87	110.42
1	D	546	PHE	N-CA-CB	5.15	119.01	110.47

There are no chirality outliers.

There are no planarity outliers.

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	3998	0	3989	58	0
1	B	3945	0	3935	50	0
1	C	3925	0	3914	79	0
1	D	3904	0	3904	78	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
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	251	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 8.

All (251) 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:CD	1:A:362:THR:HG22	2.09	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: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:A:615:ARG:HD2	1:A:636:MET:HE2	1.75	0.69
1:A:466:PHE:CD1	1:A:674:MET:HE3	2.27	0.69
1:B:357:ARG:HG3	1:B:388:VAL:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:MET:HE2	1:C:727:MET:HG3	1.75	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:B:615:ARG:HG2	1:B:636:MET:HE3	1.75	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:D:328:GLU:HG3	1:D:489:MET:HE1	1.78	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:C:678:PRO:HB3	1:C:723:MET:HE1	1.79	0.65
1:A:332:ILE:HG13	1:A:333:GLU:OE2	1.96	0.64
1:D:252:MET:HE3	1:D:253:ALA:H	1.63	0.64
1:D:610:SER:HA	1:D:625:LYS:HA	1.80	0.62
1:D:487:ALA:HA	1:D:492:ILE:HD12	1.81	0.61
1:C:466:PHE:CD1	1:C:674:MET:HE3	2.36	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:A:328:GLU:CD	1:A:362:THR:CG2	2.74	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:294:ILE:HD13	1:B:519:MET:HE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:662:PHE:C	1:D:662:PHE:CD2	2.84	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:C:495:GLU:HG2	1:C:499:GLU:HA	1.90	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
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: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:698:LEU:C	1:B:699:ASN:HD22	2.19	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:A:724:PRO:HD2	1:A:727:MET:HE2	1.93	0.50
1:A:356:ILE:HD11	1:B:356:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:519:MET:HE1	1:D:531:LEU:HD23	1.95	0.49
1:C:454:PHE:HB2	1:C:480:HIS:CE1	2.47	0.49
1:A:547:TYR:C	1:A:549:THR:H	2.20	0.49
1:C:678:PRO:HG2	1:C:727:MET:HE2	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
1:D:678:PRO:HG3	1:D:727:MET:HE2	1.95	0.48
1:C:343:THR:C	1:C:350:LEU:HD12	2.38	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:A:344:LYS:HZ2	1:A:347:ASP:HA	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:C:519:MET:HE2	1:C:535:VAL:HG21	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:466:PHE:CG	1:B:674:MET:HE2	2.51	0.45
1:D:626:LYS:O	1:D:629:VAL:HG12	2.16	0.45
1:A:412:THR:OG1	1:A:414:HIS:NE2	2.49	0.45
1:C:381:LYS:HG2	1:C:412:THR:HG22	1.97	0.45
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:A:674:MET:HE2	1:A:714:LEU:CD1	2.47	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:330:ASN:HA	1:A:333:GLU:CD	2.42	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: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:B:450:GLU:OE2	1:B:453:LYS:NZ	2.51	0.44
1:B:724:PRO:HG2	1:B:727:MET:HE2	1.99	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:D:608:ASN:N	1:D:608:ASN:ND2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:TYR:HH	1:C:509:TRP:HD1	1.67	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: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:C:418:GLU:CD	1:C:418:GLU:H	2.26	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:600:GLU:HB2	1:D:612:VAL:CG1	2.49	0.43
1:D:666:MET:HE3	1:D:666:MET:CA	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: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
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:C:636:MET:HE3	1:C:636:MET:HB2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:322:LYS:HD3	1:B:322:LYS:C	2.46	0.41
1:C:431:TYR:HH	1:C:509:TRP:CD1	2.38	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:649:LYS:HZ3	1:A:649:LYS:HG3	1.73	0.41
1:D:694:GLN:C	1:D:696:LEU:H	2.28	0.41
1:A:360:SER:HB2	1:A:409:GLU:OE1	2.20	0.41
1:B:407:TRP:CD1	1:B:407:TRP:C	2.99	0.41
1:C:398:PRO:O	1:C:399:PHE:HB2	2.21	0.41
1:D:687:GLU:H	1:D:687:GLU:CD	2.28	0.41
1:B:519:MET:HE2	1:B:535:VAL:HG21	2.03	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:C:316:PHE:CE1	1:C:364:MET:HE3	2.56	0.41
1:D:555:ILE:HD11	1:D:603:PRO:HA	2.02	0.41
1:D:636:MET:HE3	1:D:636:MET:HB2	2.01	0.41
1:D:685:THR:O	1:D:689:ILE:HG13	2.21	0.41
1:B:252:MET:HE3	1:B:253:ALA:H	1.86	0.41
1:D:350:LEU:HG	1:D:351:PRO:HD2	2.02	0.41
1:D:578:ARG:O	1:D:586:LYS:NZ	2.50	0.41
1:D:606:LEU:O	1:D:606:LEU:HD12	2.21	0.41
1:A:328:GLU:OE1	1:A:362:THR:HG22	2.19	0.40
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
1:D:407:TRP:CD1	1:D:407:TRP:C	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	30	43
1	B	475/497 (96%)	459 (97%)	14 (3%)	2 (0%)	30	43
1	C	472/497 (95%)	455 (96%)	17 (4%)	0	100	100
1	D	467/497 (94%)	445 (95%)	21 (4%)	1 (0%)	43	58
All	All	1897/1988 (95%)	1828 (96%)	64 (3%)	5 (0%)	36	50

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

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%)	439 (99%)	3 (1%)	76	88
1	B	437/450 (97%)	437 (100%)	0	100	100
1	C	434/450 (96%)	432 (100%)	2 (0%)	81	91
1	D	431/450 (96%)	426 (99%)	5 (1%)	63	81
All	All	1744/1800 (97%)	1734 (99%)	10 (1%)	78	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	ASN
1	A	338	GLU
1	A	352	GLU
1	C	347	ASP
1	C	683	ILE
1	D	546	PHE
1	D	608	ASN
1	D	664	GLU
1	D	665	VAL
1	D	691	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	395	GLN
1	A	623	ASN
1	A	667	ASN
1	A	694	GLN
1	B	383	ASN
1	B	470	ASN
1	B	570	GLN
1	B	694	GLN
1	B	699	ASN
1	C	349	ASN
1	C	667	ASN
1	D	330	ASN
1	D	383	ASN
1	D	395	GLN
1	D	408	GLN
1	D	458	ASN
1	D	470	ASN
1	D	589	HIS
1	D	608	ASN
1	D	634	GLN
1	D	667	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	A	802	-	37,39,39	4.92	11 (29%)	46,58,58	3.62	15 (32%)
3	1XK	C	802	-	37,39,39	4.84	12 (32%)	46,58,58	4.18	17 (36%)
4	BU1	A	803	-	5,5,5	0.34	0	4,4,4	0.55	0
2	PRO	C	801	-	8,8,8	0.92	1 (12%)	10,10,10	1.34	2 (20%)
3	1XK	B	802	-	37,39,39	4.93	11 (29%)	46,58,58	4.08	17 (36%)
6	HEZ	C	803	-	7,7,7	0.34	0	6,6,6	0.66	0
2	PRO	A	801	-	8,8,8	0.99	1 (12%)	10,10,10	1.32	2 (20%)
3	1XK	D	802	-	37,39,39	4.97	11 (29%)	46,58,58	3.91	14 (30%)
2	PRO	B	801	-	8,8,8	0.88	1 (12%)	10,10,10	1.53	2 (20%)
2	PRO	D	801	-	8,8,8	0.83	1 (12%)	10,10,10	1.44	2 (20%)

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	A	802	-	-	0/24/44/44	0/5/5/5
3	1XK	C	802	-	-	1/24/44/44	0/5/5/5
4	BU1	A	803	-	-	0/3/3/3	-

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	1XK	C25-N4	21.01	1.59	1.36
3	D	802	1XK	C25-N4	20.80	1.59	1.36
3	B	802	1XK	C25-N4	20.65	1.59	1.36
3	C	802	1XK	C25-N4	20.32	1.58	1.36
3	B	802	1XK	C19-C20	-13.61	1.33	1.54
3	D	802	1XK	C19-C20	-13.56	1.33	1.54
3	A	802	1XK	C19-C20	-13.05	1.34	1.54
3	C	802	1XK	C19-C20	-13.01	1.34	1.54
3	C	802	1XK	C18-N4	-9.04	1.35	1.47
3	D	802	1XK	C18-N4	-8.96	1.35	1.47
3	A	802	1XK	C18-N4	-8.89	1.35	1.47
3	B	802	1XK	C18-N4	-8.82	1.35	1.47
3	A	802	1XK	C19-C18	8.12	1.67	1.52
3	C	802	1XK	C19-C18	7.51	1.66	1.52
3	D	802	1XK	C19-C18	7.46	1.65	1.52
3	B	802	1XK	C19-C18	7.40	1.65	1.52
3	D	802	1XK	C6-N1	6.24	1.47	1.33
3	B	802	1XK	C6-N1	5.95	1.46	1.33
3	A	802	1XK	C6-N1	5.74	1.46	1.33
3	C	802	1XK	C6-N1	5.69	1.46	1.33
3	D	802	1XK	C23-C22	-5.38	1.38	1.50
3	D	802	1XK	C24-C22	-5.28	1.39	1.50
3	C	802	1XK	C23-C22	-5.28	1.39	1.50
3	C	802	1XK	C24-C22	-5.19	1.39	1.50
3	B	802	1XK	C24-C22	-5.08	1.39	1.50
3	A	802	1XK	C23-C22	-5.06	1.39	1.50
3	A	802	1XK	C24-C22	-5.03	1.39	1.50
3	B	802	1XK	C23-C22	-4.94	1.39	1.50
3	D	802	1XK	O2-C25	3.58	1.27	1.22
3	B	802	1XK	C12-C14	3.53	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	1XK	O2-C25	3.38	1.27	1.22
3	D	802	1XK	C12-C14	3.33	1.54	1.48
3	C	802	1XK	C12-C14	3.21	1.54	1.48
3	A	802	1XK	C12-C14	3.20	1.54	1.48
3	A	802	1XK	O2-C25	3.14	1.27	1.22
3	C	802	1XK	O2-C25	2.67	1.26	1.22
3	B	802	1XK	C24-C23	-2.59	1.39	1.48
3	C	802	1XK	C24-C23	-2.54	1.39	1.48
3	D	802	1XK	C24-C23	-2.54	1.39	1.48
3	A	802	1XK	C24-C23	-2.52	1.39	1.48
3	B	802	1XK	C17-C14	2.41	1.42	1.38
3	D	802	1XK	C17-C14	2.38	1.42	1.38
3	C	802	1XK	C17-C14	2.32	1.42	1.38
2	A	801	PRO	OXT-C	-2.30	1.23	1.30
2	C	801	PRO	OXT-C	-2.23	1.23	1.30
3	C	802	1XK	C3-N4	2.17	1.47	1.43
3	A	802	1XK	C17-C14	2.09	1.42	1.38
2	B	801	PRO	OXT-C	-2.04	1.24	1.30
2	D	801	PRO	OXT-C	-2.00	1.24	1.30

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	1XK	O2-C25-N4	-17.01	109.51	125.85
3	C	802	1XK	O2-C25-N4	-15.39	111.06	125.85
3	D	802	1XK	O2-C25-N4	-14.32	112.09	125.85
3	A	802	1XK	O2-C25-N4	-13.74	112.64	125.85
3	C	802	1XK	C18-N4-C25	-13.19	100.56	112.23
3	C	802	1XK	C15-N2-N3	11.66	110.82	104.41
3	D	802	1XK	C15-N2-N3	11.27	110.60	104.41
3	B	802	1XK	C15-N2-N3	11.26	110.59	104.41
3	B	802	1XK	C20-C25-N4	-11.06	102.26	109.13
3	A	802	1XK	C15-N2-N3	10.43	110.14	104.41
3	A	802	1XK	C20-C25-N4	-9.48	103.24	109.13
3	D	802	1XK	C20-C25-N4	-9.19	103.42	109.13
3	D	802	1XK	C3-N4-C25	-8.92	119.72	126.39
3	D	802	1XK	C18-N4-C25	-7.48	105.60	112.23
3	C	802	1XK	C20-C25-N4	-7.45	104.50	109.13
3	A	802	1XK	C18-N4-C25	-7.30	105.77	112.23
3	B	802	1XK	C18-N4-C25	-7.13	105.92	112.23
3	D	802	1XK	C16-N3-N2	6.85	125.52	120.03
3	C	802	1XK	C16-N3-N2	6.78	125.47	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	1XK	C16-N3-N2	6.37	125.14	120.03
3	B	802	1XK	C16-N3-N2	6.23	125.03	120.03
3	C	802	1XK	C3-N4-C25	-5.23	122.48	126.39
3	D	802	1XK	C5-N-C1	4.46	121.83	118.24
3	A	802	1XK	C3-N4-C25	-4.40	123.10	126.39
3	A	802	1XK	C18-N4-C3	4.07	126.32	120.72
3	C	802	1XK	C17-N3-N2	-4.06	109.78	112.08
3	B	802	1XK	C2-C3-N4	4.03	125.32	119.84
3	C	802	1XK	C5-N-C1	3.98	121.44	118.24
3	D	802	1XK	C17-N3-N2	-3.83	109.91	112.08
3	B	802	1XK	C17-N3-N2	-3.68	109.99	112.08
3	A	802	1XK	C16-N3-C17	-3.59	124.33	127.94
3	B	802	1XK	C3-N4-C25	3.55	129.04	126.39
3	B	802	1XK	C4-C3-N4	-3.37	115.25	119.84
3	D	802	1XK	C16-N3-C17	-3.36	124.57	127.94
3	B	802	1XK	C8-C7-N1	-3.24	106.23	113.07
3	C	802	1XK	C16-N3-C17	-3.18	124.75	127.94
3	D	802	1XK	C5-C6-N1	3.13	119.91	115.56
3	B	802	1XK	C5-N-C1	3.12	120.75	118.24
3	D	802	1XK	C19-C18-N4	3.10	107.03	102.95
3	C	802	1XK	C5-C6-N1	3.10	119.87	115.56
3	C	802	1XK	C18-N4-C3	3.05	124.91	120.72
3	C	802	1XK	C9-C10-C11	-3.04	119.80	123.50
3	B	802	1XK	C6-C5-N	2.99	122.15	117.43
3	B	802	1XK	C16-N3-C17	-2.95	124.98	127.94
2	B	801	PRO	OXT-C-O	-2.93	117.44	124.08
3	A	802	1XK	C-C1-N	2.87	120.89	116.56
3	C	802	1XK	F-C10-C11	2.80	122.25	118.28
3	A	802	1XK	C17-N3-N2	-2.74	110.53	112.08
2	D	801	PRO	OXT-C-O	-2.73	117.88	124.08
3	B	802	1XK	C9-C10-C11	-2.64	120.30	123.50
2	C	801	PRO	OXT-C-O	-2.59	118.20	124.08
3	C	802	1XK	C8-C7-N1	-2.58	107.64	113.07
3	B	802	1XK	C18-N4-C3	2.58	124.27	120.72
2	B	801	PRO	OXT-C-CA	2.51	122.00	113.51
3	D	802	1XK	C6-C5-N	2.50	121.39	117.43
3	A	802	1XK	C19-C18-N4	2.46	106.19	102.95
3	D	802	1XK	C-C1-N	2.46	120.27	116.56
3	A	802	1XK	C6-C5-N	2.44	121.29	117.43
2	A	801	PRO	OXT-C-O	-2.43	118.56	124.08
3	A	802	1XK	C-C1-C2	-2.41	118.24	121.80
2	D	801	PRO	OXT-C-CA	2.39	121.60	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	1XK	C-C1-N	2.37	120.14	116.56
3	A	802	1XK	C9-C10-C11	-2.37	120.62	123.50
3	B	802	1XK	C19-C18-N4	2.25	105.91	102.95
3	C	802	1XK	C6-C5-N	2.20	120.90	117.43
3	B	802	1XK	O1-C21-C20	-2.15	106.26	112.24
3	C	802	1XK	C14-C15-N2	-2.11	106.89	111.87
2	A	801	PRO	OXT-C-CA	2.11	120.64	113.51
3	D	802	1XK	C9-C10-C11	-2.10	120.95	123.50
3	A	802	1XK	C14-C15-N2	-2.03	107.09	111.87
2	C	801	PRO	OXT-C-CA	2.03	120.36	113.51

There are no chirality outliers.

All (12) 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
2	B	801	PRO	O-C-CA-CB
2	B	801	PRO	OXT-C-CA-CB
3	B	802	1XK	C19-C20-C22-C23
3	B	802	1XK	C19-C20-C21-O1

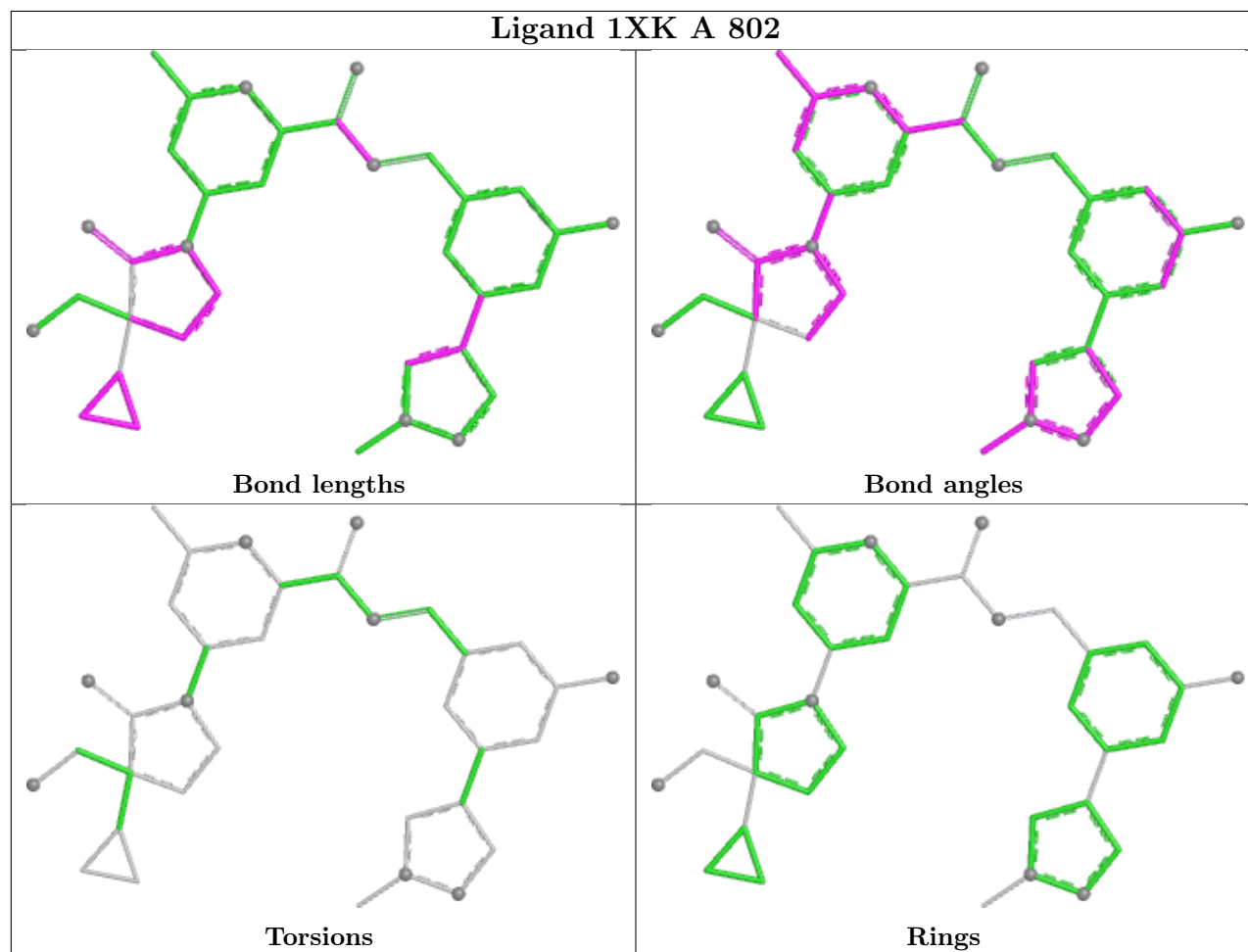
There are no ring outliers.

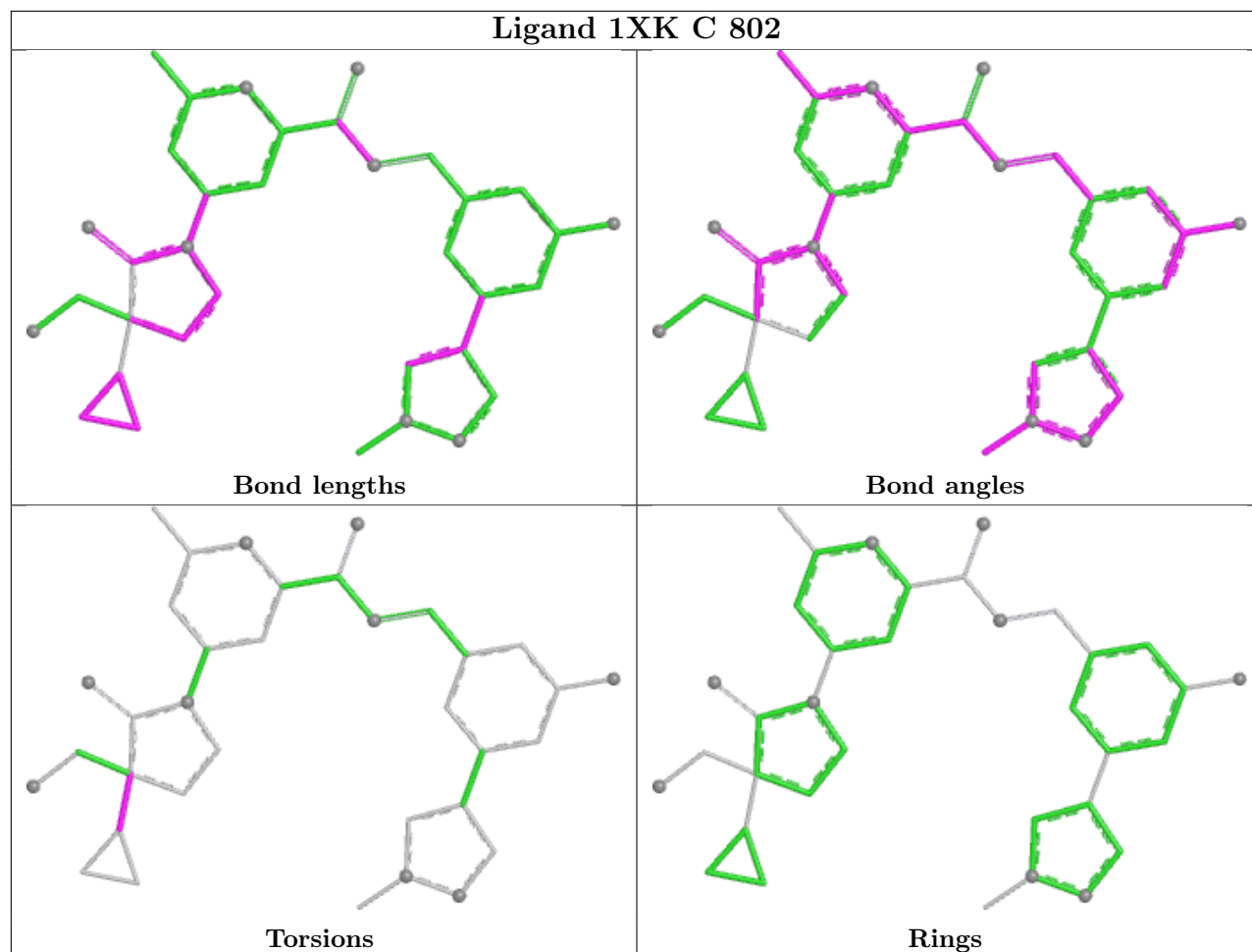
2 monomers are involved in 3 short contacts:

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

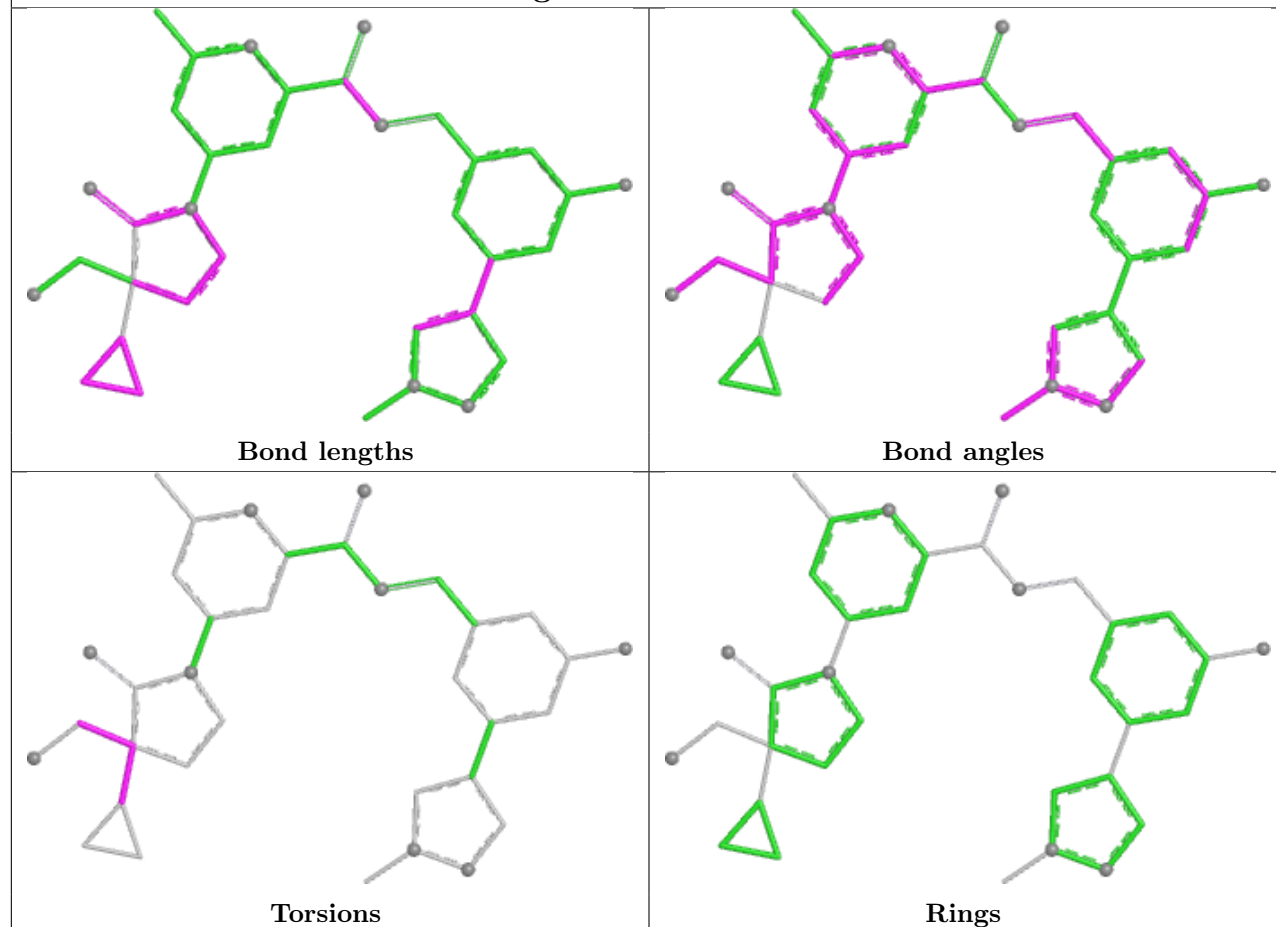
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

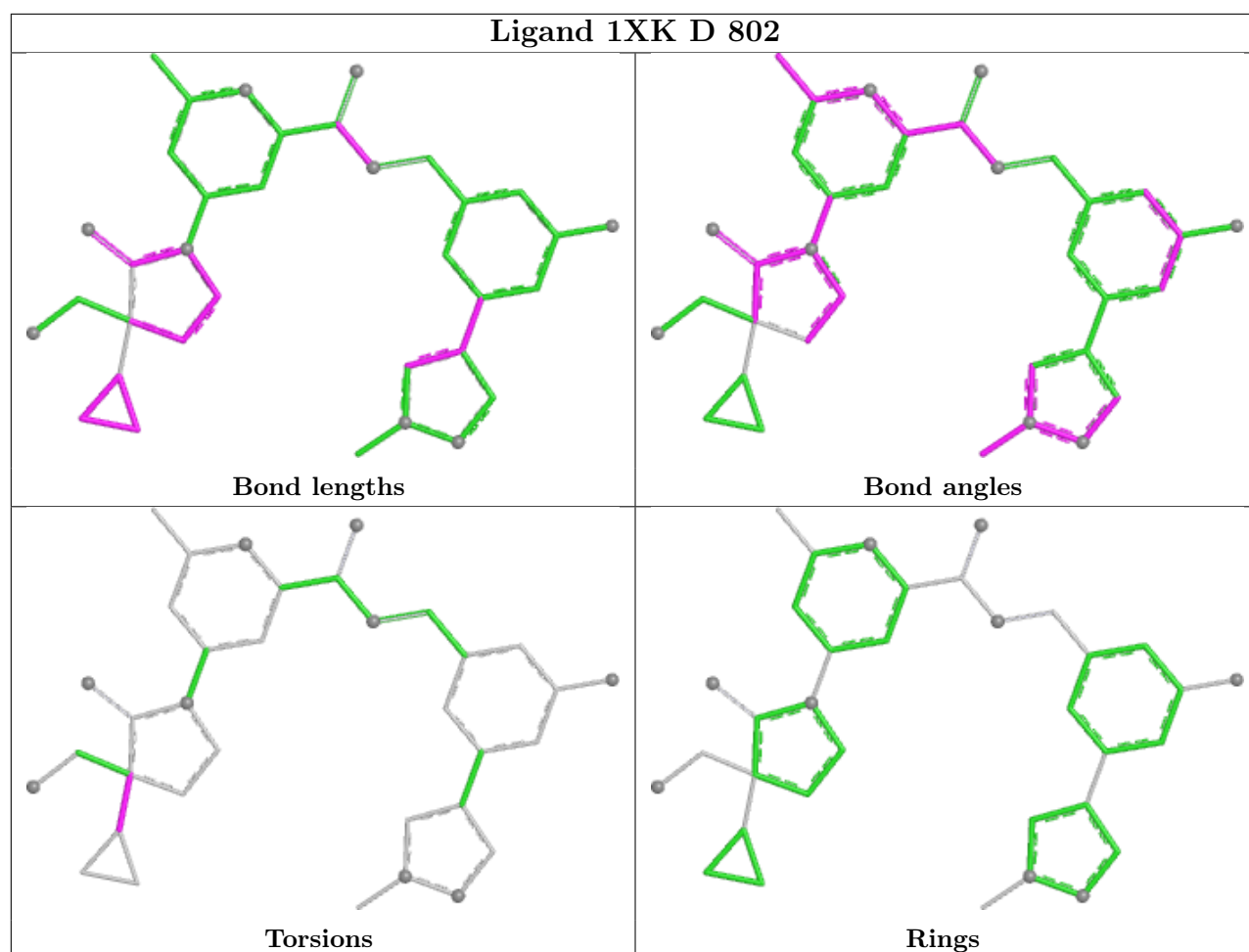
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand 1XK B 802





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	487/497 (97%)	-0.02	7 (1%) 73 69	44, 66, 101, 134	2 (0%)
1	B	481/497 (96%)	-0.06	2 (0%) 88 86	43, 68, 101, 125	2 (0%)
1	C	478/497 (96%)	0.08	5 (1%) 79 76	46, 76, 114, 137	3 (0%)
1	D	475/497 (95%)	0.12	7 (1%) 72 68	47, 75, 121, 143	5 (1%)
All	All	1921/1988 (96%)	0.03	21 (1%) 78 74	43, 71, 114, 143	12 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLU	7.7
1	C	509	TRP	3.6
1	A	331	HIS	3.4
1	D	664	GLU	3.2
1	D	547	TYR	3.0
1	D	697	SER	2.8
1	C	347	ASP	2.6
1	A	332	ILE	2.6
1	C	252	MET	2.4
1	D	707	LEU	2.4
1	B	706	THR	2.3
1	D	252	MET	2.3
1	D	553	ASN	2.2
1	D	350	LEU	2.2
1	A	392	GLU	2.2
1	A	698	LEU	2.1
1	C	393	PHE	2.1
1	A	352	GLU	2.1
1	C	346	GLY	2.1
1	A	549	THR	2.1
1	B	547	TYR	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

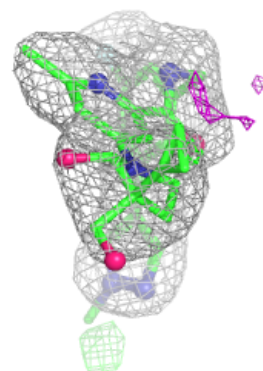
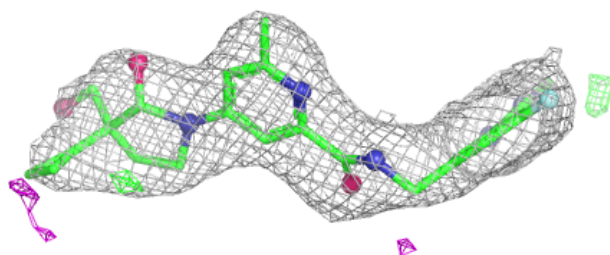
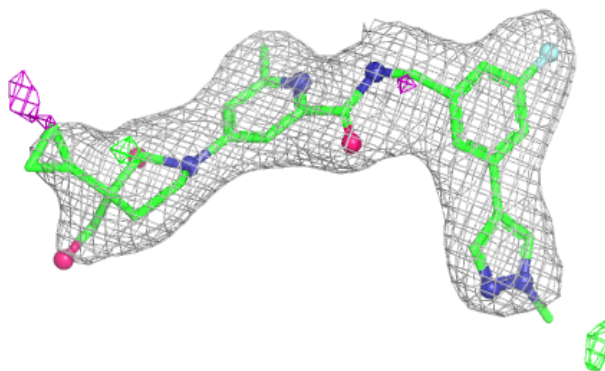
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BU1	A	803	6/6	0.80	0.14	81,85,86,90	0
6	HEZ	C	803	8/8	0.81	0.17	88,92,101,101	0
5	CL	B	803[A]	1/1	0.87	0.24	76,76,76,76	1
5	CL	B	803[B]	1/1	0.87	0.24	57,57,57,57	1
5	CL	B	804	1/1	0.87	0.17	96,96,96,96	0
5	CL	D	803	1/1	0.87	0.16	97,97,97,97	0
5	CL	A	804	1/1	0.87	0.13	101,101,101,101	0
5	CL	C	805	1/1	0.90	0.11	104,104,104,104	0
5	CL	A	805	1/1	0.91	0.12	98,98,98,98	0
5	CL	A	806	1/1	0.91	0.09	108,108,108,108	0
5	CL	C	804	1/1	0.93	0.13	94,94,94,94	0
5	CL	D	804	1/1	0.93	0.13	93,93,93,93	0
3	1XK	C	802	35/35	0.93	0.11	60,68,83,83	0
5	CL	B	805	1/1	0.94	0.08	102,102,102,102	0
3	1XK	D	802	35/35	0.94	0.09	55,73,86,89	0
3	1XK	A	802	35/35	0.94	0.09	46,57,79,87	0
2	PRO	A	801	8/8	0.95	0.08	46,57,64,64	0
2	PRO	C	801	8/8	0.95	0.09	49,60,64,65	8
2	PRO	D	801	8/8	0.96	0.09	60,73,83,84	0
2	PRO	B	801	8/8	0.96	0.08	60,73,77,79	0
3	1XK	B	802	35/35	0.96	0.08	45,58,74,81	0

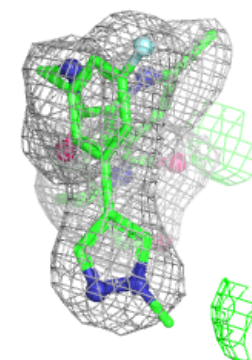
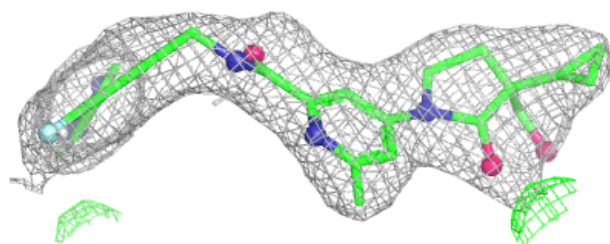
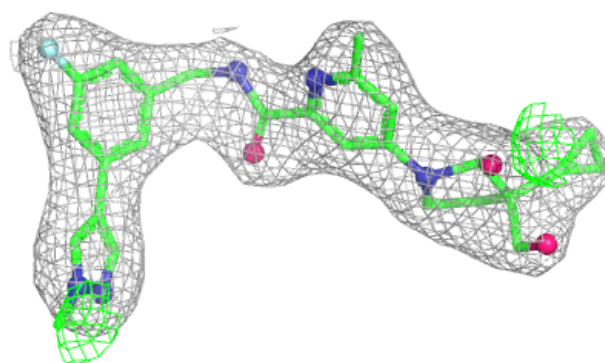
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

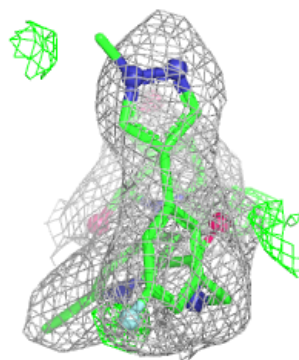
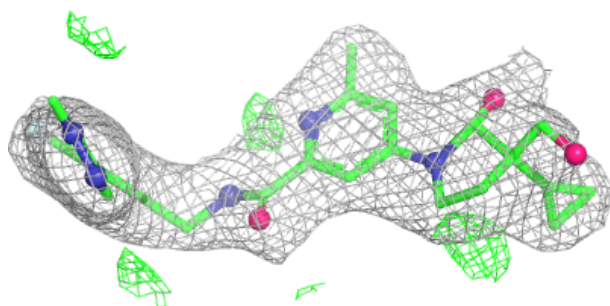
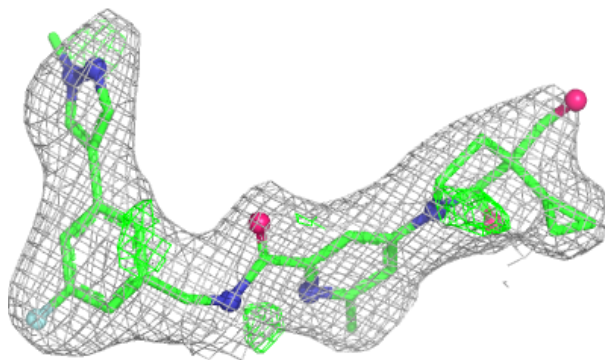
**Electron density around 1XK D 802:**

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

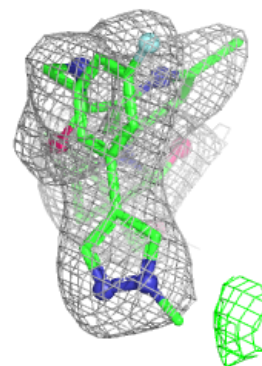
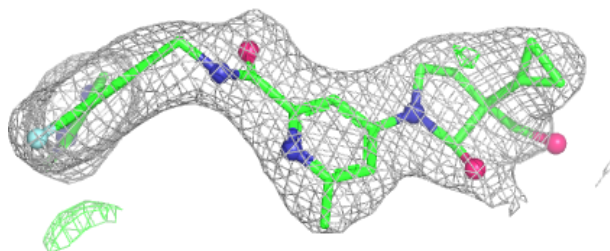
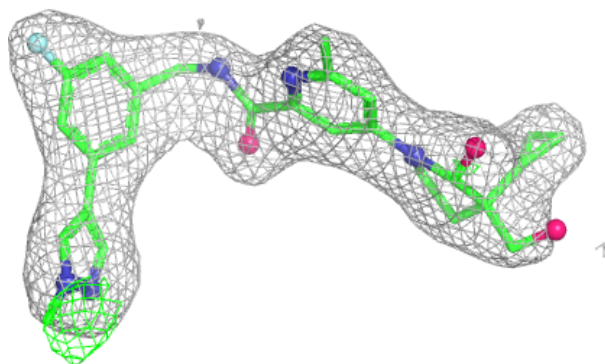


Electron density around 1XK A 802:

$2mF_o-DF_c$ (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.