



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:36 AM UTC

PDB ID : 4BGE / pdb_00004bge
Title : Crystal structure of InhA(S94A) mutant in complex with pyridomycin
Authors : Pojer, F.; Hartkoorn, R.C.; Cole, S.T.
Deposited on : 2013-03-26
Resolution : 2.25 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:

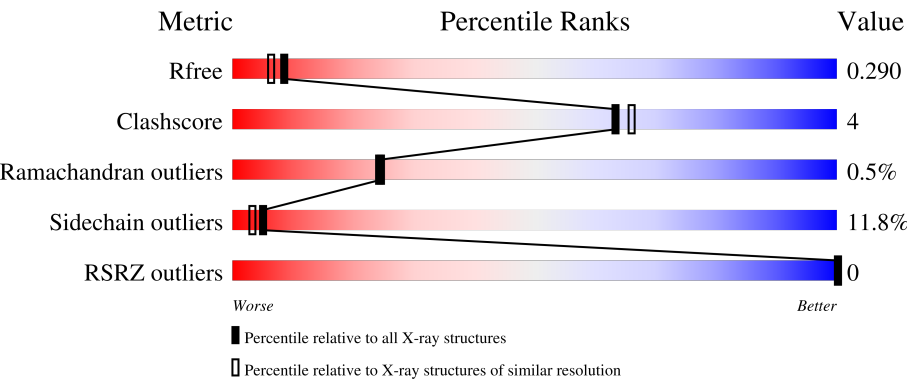
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	269	 80% 16% . .
1	B	269	 82% 14% . .
1	C	269	 80% 13% . 6%
1	D	269	 78% 13% . 6%
1	E	269	 77% 14% . 7%

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Mol	Chain	Length	Quality of chain
1	F	269	78% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12612 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.

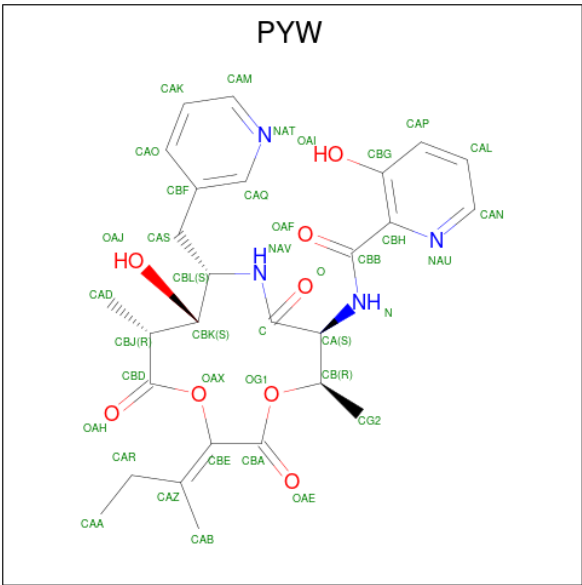
- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			
1	B	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			
1	C	254	Total	C	N	O	S	0	0	0
			1909	1210	334	356	9			
1	D	252	Total	C	N	O	S	0	0	0
			1889	1199	329	352	9			
1	E	251	Total	C	N	O	S	0	0	0
			1889	1199	331	350	9			
1	F	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	SER	engineered mutation	UNP P9WGR1
B	94	ALA	SER	engineered mutation	UNP P9WGR1
C	94	ALA	SER	engineered mutation	UNP P9WGR1
D	94	ALA	SER	engineered mutation	UNP P9WGR1
E	94	ALA	SER	engineered mutation	UNP P9WGR1
F	94	ALA	SER	engineered mutation	UNP P9WGR1

- Molecule 2 is Pyridomycin (CCD ID: PYW) (formula: C₂₇H₃₂N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	4	8		
2	B	1	Total	C	N	O	0	0
			39	27	4	8		
2	C	1	Total	C	N	O	0	0
			39	27	4	8		
2	D	1	Total	C	N	O	0	0
			39	27	4	8		
2	E	1	Total	C	N	O	0	0
			39	27	4	8		
2	F	1	Total	C	N	O	0	0
			39	27	4	8		

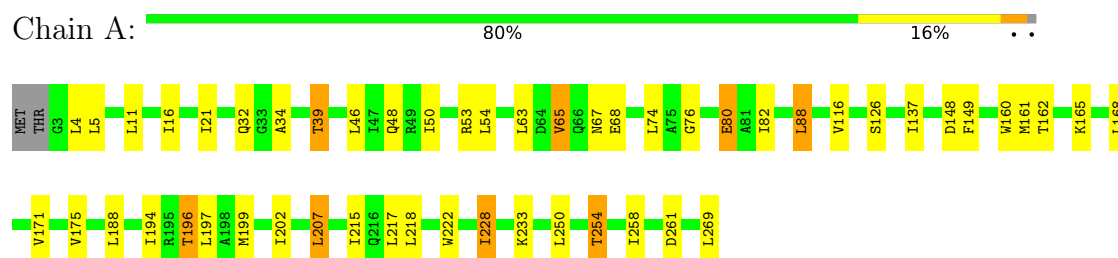
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total	O	0	0
			154	154		
3	B	114	Total	O	0	0
			114	114		
3	C	76	Total	O	0	0
			76	76		
3	D	109	Total	O	0	0
			109	109		
3	E	86	Total	O	0	0
			86	86		
3	F	188	Total	O	0	0
			188	188		

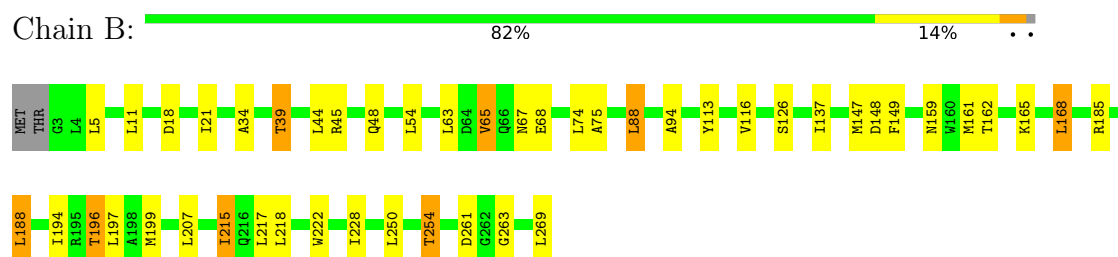
3 Residue-property plots [i](#)

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.

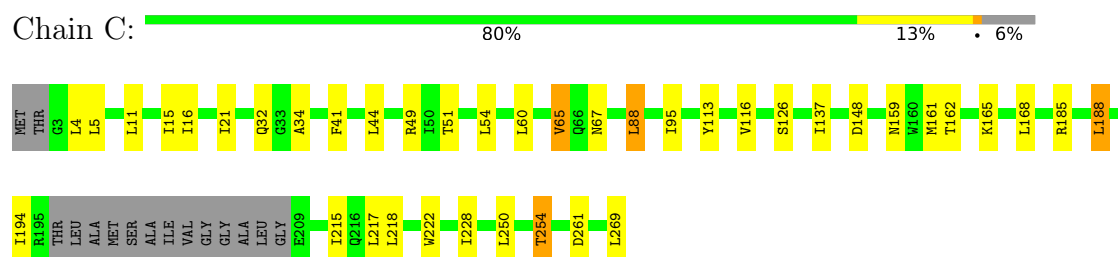
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



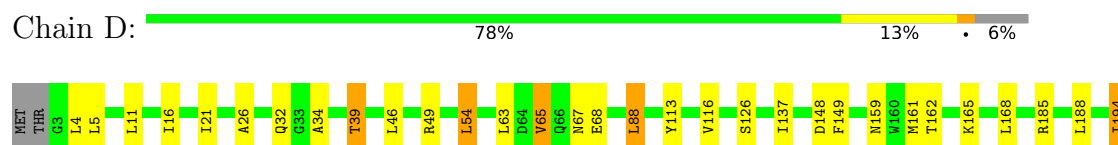
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



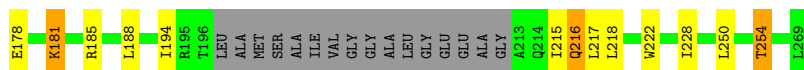
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





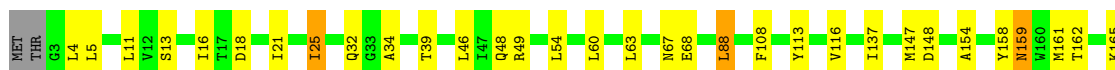
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E: 77% 14% 7%



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain F: 78% 19% 3%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.60Å 83.05Å 190.68Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	47.50 – 2.25 47.50 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.50-2.25) 77.6 (47.50-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.240 , 0.278 0.262 , 0.290	Depositor DCC
R_{free} test set	3722 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12612	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: PYW

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	0.78	0/2026	1.33	2/2750 (0.1%)
1	B	0.78	0/2026	1.34	1/2750 (0.0%)
1	C	0.76	0/1946	1.32	1/2640 (0.0%)
1	D	0.77	1/1926 (0.1%)	1.32	3/2614 (0.1%)
1	E	0.79	0/1926	1.33	0/2614
1	F	0.78	0/2026	1.31	4/2750 (0.1%)
All	All	0.77	1/11876 (0.0%)	1.32	11/16118 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	194	ILE	CG1-CD1	-5.08	1.31	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	ILE	N-CA-C	-5.97	104.81	110.42
1	B	148	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	25	ILE	CA-C-N	5.46	127.87	120.38
1	F	25	ILE	C-N-CA	5.46	127.87	120.38
1	D	49	ARG	CA-C-N	5.30	127.23	120.56
1	D	49	ARG	C-N-CA	5.30	127.23	120.56
1	D	148	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	148	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	148	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	148	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	80	GLU	CB-CG-CD	5.04	121.17	112.60

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	1988	0	2006	17	0
1	B	1988	0	2006	17	0
1	C	1909	0	1918	11	0
1	D	1889	0	1899	14	0
1	E	1889	0	1905	17	0
1	F	1988	0	2006	24	0
2	A	39	0	31	1	0
2	B	39	0	31	3	0
2	C	39	0	31	0	0
2	D	39	0	31	1	0
2	E	39	0	31	1	0
2	F	39	0	31	3	0
3	A	154	0	0	1	0
3	B	114	0	0	2	0
3	C	76	0	0	0	0
3	D	109	0	0	1	0
3	E	86	0	0	0	0
3	F	188	0	0	0	0
All	All	12612	0	11926	96	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 4.

All (96) 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:D:21:ILE:HD11	1:D:194:ILE:HD13	1.37	1.06
1:B:254:THR:HG21	3:B:2082:HOH:O	1.80	0.82
1:E:71:LEU:HD21	1:E:129:SER:HB3	1.66	0.75
1:D:149:PHE:HB2	2:D:1270:PYW:HAQ	1.67	0.75
1:A:254:THR:HG22	1:B:263:GLY:HA3	1.70	0.73
1:D:254:THR:HG21	3:D:2081:HOH:O	1.89	0.72
1:A:149:PHE:HB2	2:A:1270:PYW:HAQ	1.73	0.70
1:D:21:ILE:CD1	1:D:194:ILE:HD13	2.22	0.67
1:E:4:LEU:H	1:E:32:GLN:HE21	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:HE3	1:A:165:LYS:HE2	1.79	0.64
1:A:4:LEU:H	1:A:32:GLN:HE21	1.46	0.64
1:D:161:MET:HE3	1:D:165:LYS:HE2	1.81	0.63
1:C:4:LEU:H	1:C:32:GLN:HE21	1.46	0.62
1:D:4:LEU:H	1:D:32:GLN:HE21	1.46	0.62
1:E:44:LEU:HD11	1:E:62:GLU:HG3	1.81	0.61
1:E:161:MET:HE3	1:E:165:LYS:HE2	1.82	0.61
1:F:147:MET:HB3	2:F:1270:PYW:HAM	1.83	0.61
1:B:161:MET:HE3	1:B:165:LYS:HE2	1.82	0.60
1:A:116:VAL:HG11	1:A:160:TRP:CE3	2.36	0.60
1:F:25:ILE:HD13	1:F:239:ALA:HA	1.83	0.60
1:C:161:MET:HE3	1:C:165:LYS:HE2	1.83	0.59
1:E:178:GLU:O	1:E:181:LYS:HG2	2.06	0.56
1:E:149:PHE:HB2	2:E:1270:PYW:HAQ	1.88	0.56
1:F:11:LEU:HB2	1:F:88:LEU:HD21	1.91	0.53
1:D:11:LEU:HB2	1:D:88:LEU:HD21	1.90	0.53
1:B:11:LEU:HB2	1:B:88:LEU:HD21	1.91	0.53
1:F:5:LEU:HB3	1:F:34:ALA:HB2	1.91	0.53
1:F:21:ILE:O	1:F:25:ILE:HG12	2.08	0.53
1:F:161:MET:HE2	2:F:1270:PYW:HG21	1.92	0.52
1:C:11:LEU:HB2	1:C:88:LEU:HD21	1.91	0.52
1:E:11:LEU:HB2	1:E:88:LEU:HD21	1.91	0.51
1:A:11:LEU:HB2	1:A:88:LEU:HD21	1.91	0.51
1:E:159:ASN:HA	1:F:174:PHE:CE2	2.46	0.51
1:C:21:ILE:HD11	1:C:194:ILE:HG13	1.94	0.50
1:A:5:LEU:HB3	1:A:34:ALA:HB2	1.93	0.50
1:C:51:THR:HA	1:C:54:LEU:HD13	1.92	0.50
1:E:21:ILE:HD11	1:E:194:ILE:HG13	1.94	0.50
1:B:5:LEU:HB3	1:B:34:ALA:HB2	1.93	0.50
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.94	0.49
1:F:25:ILE:CD1	1:F:239:ALA:HA	2.43	0.49
1:E:5:LEU:HB3	1:E:34:ALA:HB2	1.94	0.49
1:B:39:THR:HG23	1:B:63:LEU:HB3	1.96	0.48
1:C:5:LEU:HB3	1:C:34:ALA:HB2	1.95	0.48
1:B:21:ILE:HD11	1:B:194:ILE:HG13	1.96	0.48
1:F:161:MET:HE3	1:F:165:LYS:HE2	1.96	0.48
1:A:171:VAL:O	1:A:175:VAL:HG23	2.14	0.48
1:A:21:ILE:HD11	1:A:194:ILE:HG13	1.95	0.47
1:E:116:VAL:HG11	1:E:160:TRP:CE3	2.48	0.47
1:C:168:LEU:HG	1:C:188:LEU:HD21	1.96	0.47
1:F:21:ILE:HD11	1:F:194:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ARG:HB3	1:F:154:ALA:HB2	1.96	0.47
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.80	0.47
1:B:149:PHE:HB2	2:B:1270:PYW:HAQ	1.96	0.46
1:B:168:LEU:HD22	1:B:188:LEU:HD11	1.97	0.46
1:B:199:MET:HE1	1:B:215:ILE:HG12	1.97	0.46
1:F:4:LEU:H	1:F:32:GLN:HE21	1.62	0.46
1:E:39:THR:HG23	1:E:63:LEU:HB3	1.98	0.45
1:E:154:ALA:HB2	1:F:173:ARG:HB3	1.98	0.45
1:C:113:TYR:HA	1:C:116:VAL:HG22	1.99	0.45
1:C:65:VAL:HG21	1:C:126:SER:HB2	1.99	0.45
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.82	0.45
1:D:222:TRP:HE1	1:D:261:ASP:HB2	1.82	0.45
1:F:108:PHE:HD1	1:F:159:ASN:HB3	1.82	0.45
1:A:202:ILE:HG22	1:A:207:LEU:HB2	1.99	0.45
1:C:222:TRP:HE1	1:C:261:ASP:HB2	1.82	0.45
1:D:113:TYR:HA	1:D:116:VAL:HG22	1.99	0.45
1:F:39:THR:HG23	1:F:63:LEU:HB3	1.98	0.44
1:B:196:THR:H	1:B:199:MET:HB2	1.83	0.44
1:B:113:TYR:HA	1:B:116:VAL:HG22	1.99	0.44
1:F:185:ARG:HA	1:F:254:THR:HG23	1.99	0.44
1:D:39:THR:HG23	1:D:63:LEU:HB3	1.99	0.44
1:F:113:TYR:HA	1:F:116:VAL:HG22	1.99	0.44
1:B:222:TRP:HE1	1:B:261:ASP:HB2	1.82	0.44
1:F:196:THR:H	1:F:199:MET:HB2	1.83	0.44
1:A:39:THR:HG23	1:A:63:LEU:HB3	2.00	0.43
1:A:196:THR:H	1:A:199:MET:HB2	1.84	0.43
1:B:147:MET:HB3	2:B:1270:PYW:HAM	2.00	0.43
1:C:185:ARG:HA	1:C:254:THR:HG23	2.00	0.43
1:B:65:VAL:HG21	1:B:126:SER:HB2	2.00	0.43
1:D:65:VAL:HG21	1:D:126:SER:HB2	2.00	0.43
1:B:185:ARG:HA	1:B:254:THR:HG23	2.01	0.43
1:F:13:SER:HA	1:F:39:THR:HB	2.00	0.43
1:E:185:ARG:HA	1:E:254:THR:HG23	2.01	0.43
1:B:94:ALA:HA	2:B:1270:PYW:HAL	2.01	0.42
1:E:63:LEU:HD13	1:E:74:LEU:HG	2.01	0.42
1:A:258:ILE:HA	3:A:2150:HOH:O	2.17	0.42
1:D:185:ARG:HA	1:D:254:THR:HG23	2.01	0.42
1:A:228:ILE:HG23	3:B:2082:HOH:O	2.21	0.41
1:F:158:TYR:HD1	2:F:1270:PYW:HAA2	1.84	0.41
1:A:65:VAL:HG21	1:A:126:SER:HB2	2.03	0.41
1:D:26:ALA:HB1	1:D:54:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:LEU:HD11	1:F:258:ILE:HG13	2.03	0.41
1:A:76:GLY:O	1:A:80:GLU:HG2	2.21	0.40
1:F:21:ILE:HG22	1:F:25:ILE:HD11	2.03	0.40
1:E:216:GLN:HE21	1:E:216:GLN:HB3	1.75	0.40
1:F:202:ILE:HG22	1:F:207:LEU:HB2	2.02	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	265/269 (98%)	250 (94%)	15 (6%)	0	100	100
1	B	265/269 (98%)	250 (94%)	13 (5%)	2 (1%)	16	14
1	C	250/269 (93%)	237 (95%)	12 (5%)	1 (0%)	30	31
1	D	248/269 (92%)	234 (94%)	13 (5%)	1 (0%)	30	31
1	E	247/269 (92%)	231 (94%)	14 (6%)	2 (1%)	16	14
1	F	265/269 (98%)	250 (94%)	14 (5%)	1 (0%)	30	31
All	All	1540/1614 (95%)	1452 (94%)	81 (5%)	7 (0%)	24	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	ALA
1	C	159	ASN
1	D	159	ASN
1	E	75	ALA
1	E	159	ASN
1	F	159	ASN
1	B	159	ASN

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	202/204 (99%)	174 (86%)	28 (14%)	3	2
1	B	202/204 (99%)	177 (88%)	25 (12%)	4	3
1	C	195/204 (96%)	175 (90%)	20 (10%)	7	5
1	D	193/204 (95%)	173 (90%)	20 (10%)	7	5
1	E	194/204 (95%)	172 (89%)	22 (11%)	5	3
1	F	202/204 (99%)	177 (88%)	25 (12%)	4	3
All	All	1188/1224 (97%)	1048 (88%)	140 (12%)	5	3

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	39	THR
1	A	46	LEU
1	A	48	GLN
1	A	50	ILE
1	A	53	ARG
1	A	54	LEU
1	A	65	VAL
1	A	67	ASN
1	A	68	GLU
1	A	74	LEU
1	A	82	ILE
1	A	88	LEU
1	A	137	ILE
1	A	162	THR
1	A	168	LEU
1	A	188	LEU
1	A	196	THR
1	A	197	LEU
1	A	207	LEU
1	A	215	ILE
1	A	217	LEU

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	228	ILE
1	A	233	LYS
1	A	250	LEU
1	A	254	THR
1	A	269	LEU
1	B	18	ASP
1	B	39	THR
1	B	44	LEU
1	B	45	ARG
1	B	48	GLN
1	B	54	LEU
1	B	65	VAL
1	B	67	ASN
1	B	68	GLU
1	B	74	LEU
1	B	88	LEU
1	B	137	ILE
1	B	162	THR
1	B	168	LEU
1	B	188	LEU
1	B	196	THR
1	B	197	LEU
1	B	207	LEU
1	B	215	ILE
1	B	217	LEU
1	B	218	LEU
1	B	228	ILE
1	B	250	LEU
1	B	254	THR
1	B	269	LEU
1	C	15	ILE
1	C	16	ILE
1	C	41	PHE
1	C	44	LEU
1	C	49	ARG
1	C	60	LEU
1	C	65	VAL
1	C	67	ASN
1	C	88	LEU
1	C	95	ILE
1	C	137	ILE

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Mol	Chain	Res	Type
1	C	162	THR
1	C	188	LEU
1	C	215	ILE
1	C	217	LEU
1	C	218	LEU
1	C	228	ILE
1	C	250	LEU
1	C	254	THR
1	C	269	LEU
1	D	16	ILE
1	D	39	THR
1	D	46	LEU
1	D	54	LEU
1	D	65	VAL
1	D	67	ASN
1	D	68	GLU
1	D	88	LEU
1	D	137	ILE
1	D	162	THR
1	D	168	LEU
1	D	188	LEU
1	D	215	ILE
1	D	217	LEU
1	D	218	LEU
1	D	228	ILE
1	D	233	LYS
1	D	250	LEU
1	D	254	THR
1	D	269	LEU
1	E	16	ILE
1	E	39	THR
1	E	48	GLN
1	E	54	LEU
1	E	65	VAL
1	E	67	ASN
1	E	68	GLU
1	E	74	LEU
1	E	88	LEU
1	E	137	ILE
1	E	162	THR
1	E	168	LEU
1	E	181	LYS

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Mol	Chain	Res	Type
1	E	188	LEU
1	E	215	ILE
1	E	216	GLN
1	E	217	LEU
1	E	218	LEU
1	E	222	TRP
1	E	228	ILE
1	E	250	LEU
1	E	254	THR
1	F	16	ILE
1	F	18	ASP
1	F	46	LEU
1	F	48	GLN
1	F	49	ARG
1	F	54	LEU
1	F	60	LEU
1	F	67	ASN
1	F	68	GLU
1	F	88	LEU
1	F	137	ILE
1	F	162	THR
1	F	168	LEU
1	F	188	LEU
1	F	196	THR
1	F	197	LEU
1	F	207	LEU
1	F	210	GLU
1	F	215	ILE
1	F	217	LEU
1	F	218	LEU
1	F	228	ILE
1	F	233	LYS
1	F	254	THR
1	F	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	106	ASN
1	A	159	ASN
1	A	172	ASN

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Mol	Chain	Res	Type
1	A	214	GLN
1	B	106	ASN
1	B	121	HIS
1	B	172	ASN
1	B	214	GLN
1	C	32	GLN
1	C	106	ASN
1	C	172	ASN
1	D	32	GLN
1	D	66	GLN
1	D	106	ASN
1	D	121	HIS
1	D	172	ASN
1	E	32	GLN
1	E	48	GLN
1	E	106	ASN
1	E	216	GLN
1	E	267	GLN
1	F	32	GLN
1	F	48	GLN
1	F	106	ASN
1	F	172	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	PYW	D	1270	-	39,41,41	1.25	3 (7%)	43,57,57	1.26	3 (6%)
2	PYW	E	1270	-	39,41,41	1.31	5 (12%)	43,57,57	1.35	4 (9%)
2	PYW	F	1270	-	39,41,41	1.28	5 (12%)	43,57,57	1.22	4 (9%)
2	PYW	A	1270	-	39,41,41	1.18	2 (5%)	43,57,57	1.28	4 (9%)
2	PYW	B	1270	-	39,41,41	1.29	4 (10%)	43,57,57	1.25	2 (4%)
2	PYW	C	1270	-	39,41,41	1.28	7 (17%)	43,57,57	1.34	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYW	D	1270	-	-	9/53/54/54	0/2/3/3
2	PYW	E	1270	-	-	14/53/54/54	0/2/3/3
2	PYW	F	1270	-	-	12/53/54/54	0/2/3/3
2	PYW	A	1270	-	-	9/53/54/54	0/2/3/3
2	PYW	B	1270	-	-	8/53/54/54	0/2/3/3
2	PYW	C	1270	-	-	10/53/54/54	0/2/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1270	PYW	C-NAV	3.31	1.41	1.34
2	A	1270	PYW	CBG-CBH	3.22	1.44	1.40
2	F	1270	PYW	C-NAV	3.11	1.40	1.34
2	B	1270	PYW	C-NAV	2.94	1.40	1.34
2	D	1270	PYW	CBG-CBH	2.88	1.44	1.40
2	F	1270	PYW	CBG-CBH	2.70	1.44	1.40
2	F	1270	PYW	CBH-NAU	2.67	1.39	1.34
2	C	1270	PYW	C-NAV	2.58	1.39	1.34
2	E	1270	PYW	CBB-N	2.58	1.40	1.34
2	C	1270	PYW	CBB-N	2.55	1.40	1.34
2	B	1270	PYW	CBK-CBL	2.52	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1270	PYW	C-NAV	2.50	1.39	1.34
2	E	1270	PYW	CBK-CBL	2.48	1.57	1.53
2	B	1270	PYW	CBG-CBH	2.47	1.43	1.40
2	D	1270	PYW	CBB-N	2.44	1.39	1.34
2	F	1270	PYW	CBB-N	2.43	1.39	1.34
2	C	1270	PYW	CBH-NAU	2.39	1.38	1.34
2	F	1270	PYW	CBK-CBL	2.36	1.57	1.53
2	C	1270	PYW	CBG-CBH	2.35	1.43	1.40
2	C	1270	PYW	CAQ-CBF	2.25	1.43	1.38
2	E	1270	PYW	CBG-CBH	2.22	1.43	1.40
2	B	1270	PYW	CBB-N	2.20	1.39	1.34
2	E	1270	PYW	CAQ-CBF	2.10	1.43	1.38
2	C	1270	PYW	CBK-CBL	2.10	1.57	1.53
2	C	1270	PYW	CAQ-NAT	2.07	1.38	1.34
2	D	1270	PYW	CBH-NAU	2.04	1.38	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1270	PYW	CB-OG1-CBA	5.49	123.89	117.33
2	C	1270	PYW	CB-OG1-CBA	5.44	123.83	117.33
2	E	1270	PYW	CB-OG1-CBA	5.38	123.75	117.33
2	A	1270	PYW	CB-OG1-CBA	4.95	123.25	117.33
2	D	1270	PYW	CB-OG1-CBA	4.89	123.17	117.33
2	F	1270	PYW	CB-OG1-CBA	4.54	122.75	117.33
2	C	1270	PYW	CBA-CBE-CAZ	3.58	128.13	124.45
2	E	1270	PYW	CBA-CBE-CAZ	3.08	127.62	124.45
2	D	1270	PYW	CBA-CBE-CAZ	2.93	127.47	124.45
2	A	1270	PYW	CBA-CBE-CAZ	2.82	127.35	124.45
2	E	1270	PYW	CA-N-CBB	2.63	126.84	121.53
2	F	1270	PYW	CBA-CBE-CAZ	2.60	127.13	124.45
2	A	1270	PYW	CBK-CBJ-CBD	2.29	115.23	110.03
2	F	1270	PYW	CB-CA-C	2.19	115.33	110.73
2	E	1270	PYW	CBK-CBJ-CBD	2.16	114.92	110.03
2	C	1270	PYW	OAE-CBA-CBE	2.09	128.59	122.46
2	A	1270	PYW	OAF-CBB-CBH	2.05	124.03	120.75
2	C	1270	PYW	OG1-CB-CA	-2.05	101.30	105.77
2	F	1270	PYW	OG1-CB-CA	-2.01	101.37	105.77
2	D	1270	PYW	OAE-CBA-CBE	2.01	128.37	122.46
2	B	1270	PYW	CBK-CBJ-CBD	2.01	114.58	110.03

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1270	PYW	CAA-CAR-CAZ-CAB
2	B	1270	PYW	CAA-CAR-CAZ-CAB
2	C	1270	PYW	CBD-CBJ-CBK-CBL
2	C	1270	PYW	CAA-CAR-CAZ-CAB
2	D	1270	PYW	CBD-CBJ-CBK-CBL
2	E	1270	PYW	OAE-CBA-CBE-OAX
2	E	1270	PYW	OG1-CBA-CBE-OAX
2	E	1270	PYW	OAE-CBA-CBE-CAZ
2	E	1270	PYW	OG1-CBA-CBE-CAZ
2	E	1270	PYW	CAA-CAR-CAZ-CAB
2	E	1270	PYW	N-CA-CB-CG2
2	E	1270	PYW	N-CBB-CBH-NAU
2	E	1270	PYW	N-CBB-CBH-CBG
2	E	1270	PYW	OAF-CBB-CBH-NAU
2	E	1270	PYW	OAF-CBB-CBH-CBG
2	F	1270	PYW	CBD-CBJ-CBK-CBL
2	F	1270	PYW	CBE-CBA-OG1-CB
2	F	1270	PYW	OAE-CBA-OG1-CB
2	F	1270	PYW	OAF-CBB-N-CA
2	F	1270	PYW	CBH-CBB-N-CA
2	A	1270	PYW	OAF-CBB-CBH-NAU
2	B	1270	PYW	OAF-CBB-CBH-NAU
2	C	1270	PYW	OAF-CBB-CBH-NAU
2	D	1270	PYW	OAF-CBB-CBH-NAU
2	F	1270	PYW	OAF-CBB-CBH-NAU
2	A	1270	PYW	N-CBB-CBH-NAU
2	B	1270	PYW	N-CBB-CBH-NAU
2	C	1270	PYW	N-CBB-CBH-NAU
2	D	1270	PYW	N-CBB-CBH-NAU
2	F	1270	PYW	N-CBB-CBH-NAU
2	C	1270	PYW	OAE-CBA-OG1-CB
2	E	1270	PYW	N-CA-CB-OG1
2	E	1270	PYW	C-CA-CB-CG2
2	E	1270	PYW	C-CA-CB-OG1
2	E	1270	PYW	OAF-CBB-N-CA
2	D	1270	PYW	CAA-CAR-CAZ-CAB
2	F	1270	PYW	CAA-CAR-CAZ-CAB
2	B	1270	PYW	CAA-CAR-CAZ-CBE
2	C	1270	PYW	CAA-CAR-CAZ-CBE
2	A	1270	PYW	CBF-CAS-CBL-NAV
2	A	1270	PYW	CAD-CBJ-CBK-CBL
2	D	1270	PYW	CAD-CBJ-CBK-CBL

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Mol	Chain	Res	Type	Atoms
2	F	1270	PYW	CAD-CBJ-CBK-CBL
2	C	1270	PYW	OAF-CBB-N-CA
2	A	1270	PYW	N-CBB-CBH-CBG
2	B	1270	PYW	N-CBB-CBH-CBG
2	C	1270	PYW	N-CBB-CBH-CBG
2	D	1270	PYW	N-CBB-CBH-CBG
2	F	1270	PYW	N-CBB-CBH-CBG
2	A	1270	PYW	CBD-CBJ-CBK-CBL
2	D	1270	PYW	CBD-CBJ-CBK-OAJ
2	F	1270	PYW	CBD-CBJ-CBK-OAJ
2	A	1270	PYW	OAF-CBB-CBH-CBG
2	B	1270	PYW	OAF-CBB-CBH-CBG
2	C	1270	PYW	OAF-CBB-CBH-CBG
2	D	1270	PYW	OAF-CBB-CBH-CBG
2	F	1270	PYW	OAF-CBB-CBH-CBG
2	C	1270	PYW	CAD-CBJ-CBK-CBL
2	A	1270	PYW	CAA-CAR-CAZ-CBE
2	D	1270	PYW	OAE-CBA-OG1-CB
2	B	1270	PYW	OAF-CBB-N-CA
2	B	1270	PYW	CBD-CBJ-CBK-CBL

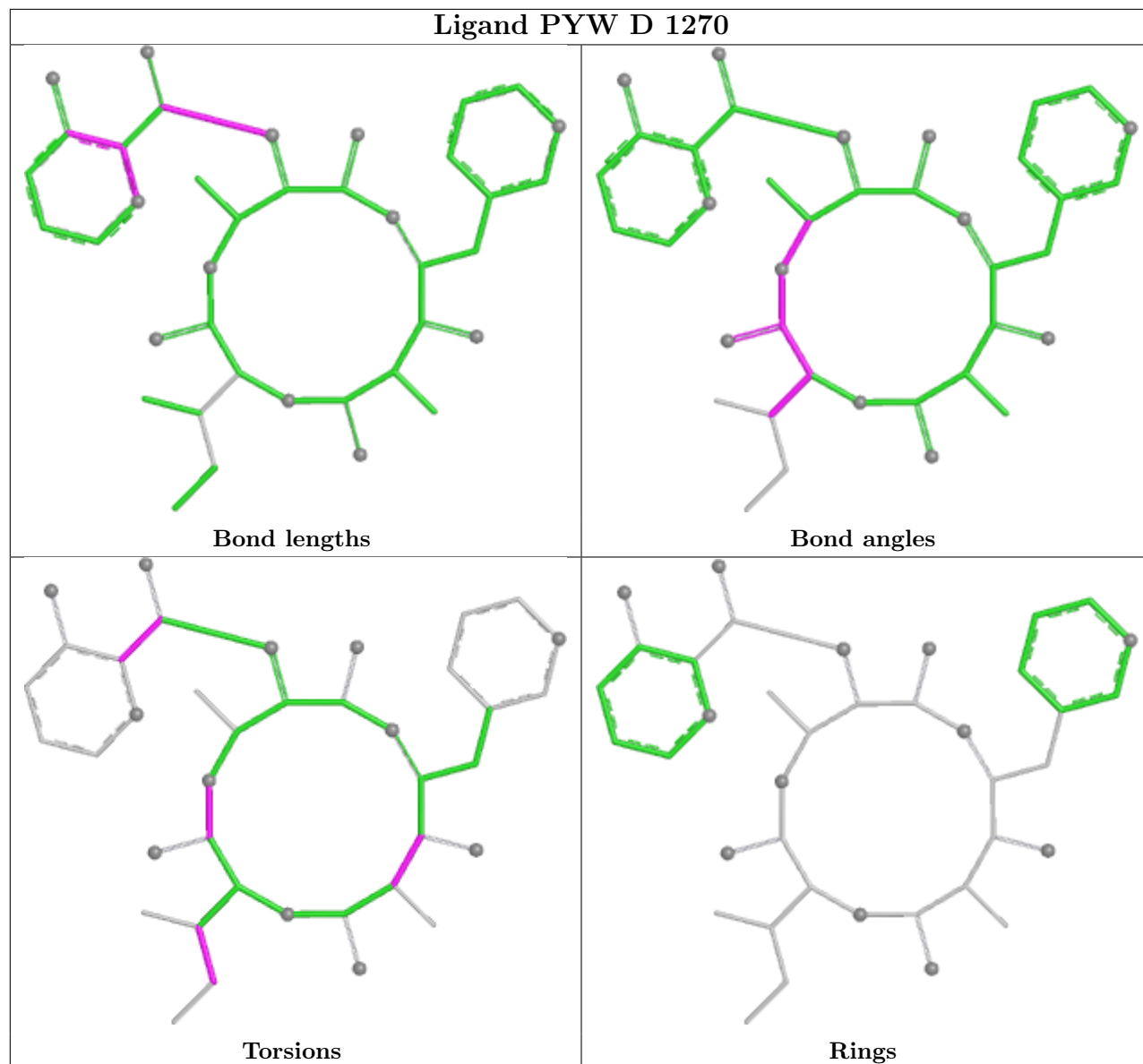
There are no ring outliers.

5 monomers are involved in 9 short contacts:

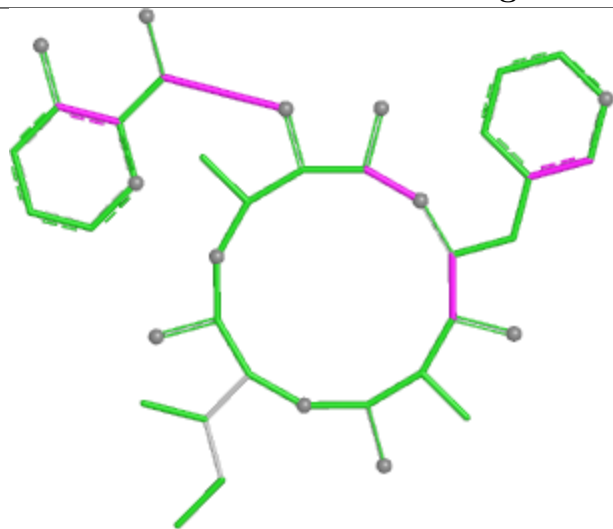
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1270	PYW	1	0
2	E	1270	PYW	1	0
2	F	1270	PYW	3	0
2	A	1270	PYW	1	0
2	B	1270	PYW	3	0

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

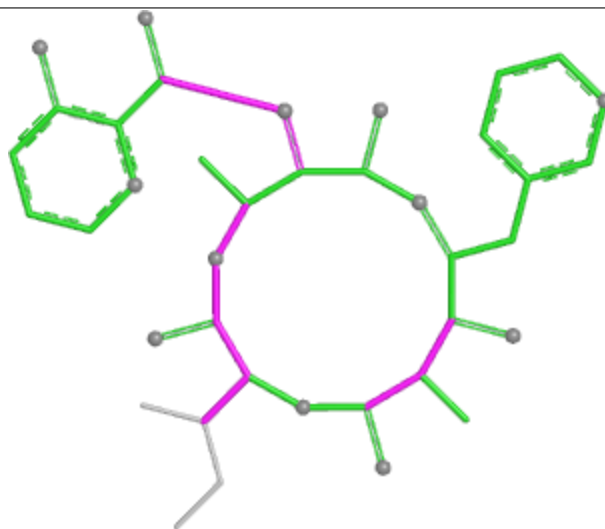
equivalents in the CSD to analyse the geometry.



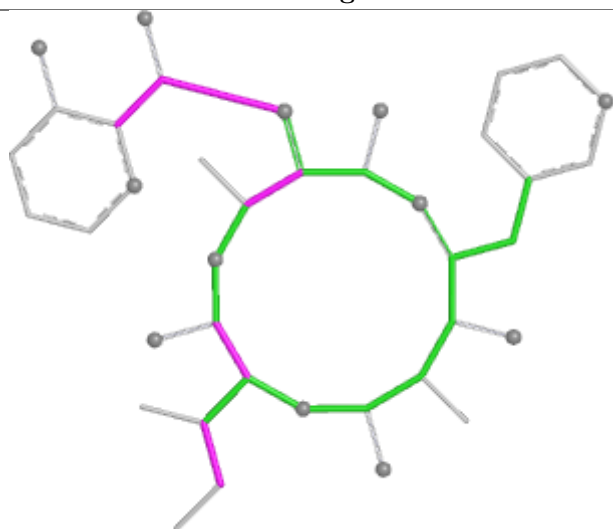
Ligand PYW E 1270



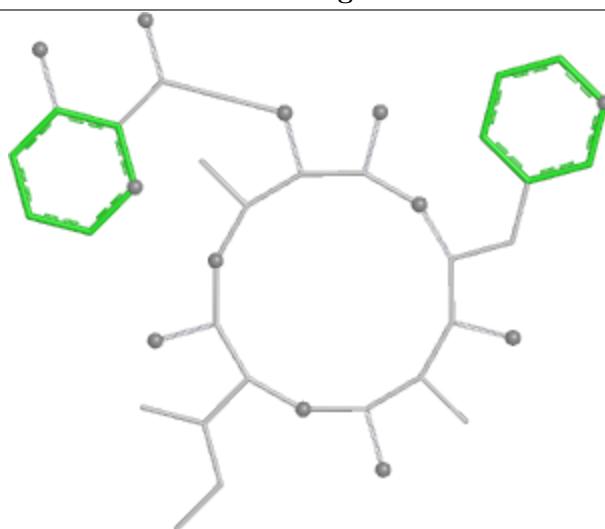
Bond lengths



Bond angles

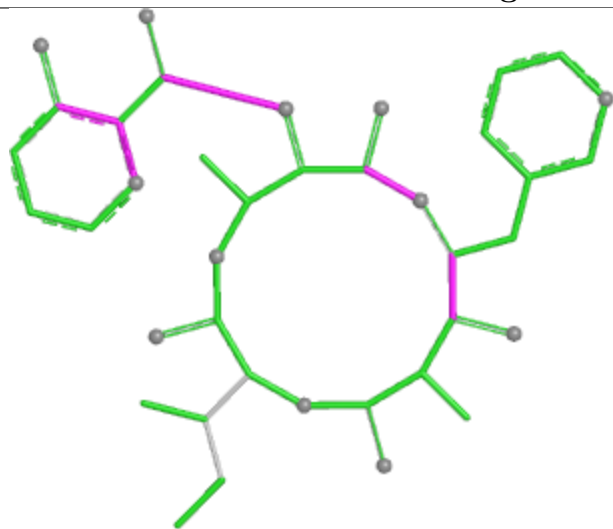


Torsions

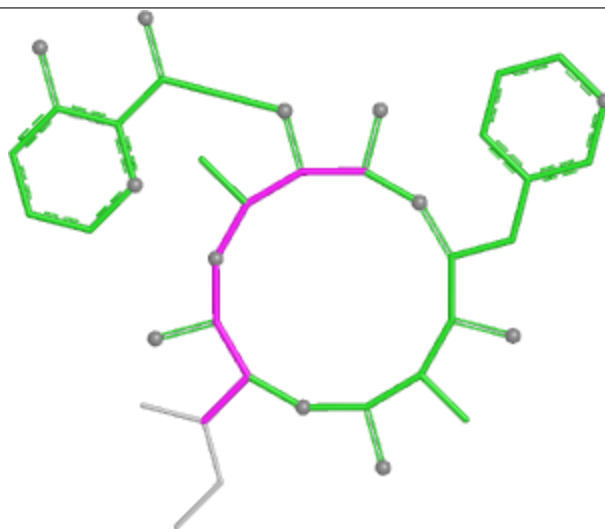


Rings

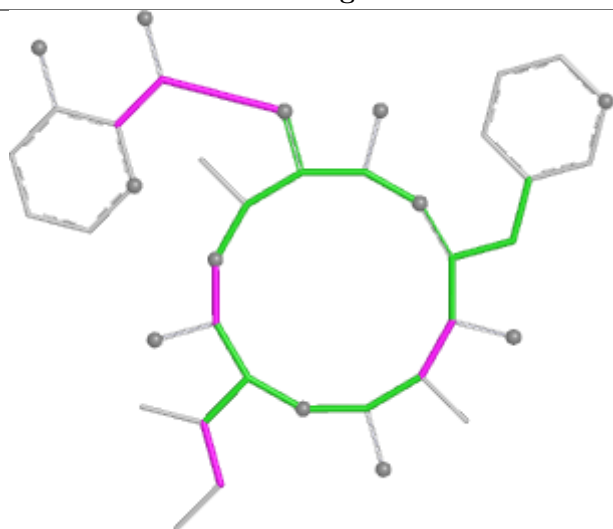
Ligand PYW F 1270



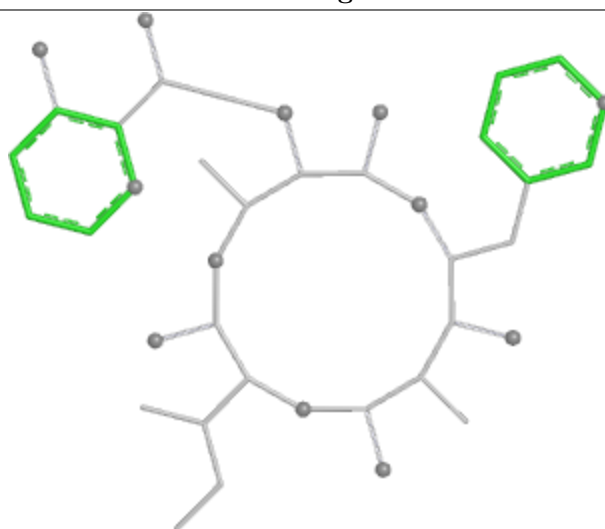
Bond lengths



Bond angles

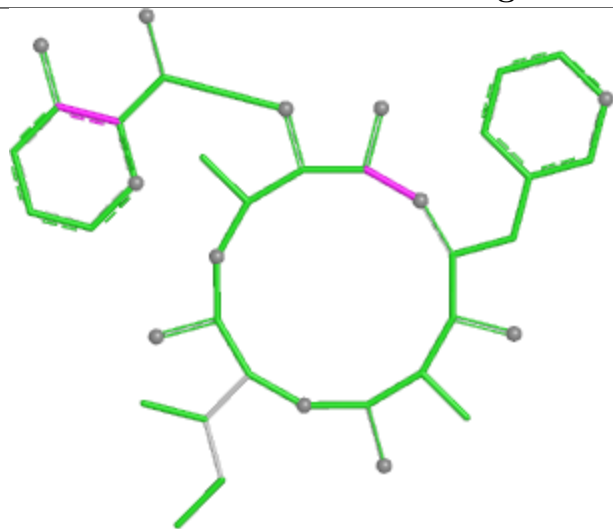


Torsions

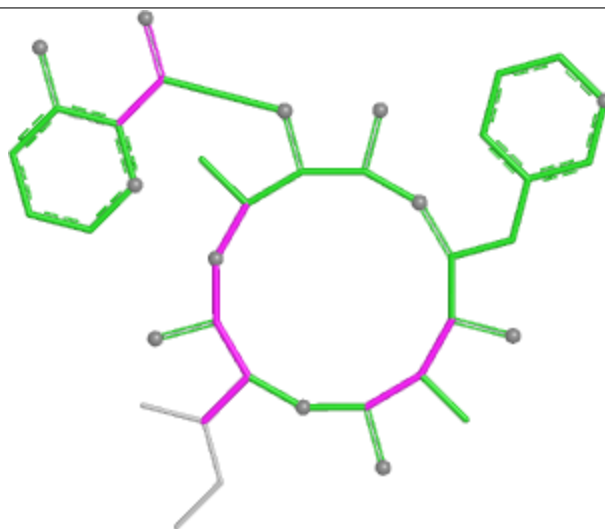


Rings

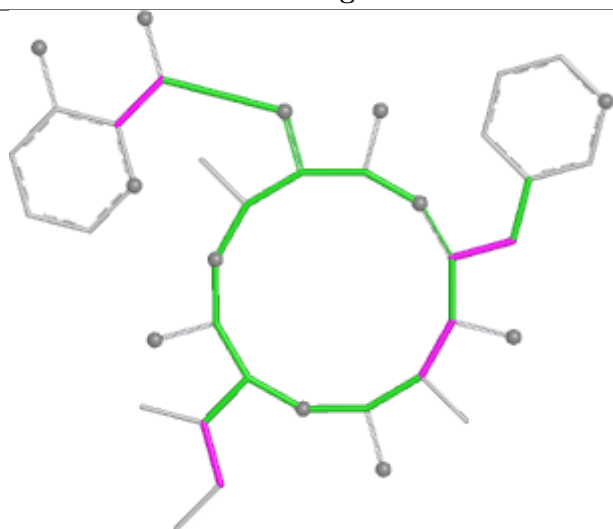
Ligand PYW A 1270



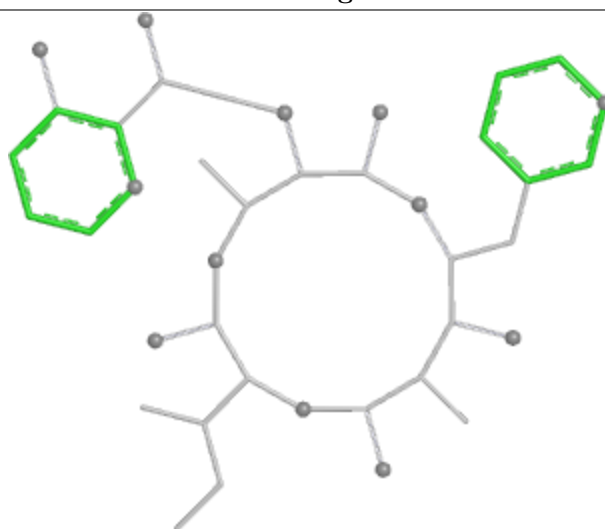
Bond lengths



Bond angles

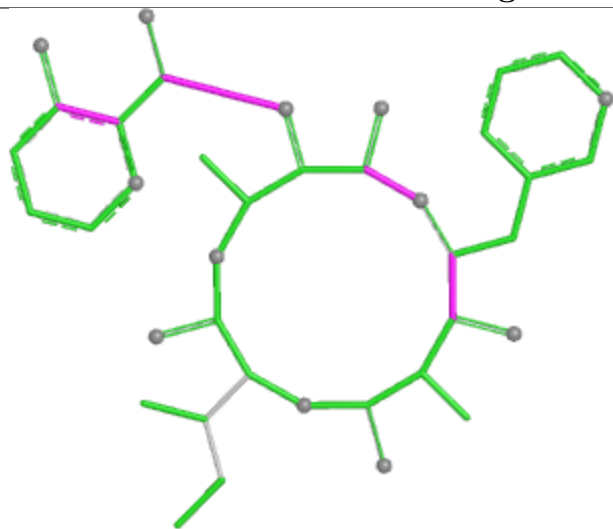


Torsions

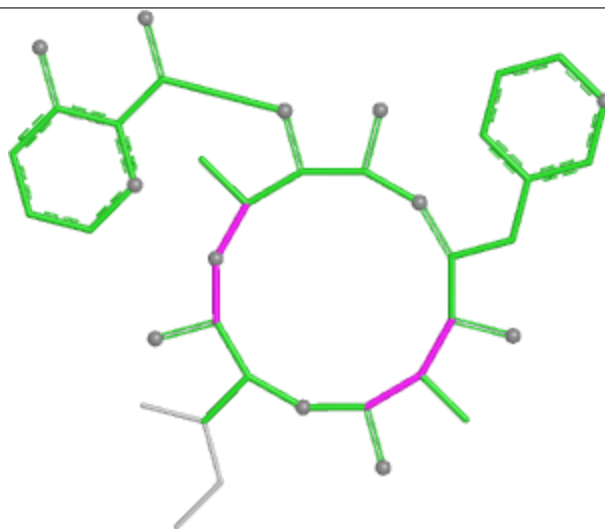


Rings

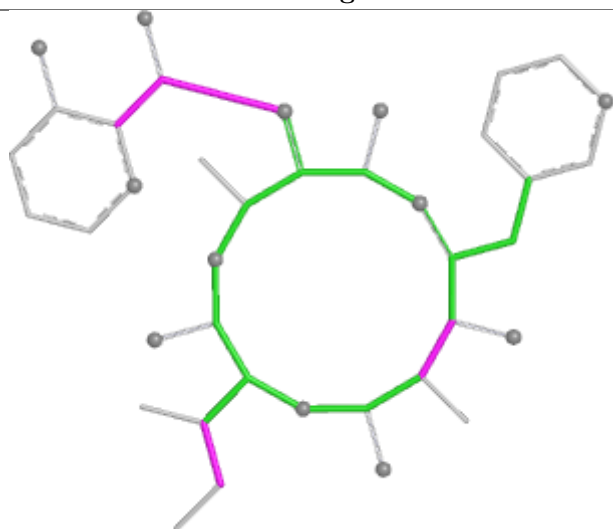
Ligand PYW B 1270



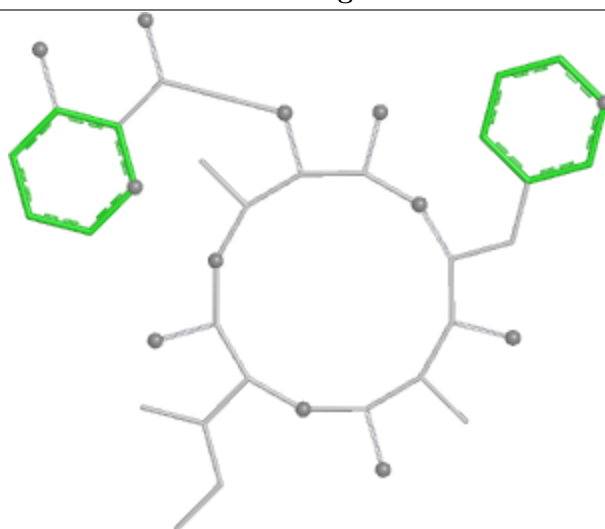
Bond lengths



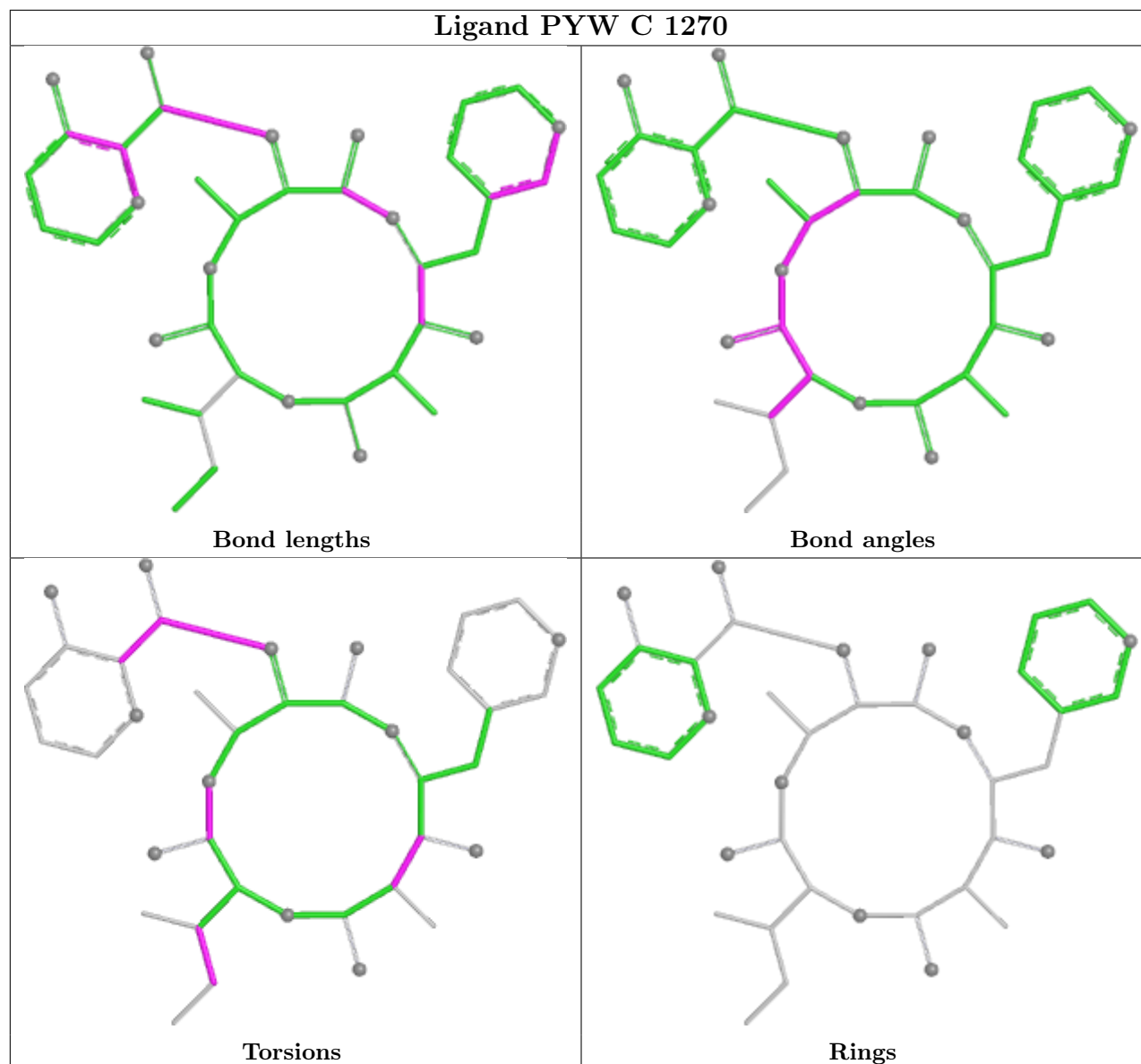
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	267/269 (99%)	-1.11	0 100 100	6, 22, 50, 66	0
1	B	267/269 (99%)	-1.12	0 100 100	5, 20, 54, 76	0
1	C	254/269 (94%)	-0.85	0 100 100	14, 36, 59, 77	0
1	D	252/269 (93%)	-0.89	0 100 100	17, 35, 58, 76	0
1	E	251/269 (93%)	-0.86	0 100 100	16, 36, 63, 75	0
1	F	267/269 (99%)	-0.80	0 100 100	17, 38, 63, 74	0
All	All	1558/1614 (96%)	-0.94	0 100 100	5, 32, 60, 77	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	PYW	C	1270	39/39	0.98	0.05	20,30,36,37	0

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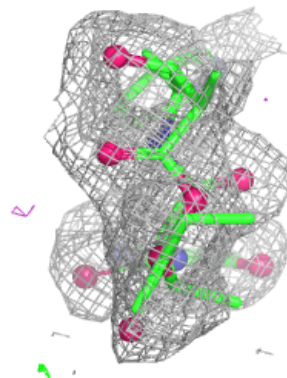
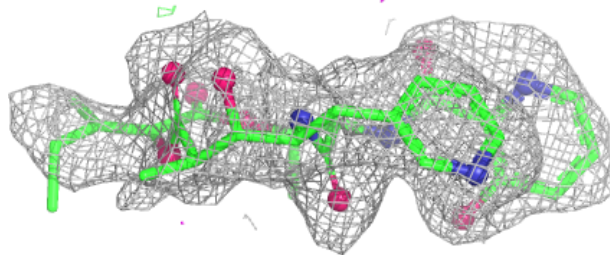
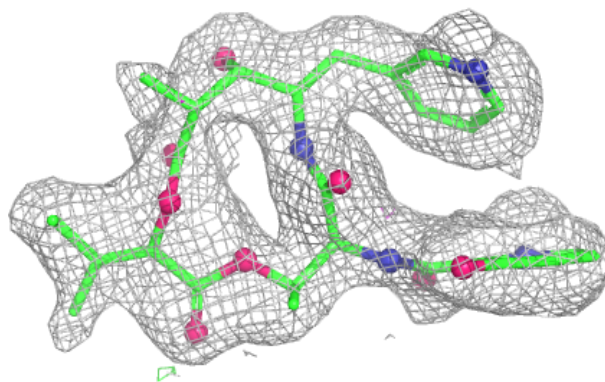
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PYW	D	1270	39/39	0.98	0.04	15,22,29,30	0
2	PYW	E	1270	39/39	0.98	0.05	26,32,40,42	0
2	PYW	F	1270	39/39	0.98	0.05	30,36,45,46	0
2	PYW	A	1270	39/39	0.99	0.03	8,16,22,26	0
2	PYW	B	1270	39/39	0.99	0.03	7,15,28,33	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.

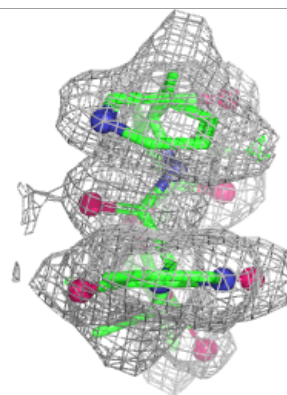
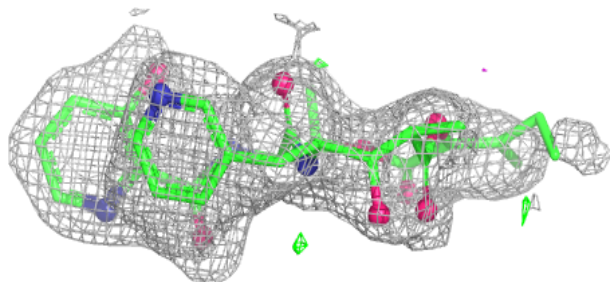
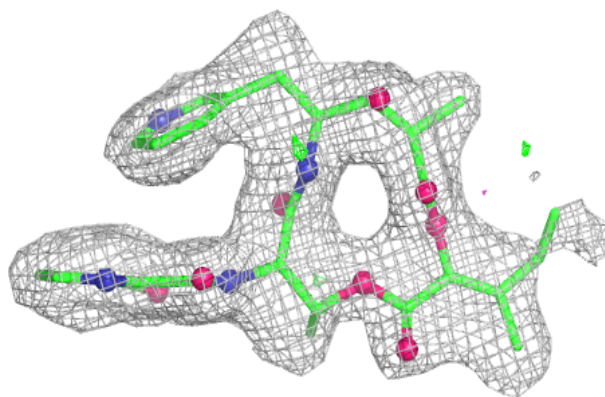
Electron density around PYW C 1270:

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

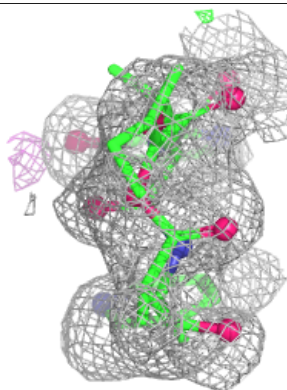
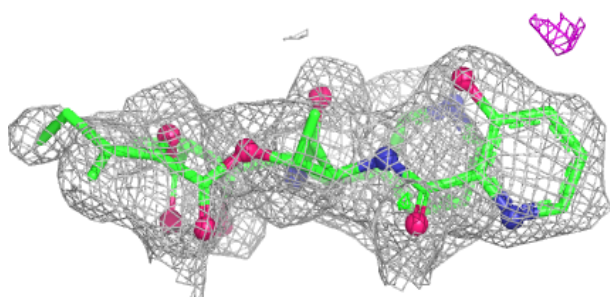
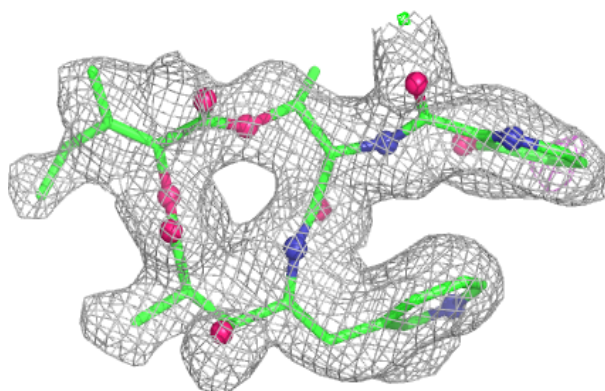


Electron density around PYW D 1270:

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

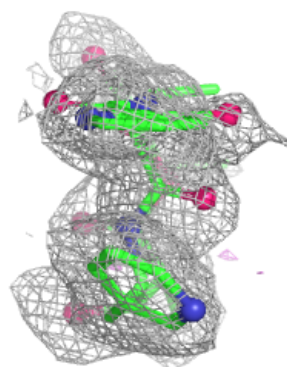
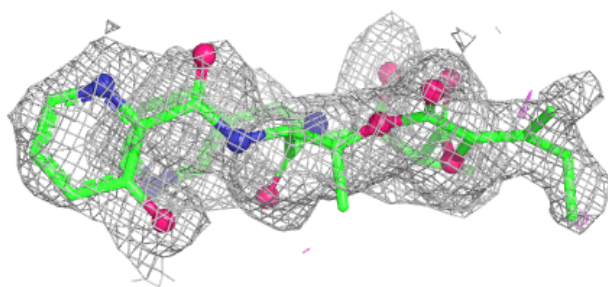
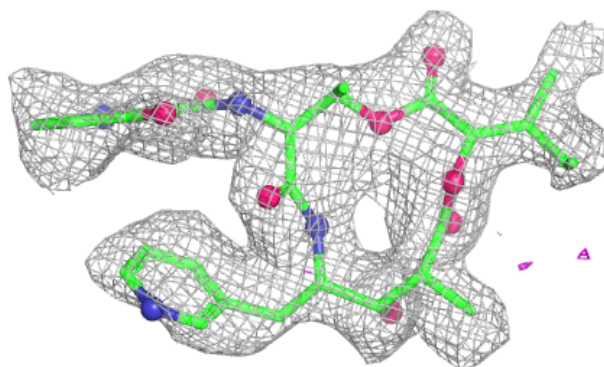
**Electron density around PYW E 1270:**

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

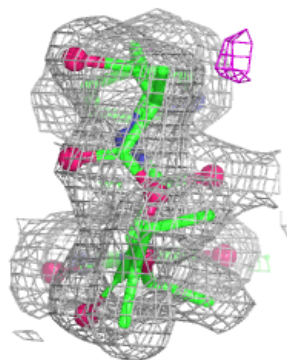
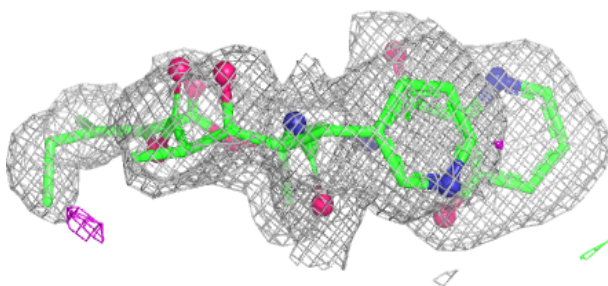
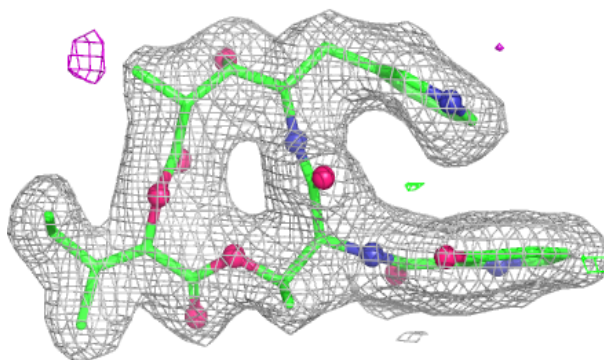


Electron density around PYW F 1270:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

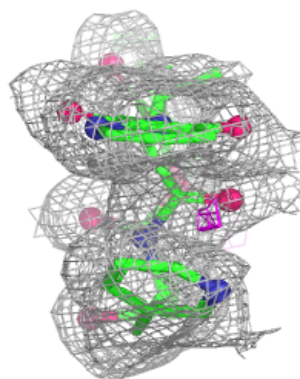
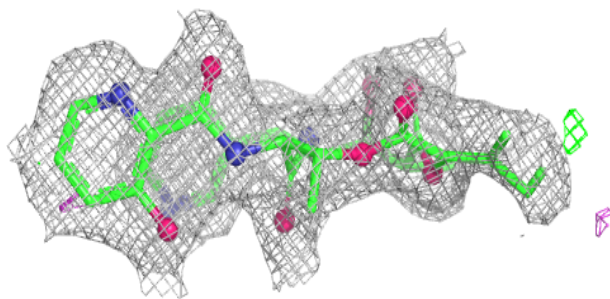
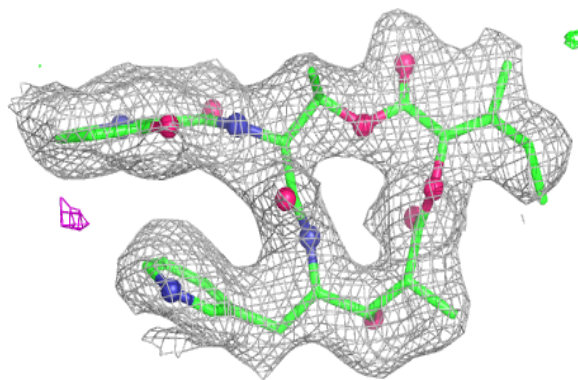
**Electron density around PYW A 1270:**

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



Electron density around PYW B 1270:

$2mF_o-DF_c$ (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.