



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 AM UTC

PDB ID : 3WI6 / pdb_00003wi6
Title : Crystal structure of MAPKAP Kinase-2 (MK2) in complex with non-selective inhibitor
Authors : Fujino, A.; Fukushima, K.; Kubota, T.; Matsumoto, Y.; Takimoto-Kamimura, M.
Deposited on : 2013-09-06
Resolution : 2.99 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

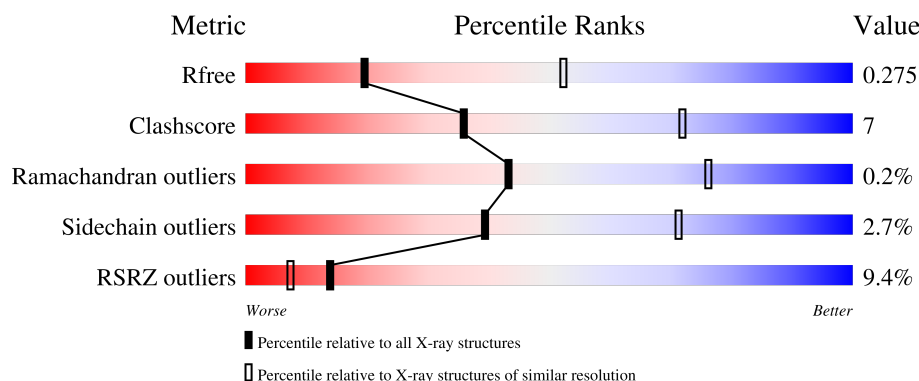
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	324	9% 71% 15% • 13%
1	B	324	8% 68% 19% • 13%
1	C	324	8% 69% 17% • 13%
1	D	324	7% 69% 17% • 13%

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Mol	Chain	Length	Quality of chain
1	E	324	
1	F	324	

2 Entry composition [i](#)

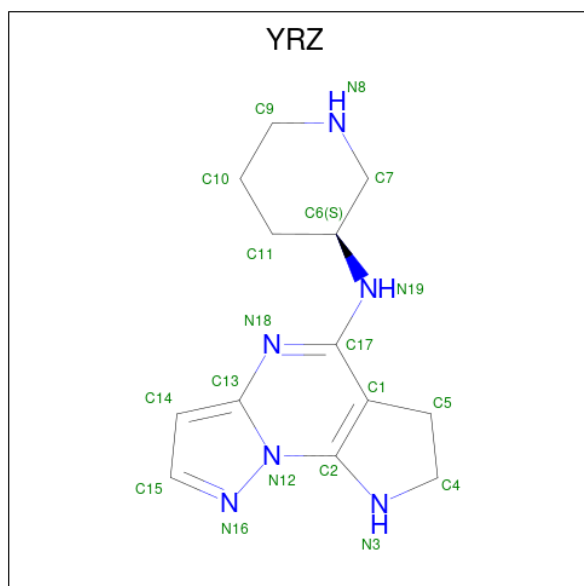
There are 2 unique types of molecules in this entry. The entry contains 13553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2233	1429	380	407	17			
1	B	283	Total	C	N	O	S	0	0	0
			2241	1433	381	410	17			
1	C	283	Total	C	N	O	S	0	0	0
			2237	1431	381	408	17			
1	D	282	Total	C	N	O	S	0	0	0
			2237	1431	380	409	17			
1	E	283	Total	C	N	O	S	0	0	0
			2249	1439	382	411	17			
1	F	283	Total	C	N	O	S	0	0	0
			2242	1434	382	409	17			

- Molecule 2 is N-[(3S)-piperidin-3-yl]-7,8-dihydro-6H-pyrazolo[1,5-a]pyrrolo[3,2-e]pyrimidin-5-amine (CCD ID: YRZ) (formula: C₁₃H₁₈N₆).

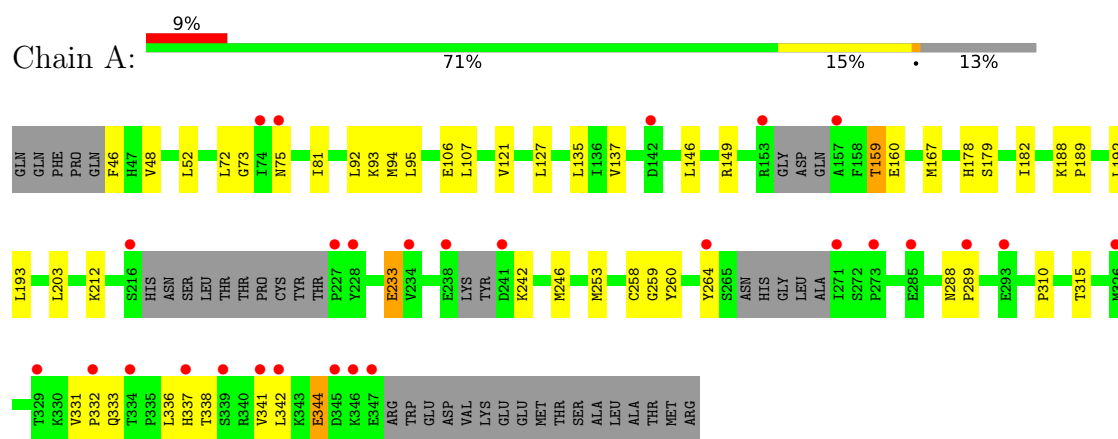


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			19	13	6		
2	B	1	Total	C	N	0	0
			19	13	6		
2	C	1	Total	C	N	0	0
			19	13	6		
2	D	1	Total	C	N	0	0
			19	13	6		
2	E	1	Total	C	N	0	0
			19	13	6		
2	F	1	Total	C	N	0	0
			19	13	6		

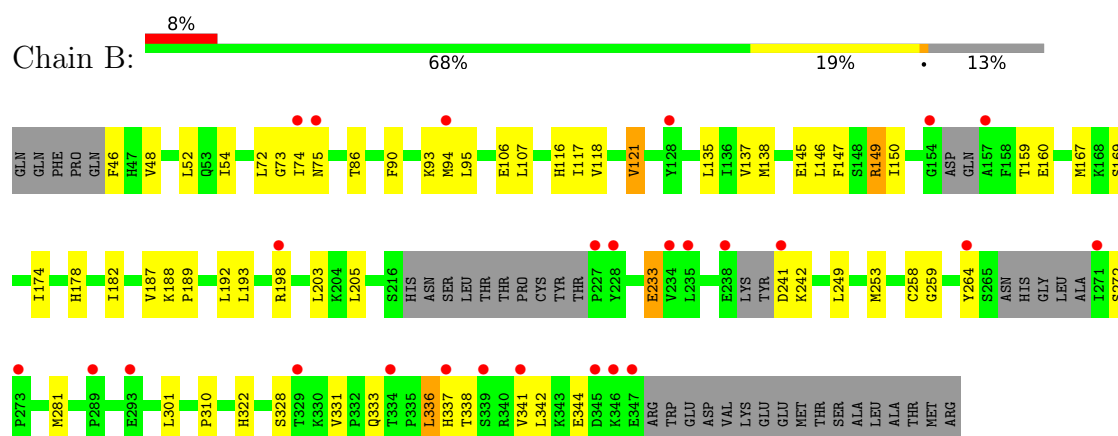
3 Residue-property plots [i](#)

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.

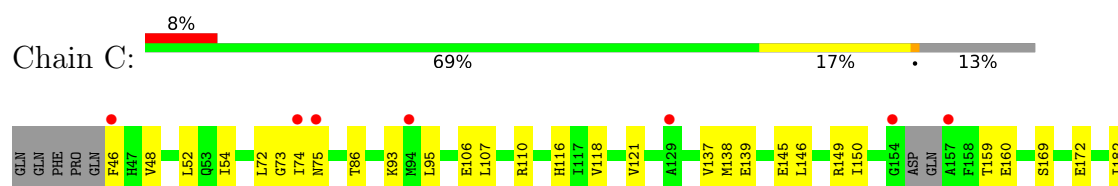
- Molecule 1: MAP kinase-activated protein kinase 2

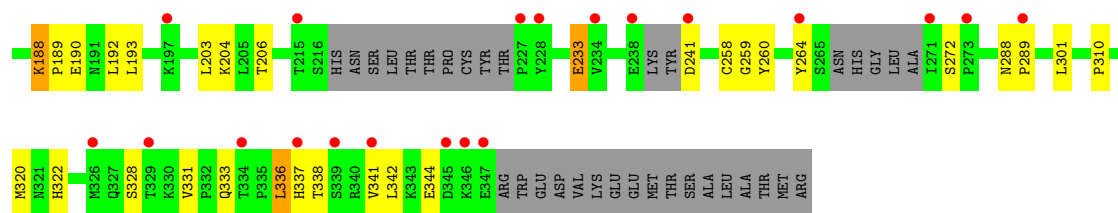


- Molecule 1: MAP kinase-activated protein kinase 2

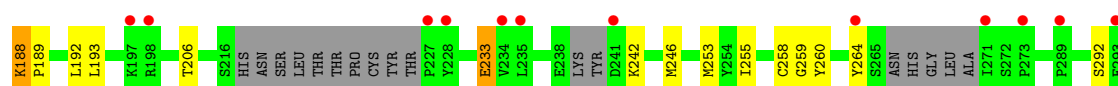


- Molecule 1: MAP kinase-activated protein kinase 2

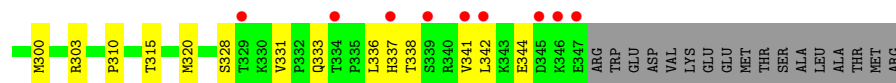
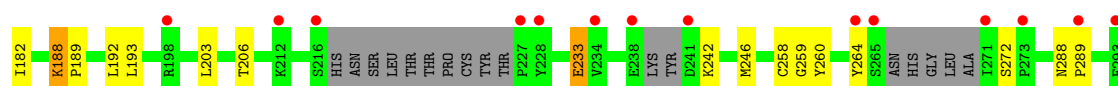
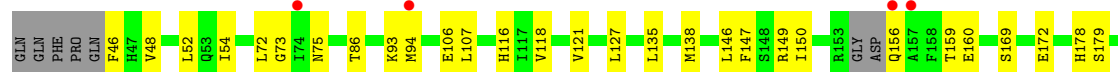




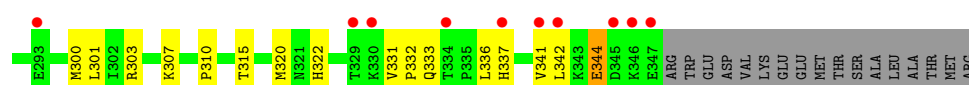
• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2



• Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	180.06Å 179.68Å 254.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.99 30.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.99) 99.3 (30.00-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.283 0.235 , 0.275	Depositor DCC
R_{free} test set	4136 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.466 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.467 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.469 for $k, h, -l$ 0.459 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.467 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13553	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: YRZ

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	1.15	1/2280 (0.0%)	0.95	1/3083 (0.0%)
1	B	1.15	2/2288 (0.1%)	0.96	1/3093 (0.0%)
1	C	1.14	2/2284 (0.1%)	0.94	1/3088 (0.0%)
1	D	1.15	4/2284 (0.2%)	0.96	1/3088 (0.0%)
1	E	1.14	1/2296 (0.0%)	0.96	1/3104 (0.0%)
1	F	1.14	3/2289 (0.1%)	0.97	1/3095 (0.0%)
All	All	1.15	13/13721 (0.1%)	0.96	6/18551 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	ILE	CA-CB	7.62	1.62	1.53
1	E	54	ILE	CA-CB	7.24	1.61	1.53
1	B	137	VAL	CA-CB	6.83	1.62	1.54
1	B	54	ILE	CA-CB	6.67	1.61	1.53
1	C	137	VAL	CA-CB	6.24	1.61	1.54
1	D	137	VAL	CA-CB	6.05	1.61	1.54
1	C	54	ILE	CA-CB	5.82	1.60	1.53
1	A	137	VAL	CA-CB	5.66	1.61	1.54
1	F	137	VAL	CA-CB	5.62	1.60	1.54
1	D	121	VAL	CA-CB	-5.57	1.47	1.54
1	F	54	ILE	CA-CB	5.39	1.59	1.53
1	D	255	ILE	C-O	-5.26	1.18	1.24
1	F	307	LYS	C-O	-5.13	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	121	VAL	CB-CA-C	-7.91	101.56	111.92
1	A	121	VAL	CB-CA-C	-6.36	103.59	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	121	VAL	CB-CA-C	-5.96	104.42	111.94
1	B	121	VAL	CB-CA-C	-5.71	104.43	111.92
1	C	121	VAL	CB-CA-C	-5.33	105.23	111.94
1	D	121	VAL	CB-CA-C	-5.12	105.21	111.92

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	2233	0	2209	30	0
1	B	2241	0	2216	39	0
1	C	2237	0	2212	35	0
1	D	2237	0	2213	34	0
1	E	2249	0	2230	33	0
1	F	2242	0	2217	36	0
2	A	19	0	18	0	0
2	B	19	0	18	0	0
2	C	19	0	18	0	0
2	D	19	0	18	0	0
2	E	19	0	18	0	0
2	F	19	0	18	1	0
All	All	13553	0	13405	197	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 (197) 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:C:337:HIS:O	1:C:341:VAL:HG23	1.81	0.81
1:E:337:HIS:O	1:E:341:VAL:HG23	1.83	0.79
1:A:337:HIS:O	1:A:341:VAL:HG23	1.83	0.78
1:D:337:HIS:O	1:D:341:VAL:HG23	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:THR:HG22	1:D:333:GLN:O	1.86	0.74
1:A:159:THR:HG22	1:A:333:GLN:O	1.87	0.73
1:E:159:THR:HG22	1:E:333:GLN:O	1.90	0.70
1:B:337:HIS:O	1:B:341:VAL:HG23	1.95	0.67
1:D:52:LEU:HD23	1:D:106:GLU:OE2	1.98	0.64
1:B:192:LEU:C	1:B:193:LEU:HD23	2.23	0.64
1:E:344:GLU:N	1:E:344:GLU:OE2	2.31	0.64
1:D:344:GLU:N	1:D:344:GLU:OE2	2.31	0.63
1:C:192:LEU:C	1:C:193:LEU:HD23	2.23	0.63
1:B:72:LEU:HD23	1:B:73:GLY:N	2.13	0.63
1:F:192:LEU:C	1:F:193:LEU:HD23	2.24	0.63
1:D:253:MET:HE1	1:D:301:LEU:CD2	2.29	0.62
1:A:344:GLU:N	1:A:344:GLU:OE2	2.33	0.61
1:C:93:LYS:HD3	1:C:138:MET:HE1	1.83	0.61
1:B:160:GLU:HA	1:B:336:LEU:HD21	1.84	0.60
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.37	0.59
1:C:110:ARG:HG2	1:E:127:LEU:HD11	1.84	0.59
1:A:127:LEU:HD11	1:D:110:ARG:HG2	1.83	0.59
1:D:72:LEU:HD23	1:D:73:GLY:N	2.18	0.59
1:F:301:LEU:HD13	1:F:322:HIS:CD2	2.37	0.59
1:B:93:LYS:HD3	1:B:138:MET:HE1	1.85	0.59
1:C:344:GLU:N	1:C:344:GLU:OE2	2.35	0.59
1:B:344:GLU:N	1:B:344:GLU:OE2	2.36	0.58
1:E:146:LEU:HD13	1:E:203:LEU:HD21	1.85	0.58
1:D:93:LYS:HD3	1:D:138:MET:HE1	1.85	0.58
1:C:160:GLU:HA	1:C:336:LEU:HD21	1.85	0.58
1:C:146:LEU:O	1:C:150:ILE:HD13	2.04	0.58
1:D:160:GLU:HA	1:D:336:LEU:HD21	1.86	0.58
1:F:337:HIS:O	1:F:341:VAL:HG23	2.04	0.57
1:D:107:LEU:HD22	1:D:182:ILE:HG12	1.86	0.57
1:C:172:GLU:HG3	1:C:320:MET:HE1	1.87	0.57
1:A:258:CYS:SG	1:A:259:GLY:N	2.78	0.57
1:B:253:MET:HE1	1:B:301:LEU:CD2	2.35	0.57
1:A:94:MET:HG2	1:A:135:LEU:HD22	1.85	0.57
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.38	0.57
1:F:344:GLU:N	1:F:344:GLU:OE2	2.37	0.56
1:F:258:CYS:SG	1:F:259:GLY:N	2.78	0.56
1:C:52:LEU:HD23	1:C:106:GLU:OE2	2.06	0.56
1:D:75:ASN:HB3	1:D:95:LEU:HD22	1.88	0.55
1:E:94:MET:HG2	1:E:135:LEU:HD22	1.88	0.55
1:E:172:GLU:HG3	1:E:320:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:HIS:CE1	1:B:242:LYS:HB2	2.42	0.54
1:D:146:LEU:O	1:D:150:ILE:HD13	2.08	0.54
1:C:146:LEU:HD13	1:C:203:LEU:HD21	1.90	0.54
1:A:160:GLU:HA	1:A:336:LEU:HD21	1.90	0.54
1:B:159:THR:HG22	1:B:333:GLN:O	2.07	0.54
1:C:107:LEU:HD22	1:C:182:ILE:HG12	1.89	0.54
1:C:338:THR:O	1:C:342:LEU:HB2	2.08	0.54
1:F:107:LEU:HD22	1:F:182:ILE:HG12	1.89	0.54
1:F:159:THR:HG22	1:F:333:GLN:O	2.07	0.53
1:D:72:LEU:HD23	1:D:73:GLY:H	1.72	0.53
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.89	0.53
1:F:72:LEU:HD23	1:F:73:GLY:N	2.24	0.53
1:B:94:MET:HG2	1:B:135:LEU:HD22	1.89	0.53
1:B:107:LEU:HD22	1:B:182:ILE:HG12	1.90	0.53
1:F:75:ASN:HB3	1:F:95:LEU:HD22	1.91	0.53
1:F:193:LEU:HD23	1:F:193:LEU:N	2.24	0.53
1:B:193:LEU:HD23	1:B:193:LEU:N	2.23	0.52
1:C:72:LEU:HD23	1:C:73:GLY:H	1.74	0.52
1:C:258:CYS:SG	1:C:260:TYR:CE2	3.02	0.52
1:C:75:ASN:HB3	1:C:95:LEU:HD22	1.92	0.52
1:D:253:MET:HE1	1:D:301:LEU:HD21	1.93	0.51
1:B:258:CYS:SG	1:B:259:GLY:N	2.84	0.51
1:A:192:LEU:C	1:A:193:LEU:HD23	2.36	0.51
1:A:179:SER:HB3	1:B:281:MET:HE2	1.93	0.51
1:A:72:LEU:HD23	1:A:73:GLY:H	1.76	0.51
1:D:328:SER:O	1:D:331:VAL:HG12	2.11	0.51
1:C:46:PHE:CE1	1:C:48:VAL:HG21	2.46	0.50
1:F:94:MET:HG2	1:F:135:LEU:HD22	1.94	0.50
1:F:147:PHE:HB3	1:F:342:LEU:HD21	1.92	0.50
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.42	0.50
1:F:93:LYS:HD3	1:F:138:MET:HE1	1.94	0.50
1:A:75:ASN:HD22	1:A:93:LYS:CE	2.25	0.49
1:E:258:CYS:SG	1:E:259:GLY:N	2.85	0.49
1:E:233:GLU:HG2	1:F:310:PRO:HG3	1.93	0.49
1:D:94:MET:HG2	1:D:135:LEU:HD22	1.93	0.49
1:E:75:ASN:HD22	1:E:93:LYS:HE3	1.78	0.49
1:F:72:LEU:HD23	1:F:73:GLY:H	1.77	0.49
1:B:52:LEU:HD23	1:B:106:GLU:OE2	2.13	0.49
1:E:46:PHE:CE1	1:E:48:VAL:HG21	2.47	0.49
1:A:246:MET:HE2	1:A:315:THR:C	2.37	0.49
1:F:160:GLU:HA	1:F:336:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PHE:CE1	1:B:48:VAL:HG21	2.48	0.49
1:D:178:HIS:CE1	1:D:242:LYS:HB2	2.47	0.49
1:D:192:LEU:C	1:D:193:LEU:HD23	2.37	0.49
1:E:179:SER:HB3	1:F:281:MET:HE2	1.95	0.49
1:E:192:LEU:C	1:E:193:LEU:HD23	2.38	0.49
1:D:310:PRO:HG3	1:F:233:GLU:HG2	1.96	0.48
1:C:159:THR:HG22	1:C:333:GLN:O	2.12	0.48
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.49	0.48
1:E:52:LEU:HD23	1:E:106:GLU:OE2	2.14	0.48
1:D:233:GLU:HG2	1:E:310:PRO:HG3	1.95	0.47
1:D:258:CYS:SG	1:D:259:GLY:N	2.87	0.47
1:C:72:LEU:HD23	1:C:73:GLY:N	2.30	0.47
1:A:178:HIS:CE1	1:A:242:LYS:HB2	2.50	0.47
1:B:75:ASN:HD22	1:B:93:LYS:HE3	1.79	0.47
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.96	0.47
1:C:258:CYS:SG	1:C:259:GLY:N	2.87	0.47
1:E:107:LEU:HD22	1:E:182:ILE:HG12	1.95	0.47
1:C:75:ASN:HD22	1:C:93:LYS:HE3	1.80	0.47
1:C:188:LYS:HB2	1:C:189:PRO:CD	2.45	0.47
1:A:46:PHE:CE1	1:A:48:VAL:HG21	2.50	0.47
1:B:188:LYS:HB2	1:B:189:PRO:CD	2.46	0.46
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.50	0.46
1:B:338:THR:O	1:B:342:LEU:HB2	2.15	0.46
1:F:253:MET:HE1	1:F:301:LEU:CD2	2.46	0.46
1:B:146:LEU:HD13	1:B:203:LEU:HD21	1.98	0.46
1:E:300:MET:HE3	1:E:303:ARG:HB2	1.97	0.46
1:D:338:THR:O	1:D:342:LEU:HB2	2.16	0.46
1:B:149:ARG:NH2	1:B:198:ARG:O	2.49	0.46
1:A:233:GLU:HG2	1:B:310:PRO:HG3	1.98	0.46
1:C:328:SER:O	1:C:331:VAL:HG12	2.16	0.46
1:E:160:GLU:HA	1:E:336:LEU:HD21	1.97	0.46
1:B:174:ILE:HD11	1:B:187:VAL:HG21	1.97	0.45
1:F:246:MET:HE2	1:F:315:THR:C	2.41	0.45
1:F:167:MET:HE1	1:F:249:LEU:HG	1.97	0.45
1:E:178:HIS:CE1	1:E:242:LYS:HB2	2.52	0.45
1:E:338:THR:O	1:E:342:LEU:HB2	2.17	0.45
1:F:46:PHE:CE1	1:F:48:VAL:HG21	2.52	0.45
1:B:328:SER:O	1:B:331:VAL:HG12	2.17	0.45
1:A:146:LEU:HD13	1:A:203:LEU:HD21	1.99	0.44
1:A:75:ASN:HD22	1:A:93:LYS:HE3	1.82	0.44
1:E:258:CYS:SG	1:E:260:TYR:CE2	3.07	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:LEU:HD23	1:F:106:GLU:OE2	2.17	0.44
1:A:75:ASN:HB3	1:A:95:LEU:HD22	2.00	0.44
1:B:116:HIS:CE1	1:B:169:SER:HB2	2.53	0.44
1:C:160:GLU:CA	1:C:336:LEU:HD21	2.47	0.43
1:E:188:LYS:HB2	1:E:189:PRO:CD	2.47	0.43
1:F:74:ILE:H	1:F:74:ILE:HD12	1.83	0.43
1:C:116:HIS:CE1	1:C:169:SER:HB2	2.53	0.43
1:C:288:ASN:HB3	1:C:289:PRO:HA	2.01	0.43
1:D:258:CYS:SG	1:D:260:TYR:CE2	3.06	0.43
1:E:147:PHE:HB3	1:E:342:LEU:HD21	2.00	0.43
1:C:74:ILE:H	1:C:74:ILE:HD12	1.83	0.43
1:F:300:MET:HE3	1:F:303:ARG:HB2	2.01	0.43
1:F:75:ASN:HD22	1:F:93:LYS:HE3	1.84	0.43
1:B:46:PHE:CE1	1:B:48:VAL:CG2	3.02	0.43
1:D:188:LYS:HB2	1:D:189:PRO:CD	2.48	0.43
1:A:81:ILE:HD13	1:A:92:LEU:HB2	2.00	0.43
1:C:190:GLU:OE1	1:C:190:GLU:N	2.49	0.43
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.99	0.43
1:C:46:PHE:CE1	1:C:48:VAL:CG2	3.02	0.42
1:D:331:VAL:HG23	1:D:332:PRO:HD2	2.01	0.42
1:E:93:LYS:HD3	1:E:138:MET:HE1	2.01	0.42
1:A:107:LEU:HD22	1:A:182:ILE:HG12	2.00	0.42
1:D:118:VAL:HB	1:D:206:THR:HG22	2.00	0.42
1:F:145:GLU:HA	1:F:193:LEU:HD22	2.00	0.42
1:B:75:ASN:HB3	1:B:95:LEU:HD22	2.00	0.42
1:C:139:GLU:OE1	1:C:204:LYS:NZ	2.47	0.42
1:D:46:PHE:CE1	1:D:48:VAL:HG21	2.54	0.42
1:E:46:PHE:CE1	1:E:48:VAL:CG2	3.03	0.42
1:E:246:MET:HE2	1:E:315:THR:C	2.45	0.42
1:D:160:GLU:CA	1:D:336:LEU:HD21	2.47	0.42
1:E:116:HIS:CE1	1:E:169:SER:HB2	2.55	0.42
1:F:118:VAL:HG21	2:F:901:YRZ:H17	2.01	0.42
1:A:167:MET:HE2	1:A:253:MET:HE3	2.01	0.42
1:D:159:THR:HG21	1:D:333:GLN:HB3	2.02	0.42
1:F:118:VAL:HB	1:F:206:THR:HG22	2.02	0.42
1:B:74:ILE:H	1:B:74:ILE:HD12	1.85	0.41
1:B:253:MET:HE1	1:B:301:LEU:HD23	2.01	0.41
1:C:145:GLU:HA	1:C:193:LEU:HD22	2.01	0.41
1:D:246:MET:HE2	1:D:315:THR:C	2.45	0.41
1:E:72:LEU:HD23	1:E:73:GLY:H	1.85	0.41
1:E:146:LEU:HD13	1:E:203:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:CYS:SG	1:A:260:TYR:CE2	3.10	0.41
1:E:118:VAL:HB	1:E:206:THR:HG22	2.02	0.41
1:E:328:SER:O	1:E:331:VAL:HG12	2.20	0.41
1:A:338:THR:O	1:A:342:LEU:HB2	2.20	0.41
1:D:172:GLU:HG3	1:D:320:MET:HE1	2.02	0.41
1:D:188:LYS:HB2	1:D:189:PRO:HD2	2.01	0.41
1:A:52:LEU:HD23	1:A:106:GLU:OE2	2.21	0.41
1:F:46:PHE:CE1	1:F:48:VAL:CG2	3.04	0.41
1:F:188:LYS:HB2	1:F:189:PRO:CD	2.51	0.41
1:F:331:VAL:HG23	1:F:332:PRO:HD2	2.03	0.41
1:B:72:LEU:HD23	1:B:73:GLY:H	1.84	0.41
1:A:331:VAL:HG23	1:A:332:PRO:HD2	2.03	0.41
1:B:192:LEU:HD21	1:B:205:LEU:HD13	2.02	0.41
1:E:288:ASN:HB3	1:E:289:PRO:HA	2.02	0.41
1:F:253:MET:HE1	1:F:301:LEU:HD21	2.02	0.41
1:B:146:LEU:O	1:B:150:ILE:HD13	2.21	0.41
1:B:147:PHE:HB3	1:B:342:LEU:HD21	2.03	0.41
1:B:167:MET:HE1	1:B:249:LEU:HG	2.02	0.41
1:F:116:HIS:CE1	1:F:169:SER:HB2	2.56	0.41
1:F:167:MET:HE2	1:F:253:MET:HE3	2.02	0.41
1:F:172:GLU:HG3	1:F:320:MET:HE1	2.02	0.41
1:E:146:LEU:O	1:E:150:ILE:HD13	2.21	0.41
1:A:75:ASN:HB3	1:A:95:LEU:CD2	2.51	0.40
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.56	0.40
1:B:145:GLU:HA	1:B:193:LEU:HD22	2.03	0.40
1:C:193:LEU:HD23	1:C:193:LEU:N	2.35	0.40
1:C:118:VAL:HB	1:C:206:THR:HG22	2.03	0.40
1:A:72:LEU:HD23	1:A:73:GLY:N	2.36	0.40
1:B:117:ILE:O	1:B:118:VAL:C	2.63	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	272/324 (84%)	258 (95%)	14 (5%)	0	100	100
1	B	273/324 (84%)	258 (94%)	14 (5%)	1 (0%)	30	65
1	C	273/324 (84%)	257 (94%)	15 (6%)	1 (0%)	30	65
1	D	272/324 (84%)	257 (94%)	15 (6%)	0	100	100
1	E	273/324 (84%)	260 (95%)	12 (4%)	1 (0%)	30	65
1	F	273/324 (84%)	261 (96%)	11 (4%)	1 (0%)	30	65
All	All	1636/1944 (84%)	1551 (95%)	81 (5%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	272	SER
1	F	272	SER
1	B	272	SER
1	C	272	SER

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	243/293 (83%)	237 (98%)	6 (2%)	42	72
1	B	244/293 (83%)	238 (98%)	6 (2%)	42	72
1	C	243/293 (83%)	236 (97%)	7 (3%)	37	70
1	D	244/293 (83%)	238 (98%)	6 (2%)	42	72
1	E	246/293 (84%)	240 (98%)	6 (2%)	43	73
1	F	244/293 (83%)	235 (96%)	9 (4%)	30	64
All	All	1464/1758 (83%)	1424 (97%)	40 (3%)	39	71

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG

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Mol	Chain	Res	Type
1	A	159	THR
1	A	212	LYS
1	A	233	GLU
1	A	264	TYR
1	A	344	GLU
1	B	86	THR
1	B	149	ARG
1	B	233	GLU
1	B	241	ASP
1	B	264	TYR
1	B	336	LEU
1	C	86	THR
1	C	149	ARG
1	C	188	LYS
1	C	233	GLU
1	C	241	ASP
1	C	264	TYR
1	C	336	LEU
1	D	149	ARG
1	D	159	THR
1	D	188	LYS
1	D	233	GLU
1	D	264	TYR
1	D	292	SER
1	E	86	THR
1	E	149	ARG
1	E	156	GLN
1	E	188	LYS
1	E	233	GLU
1	E	264	TYR
1	F	86	THR
1	F	149	ARG
1	F	156	GLN
1	F	188	LYS
1	F	193	LEU
1	F	212	LYS
1	F	233	GLU
1	F	264	TYR
1	F	344	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	68	GLN
1	A	75	ASN
1	A	80	GLN
1	A	96	GLN
1	A	175	GLN
1	A	181	ASN
1	A	304	ASN
1	B	53	GLN
1	B	75	ASN
1	B	80	GLN
1	B	87	GLN
1	B	96	GLN
1	B	175	GLN
1	B	304	ASN
1	C	53	GLN
1	C	75	ASN
1	C	80	GLN
1	C	87	GLN
1	C	96	GLN
1	C	126	ASN
1	C	175	GLN
1	C	288	ASN
1	C	304	ASN
1	D	53	GLN
1	D	68	GLN
1	D	75	ASN
1	D	80	GLN
1	D	96	GLN
1	D	126	ASN
1	D	175	GLN
1	D	304	ASN
1	E	53	GLN
1	E	68	GLN
1	E	75	ASN
1	E	80	GLN
1	E	87	GLN
1	E	96	GLN
1	E	156	GLN
1	E	175	GLN
1	E	184	HIS
1	E	200	ASN
1	E	304	ASN

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Mol	Chain	Res	Type
1	F	53	GLN
1	F	75	ASN
1	F	80	GLN
1	F	87	GLN
1	F	96	GLN
1	F	156	GLN
1	F	175	GLN
1	F	181	ASN
1	F	304	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	YRZ	B	901	-	19,22,22	1.60	3 (15%)	19,31,31	3.37	7 (36%)
2	YRZ	E	901	-	19,22,22	1.59	3 (15%)	19,31,31	3.33	7 (36%)
2	YRZ	F	901	-	19,22,22	1.59	3 (15%)	19,31,31	3.53	7 (36%)
2	YRZ	A	901	-	19,22,22	1.56	3 (15%)	19,31,31	3.36	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YRZ	C	901	-	19,22,22	1.54	2 (10%)	19,31,31	3.13	6 (31%)
2	YRZ	D	901	-	19,22,22	1.65	3 (15%)	19,31,31	3.27	7 (36%)

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	YRZ	B	901	-	-	1/4/18/18	0/4/4/4
2	YRZ	E	901	-	-	1/4/18/18	0/4/4/4
2	YRZ	F	901	-	-	1/4/18/18	0/4/4/4
2	YRZ	A	901	-	-	0/4/18/18	0/4/4/4
2	YRZ	C	901	-	-	1/4/18/18	0/4/4/4
2	YRZ	D	901	-	-	1/4/18/18	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	YRZ	C13-N12	-5.23	1.31	1.39
2	D	901	YRZ	C13-N12	-5.19	1.31	1.39
2	C	901	YRZ	C13-N12	-5.13	1.31	1.39
2	B	901	YRZ	C13-N12	-4.90	1.32	1.39
2	A	901	YRZ	C13-N12	-4.81	1.32	1.39
2	E	901	YRZ	C13-N12	-4.72	1.32	1.39
2	E	901	YRZ	N12-N16	3.17	1.43	1.37
2	A	901	YRZ	N12-N16	2.72	1.42	1.37
2	B	901	YRZ	C2-C1	2.68	1.46	1.38
2	D	901	YRZ	C2-C1	2.54	1.45	1.38
2	B	901	YRZ	N12-N16	2.50	1.42	1.37
2	C	901	YRZ	C2-C1	2.49	1.45	1.38
2	F	901	YRZ	C2-C1	2.46	1.45	1.38
2	E	901	YRZ	C2-C1	2.43	1.45	1.38
2	D	901	YRZ	N12-N16	2.41	1.41	1.37
2	F	901	YRZ	N12-N16	2.40	1.41	1.37
2	A	901	YRZ	C2-C1	2.19	1.44	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	YRZ	N12-C13-N18	8.43	127.60	121.49
2	B	901	YRZ	N12-C13-N18	8.24	127.47	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	YRZ	C15-C14-C13	8.08	110.06	104.54
2	C	901	YRZ	N12-C13-N18	7.92	127.24	121.49
2	D	901	YRZ	C15-C14-C13	7.89	109.93	104.54
2	A	901	YRZ	N12-C13-N18	7.84	127.17	121.49
2	F	901	YRZ	C15-C14-C13	7.68	109.79	104.54
2	D	901	YRZ	N12-C13-N18	7.67	127.06	121.49
2	B	901	YRZ	C15-C14-C13	7.63	109.75	104.54
2	E	901	YRZ	N12-C13-N18	7.47	126.91	121.49
2	E	901	YRZ	C15-C14-C13	7.44	109.62	104.54
2	F	901	YRZ	C2-N12-C13	-7.36	117.23	123.31
2	E	901	YRZ	C2-N12-C13	-7.12	117.43	123.31
2	C	901	YRZ	C15-C14-C13	7.11	109.39	104.54
2	A	901	YRZ	C2-N12-C13	-6.60	117.86	123.31
2	B	901	YRZ	C2-N12-C13	-6.54	117.91	123.31
2	D	901	YRZ	C2-N12-C13	-5.97	118.38	123.31
2	C	901	YRZ	C2-N12-C13	-5.81	118.52	123.31
2	F	901	YRZ	C1-C17-N18	-4.86	115.74	121.18
2	E	901	YRZ	C1-C17-N18	-4.48	116.17	121.18
2	D	901	YRZ	C1-C17-N18	-4.36	116.31	121.18
2	C	901	YRZ	C1-C17-N18	-4.18	116.50	121.18
2	B	901	YRZ	C1-C17-N18	-4.13	116.56	121.18
2	A	901	YRZ	C1-C17-N18	-4.03	116.67	121.18
2	B	901	YRZ	N19-C17-N18	2.90	124.01	119.70
2	D	901	YRZ	N19-C17-N18	2.81	123.87	119.70
2	F	901	YRZ	N19-C17-N18	2.80	123.85	119.70
2	A	901	YRZ	N19-C17-N18	2.65	123.64	119.70
2	F	901	YRZ	C14-C15-N16	-2.62	108.67	112.37
2	A	901	YRZ	C14-C15-N16	-2.58	108.72	112.37
2	E	901	YRZ	N19-C17-N18	2.57	123.51	119.70
2	D	901	YRZ	C14-C15-N16	-2.52	108.80	112.37
2	C	901	YRZ	C14-C15-N16	-2.47	108.87	112.37
2	C	901	YRZ	N19-C17-N18	2.36	123.20	119.70
2	E	901	YRZ	C14-C15-N16	-2.30	109.11	112.37
2	B	901	YRZ	C14-C15-N16	-2.29	109.12	112.37
2	E	901	YRZ	C4-C5-C1	-2.23	100.21	103.78
2	B	901	YRZ	C4-C5-C1	-2.23	100.21	103.78
2	F	901	YRZ	C4-C5-C1	-2.07	100.46	103.78
2	D	901	YRZ	C4-C5-C1	-2.01	100.55	103.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

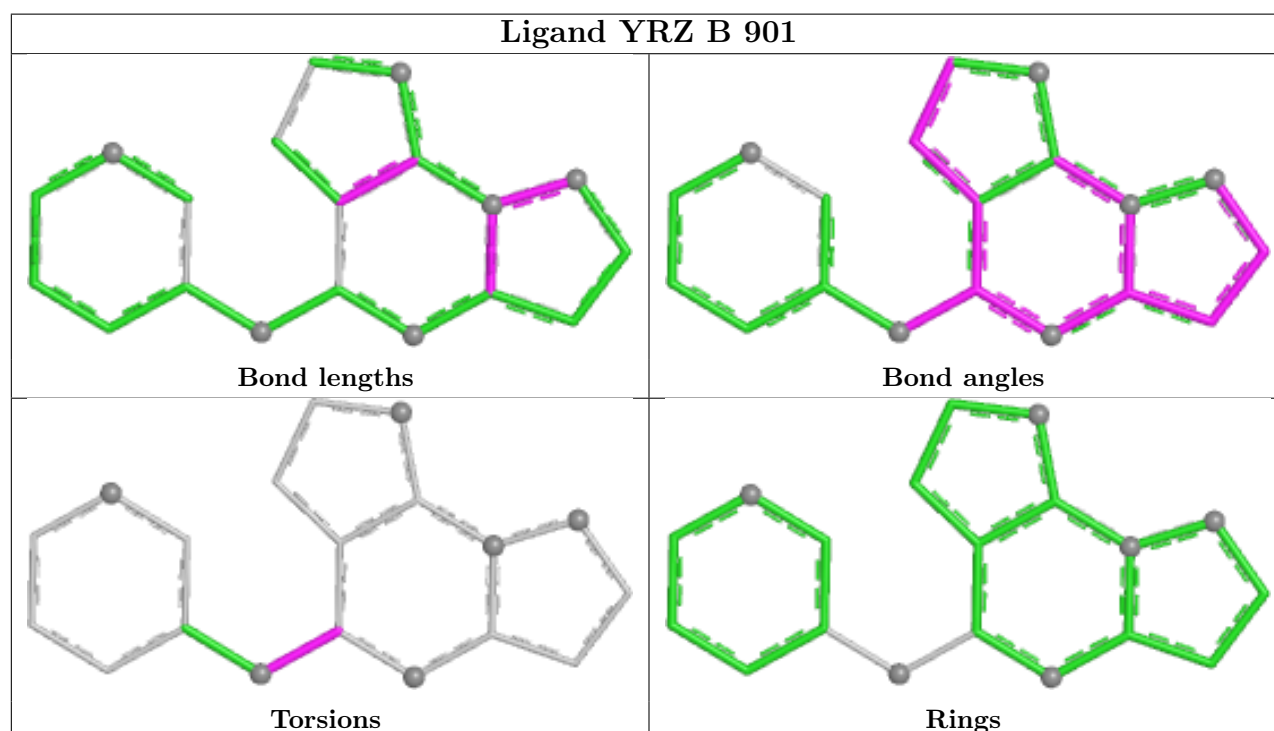
Mol	Chain	Res	Type	Atoms
2	E	901	YRZ	N18-C17-N19-C6
2	F	901	YRZ	N18-C17-N19-C6
2	B	901	YRZ	N18-C17-N19-C6
2	C	901	YRZ	N18-C17-N19-C6
2	D	901	YRZ	N18-C17-N19-C6

There are no ring outliers.

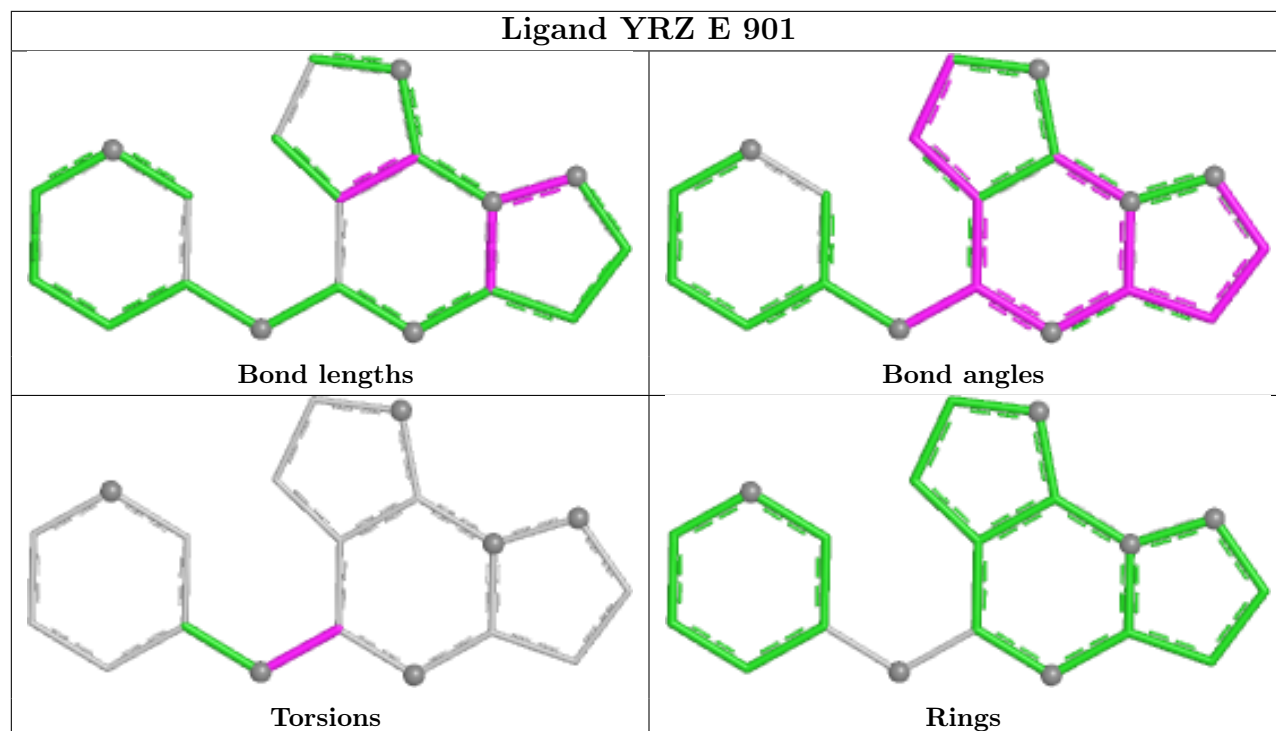
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	YRZ	1	0

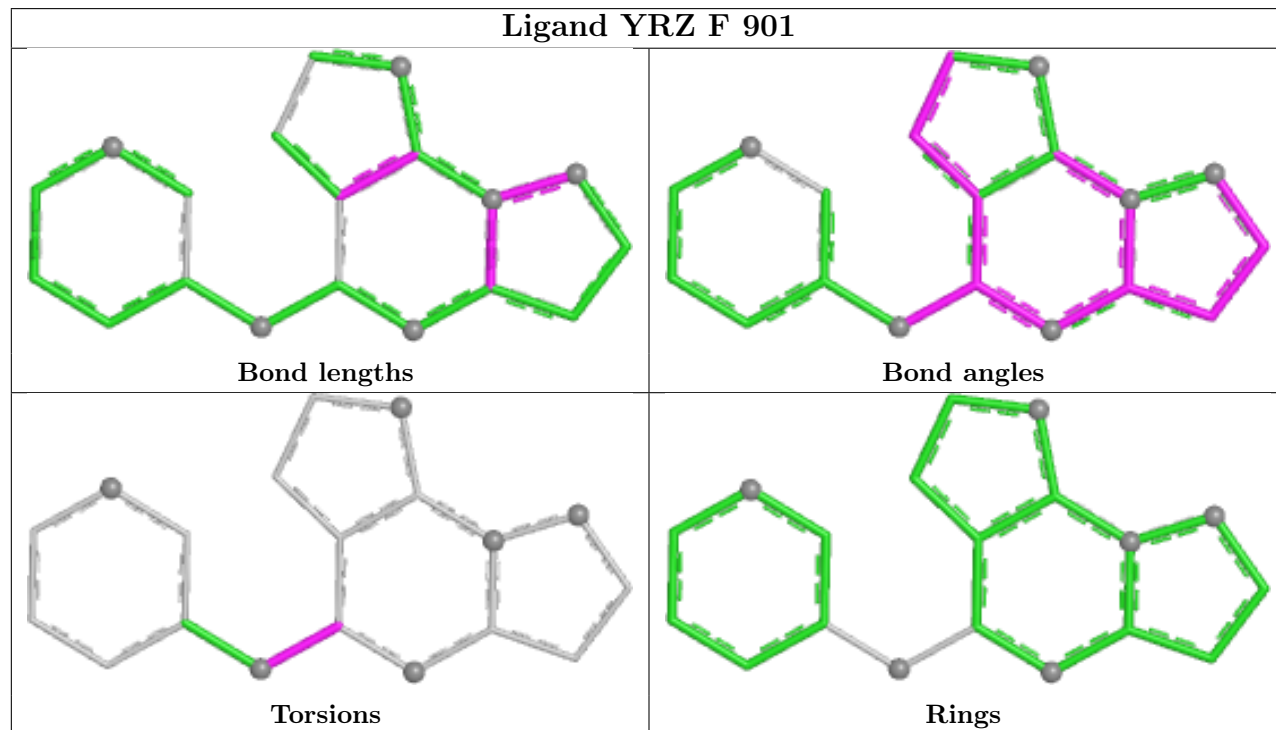
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



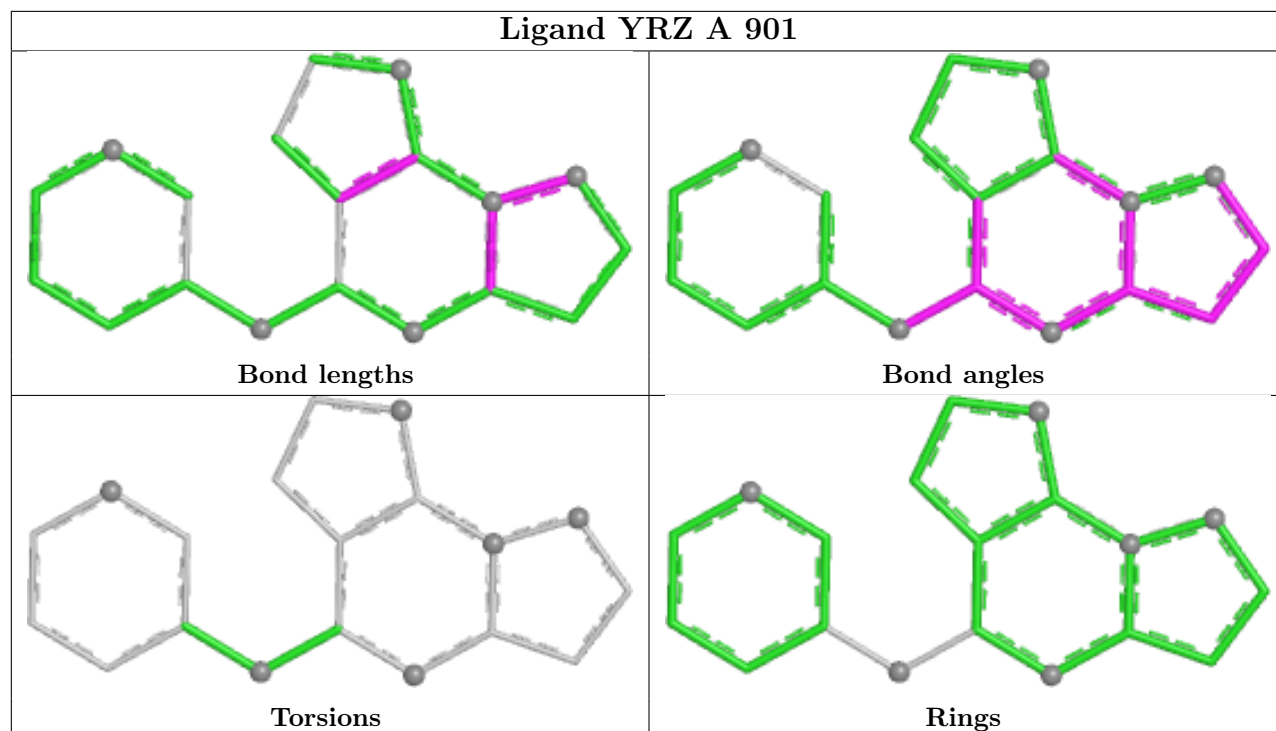
Ligand YRZ E 901



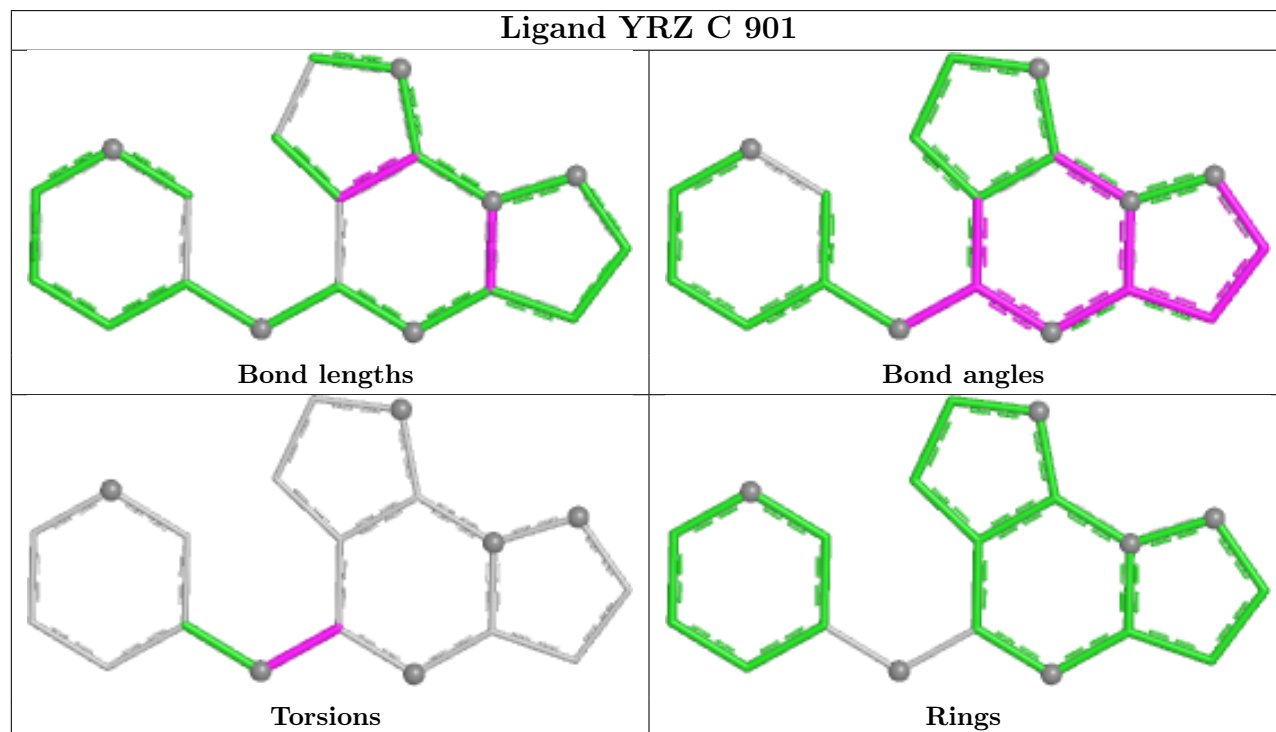
Ligand YRZ F 901

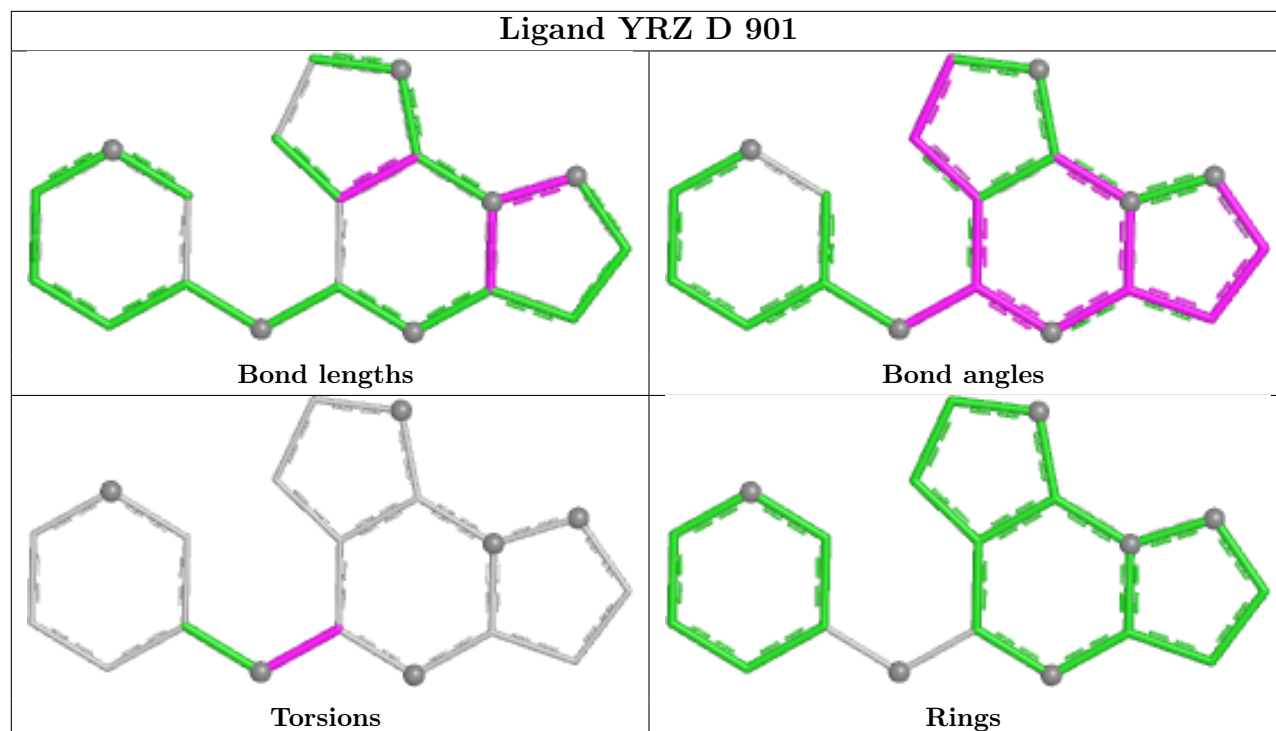


Ligand YRZ A 901



Ligand YRZ C 901





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	282/324 (87%)	0.67	28 (9%)	13 7	49, 75, 116, 133	0
1	B	283/324 (87%)	0.65	26 (9%)	14 8	49, 76, 116, 131	0
1	C	283/324 (87%)	0.65	27 (9%)	14 7	49, 76, 115, 130	0
1	D	282/324 (87%)	0.65	24 (8%)	16 8	48, 75, 113, 130	0
1	E	283/324 (87%)	0.67	27 (9%)	14 7	49, 76, 118, 132	0
1	F	283/324 (87%)	0.66	27 (9%)	14 7	49, 76, 119, 131	0
All	All	1696/1944 (87%)	0.66	159 (9%)	14 7	48, 76, 117, 133	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	271	ILE	7.5
1	B	271	ILE	7.5
1	C	271	ILE	7.0
1	C	347	GLU	7.0
1	F	271	ILE	6.8
1	A	347	GLU	6.7
1	F	347	GLU	6.6
1	E	347	GLU	6.5
1	D	271	ILE	6.4
1	D	347	GLU	6.3
1	A	271	ILE	6.2
1	B	347	GLU	6.2
1	D	157	ALA	6.1
1	E	227	PRO	6.0
1	B	227	PRO	6.0
1	D	227	PRO	5.8
1	F	227	PRO	5.5
1	C	227	PRO	5.3
1	A	157	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	227	PRO	5.1
1	C	154	GLY	5.1
1	C	157	ALA	4.3
1	B	154	GLY	4.3
1	F	329	THR	4.2
1	C	329	THR	4.0
1	D	153	ARG	4.0
1	D	234	VAL	3.9
1	D	329	THR	3.8
1	F	346	LYS	3.7
1	A	234	VAL	3.6
1	A	329	THR	3.6
1	B	329	THR	3.6
1	E	329	THR	3.6
1	D	346	LYS	3.5
1	A	273	PRO	3.5
1	B	157	ALA	3.5
1	E	346	LYS	3.4
1	E	345	ASP	3.4
1	B	273	PRO	3.4
1	E	234	VAL	3.4
1	A	153	ARG	3.3
1	C	345	ASP	3.3
1	F	345	ASP	3.3
1	C	234	VAL	3.3
1	D	264	TYR	3.2
1	E	289	PRO	3.2
1	F	234	VAL	3.2
1	E	228	TYR	3.2
1	A	346	LYS	3.2
1	B	234	VAL	3.2
1	F	273	PRO	3.2
1	E	264	TYR	3.1
1	E	334	THR	3.1
1	C	241	ASP	3.1
1	C	339	SER	3.0
1	E	241	ASP	3.0
1	E	74	ILE	3.0
1	C	346	LYS	3.0
1	F	293	GLU	3.0
1	A	264	TYR	3.0
1	F	241	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	334	THR	3.0
1	A	228	TYR	2.9
1	D	345	ASP	2.9
1	B	346	LYS	2.9
1	D	289	PRO	2.9
1	A	345	ASP	2.9
1	A	334	THR	2.9
1	C	228	TYR	2.9
1	B	241	ASP	2.9
1	D	273	PRO	2.8
1	C	264	TYR	2.8
1	F	264	TYR	2.8
1	A	74	ILE	2.8
1	E	156	GLN	2.8
1	B	74	ILE	2.7
1	B	264	TYR	2.7
1	D	74	ILE	2.7
1	A	241	ASP	2.7
1	C	273	PRO	2.7
1	A	289	PRO	2.7
1	F	289	PRO	2.7
1	B	345	ASP	2.7
1	D	339	SER	2.7
1	E	339	SER	2.7
1	C	326	MET	2.7
1	B	228	TYR	2.6
1	D	334	THR	2.6
1	E	273	PRO	2.6
1	E	94	MET	2.6
1	F	157	ALA	2.6
1	A	339	SER	2.6
1	D	241	ASP	2.6
1	C	289	PRO	2.5
1	F	156	GLN	2.5
1	E	337	HIS	2.5
1	F	198	ARG	2.4
1	D	228	TYR	2.4
1	C	74	ILE	2.4
1	A	342	LEU	2.4
1	A	285	GLU	2.4
1	F	238	GLU	2.4
1	E	157	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	265	SER	2.4
1	C	94	MET	2.4
1	F	74	ILE	2.4
1	A	75	ASN	2.3
1	F	341	VAL	2.3
1	B	339	SER	2.3
1	A	332	PRO	2.3
1	F	199	PRO	2.3
1	A	142	ASP	2.3
1	D	235	LEU	2.3
1	D	47	HIS	2.3
1	F	330	LYS	2.3
1	F	334	THR	2.3
1	C	75	ASN	2.3
1	F	288	ASN	2.2
1	E	212	LYS	2.2
1	B	94	MET	2.2
1	A	238	GLU	2.2
1	E	342	LEU	2.2
1	A	341	VAL	2.2
1	C	215	THR	2.2
1	B	238	GLU	2.2
1	F	342	LEU	2.2
1	A	337	HIS	2.2
1	F	337	HIS	2.2
1	B	334	THR	2.2
1	A	326	MET	2.2
1	B	337	HIS	2.2
1	B	289	PRO	2.2
1	C	197	LYS	2.2
1	E	238	GLU	2.2
1	E	198	ARG	2.1
1	C	337	HIS	2.1
1	A	293	GLU	2.1
1	D	198	ARG	2.1
1	D	293	GLU	2.1
1	C	341	VAL	2.1
1	B	198	ARG	2.1
1	F	75	ASN	2.1
1	F	94	MET	2.1
1	F	228	TYR	2.1
1	D	197	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	341	VAL	2.1
1	B	75	ASN	2.1
1	C	46	PHE	2.1
1	B	293	GLU	2.1
1	B	128	TYR	2.1
1	A	216	SER	2.0
1	B	341	VAL	2.0
1	E	341	VAL	2.0
1	B	235	LEU	2.0
1	C	129	ALA	2.0
1	E	293	GLU	2.0
1	E	216	SER	2.0
1	C	238	GLU	2.0
1	D	94	MET	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 oligosaccharides in this entry.

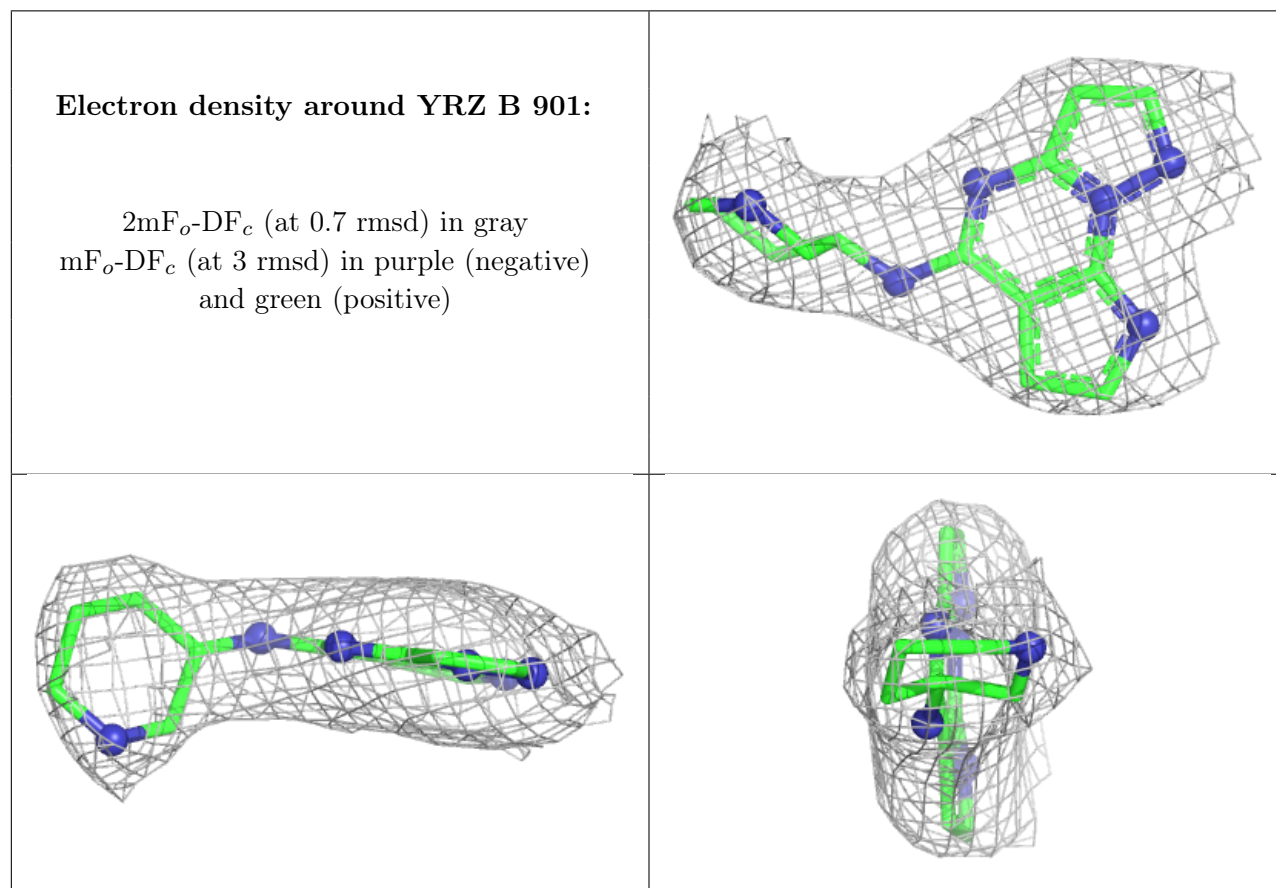
6.4 Ligands [i](#)

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
2	YRZ	B	901	19/19	0.96	0.09	72,73,76,77	0
2	YRZ	C	901	19/19	0.96	0.10	71,72,79,80	0
2	YRZ	A	901	19/19	0.97	0.09	67,68,71,73	0
2	YRZ	D	901	19/19	0.97	0.09	68,70,72,73	0
2	YRZ	E	901	19/19	0.97	0.09	66,68,74,74	0
2	YRZ	F	901	19/19	0.97	0.10	69,70,76,76	0

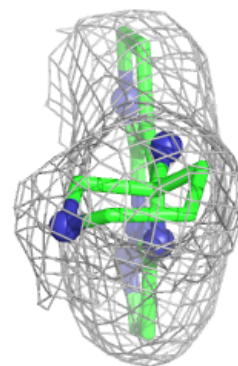
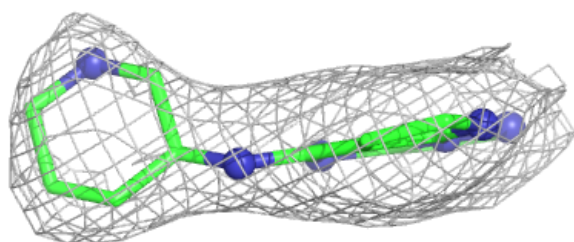
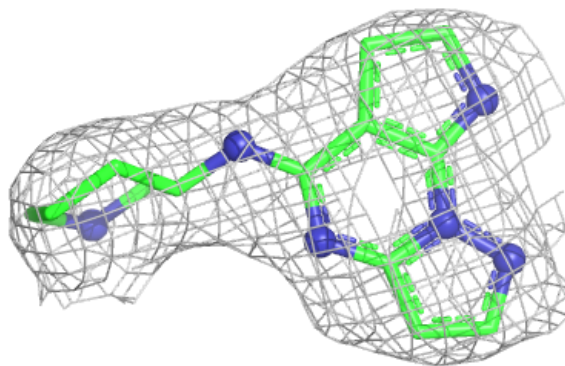
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

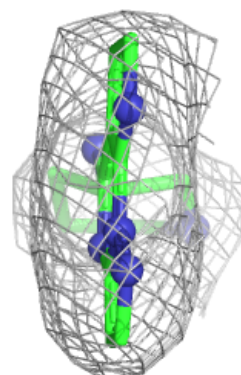
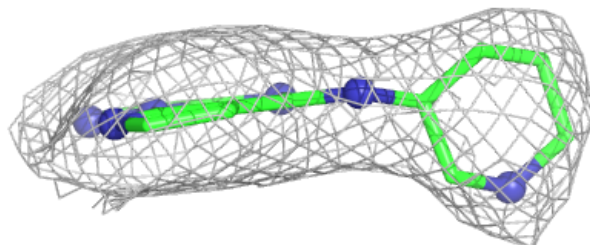
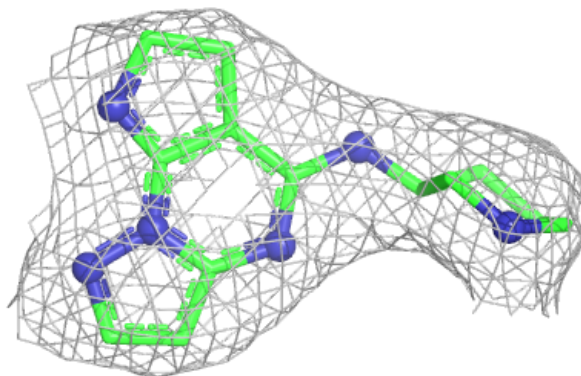


Electron density around YRZ C 901:

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

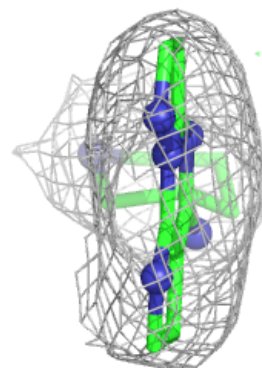
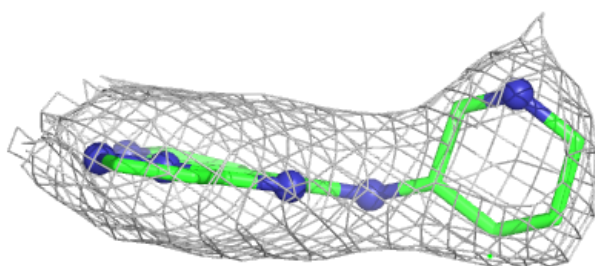
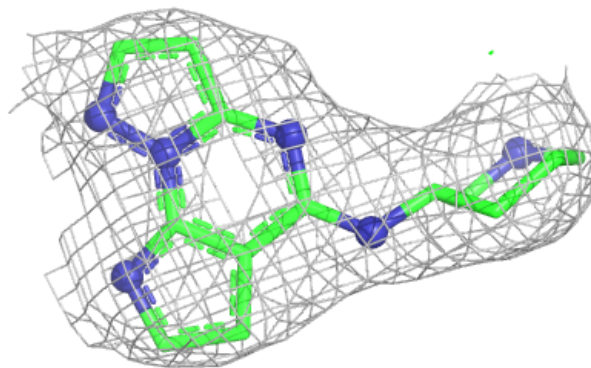
**Electron density around YRZ A 901:**

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

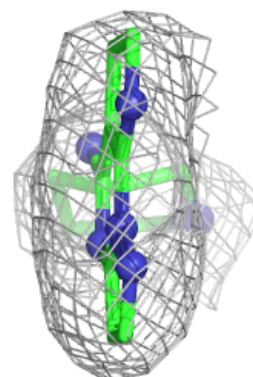
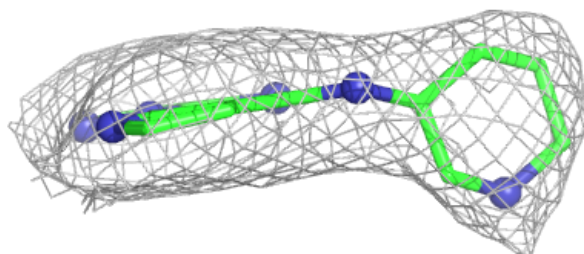
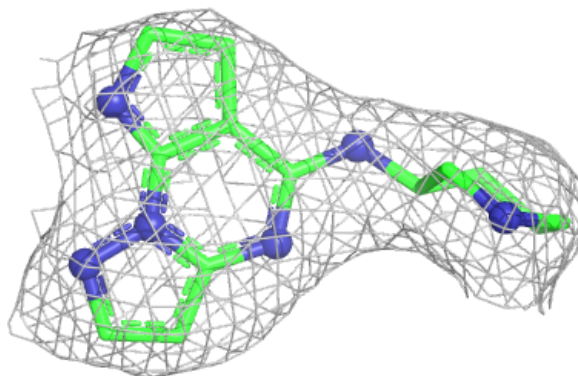


Electron density around YRZ D 901:

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

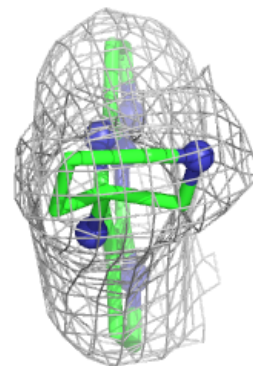
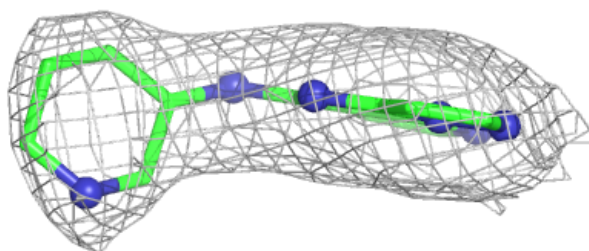
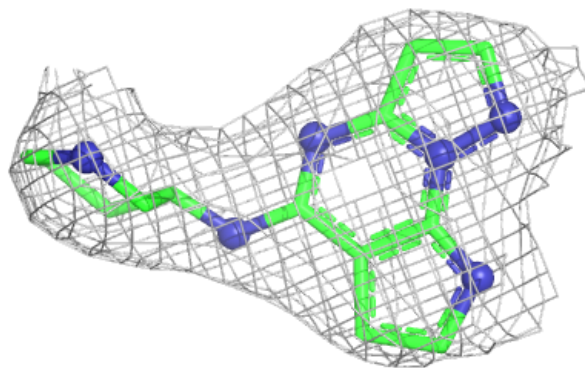
**Electron density around YRZ E 901:**

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



Electron density around YRZ F 901:

$2mF_o - DF_c$ (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.