



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:24 PM UTC

PDB ID : 5KX8 / pdb_00005kx8
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2016-07-20
Resolution : 2.67 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

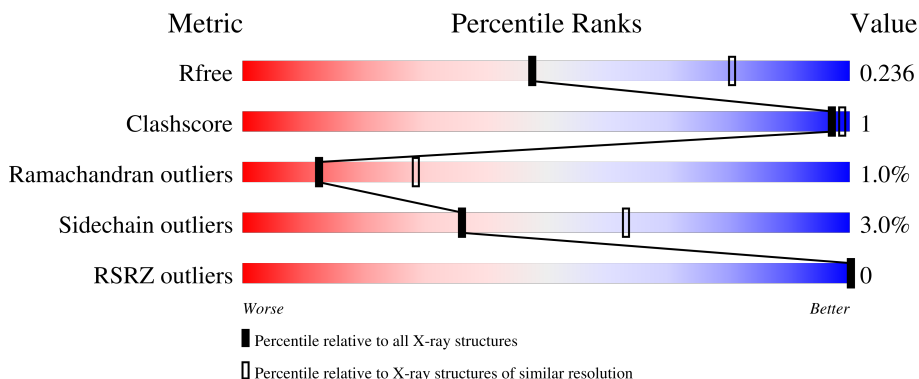
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	301	88% 6% . .
1	B	301	88% 5% . 7%
1	C	301	89% 7% .
1	D	301	89% 5% . 5%

2 Entry composition [i](#)

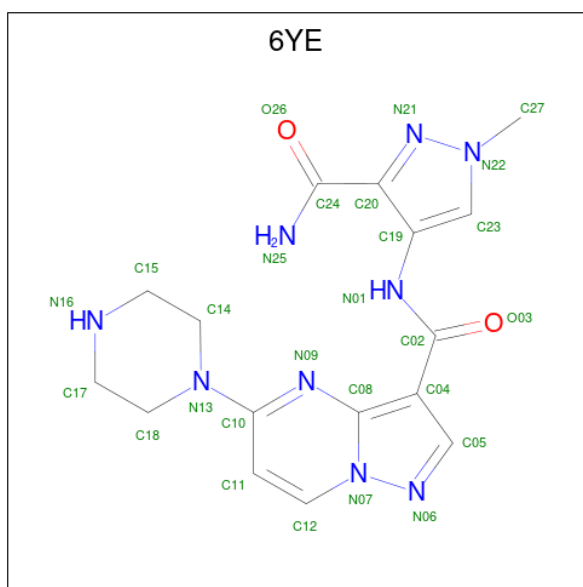
There are 3 unique types of molecules in this entry. The entry contains 9115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	3
			2262	1415	382	448	3	14			
1	B	281	Total	C	N	O	P	S	0	0	2
			2204	1381	371	435	3	14			
1	C	290	Total	C	N	O	P	S	0	0	3
			2260	1415	379	449	3	14			
1	D	286	Total	C	N	O	P	S	0	0	1
			2254	1412	380	445	3	14			

- Molecule 2 is {N}-(3-aminocarbonyl-1-methyl-pyrazol-4-yl)-5-piperazin-1-yl-pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: 6YE) (formula: C₁₆H₁₉N₉O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	16	9	2		
2	B	1	Total	C	N	O	0	0
			27	16	9	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			27	16	9	2		
2	D	1	Total	C	N	O	0	0
			27	16	9	2		

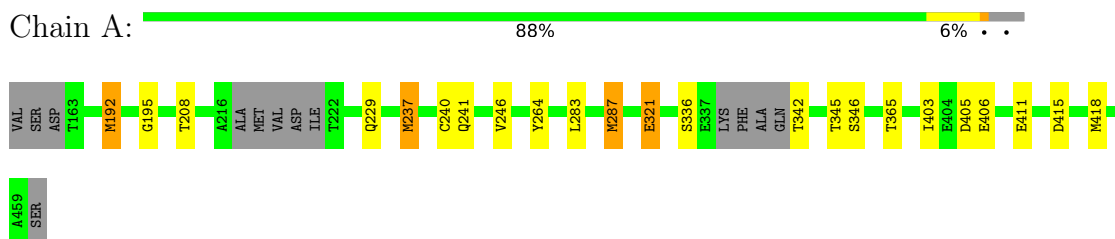
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	9	Total	O	0	0
			9	9		
3	D	8	Total	O	0	0
			8	8		

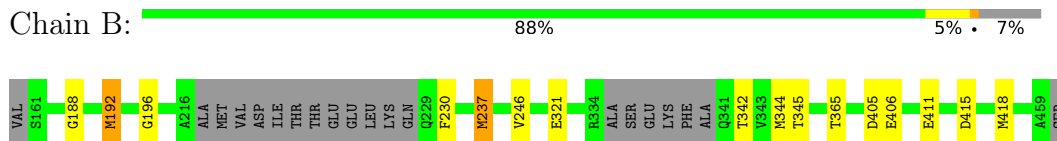
3 Residue-property plots [i](#)

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.

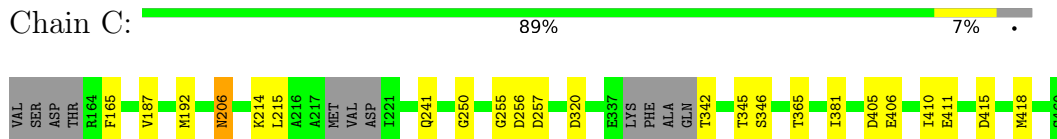
- Molecule 1: Interleukin-1 receptor-associated kinase 4



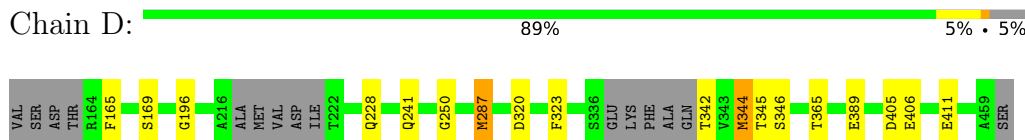
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.70Å 139.88Å 87.44Å 90.00° 125.25° 90.00°	Depositor
Resolution (Å)	45.00 – 2.67 45.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.00-2.67) 87.8 (45.00-2.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.204 , 0.233 0.210 , 0.236	Depositor DCC
R_{free} test set	2015 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 80.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.186 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9115	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2729e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP, 6YE

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	0.88	2/2266 (0.1%)	1.10	4/3053 (0.1%)
1	B	0.88	1/2207 (0.0%)	1.10	3/2972 (0.1%)
1	C	0.88	1/2264 (0.0%)	1.11	3/3051 (0.1%)
1	D	0.88	1/2258 (0.0%)	1.09	3/3042 (0.1%)
All	All	0.88	5/8995 (0.1%)	1.10	13/12118 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	MET	SD-CE	-9.23	1.56	1.79
1	A	192	MET	SD-CE	-8.85	1.57	1.79
1	B	237	MET	SD-CE	-7.21	1.61	1.79
1	D	287	MET	SD-CE	-5.74	1.65	1.79
1	A	237	MET	SD-CE	-5.17	1.66	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	ASP	CA-C-N	5.86	132.73	121.54
1	A	405	ASP	C-N-CA	5.86	132.73	121.54
1	C	405	ASP	CA-C-N	5.80	132.61	121.54
1	C	405	ASP	C-N-CA	5.80	132.61	121.54
1	A	195	GLY	N-CA-C	-5.79	104.07	112.17
1	A	240	CYS	N-CA-C	5.71	118.01	108.02
1	D	405	ASP	CA-C-N	5.71	132.45	121.54
1	D	405	ASP	C-N-CA	5.71	132.45	121.54
1	D	320	ASP	CA-CB-CG	5.67	118.28	112.60
1	B	405	ASP	CA-C-N	5.67	132.38	121.54
1	B	405	ASP	C-N-CA	5.67	132.38	121.54
1	B	230	PHE	CA-CB-CG	5.66	119.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	ASP	CA-CB-CG	5.55	118.15	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	2262	0	2221	4	0
1	B	2204	0	2155	5	0
1	C	2260	0	2212	3	0
1	D	2254	0	2216	4	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	9	0	0	0	0
3	D	8	0	0	0	0
All	All	9115	0	8804	16	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 1.

All (16) 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:287:MET:HE2	1:D:323:PHE:HB2	1.75	0.67
1:A:283:LEU:HD23	1:A:287:MET:HE2	1.86	0.57
1:B:192:MET:HG2	2:B:501:6YE:C20	2.36	0.56
1:D:287:MET:CE	1:D:323:PHE:HB2	2.40	0.49
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.95	0.48
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.95	0.48
1:A:237:MET:HE1	1:A:246:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:HE1	1:A:264:TYR:CE1	2.50	0.45
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.97	0.45
1:B:237:MET:CE	1:B:246:VAL:HG23	2.46	0.45
1:D:344:MET:HE3	1:D:344:MET:HB3	1.94	0.43
1:C:165:PHE:HB3	1:C:250:GLY:HA2	2.00	0.43
1:B:237:MET:HE1	1:B:246:VAL:O	2.19	0.43
1:C:381:ILE:HG21	1:C:410:ILE:HD11	2.01	0.43
1:B:237:MET:HE1	1:B:246:VAL:HG23	2.02	0.41
1:D:165:PHE:HB3	1:D:250:GLY:HA2	2.04	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	280/301 (93%)	266 (95%)	12 (4%)	2 (1%)	18	37
1	B	272/301 (90%)	253 (93%)	15 (6%)	4 (2%)	8	19
1	C	282/301 (94%)	265 (94%)	14 (5%)	3 (1%)	11	26
1	D	278/301 (92%)	265 (95%)	11 (4%)	2 (1%)	18	37
All	All	1112/1204 (92%)	1049 (94%)	52 (5%)	11 (1%)	12	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	406	GLU
1	D	406	GLU
1	B	321	GLU
1	C	206	ASN

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Mol	Chain	Res	Type
1	C	255	GLY
1	D	196	GLY
1	A	321	GLU
1	B	196	GLY
1	B	188	GLY

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	247/259 (95%)	238 (96%)	9 (4%)	31	57
1	B	240/259 (93%)	236 (98%)	4 (2%)	53	77
1	C	245/259 (95%)	236 (96%)	9 (4%)	30	56
1	D	246/259 (95%)	239 (97%)	7 (3%)	38	65
All	All	978/1036 (94%)	949 (97%)	29 (3%)	36	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	229	GLN
1	A	241	GLN
1	A	287	MET
1	A	321	GLU
1	A	336	SER
1	A	365	THR
1	A	403	ILE
1	A	411	GLU
1	B	192	MET
1	B	344	MET
1	B	365	THR
1	B	411	GLU
1	C	187	VAL
1	C	206	ASN
1	C	214	LYS

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Mol	Chain	Res	Type
1	C	215	LEU
1	C	241	GLN
1	C	256	ASP
1	C	257	ASP
1	C	365	THR
1	C	411	GLU
1	D	169	SER
1	D	228	GLN
1	D	241	GLN
1	D	344	MET
1	D	365	THR
1	D	389	GLU
1	D	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	297	ASN
1	A	316	ASN
1	A	451	GLN
1	B	207	ASN
1	B	297	ASN
1	B	316	ASN
1	B	390	HIS
1	B	451	GLN
1	C	179	ASN
1	C	297	ASN
1	C	316	ASN
1	C	451	GLN
1	D	178	ASN
1	D	190	ASN
1	D	286	HIS
1	D	297	ASN
1	D	316	ASN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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
1	TPO	C	345	1	8,10,11	1.25	1 (12%)	10,14,16	1.29	1 (10%)
1	TPO	D	345	1	8,10,11	1.32	1 (12%)	10,14,16	1.36	2 (20%)
1	SEP	B	346	1	8,9,10	0.75	0	7,12,14	0.77	0
1	TPO	B	345	1	8,10,11	1.09	0	10,14,16	1.30	1 (10%)
1	SEP	D	346	1	8,9,10	1.12	1 (12%)	7,12,14	0.67	0
1	TPO	B	342	1	8,10,11	0.98	1 (12%)	10,14,16	1.53	1 (10%)
1	TPO	A	345	1	8,10,11	0.99	0	10,14,16	1.25	1 (10%)
1	SEP	C	346	1	8,9,10	1.09	1 (12%)	7,12,14	0.71	0
1	SEP	A	346	1	8,9,10	0.94	0	7,12,14	1.04	1 (14%)
1	TPO	D	342	1	8,10,11	1.14	1 (12%)	10,14,16	1.52	1 (10%)
1	TPO	C	342	1	8,10,11	0.98	0	10,14,16	1.52	2 (20%)
1	TPO	A	342	1	8,10,11	1.03	1 (12%)	10,14,16	1.48	1 (10%)

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
1	TPO	C	345	1	-	2/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	B	342	1	-	2/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	D	342	1	-	2/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	P-OG1	-2.68	1.54	1.59
1	D	342	TPO	P-OG1	-2.51	1.55	1.59
1	C	345	TPO	P-OG1	-2.49	1.55	1.59
1	D	346	SEP	P-O1P	2.25	1.57	1.50
1	C	346	SEP	P-O1P	2.09	1.57	1.50
1	B	342	TPO	P-OG1	-2.01	1.56	1.59
1	A	342	TPO	P-OG1	-2.01	1.56	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	P-OG1-CB	-3.46	113.93	123.33
1	C	342	TPO	P-OG1-CB	-3.37	114.17	123.33
1	A	342	TPO	P-OG1-CB	-3.37	114.18	123.33
1	D	342	TPO	P-OG1-CB	-3.35	114.23	123.33
1	C	345	TPO	P-OG1-CB	-2.53	116.44	123.33
1	D	345	TPO	P-OG1-CB	-2.43	116.71	123.33
1	A	345	TPO	P-OG1-CB	-2.38	116.87	123.33
1	B	345	TPO	P-OG1-CB	-2.32	117.02	123.33
1	A	346	SEP	OG-CB-CA	2.22	110.30	108.14
1	D	345	TPO	O3P-P-OG1	2.09	114.00	105.85
1	C	342	TPO	O3P-P-OG1	2.04	113.82	105.85

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	C	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
1	B	342	TPO	CB-OG1-P-O3P
1	D	342	TPO	CB-OG1-P-O3P
1	A	342	TPO	C-CA-CB-CG2
1	B	342	TPO	C-CA-CB-CG2
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	O-C-CA-CB
1	D	342	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	6YE	C	501	-	29,30,30	1.30	4 (13%)	32,43,43	1.16	3 (9%)
2	6YE	A	501	-	29,30,30	1.67	4 (13%)	32,43,43	1.40	7 (21%)
2	6YE	B	501	-	29,30,30	1.29	4 (13%)	32,43,43	1.50	6 (18%)
2	6YE	D	501	-	29,30,30	1.33	5 (17%)	32,43,43	1.23	3 (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	6YE	C	501	-	-	0/16/24/24	0/4/4/4
2	6YE	A	501	-	-	2/16/24/24	0/4/4/4
2	6YE	B	501	-	-	0/16/24/24	0/4/4/4
2	6YE	D	501	-	-	0/16/24/24	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6YE	C23-C19	5.72	1.44	1.36
2	B	501	6YE	C23-C19	4.13	1.42	1.36
2	C	501	6YE	C10-N09	3.93	1.40	1.33
2	A	501	6YE	C08-N07	3.86	1.45	1.38
2	D	501	6YE	C08-N07	3.69	1.44	1.38
2	D	501	6YE	C04-C08	-3.35	1.36	1.45
2	C	501	6YE	C23-C19	3.30	1.41	1.36
2	C	501	6YE	C04-C08	-3.16	1.37	1.45
2	A	501	6YE	C10-N09	3.07	1.39	1.33
2	D	501	6YE	C23-C19	2.96	1.40	1.36
2	A	501	6YE	C05-N06	2.87	1.37	1.32
2	B	501	6YE	C08-N07	2.86	1.43	1.38
2	B	501	6YE	C04-C08	-2.65	1.38	1.45
2	D	501	6YE	C10-N09	2.35	1.37	1.33
2	D	501	6YE	C05-N06	2.31	1.36	1.32
2	B	501	6YE	C10-N09	2.26	1.37	1.33
2	C	501	6YE	C08-N07	2.23	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6YE	C17-C18-N13	4.32	118.12	109.61
2	A	501	6YE	C04-C08-N09	3.46	132.96	123.54
2	C	501	6YE	C04-C08-N09	3.38	132.72	123.54
2	B	501	6YE	C04-C08-N09	3.02	131.75	123.54
2	B	501	6YE	C23-C19-C20	-2.77	103.92	106.89
2	D	501	6YE	C04-C08-N09	2.71	130.91	123.54
2	C	501	6YE	C23-C19-C20	-2.71	103.99	106.89
2	A	501	6YE	C17-C18-N13	2.62	114.76	109.61
2	A	501	6YE	C15-C14-N13	2.61	114.75	109.61
2	C	501	6YE	C05-C04-C02	-2.52	122.14	129.45
2	A	501	6YE	C23-C19-C20	-2.47	104.24	106.89
2	A	501	6YE	C12-C11-C10	2.42	121.51	118.75
2	B	501	6YE	C15-C14-N13	2.41	114.35	109.61
2	B	501	6YE	N13-C10-N09	-2.34	114.06	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6YE	C05-C04-C02	-2.28	122.83	129.45
2	B	501	6YE	C05-C04-C02	-2.26	122.88	129.45
2	A	501	6YE	C20-N21-N22	2.18	107.47	104.36
2	D	501	6YE	C04-C02-N01	2.16	119.54	114.94
2	D	501	6YE	O03-C02-C04	-2.06	117.45	121.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6YE	N09-C10-N13-C18
2	A	501	6YE	C11-C10-N13-C18

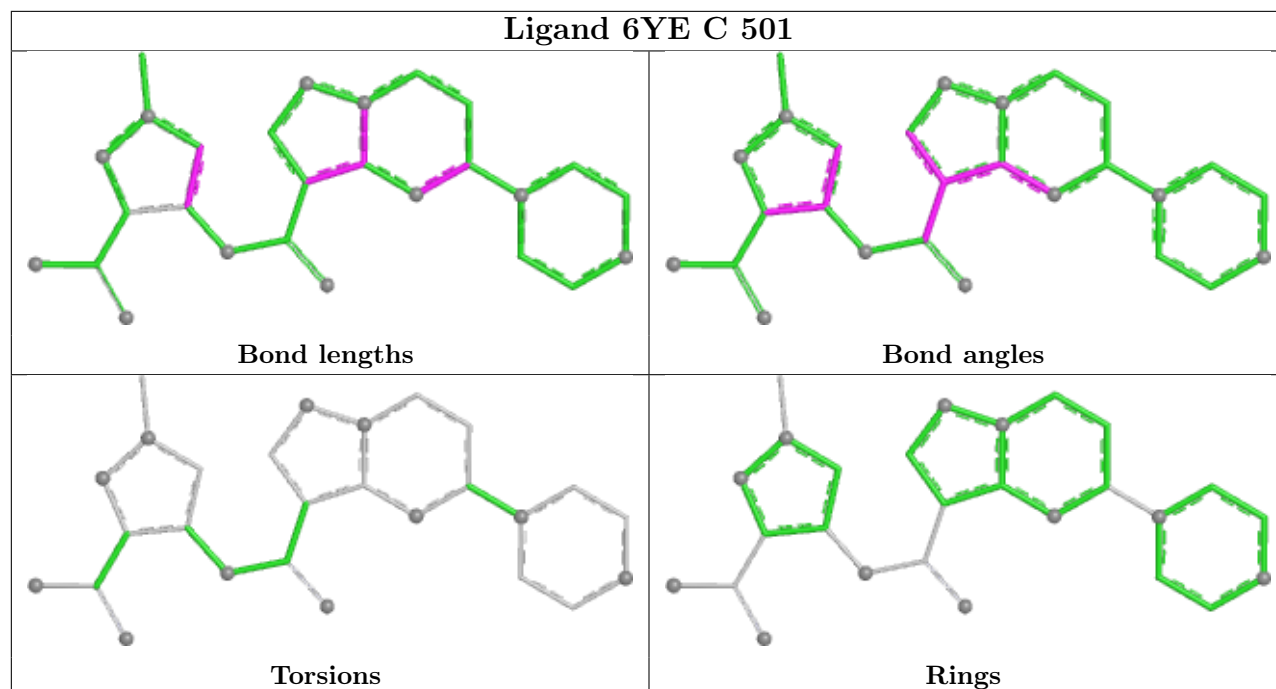
There are no ring outliers.

1 monomer is involved in 1 short contact:

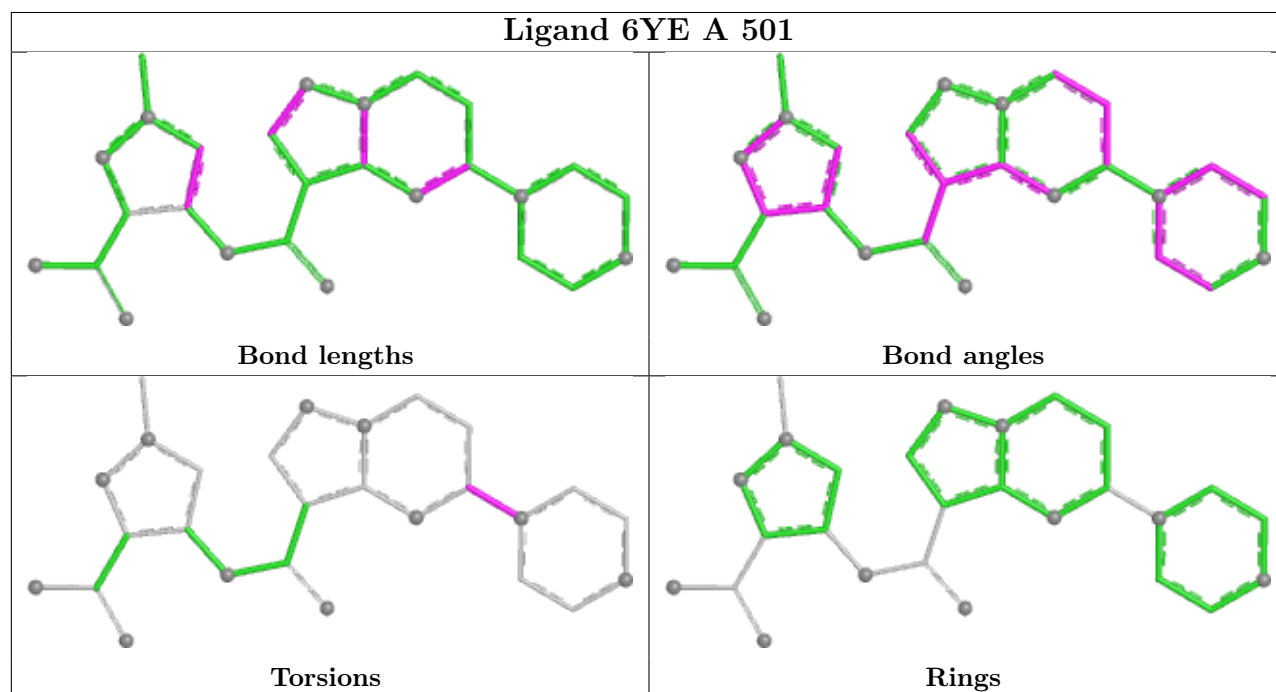
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	6YE	1	0

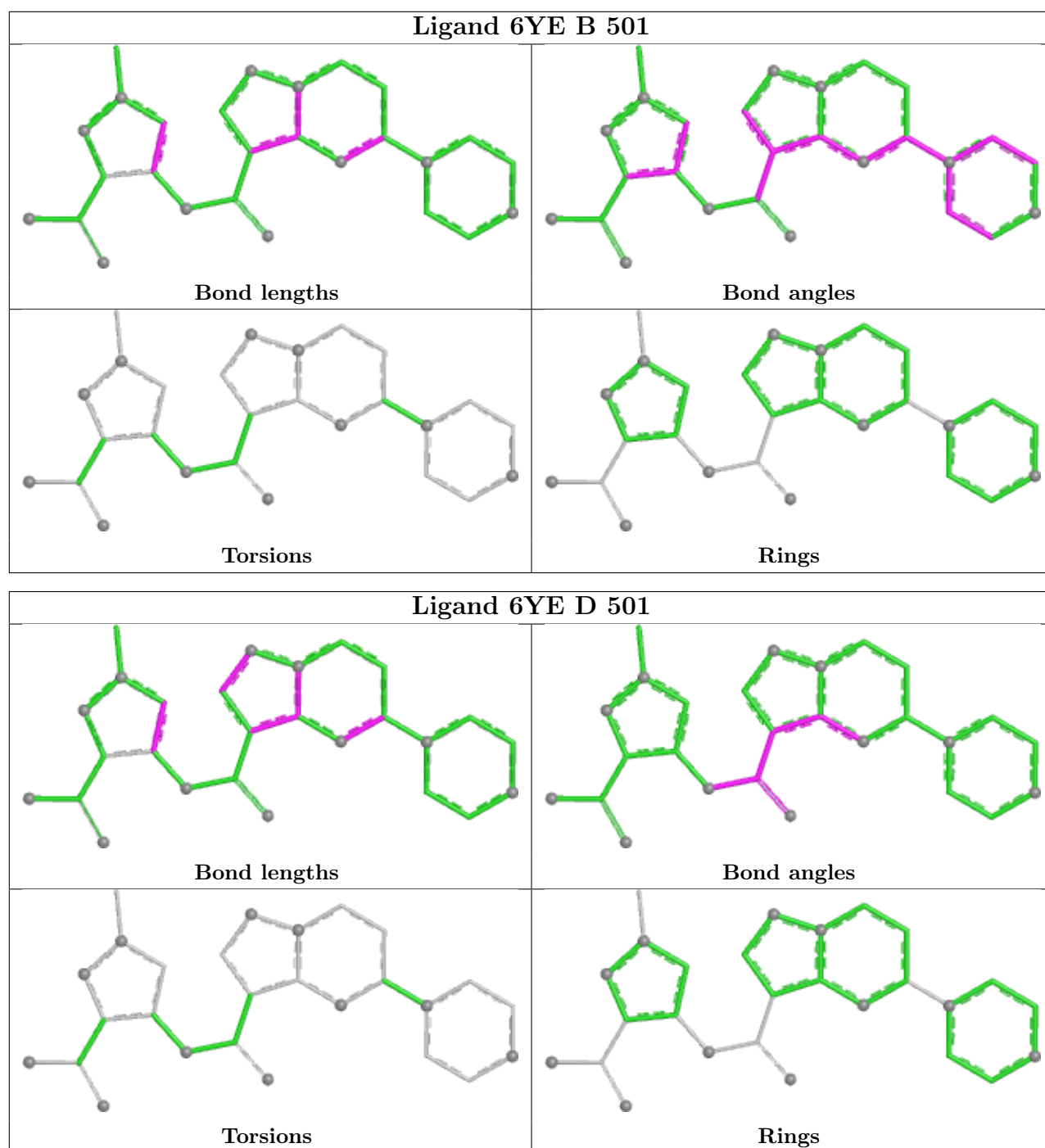
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 6YE C 501



Ligand 6YE A 501





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	285/301 (94%)	-1.13	0 100 100	45, 86, 132, 144	0
1	B	278/301 (92%)	-1.10	0 100 100	45, 80, 137, 165	0
1	C	287/301 (95%)	-1.15	0 100 100	42, 73, 112, 123	0
1	D	283/301 (94%)	-1.25	0 100 100	43, 68, 107, 141	0
All	All	1133/1204 (94%)	-1.16	0 100 100	42, 75, 128, 165	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	B	346	10/11	0.92	0.05	124,127,133,133	0
1	SEP	D	346	10/11	0.94	0.05	108,113,119,120	0
1	TPO	B	345	11/12	0.97	0.05	120,124,126,127	0
1	TPO	A	342	11/12	0.97	0.07	124,125,130,131	0
1	SEP	C	346	10/11	0.97	0.04	101,109,120,120	0
1	SEP	A	346	10/11	0.97	0.05	120,124,129,129	0
1	TPO	C	342	11/12	0.98	0.06	109,112,120,121	0
1	TPO	C	345	11/12	0.98	0.05	96,98,102,103	0
1	TPO	A	345	11/12	0.98	0.05	118,121,123,123	0
1	TPO	D	342	11/12	0.98	0.04	113,118,127,128	0
1	TPO	D	345	11/12	0.98	0.05	104,106,108,109	0
1	TPO	B	342	11/12	0.98	0.06	123,125,129,129	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

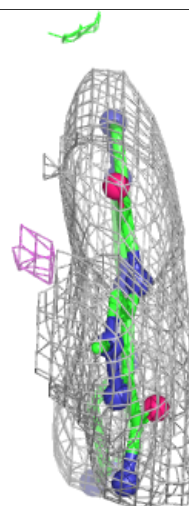
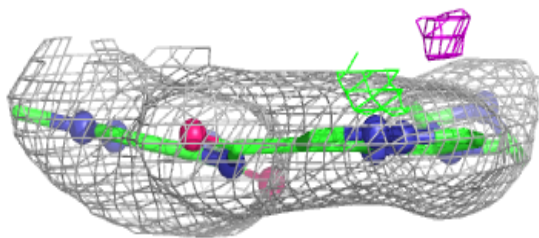
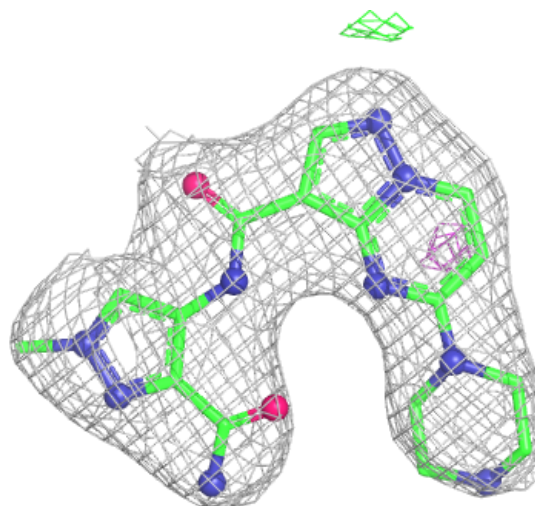
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	6YE	A	501	27/27	0.99	0.04	56,66,80,82	0
2	6YE	B	501	27/27	0.99	0.03	57,62,75,77	0
2	6YE	C	501	27/27	0.99	0.03	44,53,57,59	0
2	6YE	D	501	27/27	0.99	0.03	34,47,55,57	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.

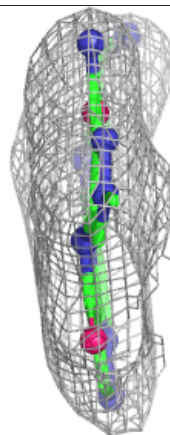
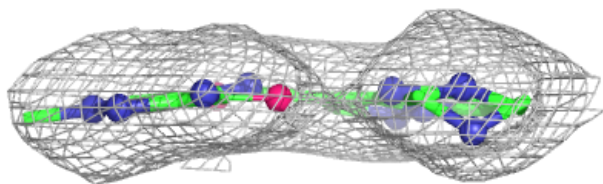
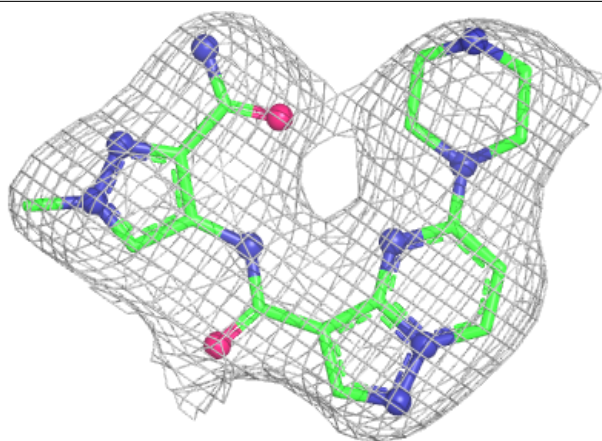
Electron density around 6YE A 501:

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



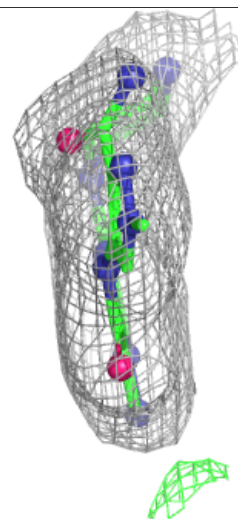
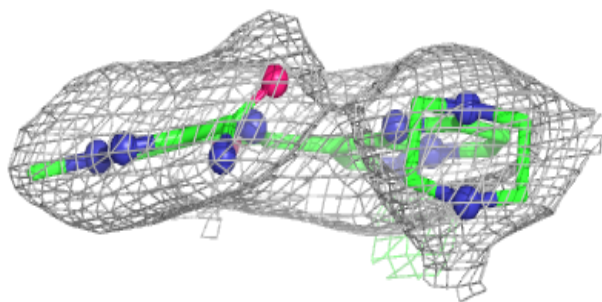
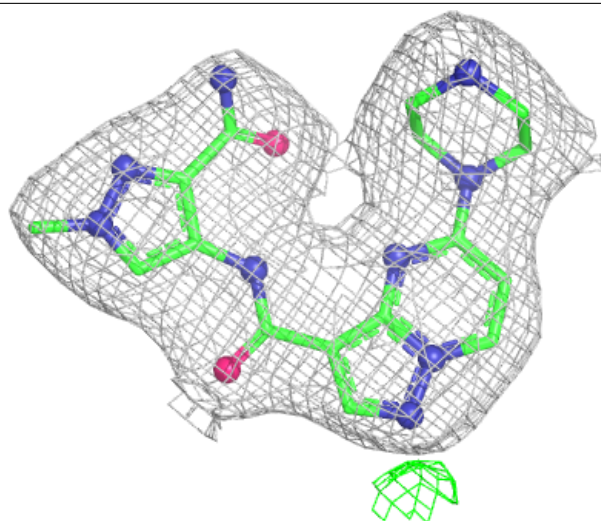
Electron density around 6YE B 501:

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



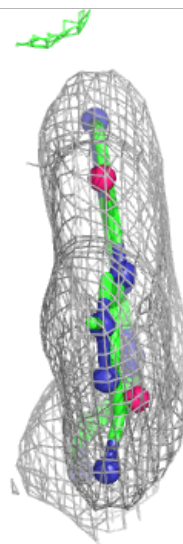
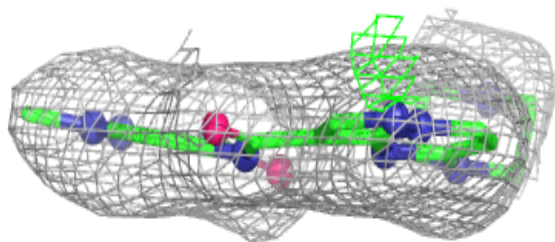
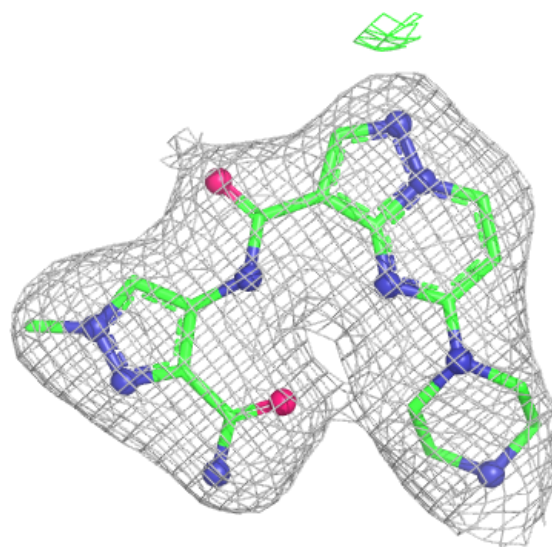
Electron density around 6YE C 501:

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



Electron density around 6YE D 501:

$2mF_o-DF_c$ (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.