



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:02 pm BST

PDB ID : 3KRY  
Title : Crystal structure of MMP-13 in complex with SC-78080  
Authors : Kiefer, J.R.; Williams, J.M.; Becker, D.P.  
Deposited on : 2009-11-19  
Resolution : 1.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

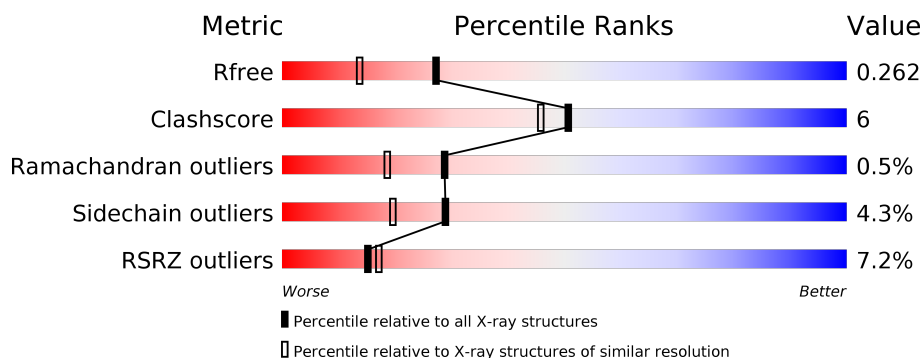
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	164	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> <div>•</div> </div>
1	B	164	<div> <div>7%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> <div>•</div> </div>
1	C	164	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> <div>•</div> </div>
1	D	164	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>8%</div> </div> <div>••</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5886 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	1	0
			1306	844	212	245	5			
1	B	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			
1	C	164	Total	C	N	O	S	0	0	0
			1304	844	212	243	5			
1	D	162	Total	C	N	O	S	0	1	0
			1292	837	207	243	5			

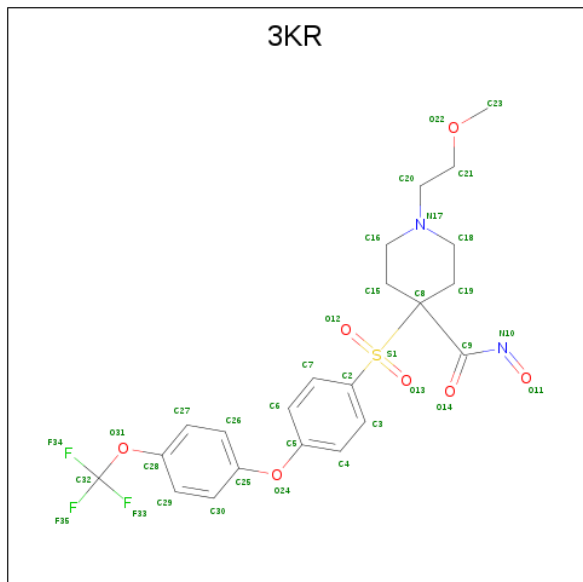
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 1-(2-methoxyethyl)-N-oxo-4-({4-[4-(trifluoromethoxy)phenoxy]phenyl}sulfonyl)piperidine-4-carboxamide (three-letter code: 3KR) (formula: C<sub>22</sub>H<sub>23</sub>F<sub>3</sub>N<sub>2</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			35	22	3	2	7	1		
4	B	1	Total	C	F	N	O	S	0	0
			35	22	3	2	7	1		
4	C	1	Total	C	F	N	O	S	0	0
			35	22	3	2	7	1		
4	D	1	Total	C	F	N	O	S	0	0
			35	22	3	2	7	1		

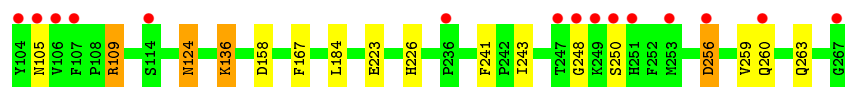
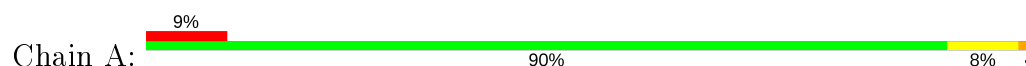
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	1
			142	142		
5	B	134	Total	O	0	1
			135	135		
5	C	114	Total	O	0	0
			114	114		
5	D	133	Total	O	0	4
			137	137		

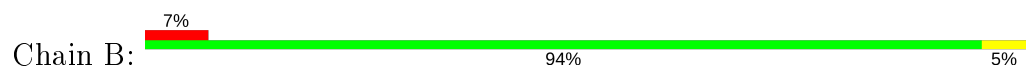
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

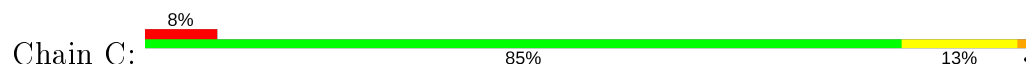
#### • Molecule 1: Collagenase 3



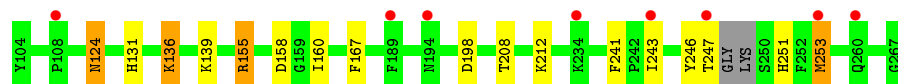
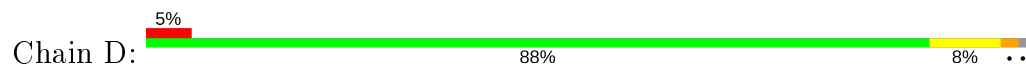
#### • Molecule 1: Collagenase 3



#### • Molecule 1: Collagenase 3



#### • Molecule 1: Collagenase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.32Å 70.02Å 69.09Å 92.42° 94.23° 104.94°	Depositor
Resolution (Å)	19.68 – 1.90 19.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.68-1.90) 95.0 (19.68-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.206 , 0.256 0.219 , 0.262	Depositor DCC
$R_{free}$ test set	2425 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CA, 3KR

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	0.42	0/1352	0.54	0/1837
1	B	0.42	0/1346	0.53	0/1829
1	C	0.43	0/1350	0.56	0/1833
1	D	0.42	0/1337	0.55	0/1817
All	All	0.42	0/5385	0.55	0/7316

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	246	TYR	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1306	0	1212	17	0
1	B	1300	0	1208	7	0
1	C	1304	0	1219	20	1
1	D	1292	0	1197	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	35	0	23	2	0
4	B	35	0	23	1	0
4	C	35	0	23	0	0
4	D	35	0	23	0	0
5	A	142	0	0	2	0
5	B	135	0	0	1	0
5	C	114	0	0	5	0
5	D	137	0	0	5	1
All	All	5886	0	4928	59	1

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 6.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG12	1:A:263:GLN:NE2	1.52	1.22
1:A:259:VAL:CG1	1:A:263:GLN:NE2	2.09	1.13
1:A:259:VAL:CG1	1:A:263:GLN:HE22	1.72	0.98
1:A:259:VAL:HG12	1:A:263:GLN:HE22	1.06	0.95
1:A:124:ASN:HD21	1:A:167:PHE:H	1.06	0.94
1:D:124:ASN:HD21	1:D:167:PHE:H	1.16	0.87
1:A:259:VAL:HG13	1:A:263:GLN:NE2	1.95	0.79
1:A:259:VAL:CG1	1:A:263:GLN:HE21	1.94	0.79
1:B:124:ASN:HD21	1:B:167:PHE:H	1.30	0.78
1:C:124:ASN:HD21	1:C:167:PHE:H	1.33	0.76
4:B:2800:3KR:H20A	5:B:519:HOH:O	1.85	0.75
1:B:241:PHE:CE2	1:B:243:ILE:HD12	2.24	0.72
1:C:254:LEU:HD23	1:C:259:VAL:HG12	1.70	0.71
1:D:208[A]:THR:HG21	1:D:212:LYS:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:HIS:NE2	5:C:294:HOH:O	2.30	0.64
1:A:259:VAL:HG13	1:A:263:GLN:HE21	1.59	0.63
1:A:124:ASN:HD21	1:A:167:PHE:N	1.89	0.62
1:C:160:ILE:O	1:C:160:ILE:HD12	2.00	0.62
1:A:124:ASN:ND2	1:A:167:PHE:H	1.88	0.61
1:B:241:PHE:CZ	1:B:243:ILE:HD12	2.36	0.60
1:A:256:ASP:O	1:A:260:GLN:HG2	2.01	0.59
1:D:124:ASN:HD22	1:D:124:ASN:C	2.05	0.59
1:D:251:HIS:NE2	5:D:429:HOH:O	2.32	0.59
1:C:248:GLY:HA2	5:C:474:HOH:O	2.01	0.59
4:A:1800:3KR:H20A	5:A:328:HOH:O	2.04	0.57
1:B:124:ASN:ND2	1:B:167:PHE:H	2.00	0.56
1:A:124:ASN:C	1:A:124:ASN:HD22	2.07	0.56
1:C:241:PHE:CE2	1:C:243:ILE:HD12	2.41	0.55
1:C:256:ASP:O	1:C:259:VAL:HG22	2.08	0.53
1:D:139:LYS:NZ	5:D:493:HOH:O	2.36	0.53
1:D:253:MET:HE2	1:D:253:MET:HA	1.91	0.53
1:B:124:ASN:HD22	1:B:124:ASN:C	2.12	0.53
1:A:136:LYS:HD3	1:A:136:LYS:N	2.25	0.52
1:C:106:VAL:HG23	1:C:107:PHE:N	2.24	0.51
1:D:253:MET:HE3	5:D:8:HOH:O	2.11	0.50
1:D:155:ARG:HD3	5:D:284:HOH:O	2.11	0.49
1:C:256:ASP:HA	1:C:259:VAL:HG22	1.94	0.49
1:D:198:ASP:HB2	5:D:346:HOH:O	2.11	0.49
1:C:259:VAL:HG21	5:C:481:HOH:O	2.13	0.49
1:C:140:LYS:NZ	5:C:473:HOH:O	2.46	0.48
1:C:106:VAL:CG2	1:C:107:PHE:N	2.77	0.48
1:A:241:PHE:CE2	1:A:243:ILE:HD12	2.49	0.48
1:C:241:PHE:HE2	1:C:243:ILE:HD12	1.80	0.47
1:D:136:LYS:HD3	1:D:136:LYS:N	2.30	0.47
1:B:188:ALA:HB3	1:B:226:HIS:HB2	1.94	0.47
1:A:184:LEU:HD23	4:A:1800:3KR:H21	1.96	0.46
1:C:124:ASN:C	1:C:124:ASN:HD22	2.19	0.45
1:C:106:VAL:HG23	1:C:107:PHE:H	1.83	0.44
1:C:124:ASN:ND2	1:C:167:PHE:H	2.08	0.43
1:C:136:LYS:HD3	1:C:136:LYS:N	2.34	0.42
1:C:170:LYS:HA	1:C:178:PHE:O	2.18	0.42
1:C:253:MET:O	1:C:253:MET:HG3	2.20	0.42
1:C:182:SER:OG	1:C:183:GLY:N	2.53	0.42
1:B:112:LYS:HA	1:B:191:PRO:HG2	2.02	0.41
5:C:294:HOH:O	1:D:131:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ASN:ND2	1:D:167:PHE:H	1.99	0.41
1:D:241:PHE:HE2	1:D:243:ILE:HD12	1.86	0.41
1:A:109:ARG:NH1	5:A:399:HOH:O	2.55	0.40
1:A:223:GLU:O	1:A:226:HIS:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:HIS:ND1	5:D:429:HOH:O[1_455]	2.18	0.02

## 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	163/164 (99%)	156 (96%)	6 (4%)	1 (1%)	25	15
1	B	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	15
1	C	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	15
1	D	159/164 (97%)	149 (94%)	10 (6%)	0	100	100
All	All	646/656 (98%)	612 (95%)	31 (5%)	3 (0%)	29	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	111	LEU
1	B	249	LYS
1	A	248	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	139/140 (99%)	132 (95%)	7 (5%)	24	15
1	B	138/140 (99%)	136 (99%)	2 (1%)	67	65
1	C	139/140 (99%)	131 (94%)	8 (6%)	20	10
1	D	138/140 (99%)	131 (95%)	7 (5%)	24	14
All	All	554/560 (99%)	530 (96%)	24 (4%)	29	19

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	109	ARG
1	A	124	ASN
1	A	136	LYS
1	A	158	ASP
1	A	250	SER
1	A	256	ASP
1	B	110	THR
1	B	124	ASN
1	C	106	VAL
1	C	112	LYS
1	C	124	ASN
1	C	136	LYS
1	C	158	ASP
1	C	210	SER
1	C	247	THR
1	C	253	MET
1	D	124	ASN
1	D	136	LYS
1	D	155	ARG
1	D	158	ASP
1	D	160	ILE
1	D	247	THR
1	D	253	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	263	GLN
1	B	124	ASN
1	C	124	ASN
1	C	194	ASN
1	C	260	GLN
1	D	124	ASN
1	D	131	HIS
1	D	194	ASN
1	D	260	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	3KR	A	1800	2	32,37,37	7.34	7 (21%)	45,54,54	2.48	10 (22%)
4	3KR	D	4800	2	32,37,37	7.63	7 (21%)	45,54,54	2.16	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	3KR	B	2800	2	32,37,37	7.45	7 (21%)	45,54,54	2.48	9 (20%)
4	3KR	C	3800	2	32,37,37	7.55	7 (21%)	45,54,54	2.19	8 (17%)

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
4	3KR	A	1800	2	-	4/28/48/48	0/3/3/3
4	3KR	D	4800	2	-	4/28/48/48	0/3/3/3
4	3KR	B	2800	2	-	4/28/48/48	0/3/3/3
4	3KR	C	3800	2	-	4/28/48/48	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4800	3KR	O13-S1	30.50	1.70	1.44
4	C	3800	3KR	O13-S1	30.06	1.70	1.44
4	B	2800	3KR	O12-S1	29.42	1.69	1.44
4	D	4800	3KR	O12-S1	29.29	1.69	1.44
4	B	2800	3KR	O13-S1	29.17	1.69	1.44
4	C	3800	3KR	O12-S1	29.15	1.69	1.44
4	A	1800	3KR	O12-S1	29.08	1.69	1.44
4	A	1800	3KR	O13-S1	28.55	1.69	1.44
4	D	4800	3KR	C2-S1	-5.70	1.70	1.76
4	C	3800	3KR	C2-S1	-5.38	1.70	1.76
4	A	1800	3KR	C2-S1	-4.52	1.71	1.76
4	B	2800	3KR	C2-S1	-4.09	1.72	1.76
4	D	4800	3KR	O24-C25	-3.22	1.32	1.39
4	B	2800	3KR	O24-C5	-3.21	1.32	1.39
4	C	3800	3KR	O24-C25	-3.03	1.33	1.39
4	D	4800	3KR	O31-C28	-2.79	1.32	1.41
4	A	1800	3KR	O24-C5	-2.78	1.33	1.39
4	B	2800	3KR	O24-C25	-2.74	1.33	1.39
4	C	3800	3KR	O31-C28	-2.65	1.32	1.41
4	A	1800	3KR	O31-C28	-2.62	1.33	1.41
4	C	3800	3KR	O24-C5	-2.51	1.34	1.39
4	B	2800	3KR	O31-C28	-2.50	1.33	1.41
4	D	4800	3KR	O24-C5	-2.46	1.34	1.39
4	A	1800	3KR	O24-C25	-2.38	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	3KR	O31-C32	2.38	1.45	1.31
4	D	4800	3KR	O31-C32	2.21	1.44	1.31
4	B	2800	3KR	O31-C32	2.16	1.43	1.31
4	C	3800	3KR	O31-C32	2.13	1.43	1.31

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2800	3KR	O13-S1-O12	-11.27	106.59	118.98
4	A	1800	3KR	O13-S1-O12	-10.77	107.15	118.98
4	C	3800	3KR	O13-S1-O12	-8.81	109.30	118.98
4	D	4800	3KR	O13-S1-O12	-8.30	109.85	118.98
4	B	2800	3KR	O13-S1-C8	6.65	114.85	107.67
4	A	1800	3KR	C20-N17-C18	5.54	125.40	111.23
4	C	3800	3KR	O13-S1-C8	5.43	113.54	107.67
4	A	1800	3KR	O13-S1-C8	5.15	113.23	107.67
4	D	4800	3KR	C20-N17-C18	4.94	123.86	111.23
4	B	2800	3KR	C20-N17-C18	4.60	123.00	111.23
4	C	3800	3KR	C20-N17-C18	4.53	122.81	111.23
4	C	3800	3KR	C19-C18-N17	-4.38	106.91	111.23
4	D	4800	3KR	C25-O24-C5	4.24	128.72	118.80
4	D	4800	3KR	O13-S1-C8	4.22	112.23	107.67
4	C	3800	3KR	C25-O24-C5	4.14	128.49	118.80
4	A	1800	3KR	C25-O24-C5	4.08	128.35	118.80
4	A	1800	3KR	C15-C16-N17	-4.03	107.26	111.23
4	C	3800	3KR	C20-N17-C16	3.93	121.29	111.23
4	A	1800	3KR	C19-C18-N17	-3.89	107.40	111.23
4	D	4800	3KR	C19-C18-N17	-3.87	107.41	111.23
4	B	2800	3KR	C25-O24-C5	3.77	127.63	118.80
4	D	4800	3KR	C20-N17-C16	3.75	120.81	111.23
4	B	2800	3KR	C15-C16-N17	-3.64	107.65	111.23
4	A	1800	3KR	O12-S1-C8	3.62	111.59	107.67
4	B	2800	3KR	C19-C18-N17	-3.61	107.67	111.23
4	A	1800	3KR	C20-N17-C16	3.39	119.91	111.23
4	B	2800	3KR	C20-N17-C16	3.20	119.41	111.23
4	D	4800	3KR	C32-O31-C28	3.17	128.47	118.01
4	C	3800	3KR	C18-N17-C16	3.05	115.69	108.83
4	A	1800	3KR	C32-O31-C28	3.04	128.04	118.01
4	D	4800	3KR	O12-S1-C8	2.83	110.73	107.67
4	D	4800	3KR	C18-N17-C16	2.80	115.12	108.83
4	B	2800	3KR	C18-N17-C16	2.49	114.43	108.83
4	C	3800	3KR	C32-O31-C28	2.45	126.08	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2800	3KR	C32-O31-C28	2.28	125.52	118.01
4	A	1800	3KR	O13-S1-C2	-2.02	105.82	108.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4800	3KR	C19-C8-S1-O13
4	B	2800	3KR	C19-C8-S1-O13
4	A	1800	3KR	C19-C8-S1-O13
4	C	3800	3KR	C19-C8-S1-O13
4	A	1800	3KR	C20-C21-O22-C23
4	D	4800	3KR	C21-C20-N17-C16
4	D	4800	3KR	C15-C8-S1-C2
4	C	3800	3KR	C15-C8-S1-C2
4	B	2800	3KR	C20-C21-O22-C23
4	C	3800	3KR	C21-C20-N17-C16
4	D	4800	3KR	C19-C8-S1-C2
4	B	2800	3KR	C15-C8-S1-C2
4	B	2800	3KR	C19-C8-S1-C2
4	A	1800	3KR	C15-C8-S1-C2
4	A	1800	3KR	C19-C8-S1-C2
4	C	3800	3KR	C19-C8-S1-C2

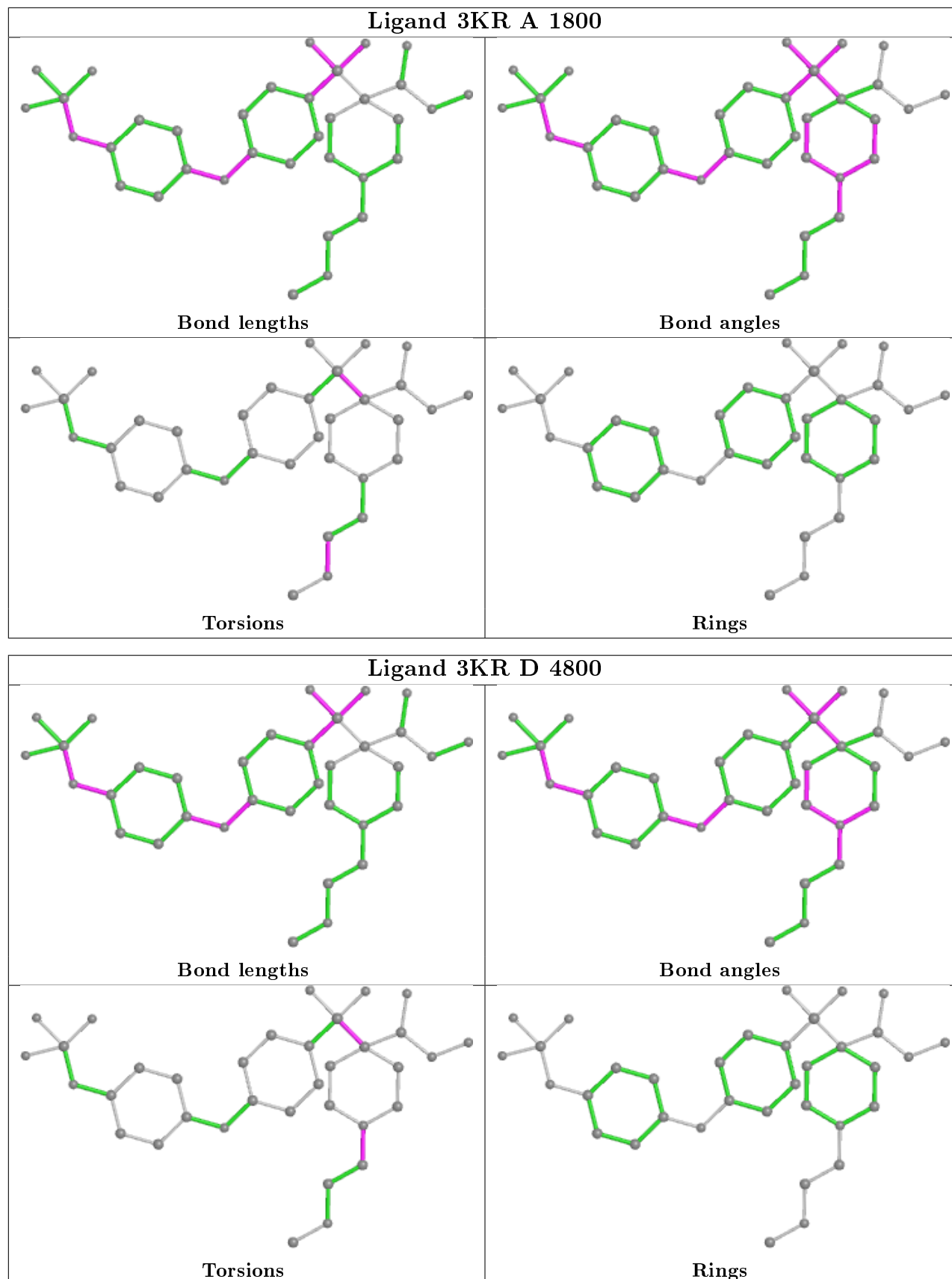
There are no ring outliers.

2 monomers are involved in 3 short contacts:

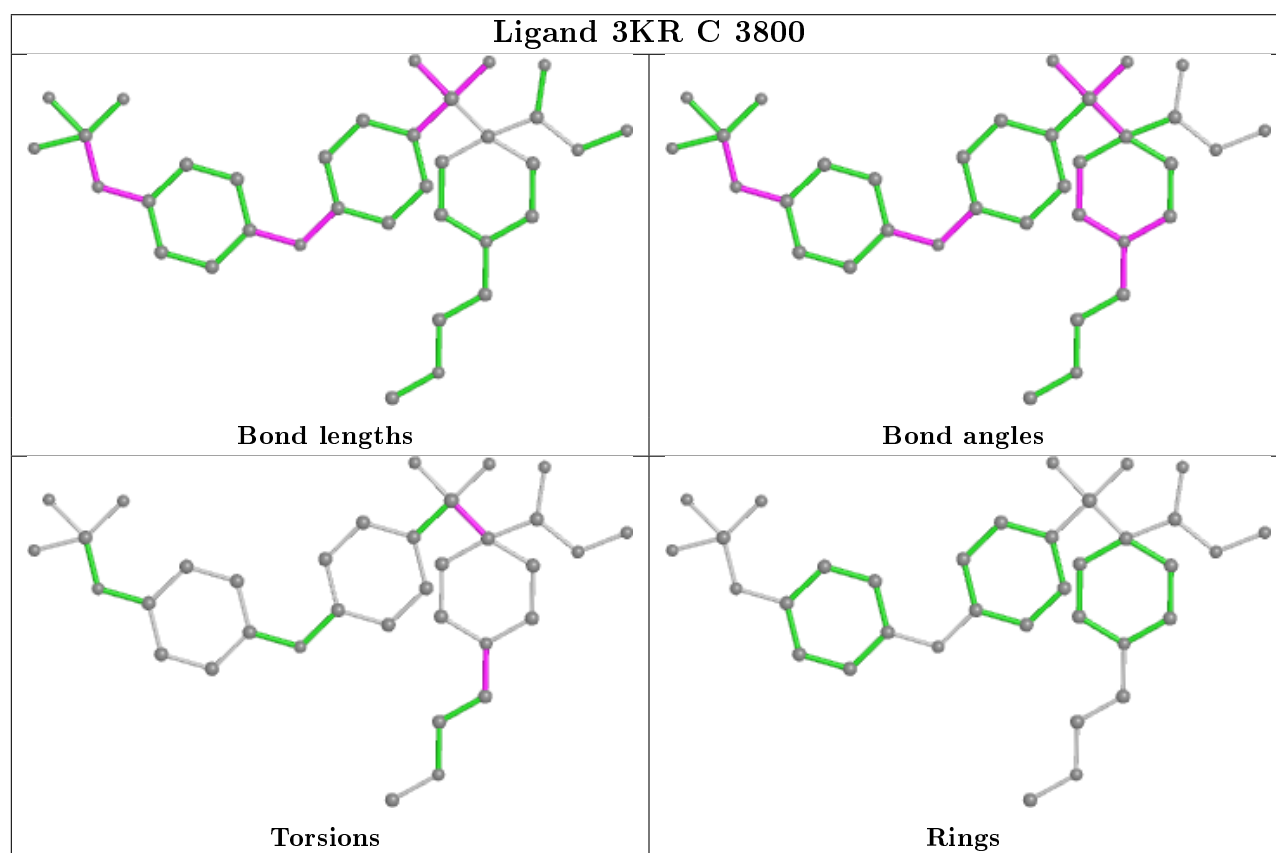
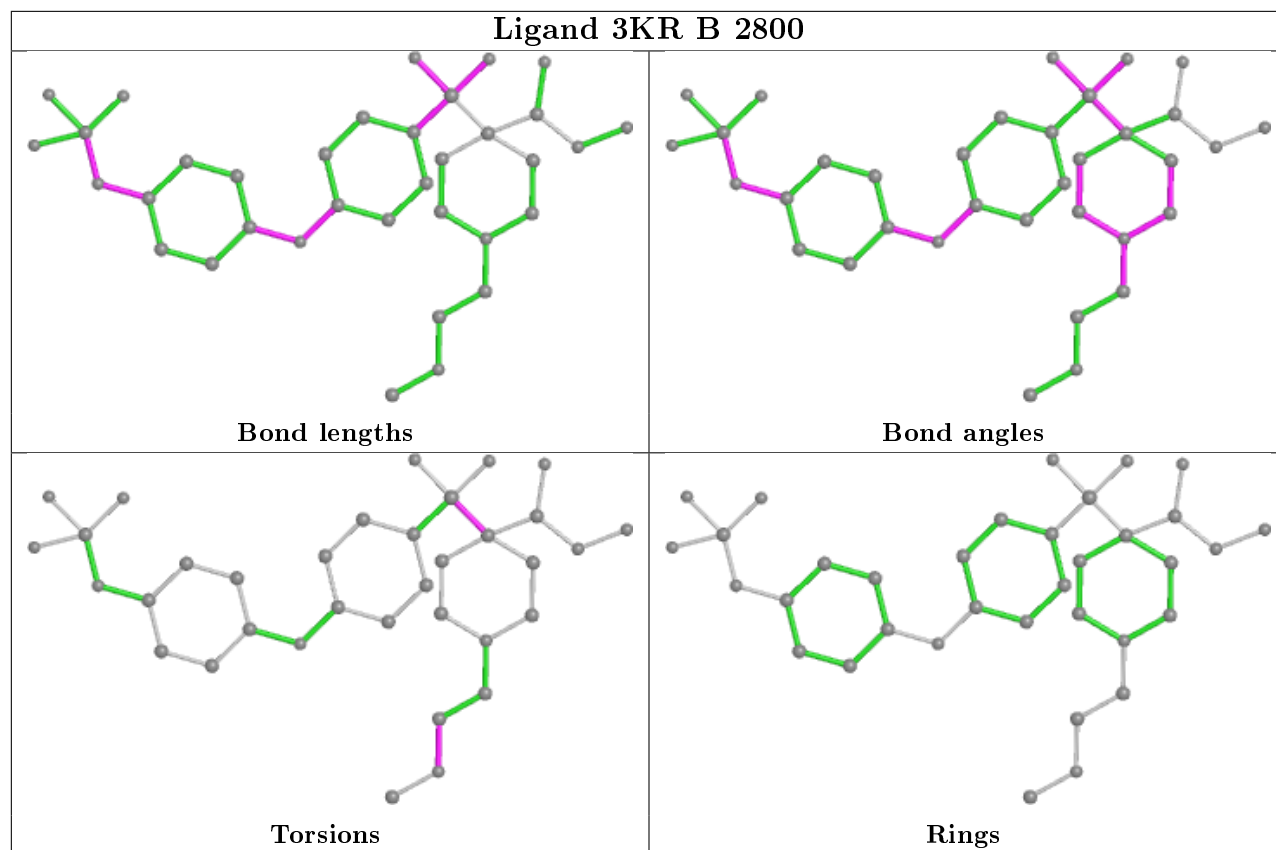
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1800	3KR	2	0
4	B	2800	3KR	1	0

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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	0.54	15 (9%) 9 10	7, 11, 23, 28	0
1	B	164/164 (100%)	0.56	11 (6%) 17 20	11, 18, 35, 41	0
1	C	164/164 (100%)	0.60	13 (7%) 12 14	14, 20, 31, 38	0
1	D	162/164 (98%)	0.46	8 (4%) 29 33	13, 20, 27, 30	0
All	All	654/656 (99%)	0.54	47 (7%) 15 17	7, 18, 28, 41	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	SER	7.8
1	A	248	GLY	7.3
1	B	250	SER	7.2
1	A	104	TYR	6.7
1	B	251	HIS	6.4
1	A	251	HIS	6.3
1	C	248	GLY	6.0
1	B	249	LYS	5.7
1	B	248	GLY	5.6
1	C	247	THR	5.5
1	A	249	LYS	5.0
1	C	108	PRO	4.7
1	D	247	THR	4.2
1	B	104	TYR	4.0
1	A	106	VAL	3.8
1	A	105	ASN	3.7
1	A	247	THR	3.7
1	B	109	ARG	3.5
1	C	111	LEU	3.4
1	B	106	VAL	2.9
1	C	195	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	108	PRO	2.8
1	A	107	PHE	2.7
1	A	236	PRO	2.7
1	A	253	MET	2.6
1	D	260	GLN	2.5
1	C	253	MET	2.5
1	B	107	PHE	2.5
1	C	250	SER	2.4
1	A	267	GLY	2.4
1	A	260	GLN	2.3
1	D	234	LYS	2.3
1	A	256	ASP	2.3
1	C	110	THR	2.2
1	C	234	LYS	2.2
1	A	114[A]	SER	2.2
1	B	253	MET	2.2
1	D	253	MET	2.2
1	C	249	LYS	2.2
1	B	108	PRO	2.1
1	D	194	ASN	2.1
1	B	114	SER	2.1
1	C	189	PHE	2.1
1	C	230	LEU	2.0
1	D	243	ILE	2.0
1	C	260	GLN	2.0
1	D	189	PHE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

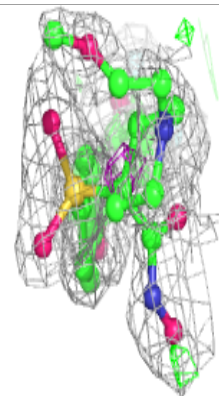
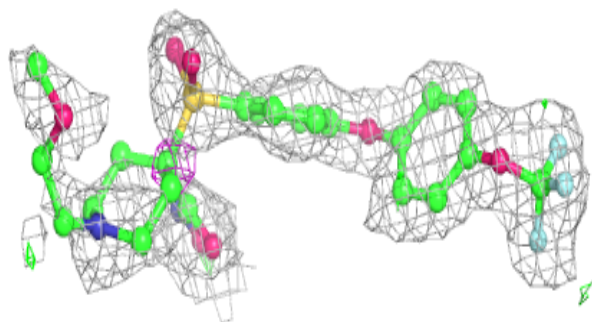
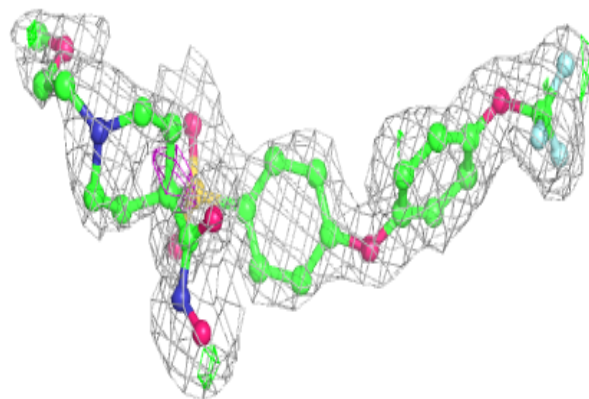
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	3KR	D	4800	35/35	0.82	0.19	20,28,42,44	0
4	3KR	C	3800	35/35	0.83	0.19	20,26,41,43	0
4	3KR	B	2800	35/35	0.89	0.16	15,21,35,36	0
4	3KR	A	1800	35/35	0.90	0.17	15,21,33,34	0
3	CA	A	1997	1/1	0.99	0.10	14,14,14,14	0
3	CA	B	2996	1/1	0.99	0.04	23,23,23,23	0
3	CA	D	4997	1/1	0.99	0.05	17,17,17,17	0
3	CA	C	3996	1/1	0.99	0.07	18,18,18,18	0
3	CA	C	3997	1/1	0.99	0.05	17,17,17,17	0
2	ZN	C	3998	1/1	1.00	0.05	15,15,15,15	0
2	ZN	A	1999	1/1	1.00	0.06	13,13,13,13	0
2	ZN	B	2998	1/1	1.00	0.04	12,12,12,12	0
2	ZN	B	2999	1/1	1.00	0.04	13,13,13,13	0
3	CA	D	4996	1/1	1.00	0.04	16,16,16,16	0
2	ZN	D	4998	1/1	1.00	0.04	14,14,14,14	0
3	CA	B	2997	1/1	1.00	0.09	14,14,14,14	0
2	ZN	D	4999	1/1	1.00	0.07	16,16,16,16	0
2	ZN	C	3999	1/1	1.00	0.05	18,18,18,18	0
2	ZN	A	1998	1/1	1.00	0.04	12,12,12,12	0
3	CA	A	1996	1/1	1.00	0.02	26,26,26,26	0

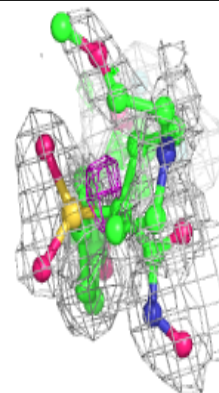
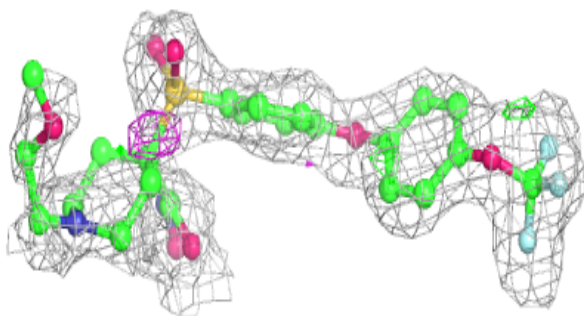
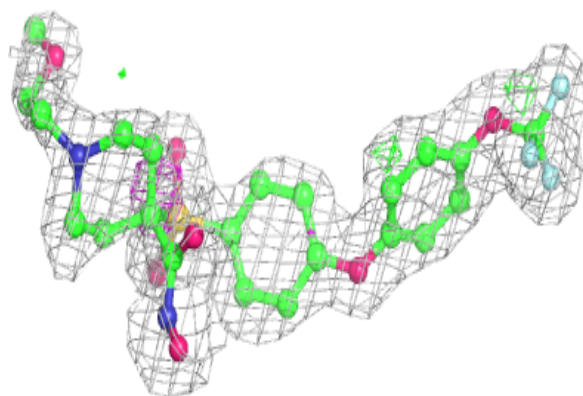
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 3KR D 4800:**

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

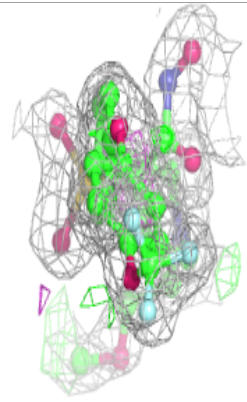
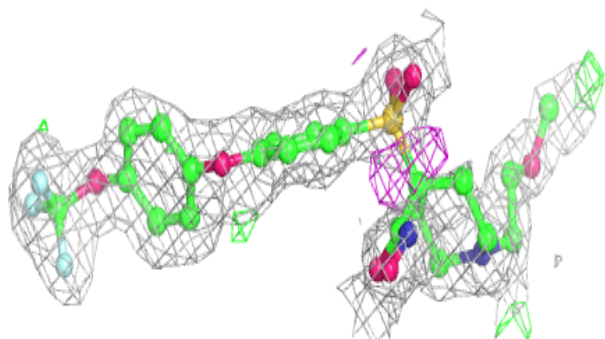
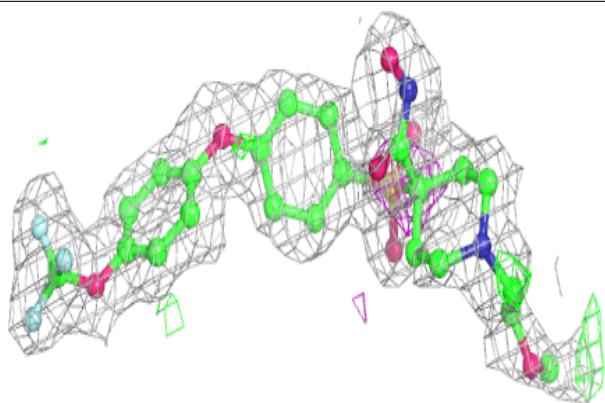
**Electron density around 3KR C 3800:**

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

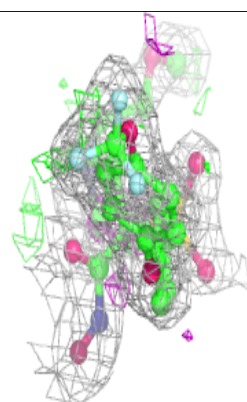
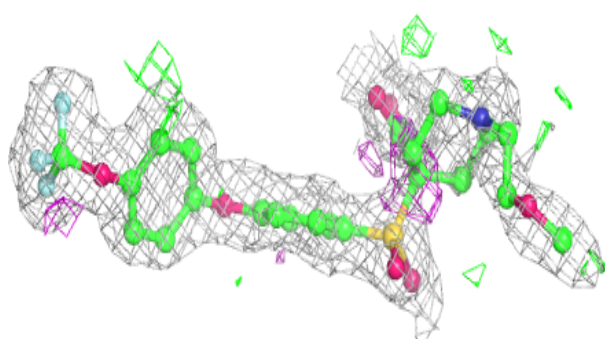
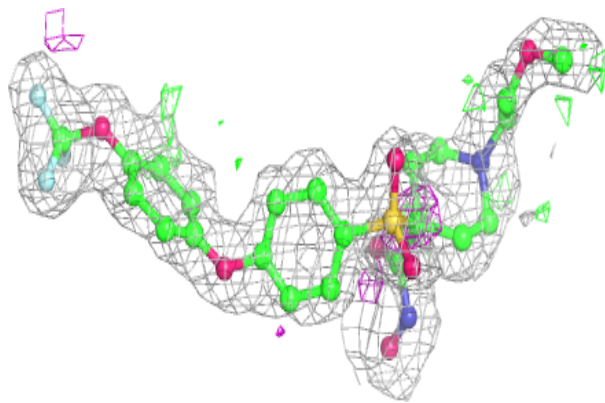


**Electron density around 3KR B 2800:**

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

**Electron density around 3KR A 1800:**

$2mF_o-DF_c$  (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.