



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 11:20 PM EST

PDB ID : 4R3U  
Title : Crystal structure of 2-Hydroxyisobutyryl-CoA Mutase  
Authors : Zahn, M.; Kurteva-Yaneva, N.; Rohwerder, T.; Straeter, N.  
Deposited on : 2014-08-18  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

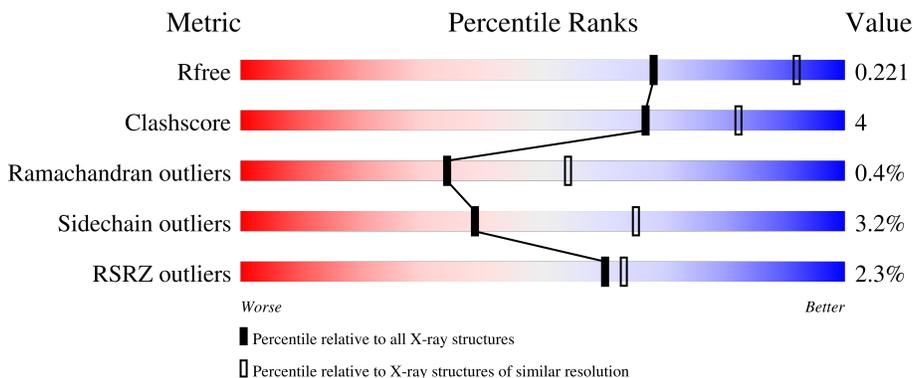
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	584	 87% 8% 5%
1	B	584	 84% 11% 5% 2%
2	C	158	 72% 10% 17% 1%
2	D	158	 71% 11% 18% 9%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11404 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 2-hydroxyisobutyryl-CoA mutase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4423	2804	755	845	19	0	0	0
1	B	555	4406	2795	753	839	19	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP I3VE77
A	-9	ALA	-	expression tag	UNP I3VE77
A	-8	SER	-	expression tag	UNP I3VE77
A	-7	HIS	-	expression tag	UNP I3VE77
A	-6	HIS	-	expression tag	UNP I3VE77
A	-5	HIS	-	expression tag	UNP I3VE77
A	-4	HIS	-	expression tag	UNP I3VE77
A	-3	HIS	-	expression tag	UNP I3VE77
A	-2	HIS	-	expression tag	UNP I3VE77
A	-1	SER	-	expression tag	UNP I3VE77
A	0	GLY	-	expression tag	UNP I3VE77
A	563	GLY	-	expression tag	UNP I3VE77
A	564	SER	-	expression tag	UNP I3VE77
A	565	ALA	-	expression tag	UNP I3VE77
A	566	TRP	-	expression tag	UNP I3VE77
A	567	SER	-	expression tag	UNP I3VE77
A	568	HIS	-	expression tag	UNP I3VE77
A	569	PRO	-	expression tag	UNP I3VE77
A	570	GLN	-	expression tag	UNP I3VE77
A	571	PHE	-	expression tag	UNP I3VE77
A	572	GLU	-	expression tag	UNP I3VE77
A	573	LYS	-	expression tag	UNP I3VE77
B	-10	MET	-	expression tag	UNP I3VE77
B	-9	ALA	-	expression tag	UNP I3VE77
B	-8	SER	-	expression tag	UNP I3VE77

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP I3VE77
B	-6	HIS	-	expression tag	UNP I3VE77
B	-5	HIS	-	expression tag	UNP I3VE77
B	-4	HIS	-	expression tag	UNP I3VE77
B	-3	HIS	-	expression tag	UNP I3VE77
B	-2	HIS	-	expression tag	UNP I3VE77
B	-1	SER	-	expression tag	UNP I3VE77
B	0	GLY	-	expression tag	UNP I3VE77
B	563	GLY	-	expression tag	UNP I3VE77
B	564	SER	-	expression tag	UNP I3VE77
B	565	ALA	-	expression tag	UNP I3VE77
B	566	TRP	-	expression tag	UNP I3VE77
B	567	SER	-	expression tag	UNP I3VE77
B	568	HIS	-	expression tag	UNP I3VE77
B	569	PRO	-	expression tag	UNP I3VE77
B	570	GLN	-	expression tag	UNP I3VE77
B	571	PHE	-	expression tag	UNP I3VE77
B	572	GLU	-	expression tag	UNP I3VE77
B	573	LYS	-	expression tag	UNP I3VE77

- Molecule 2 is a protein called 2-hydroxyisobutyryl-CoA mutase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	0	0
			982	620	176	184	2			
2	D	129	Total	C	N	O	S	0	0	0
			962	609	170	181	2			

There are 44 discrepancies between the modelled and reference sequences:

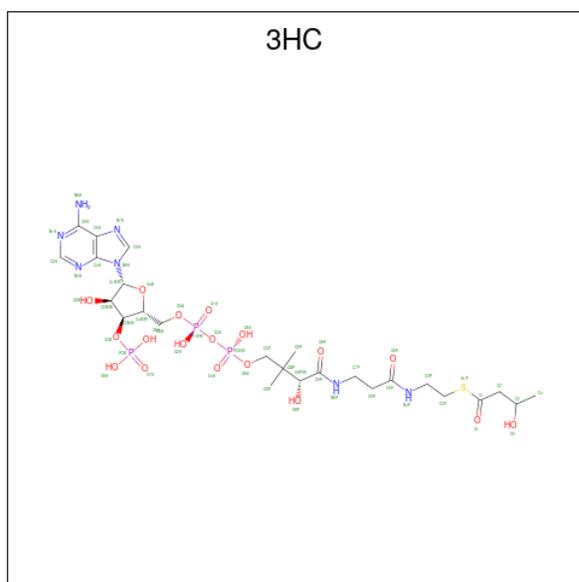
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	expression tag	UNP I3VE74
C	-9	ALA	-	expression tag	UNP I3VE74
C	-8	SER	-	expression tag	UNP I3VE74
C	-7	HIS	-	expression tag	UNP I3VE74
C	-6	HIS	-	expression tag	UNP I3VE74
C	-5	HIS	-	expression tag	UNP I3VE74
C	-4	HIS	-	expression tag	UNP I3VE74
C	-3	HIS	-	expression tag	UNP I3VE74
C	-2	HIS	-	expression tag	UNP I3VE74
C	-1	SER	-	expression tag	UNP I3VE74
C	0	GLY	-	expression tag	UNP I3VE74

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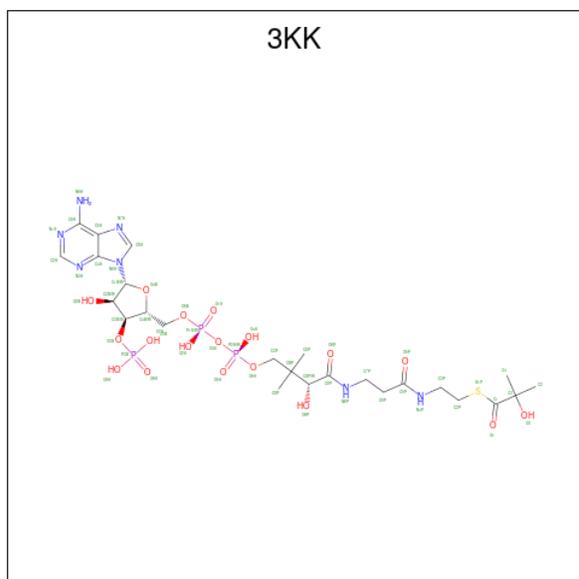
Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP I3VE74
C	138	SER	-	expression tag	UNP I3VE74
C	139	ALA	-	expression tag	UNP I3VE74
C	140	TRP	-	expression tag	UNP I3VE74
C	141	SER	-	expression tag	UNP I3VE74
C	142	HIS	-	expression tag	UNP I3VE74
C	143	PRO	-	expression tag	UNP I3VE74
C	144	GLN	-	expression tag	UNP I3VE74
C	145	PHE	-	expression tag	UNP I3VE74
C	146	GLU	-	expression tag	UNP I3VE74
C	147	LYS	-	expression tag	UNP I3VE74
D	-10	MET	-	expression tag	UNP I3VE74
D	-9	ALA	-	expression tag	UNP I3VE74
D	-8	SER	-	expression tag	UNP I3VE74
D	-7	HIS	-	expression tag	UNP I3VE74
D	-6	HIS	-	expression tag	UNP I3VE74
D	-5	HIS	-	expression tag	UNP I3VE74
D	-4	HIS	-	expression tag	UNP I3VE74
D	-3	HIS	-	expression tag	UNP I3VE74
D	-2	HIS	-	expression tag	UNP I3VE74
D	-1	SER	-	expression tag	UNP I3VE74
D	0	GLY	-	expression tag	UNP I3VE74
D	137	GLY	-	expression tag	UNP I3VE74
D	138	SER	-	expression tag	UNP I3VE74
D	139	ALA	-	expression tag	UNP I3VE74
D	140	TRP	-	expression tag	UNP I3VE74
D	141	SER	-	expression tag	UNP I3VE74
D	142	HIS	-	expression tag	UNP I3VE74
D	143	PRO	-	expression tag	UNP I3VE74
D	144	GLN	-	expression tag	UNP I3VE74
D	145	PHE	-	expression tag	UNP I3VE74
D	146	GLU	-	expression tag	UNP I3VE74
D	147	LYS	-	expression tag	UNP I3VE74

- Molecule 3 is 3-HYDROXYBUTANOYL-COENZYME A (three-letter code: 3HC) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



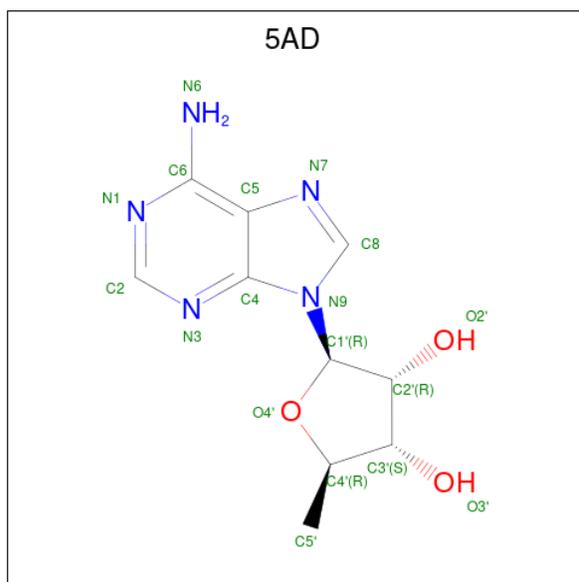
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	54	25	7	18	3	1	0	1
3	B	1	54	25	7	18	3	1	0	1

- Molecule 4 is S-{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} 2-hydroxy-2-methylpropanethioate (three-letter code: 3KK) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



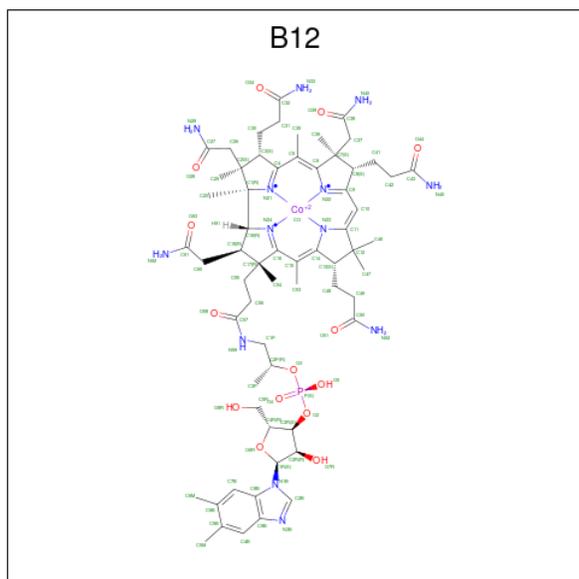
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	54	25	7	18	3	1	0	1
4	B	1	54	25	7	18	3	1	0	1

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	18	10	5	3	0	1

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

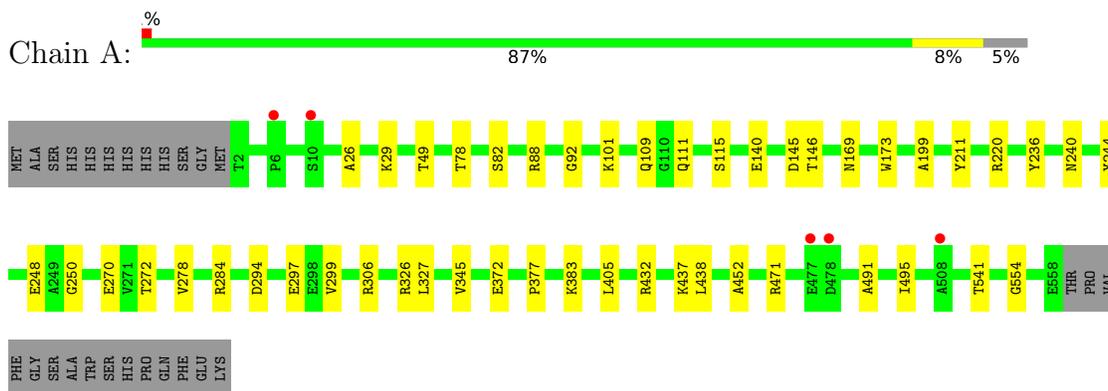
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	158	Total	O	0	5
			158	158		
7	B	16	Total	O	0	0
			16	16		
7	C	38	Total	O	0	1
			38	38		
7	D	3	Total	O	0	0
			3	3		

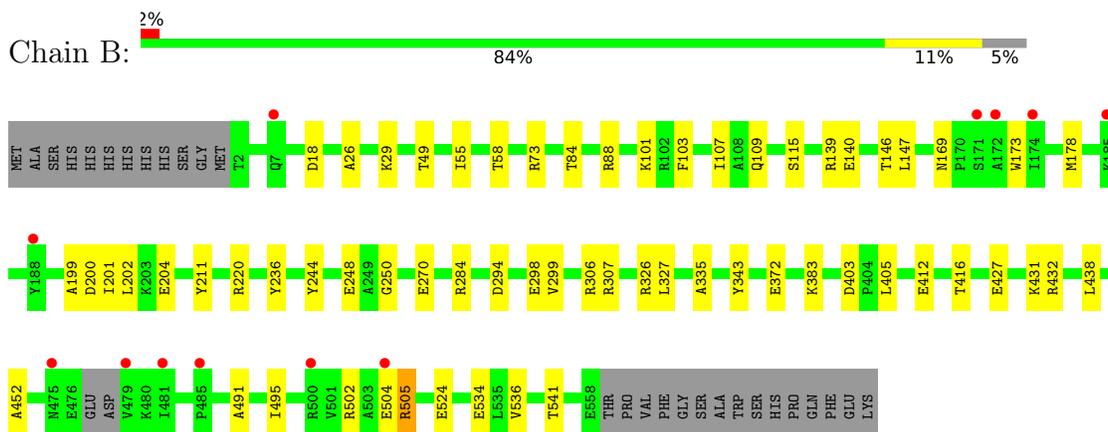
### 3 Residue-property plots [i](#)

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.

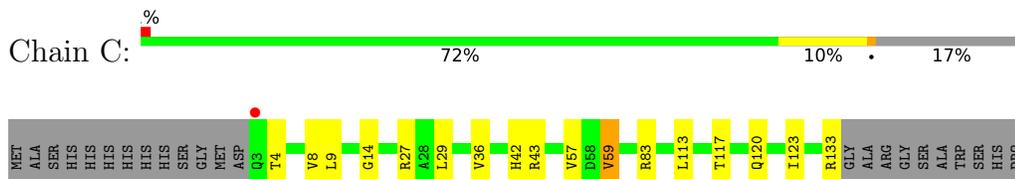
- Molecule 1: 2-hydroxyisobutyryl-CoA mutase large subunit



- Molecule 1: 2-hydroxyisobutyryl-CoA mutase large subunit



- Molecule 2: 2-hydroxyisobutyryl-CoA mutase small subunit



- Molecule 2: 2-hydroxyisobutyryl-CoA mutase small subunit





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.03Å 119.56Å 173.94Å 90.00° 91.23° 90.00°	Depositor
Resolution (Å)	24.63 – 2.50 24.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.63-2.50) 100.0 (24.63-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.50Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.168 , 0.217 0.172 , 0.221	Depositor DCC
$R_{free}$ test set	1519 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.857	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.020 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.017 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: 5AD, 3KK, 3HC, B12

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	0.54	0/4511	0.71	0/6100
1	B	0.48	0/4493	0.69	0/6074
2	C	0.56	0/992	0.70	0/1346
2	D	0.47	0/972	0.72	0/1320
All	All	0.51	0/10968	0.70	0/14840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4423	0	4391	28	0
1	B	4406	0	4380	31	0
2	C	982	0	1034	8	0
2	D	962	0	1013	9	0
3	A	54	0	38	4	0
3	B	54	0	38	0	0
4	A	54	0	38	3	0
4	B	54	0	38	0	0
5	A	18	0	13	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	91	0	88	9	0
6	D	91	0	88	7	0
7	A	158	0	0	3	0
7	B	16	0	0	1	0
7	C	38	0	0	0	0
7	D	3	0	0	0	0
All	All	11404	0	11159	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (88) 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:B:307:ARG:HH22	1:B:416:THR:HG22	1.32	0.95
1:B:178:MET:HG2	1:B:536:VAL:HG21	1.49	0.94
1:B:178:MET:CG	1:B:536:VAL:HG21	2.01	0.90
6:C:800:B12:H531	6:C:800:B12:H552	1.60	0.83
1:A:78:THR:HG21	7:A:939:HOH:O	1.82	0.79
5:A:803[C]:5AD:H8	6:C:800:B12:H372	1.65	0.79
6:D:800:B12:H552	6:D:800:B12:H531	1.64	0.77
1:A:491:ALA:O	1:A:495:ILE:HG12	1.90	0.70
1:B:307:ARG:NH2	1:B:416:THR:HG22	2.05	0.69
6:D:800:B12:H601	6:D:800:B12:H252	1.76	0.67
1:B:502:ARG:HG2	1:B:505:ARG:HH21	1.59	0.66
6:C:800:B12:H531	6:C:800:B12:C55	2.25	0.66
1:B:58:THR:OG1	1:B:416:THR:HG21	1.98	0.64
1:B:178:MET:HG2	1:B:536:VAL:CG2	2.25	0.64
6:D:800:B12:H531	6:D:800:B12:C55	2.29	0.63
1:B:178:MET:HG3	1:B:536:VAL:HG21	1.78	0.62
6:D:800:B12:H351	6:D:800:B12:H362	1.81	0.62
1:A:78:THR:HG23	4:A:802[B]:3KK:H42	1.64	0.62
2:D:77:PHE:CE1	2:D:90:VAL:HG11	2.36	0.61
6:C:800:B12:H601	6:C:800:B12:H252	1.81	0.61
6:C:800:B12:H362	6:C:800:B12:H351	1.82	0.60
1:A:92:GLY:O	5:A:803[C]:5AD:N6	2.34	0.60
2:D:77:PHE:CZ	2:D:90:VAL:HG11	2.36	0.60
5:A:803[C]:5AD:H5'3	7:A:978:HOH:O	2.01	0.59
1:A:78:THR:HG23	3:A:801[A]:3HC:H61A	1.66	0.59
1:B:299:VAL:HG11	1:B:405:LEU:HD12	1.84	0.59
1:B:147:LEU:HB2	1:B:536:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:HG2	1:A:327:LEU:HB3	1.85	0.58
1:A:299:VAL:HG11	1:A:405:LEU:HD12	1.85	0.57
1:B:306:ARG:HG2	1:B:327:LEU:HB3	1.86	0.57
1:B:412:GLU:O	1:B:416:THR:HG23	2.04	0.57
1:B:432:ARG:HB3	1:B:438:LEU:HD11	1.87	0.55
1:A:432:ARG:HB3	1:A:438:LEU:HD11	1.88	0.55
1:A:250:GLY:HA3	1:A:452:ALA:HB2	1.89	0.54
1:A:140:GLU:HB3	6:C:800:B12:H362	1.91	0.53
1:B:73:ARG:HD2	1:B:403:ASP:OD2	2.08	0.52
1:B:140:GLU:HB3	6:D:800:B12:H362	1.93	0.51
1:B:502:ARG:HG2	1:B:505:ARG:NH2	2.24	0.51
1:B:250:GLY:HA3	1:B:452:ALA:HB2	1.93	0.51
2:C:83:ARG:HG2	2:C:83:ARG:HH21	1.76	0.50
1:B:201:ILE:O	1:B:204:GLU:HB2	2.12	0.50
1:B:491:ALA:O	1:B:495:ILE:HG12	2.13	0.49
1:A:145:ASP:OD1	7:A:1003:HOH:O	2.20	0.48
1:A:372:GLU:OE1	5:A:803[C]:5AD:H3'	2.14	0.48
5:A:803[C]:5AD:C8	6:C:800:B12:H372	2.41	0.47
1:B:55:ILE:HA	7:B:913:HOH:O	2.14	0.47
1:B:88:ARG:HG2	1:B:115:SER:HB2	1.95	0.47
2:D:14:GLY:O	2:D:42:HIS:HA	2.14	0.47
1:A:146:THR:HG22	1:A:541:THR:HG22	1.96	0.47
1:A:377:PRO:HD2	5:A:803[C]:5AD:C2	2.45	0.47
2:D:29:LEU:HD23	2:D:123:ILE:HD13	1.96	0.47
2:C:14:GLY:O	2:C:42:HIS:HA	2.15	0.46
1:A:88:ARG:HG2	1:A:115:SER:HB2	1.97	0.46
1:A:294:ASP:HB3	1:A:297:GLU:HB3	1.98	0.46
1:A:240:ASN:HD21	4:A:802[B]:3KK:H14	1.81	0.45
1:B:103:PHE:O	1:B:107:ILE:HG23	2.16	0.45
2:C:8:VAL:HG13	2:C:59:VAL:HG22	1.98	0.45
1:A:109:GLN:HG3	1:A:383:LYS:HG3	1.97	0.45
1:A:240:ASN:HD21	3:A:801[A]:3HC:H61	1.82	0.44
2:C:83:ARG:HH21	2:C:83:ARG:CG	2.30	0.44
1:A:26:ALA:HA	1:A:29:LYS:HE3	1.98	0.44
1:B:109:GLN:HG3	1:B:383:LYS:HG3	2.00	0.44
2:D:119:PRO:O	2:D:123:ILE:HG12	2.17	0.44
1:A:272:THR:HG21	1:A:278:VAL:HG22	2.00	0.44
2:D:59:VAL:HG22	2:D:89:ILE:HB	2.01	0.43
1:A:236:TYR:O	1:A:284:ARG:HD2	2.17	0.43
1:B:26:ALA:HA	1:B:29:LYS:HE3	2.00	0.43
2:C:120:GLN:HA	2:C:123:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLY:HA2	1:B:431:LYS:O	2.18	0.43
1:B:236:TYR:O	1:B:284:ARG:HD2	2.18	0.42
2:D:119:PRO:HA	2:D:122:ILE:HD12	2.01	0.42
1:B:146:THR:HG22	1:B:541:THR:HG22	2.00	0.42
1:B:244:TYR:CE2	1:B:248:GLU:HG3	2.55	0.42
1:A:78:THR:OG1	1:A:82:SER:HB2	2.20	0.42
1:A:240:ASN:ND2	4:A:802[B]:3KK:H14	2.35	0.41
2:C:9:LEU:HB2	2:C:57:VAL:HG11	2.02	0.41
1:A:248:GLU:HB3	6:C:800:B12:H532	2.02	0.41
2:D:4:THR:HA	2:D:5:PRO:HD3	1.92	0.41
1:A:244:TYR:CE2	1:A:248:GLU:HG3	2.55	0.41
3:A:801[A]:3HC:HC41	6:C:800:B12:H371	2.02	0.41
1:B:294:ASP:O	1:B:298:GLU:HG2	2.21	0.41
2:C:113:LEU:HB3	2:C:117:THR:HG21	2.01	0.41
2:D:29:LEU:HB2	2:D:36:VAL:HG21	2.03	0.41
1:B:248:GLU:HB3	6:D:800:B12:H532	2.02	0.40
1:A:240:ASN:ND2	3:A:801[A]:3HC:H61	2.36	0.40
2:C:29:LEU:HB2	2:C:36:VAL:HG21	2.02	0.40
1:B:335:ALA:HB1	1:B:372:GLU:OE2	2.22	0.40
6:D:800:B12:H362	6:D:800:B12:C35	2.51	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	555/584 (95%)	533 (96%)	20 (4%)	2 (0%)	34	54
1	B	551/584 (94%)	531 (96%)	16 (3%)	4 (1%)	22	39
2	C	129/158 (82%)	125 (97%)	4 (3%)	0	100	100
2	D	127/158 (80%)	123 (97%)	4 (3%)	0	100	100
All	All	1362/1484 (92%)	1312 (96%)	44 (3%)	6 (0%)	34	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	B	169	ASN
1	A	199	ALA
1	B	199	ALA
1	B	343	TYR
1	B	200	ASP

### 5.3.2 Protein sidechains [i](#)

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	467/490 (95%)	456 (98%)	11 (2%)	49 74
1	B	465/490 (95%)	449 (97%)	16 (3%)	37 63
2	C	106/127 (84%)	101 (95%)	5 (5%)	26 49
2	D	104/127 (82%)	100 (96%)	4 (4%)	33 58
All	All	1142/1234 (92%)	1106 (97%)	36 (3%)	39 65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	101	LYS
1	A	111	GLN
1	A	173	TRP
1	A	211	TYR
1	A	220	ARG
1	A	270	GLU
1	A	326	ARG
1	A	345	VAL
1	A	437	LYS
1	A	471	ARG
1	B	18	ASP
1	B	49	THR
1	B	84	THR

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Mol	Chain	Res	Type
1	B	101	LYS
1	B	139	ARG
1	B	173	TRP
1	B	202	LEU
1	B	211	TYR
1	B	220	ARG
1	B	270	GLU
1	B	326	ARG
1	B	427	GLU
1	B	504	GLU
1	B	505	ARG
1	B	524	GLU
1	B	534	GLU
2	C	4	THR
2	C	27	ARG
2	C	43	ARG
2	C	59	VAL
2	C	133	ARG
2	D	62	VAL
2	D	104	ILE
2	D	106	LYS
2	D	111	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	B	240	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 monosaccharides in this entry.

## 5.6 Ligand geometry

7 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
5	5AD	A	803[C]	-	17,20,20	2.16	6 (35%)	15,30,30	2.51	4 (26%)
6	B12	D	800	2	90,101,101	1.02	4 (4%)	137,166,166	1.02	7 (5%)
6	B12	C	800	2	90,101,101	0.98	3 (3%)	137,166,166	1.04	6 (4%)
4	3KK	A	802[B]	-	47,56,56	1.55	6 (12%)	58,85,85	1.49	5 (8%)
3	3HC	B	801[A]	-	47,56,56	2.03	5 (10%)	59,83,83	1.73	5 (8%)
3	3HC	A	801[A]	-	47,56,56	2.05	5 (10%)	59,83,83	1.75	7 (11%)
4	3KK	B	802[B]	-	47,56,56	1.52	6 (12%)	58,85,85	1.48	4 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5AD	A	803[C]	-	-	0/0/20/20	0/3/3/3
6	B12	D	800	2	-	7/52/223/223	0/3/11/11
6	B12	C	800	2	-	7/52/223/223	0/3/11/11
4	3KK	A	802[B]	-	-	5/52/73/73	0/3/3/3
3	3HC	B	801[A]	-	-	6/51/71/71	0/3/3/3
3	3HC	A	801[A]	-	-	7/51/71/71	0/3/3/3
4	3KK	B	802[B]	-	-	4/52/73/73	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801[A]	3HC	C2A-N3A	9.50	1.47	1.32
3	A	801[A]	3HC	C2A-N3A	9.43	1.47	1.32
3	A	801[A]	3HC	C2A-N1A	7.88	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801[A]	3HC	C2A-N1A	7.75	1.48	1.33
6	D	800	B12	C14-N23	6.72	1.43	1.35
5	A	803[C]	5AD	C2-N3	6.28	1.42	1.32
6	C	800	B12	C14-N23	6.00	1.42	1.35
4	A	802[B]	3KK	C2A-N3A	6.00	1.41	1.32
4	B	802[B]	3KK	C2A-N3A	5.98	1.41	1.32
4	A	802[B]	3KK	C2A-N1A	4.73	1.42	1.33
4	B	802[B]	3KK	C2A-N1A	4.69	1.42	1.33
4	B	802[B]	3KK	O1-C1	3.23	1.23	1.20
4	A	802[B]	3KK	O1-C1	3.21	1.23	1.20
5	A	803[C]	5AD	C2-N1	3.21	1.39	1.33
6	C	800	B12	C9-N22	3.00	1.38	1.30
5	A	803[C]	5AD	C2'-C1'	-2.92	1.49	1.53
6	C	800	B12	C1P-C2P	2.85	1.58	1.51
3	A	801[A]	3HC	O4B-C1B	2.83	1.45	1.41
4	A	802[B]	3KK	O4B-C1B	2.72	1.44	1.41
4	B	802[B]	3KK	O4B-C1B	2.64	1.44	1.41
3	B	801[A]	3HC	O4B-C1B	2.61	1.44	1.41
6	D	800	B12	C1P-C2P	2.59	1.58	1.51
6	D	800	B12	C9-N22	2.53	1.37	1.30
5	A	803[C]	5AD	C6-C5	-2.33	1.34	1.43
6	D	800	B12	C16-C15	2.31	1.51	1.44
3	B	801[A]	3HC	C5A-C4A	-2.17	1.35	1.40
4	B	802[B]	3KK	C5A-C4A	-2.17	1.35	1.40
5	A	803[C]	5AD	O4'-C1'	2.15	1.44	1.41
4	A	802[B]	3KK	C5A-C4A	-2.12	1.35	1.40
4	B	802[B]	3KK	C6A-C5A	-2.12	1.35	1.43
4	A	802[B]	3KK	C6A-C5A	-2.10	1.35	1.43
3	B	801[A]	3HC	C6A-C5A	-2.09	1.35	1.43
3	A	801[A]	3HC	C5A-C4A	-2.07	1.35	1.40
3	A	801[A]	3HC	C6A-C5A	-2.07	1.35	1.43
5	A	803[C]	5AD	C5-C4	-2.07	1.35	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801[A]	3HC	N3A-C2A-N1A	-10.53	112.22	128.68
3	A	801[A]	3HC	N3A-C2A-N1A	-10.53	112.22	128.68
4	B	802[B]	3KK	N3A-C2A-N1A	-7.95	116.25	128.68
4	A	802[B]	3KK	N3A-C2A-N1A	-7.94	116.27	128.68
5	A	803[C]	5AD	N3-C2-N1	-6.23	118.94	128.68
5	A	803[C]	5AD	C5'-C4'-C3'	-5.64	109.77	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	800	B12	C2-C1-C19	-3.49	113.09	118.60
6	D	800	B12	C2-C1-C19	-3.24	113.48	118.60
5	A	803[C]	5AD	C5-C6-N6	-3.24	115.43	120.35
6	D	800	B12	C20-C1-C2	3.23	118.67	113.28
6	C	800	B12	C20-C1-C2	3.15	118.55	113.28
6	C	800	B12	C10-C9-N22	2.67	128.79	125.73
4	B	802[B]	3KK	O1-C1-S1P	2.59	124.64	122.00
6	D	800	B12	C60-C18-C17	2.56	121.95	115.74
4	A	802[B]	3KK	O1-C1-S1P	2.36	124.41	122.00
6	D	800	B12	C10-C9-N22	2.36	128.44	125.73
3	A	801[A]	3HC	C2-C1-S1P	2.31	116.49	113.63
3	A	801[A]	3HC	C2P-C3P-N4P	-2.29	107.61	112.42
3	B	801[A]	3HC	C2P-C3P-N4P	-2.29	107.61	112.42
3	A	801[A]	3HC	C1B-N9A-C4A	-2.25	122.69	126.64
5	A	803[C]	5AD	C1'-N9-C4	2.22	130.53	126.64
3	B	801[A]	3HC	C1B-N9A-C4A	-2.20	122.78	126.64
6	D	800	B12	C54-C17-C55	-2.19	105.64	109.25
6	C	800	B12	C13-C12-C11	-2.18	98.50	100.97
4	A	802[B]	3KK	C1B-N9A-C4A	-2.18	122.82	126.64
4	B	802[B]	3KK	C1B-N9A-C4A	-2.14	122.88	126.64
3	B	801[A]	3HC	C2-C1-S1P	2.14	116.27	113.63
4	A	802[B]	3KK	C2P-C3P-N4P	-2.13	107.94	112.42
4	B	802[B]	3KK	C2P-C3P-N4P	-2.13	107.94	112.42
6	C	800	B12	C35-C5-C6	2.10	125.77	122.43
6	D	800	B12	C8-C9-C10	-2.08	118.83	123.32
3	B	801[A]	3HC	O9A-P3B-O8A	2.07	115.56	107.64
4	A	802[B]	3KK	C6P-C5P-N4P	-2.07	112.94	116.42
6	D	800	B12	P-O2-C3R	2.07	126.93	119.41
3	A	801[A]	3HC	C6P-C5P-N4P	-2.06	112.95	116.42
3	A	801[A]	3HC	O9A-P3B-O8A	2.06	115.50	107.64
3	A	801[A]	3HC	C4A-C5A-N7A	-2.05	107.26	109.40
6	C	800	B12	C60-C18-C17	2.02	120.65	115.74

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801[A]	3HC	O1-C1-S1P-C2P
3	A	801[A]	3HC	C2-C1-S1P-C2P
3	B	801[A]	3HC	O1-C1-S1P-C2P
3	B	801[A]	3HC	C2-C1-S1P-C2P
4	A	802[B]	3KK	O9P-C9P-CAP-OAP

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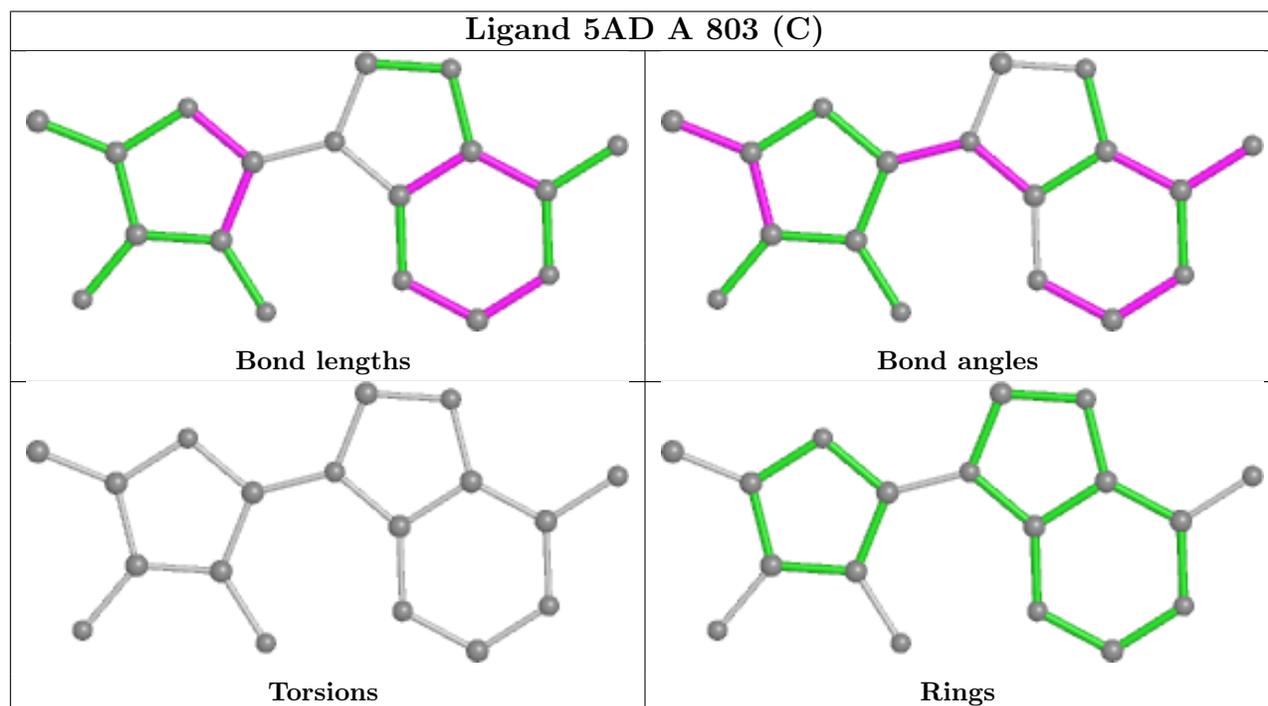
Mol	Chain	Res	Type	Atoms
4	B	802[B]	3KK	O9P-C9P-CAP-OAP
3	A	801[A]	3HC	O9P-C9P-CAP-OAP
3	B	801[A]	3HC	O9P-C9P-CAP-OAP
6	C	800	B12	C2P-O3-P-O2
6	D	800	B12	C2P-O3-P-O2
6	C	800	B12	C3-C30-C31-C32
6	D	800	B12	C3-C30-C31-C32
6	D	800	B12	C55-C56-C57-O58
6	C	800	B12	C42-C41-C8-C9
6	C	800	B12	C55-C56-C57-O58
3	A	801[A]	3HC	C3P-C2P-S1P-C1
3	B	801[A]	3HC	C3P-C2P-S1P-C1
4	A	802[B]	3KK	C3P-C2P-S1P-C1
4	B	802[B]	3KK	C3P-C2P-S1P-C1
6	D	800	B12	C55-C56-C57-N59
6	D	800	B12	C42-C41-C8-C9
3	A	801[A]	3HC	N8P-C9P-CAP-OAP
3	B	801[A]	3HC	N8P-C9P-CAP-OAP
4	A	802[B]	3KK	N8P-C9P-CAP-OAP
4	B	802[B]	3KK	N8P-C9P-CAP-OAP
6	C	800	B12	C55-C56-C57-N59
3	A	801[A]	3HC	C5B-O5B-P1A-O3A
3	B	801[A]	3HC	C5B-O5B-P1A-O3A
4	A	802[B]	3KK	C5B-O5B-P1A-O3A
4	B	802[B]	3KK	C5B-O5B-P1A-O3A
6	C	800	B12	C30-C31-C32-N33
6	D	800	B12	C30-C31-C32-N33
6	D	800	B12	C30-C31-C32-O34
3	A	801[A]	3HC	C4B-C5B-O5B-P1A
6	C	800	B12	C30-C31-C32-O34
4	A	802[B]	3KK	C4B-C5B-O5B-P1A

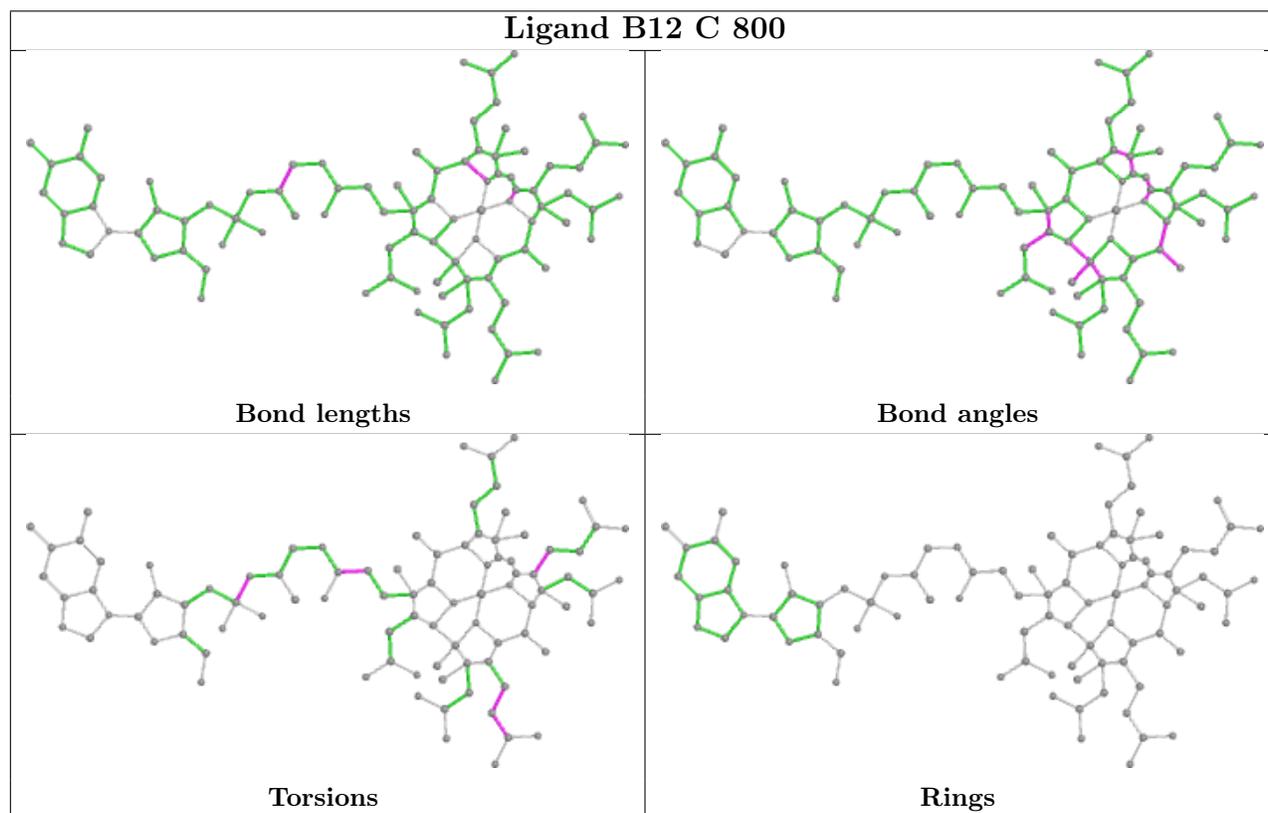
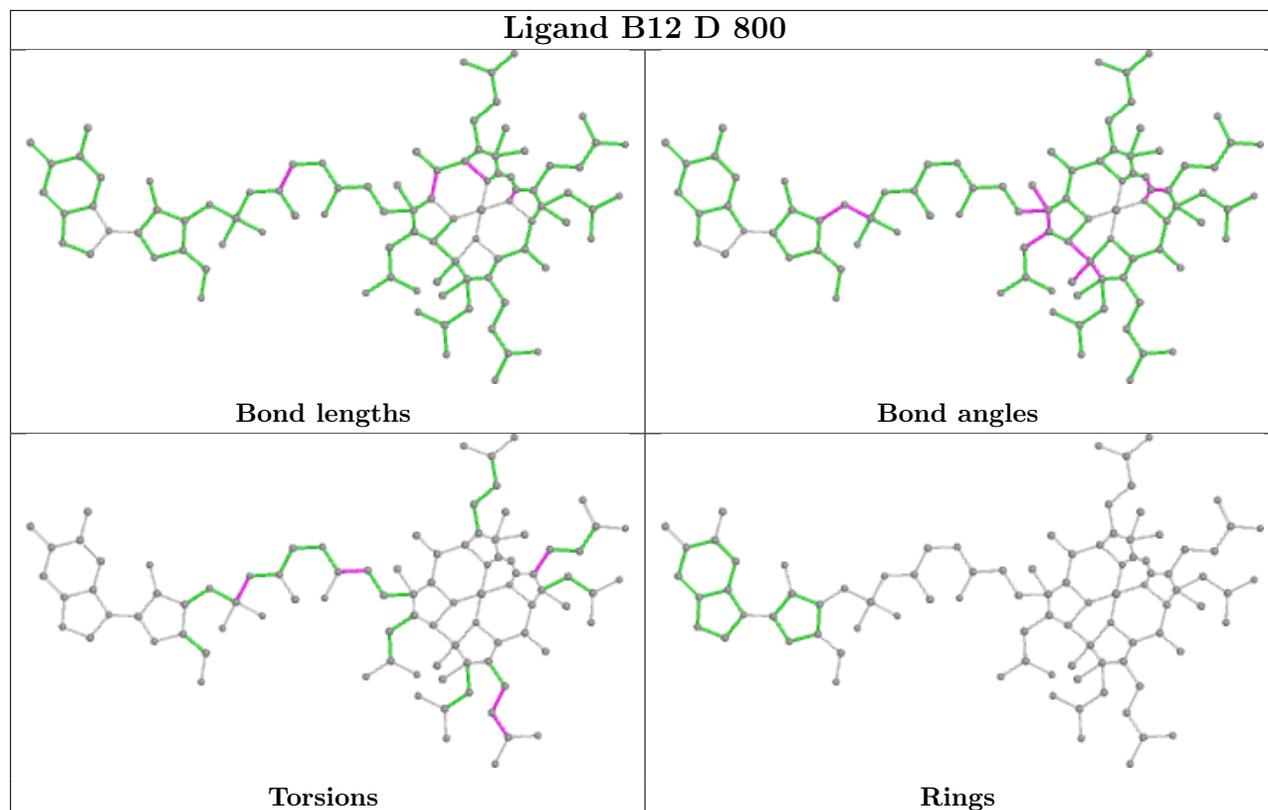
There are no ring outliers.

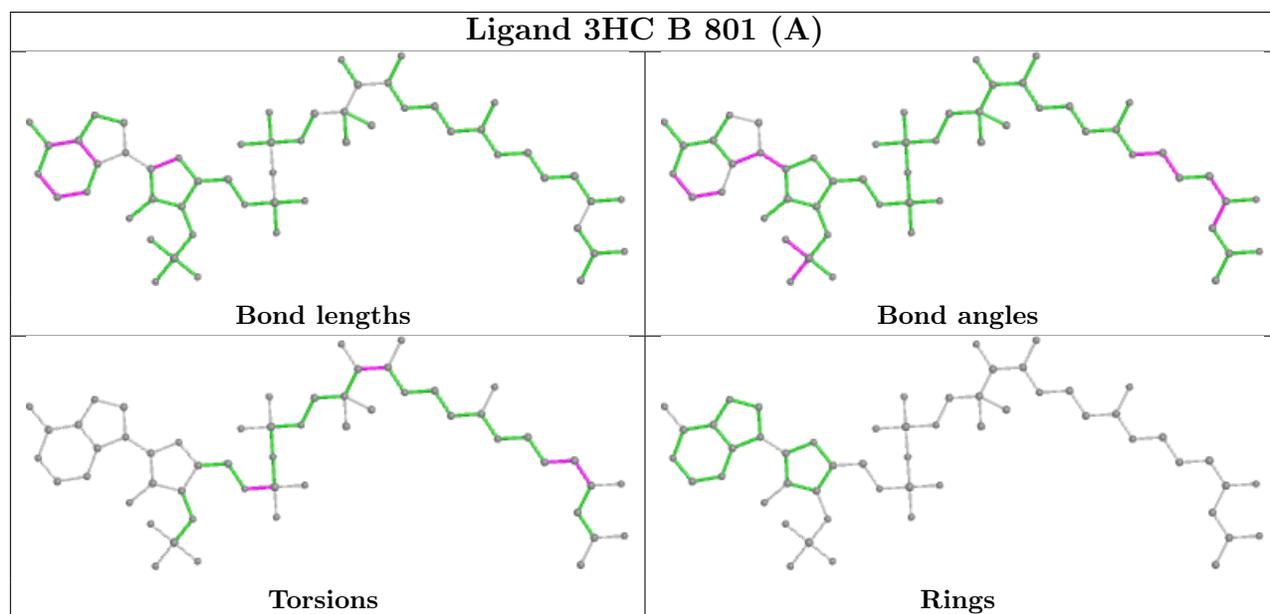
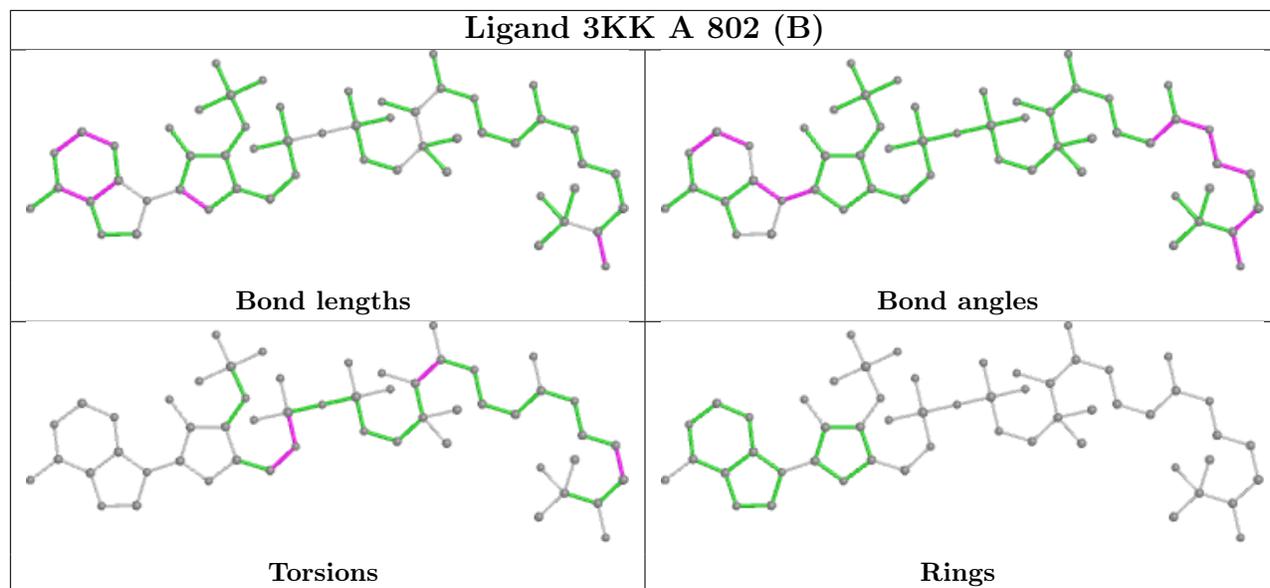
5 monomers are involved in 26 short contacts:

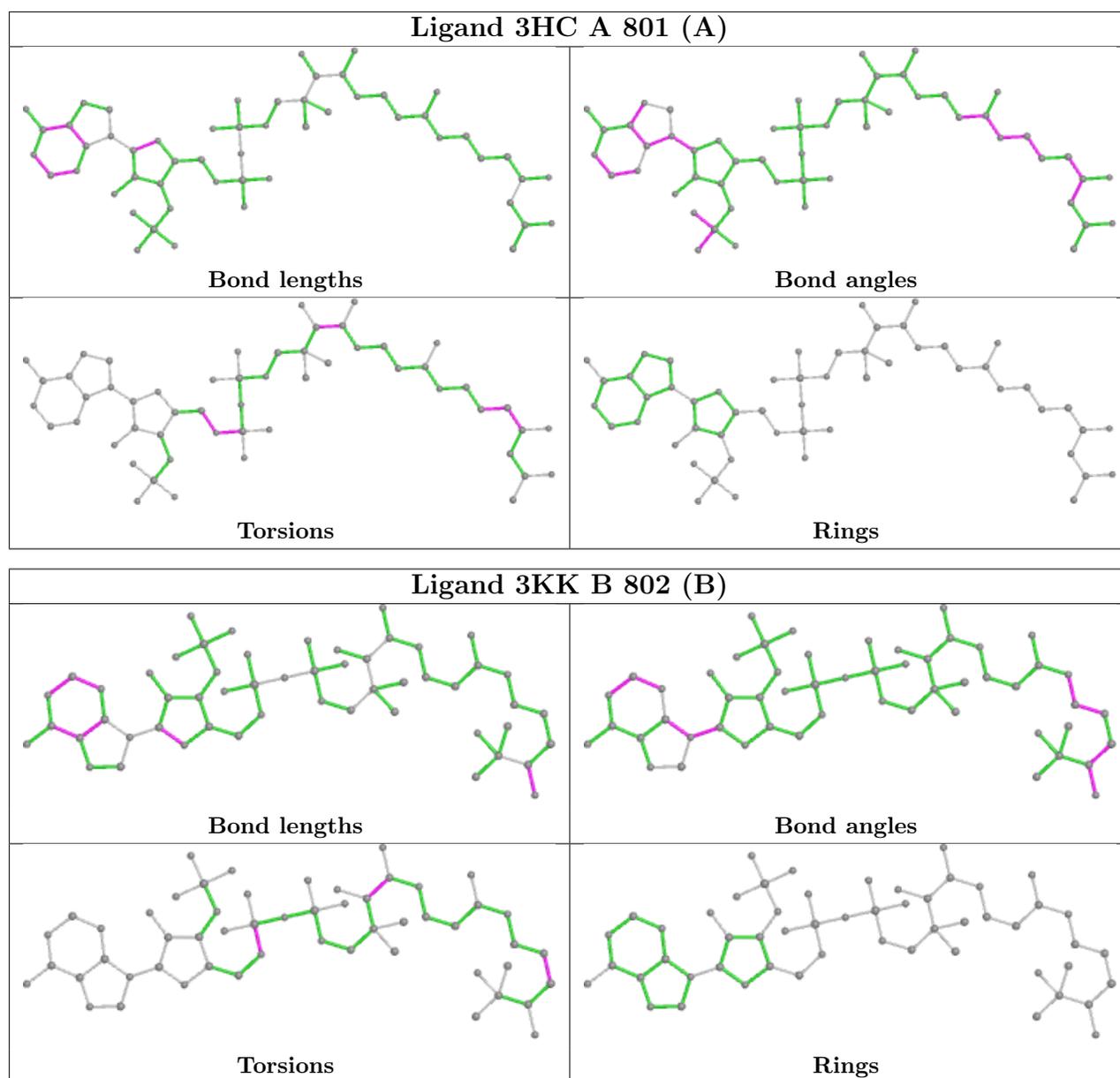
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	803[C]	5AD	6	0
6	D	800	B12	7	0
6	C	800	B12	9	0
4	A	802[B]	3KK	3	0
3	A	801[A]	3HC	4	0

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	557/584 (95%)	-0.49	5 (0%) 84 86	16, 34, 62, 97	0
1	B	555/584 (95%)	-0.06	12 (2%) 62 65	42, 56, 81, 101	0
2	C	131/158 (82%)	-0.46	1 (0%) 86 87	19, 36, 61, 73	0
2	D	129/158 (81%)	0.54	14 (10%) 5 5	54, 77, 97, 105	0
All	All	1372/1484 (92%)	-0.22	32 (2%) 60 63	16, 49, 82, 105	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	81	ASP	4.8
1	A	478	ASP	4.8
2	D	61	GLY	4.3
2	D	62	VAL	4.3
1	B	475	ASN	3.7
1	A	477	GLU	3.6
2	D	87	ASP	3.5
2	D	33	GLY	3.5
1	B	479	VAL	3.2
1	B	172	ALA	2.8
1	B	7	GLN	2.7
2	D	85	ALA	2.6
1	B	500	ARG	2.6
2	D	32	ALA	2.5
2	D	110	ARG	2.5
2	D	54	GLN	2.4
2	D	84	GLY	2.4
1	B	171	SER	2.4
1	B	174	ILE	2.3
2	D	130	VAL	2.3
1	B	188	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	106	LYS	2.3
1	B	485	PRO	2.2
1	A	6	PRO	2.2
1	A	10	SER	2.2
1	A	508	ALA	2.2
2	C	3	GLN	2.1
2	D	4	THR	2.1
2	D	59	VAL	2.1
1	B	481	ILE	2.1
1	B	185	LYS	2.0
1	B	504	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

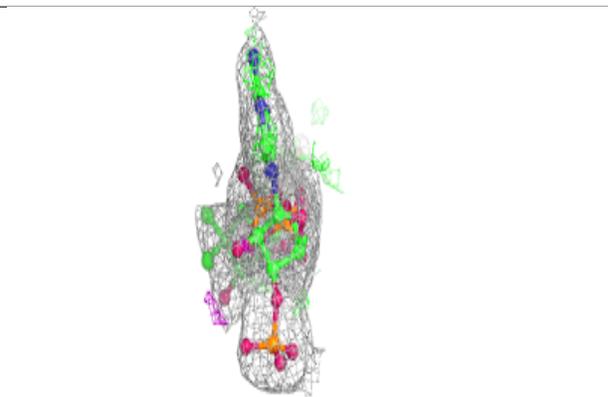
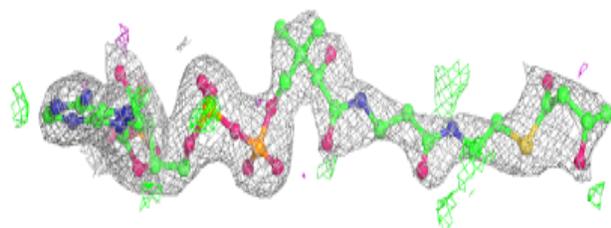
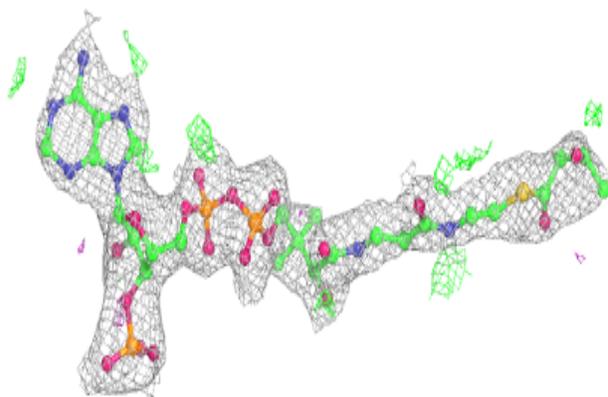
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	3HC	B	801[A]	54/54	0.94	0.14	45,55,63,65	54
4	3KK	B	802[B]	54/54	0.94	0.14	45,56,63,65	54
5	5AD	A	803[C]	18/18	0.94	0.20	17,27,31,32	18
3	3HC	A	801[A]	54/54	0.96	0.12	20,33,45,47	54
4	3KK	A	802[B]	54/54	0.96	0.12	6,32,45,47	54
6	B12	D	800	91/91	0.96	0.14	29,44,66,70	0
6	B12	C	800	91/91	0.98	0.13	14,24,35,38	0

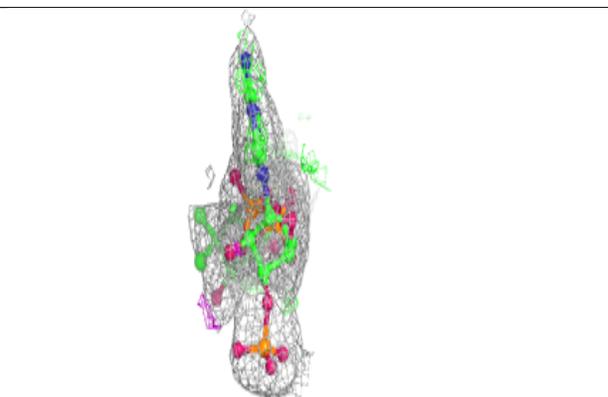
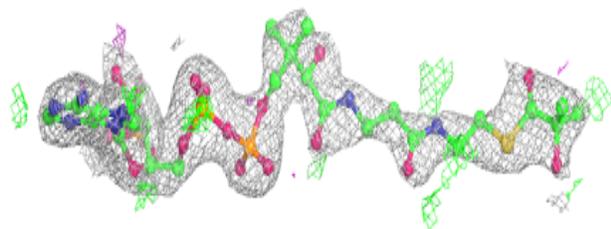
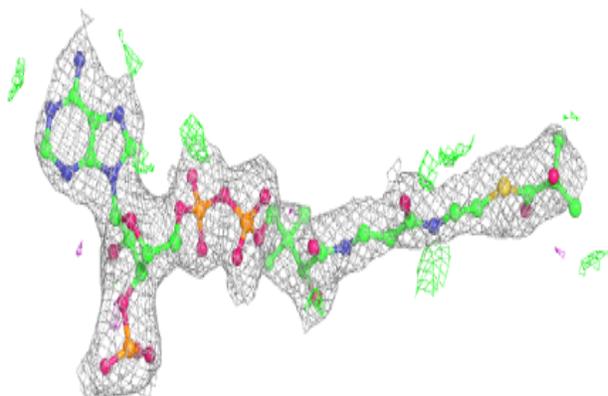
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 3HC B 801 (A):**

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

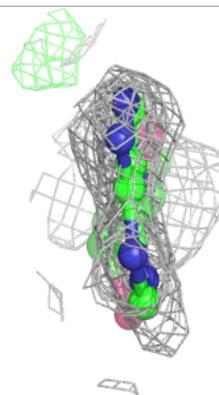
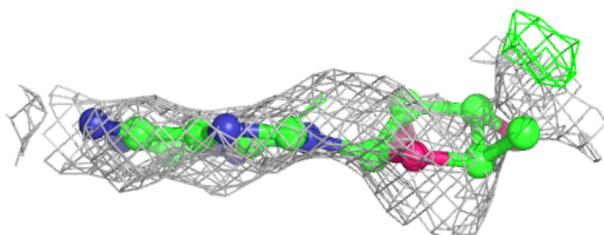
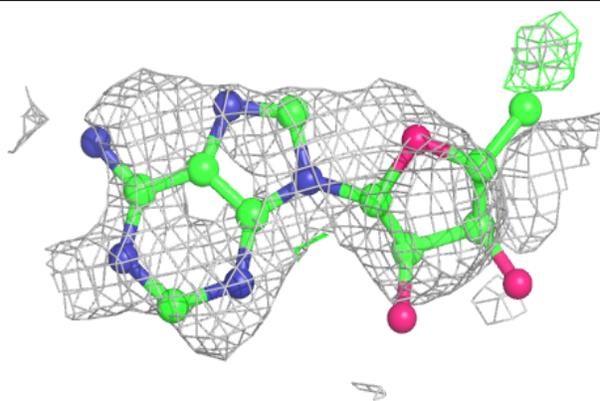
**Electron density around 3KK B 802 (B):**

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

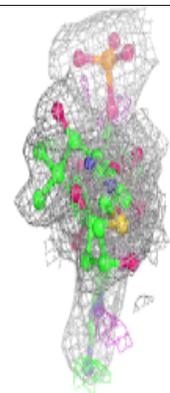
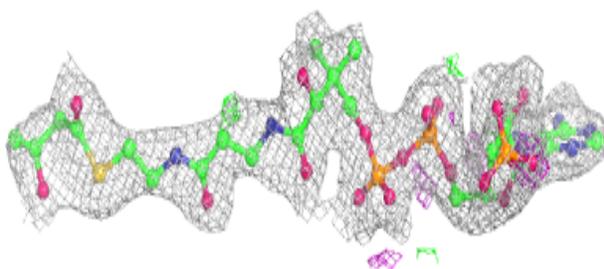
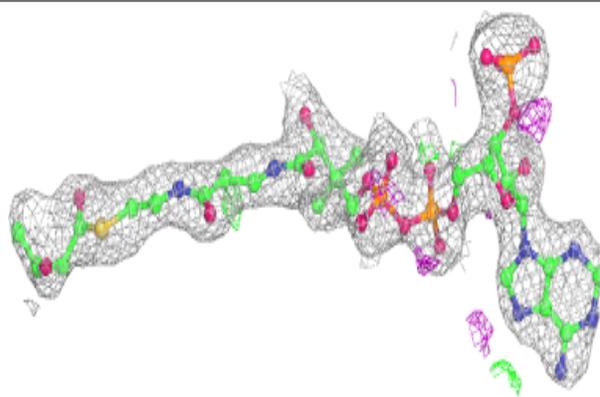


**Electron density around 5AD A 803 (C):**

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

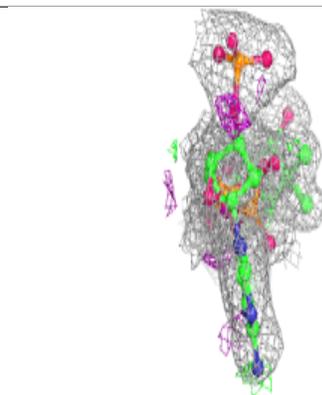
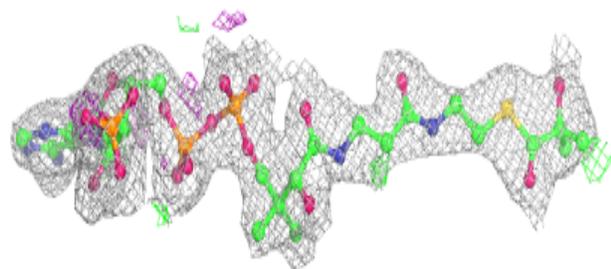
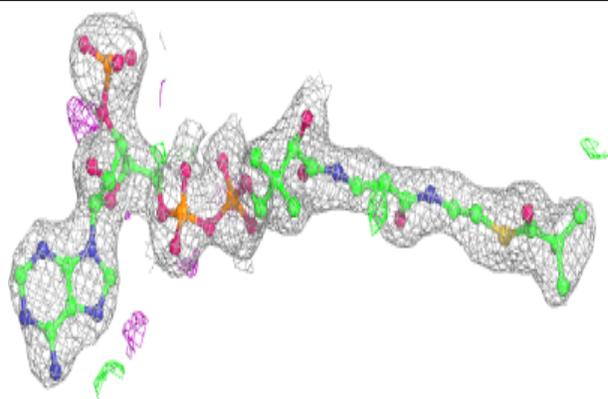
**Electron density around 3HC A 801 (A):**

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

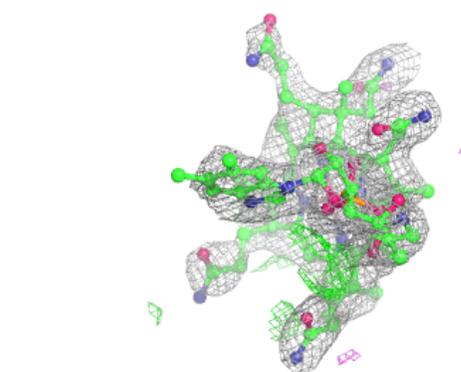
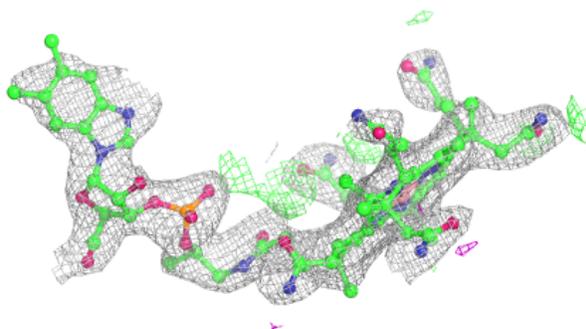
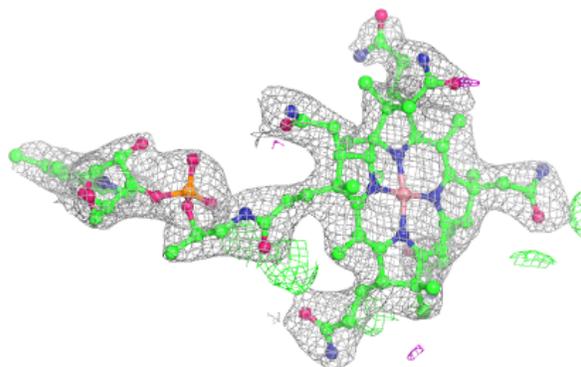


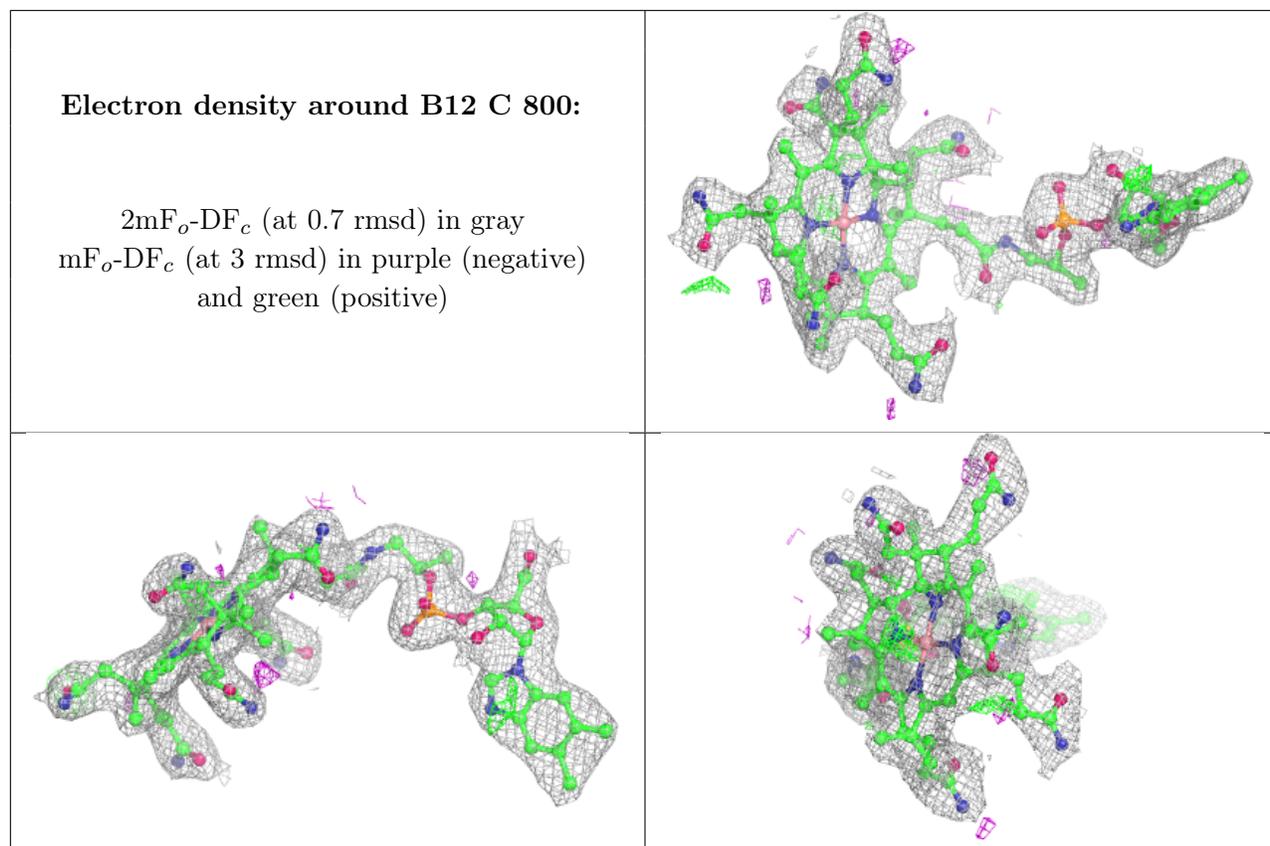
**Electron density around 3KK A 802 (B):**

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

**Electron density around B12 D 800:**

$2mF_o-DF_c$  (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.