



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:19 pm BST

PDB ID : 1XPM
Title : Crystal Structure of Staphylococcus aureus HMG-CoA Synthase with HMG-CoA and Acetoacetyl-CoA and Acetylated Cysteine
Authors : Theisen, M.J.; Misra, I.; Saadat, D.; Campobasso, N.; Miziorko, H.M.; Harrison, D.H.T.
Deposited on : 2004-10-08
Resolution : 1.60 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 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

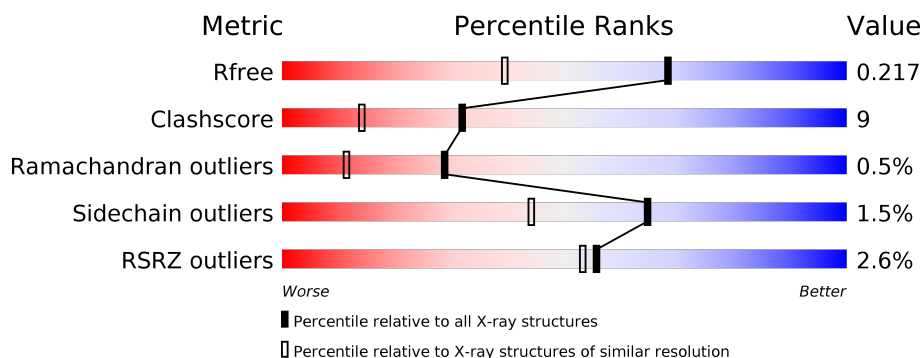
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 ≥ 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	397	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	397	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	397	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	397	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15324 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 3-hydroxy-3-methylglutaryl CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	33	0
			3458	2202	576	664	16			
1	B	389	Total	C	N	O	S	0	33	0
			3431	2188	569	658	16			
1	C	389	Total	C	N	O	S	0	33	0
			3425	2184	571	654	16			
1	D	389	Total	C	N	O	S	0	33	0
			3439	2191	571	661	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
A	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
A	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
A	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
A	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
A	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
B	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
B	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
B	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
B	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
B	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6

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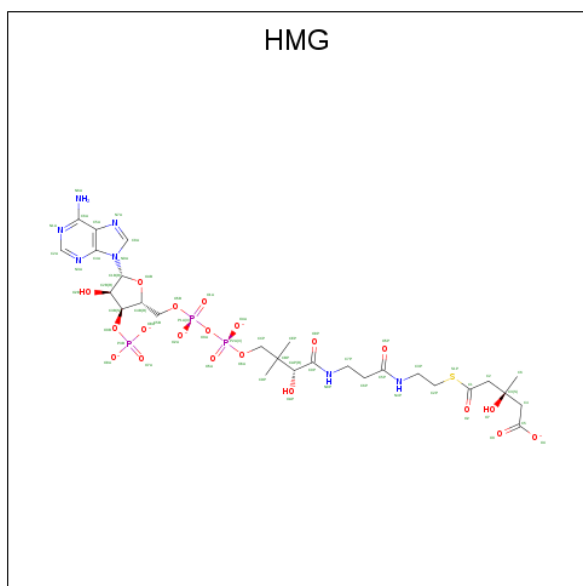
Chain	Residue	Modelled	Actual	Comment	Reference
B	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
C	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
C	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
C	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
C	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
C	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
D	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
D	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
D	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
D	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
D	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 3-HYDROXY-3-METHYLGLUTARYL-COENZYME A (three-letter code: HMG) (formula: $C_{27}H_{39}N_7O_{20}P_3S$).



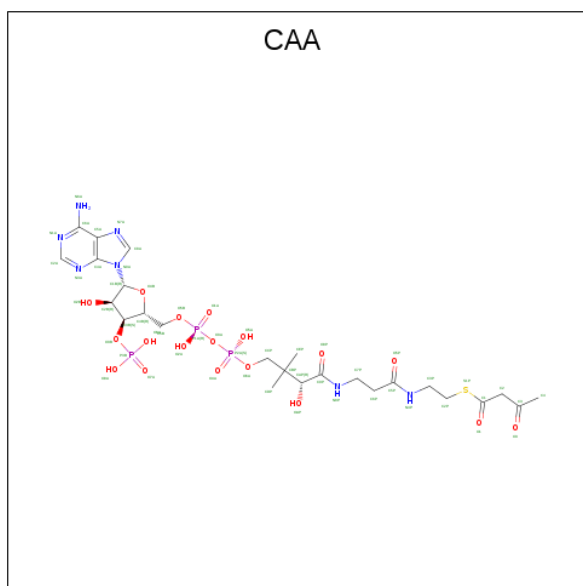
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 58 27 7 20 3 1	0	1
3	B	1	Total C N O P S 58 27 7 20 3 1	0	1
3	C	1	Total C N O P S 58 27 7 20 3 1	0	1

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	1
			58	27	7	20	3	1		

- Molecule 4 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).

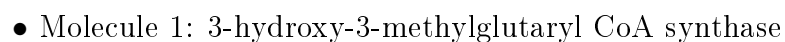
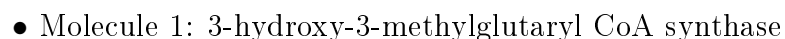
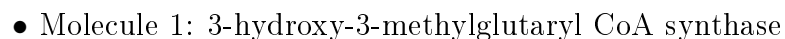


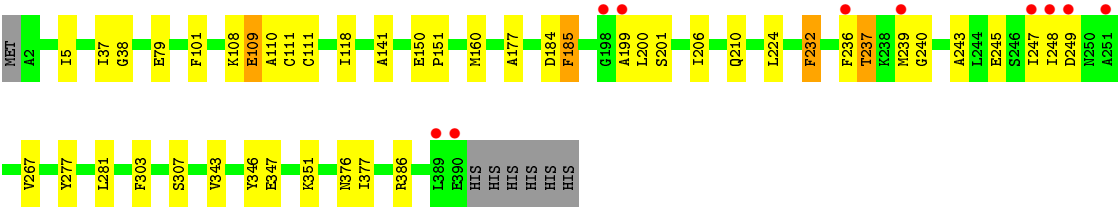
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	C	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	D	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	1
			265	265		
5	B	277	Total	O	0	1
			277	277		
5	C	278	Total	O	0	1
			278	278		
5	D	263	Total	O	0	1
			263	263		

- Molecule 1: 3-hydroxy-3-methylglutaryl CoA synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.12Å 118.77Å 121.30Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 24.96 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.60) 89.1 (24.96-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.226 0.201 , 0.217	Depositor DCC
R_{free} test set	10669 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.459 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15324	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 46.36 % 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 1.1581e-04. 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: CAA, HMG, SCY, SO4

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	4.51	9/3586 (0.3%)	1.33	15/4857 (0.3%)
1	B	1.09	3/3547 (0.1%)	0.66	3/4808 (0.1%)
1	C	1.72	6/3543 (0.2%)	0.84	6/4801 (0.1%)
1	D	1.13	3/3564 (0.1%)	0.66	3/4831 (0.1%)
All	All	2.54	21/14240 (0.1%)	0.91	27/19297 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202[A]	LYS	CD-CE	147.32	5.19	1.51
1	A	202[B]	LYS	CD-CE	147.32	5.19	1.51
1	A	202[C]	LYS	CD-CE	147.32	5.19	1.51
1	C	202[A]	LYS	CG-CD	44.16	3.02	1.52
1	C	202[B]	LYS	CG-CD	44.16	3.02	1.52
1	C	202[C]	LYS	CG-CD	44.16	3.02	1.52
1	A	249[A]	ASP	CG-OD2	43.32	2.25	1.25
1	A	249[B]	ASP	CG-OD2	43.32	2.25	1.25
1	A	249[C]	ASP	CG-OD2	43.32	2.25	1.25
1	C	249[A]	ASP	CB-CG	37.95	2.31	1.51
1	C	249[B]	ASP	CB-CG	37.95	2.31	1.51
1	C	249[C]	ASP	CB-CG	37.95	2.31	1.51
1	D	249[A]	ASP	CB-CG	37.29	2.30	1.51
1	D	249[B]	ASP	CB-CG	37.29	2.30	1.51
1	D	249[C]	ASP	CB-CG	37.29	2.30	1.51
1	B	249[A]	ASP	CB-CG	35.87	2.27	1.51
1	B	249[B]	ASP	CB-CG	35.87	2.27	1.51
1	B	249[C]	ASP	CB-CG	35.87	2.27	1.51
1	A	249[A]	ASP	CG-OD1	24.51	1.81	1.25
1	A	249[B]	ASP	CG-OD1	24.51	1.81	1.25
1	A	249[C]	ASP	CG-OD1	24.51	1.81	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249[A]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[B]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[C]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[A]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	249[B]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	249[C]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	202[A]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	A	202[B]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	A	202[C]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	C	202[A]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	C	202[B]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	C	202[C]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	A	249[A]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	A	249[B]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	A	249[C]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	B	249[A]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	B	249[B]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	B	249[C]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	D	249[A]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	D	249[B]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	D	249[C]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	C	249[A]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	C	249[B]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	C	249[C]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	A	202[A]	LYS	CD-CE-NZ	9.45	133.44	111.70
1	A	202[B]	LYS	CD-CE-NZ	9.45	133.44	111.70
1	A	202[C]	LYS	CD-CE-NZ	9.45	133.44	111.70

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	3458	0	3310	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3431	0	3252	62	0
1	C	3425	0	3257	57	0
1	D	3439	0	3277	48	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	58	0	39	5	0
3	B	58	0	39	1	0
3	C	58	0	39	4	0
3	D	58	0	39	2	0
4	A	54	0	36	0	0
4	B	54	0	36	0	0
4	C	54	0	36	4	0
4	D	54	0	36	1	0
5	A	265	0	0	6	0
5	B	277	0	0	4	0
5	C	278	0	0	5	0
5	D	263	0	0	2	0
All	All	15324	0	13396	238	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 9.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ILE:HG21	1:C:160[C]:MET:HE2	1.51	0.93
1:B:386[C]:ARG:HD3	5:B:2630:HOH:O	1.84	0.76
1:B:118:ILE:HG21	1:B:160[C]:MET:HE2	1.68	0.75
1:A:202[C]:LYS:HG3	1:A:239[C]:MET:SD	2.27	0.74
1:D:236[B]:PHE:HE1	3:D:4401[B]:HMG:H3P2	1.55	0.70
1:B:5:ILE:HG12	1:B:160[C]:MET:HE3	1.73	0.70
1:A:36:GLY:O	1:A:238[A]:LYS:HG3	1.93	0.69
1:A:36:GLY:O	1:A:238[B]:LYS:HG3	1.93	0.69
1:A:118:ILE:HG21	1:A:160[C]:MET:HE2	1.75	0.69
3:C:3401[B]:HMG:H8	3:C:3401[B]:HMG:H131	1.58	0.67
1:A:36:GLY:O	1:A:238[C]:LYS:HG3	1.96	0.65
1:A:236[B]:PHE:CZ	1:A:239[B]:MET:HB2	2.32	0.64
1:A:236[A]:PHE:CZ	1:A:239[A]:MET:HB2	2.32	0.64
1:D:236[B]:PHE:CZ	1:D:239[B]:MET:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HG21	1:B:160[C]:MET:CE	2.28	0.64
1:B:63:ILE:HD11	1:B:96:LEU:HD22	1.79	0.63
1:C:236[A]:PHE:CZ	1:C:239[A]:MET:HB2	2.33	0.63
1:C:5:ILE:HG12	1:C:160[C]:MET:HE3	1.81	0.63
1:D:236[A]:PHE:CZ	1:D:239[A]:MET:HB2	2.34	0.63
1:B:365:VAL:HG13	1:B:373:TYR:CZ	2.33	0.63
1:A:236[B]:PHE:HE1	3:A:1401[B]:HMG:H3P2	1.63	0.63
1:C:236[B]:PHE:CZ	1:C:239[B]:MET:HB2	2.34	0.63
1:B:236[A]:PHE:CZ	1:B:239[A]:MET:HB2	2.34	0.62
1:B:111[A]:SCY:CD	1:B:111[A]:SCY:H	2.13	0.62
1:C:110[A]:ALA:HB1	1:C:111[A]:SCY:CE	2.30	0.62
1:C:111[A]:SCY:H	1:C:111[A]:SCY:CD	2.13	0.62
1:B:236[B]:PHE:CZ	1:B:239[B]:MET:HB2	2.35	0.62
1:A:111[A]:SCY:H	1:A:111[A]:SCY:CD	2.13	0.61
1:C:202[C]:LYS:HG3	1:C:239[C]:MET:HE1	1.82	0.61
1:D:111[A]:SCY:CD	1:D:111[A]:SCY:H	2.14	0.60
1:B:110[A]:ALA:HB1	1:B:111[A]:SCY:CE	2.31	0.60
1:D:224:LEU:HD11	1:D:247[C]:ILE:HG22	1.82	0.60
1:C:206:ILE:O	1:C:210[B]:GLN:HG3	2.02	0.59
1:C:236[A]:PHE:CE1	1:C:239[A]:MET:HB2	2.38	0.59
1:C:236[B]:PHE:CE1	1:C:239[B]:MET:HB2	2.38	0.59
1:C:118:ILE:HG21	1:C:160[C]:MET:CE	2.30	0.58
3:C:3401[B]:HMG:H8	3:C:3401[B]:HMG:CDP	2.16	0.58
1:A:37:ILE:HG23	1:A:236[C]:PHE:CD2	2.39	0.58
1:B:236[B]:PHE:CE1	1:B:239[B]:MET:HB2	2.38	0.58
1:B:236[A]:PHE:CE1	1:B:239[A]:MET:HB2	2.38	0.57
1:C:206:ILE:O	1:C:210[A]:GLN:HG3	2.03	0.57
1:B:224:LEU:HD11	1:B:247[C]:ILE:HG22	1.85	0.57
1:D:206:ILE:O	1:D:210[B]:GLN:HG3	2.05	0.56
1:D:110[A]:ALA:HB1	1:D:111[A]:SCY:CE	2.34	0.56
1:D:206:ILE:O	1:D:210[A]:GLN:HG3	2.05	0.56
1:A:5:ILE:CD1	1:A:160[C]:MET:HE3	2.36	0.56
1:A:110[A]:ALA:HB1	1:A:111[A]:SCY:CE	2.35	0.56
1:C:129:PRO:HA	1:C:164:HIS:CD2	2.42	0.55
1:A:206:ILE:O	1:A:210[B]:GLN:HG3	2.06	0.54
1:C:237[A]:THR:HG22	1:C:267:VAL:HB	1.88	0.54
1:B:199[C]:ALA:O	1:B:200[C]:LEU:HD23	2.06	0.54
1:C:237[B]:THR:HG22	1:C:267:VAL:HB	1.88	0.54
1:C:386[C]:ARG:HD3	5:C:3773:HOH:O	2.07	0.54
1:B:206:ILE:O	1:B:210[A]:GLN:HG3	2.08	0.54
1:C:224:LEU:HD11	1:C:247[C]:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3402[A]:CAA:H141	4:C:3402[A]:CAA:HN8	1.73	0.53
1:A:206:ILE:O	1:A:210[A]:GLN:HG3	2.07	0.53
1:B:129:PRO:HA	1:B:164:HIS:CD2	2.44	0.53
1:D:199[C]:ALA:O	1:D:200[C]:LEU:HD23	2.09	0.53
1:A:118:ILE:HG21	1:A:160[C]:MET:CE	2.38	0.53
1:A:202[C]:LYS:HG3	1:A:239[C]:MET:CE	2.40	0.52
1:B:206:ILE:O	1:B:210[B]:GLN:HG3	2.09	0.52
1:D:5:ILE:CD1	1:D:160[C]:MET:HE3	2.39	0.52
1:B:5:ILE:CD1	1:B:160[C]:MET:HE3	2.40	0.52
1:B:237[A]:THR:HG22	1:B:267:VAL:HB	1.91	0.52
1:B:37:ILE:HG23	1:B:236[C]:PHE:CD2	2.45	0.52
1:C:290:GLU:OE2	1:C:331:HIS:ND1	2.42	0.52
1:C:202[C]:LYS:HG3	1:C:239[C]:MET:CE	2.40	0.51
1:D:184:ASP:HB2	1:D:201[B]:SER:HA	1.92	0.51
1:C:294:LEU:HB2	1:C:318:LEU:HD11	1.92	0.51
1:B:237[B]:THR:HG22	1:B:267:VAL:HB	1.91	0.51
1:B:386[A]:ARG:HH11	1:B:386[A]:ARG:HG3	1.76	0.51
1:B:386[B]:ARG:HH11	1:B:386[B]:ARG:HG3	1.76	0.51
1:D:184:ASP:HB2	1:D:201[A]:SER:HA	1.92	0.51
3:A:1401[B]:HMG:H131	3:A:1401[B]:HMG:H8	1.76	0.51
1:B:184:ASP:HB2	1:B:201[C]:SER:HA	1.93	0.51
1:D:386[A]:ARG:HG3	1:D:386[A]:ARG:HH11	1.76	0.50
1:D:386[B]:ARG:HG3	1:D:386[B]:ARG:HH11	1.76	0.50
4:C:3402[A]:CAA:N8P	4:C:3402[A]:CAA:H141	2.26	0.50
1:D:79:GLU:OE2	1:D:111[A]:SCY:HE2	2.12	0.50
1:A:252:ASP:O	1:A:256:GLN:HG3	2.11	0.50
1:A:245[A]:GLU:CD	1:A:248[A]:ILE:HD11	2.32	0.50
1:A:245[B]:GLU:CD	1:A:248[B]:ILE:HD11	2.32	0.50
1:B:5:ILE:CG1	1:B:160[C]:MET:HE3	2.40	0.50
1:B:184:ASP:HB2	1:B:201[B]:SER:HA	1.93	0.50
1:A:79:GLU:OE2	1:A:111[A]:SCY:HE2	2.12	0.49
4:C:3402[A]:CAA:CEP	4:C:3402[A]:CAA:HN8	2.25	0.49
1:A:224:LEU:HD11	1:A:247[C]:ILE:HG22	1.93	0.49
1:C:247[A]:ILE:HB	5:C:3749:HOH:O	2.12	0.49
1:A:386[C]:ARG:HG3	1:A:386[C]:ARG:HH11	1.78	0.49
1:C:236[C]:PHE:CZ	1:C:239[C]:MET:HB2	2.48	0.49
1:C:184:ASP:HB2	1:C:201[B]:SER:HA	1.95	0.48
1:C:247[B]:ILE:HB	5:C:3749:HOH:O	2.13	0.48
1:D:236[C]:PHE:CZ	1:D:239[C]:MET:HB2	2.49	0.48
1:B:184:ASP:HB2	1:B:201[A]:SER:HA	1.93	0.48
1:D:232[B]:PHE:N	1:D:232[B]:PHE:CD1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLY:HA3	1:D:237[B]:THR:OG1	2.13	0.48
1:D:343:VAL:O	1:D:347:GLU:HG3	2.14	0.48
1:A:5:ILE:HG12	1:A:160[C]:MET:HE3	1.96	0.48
1:C:247[A]:ILE:HG13	1:C:248[A]:ILE:N	2.28	0.48
1:D:232[A]:PHE:CD1	1:D:232[A]:PHE:N	2.82	0.48
1:C:247[B]:ILE:HG13	1:C:248[B]:ILE:N	2.28	0.48
1:B:247[A]:ILE:HG13	1:B:248[A]:ILE:N	2.29	0.47
1:D:247[A]:ILE:HG13	1:D:248[A]:ILE:N	2.28	0.47
1:B:247[B]:ILE:HG13	1:B:248[B]:ILE:N	2.29	0.47
1:C:386[A]:ARG:HH11	1:C:386[A]:ARG:HG3	1.79	0.47
1:D:247[B]:ILE:HG13	1:D:248[B]:ILE:N	2.28	0.47
1:A:386[B]:ARG:HH11	1:A:386[B]:ARG:HG3	1.78	0.47
1:D:184:ASP:HB2	1:D:201[C]:SER:HA	1.95	0.47
1:D:37:ILE:HG23	1:D:236[C]:PHE:CD2	2.50	0.47
1:A:386[A]:ARG:HG3	1:A:386[A]:ARG:HH11	1.78	0.47
1:C:141:ALA:HA	1:C:277:TYR:CE2	2.50	0.47
1:C:386[B]:ARG:HH11	1:C:386[B]:ARG:HG3	1.79	0.47
1:B:294:LEU:HB2	1:B:318:LEU:HD11	1.97	0.47
1:A:108[B]:LYS:HE2	5:A:1722:HOH:O	2.14	0.47
1:D:38:GLY:HA3	1:D:237[A]:THR:OG1	2.13	0.47
1:A:108[A]:LYS:HE2	5:A:1722:HOH:O	2.14	0.47
1:B:365:VAL:HG13	1:B:373:TYR:OH	2.15	0.47
1:D:347:GLU:HB3	1:D:351:LYS:NZ	2.30	0.47
1:A:38:GLY:HA3	1:A:237[C]:THR:OG1	2.15	0.46
1:A:355:ASP:HB2	1:A:357:GLU:HG3	1.96	0.46
1:C:232[B]:PHE:N	1:C:232[B]:PHE:CD1	2.82	0.46
1:B:38:GLY:HA3	1:B:237[B]:THR:OG1	2.15	0.46
1:A:238[C]:LYS:HD3	5:A:1633:HOH:O	2.14	0.46
1:B:343:VAL:O	1:B:347:GLU:HG3	2.16	0.46
1:C:79:GLU:OE2	1:C:111[A]:SCY:HE2	2.15	0.46
1:C:184:ASP:HB2	1:C:201[A]:SER:HA	1.96	0.46
1:C:232[A]:PHE:CD1	1:C:232[A]:PHE:N	2.83	0.46
1:C:38:GLY:HA3	1:C:237[C]:THR:OG1	2.15	0.46
1:D:245[B]:GLU:CD	1:D:248[B]:ILE:HD11	2.36	0.46
1:A:247[B]:ILE:HG13	1:A:248[B]:ILE:N	2.30	0.46
1:D:245[A]:GLU:CD	1:D:248[A]:ILE:HD11	2.36	0.46
1:A:184:ASP:HB2	1:A:201[C]:SER:HA	1.97	0.46
1:A:247[A]:ILE:HG13	1:A:248[A]:ILE:N	2.30	0.46
1:B:247[A]:ILE:HB	5:B:2671:HOH:O	2.15	0.46
1:B:245[B]:GLU:CD	1:B:248[B]:ILE:HD11	2.35	0.46
1:B:247[B]:ILE:HB	5:B:2671:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232[B]:PHE:N	1:A:232[B]:PHE:CD1	2.84	0.45
1:D:141:ALA:HA	1:D:277:TYR:CE2	2.51	0.45
1:A:236[B]:PHE:CE1	1:A:239[B]:MET:HB2	2.51	0.45
1:B:232[B]:PHE:CD1	1:B:232[B]:PHE:N	2.84	0.45
1:C:232[C]:PHE:HA	1:C:281:LEU:HD13	1.98	0.45
1:C:245[B]:GLU:CD	1:C:248[B]:ILE:HD11	2.36	0.45
1:A:232[A]:PHE:N	1:A:232[A]:PHE:CD1	2.85	0.45
1:A:240[C]:GLY:O	1:A:243:ALA:N	2.49	0.45
1:B:365:VAL:CG1	1:B:373:TYR:OH	2.65	0.45
1:B:79:GLU:OE2	1:B:111[A]:SCY:HE2	2.17	0.45
1:B:38:GLY:HA3	1:B:237[A]:THR:OG1	2.16	0.45
1:B:245[A]:GLU:CD	1:B:248[A]:ILE:HD11	2.36	0.45
1:B:294:LEU:CB	1:B:318:LEU:HD11	2.47	0.45
1:A:236[A]:PHE:CE1	1:A:239[A]:MET:HB2	2.52	0.45
3:A:1401[B]:HMG:N8P	3:A:1401[B]:HMG:H131	2.30	0.45
1:A:184:ASP:HB2	1:A:201[B]:SER:HA	1.99	0.45
1:A:38:GLY:HA3	1:A:237[B]:THR:OG1	2.17	0.45
1:C:197[B]:ASP:OD1	1:C:200[B]:LEU:HB2	2.17	0.45
1:D:232[C]:PHE:HB3	1:D:303:PHE:HB3	1.99	0.45
3:A:1401[B]:HMG:CDP	3:A:1401[B]:HMG:H8	2.30	0.45
1:B:232[A]:PHE:CD1	1:B:232[A]:PHE:N	2.85	0.45
1:D:232[C]:PHE:HA	1:D:281:LEU:HD13	1.98	0.45
1:A:184:ASP:HB2	1:A:201[A]:SER:HA	1.99	0.44
1:A:343:VAL:O	1:A:347:GLU:HG3	2.17	0.44
1:C:245[A]:GLU:CD	1:C:248[A]:ILE:HD11	2.36	0.44
1:A:232[C]:PHE:HB3	1:A:303:PHE:HB3	1.98	0.44
1:B:290:GLU:OE2	1:B:331:HIS:ND1	2.50	0.44
1:A:307:SER:OG	3:A:1401[B]:HMG:H21	2.18	0.44
1:B:38:GLY:HA3	1:B:237[C]:THR:OG1	2.17	0.44
1:D:237[B]:THR:HG22	1:D:267:VAL:HB	2.00	0.44
1:C:197[A]:ASP:OD1	1:C:200[A]:LEU:HB2	2.18	0.44
1:D:237[A]:THR:HG22	1:D:267:VAL:HB	2.00	0.44
1:A:245[B]:GLU:OE2	1:A:248[B]:ILE:HD11	2.18	0.44
1:A:67:ASP:O	1:A:71:ILE:HG13	2.18	0.44
1:B:235[B]:PRO:HG3	1:B:239[B]:MET:HG2	1.99	0.44
1:B:307:SER:OG	3:B:2401[B]:HMG:H21	2.18	0.44
1:D:245[B]:GLU:OE2	1:D:248[B]:ILE:HD11	2.18	0.44
1:D:307:SER:OG	3:D:4401[B]:HMG:H21	2.18	0.44
1:A:245[A]:GLU:OE2	1:A:248[A]:ILE:HD11	2.18	0.44
1:B:205[C]:TYR:CE1	1:B:239[C]:MET:HG3	2.52	0.44
1:B:235[A]:PRO:HG3	1:B:239[A]:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3401[B]:HMG:N8P	3:C:3401[B]:HMG:H131	2.23	0.44
1:B:150:GLU:HB3	1:B:151:PRO:HD3	2.00	0.43
1:C:38:GLY:HA3	1:C:237[B]:THR:OG1	2.18	0.43
1:D:240[C]:GLY:O	1:D:243:ALA:N	2.51	0.43
1:A:238[B]:LYS:HD3	5:A:1633:HOH:O	2.18	0.43
1:A:237[B]:THR:HG21	1:A:271:ARG:HG2	1.99	0.43
1:C:386[B]:ARG:HD3	5:C:3773:HOH:O	2.17	0.43
1:D:245[A]:GLU:OE2	1:D:248[A]:ILE:HD11	2.18	0.43
1:A:38:GLY:HA3	1:A:237[A]:THR:OG1	2.17	0.43
1:A:237[A]:THR:HG22	1:A:267:VAL:HB	2.00	0.43
1:A:376:ASN:HB3	5:A:1740:HOH:O	2.18	0.43
1:C:343:VAL:O	1:C:347:GLU:HG3	2.18	0.43
1:C:177:ALA:O	1:D:101:PHE:HA	2.17	0.43
1:A:238[A]:LYS:HD3	5:A:1633:HOH:O	2.18	0.43
1:C:366:HIS:HE1	1:C:369:ARG:NH2	2.17	0.43
1:C:386[A]:ARG:HD3	5:C:3773:HOH:O	2.17	0.43
1:A:237[A]:THR:HG21	1:A:271:ARG:HG2	1.99	0.43
1:A:239[C]:MET:O	1:A:239[C]:MET:HE2	2.18	0.43
1:B:141:ALA:HA	1:B:277:TYR:CE2	2.54	0.43
1:B:185:PHE:C	1:B:185:PHE:CD1	2.91	0.43
1:D:185:PHE:C	1:D:185:PHE:CD1	2.92	0.43
1:A:185:PHE:C	1:A:185:PHE:CD1	2.92	0.43
1:B:232[C]:PHE:HA	1:B:281:LEU:HD13	2.01	0.42
1:A:232[C]:PHE:HA	1:A:281:LEU:HD13	2.00	0.42
1:D:376:ASN:CG	1:D:377:ILE:N	2.72	0.42
1:C:118:ILE:CG2	1:C:160[C]:MET:HE2	2.35	0.42
1:C:38:GLY:HA3	1:C:237[A]:THR:OG1	2.19	0.42
1:A:101:PHE:HA	1:B:177:ALA:O	2.19	0.42
1:B:245[B]:GLU:OE2	1:B:248[B]:ILE:HD11	2.20	0.42
1:C:201[A]:SER:HB2	4:C:3402[A]:CAA:H31	2.01	0.42
1:A:237[B]:THR:HG22	1:A:267:VAL:HB	2.00	0.42
1:C:37:ILE:HG23	1:C:236[C]:PHE:CD1	2.55	0.42
1:D:150:GLU:HB3	1:D:151:PRO:HD3	2.02	0.42
1:A:239[C]:MET:HE3	1:A:242:LYS:HB2	2.02	0.42
1:C:236[C]:PHE:CE1	1:C:239[C]:MET:HB2	2.55	0.41
1:B:245[A]:GLU:OE2	1:B:248[A]:ILE:HD11	2.20	0.41
1:B:326:LEU:HA	5:B:2759:HOH:O	2.19	0.41
1:D:108[C]:LYS:HE2	5:D:4717:HOH:O	2.20	0.41
1:D:118:ILE:HD13	1:D:160[C]:MET:HE1	2.02	0.41
1:A:177:ALA:O	1:B:101:PHE:HA	2.21	0.41
1:A:308:GLY:N	1:A:309:SER:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248[B]:ILE:O	1:B:251[B]:ALA:HB3	2.19	0.41
1:C:101:PHE:HA	1:D:177:ALA:O	2.21	0.41
1:D:236[C]:PHE:CE2	1:D:239[C]:MET:HB2	2.55	0.41
1:B:248[A]:ILE:O	1:B:251[A]:ALA:HB3	2.20	0.41
1:A:150:GLU:HB3	1:A:151:PRO:HD3	2.03	0.41
1:B:232[C]:PHE:HB3	1:B:303:PHE:HB3	2.01	0.41
1:D:236[A]:PHE:HE1	4:D:4402[A]:CAA:H31	1.86	0.41
1:B:376:ASN:CG	1:B:377:ILE:N	2.74	0.41
1:D:5:ILE:HD13	1:D:160[C]:MET:HE3	2.02	0.41
1:D:236[B]:PHE:CE1	1:D:239[B]:MET:HB2	2.55	0.41
1:A:141:ALA:HA	1:A:277:TYR:CE2	2.56	0.41
1:C:5:ILE:CG1	1:C:160[C]:MET:HE3	2.50	0.40
1:C:294:LEU:CB	1:C:318:LEU:HD11	2.51	0.40
1:C:200[C]:LEU:HD23	1:C:200[C]:LEU:HA	1.96	0.40
3:C:3401[B]:HMG:CDP	3:C:3401[B]:HMG:N8P	2.80	0.40
1:A:290:GLU:HG2	1:A:326:LEU:HD13	2.03	0.40
1:C:108:LYS:HE2	5:D:4705:HOH:O	2.21	0.40
1:C:5:ILE:CD1	1:C:160[C]:MET:HE3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/397 (113%)	413 (92%)	33 (7%)	4 (1%)	17	4
1	B	448/397 (113%)	411 (92%)	36 (8%)	1 (0%)	47	26
1	C	448/397 (113%)	414 (92%)	27 (6%)	7 (2%)	9	1
1	D	449/397 (113%)	410 (91%)	35 (8%)	4 (1%)	17	4
All	All	1795/1588 (113%)	1648 (92%)	131 (7%)	16 (1%)	29	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	GLU
1	C	109	GLU
1	C	199[A]	ALA
1	C	199[B]	ALA
1	C	199[C]	ALA
1	D	237[A]	THR
1	D	237[B]	THR
1	D	237[C]	THR
1	A	109	GLU
1	C	198[A]	GLY
1	C	198[B]	GLY
1	C	198[C]	GLY
1	D	109	GLU
1	A	237[A]	THR
1	A	237[B]	THR
1	A	237[C]	THR

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	356/326 (109%)	344 (97%)	12 (3%)	37	13
1	B	345/326 (106%)	337 (98%)	8 (2%)	50	25
1	C	345/326 (106%)	337 (98%)	8 (2%)	50	25
1	D	352/326 (108%)	346 (98%)	6 (2%)	60	38
All	All	1398/1304 (107%)	1364 (98%)	34 (2%)	65	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	185	PHE
1	A	200[A]	LEU
1	A	200[B]	LEU
1	A	200[C]	LEU
1	A	232[A]	PHE

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Mol	Chain	Res	Type
1	A	232[B]	PHE
1	A	232[C]	PHE
1	A	249[A]	ASP
1	A	249[B]	ASP
1	A	249[C]	ASP
1	A	346	TYR
1	B	109	GLU
1	B	200[A]	LEU
1	B	200[B]	LEU
1	B	200[C]	LEU
1	B	232[A]	PHE
1	B	232[B]	PHE
1	B	232[C]	PHE
1	B	346	TYR
1	C	109	GLU
1	C	200[A]	LEU
1	C	200[B]	LEU
1	C	200[C]	LEU
1	C	232[A]	PHE
1	C	232[B]	PHE
1	C	232[C]	PHE
1	C	346	TYR
1	D	109	GLU
1	D	185	PHE
1	D	232[A]	PHE
1	D	232[B]	PHE
1	D	232[C]	PHE
1	D	346	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	HIS
1	A	336	ASN
1	B	325	HIS
1	C	146	ASN
1	D	325	HIS
1	D	336	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	SCY	C	111[A]	1	7,8,9	0.56	0	3,9,11	0.70	0
1	SCY	B	111[A]	1	7,8,9	0.56	0	3,9,11	0.71	0
1	SCY	D	111[A]	1	7,8,9	0.58	0	3,9,11	0.70	0
1	SCY	A	111[A]	1	7,8,9	0.58	0	3,9,11	0.71	0

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	SCY	C	111[A]	1	-	2/5/7/9	-
1	SCY	B	111[A]	1	-	2/5/7/9	-
1	SCY	D	111[A]	1	-	2/5/7/9	-
1	SCY	A	111[A]	1	-	2/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	111[A]	SCY	OCD-CD-SG-CB
1	B	111[A]	SCY	OCD-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	D	111[A]	SCY	OCD-CD-SG-CB
1	D	111[A]	SCY	CE-CD-SG-CB
1	A	111[A]	SCY	OCD-CD-SG-CB
1	C	111[A]	SCY	CE-CD-SG-CB
1	B	111[A]	SCY	CE-CD-SG-CB
1	A	111[A]	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	111[A]	SCY	3	0
1	B	111[A]	SCY	3	0
1	D	111[A]	SCY	3	0
1	A	111[A]	SCY	3	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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
4	CAA	D	4402[A]	-	47,56,56	0.70	0	60,83,83	1.29	5 (8%)
2	SO4	B	2502	-	4,4,4	0.26	0	6,6,6	0.05	0
4	CAA	C	3402[A]	-	47,56,56	0.70	0	60,83,83	1.34	5 (8%)
3	HMG	A	1401[B]	-	49,60,60	0.72	0	59,90,90	1.31	5 (8%)
2	SO4	C	3502	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	B	2501	-	4,4,4	0.29	0	6,6,6	0.06	0
3	HMG	D	4401[B]	-	49,60,60	0.74	1 (2%)	59,90,90	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAA	A	1402[A]	-	47,56,56	0.71	0	60,83,83	1.34	5 (8%)
2	SO4	D	4502	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	A	1502	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	C	3501	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	D	4501	-	4,4,4	0.28	0	6,6,6	0.07	0
3	HMG	B	2401[B]	-	49,60,60	0.72	0	59,90,90	1.34	5 (8%)
4	CAA	B	2402[A]	-	47,56,56	0.72	0	60,83,83	1.33	5 (8%)
2	SO4	A	1501	-	4,4,4	0.28	0	6,6,6	0.06	0
3	HMG	C	3401[B]	-	49,60,60	0.73	0	59,90,90	1.33	5 (8%)

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	CAA	D	4402[A]	-	-	15/50/71/71	0/3/3/3
4	CAA	C	3402[A]	-	-	21/50/71/71	0/3/3/3
3	HMG	A	1401[B]	-	-	20/54/77/77	0/3/3/3
3	HMG	D	4401[B]	-	-	11/54/77/77	0/3/3/3
4	CAA	A	1402[A]	-	-	16/50/71/71	0/3/3/3
3	HMG	B	2401[B]	-	-	18/54/77/77	0/3/3/3
4	CAA	B	2402[A]	-	-	20/50/71/71	0/3/3/3
3	HMG	C	3401[B]	-	-	19/54/77/77	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4401[B]	HMG	C1-S1P	2.19	1.81	1.76

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2402[A]	CAA	P2A-O3A-P1A	-6.40	110.85	132.83
3	B	2401[B]	HMG	P1A-O3A-P2A	-6.39	110.89	132.83
4	A	1402[A]	CAA	P2A-O3A-P1A	-6.39	110.92	132.83
4	C	3402[A]	CAA	P2A-O3A-P1A	-6.34	111.08	132.83
3	C	3401[B]	HMG	P1A-O3A-P2A	-6.28	111.28	132.83
3	A	1401[B]	HMG	P1A-O3A-P2A	-6.20	111.53	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4402[A]	CAA	P2A-O3A-P1A	-6.07	112.01	132.83
4	B	2402[A]	CAA	C2-C1-S1P	-5.56	106.76	113.69
4	C	3402[A]	CAA	C2-C1-S1P	-5.54	106.79	113.69
4	A	1402[A]	CAA	C2-C1-S1P	-5.51	106.83	113.69
3	B	2401[B]	HMG	C2-C1-S1P	-5.48	106.84	113.63
4	D	4402[A]	CAA	C2-C1-S1P	-5.42	106.94	113.69
3	A	1401[B]	HMG	C2-C1-S1P	-5.42	106.92	113.63
3	C	3401[B]	HMG	C2-C1-S1P	-5.36	106.99	113.63
3	D	4401[B]	HMG	P1A-O3A-P2A	-4.93	115.91	132.83
3	D	4401[B]	HMG	C2-C1-S1P	-4.27	108.34	113.63
4	B	2402[A]	CAA	O1-C1-S1P	3.02	126.54	122.61
4	C	3402[A]	CAA	O1-C1-S1P	2.99	126.50	122.61
4	A	1402[A]	CAA	O1-C1-S1P	2.97	126.48	122.61
3	B	2401[B]	HMG	O2-C1-S1P	2.95	126.45	122.61
3	C	3401[B]	HMG	O2-C1-S1P	2.92	126.41	122.61
4	D	4402[A]	CAA	O1-C1-S1P	2.90	126.39	122.61
3	A	1401[B]	HMG	O2-C1-S1P	2.87	126.34	122.61
3	D	4401[B]	HMG	O2-C1-S1P	2.63	126.03	122.61
4	C	3402[A]	CAA	C2P-S1P-C1	-2.39	94.43	101.87
3	B	2401[B]	HMG	C2P-S1P-C1	-2.36	94.53	101.87
3	C	3401[B]	HMG	C2P-S1P-C1	-2.32	94.64	101.87
3	A	1401[B]	HMG	C5A-C6A-N6A	2.28	123.82	120.35
4	A	1402[A]	CAA	C5A-C6A-N6A	2.27	123.81	120.35
3	C	3401[B]	HMG	C5A-C6A-N6A	2.25	123.77	120.35
3	B	2401[B]	HMG	C5A-C6A-N6A	2.21	123.72	120.35
4	C	3402[A]	CAA	C5A-C6A-N6A	2.20	123.69	120.35
4	D	4402[A]	CAA	C5A-C6A-N6A	2.19	123.68	120.35
4	B	2402[A]	CAA	C2P-S1P-C1	-2.19	95.06	101.87
3	A	1401[B]	HMG	C2P-S1P-C1	-2.19	95.07	101.87
3	D	4401[B]	HMG	C5A-C6A-N6A	2.18	123.66	120.35
4	B	2402[A]	CAA	C5A-C6A-N6A	2.16	123.64	120.35
4	D	4402[A]	CAA	C2P-S1P-C1	-2.07	95.43	101.87
4	A	1402[A]	CAA	C2P-S1P-C1	-2.03	95.54	101.87

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4402[A]	CAA	C5B-O5B-P1A-O1A
4	D	4402[A]	CAA	C5B-O5B-P1A-O2A
4	D	4402[A]	CAA	C5B-O5B-P1A-O3A
4	D	4402[A]	CAA	CCP-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
4	D	4402[A]	CAA	CCP-O6A-P2A-O5A
4	D	4402[A]	CAA	O1-C1-S1P-C2P
4	D	4402[A]	CAA	C2-C1-S1P-C2P
4	C	3402[A]	CAA	O4B-C4B-C5B-O5B
4	C	3402[A]	CAA	C5B-O5B-P1A-O1A
4	C	3402[A]	CAA	C5B-O5B-P1A-O2A
4	C	3402[A]	CAA	C5B-O5B-P1A-O3A
4	C	3402[A]	CAA	CCP-O6A-P2A-O3A
4	C	3402[A]	CAA	N8P-C9P-CAP-OAP
4	C	3402[A]	CAA	C6P-C5P-N4P-C3P
4	C	3402[A]	CAA	O5P-C5P-N4P-C3P
4	C	3402[A]	CAA	S1P-C2P-C3P-N4P
4	C	3402[A]	CAA	C3P-C2P-S1P-C1
4	C	3402[A]	CAA	O1-C1-S1P-C2P
4	C	3402[A]	CAA	C2-C1-S1P-C2P
3	A	1401[B]	HMG	C5B-O5B-P1A-O3A
3	A	1401[B]	HMG	C5B-O5B-P1A-O1A
3	A	1401[B]	HMG	C5B-O5B-P1A-O2A
3	A	1401[B]	HMG	N8P-C9P-CAP-OAP
3	A	1401[B]	HMG	C3P-C2P-S1P-C1
3	D	4401[B]	HMG	CCP-O6A-P2A-O3A
3	D	4401[B]	HMG	C5B-O5B-P1A-O3A
3	D	4401[B]	HMG	N8P-C9P-CAP-OAP
4	A	1402[A]	CAA	C5B-O5B-P1A-O3A
4	A	1402[A]	CAA	CCP-O6A-P2A-O3A
4	A	1402[A]	CAA	CCP-O6A-P2A-O5A
4	A	1402[A]	CAA	N8P-C9P-CAP-OAP
3	B	2401[B]	HMG	CCP-O6A-P2A-O3A
3	B	2401[B]	HMG	C5B-O5B-P1A-O3A
3	B	2401[B]	HMG	C5B-O5B-P1A-O1A
3	B	2401[B]	HMG	C5B-O5B-P1A-O2A
3	B	2401[B]	HMG	N8P-C9P-CAP-OAP
3	B	2401[B]	HMG	C3P-C2P-S1P-C1
3	B	2401[B]	HMG	O2-C1-S1P-C2P
3	B	2401[B]	HMG	C2-C1-S1P-C2P
4	B	2402[A]	CAA	C5B-O5B-P1A-O1A
4	B	2402[A]	CAA	C5B-O5B-P1A-O2A
4	B	2402[A]	CAA	C5B-O5B-P1A-O3A
4	B	2402[A]	CAA	CCP-O6A-P2A-O3A
4	B	2402[A]	CAA	N8P-C9P-CAP-OAP
3	C	3401[B]	HMG	CCP-O6A-P2A-O4A
3	C	3401[B]	HMG	CCP-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
3	C	3401[B]	HMG	C5B-O5B-P1A-O3A
3	C	3401[B]	HMG	C5B-O5B-P1A-O1A
3	C	3401[B]	HMG	C5B-O5B-P1A-O2A
3	C	3401[B]	HMG	O9P-C9P-CAP-CBP
3	C	3401[B]	HMG	N8P-C9P-CAP-CBP
3	C	3401[B]	HMG	N8P-C9P-CAP-OAP
3	C	3401[B]	HMG	CAP-C9P-N8P-C7P
3	C	3401[B]	HMG	C3P-C2P-S1P-C1
3	C	3401[B]	HMG	O2-C1-S1P-C2P
3	C	3401[B]	HMG	C2-C1-S1P-C2P
4	B	2402[A]	CAA	O5P-C5P-N4P-C3P
3	A	1401[B]	HMG	O4B-C4B-C5B-O5B
3	A	1401[B]	HMG	C3B-C4B-C5B-O5B
3	B	2401[B]	HMG	O4B-C4B-C5B-O5B
4	B	2402[A]	CAA	O4B-C4B-C5B-O5B
3	D	4401[B]	HMG	O5P-C5P-N4P-C3P
3	D	4401[B]	HMG	C6P-C5P-N4P-C3P
3	B	2401[B]	HMG	C6P-C5P-N4P-C3P
4	B	2402[A]	CAA	C6P-C5P-N4P-C3P
3	C	3401[B]	HMG	O9P-C9P-N8P-C7P
4	C	3402[A]	CAA	C3B-C4B-C5B-O5B
4	A	1402[A]	CAA	C3B-C4B-C5B-O5B
4	A	1402[A]	CAA	O4B-C4B-C5B-O5B
3	B	2401[B]	HMG	C3B-C4B-C5B-O5B
4	B	2402[A]	CAA	C3B-C4B-C5B-O5B
3	B	2401[B]	HMG	O5P-C5P-N4P-C3P
3	A	1401[B]	HMG	S1P-C2P-C3P-N4P
3	D	4401[B]	HMG	S1P-C2P-C3P-N4P
4	A	1402[A]	CAA	S1P-C2P-C3P-N4P
4	B	2402[A]	CAA	S1P-C2P-C3P-N4P
4	C	3402[A]	CAA	O9P-C9P-CAP-OAP
3	A	1401[B]	HMG	O9P-C9P-CAP-OAP
3	D	4401[B]	HMG	O9P-C9P-CAP-OAP
4	A	1402[A]	CAA	O9P-C9P-CAP-OAP
3	B	2401[B]	HMG	O9P-C9P-CAP-OAP
4	B	2402[A]	CAA	O9P-C9P-CAP-OAP
3	C	3401[B]	HMG	O9P-C9P-CAP-OAP
4	D	4402[A]	CAA	C3B-C4B-C5B-O5B
4	D	4402[A]	CAA	O4B-C4B-C5B-O5B
3	A	1401[B]	HMG	O5P-C5P-N4P-C3P
4	C	3402[A]	CAA	C1-C2-C3-O3
4	A	1402[A]	CAA	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	2402[A]	CAA	C1-C2-C3-O3
4	C	3402[A]	CAA	O9P-C9P-CAP-CBP
3	A	1401[B]	HMG	O9P-C9P-CAP-CBP
4	C	3402[A]	CAA	N8P-C9P-CAP-CBP
4	B	2402[A]	CAA	C3P-C2P-S1P-C1
3	A	1401[B]	HMG	O2-C1-S1P-C2P
4	B	2402[A]	CAA	O1-C1-S1P-C2P
3	A	1401[B]	HMG	C6P-C5P-N4P-C3P
4	D	4402[A]	CAA	C3B-O3B-P3B-O7A
4	C	3402[A]	CAA	C3B-O3B-P3B-O7A
3	A	1401[B]	HMG	C3B-O3B-P3B-O7A
3	D	4401[B]	HMG	C3B-O3B-P3B-O7A
3	C	3401[B]	HMG	C3B-O3B-P3B-O7A
3	A	1401[B]	HMG	C2-C1-S1P-C2P
4	B	2402[A]	CAA	C2-C1-S1P-C2P
3	A	1401[B]	HMG	CCP-O6A-P2A-O3A
3	D	4401[B]	HMG	P1A-O3A-P2A-O5A
4	D	4402[A]	CAA	CCP-O6A-P2A-O4A
3	D	4401[B]	HMG	C5B-O5B-P1A-O1A
3	D	4401[B]	HMG	C5B-O5B-P1A-O2A
4	A	1402[A]	CAA	C5B-O5B-P1A-O1A
4	A	1402[A]	CAA	C5B-O5B-P1A-O2A
4	A	1402[A]	CAA	CCP-O6A-P2A-O4A
3	B	2401[B]	HMG	CCP-O6A-P2A-O4A
4	B	2402[A]	CAA	CCP-O6A-P2A-O5A
3	C	3401[B]	HMG	CCP-O6A-P2A-O5A
4	D	4402[A]	CAA	O5P-C5P-N4P-C3P
3	C	3401[B]	HMG	CAP-CBP-CCP-O6A
3	C	3401[B]	HMG	CEP-CBP-CCP-O6A
4	D	4402[A]	CAA	C1-C2-C3-O3
3	A	1401[B]	HMG	CAP-C9P-N8P-C7P
3	C	3401[B]	HMG	CDP-CBP-CCP-O6A
3	A	1401[B]	HMG	N8P-C9P-CAP-CBP
3	A	1401[B]	HMG	O9P-C9P-N8P-C7P
4	D	4402[A]	CAA	C6P-C5P-N4P-C3P
4	A	1402[A]	CAA	C3B-O3B-P3B-O7A
3	B	2401[B]	HMG	C3B-O3B-P3B-O7A
4	B	2402[A]	CAA	C3B-O3B-P3B-O7A
3	A	1401[B]	HMG	C3B-O3B-P3B-O8A
4	A	1402[A]	CAA	C3B-O3B-P3B-O8A
4	A	1402[A]	CAA	C3B-O3B-P3B-O9A
3	B	2401[B]	HMG	C3B-O3B-P3B-O9A

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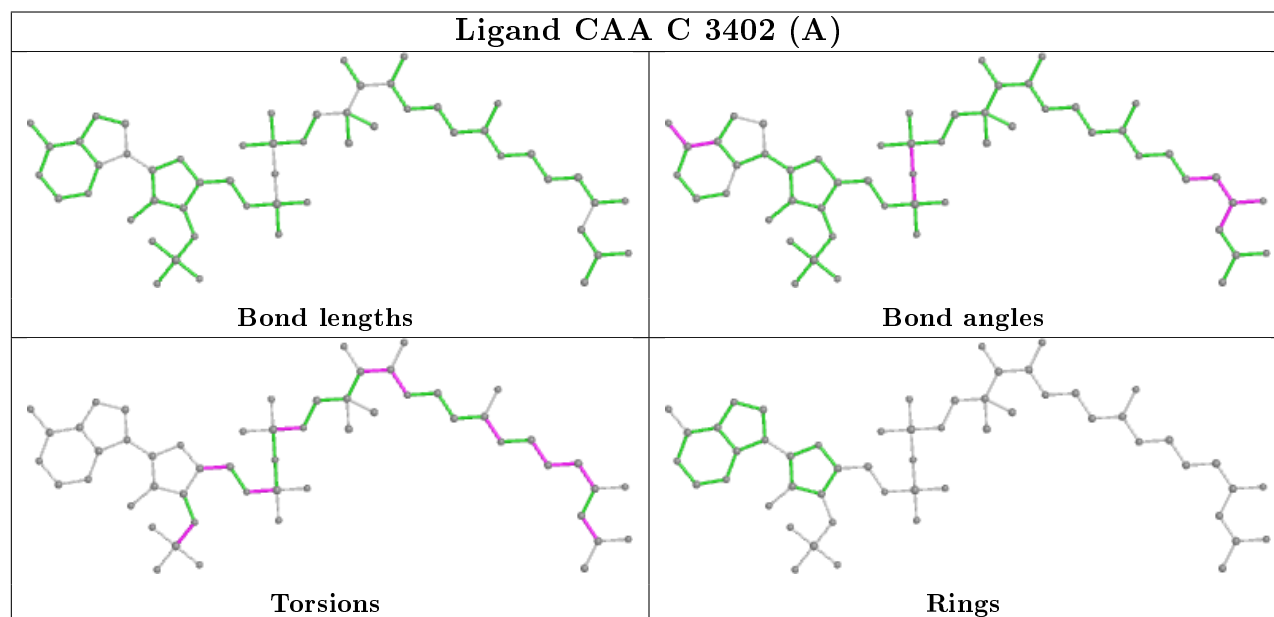
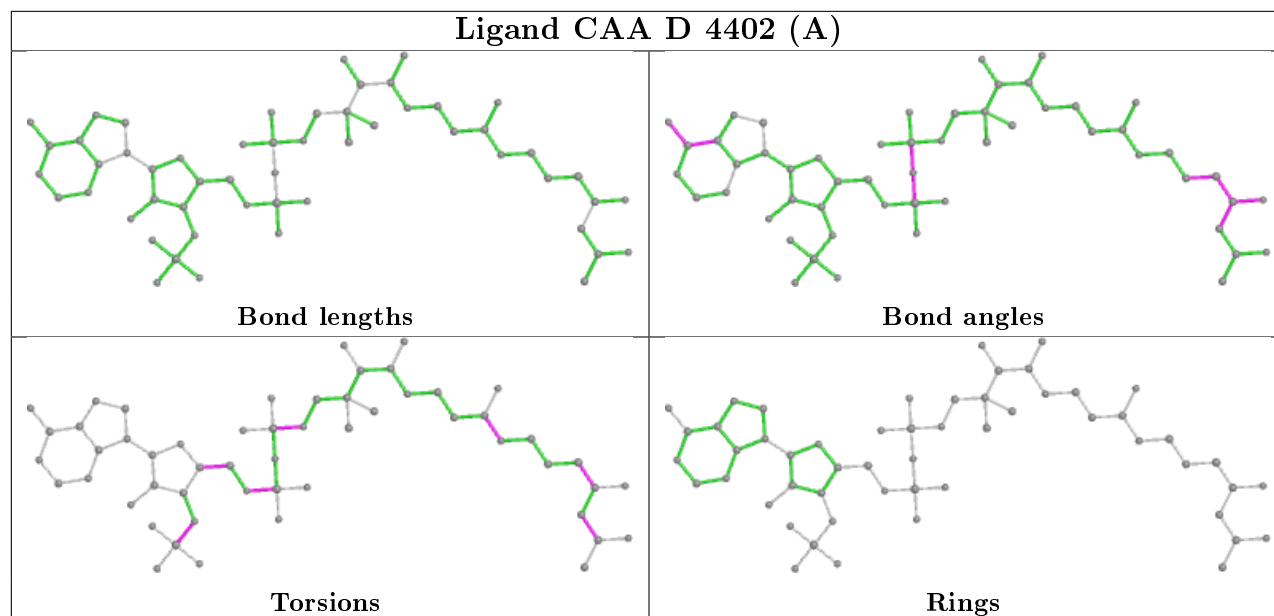
Mol	Chain	Res	Type	Atoms
4	B	2402[A]	CAA	C3B-O3B-P3B-O9A
4	D	4402[A]	CAA	C1-C2-C3-C4
4	C	3402[A]	CAA	C1-C2-C3-C4
4	A	1402[A]	CAA	C1-C2-C3-C4
4	B	2402[A]	CAA	C1-C2-C3-C4
4	C	3402[A]	CAA	CAP-C9P-N8P-C7P
3	B	2401[B]	HMG	CAP-C9P-N8P-C7P
4	B	2402[A]	CAA	CCP-O6A-P2A-O4A
3	B	2401[B]	HMG	O9P-C9P-N8P-C7P
4	C	3402[A]	CAA	O9P-C9P-N8P-C7P

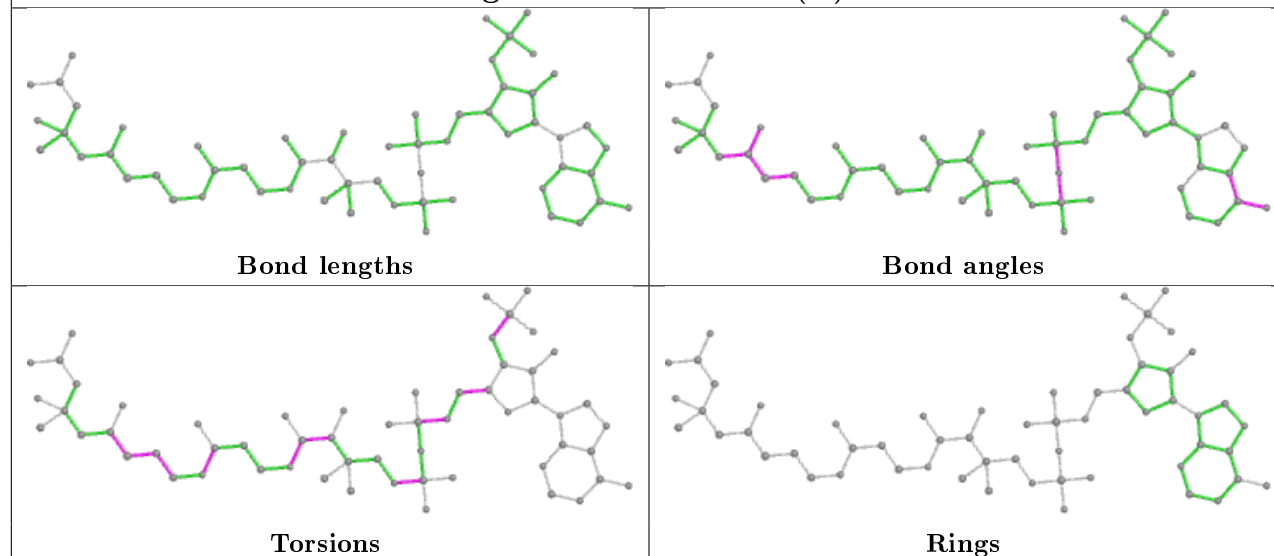
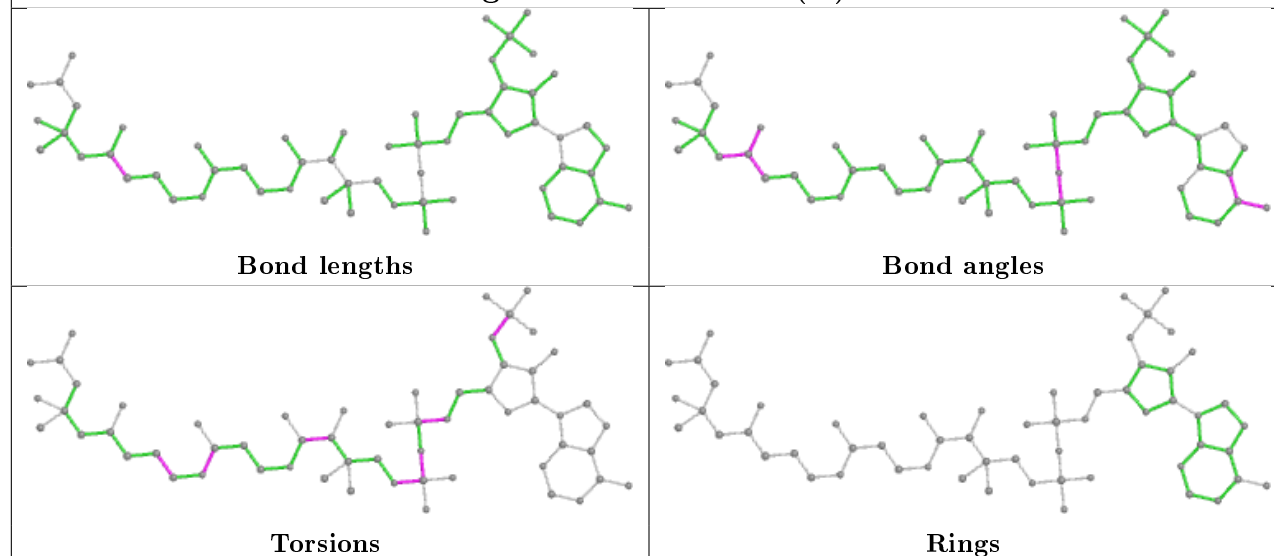
There are no ring outliers.

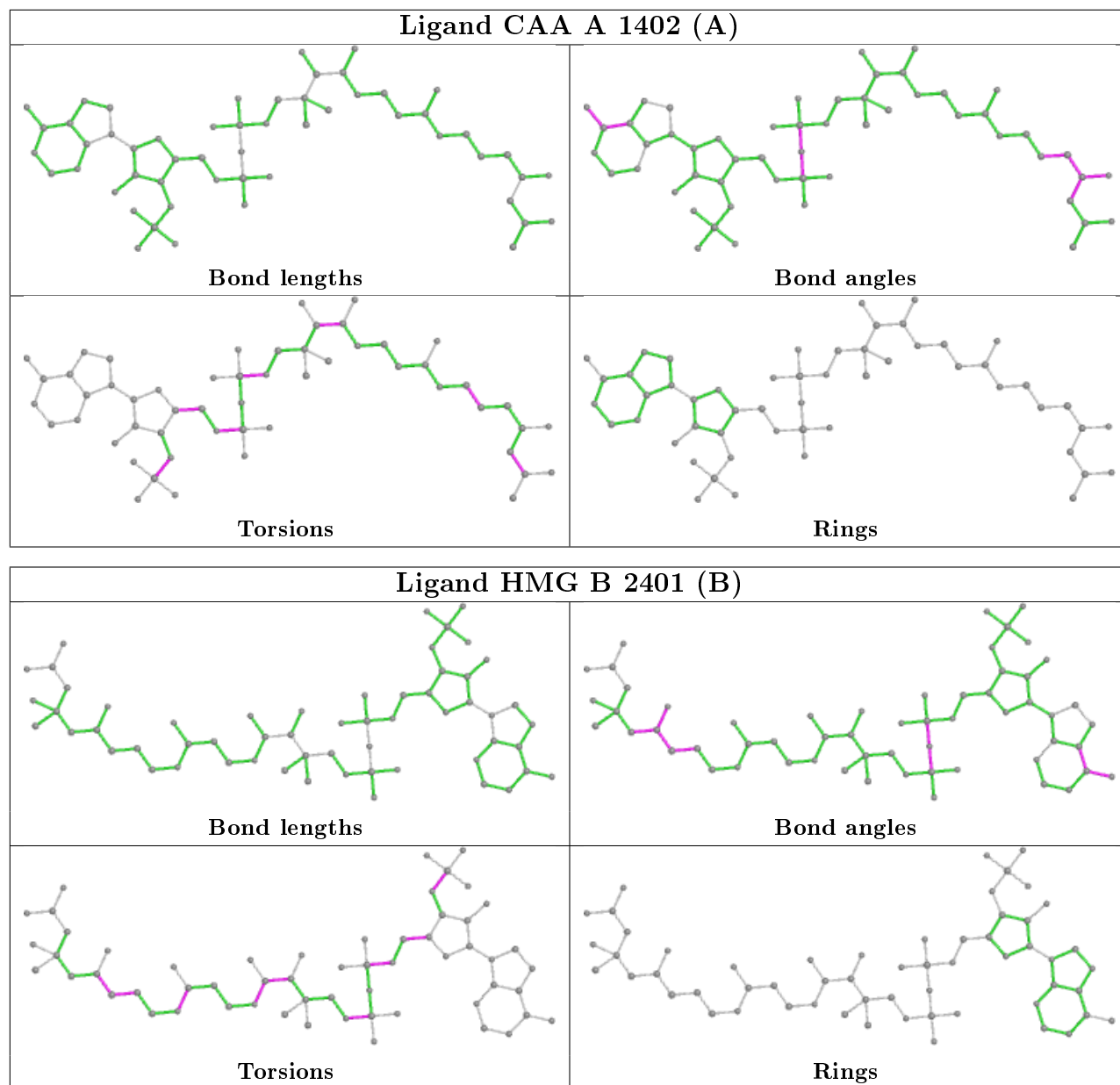
6 monomers are involved in 17 short contacts:

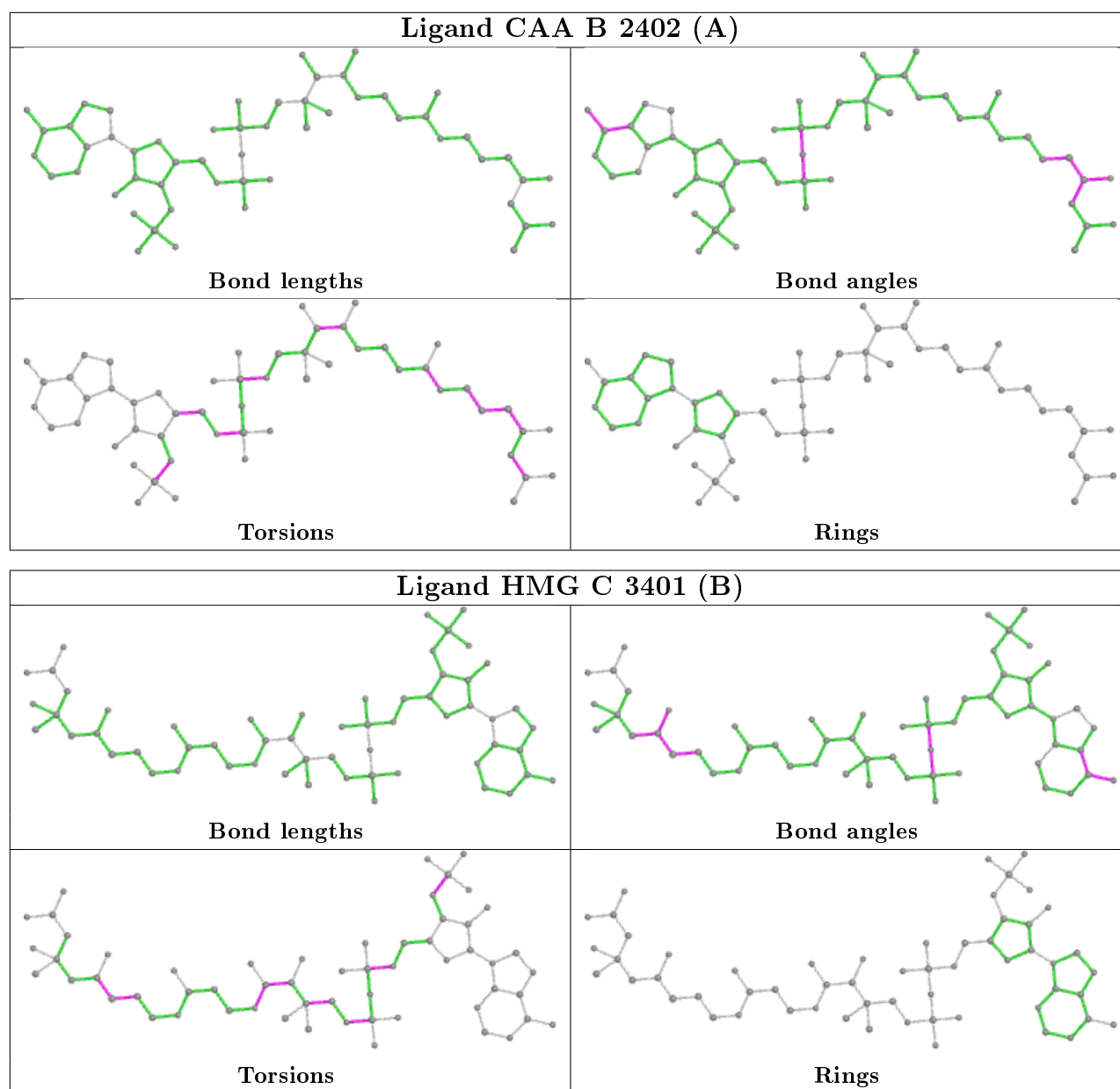
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4402[A]	CAA	1	0
4	C	3402[A]	CAA	4	0
3	A	1401[B]	HMG	5	0
3	D	4401[B]	HMG	2	0
3	B	2401[B]	HMG	1	0
3	C	3401[B]	HMG	4	0

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.



Ligand HMG A 1401 (B)**Ligand HMG D 4401 (B)**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/397 (97%)	-0.16	11 (2%) 53 50	11, 19, 32, 43	2 (0%)
1	B	388/397 (97%)	-0.17	9 (2%) 60 59	11, 18, 31, 42	2 (0%)
1	C	388/397 (97%)	-0.16	10 (2%) 56 53	11, 18, 31, 42	3 (0%)
1	D	388/397 (97%)	-0.14	10 (2%) 56 53	11, 19, 32, 45	3 (0%)
All	All	1552/1588 (97%)	-0.16	40 (2%) 56 53	11, 19, 32, 45	10 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199[A]	ALA	8.6
1	B	199[A]	ALA	7.0
1	A	199[A]	ALA	6.9
1	D	199[A]	ALA	6.3
1	C	247[A]	ILE	5.2
1	C	198[A]	GLY	5.0
1	B	389	LEU	4.7
1	A	389	LEU	4.5
1	D	389	LEU	4.3
1	B	247[A]	ILE	4.2
1	D	247[A]	ILE	4.0
1	B	390	GLU	3.8
1	C	390	GLU	3.7
1	D	390	GLU	3.6
1	C	389	LEU	3.5
1	B	198[A]	GLY	3.3
1	C	200[A]	LEU	3.2
1	A	247[A]	ILE	3.1
1	C	249[A]	ASP	2.9
1	A	198[A]	GLY	2.8
1	A	390	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	249[A]	ASP	2.7
1	D	249[A]	ASP	2.7
1	D	248[A]	ILE	2.7
1	B	232[A]	PHE	2.7
1	D	239[A]	MET	2.5
1	C	234[A]	VAL	2.5
1	C	248[A]	ILE	2.5
1	D	198[A]	GLY	2.5
1	A	238[A]	LYS	2.4
1	B	63	ILE	2.4
1	B	197[A]	ASP	2.4
1	D	251[A]	ALA	2.3
1	C	197[A]	ASP	2.3
1	B	249[A]	ASP	2.2
1	A	248[A]	ILE	2.2
1	A	239[A]	MET	2.2
1	A	240[A]	GLY	2.2
1	D	236[A]	PHE	2.1
1	A	236[A]	PHE	2.0

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	SCY	B	111[A]	9/10	0.95	0.10	12,14,22,22	9
1	SCY	C	111[A]	9/10	0.96	0.08	12,14,21,22	9
1	SCY	D	111[A]	9/10	0.97	0.07	13,14,23,24	9
1	SCY	A	111[A]	9/10	0.97	0.07	13,14,22,23	9

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,

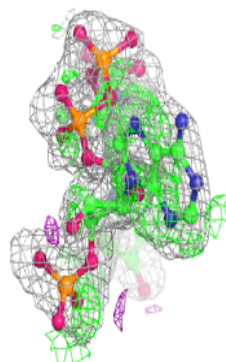
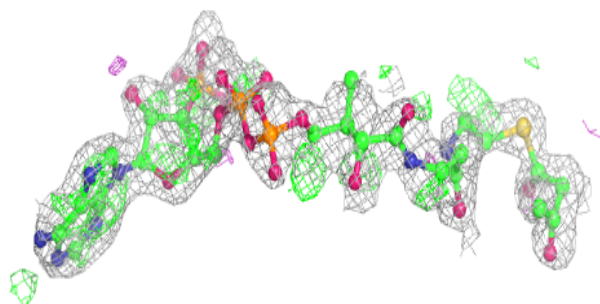
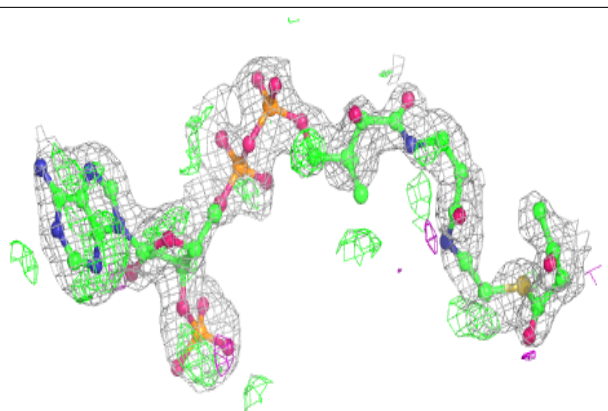
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CAA	C	3402[A]	54/54	0.82	0.19	20,30,35,35	54
3	HMG	C	3401[B]	58/58	0.82	0.18	18,28,35,35	58
4	CAA	D	4402[A]	54/54	0.83	0.17	24,29,38,39	54
3	HMG	D	4401[B]	58/58	0.84	0.17	17,27,33,34	58
4	CAA	B	2402[A]	54/54	0.85	0.17	17,29,34,35	54
3	HMG	B	2401[B]	58/58	0.85	0.17	18,28,34,35	58
4	CAA	A	1402[A]	54/54	0.88	0.16	19,28,35,36	54
3	HMG	A	1401[B]	58/58	0.88	0.16	13,27,33,34	58
2	SO4	C	3501	5/5	0.90	0.15	34,35,37,38	0
2	SO4	B	2501	5/5	0.90	0.16	36,37,40,40	0
2	SO4	D	4502	5/5	0.92	0.14	73,73,73,74	0
2	SO4	A	1502	5/5	0.92	0.14	75,75,75,75	0
2	SO4	D	4501	5/5	0.93	0.11	38,38,39,40	0
2	SO4	B	2502	5/5	0.94	0.16	80,81,81,81	0
2	SO4	A	1501	5/5	0.94	0.12	36,37,38,39	0
2	SO4	C	3502	5/5	0.94	0.20	78,78,79,79	0

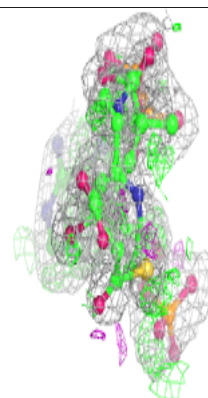
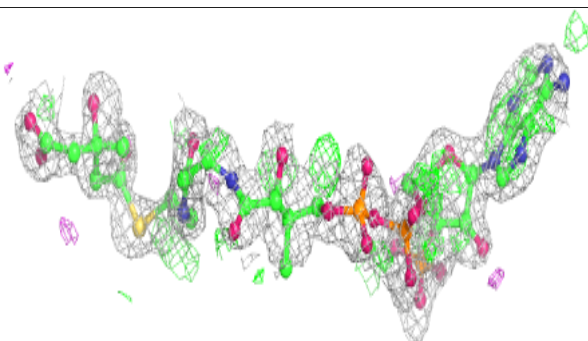
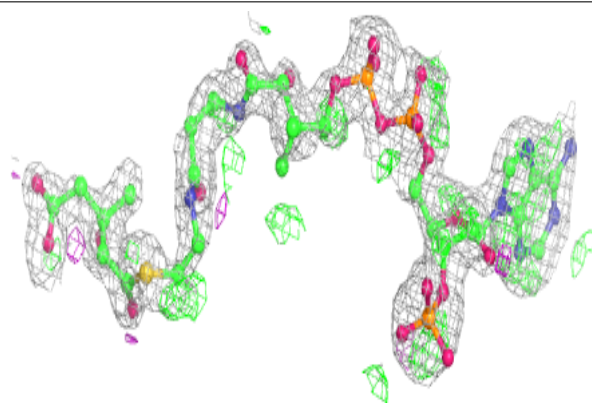
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAA C 3402 (A):

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

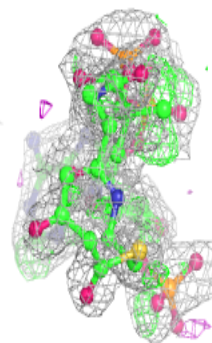
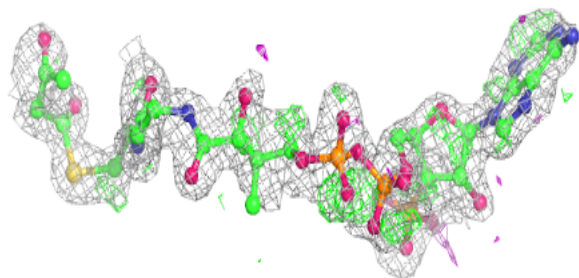
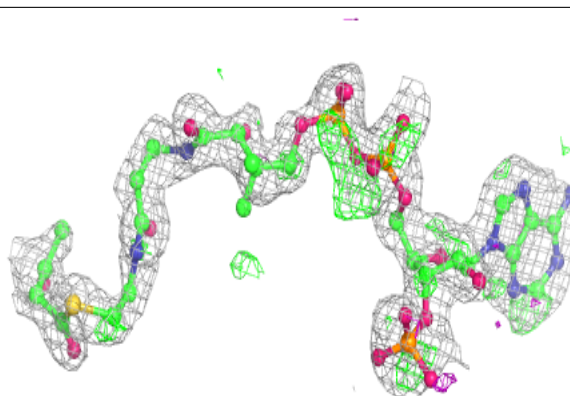
**Electron density around HMG C 3401 (B):**

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

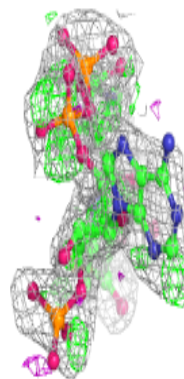
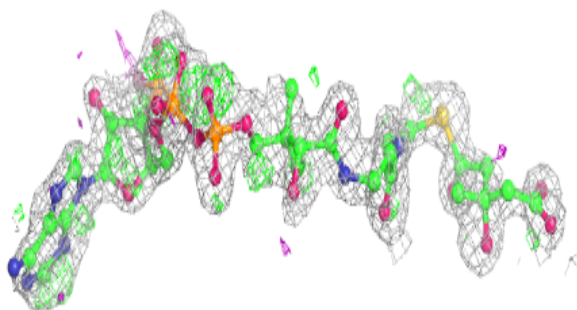
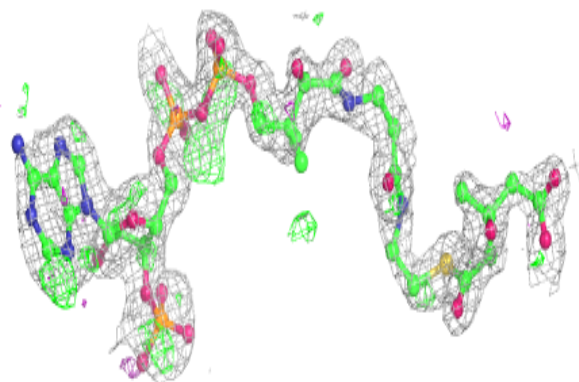


Electron density around CAA D 4402 (A):

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

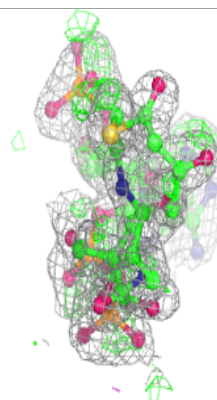
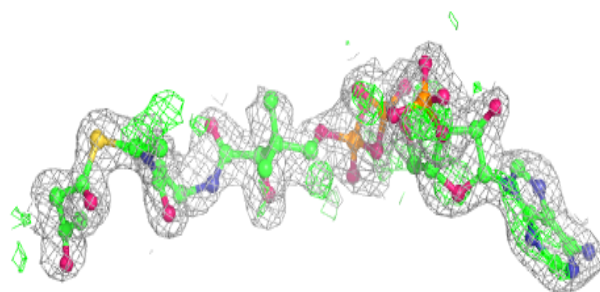
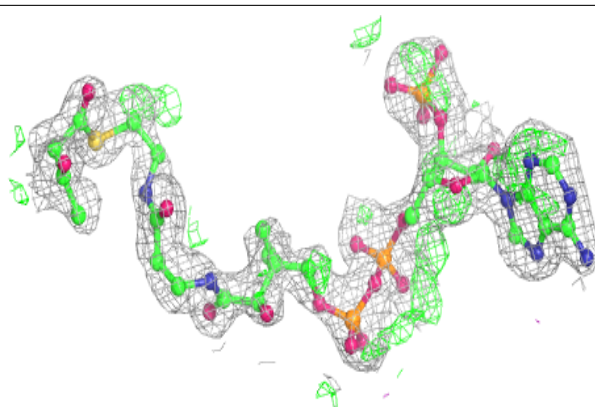
**Electron density around HMG D 4401 (B):**

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

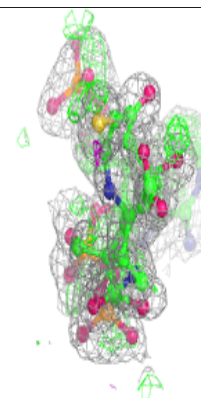
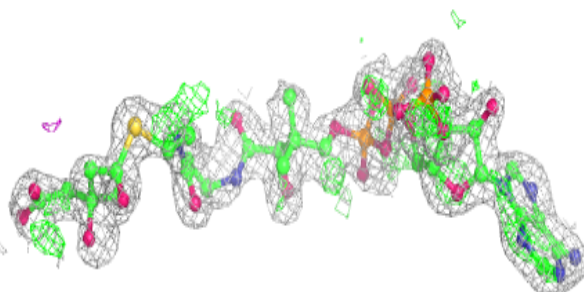
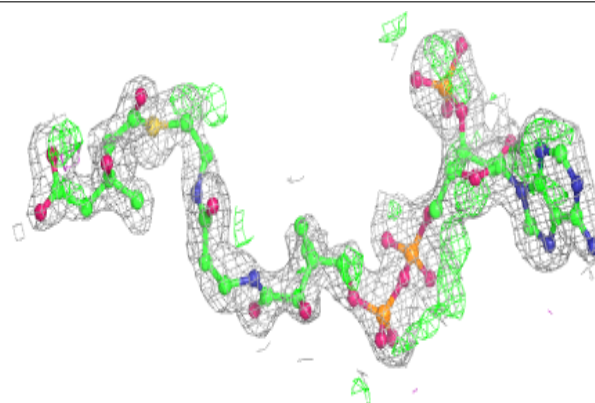


Electron density around CAA B 2402 (A):

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

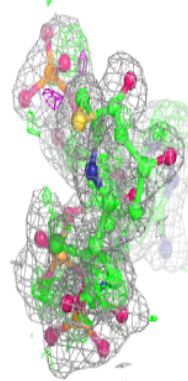
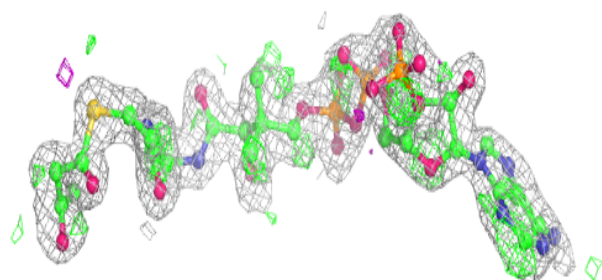
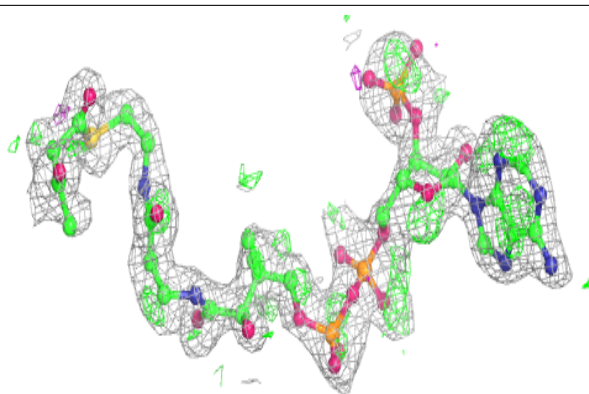
**Electron density around HMG B 2401 (B):**

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

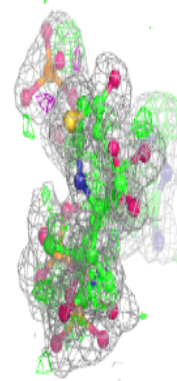
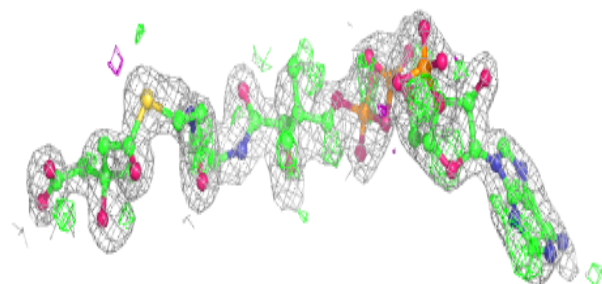
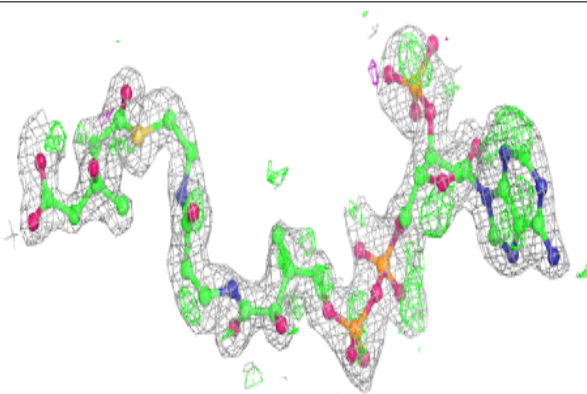


Electron density around CAA A 1402 (A):

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

**Electron density around HMG A 1401 (B):**

$2mF_o-DF_c$ (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.