



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 01:28 PM EST

PDB ID : 3SXN
Title : Mycobacterium tuberculosis Eis protein initiates modulation of host immune responses by acetylation of DUSP16/MKP-7
Authors : Kim, K.H.; An, D.R.; Yoon, J.Y.; Kim, H.S.; Yoon, H.J.; Song, J.S.; Im, H.N.; Kim, J.; Kim, D.J.; Lee, S.J.; Kim, H.J.; Lee, J.Y.; Suh, S.W.
Deposited on : 2011-07-15
Resolution : 2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

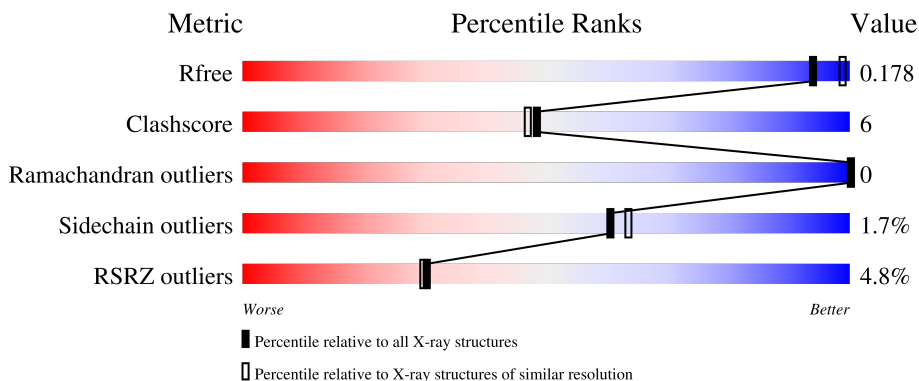
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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.



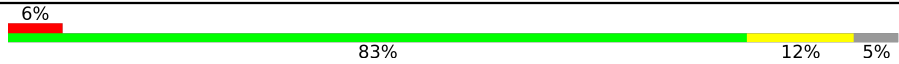

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	 4% 86% 9% • 5%
1	B	422	 4% 82% 13% • 5%
1	C	422	 5% 84% 11% 5%
1	D	422	 4% 87% 8% 5%

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Mol	Chain	Length	Quality of chain
1	E	422	 6% 83% 12% 5%
1	F	422	 5% 83% 11% 5%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20893 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 Enhanced intracellular survival protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3100	1946	568	578	8	0	0	0
1	B	402	3100	1946	568	578	8	0	0	0
1	C	402	3100	1946	568	578	8	0	0	0
1	D	402	3100	1946	568	578	8	0	0	0
1	E	402	3100	1946	568	578	8	0	0	0
1	F	402	3100	1946	568	578	8	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A0QY29
A	-18	GLY	-	expression tag	UNP A0QY29
A	-17	SER	-	expression tag	UNP A0QY29
A	-16	SER	-	expression tag	UNP A0QY29
A	-15	HIS	-	expression tag	UNP A0QY29
A	-14	HIS	-	expression tag	UNP A0QY29
A	-13	HIS	-	expression tag	UNP A0QY29
A	-12	HIS	-	expression tag	UNP A0QY29
A	-11	HIS	-	expression tag	UNP A0QY29
A	-10	HIS	-	expression tag	UNP A0QY29
A	-9	SER	-	expression tag	UNP A0QY29
A	-8	SER	-	expression tag	UNP A0QY29
A	-7	GLY	-	expression tag	UNP A0QY29
A	-6	LEU	-	expression tag	UNP A0QY29
A	-5	VAL	-	expression tag	UNP A0QY29
A	-4	PRO	-	expression tag	UNP A0QY29
A	-3	ARG	-	expression tag	UNP A0QY29

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0QY29
A	-1	SER	-	expression tag	UNP A0QY29
A	0	HIS	-	expression tag	UNP A0QY29
B	-19	MET	-	expression tag	UNP A0QY29
B	-18	GLY	-	expression tag	UNP A0QY29
B	-17	SER	-	expression tag	UNP A0QY29
B	-16	SER	-	expression tag	UNP A0QY29
B	-15	HIS	-	expression tag	UNP A0QY29
B	-14	HIS	-	expression tag	UNP A0QY29
B	-13	HIS	-	expression tag	UNP A0QY29
B	-12	HIS	-	expression tag	UNP A0QY29
B	-11	HIS	-	expression tag	UNP A0QY29
B	-10	HIS	-	expression tag	UNP A0QY29
B	-9	SER	-	expression tag	UNP A0QY29
B	-8	SER	-	expression tag	UNP A0QY29
B	-7	GLY	-	expression tag	UNP A0QY29
B	-6	LEU	-	expression tag	UNP A0QY29
B	-5	VAL	-	expression tag	UNP A0QY29
B	-4	PRO	-	expression tag	UNP A0QY29
B	-3	ARG	-	expression tag	UNP A0QY29
B	-2	GLY	-	expression tag	UNP A0QY29
B	-1	SER	-	expression tag	UNP A0QY29
B	0	HIS	-	expression tag	UNP A0QY29
C	-19	MET	-	expression tag	UNP A0QY29
C	-18	GLY	-	expression tag	UNP A0QY29
C	-17	SER	-	expression tag	UNP A0QY29
C	-16	SER	-	expression tag	UNP A0QY29
C	-15	HIS	-	expression tag	UNP A0QY29
C	-14	HIS	-	expression tag	UNP A0QY29
C	-13	HIS	-	expression tag	UNP A0QY29
C	-12	HIS	-	expression tag	UNP A0QY29
C	-11	HIS	-	expression tag	UNP A0QY29
C	-10	HIS	-	expression tag	UNP A0QY29
C	-9	SER	-	expression tag	UNP A0QY29
C	-8	SER	-	expression tag	UNP A0QY29
C	-7	GLY	-	expression tag	UNP A0QY29
C	-6	LEU	-	expression tag	UNP A0QY29
C	-5	VAL	-	expression tag	UNP A0QY29
C	-4	PRO	-	expression tag	UNP A0QY29
C	-3	ARG	-	expression tag	UNP A0QY29
C	-2	GLY	-	expression tag	UNP A0QY29
C	-1	SER	-	expression tag	UNP A0QY29

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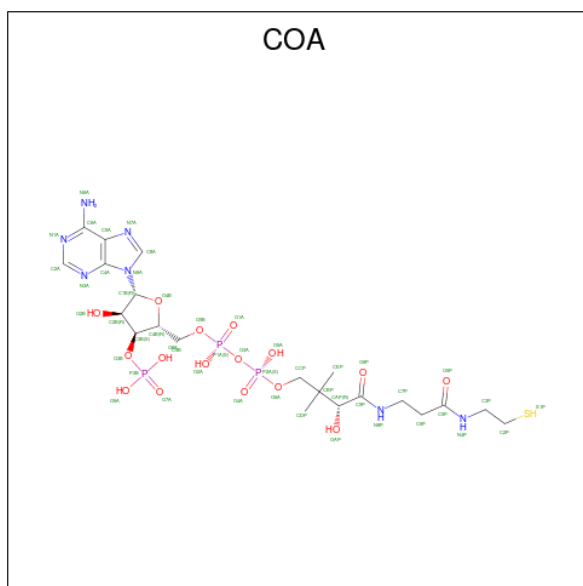
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0QY29
D	-19	MET	-	expression tag	UNP A0QY29
D	-18	GLY	-	expression tag	UNP A0QY29
D	-17	SER	-	expression tag	UNP A0QY29
D	-16	SER	-	expression tag	UNP A0QY29
D	-15	HIS	-	expression tag	UNP A0QY29
D	-14	HIS	-	expression tag	UNP A0QY29
D	-13	HIS	-	expression tag	UNP A0QY29
D	-12	HIS	-	expression tag	UNP A0QY29
D	-11	HIS	-	expression tag	UNP A0QY29
D	-10	HIS	-	expression tag	UNP A0QY29
D	-9	SER	-	expression tag	UNP A0QY29
D	-8	SER	-	expression tag	UNP A0QY29
D	-7	GLY	-	expression tag	UNP A0QY29
D	-6	LEU	-	expression tag	UNP A0QY29
D	-5	VAL	-	expression tag	UNP A0QY29
D	-4	PRO	-	expression tag	UNP A0QY29
D	-3	ARG	-	expression tag	UNP A0QY29
D	-2	GLY	-	expression tag	UNP A0QY29
D	-1	SER	-	expression tag	UNP A0QY29
D	0	HIS	-	expression tag	UNP A0QY29
E	-19	MET	-	expression tag	UNP A0QY29
E	-18	GLY	-	expression tag	UNP A0QY29
E	-17	SER	-	expression tag	UNP A0QY29
E	-16	SER	-	expression tag	UNP A0QY29
E	-15	HIS	-	expression tag	UNP A0QY29
E	-14	HIS	-	expression tag	UNP A0QY29
E	-13	HIS	-	expression tag	UNP A0QY29
E	-12	HIS	-	expression tag	UNP A0QY29
E	-11	HIS	-	expression tag	UNP A0QY29
E	-10	HIS	-	expression tag	UNP A0QY29
E	-9	SER	-	expression tag	UNP A0QY29
E	-8	SER	-	expression tag	UNP A0QY29
E	-7	GLY	-	expression tag	UNP A0QY29
E	-6	LEU	-	expression tag	UNP A0QY29
E	-5	VAL	-	expression tag	UNP A0QY29
E	-4	PRO	-	expression tag	UNP A0QY29
E	-3	ARG	-	expression tag	UNP A0QY29
E	-2	GLY	-	expression tag	UNP A0QY29
E	-1	SER	-	expression tag	UNP A0QY29
E	0	HIS	-	expression tag	UNP A0QY29
F	-19	MET	-	expression tag	UNP A0QY29

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP A0QY29
F	-17	SER	-	expression tag	UNP A0QY29
F	-16	SER	-	expression tag	UNP A0QY29
F	-15	HIS	-	expression tag	UNP A0QY29
F	-14	HIS	-	expression tag	UNP A0QY29
F	-13	HIS	-	expression tag	UNP A0QY29
F	-12	HIS	-	expression tag	UNP A0QY29
F	-11	HIS	-	expression tag	UNP A0QY29
F	-10	HIS	-	expression tag	UNP A0QY29
F	-9	SER	-	expression tag	UNP A0QY29
F	-8	SER	-	expression tag	UNP A0QY29
F	-7	GLY	-	expression tag	UNP A0QY29
F	-6	LEU	-	expression tag	UNP A0QY29
F	-5	VAL	-	expression tag	UNP A0QY29
F	-4	PRO	-	expression tag	UNP A0QY29
F	-3	ARG	-	expression tag	UNP A0QY29
F	-2	GLY	-	expression tag	UNP A0QY29
F	-1	SER	-	expression tag	UNP A0QY29
F	0	HIS	-	expression tag	UNP A0QY29

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		


- Molecule 3 is water.

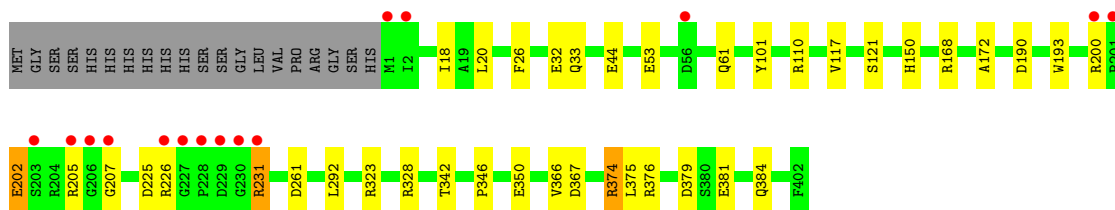
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	396	Total	O	0	0
			396	396		
3	B	394	Total	O	0	0
			394	394		
3	C	349	Total	O	0	0
			349	349		
3	D	361	Total	O	0	0
			361	361		
3	E	234	Total	O	0	0
			234	234		
3	F	271	Total	O	0	0
			271	271		

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.

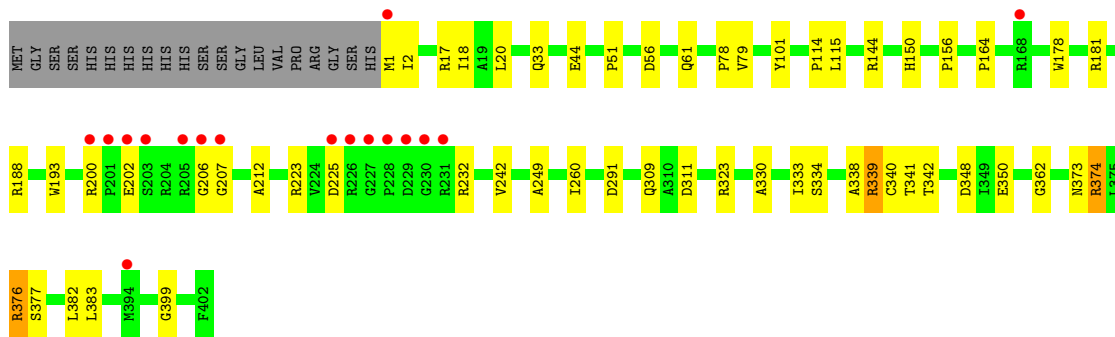
- Molecule 1: Enhanced intracellular survival protein

Chain A: 




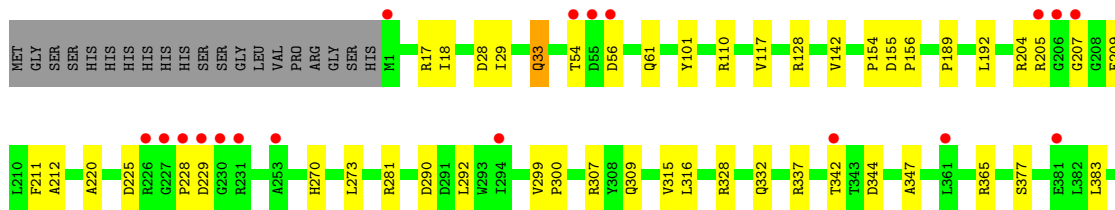
- Molecule 1: Enhanced intracellular survival protein

Chain B: 



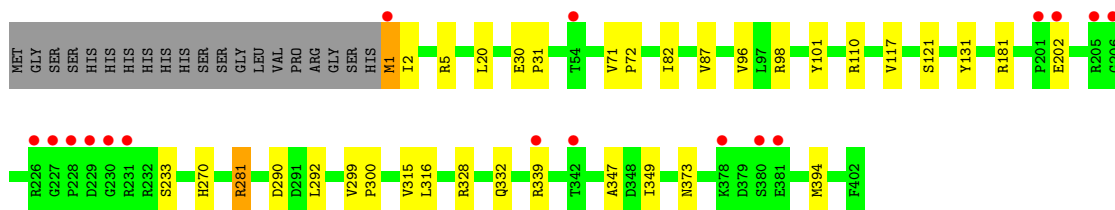
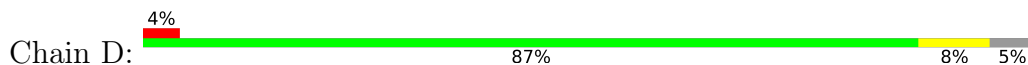
- Molecule 1: Enhanced intracellular survival protein

Chain C: 

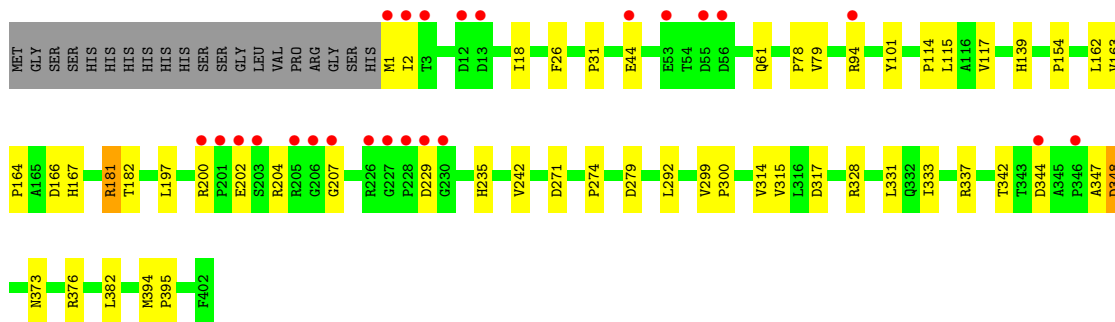
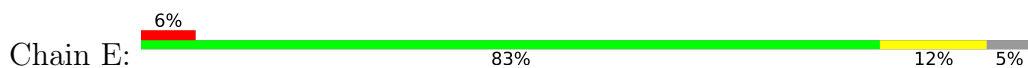




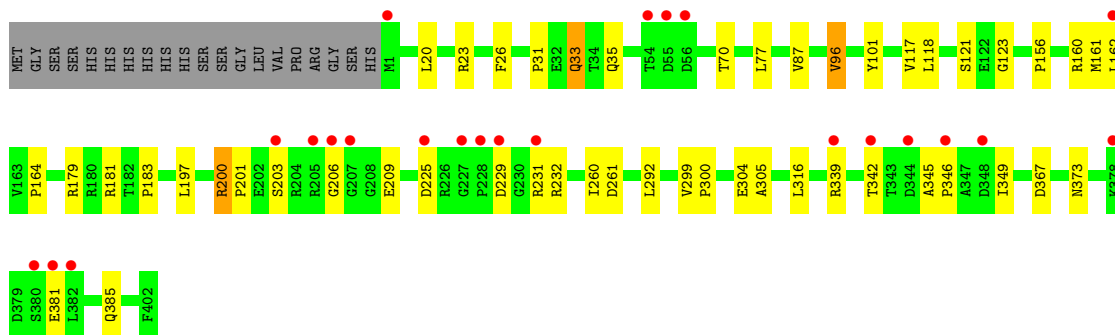
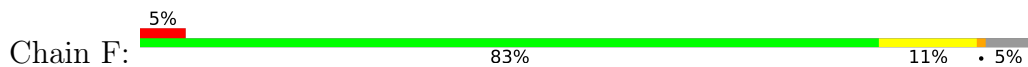
- Molecule 1: Enhanced intracellular survival protein



- Molecule 1: Enhanced intracellular survival protein



- Molecule 1: Enhanced intracellular survival protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.74Å 126.52Å 238.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 29.85 – 2.02	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.03) 92.0 (29.85-2.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.03Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.181 , 0.217 0.178 , 0.178	Depositor DCC
R_{free} test set	20113 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtrriage
Anisotropy	0.430	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20893	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0.48	0/3172	0.63	3/4321 (0.1%)
1	B	0.46	0/3172	0.62	4/4321 (0.1%)
1	C	0.36	0/3172	0.55	0/4321
1	D	0.39	0/3172	0.56	1/4321 (0.0%)
1	E	0.34	0/3172	0.54	0/4321
1	F	0.34	0/3172	0.55	0/4321
All	All	0.40	0/19032	0.57	8/25926 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	374	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	374	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	323	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	323	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	323	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	281	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	291	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3100	0	3020	35	0
1	B	3100	0	3020	41	0
1	C	3100	0	3020	38	0
1	D	3100	0	3020	43	0
1	E	3100	0	3020	35	0
1	F	3100	0	3020	36	0
2	A	48	0	32	4	0
2	B	48	0	31	0	0
2	C	48	0	32	4	0
2	D	48	0	31	4	0
2	E	48	0	32	1	0
2	F	48	0	32	6	0
3	A	396	0	0	6	0
3	B	394	0	0	8	0
3	C	349	0	0	6	0
3	D	361	0	0	8	0
3	E	234	0	0	2	0
3	F	271	0	0	4	0
All	All	20893	0	18310	222	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 6.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH11	1:A:231:ARG:CG	1.68	1.06
1:A:231:ARG:HG3	1:A:231:ARG:NH1	1.56	1.03
1:E:1:MET:CB	1:E:2:ILE:HA	1.92	0.99
1:E:1:MET:HB3	1:E:2:ILE:CA	1.92	0.97
1:E:1:MET:HB3	1:E:2:ILE:HA	1.00	0.97
1:C:290:ASP:OD1	1:D:281:ARG:HD2	1.68	0.93
1:C:281:ARG:HD2	1:D:290:ASP:OD1	1.73	0.88
1:D:110:ARG:HD3	3:D:852:HOH:O	1.73	0.87
1:A:231:ARG:HH11	1:A:231:ARG:HG3	0.75	0.84
1:C:33:GLN:HE21	1:C:33:GLN:H	1.30	0.79
2:C:500:COA:H2A	2:C:500:COA:H122	1.64	0.78
1:D:1:MET:H3	1:D:2:ILE:HA	1.50	0.76
1:B:1:MET:HG3	3:B:984:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA2	1:A:225:ASP:HB3	1.72	0.72
1:A:33:GLN:OE1	1:A:200:ARG:NH2	2.23	0.72
1:D:87:VAL:HG21	1:D:96:VAL:HG23	1.70	0.72
1:F:206:GLY:O	1:F:225:ASP:HB2	1.90	0.71
2:C:500:COA:H2A	2:C:500:COA:CCP	2.22	0.70
1:C:344:ASP:HB2	3:C:625:HOH:O	1.92	0.69
1:D:96:VAL:HG22	3:D:809:HOH:O	1.93	0.68
1:B:350:GLU:HB2	1:B:376:ARG:HG2	1.75	0.67
1:C:28:ASP:CG	1:C:29:ILE:H	1.98	0.66
1:A:374:ARG:HD2	3:A:961:HOH:O	1.94	0.66
1:A:110:ARG:NH1	3:A:864:HOH:O	2.28	0.65
1:D:87:VAL:CG2	1:D:96:VAL:HG23	2.26	0.65
1:C:307:ARG:NH2	1:C:337:ARG:HH22	1.94	0.65
1:E:204:ARG:HG2	1:E:207:GLY:HA2	1.80	0.64
1:C:290:ASP:OD1	1:D:281:ARG:CD	2.44	0.64
1:B:309:GLN:NE2	3:B:880:HOH:O	2.31	0.64
1:A:121:SER:HB3	2:A:500:COA:H21	1.79	0.64
1:E:79:VAL:HG12	1:E:115:LEU:HB2	1.81	0.63
1:B:202:GLU:H	1:B:202:GLU:CD	2.02	0.63
1:A:117:VAL:HB	1:A:292:LEU:HD11	1.82	0.62
1:B:207:GLY:O	1:B:223:ARG:HB3	1.99	0.62
1:A:366:VAL:HG13	1:A:375:LEU:HD23	1.83	0.61
1:A:328:ARG:NH1	1:A:346:PRO:HA	2.16	0.61
1:C:307:ARG:NH2	1:C:337:ARG:NH2	2.50	0.60
1:E:44:GLU:H	1:E:44:GLU:CD	2.03	0.59
1:C:209:GLU:HB2	1:F:23:ARG:NH2	2.18	0.59
1:A:53:GLU:H	1:A:53:GLU:CD	2.06	0.59
1:B:311:ASP:OD1	1:B:334:SER:HA	2.03	0.59
1:A:200:ARG:HG2	1:A:202:GLU:OE2	2.03	0.58
1:F:209:GLU:HG2	3:F:850:HOH:O	2.02	0.58
1:E:181:ARG:CZ	1:E:242:VAL:O	2.52	0.58
1:A:32:GLU:HG2	3:A:743:HOH:O	2.03	0.58
1:B:156:PRO:HG2	1:B:249:ALA:HB2	1.84	0.58
1:C:228:PRO:HA	1:C:229:ASP:OD1	2.04	0.57
1:D:87:VAL:CG1	1:D:96:VAL:HG21	2.35	0.57
1:C:204:ARG:O	1:C:205:ARG:HB2	2.04	0.57
1:D:1:MET:N	1:D:2:ILE:HA	2.14	0.57
1:F:181:ARG:NH1	1:F:181:ARG:HB3	2.20	0.56
1:B:164:PRO:HG3	1:B:212:ALA:HB2	1.87	0.56
1:F:87:VAL:HG23	2:F:500:COA:H132	1.88	0.56
1:D:121:SER:HB3	2:D:500:COA:H21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:CB	1:D:2:ILE:HA	2.35	0.56
1:F:121:SER:CB	2:F:500:COA:H21	2.36	0.55
1:E:164:PRO:HB2	1:E:197:LEU:HD22	1.89	0.55
1:A:231:ARG:CG	1:A:231:ARG:NH1	2.40	0.55
1:E:163:VAL:HG13	1:E:166:ASP:HB2	1.89	0.55
2:D:500:COA:H141	2:D:500:COA:O5P	2.07	0.55
1:C:207:GLY:HA2	1:C:225:ASP:HB3	1.89	0.54
1:F:121:SER:HB3	2:F:500:COA:H21	1.88	0.54
1:F:121:SER:OG	2:F:500:COA:H21	2.07	0.54
1:E:299:VAL:HB	1:E:300:PRO:HD3	1.88	0.54
1:D:87:VAL:HG13	1:D:96:VAL:HG21	1.88	0.54
1:C:33:GLN:H	1:C:33:GLN:NE2	2.05	0.53
1:B:339:ARG:HH11	1:B:339:ARG:HG3	1.73	0.53
1:F:304:GLU:OE1	1:F:339:ARG:HD2	2.08	0.53
1:A:374:ARG:HD3	1:B:150:HIS:CE1	2.44	0.53
1:E:181:ARG:NH2	1:E:242:VAL:O	2.42	0.52
1:B:339:ARG:HH11	1:B:339:ARG:CG	2.21	0.52
1:E:139:HIS:HB2	3:E:820:HOH:O	2.08	0.52
1:B:333:ILE:HG12	1:B:338:ALA:HB2	1.92	0.52
1:C:228:PRO:HA	1:C:229:ASP:CG	2.29	0.52
1:F:96:VAL:HG13	3:F:772:HOH:O	2.09	0.52
1:B:33:GLN:OE1	1:B:200:ARG:NH2	2.43	0.52
1:F:26:PHE:CZ	2:F:500:COA:O5P	2.62	0.52
1:F:345:ALA:HB1	1:F:346:PRO:HD2	1.91	0.52
1:D:315:VAL:HB	1:D:347:ALA:HA	1.93	0.51
1:F:118:LEU:C	1:F:118:LEU:HD12	2.31	0.51
1:E:26:PHE:CZ	2:E:500:COA:O5P	2.64	0.51
2:C:500:COA:H61	3:C:689:HOH:O	2.08	0.51
1:A:33:GLN:CD	1:A:200:ARG:HH22	2.13	0.51
1:F:20:LEU:C	1:F:20:LEU:HD23	2.30	0.51
1:C:110:ARG:HD3	3:C:925:HOH:O	2.10	0.51
1:F:381:GLU:O	1:F:385:GLN:HG3	2.11	0.50
1:A:168:ARG:HH22	1:A:190:ASP:CG	2.13	0.50
1:B:33:GLN:OE1	1:B:200:ARG:NE	2.43	0.50
1:D:1:MET:HB2	1:D:2:ILE:CA	2.41	0.50
1:E:315:VAL:H	1:E:348:ASP:HB2	1.77	0.50
1:A:121:SER:CB	2:A:500:COA:H21	2.41	0.50
1:D:1:MET:HB2	1:D:2:ILE:HA	1.93	0.50
1:D:181:ARG:O	1:D:394:MET:SD	2.69	0.50
1:F:299:VAL:HB	1:F:300:PRO:HD3	1.94	0.50
1:D:31:PRO:HB3	1:D:202:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD22	1:E:167:HIS:CE1	2.46	0.49
1:F:33:GLN:NE2	1:F:33:GLN:H	2.11	0.49
1:D:82:ILE:HD11	1:D:131:TYR:OH	2.12	0.49
1:F:161:MET:O	1:F:162:LEU:HD23	2.12	0.49
1:F:231:ARG:HB3	1:F:261:ASP:OD2	2.13	0.49
1:D:316:LEU:O	1:D:328:ARG:HA	2.13	0.49
1:C:315:VAL:HB	1:C:347:ALA:HA	1.95	0.48
1:F:77:LEU:HD21	1:F:305:ALA:HB1	1.94	0.48
1:F:31:PRO:O	1:F:35:GLN:HG3	2.14	0.48
1:B:44:GLU:H	1:B:44:GLU:CD	2.17	0.48
1:B:348:ASP:HB3	1:B:382:LEU:HD23	1.96	0.48
1:C:316:LEU:O	1:C:328:ARG:HA	2.14	0.48
1:A:20:LEU:C	1:A:20:LEU:HD23	2.34	0.47
1:B:51:PRO:HD2	3:B:950:HOH:O	2.13	0.47
1:A:384:GLN:HA	3:A:735:HOH:O	2.13	0.47
1:B:206:GLY:O	1:B:225:ASP:HB2	2.14	0.47
1:D:82:ILE:HD12	1:D:117:VAL:O	2.15	0.47
1:B:373:ASN:HB2	3:B:815:HOH:O	2.14	0.47
1:C:154:PRO:C	1:C:156:PRO:HD3	2.34	0.47
1:D:299:VAL:HB	1:D:300:PRO:HD3	1.96	0.47
1:E:279:ASP:OD1	1:F:123:GLY:HA3	2.14	0.47
2:A:500:COA:H61	3:A:685:HOH:O	2.14	0.47
1:B:200:ARG:HG2	1:B:200:ARG:HH11	1.78	0.47
1:A:26:PHE:CZ	2:A:500:COA:O5P	2.68	0.47
1:E:317:ASP:HB2	1:E:347:ALA:CB	2.44	0.47
1:B:181:ARG:CZ	1:B:242:VAL:O	2.63	0.46
1:D:98:ARG:NH1	2:D:500:COA:O9A	2.40	0.46
1:C:18:ILE:HA	1:C:61:GLN:OE1	2.16	0.46
1:B:200:ARG:HG2	1:B:200:ARG:NH1	2.30	0.46
1:C:56:ASP:HA	3:C:943:HOH:O	2.15	0.46
1:D:121:SER:CB	2:D:500:COA:H21	2.46	0.46
1:A:350:GLU:HB2	1:A:376:ARG:HB2	1.98	0.46
1:B:232:ARG:HB3	1:B:260:ILE:HD13	1.97	0.46
1:D:30:GLU:HB3	1:D:31:PRO:HD2	1.98	0.46
1:E:200:ARG:HB3	1:E:202:GLU:OE1	2.15	0.46
1:E:18:ILE:HA	1:E:61:GLN:OE1	2.16	0.45
1:E:31:PRO:HG3	1:E:202:GLU:HB2	1.98	0.45
1:C:155:ASP:N	1:C:156:PRO:HD3	2.32	0.45
1:E:78:PRO:O	1:E:114:PRO:HD2	2.16	0.45
1:B:17:ARG:HD3	1:B:56:ASP:O	2.17	0.45
1:E:235:HIS:HE1	3:E:802:HOH:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:CD	3:A:961:HOH:O	2.60	0.45
1:B:339:ARG:NH1	1:B:341:THR:HG21	2.32	0.45
1:C:128:ARG:CZ	2:C:500:COA:H1B	2.47	0.45
1:F:232:ARG:HB3	1:F:260:ILE:HD13	1.99	0.45
1:E:182:THR:HG23	1:E:394:MET:SD	2.57	0.45
1:C:270:HIS:HD2	3:C:853:HOH:O	2.00	0.44
1:D:394:MET:CE	3:D:655:HOH:O	2.64	0.44
1:A:231:ARG:NH1	1:A:261:ASP:OD2	2.50	0.44
1:A:379:ASP:OD1	1:A:381:GLU:HB2	2.17	0.44
1:C:17:ARG:CZ	1:C:56:ASP:O	2.66	0.44
1:E:182:THR:HA	1:E:394:MET:SD	2.58	0.44
1:B:164:PRO:HD2	3:B:640:HOH:O	2.17	0.44
1:B:188:ARG:HD3	1:B:193:TRP:CE2	2.52	0.44
1:F:200:ARG:HA	1:F:201:PRO:HD3	1.90	0.44
1:C:117:VAL:HB	1:C:292:LEU:HD11	1.99	0.44
1:C:142:VAL:HG21	1:C:273:LEU:HD21	2.00	0.44
1:D:20:LEU:C	1:D:20:LEU:HD23	2.38	0.44
1:D:332:GLN:CD	1:D:339:ARG:NH1	2.70	0.44
1:C:28:ASP:CG	1:C:29:ILE:N	2.68	0.44
1:C:209:GLU:HB2	1:F:23:ARG:HH21	1.80	0.44
1:C:377:SER:HB3	1:C:383:LEU:HG	1.99	0.43
1:A:18:ILE:HA	1:A:61:GLN:OE1	2.17	0.43
1:D:181:ARG:CZ	3:D:856:HOH:O	2.66	0.43
1:D:5:ARG:HD3	3:D:953:HOH:O	2.18	0.43
1:F:87:VAL:HG13	1:F:96:VAL:HG21	2.01	0.43
1:D:117:VAL:HB	1:D:292:LEU:HD11	2.00	0.43
1:E:271:ASP:O	1:E:274:PRO:HD2	2.19	0.43
1:F:20:LEU:HD23	1:F:20:LEU:O	2.19	0.43
1:F:203:SER:HB3	3:F:695:HOH:O	2.18	0.43
1:A:231:ARG:HA	1:A:231:ARG:HD2	1.72	0.43
1:E:117:VAL:HB	1:E:292:LEU:HD11	1.99	0.43
1:F:70:THR:O	1:F:183:PRO:HA	2.18	0.43
1:B:20:LEU:C	1:B:20:LEU:HD23	2.38	0.43
1:E:328:ARG:HH21	1:E:344:ASP:HB2	1.83	0.43
1:E:314:VAL:HG12	1:E:382:LEU:HD21	2.00	0.43
2:F:500:COA:H61	3:F:654:HOH:O	2.19	0.43
1:A:150:HIS:NE2	1:B:374:ARG:HD3	2.33	0.42
1:C:309:GLN:HG2	3:C:850:HOH:O	2.19	0.42
1:F:164:PRO:HB2	1:F:197:LEU:CD2	2.49	0.42
1:A:44:GLU:H	1:A:44:GLU:CD	2.22	0.42
1:B:144:ARG:HD3	1:B:260:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ARG:NH2	3:D:856:HOH:O	2.52	0.42
1:D:87:VAL:HG11	1:D:96:VAL:CG2	2.50	0.42
1:F:316:LEU:HD12	1:F:349:ILE:HB	2.01	0.42
1:C:299:VAL:HB	1:C:300:PRO:HD3	2.00	0.42
1:B:18:ILE:HA	1:B:61:GLN:OE1	2.20	0.42
1:B:78:PRO:O	1:B:114:PRO:HD2	2.20	0.42
1:C:212:ALA:HA	1:C:220:ALA:O	2.20	0.42
1:D:316:LEU:HD23	1:D:349:ILE:HB	2.02	0.42
1:A:172:ALA:HA	1:A:193:TRP:CZ2	2.55	0.42
1:C:365:ARG:HD3	1:D:270:HIS:CG	2.55	0.42
1:D:71:VAL:HB	1:D:72:PRO:CD	2.50	0.42
1:F:181:ARG:HB3	1:F:181:ARG:CZ	2.49	0.42
1:A:20:LEU:HD23	1:A:20:LEU:O	2.19	0.41
1:B:44:GLU:HG3	3:B:949:HOH:O	2.20	0.41
1:B:181:ARG:NH2	3:B:779:HOH:O	2.53	0.41
1:D:332:GLN:CD	1:D:339:ARG:HH11	2.23	0.41
1:E:394:MET:HG2	1:E:395:PRO:HD2	2.02	0.41
1:E:44:GLU:CD	1:E:44:GLU:N	2.71	0.41
1:D:82:ILE:HD12	1:D:82:ILE:H	1.85	0.41
1:B:178:TRP:CH2	1:B:399:GLY:HA2	2.55	0.41
1:D:87:VAL:CG1	1:D:96:VAL:CG2	2.98	0.41
1:D:394:MET:HE3	3:D:655:HOH:O	2.20	0.41
1:C:54:THR:O	1:C:54:THR:HG22	2.21	0.41
1:D:181:ARG:O	1:D:394:MET:CE	2.68	0.41
1:F:229:ASP:N	1:F:229:ASP:OD1	2.53	0.41
1:A:33:GLN:CD	1:A:200:ARG:NH2	2.73	0.41
1:B:79:VAL:HG12	1:B:115:LEU:HB2	2.02	0.41
1:C:204:ARG:O	1:C:205:ARG:CB	2.67	0.41
1:D:87:VAL:CG2	1:D:96:VAL:CG2	2.98	0.41
1:D:373:ASN:ND2	3:D:799:HOH:O	2.54	0.41
1:E:154:PRO:HG3	1:F:373:ASN:ND2	2.36	0.41
1:E:317:ASP:HB2	1:E:347:ALA:HB2	2.03	0.41
1:F:117:VAL:HB	1:F:292:LEU:HD11	2.02	0.41
1:A:205:ARG:O	1:A:205:ARG:HG3	2.20	0.41
1:A:226:ARG:NH1	1:C:205:ARG:HH12	2.18	0.41
1:B:339:ARG:CG	1:B:339:ARG:NH1	2.81	0.41
1:B:1:MET:HG2	1:B:2:ILE:N	2.36	0.40
1:B:330:ALA:O	1:B:340:CYS:HA	2.21	0.40
1:E:242:VAL:O	1:E:242:VAL:HG23	2.20	0.40
1:C:189:PRO:HD2	1:C:192:LEU:HD12	2.02	0.40
1:B:362:GLY:HA2	3:B:861:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB3	1:B:383:LEU:HG	2.03	0.40
1:C:211:PHE:CE1	1:F:23:ARG:HG2	2.56	0.40
1:E:333:ILE:HA	1:E:337:ARG:O	2.21	0.40
1:E:373:ASN:ND2	1:E:376:ARG:HG2	2.35	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	400/422 (95%)	393 (98%)	7 (2%)	0	100	100
1	B	400/422 (95%)	396 (99%)	4 (1%)	0	100	100
1	C	400/422 (95%)	393 (98%)	7 (2%)	0	100	100
1	D	400/422 (95%)	396 (99%)	4 (1%)	0	100	100
1	E	400/422 (95%)	390 (98%)	10 (2%)	0	100	100
1	F	400/422 (95%)	395 (99%)	5 (1%)	0	100	100
All	All	2400/2532 (95%)	2363 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/328 (95%)	306 (98%)	5 (2%)	62	66
1	B	311/328 (95%)	307 (99%)	4 (1%)	69	72
1	C	311/328 (95%)	307 (99%)	4 (1%)	69	72
1	D	311/328 (95%)	308 (99%)	3 (1%)	76	80
1	E	311/328 (95%)	304 (98%)	7 (2%)	50	51
1	F	311/328 (95%)	302 (97%)	9 (3%)	42	41
All	All	1866/1968 (95%)	1834 (98%)	32 (2%)	60	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	TYR
1	A	202	GLU
1	A	231	ARG
1	A	342	THR
1	A	367	ASP
1	B	101	TYR
1	B	339	ARG
1	B	342	THR
1	B	376	ARG
1	C	33	GLN
1	C	101	TYR
1	C	332	GLN
1	C	342	THR
1	D	1	MET
1	D	101	TYR
1	D	233	SER
1	E	94	ARG
1	E	101	TYR
1	E	181	ARG
1	E	229	ASP
1	E	331	LEU
1	E	342	THR
1	E	348	ASP
1	F	33	GLN
1	F	96	VAL
1	F	101	TYR
1	F	156	PRO
1	F	160	ARG
1	F	179	ARG
1	F	200	ARG

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Mol	Chain	Res	Type
1	F	342	THR
1	F	367	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	B	309	GLN
1	C	33	GLN
1	C	235	HIS
1	C	270	HIS
1	C	385	GLN
1	D	235	HIS
1	D	385	GLN
1	E	167	HIS
1	E	373	ASN
1	F	33	GLN
1	F	385	GLN

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 [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	B	500	-	41,50,50	1.78	13 (31%)	52,75,75	2.87	17 (32%)
2	COA	D	500	-	41,50,50	1.73	12 (29%)	52,75,75	2.84	15 (28%)
2	COA	C	500	-	41,50,50	2.16	13 (31%)	52,75,75	2.29	15 (28%)
2	COA	E	500	-	41,50,50	1.45	9 (21%)	52,75,75	2.91	15 (28%)
2	COA	A	500	-	41,50,50	1.82	13 (31%)	52,75,75	2.76	14 (26%)
2	COA	F	500	-	41,50,50	1.70	14 (34%)	52,75,75	2.75	17 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	500	-	-	8/44/64/64	0/3/3/3
2	COA	D	500	-	-	9/44/64/64	0/3/3/3
2	COA	C	500	-	-	9/44/64/64	0/3/3/3
2	COA	E	500	-	-	9/44/64/64	0/3/3/3
2	COA	A	500	-	-	11/44/64/64	0/3/3/3
2	COA	F	500	-	-	13/44/64/64	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	COA	C4A-N3A	-5.66	1.27	1.35
2	C	500	COA	O5P-C5P	-4.60	1.13	1.23
2	C	500	COA	C3P-N4P	-4.16	1.36	1.46
2	D	500	COA	C5P-N4P	-3.58	1.25	1.33
2	B	500	COA	O5P-C5P	-3.26	1.16	1.23
2	A	500	COA	C6P-C5P	-3.24	1.45	1.51
2	A	500	COA	O5P-C5P	-3.20	1.16	1.23
2	C	500	COA	P3B-O9A	-3.17	1.42	1.54
2	C	500	COA	C2A-N3A	-3.16	1.27	1.32
2	D	500	COA	P2A-O5A	-3.09	1.40	1.55
2	B	500	COA	P2A-O5A	-3.06	1.41	1.55
2	C	500	COA	C5P-N4P	-3.04	1.26	1.33
2	B	500	COA	P1A-O2A	-3.00	1.41	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	COA	P2A-O5A	-2.99	1.41	1.55
2	A	500	COA	P3B-O8A	-2.97	1.43	1.54
2	A	500	COA	P2A-O5A	-2.95	1.41	1.55
2	D	500	COA	P1A-O2A	-2.88	1.41	1.55
2	A	500	COA	P1A-O2A	-2.87	1.41	1.55
2	A	500	COA	C3P-N4P	-2.87	1.39	1.46
2	D	500	COA	P2A-O4A	-2.82	1.40	1.50
2	B	500	COA	C3P-N4P	-2.78	1.39	1.46
2	D	500	COA	C5A-N7A	-2.78	1.29	1.39
2	B	500	COA	P2A-O4A	-2.77	1.41	1.50
2	F	500	COA	C3P-N4P	-2.76	1.39	1.46
2	A	500	COA	O9P-C9P	-2.75	1.17	1.23
2	C	500	COA	O9P-C9P	-2.74	1.18	1.23
2	F	500	COA	P2A-O5A	-2.67	1.42	1.55
2	C	500	COA	P3B-O8A	-2.66	1.44	1.54
2	C	500	COA	P1A-O2A	-2.66	1.42	1.55
2	A	500	COA	C4A-N3A	-2.64	1.32	1.35
2	B	500	COA	P3B-O9A	-2.63	1.44	1.54
2	F	500	COA	P1A-O2A	-2.62	1.43	1.55
2	F	500	COA	C4A-N3A	-2.60	1.32	1.35
2	E	500	COA	P2A-O5A	-2.54	1.43	1.55
2	A	500	COA	C5A-N7A	-2.54	1.30	1.39
2	D	500	COA	C4A-N3A	-2.52	1.32	1.35
2	F	500	COA	C5A-N7A	-2.51	1.30	1.39
2	B	500	COA	C5A-N7A	-2.51	1.30	1.39
2	A	500	COA	P3B-O9A	-2.50	1.45	1.54
2	B	500	COA	P3B-O8A	-2.48	1.45	1.54
2	B	500	COA	C7P-N8P	-2.48	1.40	1.46
2	F	500	COA	C6P-C5P	-2.48	1.46	1.51
2	F	500	COA	C7P-N8P	-2.46	1.40	1.46
2	A	500	COA	P2A-O4A	-2.46	1.42	1.50
2	B	500	COA	C6P-C5P	-2.43	1.46	1.51
2	F	500	COA	P3B-O9A	-2.43	1.45	1.54
2	C	500	COA	P2A-O4A	-2.42	1.42	1.50
2	B	500	COA	P1A-O1A	-2.42	1.42	1.50
2	E	500	COA	P1A-O2A	-2.40	1.44	1.55
2	F	500	COA	P3B-O8A	-2.38	1.45	1.54
2	E	500	COA	P3B-O8A	-2.37	1.45	1.54
2	B	500	COA	O9P-C9P	-2.37	1.18	1.23
2	A	500	COA	P1A-O1A	-2.37	1.42	1.50
2	D	500	COA	CEP-CBP	-2.36	1.48	1.53
2	F	500	COA	C2B-C1B	-2.34	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	COA	C5A-N7A	-2.32	1.31	1.39
2	D	500	COA	O5P-C5P	-2.30	1.18	1.23
2	F	500	COA	O9P-C9P	-2.29	1.18	1.23
2	E	500	COA	O9P-C9P	-2.28	1.18	1.23
2	E	500	COA	P3B-O9A	-2.27	1.46	1.54
2	D	500	COA	O9P-C9P	-2.26	1.18	1.23
2	C	500	COA	P1A-O1A	-2.24	1.43	1.50
2	B	500	COA	CEP-CBP	-2.22	1.48	1.53
2	E	500	COA	C6P-C5P	-2.21	1.47	1.51
2	C	500	COA	C2P-S1P	-2.19	1.73	1.80
2	D	500	COA	P3B-O8A	-2.17	1.46	1.54
2	F	500	COA	O5P-C5P	-2.16	1.18	1.23
2	D	500	COA	C3P-N4P	-2.12	1.41	1.46
2	F	500	COA	O4B-C4B	-2.10	1.40	1.45
2	E	500	COA	P2A-O4A	-2.05	1.43	1.50
2	F	500	COA	P1A-O1A	-2.03	1.43	1.50
2	D	500	COA	C2P-S1P	-2.02	1.73	1.80
2	A	500	COA	P3B-O7A	-2.02	1.44	1.50
2	E	500	COA	O5P-C5P	-2.01	1.19	1.23

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	COA	CEP-CBP-CAP	-10.35	90.87	108.82
2	E	500	COA	CEP-CBP-CCP	10.25	124.95	108.23
2	A	500	COA	CEP-CBP-CAP	-10.11	91.30	108.82
2	D	500	COA	CEP-CBP-CAP	-9.41	92.51	108.82
2	B	500	COA	CEP-CBP-CAP	-9.27	92.75	108.82
2	F	500	COA	CEP-CBP-CAP	-9.01	93.20	108.82
2	B	500	COA	CDP-CBP-CAP	-8.83	93.50	108.82
2	F	500	COA	CEP-CBP-CCP	8.60	122.26	108.23
2	A	500	COA	CEP-CBP-CCP	7.98	121.25	108.23
2	D	500	COA	CDP-CBP-CCP	7.47	120.41	108.23
2	A	500	COA	CDP-CBP-CAP	-7.43	95.94	108.82
2	D	500	COA	CDP-CBP-CAP	-7.43	95.95	108.82
2	F	500	COA	CDP-CBP-CAP	-7.02	96.64	108.82
2	E	500	COA	CDP-CBP-CAP	-6.85	96.94	108.82
2	A	500	COA	CEP-CBP-CDP	6.48	122.38	109.17
2	C	500	COA	C3P-N4P-C5P	-6.42	110.91	122.84
2	B	500	COA	CEP-CBP-CDP	6.41	122.23	109.17
2	F	500	COA	CDP-CBP-CCP	6.36	118.60	108.23
2	B	500	COA	CEP-CBP-CCP	6.35	118.59	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	COA	CEP-CBP-CDP	6.20	121.80	109.17
2	C	500	COA	C2A-N1A-C6A	5.91	128.87	118.75
2	B	500	COA	CDP-CBP-CCP	5.82	117.72	108.23
2	D	500	COA	CEP-CBP-CCP	5.72	117.56	108.23
2	D	500	COA	O6A-CCP-CBP	5.69	119.69	110.55
2	D	500	COA	CEP-CBP-CDP	5.64	120.65	109.17
2	B	500	COA	C7P-N8P-C9P	5.53	132.46	122.59
2	C	500	COA	O6A-CCP-CBP	5.29	119.05	110.55
2	C	500	COA	O5P-C5P-N4P	-5.20	113.20	123.01
2	C	500	COA	N3A-C2A-N1A	-5.03	120.82	128.68
2	C	500	COA	C6P-C5P-N4P	4.97	124.79	116.42
2	B	500	COA	C6P-C5P-N4P	4.47	123.95	116.42
2	F	500	COA	O5P-C5P-C6P	-4.46	113.86	122.02
2	A	500	COA	CDP-CBP-CCP	4.37	115.35	108.23
2	D	500	COA	C2P-C3P-N4P	-4.34	102.39	112.31
2	F	500	COA	CEP-CBP-CDP	4.34	118.01	109.17
2	E	500	COA	C6P-C5P-N4P	4.08	123.28	116.42
2	E	500	COA	C2P-C3P-N4P	3.90	121.21	112.31
2	E	500	COA	O5P-C5P-C6P	-3.87	114.94	122.02
2	A	500	COA	O6A-CCP-CBP	3.80	116.66	110.55
2	E	500	COA	C7P-C6P-C5P	-3.73	106.14	112.36
2	A	500	COA	C6P-C5P-N4P	3.72	122.68	116.42
2	F	500	COA	C6P-C5P-N4P	3.67	122.61	116.42
2	D	500	COA	C4A-C5A-N7A	-3.63	105.62	109.40
2	D	500	COA	O5P-C5P-N4P	-3.61	116.20	123.01
2	B	500	COA	C3P-N4P-C5P	3.38	129.11	122.84
2	A	500	COA	O5P-C5P-C6P	-3.36	115.86	122.02
2	B	500	COA	C7P-C6P-C5P	-3.36	106.76	112.36
2	F	500	COA	C6P-C7P-N8P	-3.34	105.14	111.90
2	D	500	COA	O9A-P3B-O8A	3.34	120.40	107.64
2	C	500	COA	O4B-C1B-C2B	-3.11	102.38	106.93
2	F	500	COA	C4A-C5A-N7A	-3.09	106.17	109.40
2	F	500	COA	O6A-CCP-CBP	3.04	115.44	110.55
2	A	500	COA	C4A-C5A-N7A	-3.01	106.26	109.40
2	A	500	COA	OAP-CAP-CBP	2.98	117.26	110.25
2	A	500	COA	N3A-C2A-N1A	-2.92	124.11	128.68
2	E	500	COA	OAP-CAP-CBP	2.90	117.07	110.25
2	F	500	COA	P2A-O3A-P1A	-2.88	122.95	132.83
2	F	500	COA	OAP-CAP-CBP	2.88	117.03	110.25
2	D	500	COA	OAP-CAP-CBP	2.87	117.02	110.25
2	B	500	COA	N3A-C2A-N1A	-2.78	124.33	128.68
2	C	500	COA	C5A-C6A-N1A	-2.78	114.06	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	COA	C7P-C6P-C5P	-2.76	107.76	112.36
2	B	500	COA	O5P-C5P-C6P	-2.76	116.97	122.02
2	E	500	COA	N3A-C2A-N1A	-2.76	124.37	128.68
2	B	500	COA	OAP-CAP-CBP	2.74	116.70	110.25
2	E	500	COA	CDP-CBP-CCP	2.68	112.61	108.23
2	E	500	COA	C4A-C5A-N7A	-2.64	106.65	109.40
2	D	500	COA	P2A-O3A-P1A	-2.63	123.79	132.83
2	C	500	COA	C5A-C6A-N6A	2.62	124.34	120.35
2	E	500	COA	C7P-N8P-C9P	-2.52	118.08	122.59
2	C	500	COA	C7P-N8P-C9P	2.52	127.08	122.59
2	E	500	COA	O6A-CCP-CBP	2.52	114.60	110.55
2	F	500	COA	O9A-P3B-O8A	2.50	117.19	107.64
2	C	500	COA	C2P-C3P-N4P	-2.47	106.65	112.31
2	B	500	COA	O5A-P2A-O4A	2.44	124.29	112.24
2	F	500	COA	N3A-C2A-N1A	-2.38	124.95	128.68
2	C	500	COA	C1B-N9A-C4A	-2.38	122.46	126.64
2	C	500	COA	P2A-O3A-P1A	-2.35	124.75	132.83
2	C	500	COA	C4A-C5A-N7A	2.30	111.79	109.40
2	C	500	COA	O5A-P2A-O4A	2.27	123.46	112.24
2	D	500	COA	O5A-P2A-O4A	2.24	123.32	112.24
2	B	500	COA	C4A-C5A-N7A	-2.22	107.09	109.40
2	F	500	COA	C7P-C6P-C5P	-2.20	108.70	112.36
2	F	500	COA	N6A-C6A-N1A	2.15	123.04	118.57
2	D	500	COA	O5A-P2A-O6A	-2.13	97.85	107.75
2	B	500	COA	O5P-C5P-N4P	-2.11	119.03	123.01
2	B	500	COA	O5B-C5B-C4B	2.09	116.20	108.99
2	B	500	COA	O6A-CCP-CBP	2.09	113.90	110.55
2	A	500	COA	O9A-P3B-O8A	2.07	115.54	107.64
2	E	500	COA	C2A-N1A-C6A	2.06	122.28	118.75
2	F	500	COA	O4B-C1B-C2B	-2.05	103.93	106.93
2	A	500	COA	C1B-N9A-C4A	-2.03	123.07	126.64
2	D	500	COA	N3A-C2A-N1A	-2.00	125.55	128.68

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	COA	C5B-O5B-P1A-O1A
2	A	500	COA	CDP-CBP-CCP-O6A
2	A	500	COA	CAP-CBP-CCP-O6A
2	A	500	COA	CAP-C9P-N8P-C7P
2	A	500	COA	C6P-C5P-N4P-C3P

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Mol	Chain	Res	Type	Atoms
2	A	500	COA	O5P-C5P-N4P-C3P
2	B	500	COA	C5B-O5B-P1A-O1A
2	B	500	COA	N8P-C9P-CAP-OAP
2	B	500	COA	C6P-C5P-N4P-C3P
2	B	500	COA	O5P-C5P-N4P-C3P
2	C	500	COA	C5B-O5B-P1A-O1A
2	C	500	COA	C5B-O5B-P1A-O2A
2	C	500	COA	C6P-C5P-N4P-C3P
2	C	500	COA	O5P-C5P-N4P-C3P
2	C	500	COA	S1P-C2P-C3P-N4P
2	D	500	COA	C5B-O5B-P1A-O1A
2	D	500	COA	CDP-CBP-CCP-O6A
2	D	500	COA	CAP-CBP-CCP-O6A
2	D	500	COA	C5P-C6P-C7P-N8P
2	D	500	COA	S1P-C2P-C3P-N4P
2	E	500	COA	C5B-O5B-P1A-O1A
2	E	500	COA	CAP-C9P-N8P-C7P
2	E	500	COA	C5P-C6P-C7P-N8P
2	E	500	COA	C6P-C5P-N4P-C3P
2	E	500	COA	O5P-C5P-N4P-C3P
2	F	500	COA	C3B-O3B-P3B-O8A
2	F	500	COA	C5B-O5B-P1A-O1A
2	F	500	COA	C6P-C5P-N4P-C3P
2	F	500	COA	O5P-C5P-N4P-C3P
2	F	500	COA	S1P-C2P-C3P-N4P
2	D	500	COA	O5P-C5P-N4P-C3P
2	D	500	COA	C6P-C5P-N4P-C3P
2	A	500	COA	O9P-C9P-N8P-C7P
2	E	500	COA	O9P-C9P-N8P-C7P
2	B	500	COA	CDP-CBP-CCP-O6A
2	E	500	COA	CDP-CBP-CCP-O6A
2	F	500	COA	CDP-CBP-CCP-O6A
2	A	500	COA	C5P-C6P-C7P-N8P
2	F	500	COA	C5P-C6P-C7P-N8P
2	B	500	COA	O9P-C9P-CAP-OAP
2	F	500	COA	C3B-O3B-P3B-O7A
2	F	500	COA	C5B-O5B-P1A-O3A
2	A	500	COA	C5B-O5B-P1A-O2A
2	B	500	COA	C5B-O5B-P1A-O2A
2	D	500	COA	C5B-O5B-P1A-O2A
2	E	500	COA	C5B-O5B-P1A-O2A
2	F	500	COA	C5B-O5B-P1A-O2A

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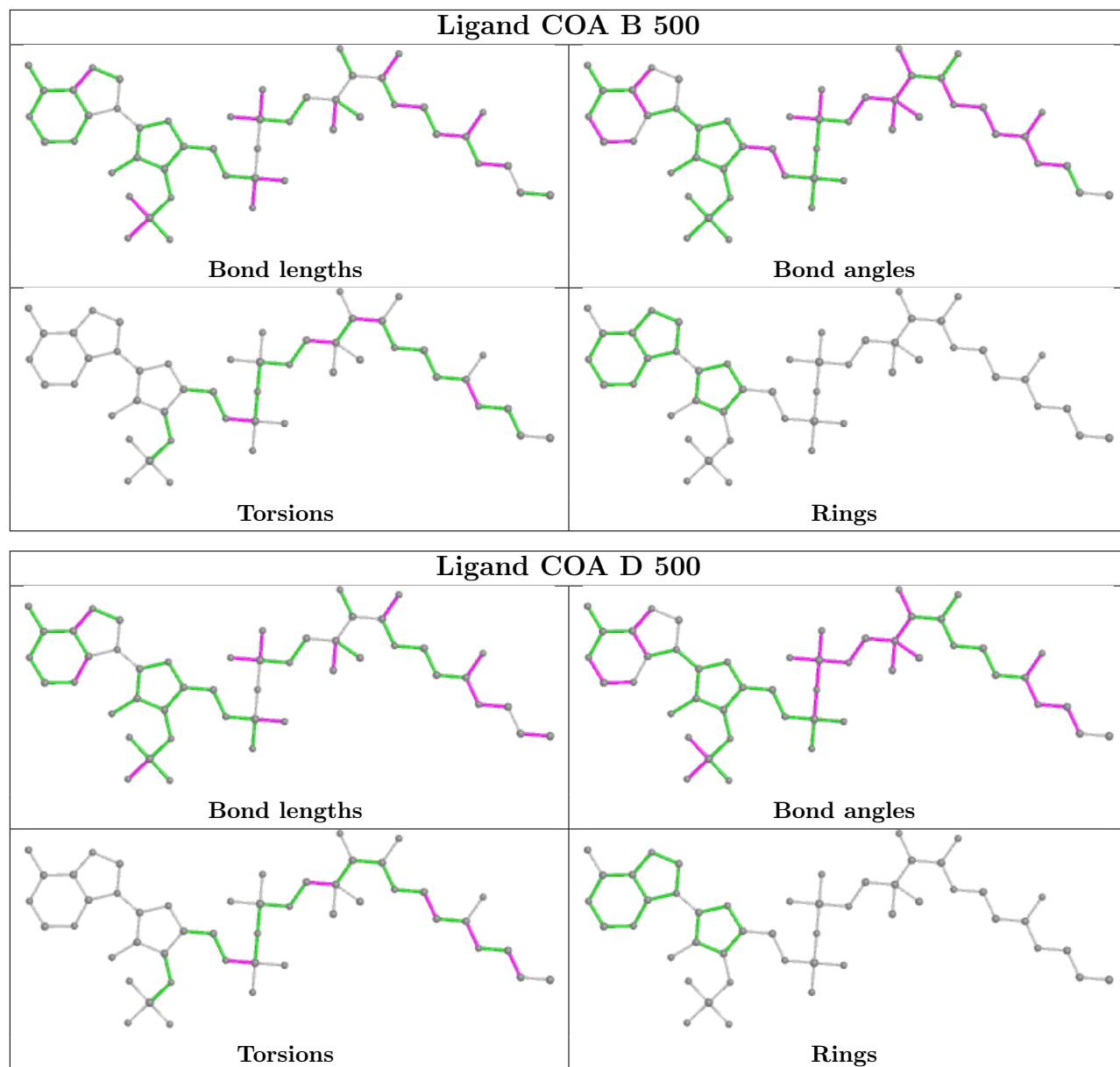
Mol	Chain	Res	Type	Atoms
2	C	500	COA	CDP-CBP-CCP-O6A
2	C	500	COA	CEP-CBP-CCP-O6A
2	F	500	COA	CAP-C9P-N8P-C7P
2	F	500	COA	O9P-C9P-N8P-C7P
2	C	500	COA	O9P-C9P-N8P-C7P
2	A	500	COA	C2P-C3P-N4P-C5P
2	F	500	COA	C2P-C3P-N4P-C5P
2	A	500	COA	C5B-O5B-P1A-O3A
2	B	500	COA	C5B-O5B-P1A-O3A
2	C	500	COA	C5B-O5B-P1A-O3A
2	D	500	COA	C5B-O5B-P1A-O3A
2	E	500	COA	C5B-O5B-P1A-O3A

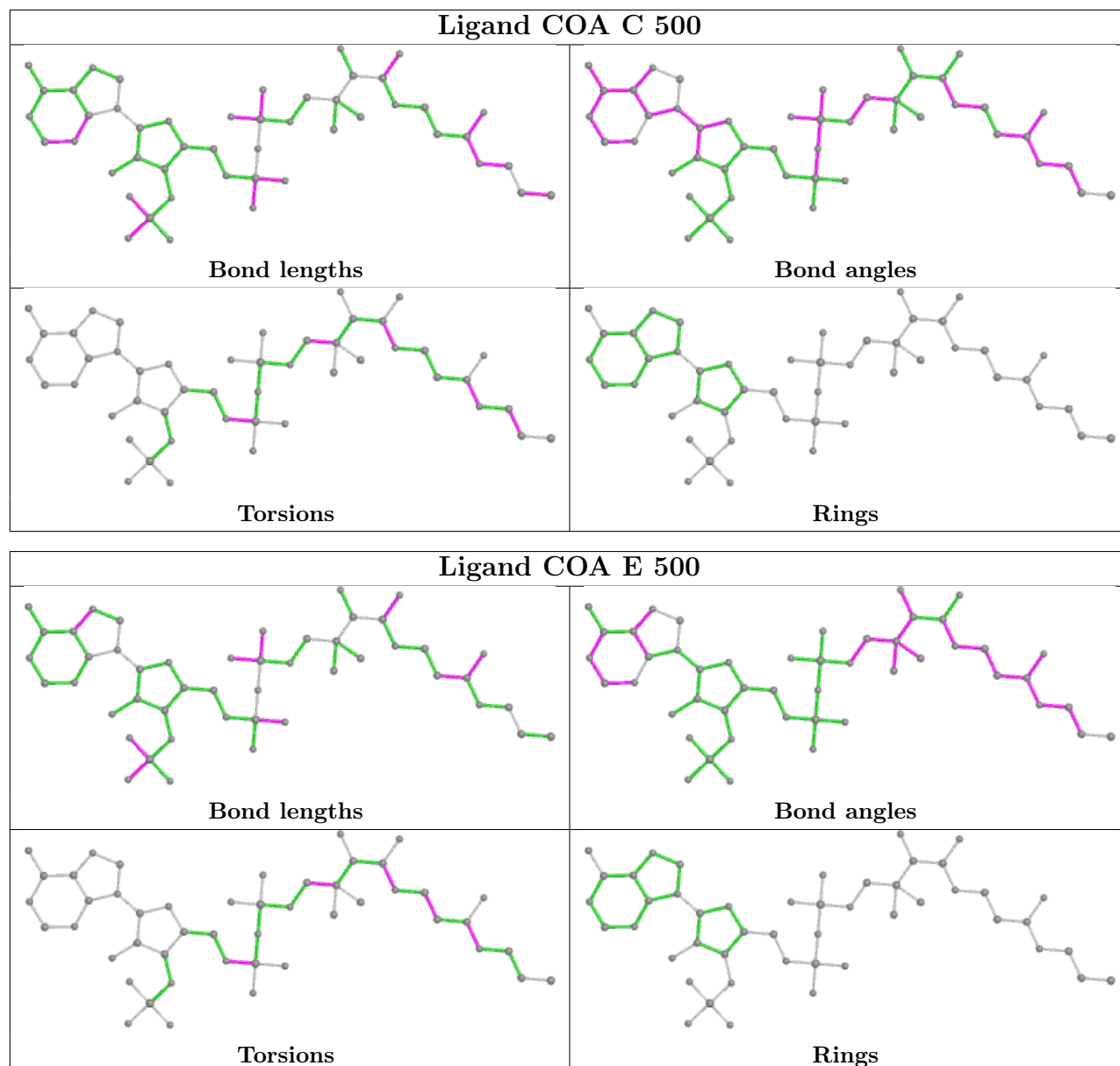
There are no ring outliers.

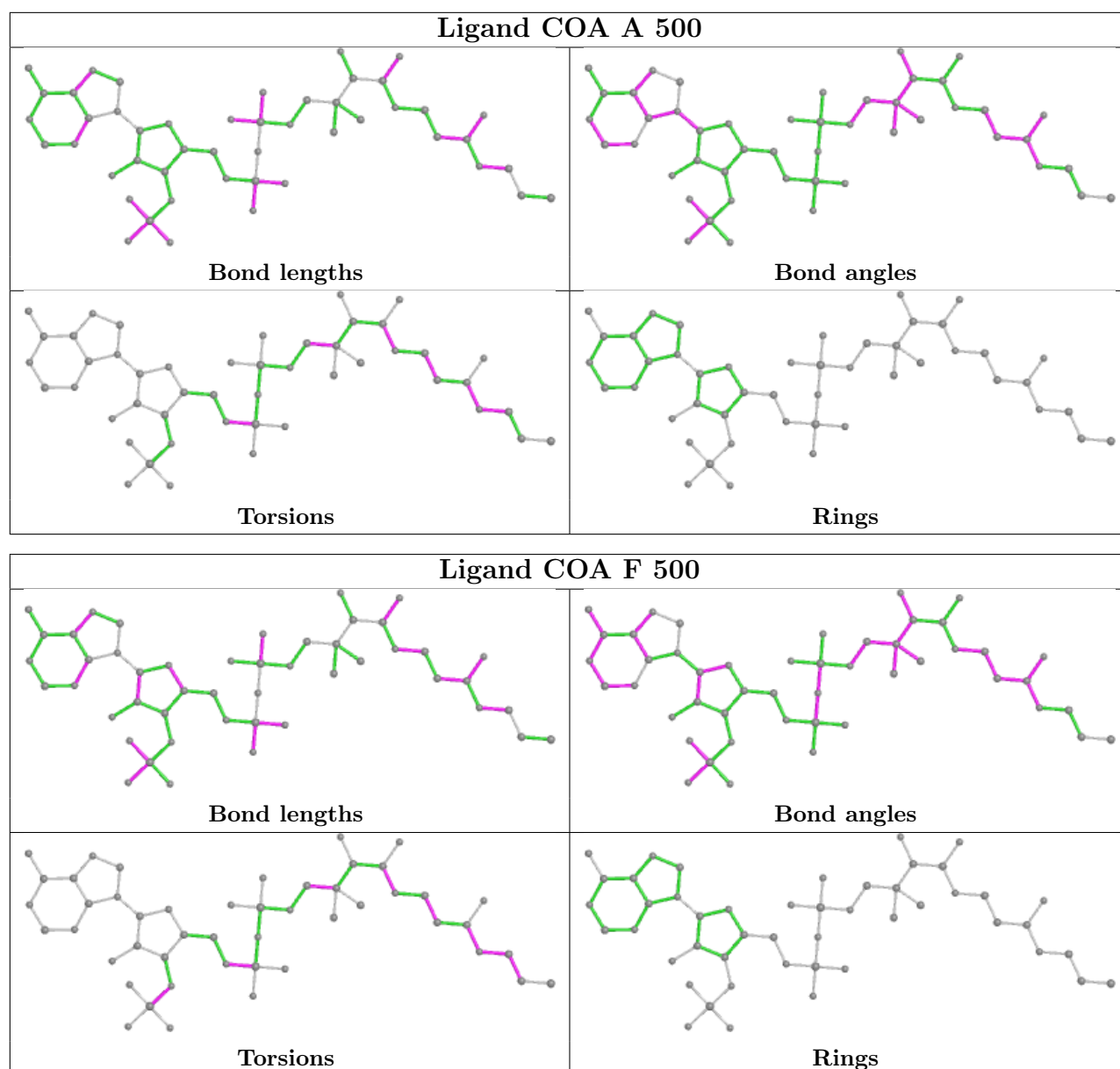
5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	COA	4	0
2	C	500	COA	4	0
2	E	500	COA	1	0
2	A	500	COA	4	0
2	F	500	COA	6	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, 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	402/422 (95%)	-0.13	15 (3%) 41 41	17, 25, 46, 83	0
1	B	402/422 (95%)	-0.03	17 (4%) 36 35	17, 25, 50, 82	0
1	C	402/422 (95%)	-0.02	19 (4%) 31 31	19, 28, 55, 81	0
1	D	402/422 (95%)	-0.16	17 (4%) 36 35	15, 27, 49, 73	0
1	E	402/422 (95%)	0.06	24 (5%) 21 21	22, 34, 58, 77	0
1	F	402/422 (95%)	0.05	23 (5%) 23 23	22, 32, 57, 80	0
All	All	2412/2532 (95%)	-0.04	115 (4%) 30 30	15, 29, 54, 83	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	10.3
1	F	206	GLY	8.8
1	E	206	GLY	8.2
1	F	205	ARG	7.1
1	B	227	GLY	6.8
1	F	228	PRO	6.7
1	F	1	MET	6.3
1	B	228	PRO	6.2
1	D	228	PRO	6.2
1	E	228	PRO	6.2
1	A	203	SER	6.2
1	C	227	GLY	6.1
1	C	228	PRO	6.0
1	B	1	MET	5.7
1	E	203	SER	5.7
1	E	227	GLY	5.7
1	B	205	ARG	5.6
1	C	1	MET	5.5
1	A	227	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	227	GLY	5.1
1	C	207	GLY	4.8
1	B	206	GLY	4.7
1	C	206	GLY	4.7
1	B	230	GLY	4.5
1	F	56	ASP	4.5
1	C	229	ASP	4.5
1	E	1	MET	4.4
1	B	207	GLY	4.3
1	B	231	ARG	4.3
1	F	227	GLY	4.3
1	A	205	ARG	4.3
1	A	206	GLY	4.2
1	F	381	GLU	4.2
1	C	205	ARG	4.0
1	D	205	ARG	4.0
1	B	229	ASP	3.9
1	B	203	SER	3.9
1	F	231	ARG	3.9
1	D	1	MET	3.9
1	E	205	ARG	3.8
1	F	229	ASP	3.8
1	B	226	ARG	3.8
1	A	229	ASP	3.8
1	E	229	ASP	3.7
1	A	1	MET	3.6
1	F	54	THR	3.6
1	A	231	ARG	3.6
1	F	344	ASP	3.6
1	C	231	ARG	3.3
1	D	378	LYS	3.2
1	E	3	THR	3.2
1	C	381	GLU	3.2
1	E	56	ASP	3.2
1	C	394	MET	3.2
1	F	346	PRO	3.2
1	A	56	ASP	3.1
1	E	202	GLU	3.1
1	B	394	MET	3.1
1	C	226	ARG	3.0
1	E	230	GLY	3.0
1	D	206	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	55	ASP	2.9
1	F	207	GLY	2.9
1	E	346	PRO	2.8
1	D	380	SER	2.8
1	F	203	SER	2.7
1	B	202	GLU	2.7
1	E	200	ARG	2.7
1	A	230	GLY	2.6
1	D	202	GLU	2.6
1	D	54	THR	2.6
1	C	56	ASP	2.6
1	D	230	GLY	2.5
1	C	55	ASP	2.5
1	E	207	GLY	2.5
1	C	294	ILE	2.5
1	D	381	GLU	2.5
1	E	53	GLU	2.5
1	F	382	LEU	2.5
1	E	44	GLU	2.4
1	D	229	ASP	2.4
1	A	201	PRO	2.4
1	A	200	ARG	2.3
1	E	226	ARG	2.3
1	F	348	ASP	2.3
1	F	380	SER	2.3
1	F	342	THR	2.3
1	B	200	ARG	2.3
1	D	339	ARG	2.3
1	F	162	LEU	2.3
1	F	378	LYS	2.3
1	E	55	ASP	2.3
1	E	2	ILE	2.2
1	A	207	GLY	2.2
1	C	230	GLY	2.2
1	E	12	ASP	2.2
1	C	342	THR	2.2
1	D	201	PRO	2.2
1	E	344	ASP	2.2
1	F	339	ARG	2.2
1	E	13	ASP	2.2
1	D	226	ARG	2.2
1	E	94	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	PRO	2.1
1	A	226	ARG	2.1
1	B	168	ARG	2.1
1	C	361	LEU	2.1
1	B	225	ASP	2.1
1	F	225	ASP	2.1
1	E	201	PRO	2.0
1	C	54	THR	2.0
1	D	231	ARG	2.0
1	A	2	ILE	2.0
1	C	253	ALA	2.0
1	D	342	THR	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](#)

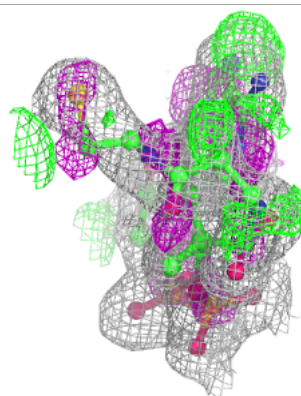
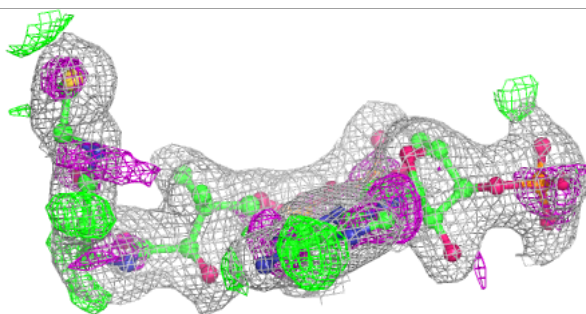
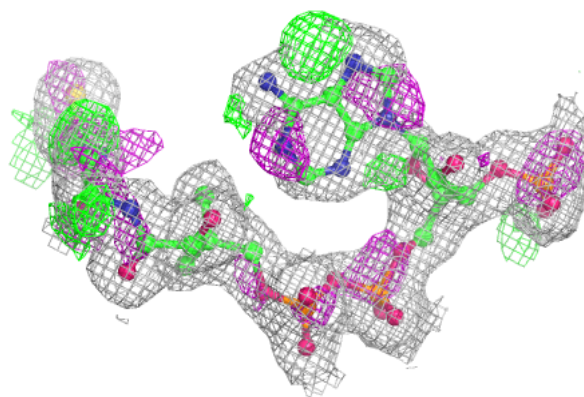
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	C	500	48/48	0.92	0.14	16,24,35,42	0
2	COA	F	500	48/48	0.93	0.16	16,24,35,42	0
2	COA	D	500	48/48	0.94	0.12	16,24,35,42	0
2	COA	E	500	48/48	0.94	0.15	16,24,35,42	0
2	COA	B	500	48/48	0.94	0.10	16,24,35,42	0
2	COA	A	500	48/48	0.95	0.12	16,24,35,42	0

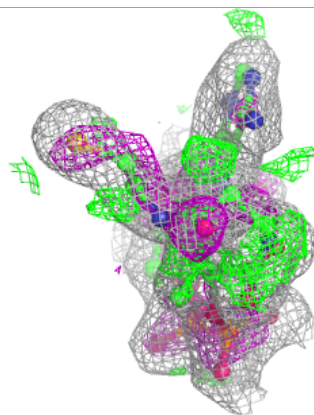
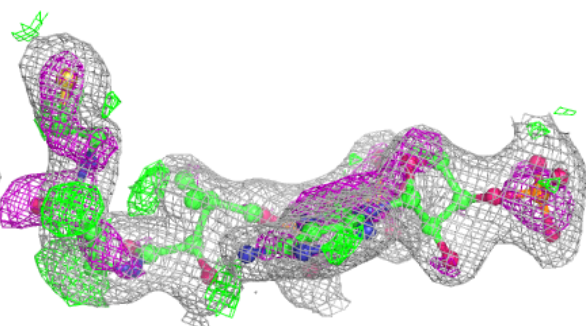
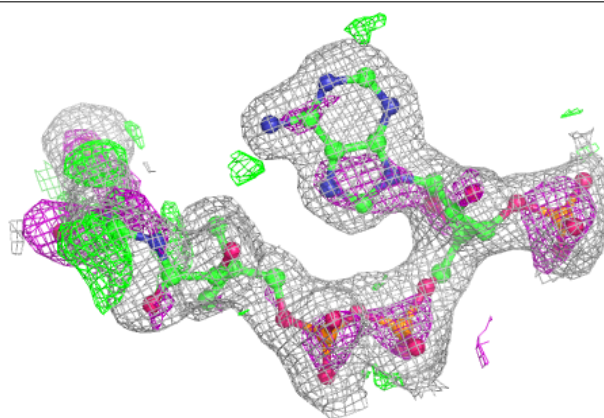
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA C 500:

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

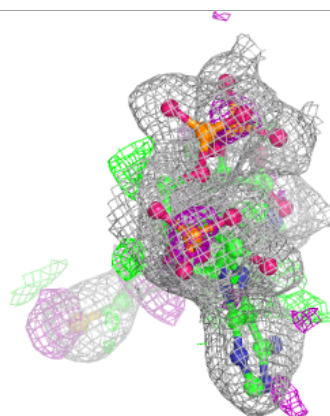
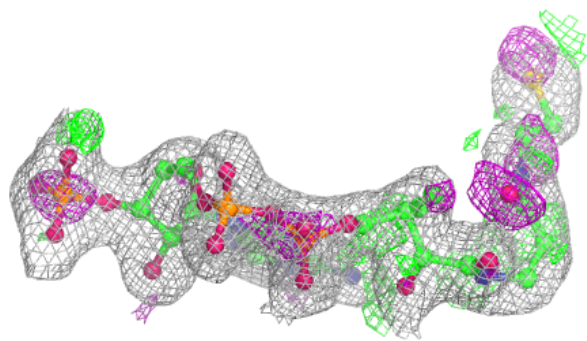
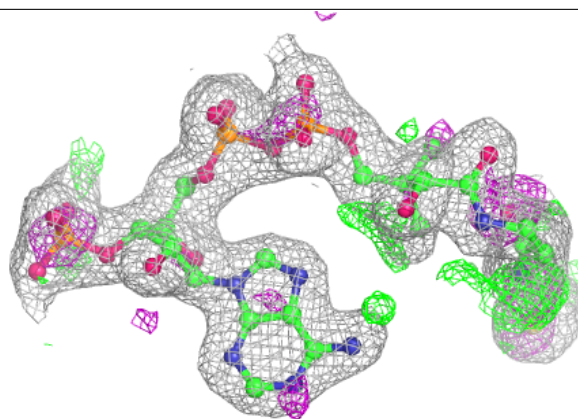
**Electron density around COA F 500:**

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

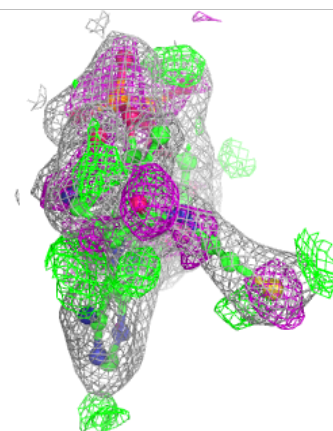
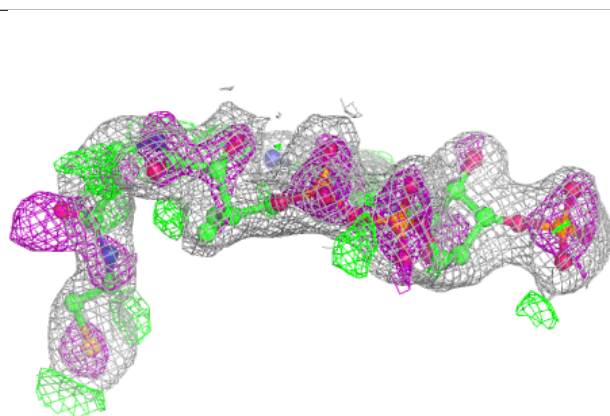
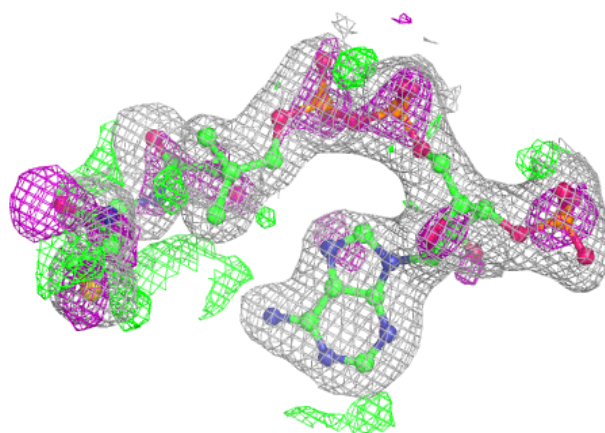


Electron density around COA D 500:

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

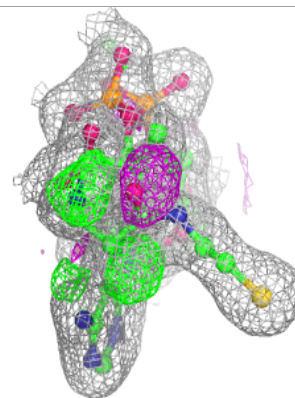
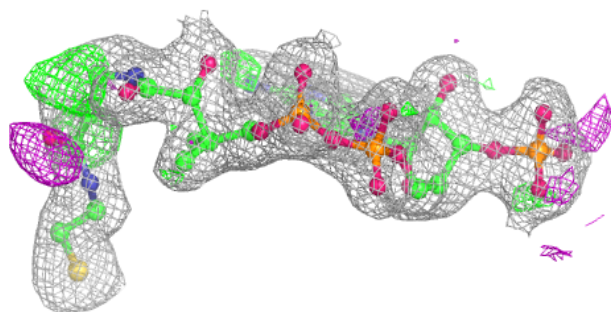
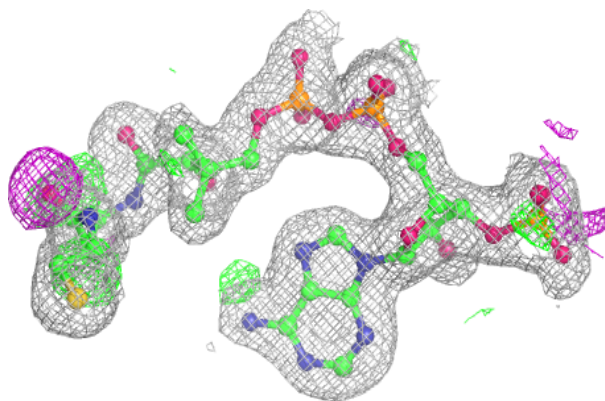
**Electron density around COA E 500:**

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

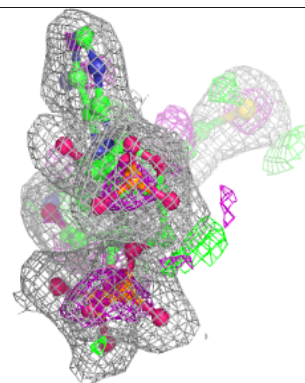
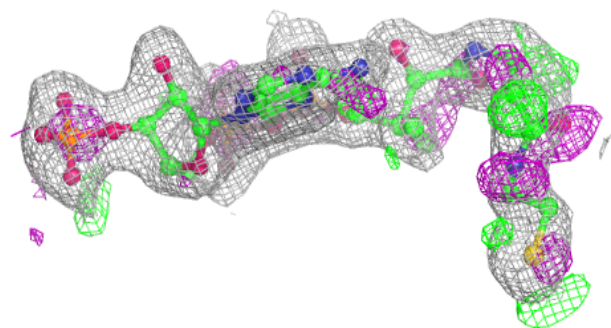
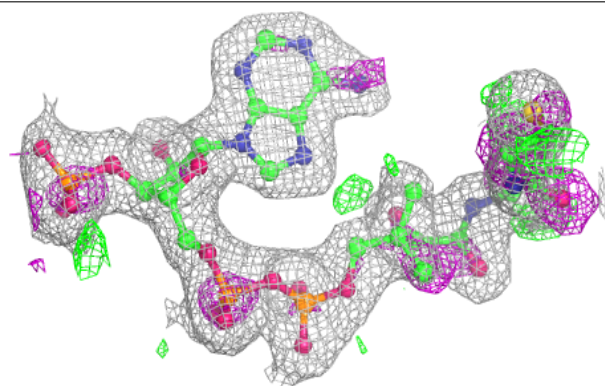


Electron density around COA B 500:

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

**Electron density around COA A 500:**

$2mF_o-DF_c$ (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.