Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 03:12 am BST

PDB ID	:	4A2U
Title	:	CRP(CAP) from Myco. Tuberculosis, with cAMP
Authors	:	Gallagher, D.T.; Reddy, P.T.
Deposited on	:	2011-09-28
Resolution	:	2.63 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:

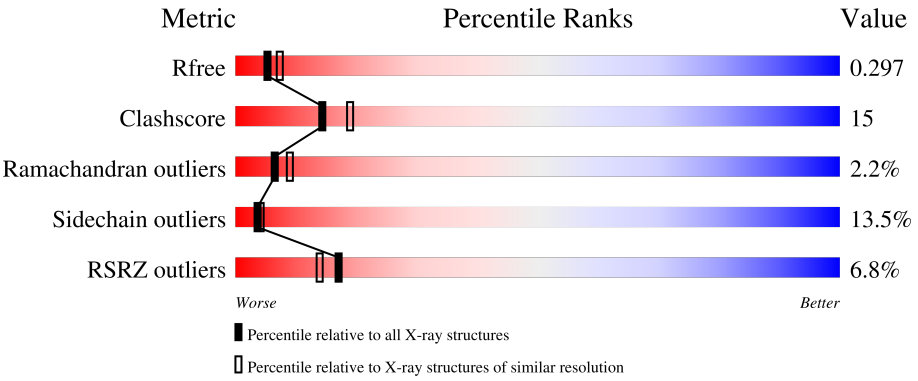
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	227	3% 59% 35% 5%
1	B	227	5% 66% 29%
1	C	227	4% 63% 30% 6%
1	D	227	15% 52% 33% 7% 8%
1	E	227	17% 59% 34% 5%

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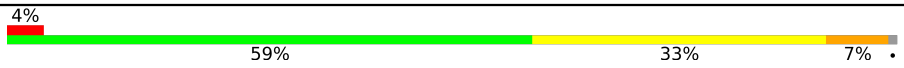
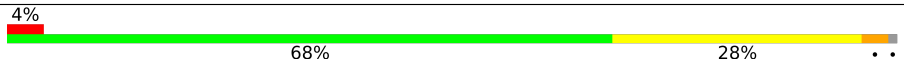
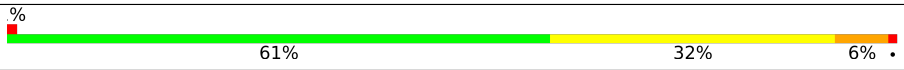
Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14105 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 PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1745	1085	331	325	4			
1	B	224	Total	C	N	O	S	0	0	0
			1745	1085	331	325	4			
1	C	224	Total	C	N	O	S	0	0	0
			1745	1085	331	325	4			
1	D	208	Total	C	N	O	S	0	0	0
			1624	1008	311	302	3			
1	E	224	Total	C	N	O	S	0	0	0
			1745	1085	331	325	4			
1	F	225	Total	C	N	O	S	0	0	0
			1750	1088	332	326	4			
1	G	224	Total	C	N	O	S	0	0	0
			1745	1085	331	325	4			
1	H	227	Total	C	N	O	S	0	0	0
			1765	1096	336	329	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O69644
A	-1	SER	-	expression tag	UNP O69644
A	0	HIS	-	expression tag	UNP O69644
B	-2	GLY	-	expression tag	UNP O69644
B	-1	SER	-	expression tag	UNP O69644
B	0	HIS	-	expression tag	UNP O69644
C	-2	GLY	-	expression tag	UNP O69644
C	-1	SER	-	expression tag	UNP O69644
C	0	HIS	-	expression tag	UNP O69644
D	-2	GLY	-	expression tag	UNP O69644
D	-1	SER	-	expression tag	UNP O69644
D	0	HIS	-	expression tag	UNP O69644

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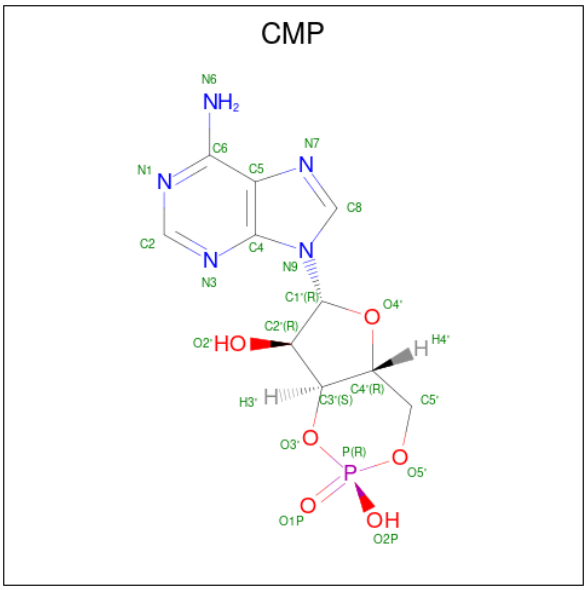
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP O69644
E	-1	SER	-	expression tag	UNP O69644
E	0	HIS	-	expression tag	UNP O69644
F	-2	GLY	-	expression tag	UNP O69644
F	-1	SER	-	expression tag	UNP O69644
F	0	HIS	-	expression tag	UNP O69644
G	-2	GLY	-	expression tag	UNP O69644
G	-1	SER	-	expression tag	UNP O69644
G	0	HIS	-	expression tag	UNP O69644
H	-2	GLY	-	expression tag	UNP O69644
H	-1	SER	-	expression tag	UNP O69644
H	0	HIS	-	expression tag	UNP O69644

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	G	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	H	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 3 is water.

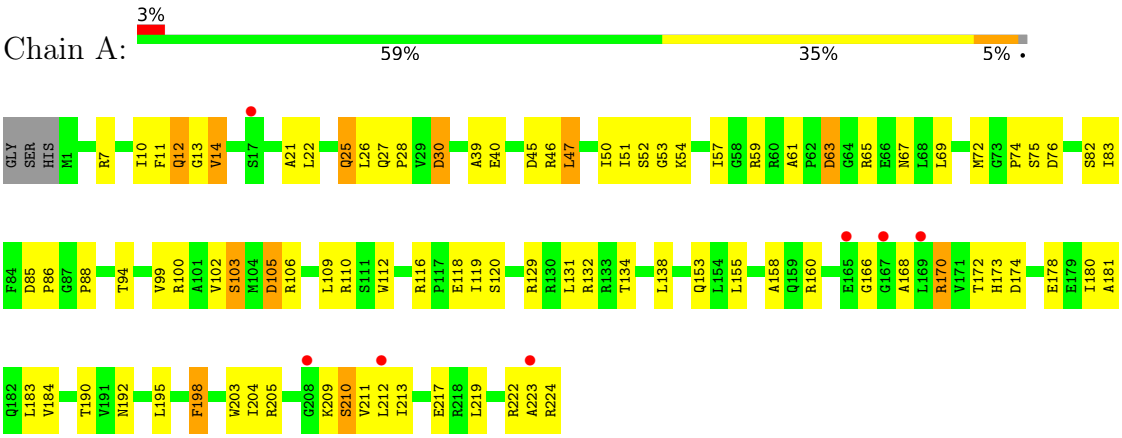
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	10	Total	O	0	0
			10	10		
3	C	7	Total	O	0	0
			7	7		
3	D	1	Total	O	0	0
			1	1		
3	E	6	Total	O	0	0
			6	6		
3	F	11	Total	O	0	0
			11	11		
3	G	9	Total	O	0	0
			9	9		
3	H	16	Total	O	0	0
			16	16		

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.

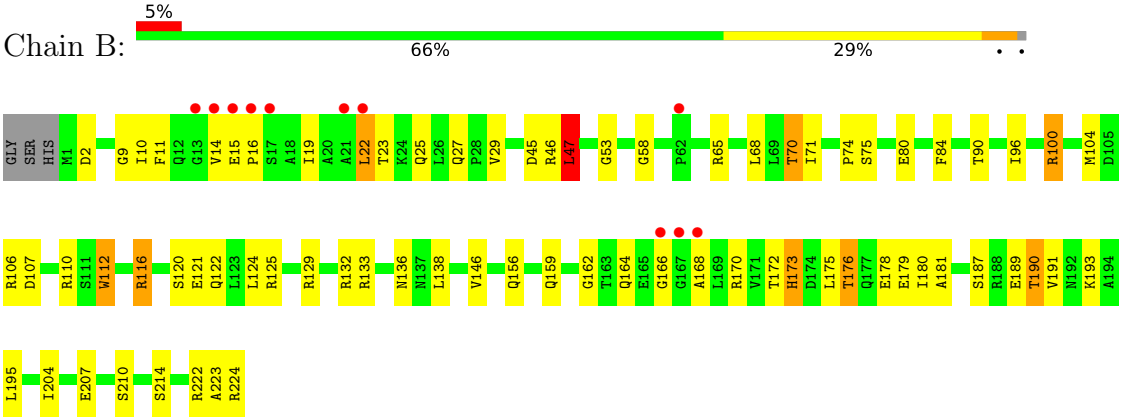
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

Chain A:



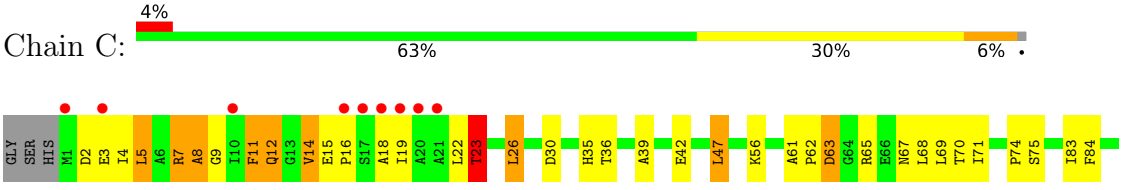
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

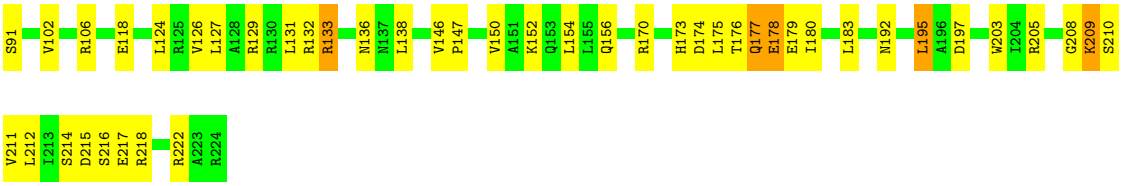
Chain B:



• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

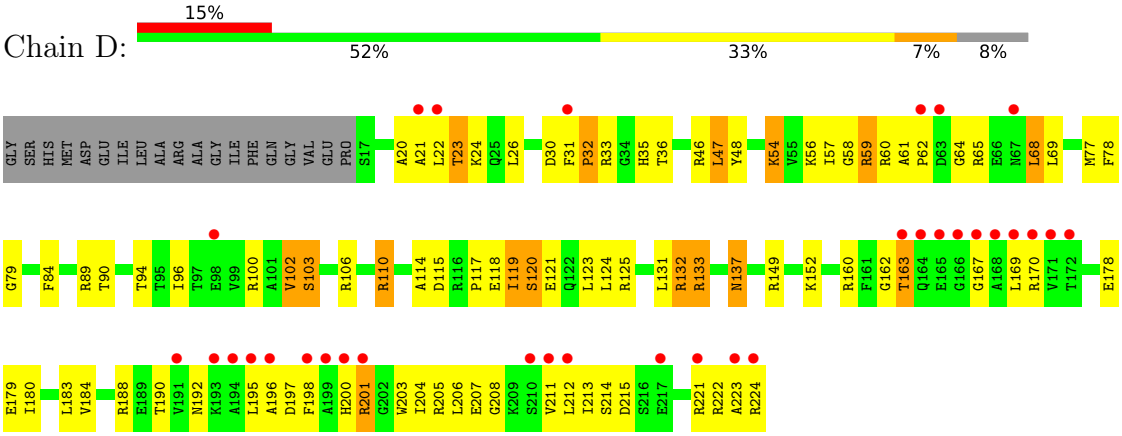
Chain C:





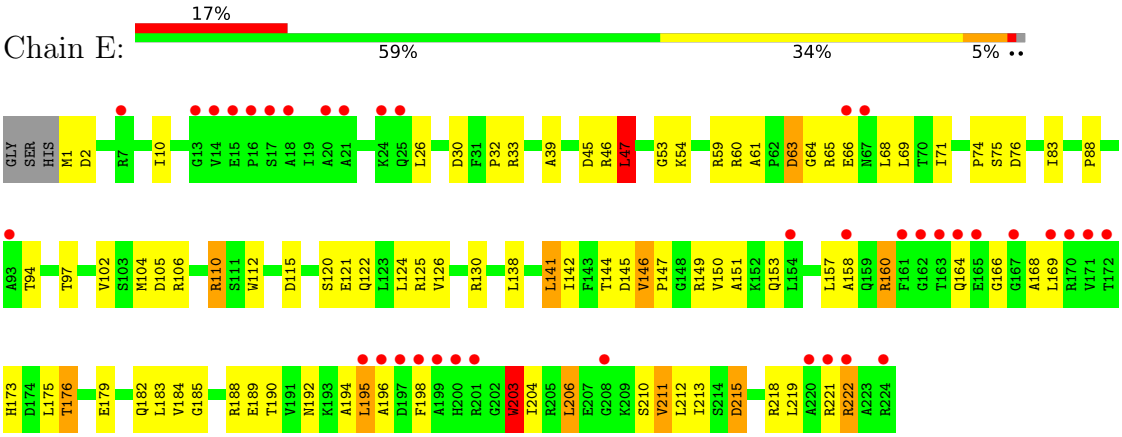
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

Chain D:



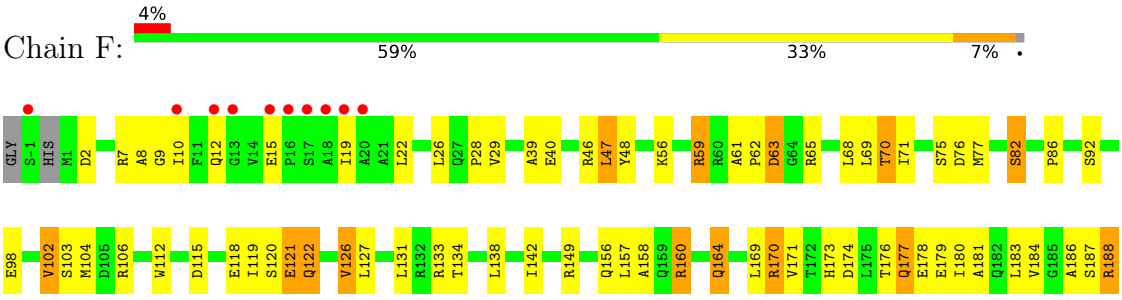
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

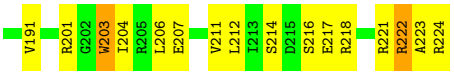
Chain E:



• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

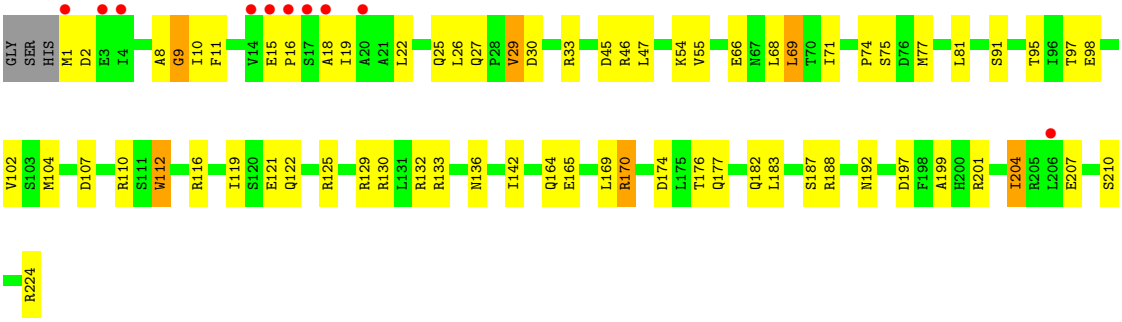
Chain F:





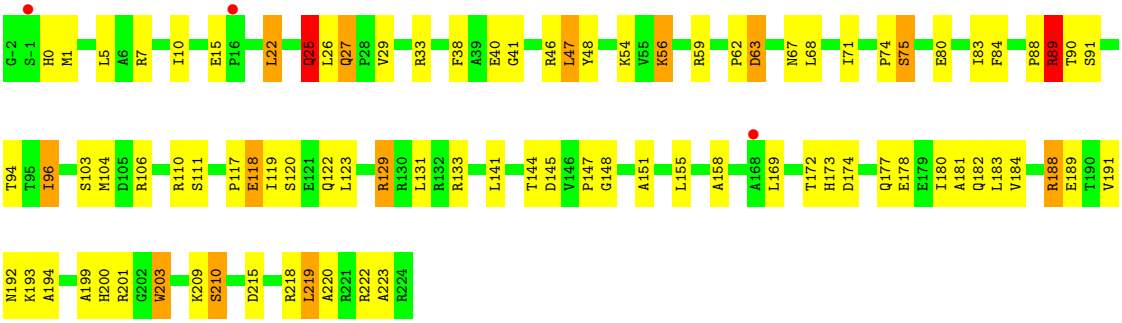
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

Chain G:



• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/ FNR-FAMILY)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.33Å 67.80Å 104.88Å 84.41° 83.46° 80.14°	Depositor
Resolution (Å)	16.00 – 2.63 29.48 – 2.58	Depositor EDS
% Data completeness (in resolution range)	86.1 (16.00-2.63) 82.5 (29.48-2.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.288 0.196 , 0.297	Depositor DCC
R_{free} test set	2389 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CMP

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	0.55	2/1770 (0.1%)	0.74	0/2388
1	B	0.60	1/1770 (0.1%)	0.84	1/2388 (0.0%)
1	C	0.55	1/1770 (0.1%)	0.79	1/2388 (0.0%)
1	D	0.51	0/1647	0.73	0/2222
1	E	0.51	2/1770 (0.1%)	0.74	1/2388 (0.0%)
1	F	0.57	1/1774 (0.1%)	0.78	1/2392 (0.0%)
1	G	0.62	1/1770 (0.1%)	0.87	2/2388 (0.1%)
1	H	0.58	1/1790 (0.1%)	0.85	3/2413 (0.1%)
All	All	0.56	9/14061 (0.1%)	0.80	9/18967 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	TRP	CD2-CE2	5.45	1.47	1.41
1	G	112	TRP	CD2-CE2	5.33	1.47	1.41
1	H	203	TRP	CD2-CE2	5.32	1.47	1.41
1	A	203	TRP	CD2-CE2	5.24	1.47	1.41
1	E	203	TRP	CD2-CE2	5.22	1.47	1.41
1	F	203	TRP	CD2-CE2	5.14	1.47	1.41
1	C	203	TRP	CD2-CE2	5.04	1.47	1.41
1	A	112	TRP	CD2-CE2	5.04	1.47	1.41
1	B	112	TRP	CD2-CE2	5.02	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	47	LEU	CA-CB-CG	6.97	131.34	115.30
1	H	183	LEU	CA-CB-CG	6.49	130.24	115.30
1	E	47	LEU	CA-CB-CG	6.26	129.70	115.30
1	H	47	LEU	CA-CB-CG	6.17	129.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	169	LEU	CA-CB-CG	6.07	129.25	115.30
1	G	45	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	47	LEU	CA-CB-CG	5.89	128.86	115.30
1	C	47	LEU	CA-CB-CG	5.62	128.23	115.30
1	H	89	ARG	NE-CZ-NH1	5.25	122.92	120.30

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	1745	0	1784	53	0
1	B	1745	0	1784	58	0
1	C	1745	0	1784	63	0
1	D	1624	0	1661	63	0
1	E	1745	0	1784	59	0
1	F	1750	0	1788	53	0
1	G	1745	0	1784	52	0
1	H	1765	0	1801	58	0
2	A	22	0	11	2	0
2	B	22	0	11	2	0
2	C	22	0	11	1	0
2	D	22	0	11	1	0
2	E	22	0	11	1	0
2	F	22	0	11	1	0
2	G	22	0	11	4	0
2	H	22	0	11	2	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0
3	C	7	0	0	0	0
3	D	1	0	0	1	0
3	E	6	0	0	0	0
3	F	11	0	0	0	0
3	G	9	0	0	0	0
3	H	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14105	0	14258	438	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 15.

All (438) 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)
2:G:280:CMP:H2	2:G:280:CMP:C2	0.97	1.50
2:C:280:CMP:H2	2:C:280:CMP:C2	0.97	1.49
2:F:280:CMP:C2	2:F:280:CMP:H2	0.97	1.49
2:B:280:CMP:H2	2:B:280:CMP:C2	0.97	1.48
2:A:280:CMP:C2	2:A:280:CMP:H2	0.97	1.48
2:E:280:CMP:H2	2:E:280:CMP:C2	0.97	1.48
2:D:280:CMP:C2	2:D:280:CMP:H2	0.97	1.48
2:H:280:CMP:H2	2:H:280:CMP:C2	0.97	1.47
1:G:97:THR:HG22	1:G:98:GLU:O	1.50	1.10
1:C:177:GLN:HE21	1:C:177:GLN:HA	1.02	1.09
1:D:133:ARG:HB2	1:D:133:ARG:NH1	1.76	1.01
1:F:71:ILE:HD12	1:F:183:LEU:HD21	1.46	0.96
1:C:177:GLN:HA	1:C:177:GLN:NE2	1.82	0.91
1:G:71:ILE:CD1	1:G:183:LEU:HD21	2.01	0.90
1:G:130:ARG:HD3	2:G:280:CMP:C2	2.07	0.90
1:D:31:PHE:HE1	1:D:35:HIS:HD2	1.19	0.89
1:G:10:ILE:HG12	1:G:112:TRP:HZ3	1.37	0.89
1:E:110:ARG:HH11	1:E:110:ARG:HB3	1.38	0.89
1:D:31:PHE:CE1	1:D:35:HIS:HD2	1.90	0.89
1:E:122:GLN:HE22	1:E:125:ARG:HD3	1.38	0.88
1:C:71:ILE:HD13	1:C:175:LEU:HD21	1.59	0.84
1:B:133:ARG:HD2	1:B:156:GLN:OE1	1.77	0.83
1:D:133:ARG:HB2	1:D:133:ARG:HH11	1.39	0.83
1:A:83:ILE:HG21	1:A:109:LEU:HD23	1.61	0.82
1:H:56:LYS:HD2	1:H:96:ILE:HD11	1.62	0.81
1:C:177:GLN:HE21	1:C:177:GLN:CA	1.90	0.81
1:H:172:THR:HG22	1:H:210:SER:HB3	1.63	0.80
1:E:121:GLU:HA	1:E:124:LEU:HD12	1.63	0.80
1:D:46:ARG:HH11	1:D:103:SER:HB3	1.47	0.79
1:B:45:ASP:HB3	1:C:42:GLU:HG2	1.63	0.79
1:G:54:LYS:HE2	1:G:174:ASP:OD2	1.83	0.79
1:E:122:GLN:NE2	1:E:125:ARG:HD3	1.99	0.78
1:C:26:LEU:HD12	1:C:102:VAL:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ARG:HD3	2:G:280:CMP:H2	1.66	0.77
1:D:46:ARG:NH1	1:D:103:SER:HB3	2.01	0.76
1:F:206:LEU:HD23	1:F:211:VAL:HG22	1.67	0.75
1:A:83:ILE:HG23	1:A:106:ARG:HG3	1.69	0.75
1:F:164:GLN:H	1:F:164:GLN:HE21	1.35	0.75
1:A:14:VAL:CG1	1:A:116:ARG:HD3	2.17	0.75
1:B:116:ARG:CG	1:B:116:ARG:HH11	2.00	0.74
1:C:132:ARG:HG3	1:D:90:THR:CG2	2.16	0.74
1:C:132:ARG:HG3	1:D:90:THR:HG22	1.70	0.74
1:B:14:VAL:HG23	1:B:19:ILE:HG12	1.70	0.74
1:G:74:PRO:O	1:G:75:SER:HB2	1.88	0.73
1:C:71:ILE:CD1	1:C:175:LEU:HD21	2.18	0.73
1:D:31:PHE:HE1	1:D:35:HIS:CD2	2.07	0.72
1:G:11:PHE:CD1	1:G:19:ILE:HG23	2.24	0.72
1:H:155:LEU:O	1:H:158:ALA:HB3	1.88	0.72
1:G:71:ILE:HD12	1:G:183:LEU:HD21	1.70	0.72
1:H:180:ILE:O	1:H:184:VAL:HG23	1.89	0.72
1:A:59:ARG:NH2	1:B:136:ASN:OD1	2.23	0.71
1:G:10:ILE:HG12	1:G:112:TRP:CZ3	2.25	0.70
1:E:146:VAL:O	1:E:150:VAL:HG23	1.92	0.70
1:E:26:LEU:HD13	1:E:102:VAL:HG21	1.71	0.70
1:C:174:ASP:HA	1:C:209:LYS:HB3	1.73	0.70
1:D:180:ILE:O	1:D:184:VAL:HG23	1.91	0.70
1:C:215:ASP:OD2	1:C:218:ARG:HD2	1.91	0.69
1:B:116:ARG:HH11	1:B:116:ARG:HG2	1.55	0.69
1:D:119:ILE:O	1:D:123:LEU:HG	1.91	0.69
1:E:198:PHE:HB3	1:E:204:ILE:HG12	1.74	0.69
1:B:9:GLY:O	1:B:122:GLN:HB3	1.93	0.69
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.55	0.69
1:H:0:HIS:C	1:H:1:MET:H2	1.97	0.69
1:A:106:ARG:O	1:A:110:ARG:HG2	1.93	0.68
1:C:83:ILE:HG23	1:C:106:ARG:HG2	1.76	0.68
1:B:110:ARG:HD2	1:C:35:HIS:HE1	1.58	0.68
1:G:27:GLN:HE21	1:G:29:VAL:HG22	1.60	0.67
1:H:96:ILE:O	1:H:96:ILE:HG22	1.94	0.67
1:G:22:LEU:HD13	1:G:112:TRP:HE1	1.58	0.67
1:F:133:ARG:HE	1:F:156:GLN:NE2	1.93	0.67
1:F:181:ALA:HA	1:F:191:VAL:HG21	1.75	0.67
1:F:40:GLU:H	1:F:92:SER:HB3	1.59	0.67
1:D:110:ARG:HB3	1:D:110:ARG:HH11	1.59	0.66
3:A:2005:HOH:O	1:B:65:ARG:NH2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:PRO:O	1:H:75:SER:HB2	1.95	0.66
1:G:125:ARG:NH2	1:G:129:ARG:HE	1.94	0.66
1:C:133:ARG:HH12	1:C:156:GLN:HG2	1.61	0.66
1:H:147:PRO:HB2	1:H:222:ARG:NH1	2.12	0.65
1:A:88:PRO:O	1:B:132:ARG:NH2	2.29	0.65
1:C:192:ASN:HA	1:C:195:LEU:HD12	1.77	0.65
1:F:204:ILE:HA	1:F:212:LEU:O	1.96	0.65
1:B:11:PHE:CE1	1:B:112:TRP:CH2	2.85	0.65
1:C:36:THR:O	1:C:36:THR:HG22	1.94	0.65
1:B:11:PHE:CE1	1:B:112:TRP:HH2	2.14	0.65
1:C:14:VAL:HG23	1:C:15:GLU:H	1.61	0.65
1:C:56:LYS:HB2	1:C:68:LEU:HD22	1.78	0.65
1:E:168:ALA:HB3	1:E:213:ILE:O	1.96	0.65
1:A:30:ASP:OD2	1:A:100:ARG:HD3	1.97	0.64
1:A:174:ASP:HA	1:A:209:LYS:HB3	1.79	0.64
1:H:148:GLY:O	1:H:151:ALA:HB3	1.98	0.64
1:A:172:THR:HG23	1:A:210:SER:HB2	1.80	0.64
1:B:125:ARG:O	1:B:129:ARG:HG3	1.98	0.64
1:B:74:PRO:O	1:B:75:SER:HB2	1.98	0.64
1:C:39:ALA:HB3	1:C:42:GLU:OE2	1.98	0.63
1:B:191:VAL:O	1:B:195:LEU:HD12	1.99	0.63
1:E:204:ILE:HG22	1:E:213:ILE:HA	1.81	0.63
1:E:150:VAL:HG11	1:E:194:ALA:HB1	1.79	0.63
1:B:146:VAL:HG11	1:B:190:THR:CG2	2.29	0.62
1:D:47:LEU:HD11	1:D:77:MET:SD	2.39	0.62
1:B:11:PHE:HE1	1:B:112:TRP:HH2	1.47	0.62
1:C:176:THR:HG22	1:C:178:GLU:H	1.65	0.62
1:G:47:LEU:HD21	1:G:77:MET:HE2	1.81	0.62
1:E:176:THR:H	1:E:179:GLU:HB2	1.64	0.62
1:C:176:THR:HB	1:C:179:GLU:HG3	1.82	0.62
1:G:16:PRO:HA	1:G:19:ILE:HD12	1.81	0.62
1:A:74:PRO:O	1:A:75:SER:HB2	1.99	0.62
1:F:170:ARG:HH21	1:F:212:LEU:HB2	1.65	0.62
1:G:81:LEU:HD21	1:H:131:LEU:HD23	1.81	0.61
1:C:61:ALA:HB1	1:C:62:PRO:HD2	1.80	0.61
1:F:112:TRP:HB3	1:F:119:ILE:CD1	2.31	0.61
1:D:114:ALA:O	1:F:221:ARG:NH1	2.33	0.61
1:C:2:ASP:OD1	1:C:23:THR:HG21	2.01	0.61
1:F:76:ASP:CG	1:F:160:ARG:HH21	2.04	0.61
1:A:153:GLN:HE21	1:A:183:LEU:HD13	1.65	0.61
1:B:146:VAL:HG11	1:B:190:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:HB2	1:D:133:ARG:CZ	2.32	0.60
1:A:7:ARG:HA	1:A:12:GLN:HE22	1.67	0.60
1:D:137:ASN:N	1:D:137:ASN:HD22	1.98	0.60
1:D:203:TRP:HD1	1:D:215:ASP:HB3	1.66	0.60
1:G:22:LEU:HA	1:G:25:GLN:HE21	1.67	0.60
1:H:83:ILE:HG22	1:H:83:ILE:O	2.01	0.60
1:E:120:SER:HB3	1:F:120:SER:HB3	1.84	0.60
1:B:162:GLY:HA2	1:B:170:ARG:O	2.02	0.59
1:D:149:ARG:HB3	1:D:184:VAL:HG13	1.84	0.59
1:F:176:THR:HG22	1:F:178:GLU:H	1.67	0.59
1:G:165:GLU:OE2	1:G:170:ARG:NH1	2.36	0.59
1:G:197:ASP:OD1	1:G:201:ARG:HD2	2.02	0.59
1:A:46:ARG:NH1	1:A:103:SER:OG	2.34	0.59
1:D:133:ARG:HH11	1:D:133:ARG:CB	2.12	0.59
1:E:45:ASP:HB2	1:E:106:ARG:HB2	1.84	0.59
1:C:16:PRO:HG3	1:E:88:PRO:HG3	1.85	0.58
1:B:173:HIS:O	1:B:175:LEU:HG	2.04	0.58
1:D:152:LYS:HG3	1:D:223:ALA:HB1	1.86	0.58
1:F:26:LEU:HD22	1:F:104:MET:HB3	1.86	0.58
1:H:201:ARG:HD3	1:H:203:TRP:CE2	2.39	0.58
1:G:11:PHE:HD1	1:G:19:ILE:HG23	1.66	0.58
1:E:153:GLN:HE21	1:E:183:LEU:HD13	1.69	0.57
1:E:169:LEU:O	1:E:212:LEU:HA	2.03	0.57
1:H:0:HIS:C	1:H:1:MET:N	2.57	0.57
1:B:121:GLU:HG2	1:B:124:LEU:HD12	1.84	0.57
1:D:203:TRP:CD1	1:D:215:ASP:HB3	2.39	0.57
1:F:188:ARG:NH2	1:H:7:ARG:HD2	2.19	0.57
1:A:173:HIS:CE1	1:A:209:LYS:O	2.57	0.57
1:B:189:GLU:HG3	1:B:190:THR:N	2.19	0.57
1:D:31:PHE:CE1	1:D:35:HIS:CD2	2.82	0.57
1:F:164:GLN:HE21	1:F:164:GLN:N	2.01	0.57
1:C:192:ASN:HA	1:C:195:LEU:CD1	2.35	0.57
1:F:149:ARG:HB2	1:F:184:VAL:HG13	1.88	0.56
1:D:56:LYS:HB2	1:D:68:LEU:HD13	1.86	0.56
1:G:107:ASP:OD2	1:G:110:ARG:NH1	2.38	0.56
1:B:176:THR:CG2	1:B:178:GLU:H	2.17	0.56
1:B:47:LEU:C	1:B:47:LEU:HD23	2.25	0.56
1:C:7:ARG:O	1:C:9:GLY:N	2.38	0.56
1:A:7:ARG:HA	1:A:12:GLN:NE2	2.21	0.56
1:B:46:ARG:HG2	1:B:46:ARG:NH1	2.18	0.55
1:B:181:ALA:HA	1:B:191:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:LEU:HG	1:H:182:GLN:HB2	1.88	0.55
1:C:16:PRO:HB3	1:E:88:PRO:HB3	1.89	0.55
1:H:158:ALA:HB1	1:H:169:LEU:HD11	1.88	0.55
1:H:215:ASP:O	1:H:219:LEU:HB2	2.07	0.54
1:F:28:PRO:HA	1:F:102:VAL:HG23	1.89	0.54
1:H:38:PHE:CD1	1:H:89:ARG:HD3	2.42	0.54
1:H:33:ARG:HH22	1:H:209:LYS:HE3	1.72	0.54
1:F:61:ALA:HB3	1:F:65:ARG:HB2	1.90	0.54
1:D:221:ARG:O	1:D:224:ARG:HB2	2.07	0.54
1:C:173:HIS:CD2	1:C:175:LEU:HB2	2.43	0.54
1:E:203:TRP:HD1	1:E:215:ASP:HB3	1.73	0.54
1:E:83:ILE:HG23	1:E:106:ARG:HG3	1.90	0.53
1:E:175:LEU:HB3	1:E:179:GLU:CB	2.38	0.53
1:E:195:LEU:HG	1:E:196:ALA:N	2.24	0.53
1:G:47:LEU:HD11	1:G:77:MET:HE2	1.91	0.53
1:E:65:ARG:HH22	1:E:188:ARG:HD2	1.72	0.53
1:E:74:PRO:O	1:E:75:SER:HB2	2.08	0.53
1:G:26:LEU:HD12	1:G:26:LEU:H	1.73	0.53
1:A:47:LEU:C	1:A:47:LEU:HD23	2.29	0.53
1:C:152:LYS:HG2	1:C:156:GLN:HE21	1.74	0.53
1:E:219:LEU:O	1:E:222:ARG:HB3	2.09	0.53
1:G:69:LEU:HD23	2:G:280:CMP:N7	2.24	0.53
1:B:106:ARG:O	1:B:110:ARG:HG2	2.09	0.53
1:D:54:LYS:HD2	1:D:54:LYS:N	2.24	0.53
1:D:196:ALA:C	1:D:198:PHE:H	2.12	0.53
1:H:155:LEU:HD11	1:H:220:ALA:HB2	1.91	0.53
1:H:83:ILE:O	1:H:83:ILE:CG2	2.56	0.52
1:C:15:GLU:HB2	1:C:18:ALA:HB3	1.92	0.52
1:D:22:LEU:C	1:D:24:LYS:H	2.12	0.52
1:G:142:ILE:HD11	1:H:141:LEU:HD11	1.91	0.52
1:G:122:GLN:OE1	1:G:125:ARG:HD3	2.09	0.52
1:B:70:THR:O	1:B:71:ILE:HD13	2.10	0.52
1:F:12:GLN:O	1:F:122:GLN:HG2	2.10	0.52
1:G:107:ASP:OD1	1:G:110:ARG:HD3	2.10	0.51
1:F:221:ARG:HG2	1:F:224:ARG:NH1	2.24	0.51
1:H:117:PRO:O	1:H:120:SER:HB2	2.10	0.51
1:H:129:ARG:O	1:H:133:ARG:HG3	2.11	0.51
1:C:74:PRO:O	1:C:75:SER:HB3	2.10	0.51
1:A:178:GLU:O	1:A:181:ALA:HB3	2.10	0.50
1:F:40:GLU:OE2	1:F:59:ARG:NH1	2.45	0.50
1:B:133:ARG:NH1	1:B:156:GLN:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:HG23	1:D:170:ARG:HD2	1.93	0.50
1:H:26:LEU:HD22	1:H:104:MET:HB3	1.93	0.50
1:B:207:GLU:O	1:B:210:SER:HB3	2.11	0.50
1:G:136:ASN:OD1	1:H:59:ARG:NH2	2.43	0.50
1:G:197:ASP:O	1:G:201:ARG:HG3	2.11	0.50
1:A:54:LYS:HA	1:A:72:MET:O	2.12	0.50
1:B:122:GLN:OE1	1:B:125:ARG:NE	2.38	0.50
1:B:176:THR:HG22	1:B:179:GLU:H	1.76	0.50
1:C:63:ASP:CG	1:C:65:ARG:HE	2.14	0.50
1:D:59:ARG:HD2	1:D:69:LEU:HD11	1.93	0.50
1:E:59:ARG:HG2	1:E:60:ARG:H	1.76	0.50
1:E:65:ARG:NH2	1:E:188:ARG:HD2	2.27	0.50
1:G:121:GLU:OE2	1:H:110:ARG:NH2	2.44	0.50
1:A:138:LEU:C	1:A:138:LEU:HD23	2.32	0.50
1:D:30:ASP:OD1	1:D:100:ARG:HD2	2.12	0.50
1:G:47:LEU:HD11	1:G:77:MET:CE	2.42	0.50
1:H:119:ILE:O	1:H:123:LEU:HG	2.12	0.50
1:B:10:ILE:HG13	1:B:11:PHE:N	2.26	0.50
1:A:14:VAL:HG13	1:A:116:ARG:HD3	1.92	0.49
1:B:110:ARG:HD2	1:C:35:HIS:CE1	2.45	0.49
1:E:141:LEU:HD11	1:F:142:ILE:HG12	1.94	0.49
1:F:46:ARG:HG2	1:F:48:TYR:CE1	2.47	0.49
1:F:133:ARG:HE	1:F:156:GLN:HE21	1.59	0.49
1:C:69:LEU:O	1:C:70:THR:HB	2.12	0.49
1:C:150:VAL:O	1:C:154:LEU:HG	2.12	0.49
1:F:222:ARG:HD2	1:F:222:ARG:O	2.12	0.49
1:H:41:GLY:HA2	1:H:88:PRO:HB2	1.94	0.49
1:H:96:ILE:O	1:H:96:ILE:CG2	2.61	0.49
1:C:127:LEU:HD12	1:D:124:LEU:HD23	1.93	0.49
1:H:74:PRO:O	1:H:75:SER:CB	2.61	0.49
1:A:22:LEU:O	1:A:26:LEU:HG	2.12	0.49
1:A:217:GLU:C	1:A:219:LEU:H	2.15	0.49
1:E:47:LEU:HB2	1:E:83:ILE:HD12	1.95	0.49
1:G:74:PRO:O	1:G:75:SER:CB	2.61	0.49
1:A:170:ARG:O	1:A:170:ARG:HG3	2.13	0.48
1:C:26:LEU:HD12	1:C:102:VAL:CG2	2.40	0.48
1:E:144:THR:HG22	1:E:149:ARG:HG3	1.94	0.48
1:F:221:ARG:HG2	1:F:224:ARG:HH11	1.76	0.48
1:E:175:LEU:HD22	1:E:179:GLU:HG2	1.96	0.48
1:G:125:ARG:NH2	1:G:129:ARG:NE	2.60	0.48
1:D:46:ARG:HG2	1:D:48:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:HH11	1:D:103:SER:CB	2.23	0.48
1:C:11:PHE:HB2	1:C:14:VAL:HG21	1.95	0.48
1:F:122:GLN:O	1:F:126:VAL:HG12	2.14	0.48
1:F:158:ALA:HB1	1:F:169:LEU:HD13	1.96	0.48
1:H:188:ARG:HD2	1:H:192:ASN:HD21	1.79	0.48
1:A:63:ASP:OD1	1:A:63:ASP:N	2.47	0.48
1:A:219:LEU:HA	1:A:222:ARG:HB3	1.95	0.48
1:B:11:PHE:HE1	1:B:112:TRP:CH2	2.25	0.48
1:C:173:HIS:HD2	1:C:175:LEU:N	2.12	0.48
1:C:208:GLY:C	1:C:210:SER:H	2.16	0.48
1:A:120:SER:HB3	1:B:120:SER:HB3	1.95	0.48
1:E:126:VAL:O	1:E:130:ARG:HG3	2.14	0.48
1:C:173:HIS:CD2	1:C:175:LEU:H	2.32	0.48
1:D:60:ARG:HE	1:D:64:GLY:HA2	1.79	0.48
1:E:183:LEU:C	1:E:185:GLY:H	2.18	0.48
1:C:138:LEU:C	1:C:138:LEU:HD23	2.34	0.47
1:D:179:GLU:O	1:D:183:LEU:HD12	2.14	0.47
1:D:205:ARG:HA	3:D:2001:HOH:O	2.13	0.47
1:C:5:LEU:O	1:C:11:PHE:HE1	1.96	0.47
1:A:204:ILE:HA	1:A:212:LEU:O	2.14	0.47
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.27	0.47
1:D:48:TYR:O	1:D:78:PHE:N	2.42	0.47
1:G:170:ARG:NH2	1:G:207:GLU:OE1	2.47	0.47
1:C:71:ILE:HD12	1:C:183:LEU:HD11	1.97	0.47
1:E:66:GLU:OE1	1:E:182:GLN:NE2	2.47	0.47
1:G:132:ARG:HG2	1:H:90:THR:HG22	1.97	0.47
1:C:19:ILE:O	1:C:23:THR:HB	2.15	0.46
1:F:176:THR:HB	1:F:179:GLU:H	1.80	0.46
1:G:188:ARG:HD2	1:G:192:ASN:HD21	1.79	0.46
1:F:188:ARG:HH22	1:H:7:ARG:HD2	1.80	0.46
1:G:97:THR:O	1:G:98:GLU:C	2.53	0.46
1:H:215:ASP:OD2	1:H:218:ARG:HB3	2.14	0.46
1:D:79:GLY:O	1:D:89:ARG:NH1	2.48	0.46
1:E:61:ALA:C	1:E:63:ASP:N	2.69	0.46
1:B:80:GLU:HB2	1:B:84:PHE:CE2	2.50	0.46
1:E:153:GLN:O	1:E:157:LEU:HB2	2.15	0.46
1:E:206:LEU:HG	1:E:211:VAL:HG23	1.97	0.46
1:H:201:ARG:HB3	1:H:203:TRP:CD1	2.51	0.46
1:A:219:LEU:O	1:A:223:ALA:N	2.46	0.46
1:B:74:PRO:O	1:B:75:SER:CB	2.64	0.46
1:F:157:LEU:HD23	1:F:157:LEU:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:HG22	1:B:178:GLU:N	2.31	0.46
1:D:23:THR:HG22	1:D:26:LEU:HD21	1.98	0.46
1:H:118:GLU:O	1:H:122:GLN:HG2	2.16	0.46
1:H:178:GLU:O	1:H:181:ALA:HB3	2.15	0.46
1:H:181:ALA:HA	1:H:191:VAL:HG21	1.97	0.46
1:H:199:ALA:C	1:H:201:ARG:H	2.18	0.46
1:E:175:LEU:HB3	1:E:179:GLU:HB2	1.97	0.46
1:H:56:LYS:HB3	1:H:96:ILE:HG13	1.98	0.46
1:E:146:VAL:N	1:E:147:PRO:HD2	2.30	0.46
1:H:155:LEU:HD23	1:H:155:LEU:HA	1.72	0.46
1:H:178:GLU:O	1:H:181:ALA:N	2.50	0.46
1:H:62:PRO:HG2	1:H:63:ASP:OD1	2.16	0.45
1:D:57:ILE:O	1:D:69:LEU:N	2.44	0.45
1:F:63:ASP:OD1	1:F:63:ASP:N	2.48	0.45
1:G:207:GLU:O	1:G:210:SER:HB3	2.16	0.45
1:A:166:GLY:C	1:A:168:ALA:H	2.20	0.45
1:C:84:PHE:O	1:D:125:ARG:HG3	2.17	0.45
1:C:180:ILE:O	1:C:183:LEU:HB2	2.17	0.45
1:H:173:HIS:O	1:H:174:ASP:HB2	2.17	0.45
1:A:11:PHE:C	1:A:13:GLY:H	2.21	0.45
1:A:180:ILE:O	1:A:184:VAL:HG23	2.17	0.45
1:C:132:ARG:HG3	1:D:90:THR:HG21	1.94	0.45
1:F:7:ARG:HA	1:F:12:GLN:HE21	1.81	0.45
1:F:173:HIS:O	1:F:174:ASP:HB2	2.16	0.45
1:A:198:PHE:N	1:A:198:PHE:CD1	2.84	0.45
1:B:176:THR:HG23	1:B:178:GLU:H	1.81	0.45
1:H:147:PRO:HB2	1:H:222:ARG:HH12	1.80	0.45
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.66	0.45
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.81	0.44
1:D:48:TYR:O	1:D:77:MET:HA	2.17	0.44
1:A:10:ILE:HG23	1:A:119:ILE:HG23	2.00	0.44
1:A:57:ILE:HD13	1:A:72:MET:HE3	1.99	0.44
1:B:58:GLY:HA2	1:B:68:LEU:HD23	1.99	0.44
1:F:160:ARG:HD2	1:F:160:ARG:O	2.17	0.44
1:H:220:ALA:HA	1:H:223:ALA:HB3	1.99	0.44
1:G:47:LEU:C	1:G:47:LEU:HD23	2.38	0.44
1:H:46:ARG:HG3	1:H:48:TYR:CZ	2.53	0.44
1:D:205:ARG:HH12	1:D:207:GLU:HG3	1.83	0.44
1:H:144:THR:HG22	1:H:145:ASP:O	2.17	0.44
1:A:168:ALA:HB1	1:A:213:ILE:O	2.16	0.44
1:F:39:ALA:HA	1:F:92:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:GLU:OE1	2:H:280:CMP:O2'	2.31	0.44
1:A:51:ILE:HG22	1:A:52:SER:N	2.33	0.44
1:C:56:LYS:HD2	1:C:68:LEU:HD21	1.99	0.44
1:D:204:ILE:HG22	1:D:213:ILE:HG23	1.99	0.44
1:E:153:GLN:NE2	1:E:183:LEU:HD13	2.33	0.44
1:E:192:ASN:HA	1:E:195:LEU:HD23	2.00	0.44
1:F:19:ILE:HA	1:F:22:LEU:HD12	1.99	0.44
1:F:181:ALA:HB1	1:F:186:ALA:O	2.18	0.44
1:H:22:LEU:O	1:H:25:GLN:HB2	2.17	0.44
1:D:26:LEU:HD22	1:D:102:VAL:HG11	1.99	0.44
1:B:138:LEU:HD13	3:B:2009:HOH:O	2.17	0.43
1:B:189:GLU:HG3	1:B:190:THR:H	1.83	0.43
1:C:170:ARG:CZ	1:C:212:LEU:HD13	2.48	0.43
1:H:22:LEU:N	1:H:22:LEU:HD23	2.33	0.43
1:B:173:HIS:CE1	1:B:180:ILE:HD11	2.52	0.43
1:H:40:GLU:HG3	1:H:91:SER:HA	2.00	0.43
1:A:172:THR:HA	1:A:210:SER:HB2	2.00	0.43
1:E:76:ASP:OD1	1:E:160:ARG:NH2	2.51	0.43
1:E:151:ALA:HB1	1:E:219:LEU:HG	2.00	0.43
1:A:50:ILE:HD12	1:A:76:ASP:HB2	2.00	0.43
1:E:218:ARG:HA	1:E:221:ARG:HB2	2.01	0.43
1:G:22:LEU:CA	1:G:25:GLN:HE21	2.30	0.43
1:G:26:LEU:HD23	1:G:104:MET:HB3	2.00	0.43
1:B:116:ARG:CG	1:B:116:ARG:NH1	2.68	0.43
1:A:192:ASN:HA	1:A:195:LEU:HG	2.01	0.43
1:E:150:VAL:HG11	1:E:194:ALA:CB	2.48	0.43
1:F:76:ASP:OD2	1:F:160:ARG:NH2	2.48	0.43
1:C:3:GLU:HG2	1:E:39:ALA:CB	2.49	0.43
1:C:11:PHE:HB2	1:C:14:VAL:CG2	2.49	0.43
1:F:201:ARG:HD3	1:F:203:TRP:CZ2	2.54	0.43
1:A:45:ASP:O	1:A:105:ASP:HB2	2.18	0.43
1:E:61:ALA:C	1:E:63:ASP:H	2.21	0.43
1:C:19:ILE:HD13	1:C:19:ILE:HA	1.89	0.43
1:D:132:ARG:O	1:D:133:ARG:C	2.57	0.43
1:E:59:ARG:CG	1:E:60:ARG:H	2.32	0.43
1:B:176:THR:HB	1:B:179:GLU:OE1	2.19	0.42
1:C:5:LEU:O	1:C:8:ALA:HB2	2.19	0.42
1:D:201:ARG:HB3	1:D:203:TRP:CZ3	2.54	0.42
1:E:45:ASP:O	1:E:105:ASP:HA	2.19	0.42
1:B:80:GLU:OE1	2:B:280:CMP:O2'	2.35	0.42
1:E:138:LEU:C	1:E:138:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ARG:HB2	1:E:184:VAL:HG23	2.00	0.42
1:H:1:MET:CE	3:H:2003:HOH:O	2.66	0.42
1:E:26:LEU:HD13	1:E:102:VAL:CG2	2.46	0.42
1:C:192:ASN:N	1:C:192:ASN:HD22	2.17	0.42
1:A:82:SER:O	1:A:86:PRO:HA	2.19	0.42
1:F:127:LEU:HD23	1:F:127:LEU:HA	1.89	0.42
1:F:180:ILE:O	1:F:183:LEU:HB2	2.20	0.42
1:G:116:ARG:HB2	1:G:119:ILE:HD12	2.00	0.42
1:C:61:ALA:CB	1:C:63:ASP:OD1	2.68	0.42
1:C:71:ILE:HG13	1:C:183:LEU:HD21	2.02	0.42
1:D:61:ALA:HB1	1:D:62:PRO:HD2	2.01	0.42
1:D:162:GLY:HA2	1:D:170:ARG:O	2.19	0.42
1:E:71:ILE:CD1	1:E:183:LEU:HD21	2.49	0.42
1:E:110:ARG:NH2	1:F:121:GLU:OE2	2.50	0.42
1:G:8:ALA:O	1:G:9:GLY:C	2.57	0.42
1:G:199:ALA:HA	1:G:204:ILE:O	2.18	0.42
1:A:69:LEU:HD23	2:A:280:CMP:N7	2.35	0.42
1:D:32:PRO:HB2	1:D:33:ARG:H	1.73	0.42
1:D:117:PRO:O	1:D:120:SER:HB2	2.18	0.42
1:A:39:ALA:O	1:A:40:GLU:C	2.57	0.42
1:G:122:GLN:HA	1:G:122:GLN:NE2	2.35	0.42
1:D:58:GLY:HA2	1:D:68:LEU:HA	2.02	0.41
1:F:69:LEU:O	1:F:70:THR:HB	2.20	0.41
1:G:68:LEU:HD23	1:G:68:LEU:HA	1.86	0.41
1:F:8:ALA:O	1:F:9:GLY:C	2.59	0.41
1:F:82:SER:O	1:F:86:PRO:HA	2.19	0.41
1:F:176:THR:C	1:F:178:GLU:N	2.73	0.41
1:A:61:ALA:N	1:A:65:ARG:O	2.29	0.41
1:C:146:VAL:N	1:C:147:PRO:CD	2.83	0.41
1:D:195:LEU:HA	1:D:198:PHE:HD2	1.85	0.41
1:E:184:VAL:O	1:E:184:VAL:HG22	2.20	0.41
1:F:40:GLU:OE2	1:F:59:ARG:HD2	2.20	0.41
1:G:176:THR:HG22	1:G:177:GLN:N	2.36	0.41
1:C:26:LEU:HB2	1:C:102:VAL:HG22	2.01	0.41
1:F:56:LYS:HE3	1:F:68:LEU:HD21	2.02	0.41
1:A:155:LEU:O	1:A:158:ALA:HB3	2.20	0.41
1:C:124:LEU:HD13	1:D:84:PHE:CE1	2.55	0.41
1:A:210:SER:OG	1:A:211:VAL:N	2.53	0.41
1:B:47:LEU:HD22	1:B:104:MET:HG2	2.02	0.41
1:B:176:THR:HG22	1:B:178:GLU:H	1.83	0.41
1:C:136:ASN:OD1	1:D:59:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LEU:HA	1:D:198:PHE:CD2	2.56	0.41
1:E:141:LEU:HD23	1:E:149:ARG:NH1	2.35	0.41
1:F:112:TRP:HB3	1:F:119:ILE:HD13	2.00	0.41
1:F:191:VAL:O	1:F:191:VAL:HG12	2.21	0.41
1:G:68:LEU:HG	1:G:182:GLN:HB3	2.01	0.41
1:A:21:ALA:O	1:A:25:GLN:NE2	2.53	0.41
1:B:166:GLY:C	1:B:168:ALA:H	2.23	0.41
1:D:106:ARG:O	1:D:110:ARG:HG3	2.20	0.41
1:H:15:GLU:O	1:H:15:GLU:HG2	2.19	0.41
1:B:19:ILE:HA	1:B:22:LEU:HD11	2.03	0.41
1:B:53:GLY:O	1:B:74:PRO:HD3	2.20	0.41
1:D:84:PHE:HZ	1:D:123:LEU:HD13	1.86	0.41
1:D:118:GLU:O	1:D:119:ILE:C	2.59	0.41
1:D:205:ARG:HH21	1:D:212:LEU:HD22	1.86	0.41
1:E:53:GLY:O	1:E:74:PRO:HD3	2.21	0.41
1:G:66:GLU:O	1:G:182:GLN:HG2	2.20	0.41
1:A:53:GLY:HA3	1:A:99:VAL:HG22	2.02	0.41
1:D:118:GLU:O	1:D:121:GLU:N	2.54	0.41
1:G:55:VAL:HA	1:G:95:THR:HA	2.03	0.41
1:H:67:ASN:O	1:H:68:LEU:HD23	2.21	0.41
1:A:85:ASP:OD2	1:B:132:ARG:HD2	2.21	0.40
1:B:14:VAL:O	1:B:15:GLU:C	2.59	0.40
1:B:16:PRO:HA	1:B:19:ILE:HG13	2.02	0.40
1:G:116:ARG:HB2	1:G:119:ILE:CD1	2.51	0.40
1:A:132:ARG:HG3	1:B:90:THR:HG22	2.03	0.40
1:E:168:ALA:CB	1:E:213:ILE:O	2.67	0.40
1:D:23:THR:HA	1:D:26:LEU:HG	2.01	0.40
1:E:158:ALA:C	1:E:160:ARG:H	2.25	0.40
1:F:158:ALA:HA	1:F:171:VAL:HG22	2.03	0.40
1:G:18:ALA:HB1	1:G:116:ARG:HH21	1.85	0.40
1:A:198:PHE:N	1:A:198:PHE:HD1	2.20	0.40
1:C:222:ARG:HA	1:C:222:ARG:HD2	1.86	0.40
1:A:27:GLN:HA	1:A:28:PRO:HD2	1.99	0.40
1:E:153:GLN:NE2	1:E:183:LEU:HD22	2.36	0.40
1:H:27:GLN:NE2	1:H:27:GLN:H	2.19	0.40
1:H:84:PHE:CZ	1:H:123:LEU:HD13	2.56	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	222/227 (98%)	195 (88%)	25 (11%)	2 (1%)	17	26
1	B	222/227 (98%)	203 (91%)	17 (8%)	2 (1%)	17	26
1	C	222/227 (98%)	191 (86%)	26 (12%)	5 (2%)	6	8
1	D	206/227 (91%)	171 (83%)	25 (12%)	10 (5%)	2	2
1	E	222/227 (98%)	171 (77%)	42 (19%)	9 (4%)	3	3
1	F	222/227 (98%)	202 (91%)	15 (7%)	5 (2%)	6	8
1	G	222/227 (98%)	202 (91%)	19 (9%)	1 (0%)	29	43
1	H	223/227 (98%)	190 (85%)	28 (13%)	5 (2%)	6	9
All	All	1761/1816 (97%)	1525 (87%)	197 (11%)	39 (2%)	6	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	ALA
1	C	8	ALA
1	D	211	VAL
1	E	10	ILE
1	E	32	PRO
1	F	188	ARG
1	A	12	GLN
1	C	23	THR
1	C	217	GLU
1	D	23	THR
1	E	64	GLY
1	F	177	GLN
1	G	9	GLY
1	H	10	ILE
1	H	193	LYS
1	A	210	SER
1	D	20	ALA

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Mol	Chain	Res	Type
1	D	32	PRO
1	D	208	GLY
1	E	215	ASP
1	H	25	GLN
1	B	70	THR
1	C	12	GLN
1	C	14	VAL
1	D	21	ALA
1	D	206	LEU
1	E	166	GLY
1	E	189	GLU
1	F	223	ALA
1	H	194	ALA
1	F	70	THR
1	D	197	ASP
1	E	2	ASP
1	E	63	ASP
1	E	145	ASP
1	F	216	SER
1	H	75	SER
1	D	167	GLY
1	D	119	ILE

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	183/185 (99%)	164 (90%)	19 (10%)	7 9
1	B	183/185 (99%)	160 (87%)	23 (13%)	4 5
1	C	183/185 (99%)	156 (85%)	27 (15%)	3 3
1	D	171/185 (92%)	143 (84%)	28 (16%)	2 2
1	E	183/185 (99%)	156 (85%)	27 (15%)	3 3
1	F	183/185 (99%)	150 (82%)	33 (18%)	1 1
1	G	183/185 (99%)	167 (91%)	16 (9%)	10 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	185/185 (100%)	161 (87%)	24 (13%)	4 5
All	All	1454/1480 (98%)	1257 (86%)	197 (14%)	4 4

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	25	GLN
1	A	30	ASP
1	A	47	LEU
1	A	63	ASP
1	A	67	ASN
1	A	94	THR
1	A	102	VAL
1	A	103	SER
1	A	105	ASP
1	A	118	GLU
1	A	131	LEU
1	A	134	THR
1	A	160	ARG
1	A	170	ARG
1	A	190	THR
1	A	198	PHE
1	A	205	ARG
1	A	224	ARG
1	B	2	ASP
1	B	22	LEU
1	B	23	THR
1	B	25	GLN
1	B	27	GLN
1	B	29	VAL
1	B	47	LEU
1	B	96	ILE
1	B	100	ARG
1	B	107	ASP
1	B	116	ARG
1	B	159	GLN
1	B	164	GLN
1	B	172	THR
1	B	173	HIS
1	B	176	THR
1	B	187	SER

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Mol	Chain	Res	Type
1	B	190	THR
1	B	193	LYS
1	B	204	ILE
1	B	214	SER
1	B	222	ARG
1	B	224	ARG
1	C	4	ILE
1	C	5	LEU
1	C	7	ARG
1	C	11	PHE
1	C	12	GLN
1	C	22	LEU
1	C	23	THR
1	C	26	LEU
1	C	30	ASP
1	C	47	LEU
1	C	63	ASP
1	C	67	ASN
1	C	91	SER
1	C	118	GLU
1	C	126	VAL
1	C	129	ARG
1	C	131	LEU
1	C	133	ARG
1	C	177	GLN
1	C	178	GLU
1	C	195	LEU
1	C	197	ASP
1	C	205	ARG
1	C	209	LYS
1	C	211	VAL
1	C	214	SER
1	C	216	SER
1	D	36	THR
1	D	47	LEU
1	D	54	LYS
1	D	59	ARG
1	D	65	ARG
1	D	68	LEU
1	D	94	THR
1	D	96	ILE
1	D	102	VAL

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Mol	Chain	Res	Type
1	D	103	SER
1	D	110	ARG
1	D	115	ASP
1	D	120	SER
1	D	131	LEU
1	D	132	ARG
1	D	133	ARG
1	D	137	ASN
1	D	160	ARG
1	D	163	THR
1	D	169	LEU
1	D	178	GLU
1	D	188	ARG
1	D	190	THR
1	D	192	ASN
1	D	200	HIS
1	D	201	ARG
1	D	214	SER
1	D	222	ARG
1	E	1	MET
1	E	30	ASP
1	E	33	ARG
1	E	46	ARG
1	E	47	LEU
1	E	54	LYS
1	E	68	LEU
1	E	69	LEU
1	E	94	THR
1	E	97	THR
1	E	104	MET
1	E	110	ARG
1	E	115	ASP
1	E	141	LEU
1	E	142	ILE
1	E	146	VAL
1	E	160	ARG
1	E	164	GLN
1	E	173	HIS
1	E	176	THR
1	E	190	THR
1	E	195	LEU
1	E	203	TRP

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Mol	Chain	Res	Type
1	E	206	LEU
1	E	210	SER
1	E	211	VAL
1	E	222	ARG
1	F	2	ASP
1	F	10	ILE
1	F	15	GLU
1	F	29	VAL
1	F	47	LEU
1	F	59	ARG
1	F	62	PRO
1	F	63	ASP
1	F	75	SER
1	F	77	MET
1	F	82	SER
1	F	98	GLU
1	F	102	VAL
1	F	103	SER
1	F	106	ARG
1	F	115	ASP
1	F	118	GLU
1	F	121	GLU
1	F	122	GLN
1	F	126	VAL
1	F	131	LEU
1	F	134	THR
1	F	138	LEU
1	F	160	ARG
1	F	164	GLN
1	F	170	ARG
1	F	177	GLN
1	F	187	SER
1	F	207	GLU
1	F	214	SER
1	F	217	GLU
1	F	218	ARG
1	F	222	ARG
1	G	1	MET
1	G	2	ASP
1	G	15	GLU
1	G	29	VAL
1	G	30	ASP

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Mol	Chain	Res	Type
1	G	33	ARG
1	G	46	ARG
1	G	69	LEU
1	G	91	SER
1	G	102	VAL
1	G	133	ARG
1	G	164	GLN
1	G	170	ARG
1	G	187	SER
1	G	204	ILE
1	G	224	ARG
1	H	5	LEU
1	H	22	LEU
1	H	25	GLN
1	H	27	GLN
1	H	29	VAL
1	H	47	LEU
1	H	54	LYS
1	H	56	LYS
1	H	63	ASP
1	H	71	ILE
1	H	89	ARG
1	H	94	THR
1	H	96	ILE
1	H	103	SER
1	H	106	ARG
1	H	111	SER
1	H	118	GLU
1	H	129	ARG
1	H	177	GLN
1	H	188	ARG
1	H	189	GLU
1	H	200	HIS
1	H	210	SER
1	H	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	25	GLN
1	A	153	GLN

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Mol	Chain	Res	Type
1	A	159	GLN
1	A	164	GLN
1	B	35	HIS
1	B	137	ASN
1	B	164	GLN
1	C	35	HIS
1	C	67	ASN
1	C	137	ASN
1	C	156	GLN
1	C	173	HIS
1	C	177	GLN
1	C	192	ASN
1	D	25	GLN
1	D	35	HIS
1	D	137	ASN
1	D	153	GLN
1	D	164	GLN
1	D	182	GLN
1	E	27	GLN
1	E	35	HIS
1	E	122	GLN
1	E	153	GLN
1	F	12	GLN
1	F	156	GLN
1	F	159	GLN
1	F	164	GLN
1	G	25	GLN
1	G	27	GLN
1	G	35	HIS
1	G	67	ASN
1	G	192	ASN
1	H	27	GLN
1	H	137	ASN
1	H	177	GLN
1	H	182	GLN

5.3.3 RNA

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)

8 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	CMP	C	280	-	22,25,25	1.49	3 (13%)	24,39,39	2.74	8 (33%)
2	CMP	E	280	-	22,25,25	1.48	4 (18%)	24,39,39	1.86	5 (20%)
2	CMP	B	280	-	22,25,25	1.27	3 (13%)	24,39,39	2.06	6 (25%)
2	CMP	D	280	-	22,25,25	1.34	3 (13%)	24,39,39	1.99	7 (29%)
2	CMP	G	280	-	22,25,25	1.45	3 (13%)	24,39,39	1.95	7 (29%)
2	CMP	F	280	-	22,25,25	1.50	3 (13%)	24,39,39	2.95	12 (50%)
2	CMP	H	280	-	22,25,25	1.34	4 (18%)	24,39,39	2.35	9 (37%)
2	CMP	A	280	-	22,25,25	1.40	4 (18%)	24,39,39	2.04	6 (25%)

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	CMP	C	280	-	-	0/0/31/31	0/4/4/4
2	CMP	E	280	-	-	0/0/31/31	0/4/4/4
2	CMP	B	280	-	-	0/0/31/31	0/4/4/4
2	CMP	D	280	-	-	0/0/31/31	0/4/4/4
2	CMP	G	280	-	-	0/0/31/31	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	F	280	-	-	0/0/31/31	0/4/4/4
2	CMP	H	280	-	-	0/0/31/31	0/4/4/4
2	CMP	A	280	-	-	0/0/31/31	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	280	CMP	P-O3'	3.95	1.64	1.57
2	F	280	CMP	O5'-C5'	-3.95	1.40	1.46
2	G	280	CMP	P-O5'	3.84	1.62	1.57
2	A	280	CMP	P-O5'	3.73	1.61	1.57
2	C	280	CMP	O5'-C5'	-2.98	1.41	1.46
2	D	280	CMP	P-O5'	2.97	1.61	1.57
2	B	280	CMP	P-O3'	2.96	1.62	1.57
2	F	280	CMP	P-O3'	2.84	1.62	1.57
2	D	280	CMP	C5-C4	2.72	1.48	1.40
2	B	280	CMP	P-O5'	2.69	1.60	1.57
2	E	280	CMP	P-O5'	2.67	1.60	1.57
2	D	280	CMP	O4'-C1'	2.56	1.44	1.41
2	E	280	CMP	O3'-C3'	-2.55	1.40	1.44
2	E	280	CMP	O5'-C5'	-2.53	1.42	1.46
2	G	280	CMP	O5'-C5'	-2.53	1.42	1.46
2	H	280	CMP	C5-C4	2.51	1.47	1.40
2	F	280	CMP	C2'-C1'	-2.32	1.50	1.53
2	E	280	CMP	C5-C4	2.30	1.47	1.40
2	A	280	CMP	C5-C4	2.21	1.46	1.40
2	C	280	CMP	C5-C4	2.15	1.46	1.40
2	H	280	CMP	O4'-C1'	2.13	1.44	1.41
2	A	280	CMP	O4'-C1'	2.13	1.44	1.41
2	H	280	CMP	O3'-C3'	-2.12	1.41	1.44
2	A	280	CMP	O3'-C3'	-2.10	1.41	1.44
2	H	280	CMP	P-O3'	2.06	1.61	1.57
2	B	280	CMP	C5-C4	2.05	1.46	1.40
2	G	280	CMP	O4'-C1'	2.00	1.43	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	280	CMP	O3'-C3'-C4'	-9.91	103.23	110.71
2	H	280	CMP	O3'-C3'-C4'	-7.01	105.42	110.71
2	C	280	CMP	O3'-C3'-C4'	-6.83	105.55	110.71
2	C	280	CMP	O3'-C3'-C2'	6.02	121.51	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	280	CMP	O5'-P-O3'	-5.80	97.68	105.68
2	B	280	CMP	O2P-P-O1P	5.02	124.45	108.73
2	A	280	CMP	O2P-P-O1P	4.68	123.39	108.73
2	H	280	CMP	O2P-P-O1P	4.67	123.37	108.73
2	E	280	CMP	O2P-P-O1P	4.42	122.56	108.73
2	H	280	CMP	O5'-P-O3'	-4.36	99.67	105.68
2	F	280	CMP	N3-C2-N1	-4.34	121.90	128.68
2	G	280	CMP	O2P-P-O1P	4.28	122.12	108.73
2	D	280	CMP	N3-C2-N1	-4.27	122.00	128.68
2	E	280	CMP	O3'-C3'-C4'	-4.24	107.51	110.71
2	A	280	CMP	O5'-P-O3'	-4.22	99.86	105.68
2	B	280	CMP	O3'-C3'-C2'	4.19	119.71	115.61
2	F	280	CMP	O5'-P-O3'	-4.15	99.96	105.68
2	A	280	CMP	N3-C2-N1	-3.97	122.47	128.68
2	G	280	CMP	N3-C2-N1	-3.95	122.50	128.68
2	F	280	CMP	O2P-P-O1P	3.89	120.91	108.73
2	B	280	CMP	N3-C2-N1	-3.88	122.62	128.68
2	D	280	CMP	C2-N1-C6	3.86	125.36	118.75
2	C	280	CMP	N3-C2-N1	-3.64	122.98	128.68
2	E	280	CMP	N3-C2-N1	-3.50	123.21	128.68
2	D	280	CMP	O2P-P-O1P	3.36	119.27	108.73
2	C	280	CMP	O5'-P-O1P	3.34	118.14	110.44
2	A	280	CMP	C2-N1-C6	3.34	124.46	118.75
2	D	280	CMP	O5'-P-O3'	-3.30	101.13	105.68
2	B	280	CMP	O3'-C3'-C4'	-3.25	108.26	110.71
2	G	280	CMP	C4-C5-N7	-3.18	106.08	109.40
2	H	280	CMP	N3-C2-N1	-3.15	123.75	128.68
2	G	280	CMP	C2-N1-C6	2.96	123.81	118.75
2	G	280	CMP	O3'-C3'-C4'	-2.90	108.52	110.71
2	B	280	CMP	C4-C5-N7	-2.86	106.42	109.40
2	A	280	CMP	N6-C6-N1	2.85	124.50	118.57
2	C	280	CMP	O2P-P-O1P	2.85	117.66	108.73
2	D	280	CMP	O3'-C3'-C4'	-2.84	108.56	110.71
2	F	280	CMP	O2P-P-O3'	2.83	113.62	107.04
2	F	280	CMP	O3'-C3'-C2'	2.82	118.37	115.61
2	C	280	CMP	O2P-P-O5'	-2.79	100.34	107.16
2	F	280	CMP	O5'-C5'-C4'	-2.77	99.25	105.71
2	A	280	CMP	O4'-C4'-C3'	-2.75	98.97	104.87
2	C	280	CMP	C4-C5-N7	-2.75	106.53	109.40
2	B	280	CMP	C2-N1-C6	2.74	123.44	118.75
2	H	280	CMP	C4-C5-N7	-2.51	106.79	109.40
2	G	280	CMP	C5-C6-N6	2.49	124.14	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	280	CMP	C5'-C4'-C3'	-2.43	107.57	112.49
2	G	280	CMP	O3'-C3'-C2'	2.38	117.94	115.61
2	F	280	CMP	C2-N1-C6	2.36	122.79	118.75
2	H	280	CMP	C2-N1-C6	2.30	122.69	118.75
2	D	280	CMP	C5-C6-N1	-2.28	115.18	120.35
2	E	280	CMP	N6-C6-N1	2.22	123.19	118.57
2	H	280	CMP	C5'-C4'-C3'	-2.21	108.01	112.49
2	F	280	CMP	C4-C5-N7	-2.18	107.13	109.40
2	D	280	CMP	N6-C6-N1	2.12	122.97	118.57
2	F	280	CMP	N6-C6-N1	2.11	122.94	118.57
2	F	280	CMP	O2P-P-O5'	-2.09	102.06	107.16
2	H	280	CMP	C5-C6-N6	2.01	123.41	120.35
2	E	280	CMP	O2P-P-O5'	-2.01	102.25	107.16
2	H	280	CMP	O3'-C3'-C2'	2.00	117.57	115.61

There are no chirality outliers.

There are no torsion outliers.

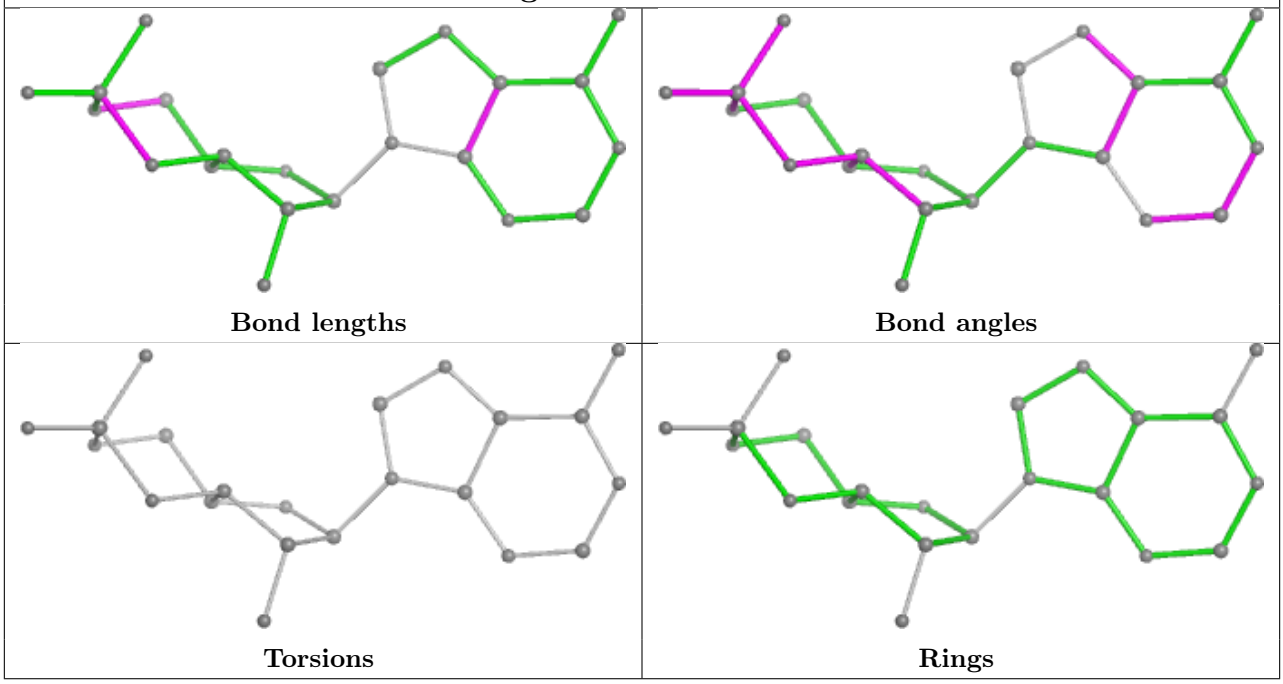
There are no ring outliers.

8 monomers are involved in 14 short contacts:

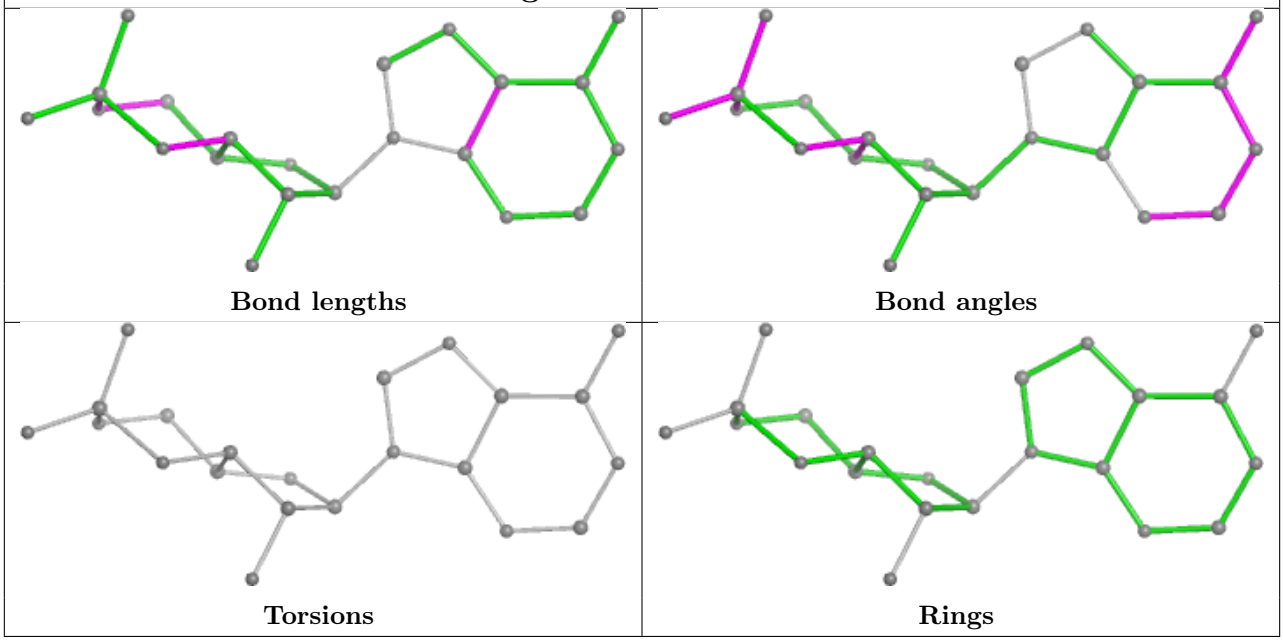
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	280	CMP	1	0
2	E	280	CMP	1	0
2	B	280	CMP	2	0
2	D	280	CMP	1	0
2	G	280	CMP	4	0
2	F	280	CMP	1	0
2	H	280	CMP	2	0
2	A	280	CMP	2	0

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 then 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.

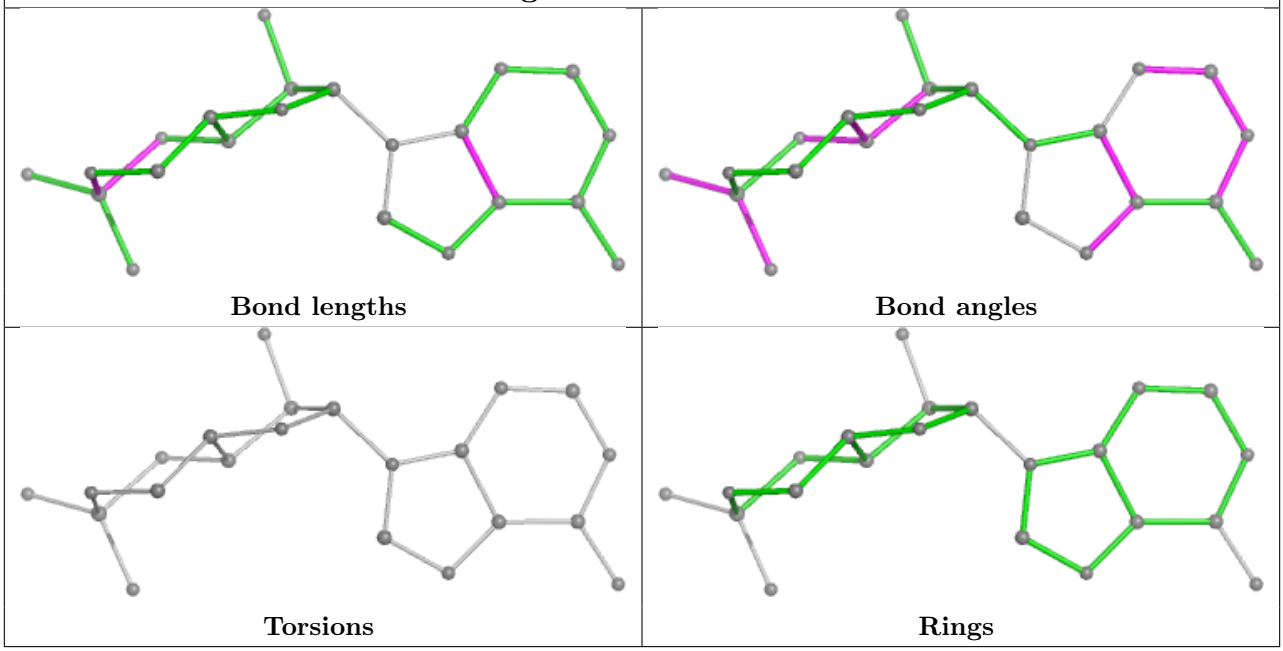
Ligand CMP C 280



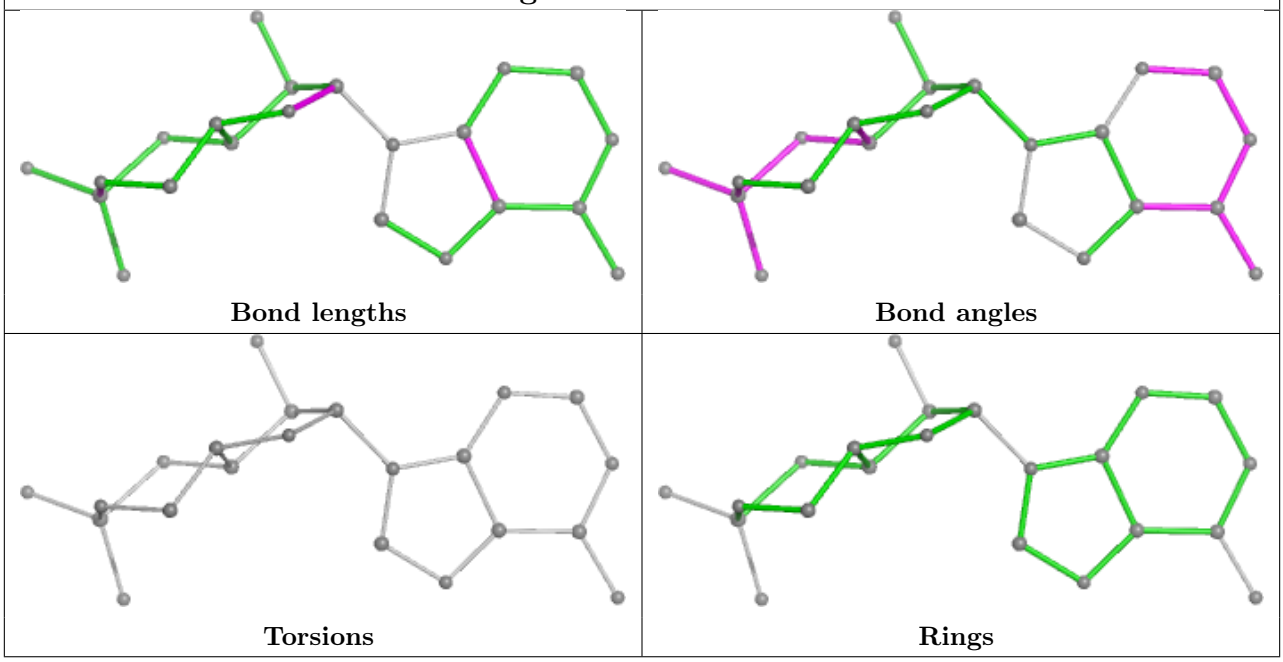
Ligand CMP E 280



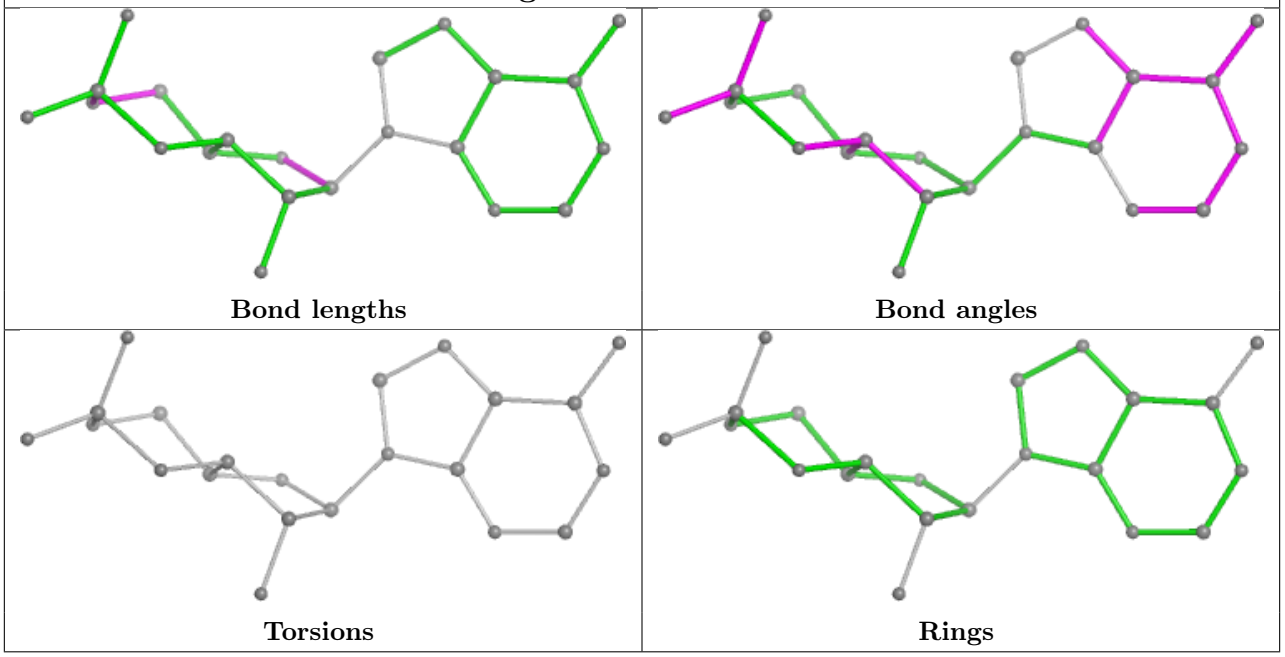
Ligand CMP B 280



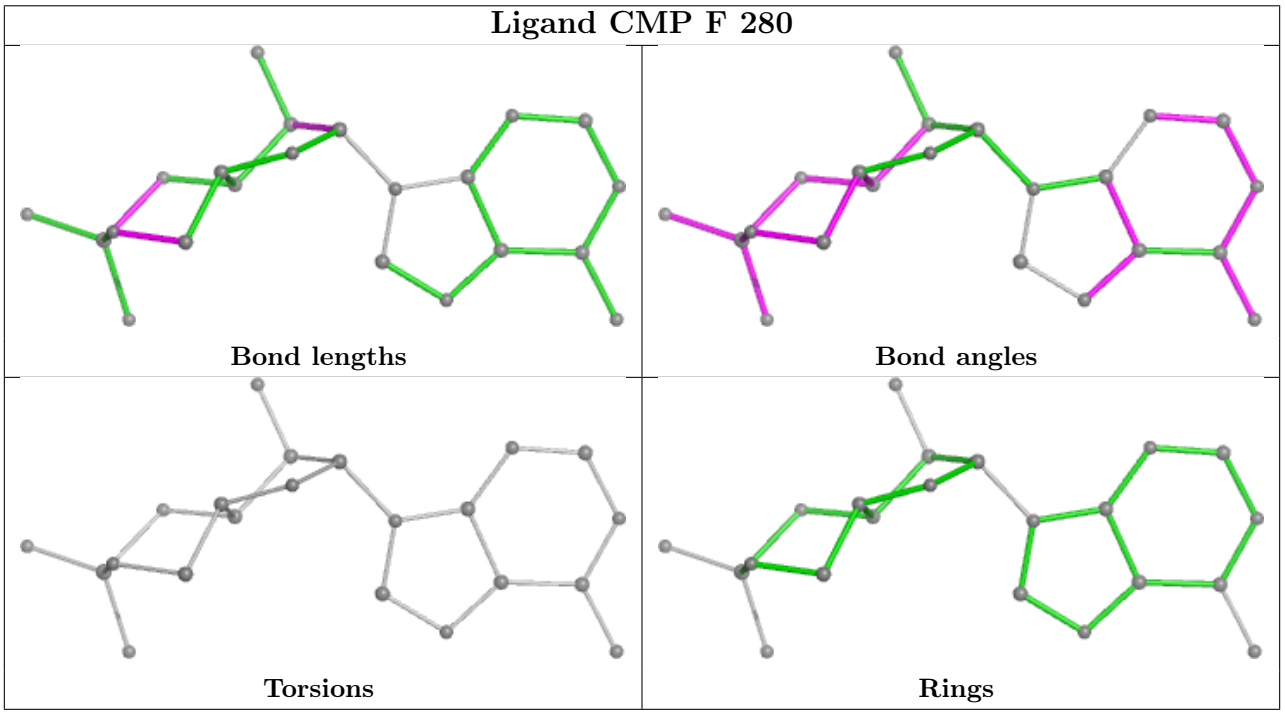
Ligand CMP D 280



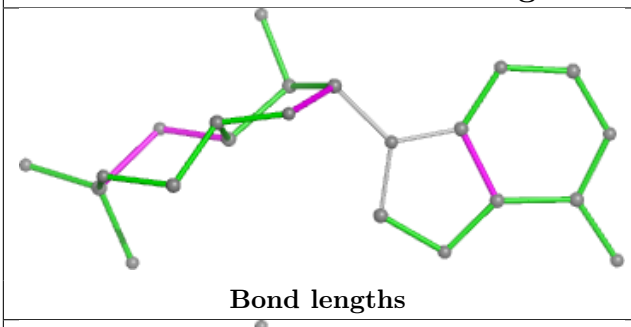
Ligand CMP G 280



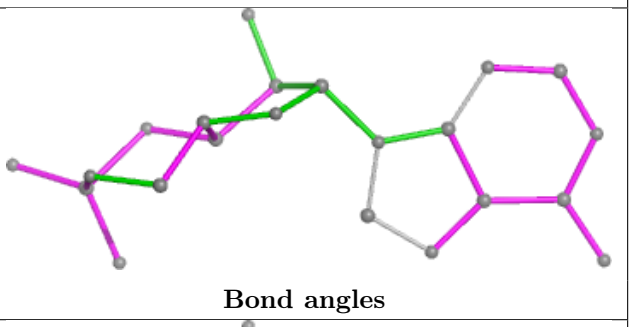
Ligand CMP F 280



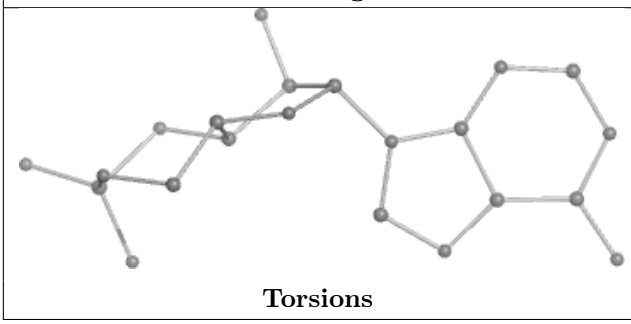
Ligand CMP H 280



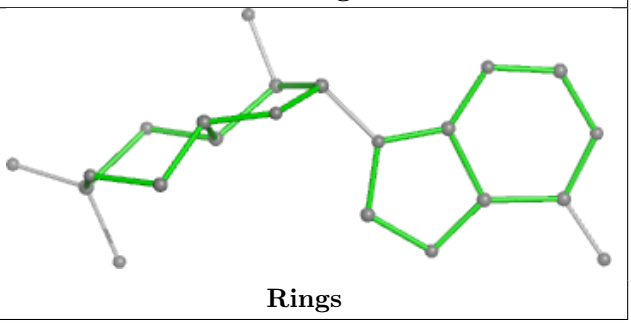
Bond lengths



Bond angles

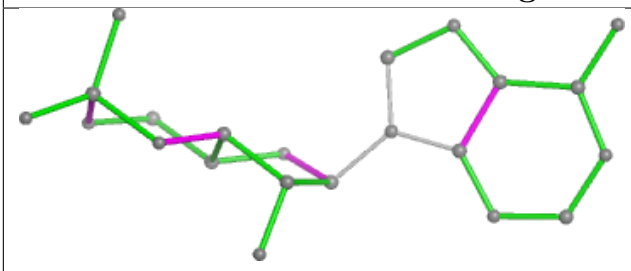


Torsions

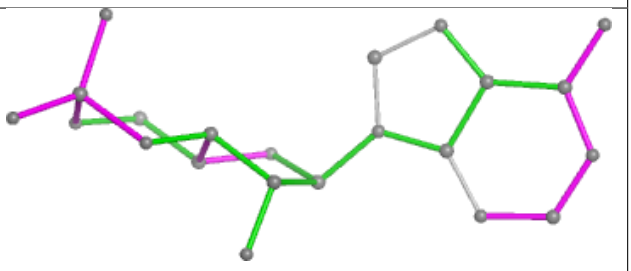


Rings

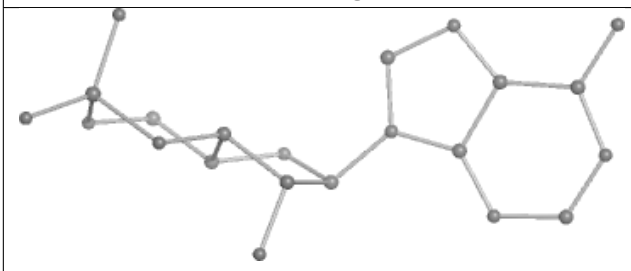
Ligand CMP A 280



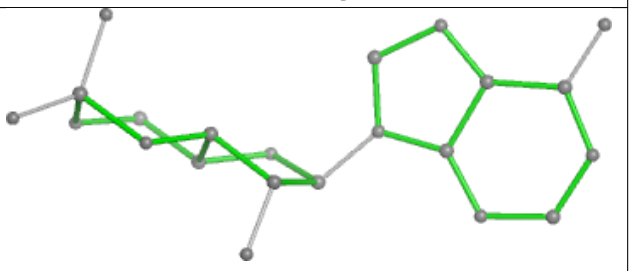
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	0:HIS	C	1:MET	N	2.57

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	224/227 (98%)	0.08	7 (3%) 49 45	36, 68, 105, 123	0
1	B	224/227 (98%)	0.06	11 (4%) 29 25	36, 53, 90, 113	0
1	C	224/227 (98%)	0.01	9 (4%) 38 35	42, 59, 110, 137	0
1	D	208/227 (91%)	0.74	33 (15%) 1 1	44, 83, 117, 144	0
1	E	224/227 (98%)	0.75	38 (16%) 1 1	43, 82, 122, 145	0
1	F	225/227 (99%)	-0.00	10 (4%) 34 31	36, 52, 96, 117	0
1	G	224/227 (98%)	0.02	10 (4%) 33 30	33, 53, 93, 117	0
1	H	227/227 (100%)	0.06	3 (1%) 77 75	34, 60, 93, 116	0
All	All	1780/1816 (98%)	0.21	121 (6%) 17 14	33, 63, 109, 145	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	196	ALA	8.5
1	D	165	GLU	7.1
1	E	162	GLY	6.8
1	D	166	GLY	6.6
1	E	198	PHE	6.6
1	C	19	ILE	6.3
1	B	14	VAL	6.2
1	F	18	ALA	6.2
1	B	13	GLY	6.1
1	E	20	ALA	5.9
1	D	195	LEU	5.9
1	F	17	SER	5.8
1	E	200	HIS	5.8
1	F	-1	SER	5.8
1	D	211	VAL	5.7
1	C	18	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	199	ALA	5.6
1	F	19	ILE	5.4
1	D	212	LEU	5.3
1	C	16	PRO	5.3
1	D	210	SER	5.3
1	C	17	SER	5.1
1	E	170	ARG	5.1
1	E	172	THR	5.1
1	E	164	GLN	5.0
1	E	21	ALA	4.8
1	E	163	THR	4.7
1	C	20	ALA	4.7
1	E	17	SER	4.6
1	D	170	ARG	4.5
1	G	14	VAL	4.5
1	D	168	ALA	4.4
1	E	16	PRO	4.3
1	D	172	THR	4.2
1	E	224	ARG	4.1
1	G	15	GLU	4.1
1	D	167	GLY	4.1
1	D	217	GLU	4.1
1	E	158	ALA	4.1
1	D	224	ARG	4.0
1	B	16	PRO	4.0
1	F	12	GLN	4.0
1	E	171	VAL	3.9
1	D	164	GLN	3.9
1	C	10	ILE	3.9
1	E	24	LYS	3.9
1	E	13	GLY	3.9
1	B	22	LEU	3.9
1	B	168	ALA	3.8
1	D	196	ALA	3.8
1	F	13	GLY	3.8
1	C	3	GLU	3.8
1	E	222	ARG	3.7
1	G	206	LEU	3.7
1	E	169	LEU	3.7
1	B	15	GLU	3.7
1	E	25	GLN	3.7
1	D	62	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLU	3.6
1	E	15	GLU	3.6
1	G	17	SER	3.6
1	E	208	GLY	3.5
1	C	1	MET	3.5
1	D	223	ALA	3.5
1	D	200	HIS	3.4
1	A	208	GLY	3.4
1	A	17	SER	3.4
1	D	163	THR	3.4
1	B	17	SER	3.3
1	G	20	ALA	3.2
1	G	16	PRO	3.2
1	D	193	LYS	3.1
1	F	10	ILE	3.1
1	E	14	VAL	3.1
1	E	167	GLY	3.0
1	E	221	ARG	3.0
1	D	67	ASN	3.0
1	B	167	GLY	2.9
1	D	63	ASP	2.9
1	E	197	ASP	2.9
1	B	62	PRO	2.8
1	D	201	ARG	2.8
1	D	171	VAL	2.8
1	C	21	ALA	2.7
1	E	220	ALA	2.7
1	A	212	LEU	2.7
1	G	4	ILE	2.7
1	D	22	LEU	2.7
1	E	18	ALA	2.6
1	F	20	ALA	2.6
1	D	169	LEU	2.6
1	A	167	GLY	2.6
1	D	194	ALA	2.6
1	E	195	LEU	2.6
1	H	16	PRO	2.6
1	E	93	ALA	2.4
1	D	191	VAL	2.4
1	G	1	MET	2.4
1	D	21	ALA	2.4
1	G	18	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	31	PHE	2.4
1	D	221	ARG	2.4
1	E	7	ARG	2.4
1	F	16	PRO	2.3
1	A	223	ALA	2.3
1	D	199	ALA	2.3
1	E	201	ARG	2.3
1	B	21	ALA	2.2
1	D	98	GLU	2.2
1	A	169	LEU	2.2
1	A	165	GLU	2.2
1	B	166	GLY	2.2
1	D	198	PHE	2.2
1	H	168	ALA	2.1
1	E	67	ASN	2.1
1	E	66	GLU	2.1
1	G	3	GLU	2.1
1	E	154	LEU	2.0
1	F	15	GLU	2.0
1	H	-1	SER	2.0
1	E	161	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	CMP	D	280	22/22	0.97	0.17	47,52,57,61	0
2	CMP	H	280	22/22	0.97	0.20	36,42,47,47	0

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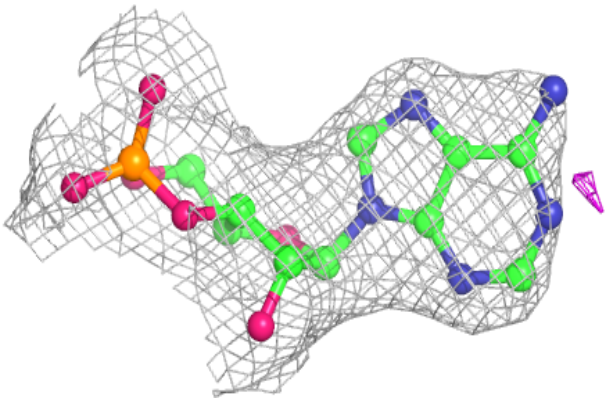
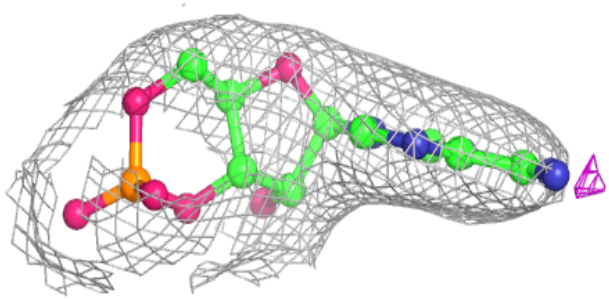
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CMP	A	280	22/22	0.98	0.17	39,44,50,55	0
2	CMP	E	280	22/22	0.98	0.18	40,45,58,59	0
2	CMP	F	280	22/22	0.98	0.20	35,41,44,47	0
2	CMP	B	280	22/22	0.98	0.23	36,41,47,49	0
2	CMP	G	280	22/22	0.99	0.20	34,38,42,43	0
2	CMP	C	280	22/22	0.99	0.20	40,47,51,52	0

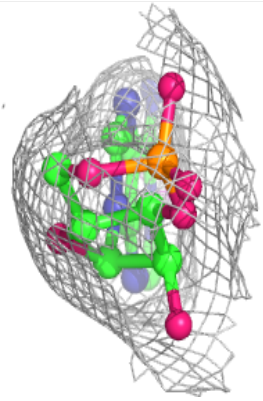
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CMP D 280:

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

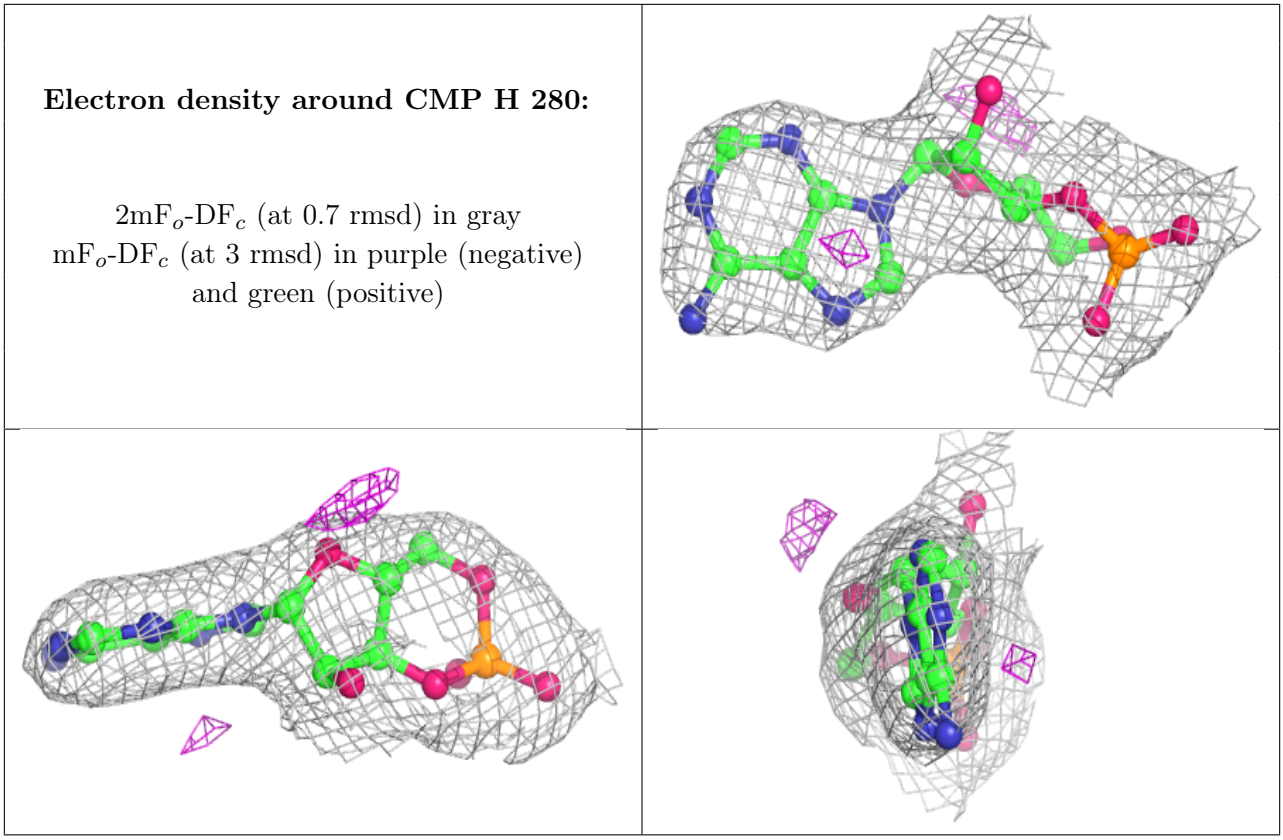






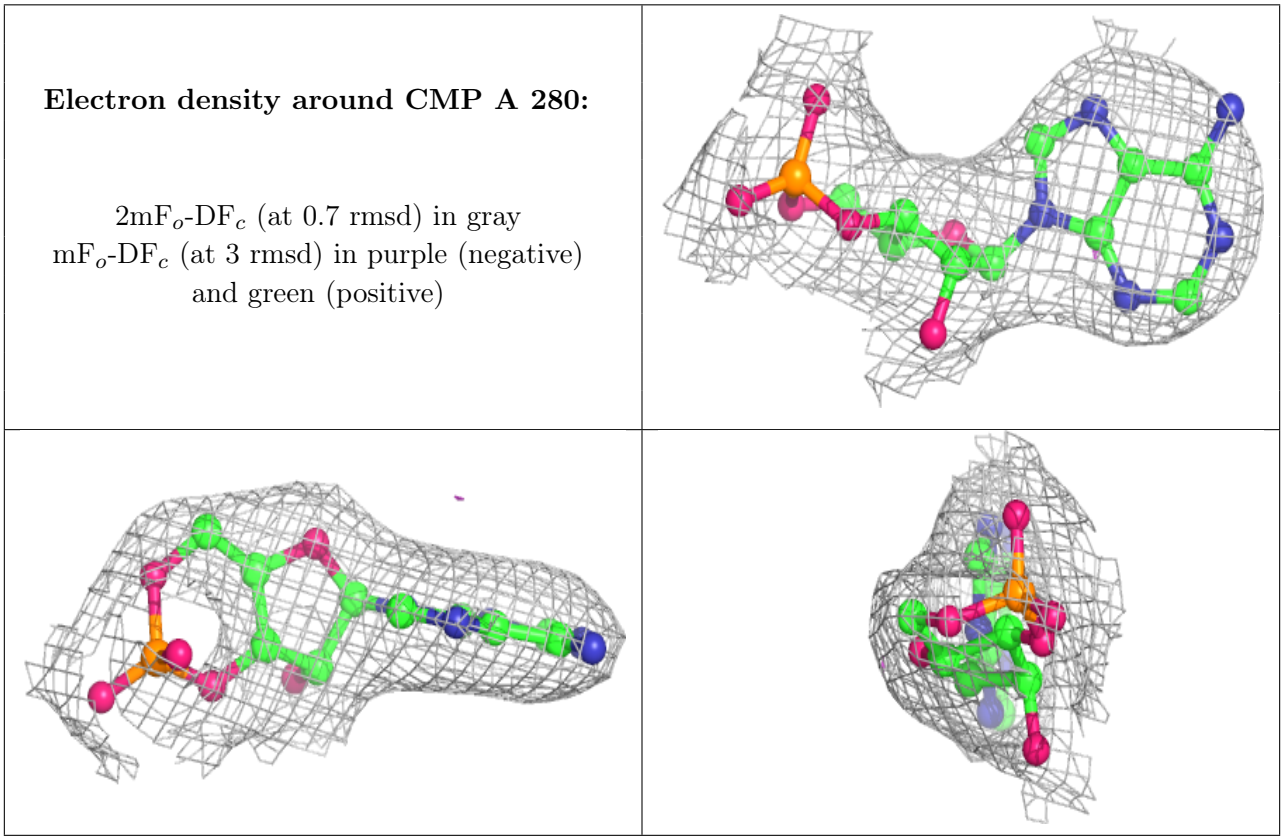
Electron density around CMP H 280:

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



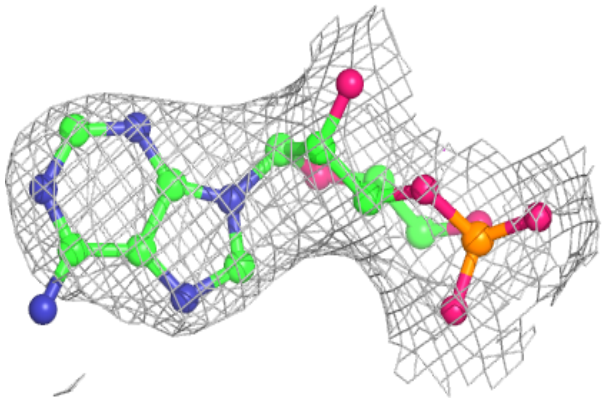
Electron density around CMP A 280:

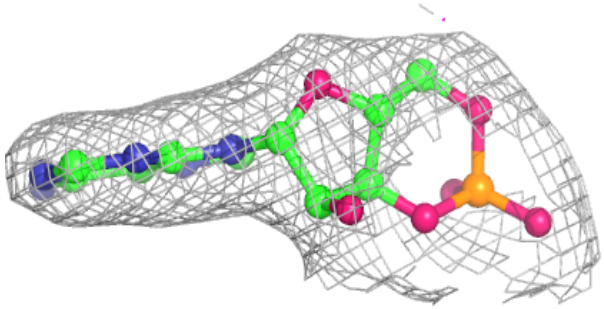
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

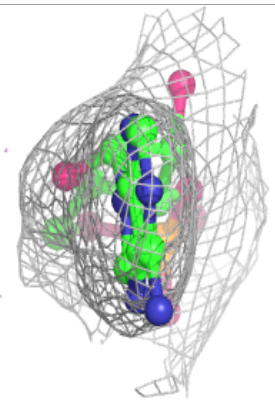


Electron density around CMP E 280:

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

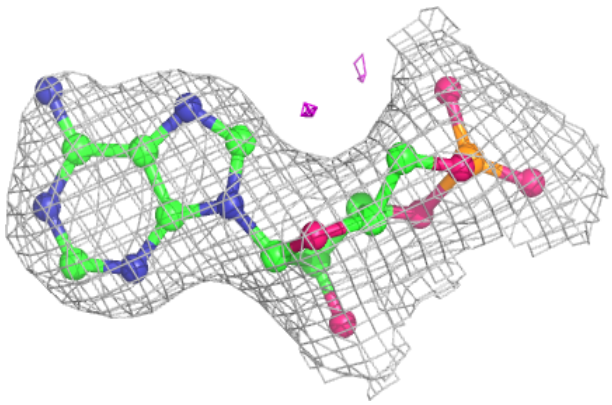


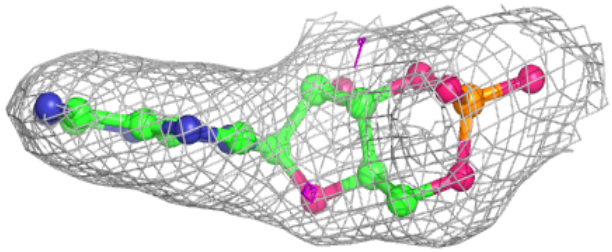


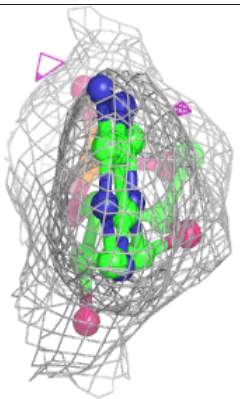


Electron density around CMP F 280:

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

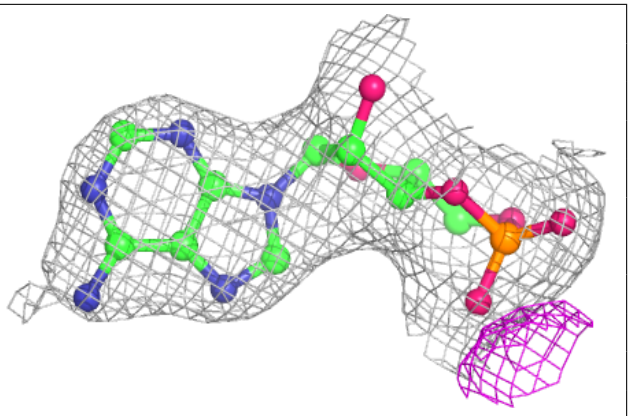


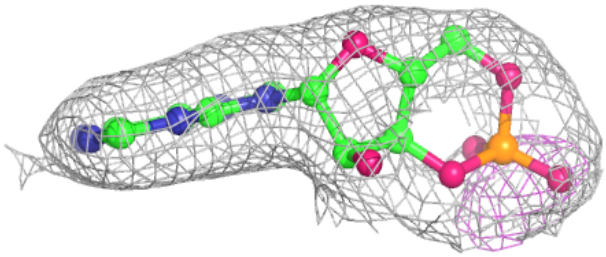


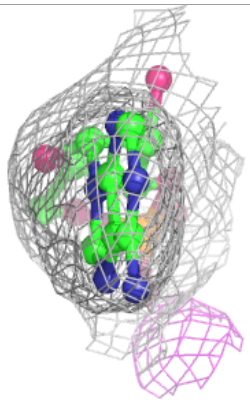


Electron density around CMP B 280:

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

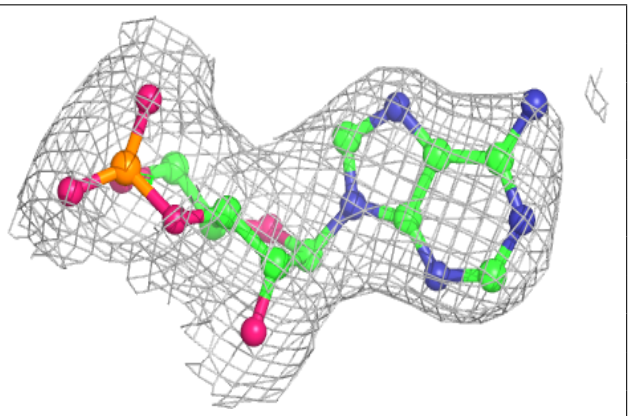


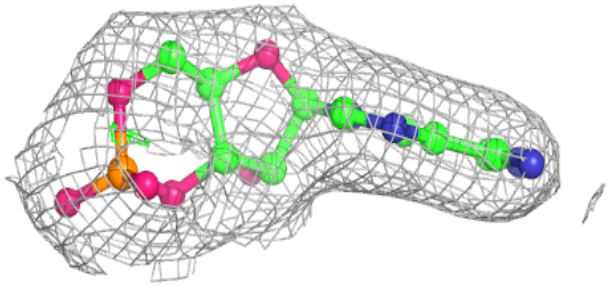


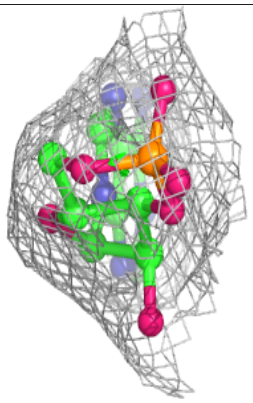


Electron density around CMP G 280:

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

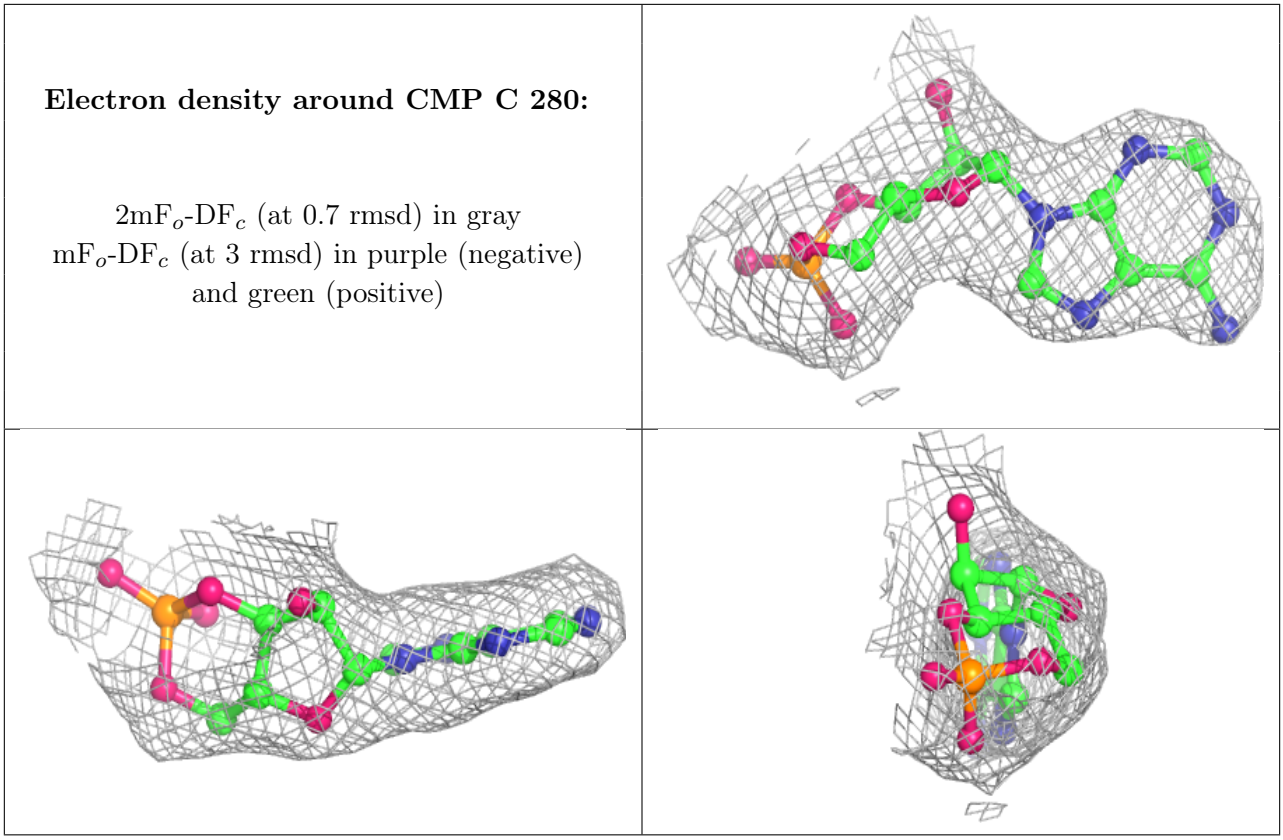






Electron density around CMP C 280:

$2mF_o$-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.