Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 12:18 AM EDT

PDB ID	:	2H12
Title	:	Structure of Acetobacter aceti citrate synthase complexed with oxaloacetate and carboxymethyldethia coenzyme A (CMX)
Authors	:	Starks, C.M.; Kappock, T.J.
Deposited on	:	2006-05-15
Resolution	:	1.85 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 (i) 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 (i)) were used in the production of this report:

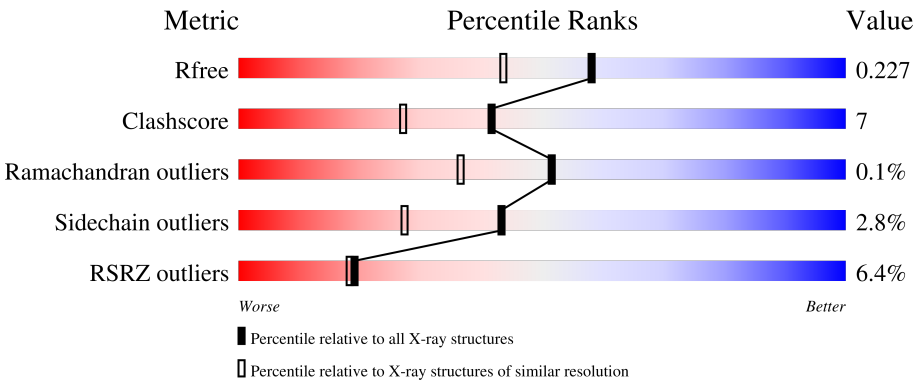
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	436	4% 83% 12% •
1	B	436	7% 87% 10% •
1	C	436	5% 85% 11% • •
1	D	436	9% 85% 11% •
1	E	436	7% 85% 11% • •

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Mol	Chain	Length	Quality of chain
1	F	436	6% 83% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5040	-	-	-	X
3	SO4	A	5047	-	-	-	X
3	SO4	A	5052	-	-	-	X
3	SO4	B	5053	-	-	-	X
3	SO4	C	5041	-	-	X	X
3	SO4	E	5037	-	-	-	X
3	SO4	E	5043	-	-	-	X
3	SO4	F	5044	-	-	-	X
3	SO4	F	5051	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23521 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.

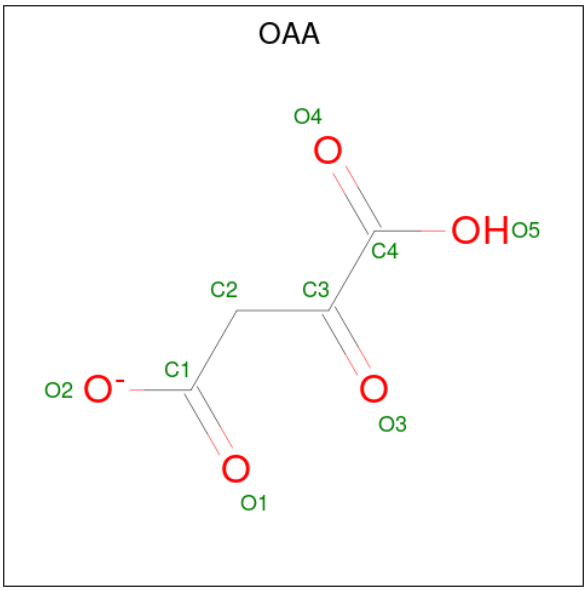
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3258	2086	563	592	17	0	0	0
1	B	426	3313	2119	572	605	17	0	0	0
1	C	426	3315	2121	572	605	17	0	0	0
1	D	417	3253	2083	562	591	17	0	0	0
1	E	426	3315	2121	572	605	17	0	0	0
1	F	420	3273	2095	565	596	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

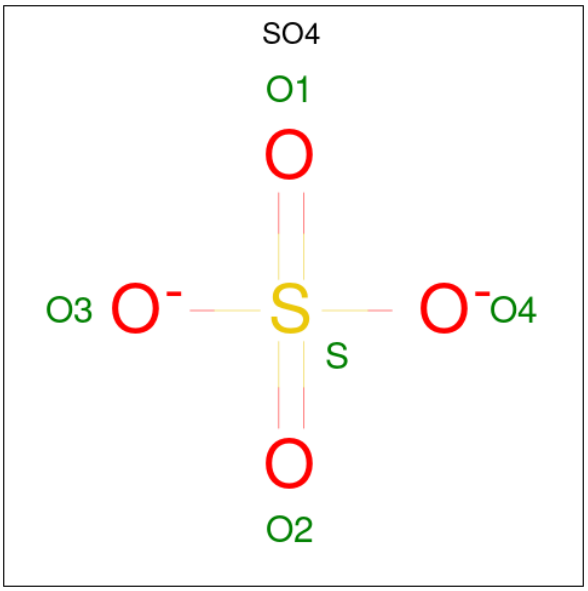
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	ASP	SEE REMARK 999	UNP P20901
A	106	ALA	VAL	SEE REMARK 999	UNP P20901
B	85	ALA	ASP	SEE REMARK 999	UNP P20901
B	106	ALA	VAL	SEE REMARK 999	UNP P20901
C	85	ALA	ASP	SEE REMARK 999	UNP P20901
C	106	ALA	VAL	SEE REMARK 999	UNP P20901
D	85	ALA	ASP	SEE REMARK 999	UNP P20901
D	106	ALA	VAL	SEE REMARK 999	UNP P20901
E	85	ALA	ASP	SEE REMARK 999	UNP P20901
E	106	ALA	VAL	SEE REMARK 999	UNP P20901
F	85	ALA	ASP	SEE REMARK 999	UNP P20901
F	106	ALA	VAL	SEE REMARK 999	UNP P20901

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			9	4	5			
2	B	1	Total	C	O		0	0
			9	4	5			
2	C	1	Total	C	O		0	0
			9	4	5			
2	D	1	Total	C	O		0	0
			9	4	5			
2	E	1	Total	C	O		0	0
			9	4	5			
2	F	1	Total	C	O		0	0
			9	4	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0

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

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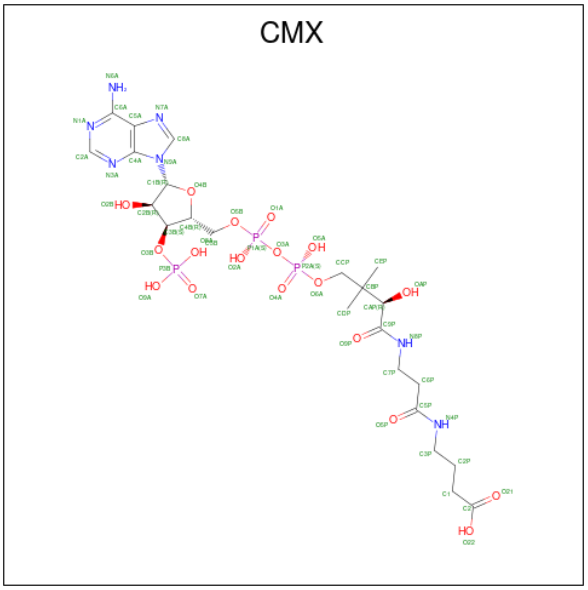
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0

- Molecule 4 is CARBOXYMETHYLDETHIA COENZYME *A (three-letter code: CMX) (formula: $C_{23}H_{38}N_7O_{18}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	51	23	7	18	3	0	0
			Total	C	N	O	P		
4	B	1	51	23	7	18	3	0	0
			Total	C	N	O	P		
4	C	1	51	23	7	18	3	0	0
			Total	C	N	O	P		
4	D	1	51	23	7	18	3	0	0
			Total	C	N	O	P		
4	E	1	51	23	7	18	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	F	1	51	23	7	18	3	0	0

- Molecule 5 is water.

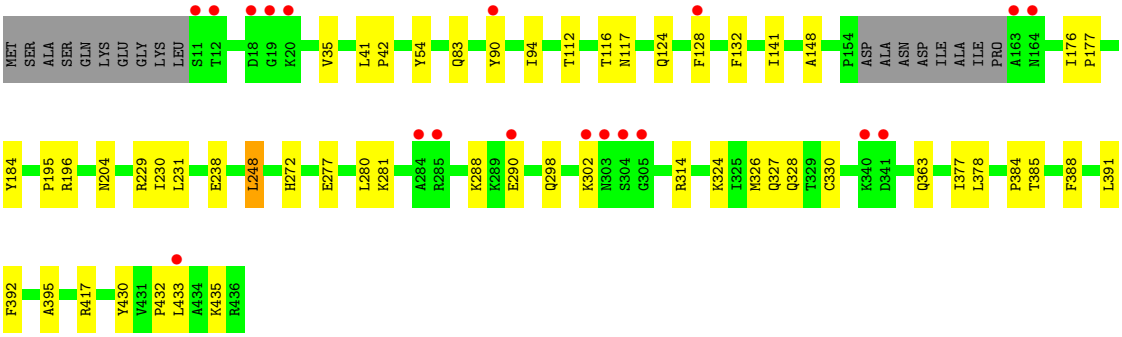
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	561	561	561	0	0
5	B	555	555	555	0	0
5	C	526	526	526	0	0
5	D	499	499	499	0	0
5	E	547	547	547	0	0
5	F	541	541	541	0	0

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.

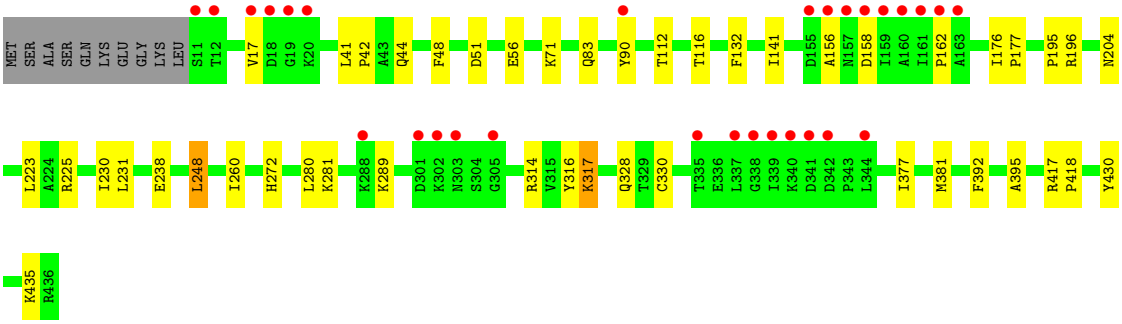
• Molecule 1: Citrate synthase

Chain A:



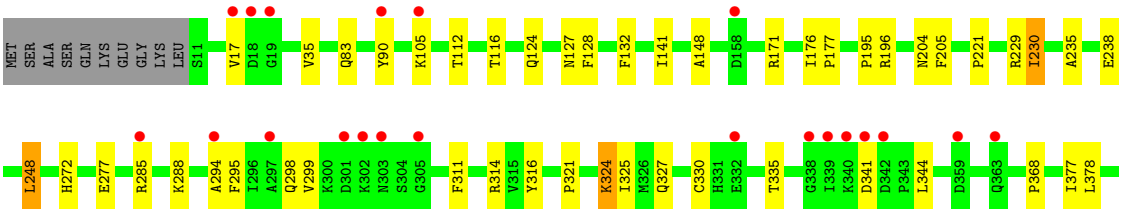
• Molecule 1: Citrate synthase

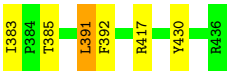
Chain B:



• Molecule 1: Citrate synthase

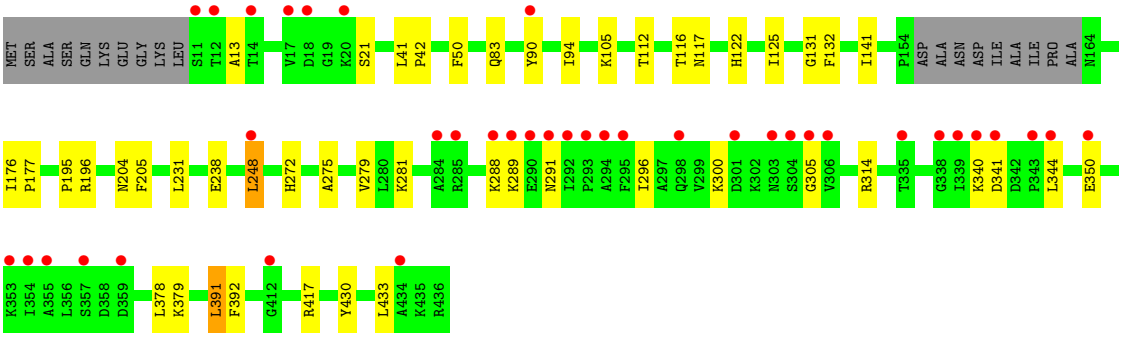
Chain C:





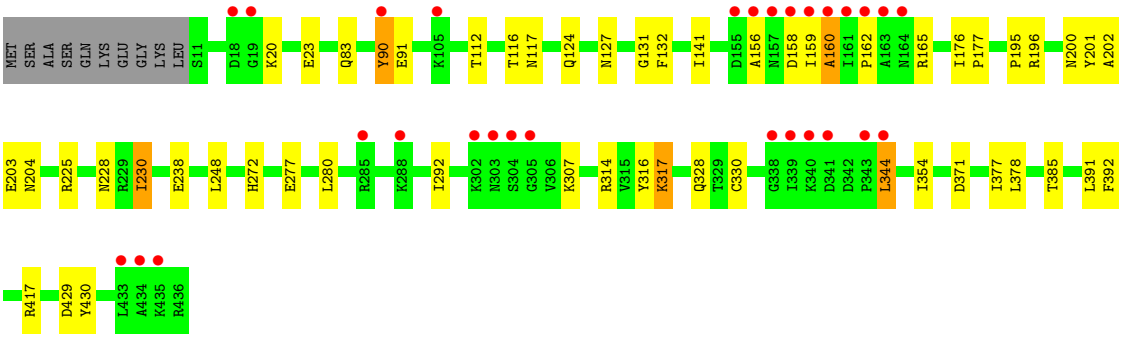
- Molecule 1: Citrate synthase

Chain D:



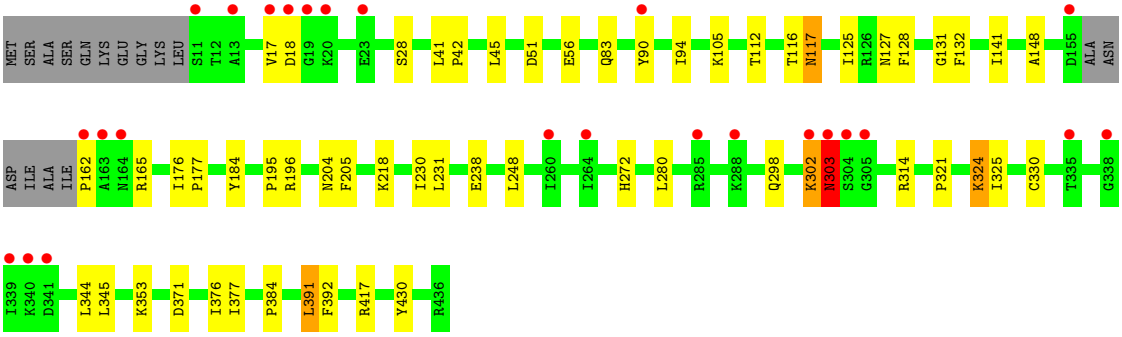
- Molecule 1: Citrate synthase

Chain E:



- Molecule 1: Citrate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	170.66Å 125.69Å 150.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 1.85 39.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.28-1.85) 99.6 (39.28-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.60 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.231 0.192 , 0.227	Depositor DCC
R_{free} test set	13558 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23521	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, OAA, CMX

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	0.39	0/3332	0.68	0/4517
1	B	0.39	0/3388	0.69	1/4596 (0.0%)
1	C	0.39	0/3391	0.69	0/4601
1	D	0.39	0/3327	0.70	0/4510
1	E	0.40	0/3391	0.68	0/4601
1	F	0.39	0/3348	0.68	0/4539
All	All	0.39	0/20177	0.68	1/27364 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	PRO	N-CA-CB	5.19	109.53	103.30

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	3258	0	3271	53	0
1	B	3313	0	3319	40	0
1	C	3315	0	3325	49	0
1	D	3253	0	3266	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3315	0	3325	61	0
1	F	3273	0	3283	59	0
2	A	9	0	2	0	0
2	B	9	0	2	0	0
2	C	9	0	2	0	0
2	D	9	0	2	0	0
2	E	9	0	2	0	0
2	F	9	0	2	0	0
3	A	35	0	0	0	0
3	B	45	0	0	2	0
3	C	30	0	0	4	0
3	D	30	0	0	0	0
3	E	35	0	0	1	0
3	F	30	0	0	1	0
4	A	51	0	33	0	0
4	B	51	0	33	0	0
4	C	51	0	33	2	0
4	D	51	0	33	0	0
4	E	51	0	33	1	0
4	F	51	0	33	1	0
5	A	561	0	0	8	1
5	B	555	0	0	9	0
5	C	526	0	0	5	1
5	D	499	0	0	5	0
5	E	547	0	0	10	0
5	F	541	0	0	13	2
All	All	23521	0	19999	282	2

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 7.

All (282) 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:90:TYR:CE1	1:A:231:LEU:HB3	1.88	1.08
1:E:159:ILE:HB	1:E:165:ARG:HH21	1.18	1.02
1:F:90:TYR:CE2	1:F:94:ILE:HD11	1.94	1.01
1:F:280:LEU:HD11	1:F:344:LEU:HD21	1.39	0.99
1:E:159:ILE:HG22	5:E:5226:HOH:O	1.66	0.95
1:E:90:TYR:CD2	1:E:228:ASN:OD1	2.24	0.91
3:F:5038:SO4:O2	5:F:5521:HOH:O	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:TYR:CE1	1:E:201:TYR:HB3	2.08	0.88
1:F:90:TYR:HE2	1:F:94:ILE:HD11	1.40	0.86
1:E:90:TYR:CD1	1:E:201:TYR:HB3	2.11	0.86
1:E:165:ARG:HD2	5:E:5564:HOH:O	1.76	0.85
1:D:90:TYR:CE1	1:D:231:LEU:HB3	2.12	0.85
1:D:90:TYR:HE1	1:D:231:LEU:C	1.81	0.84
1:E:90:TYR:CE2	1:E:202:ALA:HB2	2.11	0.84
1:A:90:TYR:HE1	1:A:231:LEU:C	1.80	0.84
1:C:171:ARG:NH2	3:C:5041:SO4:O1	2.12	0.82
3:C:5041:SO4:O4	5:C:5532:HOH:O	1.97	0.82
1:E:162:PRO:HA	5:E:5564:HOH:O	1.78	0.81
1:B:90:TYR:CE1	1:B:231:LEU:HB3	2.16	0.81
1:E:430:TYR:H	1:F:83:GLN:NE2	1.77	0.80
1:E:307:LYS:HE3	5:E:5407:HOH:O	1.80	0.79
1:E:90:TYR:OH	1:E:200:ASN:OD1	2.01	0.79
1:A:90:TYR:CE1	1:A:231:LEU:CB	2.66	0.77
1:A:83:GLN:NE2	1:B:430:TYR:H	1.81	0.77
1:C:205:PHE:HE2	1:C:391:LEU:HD13	1.50	0.77
1:F:321:PRO:O	1:F:324:LYS:HG3	1.85	0.77
1:F:302:LYS:O	1:F:303:ASN:HB3	1.83	0.76
1:D:90:TYR:CE1	1:D:231:LEU:C	2.58	0.76
1:C:321:PRO:HA	1:C:324:LYS:HD3	1.68	0.75
1:D:90:TYR:HE1	1:D:231:LEU:O	1.69	0.75
1:C:324:LYS:HG2	1:C:325:ILE:N	2.02	0.74
1:D:340:LYS:HG3	1:D:341:ASP:H	1.54	0.73
1:C:83:GLN:NE2	1:D:430:TYR:H	1.87	0.73
1:C:430:TYR:H	1:D:83:GLN:NE2	1.86	0.73
1:E:90:TYR:OH	1:E:200:ASN:CG	2.28	0.72
1:E:90:TYR:CE2	1:E:202:ALA:CB	2.73	0.71
1:A:430:TYR:H	1:B:83:GLN:NE2	1.88	0.71
1:E:83:GLN:NE2	1:F:430:TYR:H	1.89	0.70
1:B:44:GLN:NE2	5:B:5605:HOH:O	2.23	0.70
1:A:90:TYR:CE1	1:A:231:LEU:C	2.65	0.70
1:E:176:ILE:HG22	1:E:177:PRO:HD3	1.74	0.69
1:F:165:ARG:HD2	5:F:5289:HOH:O	1.91	0.69
1:D:205:PHE:HE2	1:D:391:LEU:HD13	1.57	0.69
1:A:298:GLN:NE2	5:A:5453:HOH:O	2.24	0.69
1:F:125:ILE:HD13	1:F:128:PHE:HE1	1.57	0.68
1:B:196:ARG:H	1:B:204:ASN:ND2	1.92	0.67
1:D:289:LYS:HG3	1:D:350:GLU:HG2	1.75	0.67
1:E:90:TYR:CE2	5:E:5295:HOH:O	2.47	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HE3	5:B:5580:HOH:O	1.95	0.66
1:F:125:ILE:HD13	1:F:128:PHE:CE1	2.31	0.65
1:D:340:LYS:HG3	1:D:341:ASP:N	2.11	0.65
1:C:112:THR:O	1:C:116:THR:HG23	1.96	0.64
1:F:90:TYR:CE2	1:F:94:ILE:CD1	2.77	0.64
1:C:196:ARG:H	1:C:204:ASN:ND2	1.96	0.64
1:A:90:TYR:CD2	1:A:94:ILE:HD11	2.34	0.63
1:A:90:TYR:CE2	1:A:94:ILE:HD11	2.32	0.63
1:F:196:ARG:H	1:F:204:ASN:ND2	1.97	0.63
1:B:90:TYR:CD1	1:B:231:LEU:HD13	2.34	0.63
1:A:90:TYR:CD1	1:A:231:LEU:HB3	2.32	0.63
1:D:205:PHE:CE2	1:D:391:LEU:HD13	2.33	0.63
1:A:128:PHE:CZ	1:A:148:ALA:HB1	2.33	0.63
1:F:90:TYR:CD2	1:F:94:ILE:HD11	2.33	0.62
1:A:90:TYR:CD1	1:A:231:LEU:CB	2.82	0.62
1:C:248:LEU:HD12	1:D:248:LEU:HD12	1.81	0.62
1:E:176:ILE:CG2	1:E:177:PRO:HD3	2.29	0.62
1:A:302:LYS:HG2	5:A:5585:HOH:O	2.00	0.62
1:C:230:ILE:HD11	1:C:377:ILE:CG2	2.29	0.62
1:B:281:LYS:HG3	5:B:5576:HOH:O	1.99	0.62
1:D:90:TYR:CE1	1:D:231:LEU:CB	2.82	0.61
1:A:83:GLN:HE22	1:B:430:TYR:H	1.46	0.61
1:A:385:THR:HG21	5:A:5220:HOH:O	2.00	0.61
1:F:112:THR:O	1:F:116:THR:HG23	2.00	0.61
1:F:90:TYR:CD1	1:F:231:LEU:HB3	2.36	0.60
1:C:196:ARG:H	1:C:204:ASN:HD21	1.49	0.60
1:B:176:ILE:HG22	1:B:177:PRO:HD3	1.83	0.60
1:E:429:ASP:HA	1:F:83:GLN:HE22	1.66	0.60
1:D:112:THR:O	1:D:116:THR:HG23	2.02	0.60
1:D:196:ARG:H	1:D:204:ASN:ND2	1.99	0.60
1:F:90:TYR:CE1	1:F:231:LEU:HB3	2.36	0.60
1:E:90:TYR:CE1	1:E:201:TYR:CB	2.83	0.60
1:A:363:GLN:HE21	1:A:363:GLN:HA	1.67	0.60
1:C:17:VAL:HG12	1:D:13:ALA:CB	2.31	0.59
1:C:17:VAL:HG12	1:D:13:ALA:HB2	1.84	0.59
1:D:176:ILE:HG22	1:D:177:PRO:HD3	1.85	0.59
1:C:230:ILE:HD11	1:C:377:ILE:HG21	1.84	0.59
1:F:324:LYS:HD2	1:F:325:ILE:HG13	1.84	0.59
1:C:430:TYR:H	1:D:83:GLN:HE22	1.51	0.58
1:D:90:TYR:CD2	1:D:94:ILE:HD11	2.38	0.58
1:A:176:ILE:HG22	1:A:177:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ALA:O	5:B:5604:HOH:O	2.17	0.57
1:E:132:PHE:CZ	1:E:141:ILE:HA	2.39	0.57
1:C:321:PRO:O	1:C:324:LYS:HE2	2.03	0.57
1:A:90:TYR:HE1	1:A:231:LEU:O	1.88	0.57
1:A:277:GLU:HG3	1:A:385:THR:HG22	1.86	0.57
1:E:277:GLU:HG3	1:E:385:THR:HG22	1.86	0.57
1:A:184:TYR:CE1	1:A:384:PRO:HG3	2.40	0.56
1:E:430:TYR:H	1:F:83:GLN:HE22	1.50	0.56
1:A:288:LYS:HG3	1:A:290:GLU:HG2	1.87	0.56
1:A:432:PRO:HD2	1:A:435:LYS:HD2	1.85	0.56
1:C:324:LYS:HE3	5:C:5296:HOH:O	2.04	0.56
1:B:176:ILE:CG2	1:B:177:PRO:HD3	2.35	0.56
1:B:196:ARG:H	1:B:204:ASN:HD21	1.52	0.56
1:D:90:TYR:CD1	1:D:231:LEU:CB	2.88	0.56
1:D:176:ILE:CG2	1:D:177:PRO:HD3	2.35	0.56
1:F:324:LYS:HG2	5:F:5571:HOH:O	2.04	0.56
1:E:112:THR:O	1:E:116:THR:HG23	2.06	0.56
1:D:196:ARG:H	1:D:204:ASN:HD21	1.54	0.56
1:F:165:ARG:CD	5:F:5289:HOH:O	2.51	0.56
1:F:196:ARG:H	1:F:204:ASN:HD21	1.54	0.56
1:F:330:CYS:SG	1:F:377:ILE:HG13	2.46	0.56
1:C:229:ARG:NH2	5:C:5428:HOH:O	2.40	0.55
1:F:321:PRO:O	1:F:324:LYS:HE2	2.05	0.55
1:B:90:TYR:CZ	1:B:231:LEU:HB3	2.42	0.55
1:E:90:TYR:HD2	1:E:228:ASN:HA	1.70	0.55
1:A:281:LYS:HG3	5:A:5220:HOH:O	2.07	0.55
1:C:176:ILE:HG22	1:C:177:PRO:HD3	1.89	0.55
1:F:298:GLN:NE2	5:F:5221:HOH:O	2.39	0.55
1:E:90:TYR:CE1	1:E:91:GLU:OE1	2.61	0.54
1:E:23:GLU:HG3	5:E:5579:HOH:O	2.08	0.54
1:B:435:LYS:HE2	5:B:5419:HOH:O	2.07	0.54
1:E:316:TYR:O	1:E:317:LYS:HD2	2.08	0.54
1:C:335:THR:HA	5:C:5267:HOH:O	2.07	0.54
1:E:83:GLN:HE22	1:F:430:TYR:H	1.56	0.54
1:F:17:VAL:O	1:F:18:ASP:HB2	2.06	0.54
1:A:326:MET:O	1:A:377:ILE:HD11	2.08	0.53
1:B:41:LEU:HB3	1:B:42:PRO:HD3	1.91	0.53
1:D:305:GLY:HA2	5:D:5535:HOH:O	2.08	0.53
1:D:379:LYS:HG3	5:D:5405:HOH:O	2.08	0.53
1:A:230:ILE:HD11	1:A:377:ILE:HG21	1.90	0.53
1:A:176:ILE:CG2	1:A:177:PRO:HD3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD11	1:B:377:ILE:HG21	1.90	0.52
1:F:280:LEU:CD1	1:F:344:LEU:HD21	2.25	0.52
1:F:184:TYR:CE1	1:F:384:PRO:HG3	2.45	0.52
1:F:230:ILE:HD11	1:F:377:ILE:HG21	1.92	0.52
1:E:90:TYR:CE2	1:E:228:ASN:OD1	2.61	0.52
1:C:105:LYS:HE3	5:C:5477:HOH:O	2.08	0.52
1:F:218:LYS:HD2	5:F:5546:HOH:O	2.10	0.52
1:F:324:LYS:NZ	5:F:5571:HOH:O	2.42	0.52
1:F:205:PHE:HE2	1:F:391:LEU:HD13	1.74	0.52
1:B:112:THR:O	1:B:116:THR:HG23	2.09	0.52
1:E:90:TYR:HH	1:E:200:ASN:CG	2.10	0.52
1:A:433:LEU:HD23	5:A:5419:HOH:O	2.10	0.52
1:B:316:TYR:O	1:B:317:LYS:HD2	2.09	0.52
1:C:128:PHE:CZ	1:C:148:ALA:HB1	2.45	0.52
1:A:196:ARG:H	1:A:204:ASN:ND2	2.09	0.51
1:D:41:LEU:HB3	1:D:42:PRO:HD3	1.92	0.51
1:D:90:TYR:CE2	1:D:94:ILE:HD11	2.45	0.51
1:D:288:LYS:HG2	1:D:291:ASN:ND2	2.25	0.51
1:E:200:ASN:OD1	1:E:203:GLU:HG3	2.10	0.51
1:E:330:CYS:SG	1:E:377:ILE:HG13	2.51	0.51
1:A:330:CYS:SG	1:A:377:ILE:HG13	2.51	0.51
1:F:195:PRO:HA	1:F:204:ASN:HD21	1.75	0.51
1:E:196:ARG:H	1:E:204:ASN:ND2	2.08	0.51
1:D:90:TYR:CD1	1:D:231:LEU:HB3	2.46	0.50
1:A:417:ARG:HB3	1:B:314:ARG:HG2	1.91	0.50
1:C:330:CYS:SG	1:C:377:ILE:HG13	2.51	0.50
1:F:117:ASN:ND2	5:F:5512:HOH:O	2.44	0.50
1:F:302:LYS:O	1:F:303:ASN:CB	2.55	0.50
1:A:314:ARG:HG2	1:B:417:ARG:HB3	1.94	0.50
1:E:90:TYR:CD2	1:E:228:ASN:HA	2.45	0.50
1:F:176:ILE:HG22	1:F:177:PRO:HD3	1.93	0.50
1:B:195:PRO:HA	1:B:204:ASN:HD21	1.76	0.50
1:A:327:GLN:O	1:A:330:CYS:HB2	2.11	0.50
1:D:90:TYR:CD1	1:D:231:LEU:HB2	2.47	0.49
1:A:90:TYR:CD1	1:A:231:LEU:HB2	2.47	0.49
1:F:205:PHE:CE2	1:F:391:LEU:HD13	2.48	0.49
1:F:324:LYS:CE	5:F:5504:HOH:O	2.59	0.49
1:E:159:ILE:HB	1:E:165:ARG:NH2	2.04	0.49
1:B:132:PHE:CZ	1:B:141:ILE:HA	2.48	0.49
1:B:435:LYS:NZ	5:B:5419:HOH:O	2.45	0.49
1:E:314:ARG:HG2	1:F:417:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:NH1	3:B:5048:SO4:O3	2.40	0.48
1:E:159:ILE:HG13	1:E:160:ALA:N	2.28	0.48
1:A:324:LYS:NZ	5:A:5582:HOH:O	2.45	0.48
1:D:195:PRO:HA	1:D:204:ASN:HD21	1.77	0.48
1:A:324:LYS:CE	5:A:5582:HOH:O	2.62	0.48
1:D:391:LEU:HD12	1:D:391:LEU:O	2.13	0.48
1:D:132:PHE:CZ	1:D:141:ILE:HA	2.48	0.48
1:E:378:LEU:HD22	1:E:391:LEU:HD13	1.96	0.48
1:E:90:TYR:HH	1:E:202:ALA:H	1.61	0.48
1:A:41:LEU:HB3	1:A:42:PRO:HD3	1.95	0.48
1:C:295:PHE:HA	1:C:298:GLN:HE21	1.79	0.48
1:D:340:LYS:CG	1:D:341:ASP:H	2.24	0.48
1:D:340:LYS:CG	1:D:341:ASP:N	2.77	0.47
1:F:128:PHE:CZ	1:F:148:ALA:HB1	2.49	0.47
1:A:430:TYR:H	1:B:83:GLN:HE22	1.61	0.47
1:F:162:PRO:HA	5:F:5289:HOH:O	2.13	0.47
1:C:83:GLN:HE22	1:D:430:TYR:H	1.58	0.47
1:A:229:ARG:NH2	5:A:5246:HOH:O	2.27	0.47
1:D:122:HIS:O	1:D:125:ILE:HB	2.14	0.47
1:F:230:ILE:HD11	1:F:377:ILE:CG2	2.45	0.47
1:B:435:LYS:CE	5:B:5419:HOH:O	2.62	0.47
1:C:195:PRO:HA	1:C:204:ASN:HD21	1.80	0.47
1:E:90:TYR:CE1	1:E:91:GLU:CD	2.88	0.47
1:A:248:LEU:HD12	1:B:248:LEU:HD12	1.97	0.47
1:A:378:LEU:HD22	1:A:391:LEU:HD13	1.95	0.47
1:B:90:TYR:OH	1:B:395:ALA:HA	2.14	0.47
1:C:277:GLU:HG3	1:C:385:THR:HG22	1.96	0.47
1:C:294:ALA:O	1:C:298:GLN:HG3	2.14	0.47
1:E:90:TYR:CZ	1:E:202:ALA:N	2.72	0.47
1:F:132:PHE:CZ	1:F:141:ILE:HA	2.50	0.47
1:A:196:ARG:H	1:A:204:ASN:HD21	1.62	0.47
1:C:221:PRO:HB2	3:C:5046:SO4:O1	2.14	0.47
1:C:277:GLU:HG3	1:C:385:THR:CG2	2.45	0.47
1:D:296:ILE:HG22	1:D:300:LYS:HE3	1.97	0.47
1:F:353:LYS:HE3	5:F:5576:HOH:O	2.15	0.47
1:C:383:ILE:HD13	1:C:391:LEU:CD2	2.45	0.46
1:E:159:ILE:HG23	5:E:5434:HOH:O	2.14	0.46
1:F:41:LEU:HB3	1:F:42:PRO:HD3	1.98	0.46
1:A:132:PHE:CZ	1:A:141:ILE:HA	2.51	0.46
1:B:330:CYS:SG	1:B:377:ILE:HG13	2.56	0.46
1:C:132:PHE:CZ	1:C:141:ILE:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LYS:HE2	5:D:5327:HOH:O	2.15	0.46
1:E:292:ILE:HG21	1:E:354:ILE:HD13	1.98	0.45
1:C:324:LYS:HG2	1:C:325:ILE:HG13	1.99	0.45
1:F:17:VAL:HG12	1:F:45:LEU:HD13	1.98	0.45
1:C:383:ILE:HD13	1:C:391:LEU:HD23	1.98	0.45
1:E:90:TYR:CD1	1:E:91:GLU:OE1	2.69	0.45
1:E:195:PRO:HA	1:E:204:ASN:HD21	1.82	0.45
1:D:105:LYS:CE	5:D:5327:HOH:O	2.65	0.45
1:E:230:ILE:CG2	1:E:391:LEU:HD21	2.47	0.45
1:C:171:ARG:CZ	3:C:5041:SO4:O1	2.64	0.45
1:A:90:TYR:OH	1:A:395:ALA:HA	2.17	0.45
1:A:195:PRO:HA	1:A:204:ASN:HD21	1.82	0.45
1:C:316:TYR:CZ	1:C:321:PRO:HD2	2.52	0.45
3:B:5045:SO4:O2	5:B:5575:HOH:O	2.21	0.44
1:A:280:LEU:HD22	1:A:388:PHE:HE2	1.82	0.44
1:C:299:VAL:HG13	4:C:5003:CMX:H2A	1.98	0.44
1:E:225:ARG:NH1	3:E:5050:SO4:O3	2.45	0.44
1:A:363:GLN:HA	1:A:363:GLN:NE2	2.31	0.44
1:C:311:PHE:CE1	1:C:368:PRO:HG3	2.53	0.44
1:F:324:LYS:CD	5:F:5560:HOH:O	2.65	0.44
1:C:205:PHE:CE2	1:C:391:LEU:HD13	2.41	0.44
1:E:371:ASP:OD2	4:E:5005:CMX:O22	2.36	0.44
1:F:90:TYR:CD1	1:F:231:LEU:CB	3.00	0.44
1:D:90:TYR:O	1:D:94:ILE:HG13	2.18	0.44
1:E:280:LEU:HD11	1:E:344:LEU:HD23	2.00	0.43
1:C:299:VAL:CG1	4:C:5003:CMX:H2A	2.48	0.43
1:F:51:ASP:OD1	1:F:56:GLU:OE1	2.35	0.43
1:E:430:TYR:H	1:F:83:GLN:HE21	1.64	0.43
1:D:378:LEU:HD22	1:D:391:LEU:HD23	2.00	0.43
1:E:20:LYS:HE3	5:E:5519:HOH:O	2.17	0.43
1:E:131:GLY:HA2	1:F:127:ASN:HB2	1.99	0.43
1:F:90:TYR:CE2	1:F:94:ILE:CG1	3.01	0.43
1:C:176:ILE:CG2	1:C:177:PRO:HD3	2.48	0.43
1:C:127:ASN:HB2	1:D:131:GLY:HA2	2.00	0.43
1:D:281:LYS:HD3	5:D:5332:HOH:O	2.18	0.43
1:E:417:ARG:HB3	1:F:314:ARG:HG2	2.00	0.43
1:E:391:LEU:C	1:E:391:LEU:HD23	2.39	0.43
1:E:127:ASN:HB2	1:F:131:GLY:HA2	2.01	0.42
1:A:54:TYR:O	1:B:418:PRO:HA	2.19	0.42
1:B:230:ILE:HD11	1:B:377:ILE:CG2	2.49	0.42
1:B:51:ASP:OD1	1:B:56:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TYR:C	1:B:317:LYS:HD2	2.40	0.42
1:A:35:VAL:HG12	1:B:48:PHE:HB2	2.01	0.42
1:C:324:LYS:HG2	1:C:325:ILE:H	1.82	0.42
1:A:277:GLU:HG3	1:A:385:THR:CG2	2.49	0.42
1:B:90:TYR:CD1	1:B:231:LEU:HB3	2.53	0.42
1:E:307:LYS:CE	5:E:5407:HOH:O	2.52	0.42
1:B:158:ASP:HA	5:B:5312:HOH:O	2.20	0.42
1:E:156:ALA:C	1:E:158:ASP:H	2.21	0.42
1:F:324:LYS:HE3	5:F:5504:HOH:O	2.19	0.42
1:F:321:PRO:O	1:F:324:LYS:CG	2.62	0.42
1:C:417:ARG:HB3	1:D:314:ARG:HG2	2.02	0.42
1:D:275:ALA:O	1:D:279:VAL:HG23	2.20	0.42
1:A:128:PHE:HE2	1:B:132:PHE:CE1	2.38	0.41
1:C:378:LEU:HD22	1:C:391:LEU:HD23	2.01	0.41
1:A:112:THR:O	1:A:116:THR:HG23	2.20	0.41
1:E:328:GLN:NE2	5:E:5498:HOH:O	2.48	0.41
1:F:345:LEU:HA	1:F:376:ILE:HD13	2.03	0.41
1:B:223:LEU:HD22	1:B:381:MET:HG2	2.02	0.41
1:C:35:VAL:CG2	1:D:50:PHE:HB2	2.51	0.41
1:C:314:ARG:HG2	1:D:417:ARG:HB3	2.02	0.41
1:E:277:GLU:HG3	1:E:385:THR:CG2	2.48	0.41
1:E:196:ARG:H	1:E:204:ASN:HD21	1.68	0.41
1:A:280:LEU:HD22	1:A:388:PHE:CE2	2.55	0.41
1:A:330:CYS:SG	1:A:377:ILE:CG1	3.09	0.40
1:F:371:ASP:OD2	4:F:5006:CMX:O22	2.39	0.40
1:B:90:TYR:CE1	1:B:231:LEU:HD13	2.56	0.40
1:C:90:TYR:HE1	1:C:235:ALA:HB2	1.86	0.40
1:C:327:GLN:O	1:C:330:CYS:HB2	2.21	0.40
1:E:156:ALA:C	1:E:158:ASP:N	2.75	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:5541:HOH:O	5:F:5575:HOH:O[2_554]	1.99	0.21
5:A:5597:HOH:O	5:F:5226:HOH:O[4_445]	2.19	0.01

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	414/436 (95%)	407 (98%)	7 (2%)	0	100	100
1	B	424/436 (97%)	416 (98%)	8 (2%)	0	100	100
1	C	424/436 (97%)	416 (98%)	8 (2%)	0	100	100
1	D	413/436 (95%)	403 (98%)	10 (2%)	0	100	100
1	E	424/436 (97%)	413 (97%)	10 (2%)	1 (0%)	47	33
1	F	416/436 (95%)	406 (98%)	8 (2%)	2 (0%)	29	15
All	All	2515/2616 (96%)	2461 (98%)	51 (2%)	3 (0%)	51	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	160	ALA
1	F	303	ASN
1	F	302	LYS

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	340/354 (96%)	333 (98%)	7 (2%)	53	38
1	B	345/354 (98%)	335 (97%)	10 (3%)	42	26
1	C	346/354 (98%)	334 (96%)	12 (4%)	36	18
1	D	340/354 (96%)	331 (97%)	9 (3%)	46	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	346/354 (98%)	336 (97%)	10 (3%)	42	26
1	F	342/354 (97%)	332 (97%)	10 (3%)	42	26
All	All	2059/2124 (97%)	2001 (97%)	58 (3%)	43	27

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	124	GLN
1	A	238	GLU
1	A	248	LEU
1	A	272	HIS
1	A	328	GLN
1	A	392	PHE
1	B	17	VAL
1	B	238	GLU
1	B	248	LEU
1	B	260	ILE
1	B	272	HIS
1	B	280	LEU
1	B	289	LYS
1	B	317	LYS
1	B	328	GLN
1	B	392	PHE
1	C	124	GLN
1	C	230	ILE
1	C	238	GLU
1	C	248	LEU
1	C	272	HIS
1	C	285	ARG
1	C	288	LYS
1	C	324	LYS
1	C	341	ASP
1	C	344	LEU
1	C	391	LEU
1	C	392	PHE
1	D	21	SER
1	D	117	ASN
1	D	238	GLU
1	D	248	LEU
1	D	272	HIS

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Mol	Chain	Res	Type
1	D	344	LEU
1	D	391	LEU
1	D	392	PHE
1	D	433	LEU
1	E	90	TYR
1	E	117	ASN
1	E	124	GLN
1	E	230	ILE
1	E	238	GLU
1	E	248	LEU
1	E	272	HIS
1	E	317	LYS
1	E	344	LEU
1	E	392	PHE
1	F	28	SER
1	F	105	LYS
1	F	117	ASN
1	F	238	GLU
1	F	248	LEU
1	F	272	HIS
1	F	303	ASN
1	F	324	LYS
1	F	391	LEU
1	F	392	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	204	ASN
1	A	239	GLN
1	A	363	GLN
1	B	83	GLN
1	B	117	ASN
1	B	164	ASN
1	B	204	ASN
1	C	44	GLN
1	C	83	GLN
1	C	204	ASN
1	C	239	GLN
1	C	298	GLN
1	D	83	GLN

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Mol	Chain	Res	Type
1	D	204	ASN
1	D	239	GLN
1	D	291	ASN
1	D	298	GLN
1	E	83	GLN
1	E	204	ASN
1	E	239	GLN
1	E	303	ASN
1	F	83	GLN
1	F	127	ASN
1	F	204	ASN
1	F	298	GLN
1	F	303	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

53 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	$\#\|Z\| > 2$
3	SO4	E	5023	-	4,4,4	0.62	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	F	5044	-	4,4,4	0.64	0	6,6,6	0.09	0
3	SO4	B	5013	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	E	5025	-	4,4,4	0.62	0	6,6,6	0.05	0
4	CMX	A	5001	-	45,53,53	1.07	3 (6%)	57,79,79	1.05	2 (3%)
3	SO4	B	5039	-	4,4,4	0.63	0	6,6,6	0.09	0
4	CMX	D	5004	-	45,53,53	1.08	3 (6%)	57,79,79	1.04	3 (5%)
3	SO4	A	5047	1	4,4,4	0.63	0	6,6,6	0.15	0
3	SO4	D	5021	-	4,4,4	0.62	0	6,6,6	0.07	0
3	SO4	A	5040	-	4,4,4	0.64	0	6,6,6	0.09	0
3	SO4	D	5028	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	B	5053	-	4,4,4	0.64	0	6,6,6	0.06	0
3	SO4	D	5018	-	4,4,4	0.63	0	6,6,6	0.07	0
3	SO4	A	5052	-	4,4,4	0.64	0	6,6,6	0.07	0
3	SO4	A	5029	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	E	5037	-	4,4,4	0.63	0	6,6,6	0.07	0
2	OAA	C	5009	-	8,8,8	1.19	0	9,10,10	1.25	1 (11%)
4	CMX	E	5005	-	45,53,53	1.08	3 (6%)	57,79,79	1.07	3 (5%)
3	SO4	C	5041	-	4,4,4	0.63	0	6,6,6	0.17	0
3	SO4	D	5049	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	E	5043	-	4,4,4	0.65	0	6,6,6	0.07	0
3	SO4	E	5050	-	4,4,4	0.63	0	6,6,6	0.08	0
4	CMX	B	5002	-	45,53,53	1.08	3 (6%)	57,79,79	1.04	2 (3%)
3	SO4	F	5026	-	4,4,4	0.63	0	6,6,6	0.06	0
3	SO4	F	5038	-	4,4,4	0.61	0	6,6,6	0.09	0
3	SO4	C	5046	-	4,4,4	0.63	0	6,6,6	0.06	0
3	SO4	E	5024	-	4,4,4	0.62	0	6,6,6	0.07	0
3	SO4	C	5019	-	4,4,4	0.63	0	6,6,6	0.07	0
4	CMX	C	5003	-	45,53,53	1.08	3 (6%)	57,79,79	1.07	2 (3%)
2	OAA	F	5012	-	8,8,8	1.18	0	9,10,10	1.44	1 (11%)
3	SO4	B	5016	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	C	5020	-	4,4,4	0.63	0	6,6,6	0.06	0
3	SO4	F	5051	-	4,4,4	0.63	0	6,6,6	0.07	0
3	SO4	A	5015	-	4,4,4	0.62	0	6,6,6	0.04	0
3	SO4	E	5033	-	4,4,4	0.62	0	6,6,6	0.06	0
3	SO4	A	5014	-	4,4,4	0.62	0	6,6,6	0.06	0
2	OAA	A	5007	-	8,8,8	1.17	0	9,10,10	1.29	1 (11%)
3	SO4	F	5034	-	4,4,4	0.62	0	6,6,6	0.05	0
2	OAA	E	5011	-	8,8,8	1.19	0	9,10,10	1.24	1 (11%)
3	SO4	C	5027	-	4,4,4	0.62	0	6,6,6	0.05	0
3	SO4	B	5017	-	4,4,4	0.63	0	6,6,6	0.10	0
3	SO4	B	5030	-	4,4,4	0.63	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CMX	F	5006	-	45,53,53	1.08	3 (6%)	57,79,79	1.07	2 (3%)
3	SO4	B	5045	-	4,4,4	0.63	0	6,6,6	0.07	0
3	SO4	D	5032	-	4,4,4	0.63	0	6,6,6	0.07	0
3	SO4	F	5022	-	4,4,4	0.63	0	6,6,6	0.04	0
3	SO4	B	5048	-	4,4,4	0.63	0	6,6,6	0.06	0
3	SO4	A	5035	-	4,4,4	0.63	0	6,6,6	0.07	0
2	OAA	B	5008	-	8,8,8	1.17	0	9,10,10	1.40	1 (11%)
3	SO4	D	5042	-	4,4,4	0.63	0	6,6,6	0.10	0
2	OAA	D	5010	-	8,8,8	1.19	0	9,10,10	1.39	1 (11%)
3	SO4	C	5031	-	4,4,4	0.63	0	6,6,6	0.05	0
3	SO4	B	5036	-	4,4,4	0.62	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OAA	A	5007	-	-	0/8/8/8	-
2	OAA	E	5011	-	-	0/8/8/8	-
4	CMX	F	5006	-	-	6/47/67/67	0/3/3/3
4	CMX	C	5003	-	-	5/47/67/67	0/3/3/3
4	CMX	A	5001	-	-	6/47/67/67	0/3/3/3
2	OAA	F	5012	-	-	0/8/8/8	-
4	CMX	D	5004	-	-	6/47/67/67	0/3/3/3
2	OAA	C	5009	-	-	0/8/8/8	-
2	OAA	B	5008	-	-	0/8/8/8	-
4	CMX	E	5005	-	-	6/47/67/67	0/3/3/3
2	OAA	D	5010	-	-	0/8/8/8	-
4	CMX	B	5002	-	-	6/47/67/67	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5002	CMX	P2A-O4A	2.94	1.61	1.50
4	C	5003	CMX	P2A-O4A	2.94	1.61	1.50
4	A	5001	CMX	P1A-O1A	2.93	1.61	1.50
4	E	5005	CMX	P1A-O1A	2.92	1.61	1.50
4	D	5004	CMX	P2A-O4A	2.92	1.61	1.50
4	E	5005	CMX	P2A-O4A	2.92	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5003	CMX	P1A-O1A	2.92	1.61	1.50
4	B	5002	CMX	P1A-O1A	2.91	1.61	1.50
4	D	5004	CMX	P1A-O1A	2.91	1.61	1.50
4	F	5006	CMX	P2A-O4A	2.90	1.61	1.50
4	F	5006	CMX	P1A-O1A	2.90	1.61	1.50
4	A	5001	CMX	P2A-O4A	2.87	1.61	1.50
4	B	5002	CMX	O4B-C1B	2.48	1.44	1.41
4	C	5003	CMX	O4B-C1B	2.44	1.44	1.41
4	D	5004	CMX	O4B-C1B	2.41	1.44	1.41
4	F	5006	CMX	O4B-C1B	2.38	1.44	1.41
4	E	5005	CMX	O4B-C1B	2.37	1.44	1.41
4	A	5001	CMX	O4B-C1B	2.32	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5006	CMX	N3A-C2A-N1A	-4.51	121.62	128.68
4	C	5003	CMX	N3A-C2A-N1A	-4.46	121.70	128.68
4	B	5002	CMX	N3A-C2A-N1A	-4.44	121.75	128.68
4	D	5004	CMX	N3A-C2A-N1A	-4.39	121.81	128.68
4	A	5001	CMX	N3A-C2A-N1A	-4.38	121.83	128.68
4	E	5005	CMX	N3A-C2A-N1A	-4.35	121.88	128.68
2	F	5012	OAA	O4-C4-C3	-3.32	117.29	121.72
2	B	5008	OAA	O4-C4-C3	-3.18	117.47	121.72
2	D	5010	OAA	O4-C4-C3	-3.16	117.50	121.72
4	F	5006	CMX	P2A-O3A-P1A	-2.86	123.02	132.83
2	A	5007	OAA	O4-C4-C3	-2.86	117.91	121.72
2	C	5009	OAA	O4-C4-C3	-2.83	117.94	121.72
4	E	5005	CMX	P2A-O3A-P1A	-2.71	123.51	132.83
4	C	5003	CMX	P2A-O3A-P1A	-2.71	123.51	132.83
4	A	5001	CMX	P2A-O3A-P1A	-2.70	123.56	132.83
4	B	5002	CMX	P2A-O3A-P1A	-2.64	123.76	132.83
2	E	5011	OAA	O4-C4-C3	-2.64	118.19	121.72
4	D	5004	CMX	P2A-O3A-P1A	-2.50	124.25	132.83
4	E	5005	CMX	O6A-CCP-CBP	-2.02	107.31	110.55
4	D	5004	CMX	O21-C2-C1	-2.01	116.61	123.08

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5001	CMX	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
4	A	5001	CMX	C5B-O5B-P1A-O2A
4	B	5002	CMX	C5B-O5B-P1A-O1A
4	B	5002	CMX	C5B-O5B-P1A-O2A
4	C	5003	CMX	C5B-O5B-P1A-O1A
4	C	5003	CMX	C5B-O5B-P1A-O2A
4	D	5004	CMX	C5B-O5B-P1A-O1A
4	D	5004	CMX	C5B-O5B-P1A-O2A
4	E	5005	CMX	C5B-O5B-P1A-O1A
4	E	5005	CMX	C5B-O5B-P1A-O2A
4	F	5006	CMX	C5B-O5B-P1A-O2A
4	F	5006	CMX	C5B-O5B-P1A-O1A
4	A	5001	CMX	P1A-O3A-P2A-O5A
4	E	5005	CMX	P1A-O3A-P2A-O5A
4	F	5006	CMX	P1A-O3A-P2A-O5A
4	D	5004	CMX	C2P-C1-C2-O22
4	B	5002	CMX	C2P-C1-C2-O22
4	E	5005	CMX	C2P-C1-C2-O22
4	A	5001	CMX	C2P-C1-C2-O22
4	D	5004	CMX	C2P-C1-C2-O21
4	C	5003	CMX	C2P-C1-C2-O22
4	E	5005	CMX	C2P-C1-C2-O21
4	A	5001	CMX	C2P-C1-C2-O21
4	F	5006	CMX	C2P-C1-C2-O22
4	B	5002	CMX	C2P-C1-C2-O21
4	F	5006	CMX	C2P-C1-C2-O21
4	C	5003	CMX	C2P-C1-C2-O21
4	A	5001	CMX	C5B-O5B-P1A-O3A
4	B	5002	CMX	C5B-O5B-P1A-O3A
4	C	5003	CMX	C5B-O5B-P1A-O3A
4	D	5004	CMX	C5B-O5B-P1A-O3A
4	E	5005	CMX	C5B-O5B-P1A-O3A
4	F	5006	CMX	C5B-O5B-P1A-O3A
4	B	5002	CMX	P1A-O3A-P2A-O5A
4	D	5004	CMX	P1A-O3A-P2A-O5A

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5005	CMX	1	0
3	C	5041	SO4	3	0
3	E	5050	SO4	1	0

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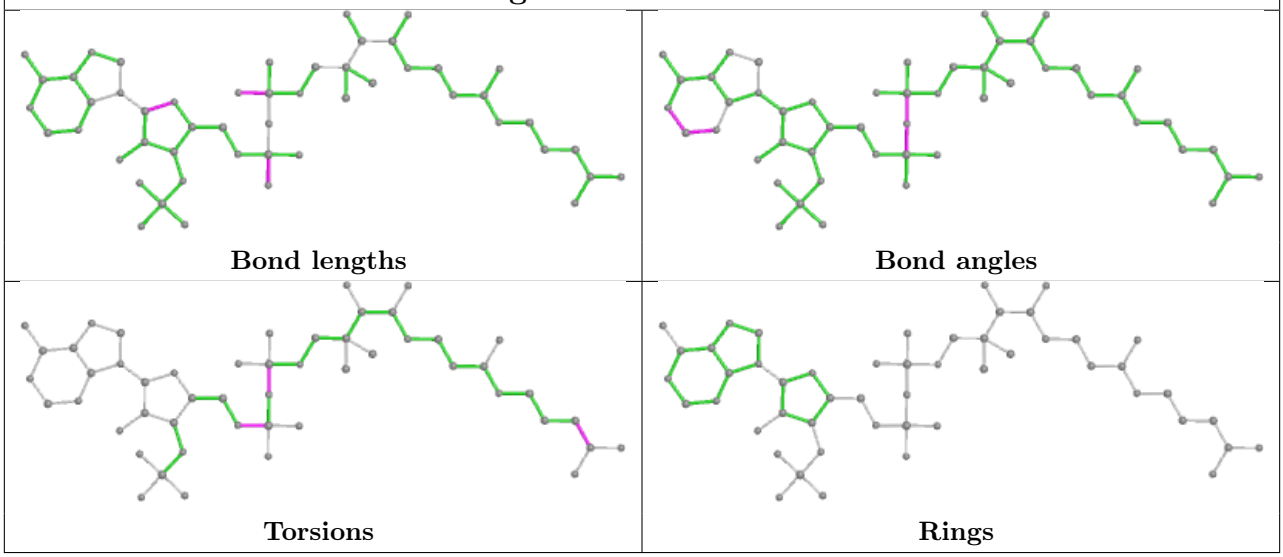
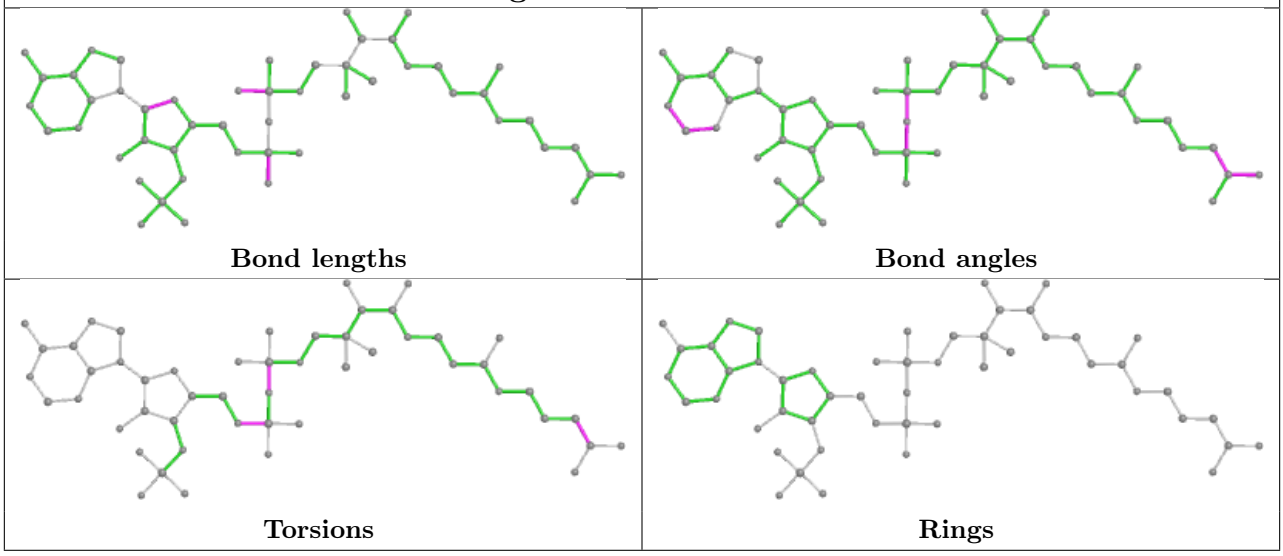
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5038	SO4	1	0
3	C	5046	SO4	1	0
4	C	5003	CMX	2	0
4	F	5006	CMX	1	0
3	B	5045	SO4	1	0
3	B	5048	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

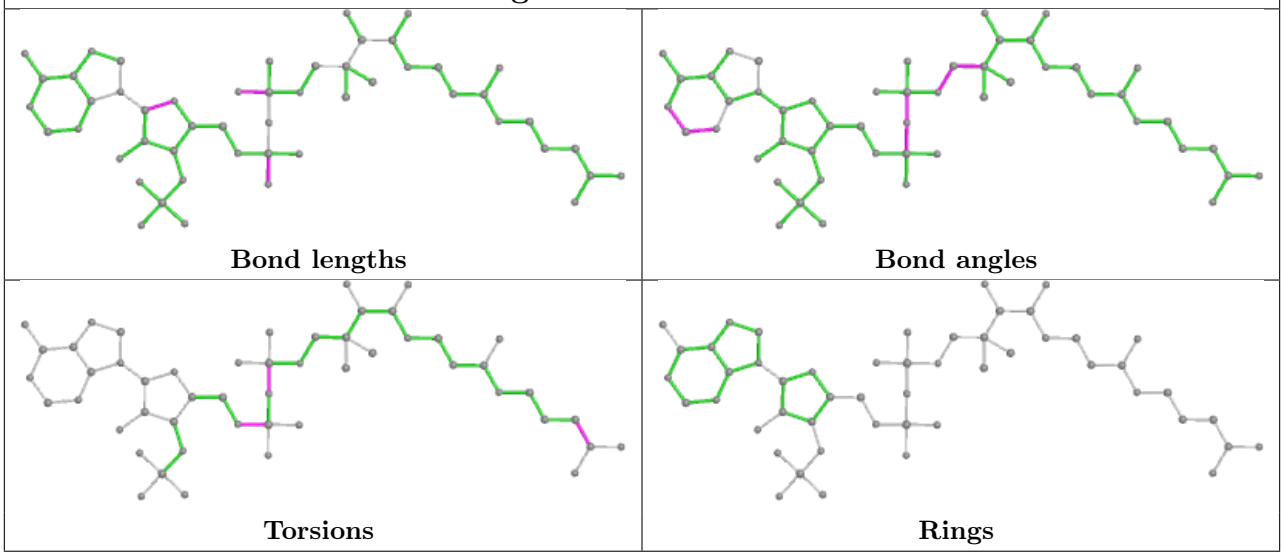
Ligand CMX A 5001



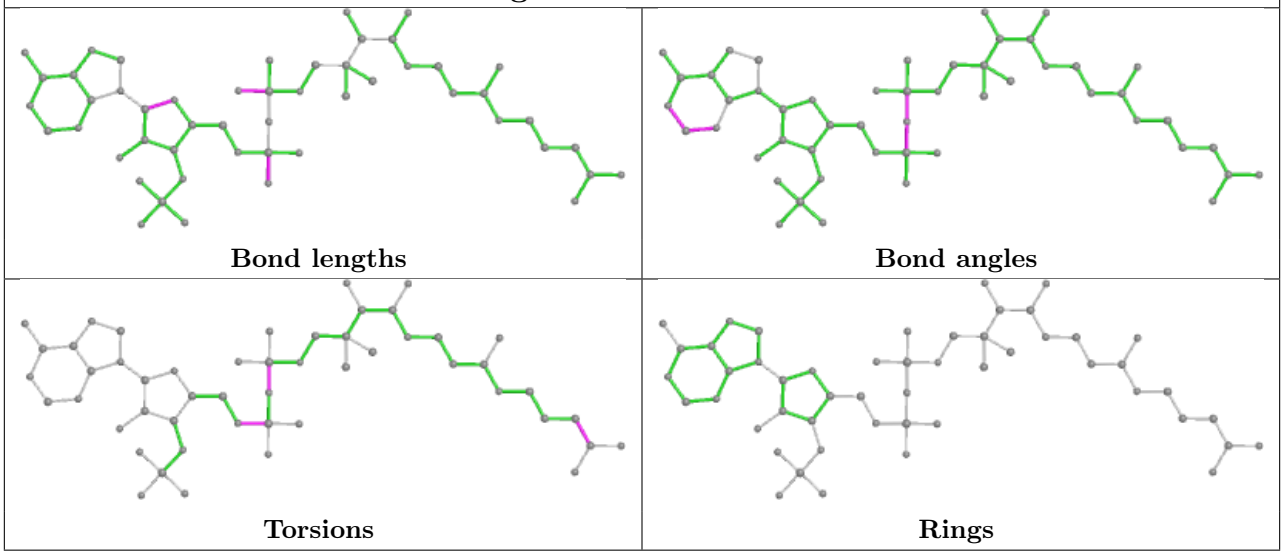
Ligand CMX D 5004



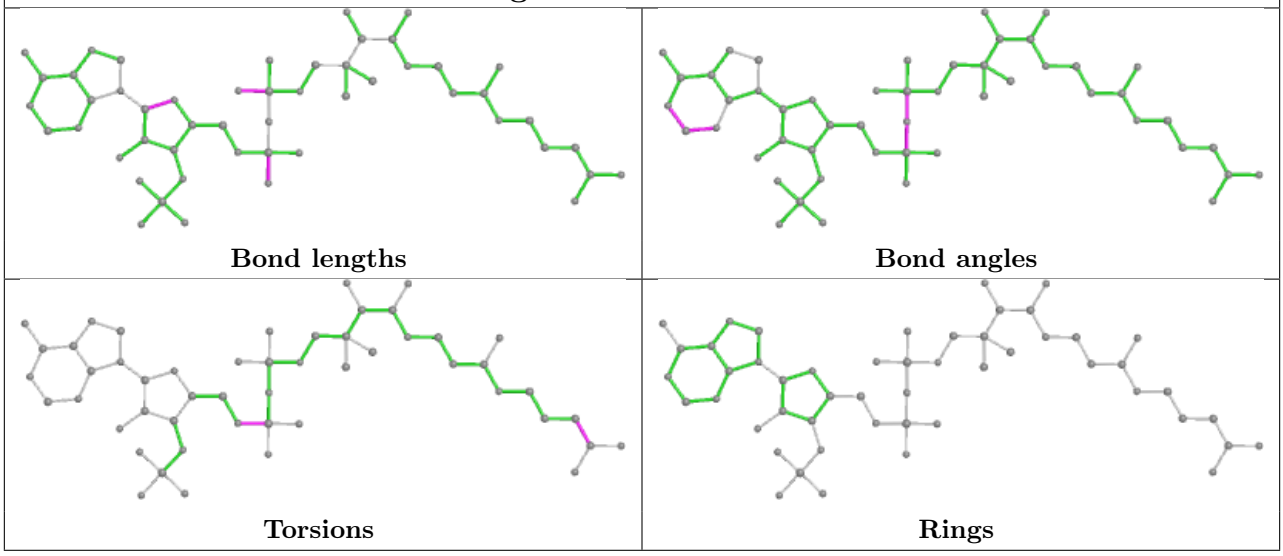
Ligand CMX E 5005



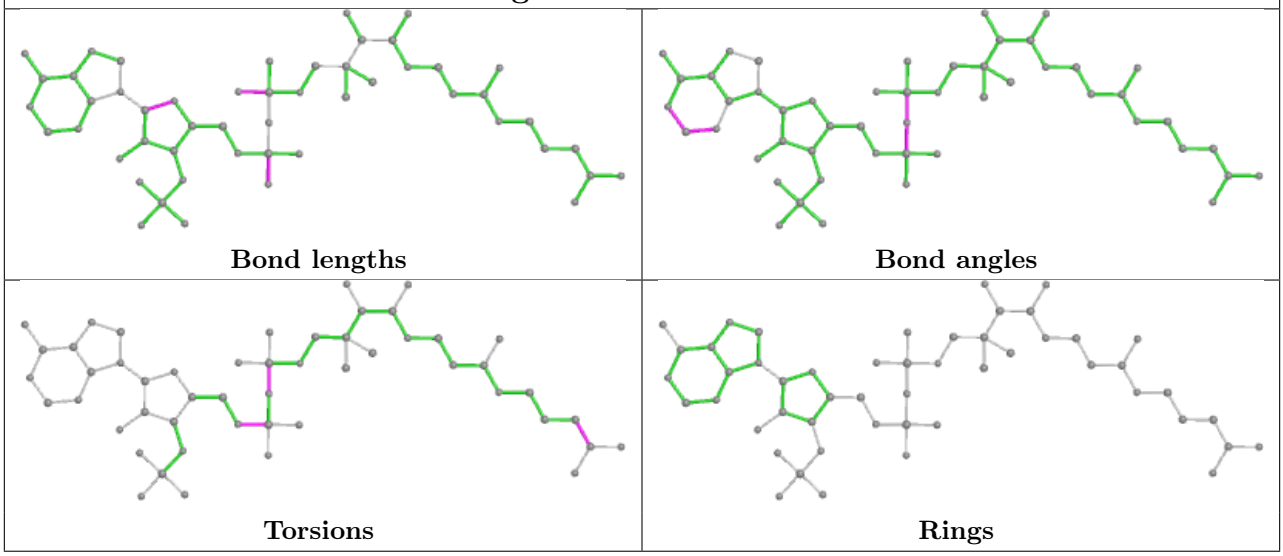
Ligand CMX B 5002



Ligand CMX C 5003



Ligand CMX F 5006



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	418/436 (95%)	0.15	19 (4%)	33	32	15, 22, 39, 57	0
1	B	426/436 (97%)	0.27	29 (6%)	17	16	16, 23, 45, 59	0
1	C	426/436 (97%)	0.23	21 (4%)	29	28	16, 23, 47, 60	0
1	D	417/436 (95%)	0.37	39 (9%)	8	8	16, 24, 49, 66	0
1	E	426/436 (97%)	0.31	29 (6%)	17	16	15, 22, 46, 63	0
1	F	420/436 (96%)	0.23	25 (5%)	21	21	15, 23, 43, 58	0
All	All	2533/2616 (96%)	0.26	162 (6%)	19	18	15, 23, 46, 66	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	159	ILE	13.9
1	E	90	TYR	7.8
1	B	161	ILE	7.4
1	B	303	ASN	6.9
1	F	303	ASN	6.9
1	E	158	ASP	6.8
1	F	18	ASP	6.6
1	A	18	ASP	6.6
1	E	161	ILE	6.2
1	D	90	TYR	5.9
1	A	90	TYR	5.8
1	A	163	ALA	5.7
1	E	18	ASP	5.7
1	C	303	ASN	5.7
1	C	341	ASP	5.6
1	E	303	ASN	5.4
1	B	156	ALA	5.4
1	F	90	TYR	5.3
1	B	163	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	302	LYS	5.1
1	F	340	LYS	5.1
1	E	156	ALA	5.1
1	D	303	ASN	5.0
1	D	289	LYS	5.0
1	D	304	SER	4.9
1	F	163	ALA	4.8
1	D	290	GLU	4.6
1	D	339	ILE	4.6
1	B	90	TYR	4.5
1	E	157	ASN	4.5
1	B	338	GLY	4.5
1	D	18	ASP	4.5
1	E	340	LYS	4.4
1	F	155	ASP	4.4
1	A	302	LYS	4.4
1	C	18	ASP	4.4
1	F	302	LYS	4.4
1	B	19	GLY	4.4
1	E	162	PRO	4.3
1	D	338	GLY	4.3
1	B	158	ASP	4.3
1	F	19	GLY	4.3
1	C	340	LYS	4.2
1	B	162	PRO	4.2
1	B	159	ILE	4.2
1	E	163	ALA	4.2
1	F	304	SER	4.2
1	E	160	ALA	4.1
1	A	303	ASN	4.1
1	B	160	ALA	4.1
1	B	18	ASP	4.1
1	B	340	LYS	4.0
1	C	339	ILE	4.0
1	D	340	LYS	4.0
1	E	155	ASP	4.0
1	C	305	GLY	3.9
1	C	90	TYR	3.8
1	A	433	LEU	3.8
1	E	343	PRO	3.7
1	B	341	ASP	3.7
1	E	305	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	285	ARG	3.7
1	E	341	ASP	3.7
1	A	340	LYS	3.5
1	F	285	ARG	3.5
1	F	162	PRO	3.5
1	D	344	LEU	3.5
1	E	19	GLY	3.5
1	D	341	ASP	3.4
1	D	288	LYS	3.4
1	D	294	ALA	3.3
1	D	291	ASN	3.3
1	B	11	SER	3.3
1	B	344	LEU	3.3
1	A	285	ARG	3.3
1	B	302	LYS	3.3
1	C	19	GLY	3.2
1	B	305	GLY	3.2
1	B	157	ASN	3.2
1	A	19	GLY	3.2
1	C	342	ASP	3.2
1	C	363	GLN	3.1
1	C	338	GLY	3.1
1	E	434	ALA	3.1
1	E	302	LYS	3.0
1	C	297	ALA	3.0
1	F	341	ASP	2.9
1	C	359	ASP	2.9
1	A	164	ASN	2.9
1	D	293	PRO	2.9
1	C	158	ASP	2.9
1	C	294	ALA	2.9
1	D	20	LYS	2.9
1	D	305	GLY	2.8
1	B	301	ASP	2.7
1	F	288	LYS	2.7
1	D	343	PRO	2.7
1	B	337	LEU	2.7
1	D	357	SER	2.7
1	E	435	LYS	2.7
1	F	17	VAL	2.7
1	D	301	ASP	2.6
1	A	11	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	339	ILE	2.6
1	B	17	VAL	2.6
1	D	11	SER	2.6
1	E	288	LYS	2.6
1	D	292	ILE	2.5
1	D	412	GLY	2.5
1	E	344	LEU	2.5
1	B	342	ASP	2.5
1	B	339	ILE	2.5
1	C	17	VAL	2.5
1	A	304	SER	2.5
1	C	332	GLU	2.4
1	E	304	SER	2.4
1	B	20	LYS	2.4
1	F	164	ASN	2.4
1	A	12	THR	2.4
1	B	12	THR	2.4
1	B	288	LYS	2.4
1	F	23	GLU	2.4
1	F	305	GLY	2.4
1	E	105	LYS	2.4
1	D	284	ALA	2.4
1	A	341	ASP	2.3
1	B	155	ASP	2.3
1	A	290	GLU	2.3
1	F	339	ILE	2.3
1	C	285	ARG	2.3
1	D	298	GLN	2.3
1	A	20	LYS	2.3
1	C	105	LYS	2.3
1	D	295	PHE	2.3
1	C	301	ASP	2.3
1	A	284	ALA	2.3
1	D	434	ALA	2.3
1	E	285	ARG	2.3
1	F	338	GLY	2.2
1	D	17	VAL	2.2
1	D	359	ASP	2.2
1	F	20	LYS	2.2
1	F	260	ILE	2.2
1	A	305	GLY	2.2
1	F	335	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	164	ASN	2.2
1	D	335	THR	2.2
1	A	128	PHE	2.2
1	D	354	ILE	2.1
1	D	353	LYS	2.1
1	D	306	VAL	2.1
1	D	350	GLU	2.1
1	E	338	GLY	2.1
1	F	13	ALA	2.1
1	D	248	LEU	2.1
1	F	11	SER	2.1
1	F	264	ILE	2.1
1	D	14	THR	2.0
1	D	355	ALA	2.0
1	D	12	THR	2.0
1	E	433	LEU	2.0
1	B	335	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
3	SO4	E	5043	5/5	0.57	0.46	51,54,58,59	0
3	SO4	D	5049	5/5	0.59	0.33	72,73,74,75	0
3	SO4	A	5047	5/5	0.64	0.41	54,56,59,60	0
3	SO4	C	5041	5/5	0.68	0.44	61,62,63,64	0
3	SO4	B	5039	5/5	0.69	0.38	53,54,57,58	0
3	SO4	E	5037	5/5	0.71	0.46	55,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	5052	5/5	0.73	0.51	57,58,60,61	0
3	SO4	B	5048	5/5	0.76	0.40	58,60,62,62	0
3	SO4	B	5053	5/5	0.76	0.41	55,57,59,59	0
3	SO4	F	5044	5/5	0.76	0.44	56,57,58,59	0
3	SO4	F	5051	5/5	0.78	0.43	50,53,55,56	0
3	SO4	A	5040	5/5	0.79	0.41	54,54,57,57	0
3	SO4	D	5042	5/5	0.81	0.43	55,56,57,57	0
3	SO4	E	5050	5/5	0.81	0.34	59,59,60,60	0
3	SO4	F	5038	5/5	0.82	0.51	61,61,62,64	0
3	SO4	B	5045	5/5	0.83	0.42	58,58,59,62	0
3	SO4	A	5035	5/5	0.83	0.45	59,60,60,63	0
3	SO4	C	5046	5/5	0.84	0.42	62,63,64,65	0
3	SO4	B	5036	5/5	0.85	0.39	52,55,56,56	0
3	SO4	C	5027	5/5	0.89	0.27	69,70,71,71	0
3	SO4	C	5031	5/5	0.90	0.23	63,65,66,66	0
3	SO4	A	5029	5/5	0.91	0.19	52,52,54,55	0
4	CMX	B	5002	51/51	0.93	0.11	19,26,41,43	0
4	CMX	C	5003	51/51	0.93	0.10	18,25,39,42	0
4	CMX	E	5005	51/51	0.93	0.10	17,22,38,41	0
4	CMX	F	5006	51/51	0.93	0.11	18,22,37,40	0
3	SO4	B	5030	5/5	0.94	0.14	43,43,46,48	0
3	SO4	F	5034	5/5	0.94	0.18	51,52,53,54	0
3	SO4	D	5032	5/5	0.94	0.20	45,47,49,50	0
4	CMX	A	5001	51/51	0.95	0.10	16,23,41,42	0
4	CMX	D	5004	51/51	0.95	0.10	20,25,43,48	0
3	SO4	E	5033	5/5	0.96	0.18	46,47,47,50	0
3	SO4	D	5028	5/5	0.96	0.18	58,59,59,60	0
2	OAA	F	5012	9/9	0.97	0.11	16,18,22,23	0
3	SO4	B	5017	5/5	0.97	0.11	36,39,40,41	0
2	OAA	A	5007	9/9	0.97	0.14	19,20,24,24	0
2	OAA	B	5008	9/9	0.97	0.12	17,20,22,23	0
2	OAA	C	5009	9/9	0.97	0.13	19,20,22,23	0
2	OAA	D	5010	9/9	0.97	0.12	20,21,24,26	0
2	OAA	E	5011	9/9	0.98	0.14	16,18,23,23	0
3	SO4	A	5015	5/5	0.98	0.07	26,27,29,29	0
3	SO4	E	5024	5/5	0.98	0.18	42,43,44,46	0
3	SO4	E	5025	5/5	0.98	0.07	24,26,29,31	0
3	SO4	F	5022	5/5	0.98	0.08	23,23,25,29	0
3	SO4	C	5019	5/5	0.99	0.06	26,26,30,30	0
3	SO4	D	5018	5/5	0.99	0.09	28,28,31,31	0
3	SO4	D	5021	5/5	0.99	0.06	26,30,32,34	0
3	SO4	C	5020	5/5	0.99	0.09	27,30,31,33	0

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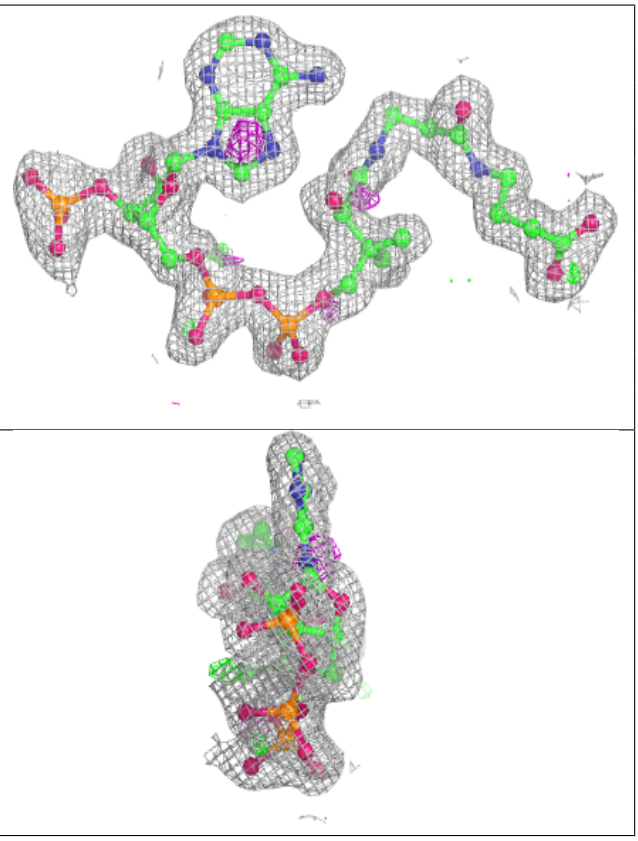
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	5013	5/5	0.99	0.04	24,25,26,30	0
3	SO4	B	5016	5/5	0.99	0.06	22,23,24,30	0
3	SO4	A	5014	5/5	0.99	0.05	25,28,32,33	0
3	SO4	F	5026	5/5	0.99	0.06	25,29,31,32	0
3	SO4	E	5023	5/5	0.99	0.07	23,27,29,29	0

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.

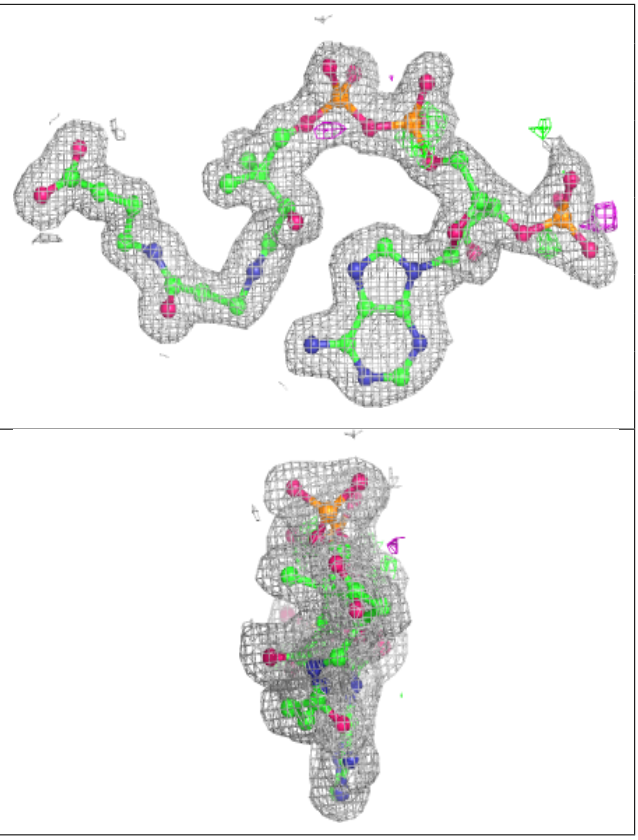
Electron density around CMX B 5002:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



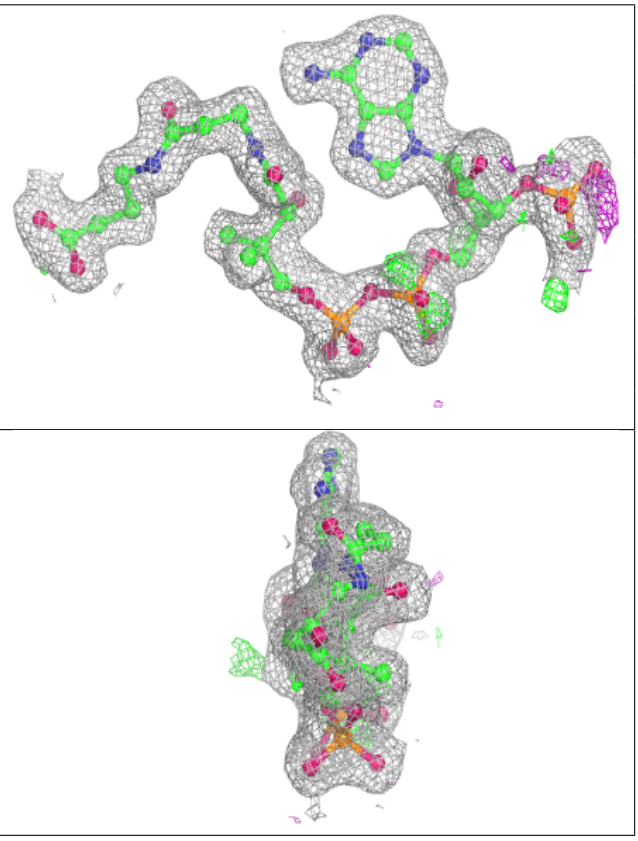
Electron density around CMX C 5003:

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



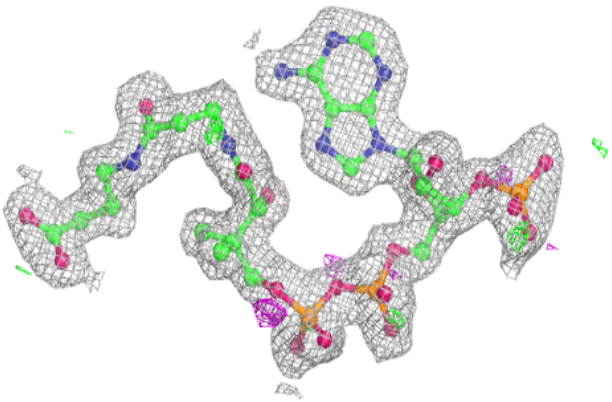
Electron density around CMX E 5005:

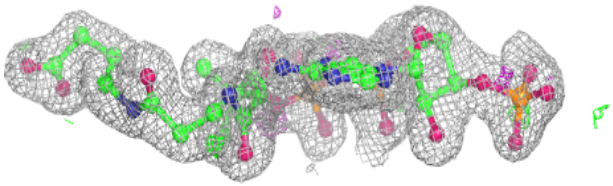
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

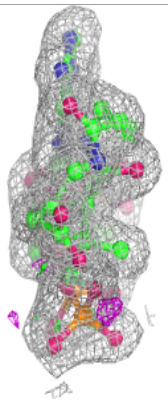


Electron density around CMX F 5006:

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

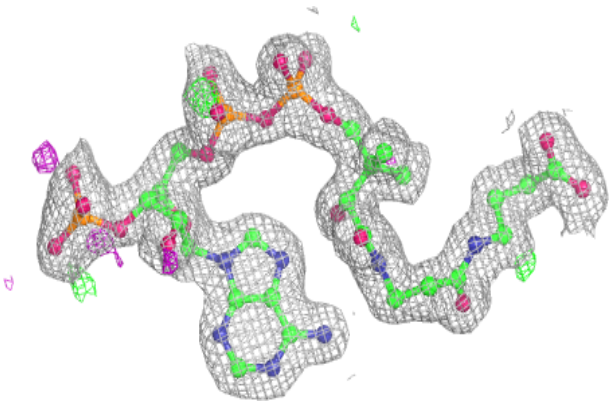


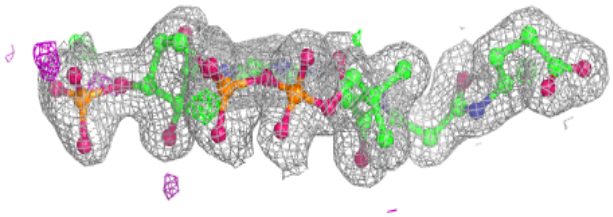


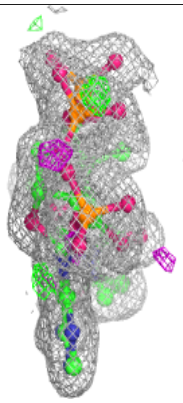


Electron density around CMX A 5001:

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

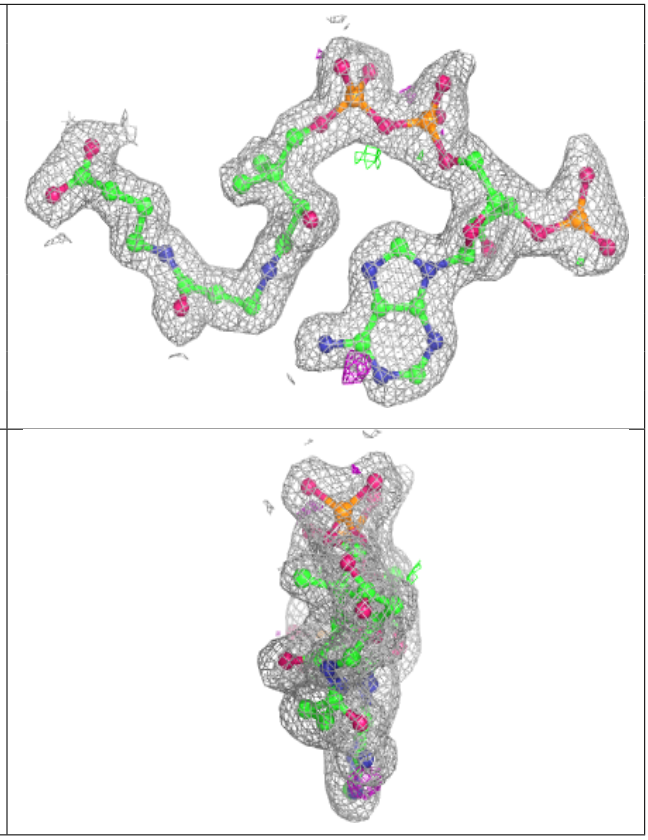






Electron density around CMX D 5004:

$2mF_o$-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.