Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 AM UTC

PDB ID	:	2H12 / pdb_00002h12
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 ⓘ 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:

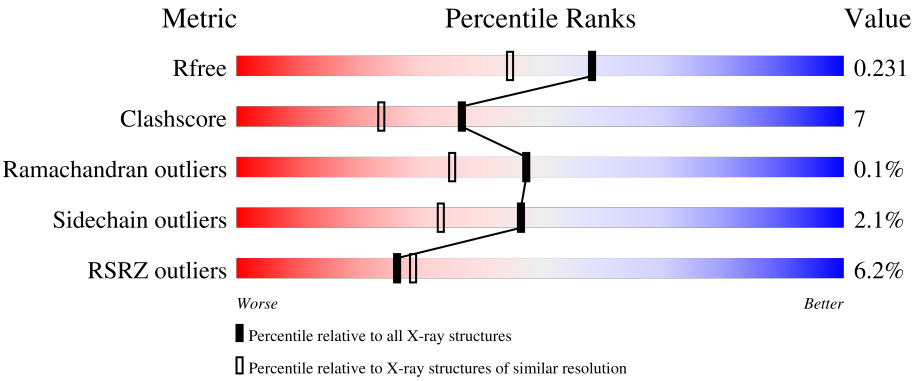
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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% 80% 15%
1	B	436	7% 83% 14%
1	C	436	8% 81% 15%
1	D	436	7% 80% 14%
1	E	436	5% 81% 15%

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Mol	Chain	Length	Quality of chain
1	F	436	

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	C	5041	-	-	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.

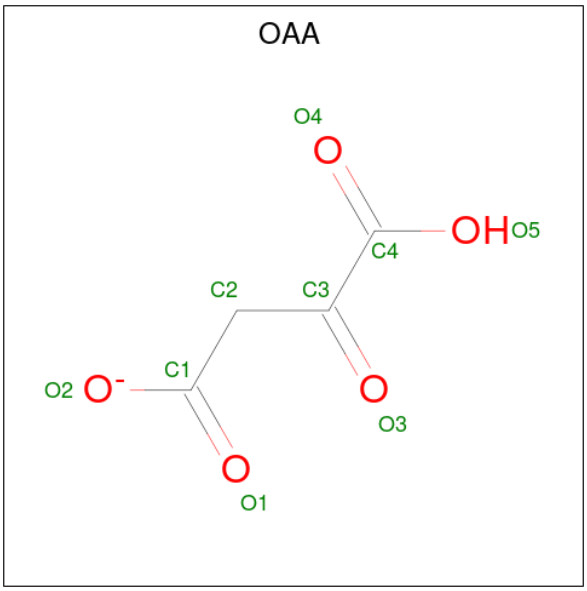
- Molecule 1 is a protein called Citrate synthase.

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

There are 12 discrepancies between the modelled and reference sequences:

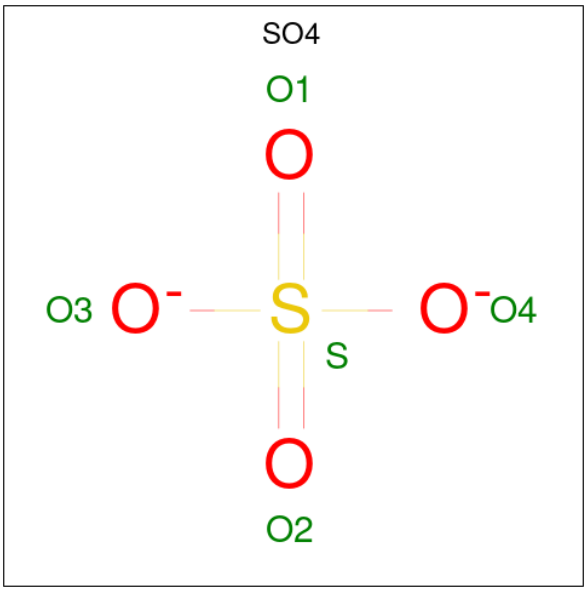
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	ASP	SEE REMARK 999	UNP P20901
A	106	ALA	VAL	SEE REMARK 999	UNP P20901
B	85	ALA	ASP	SEE REMARK 999	UNP P20901
B	106	ALA	VAL	SEE REMARK 999	UNP P20901
C	85	ALA	ASP	SEE REMARK 999	UNP P20901
C	106	ALA	VAL	SEE REMARK 999	UNP P20901
D	85	ALA	ASP	SEE 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 (CCD ID: OAA) (formula: $C_4H_3O_5$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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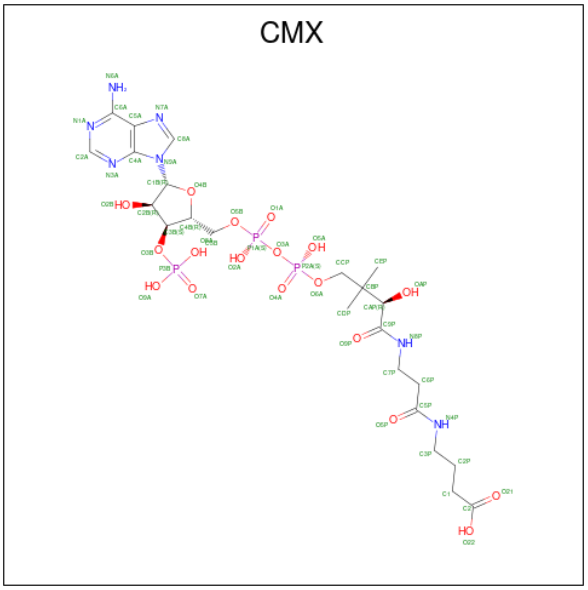
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

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



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

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

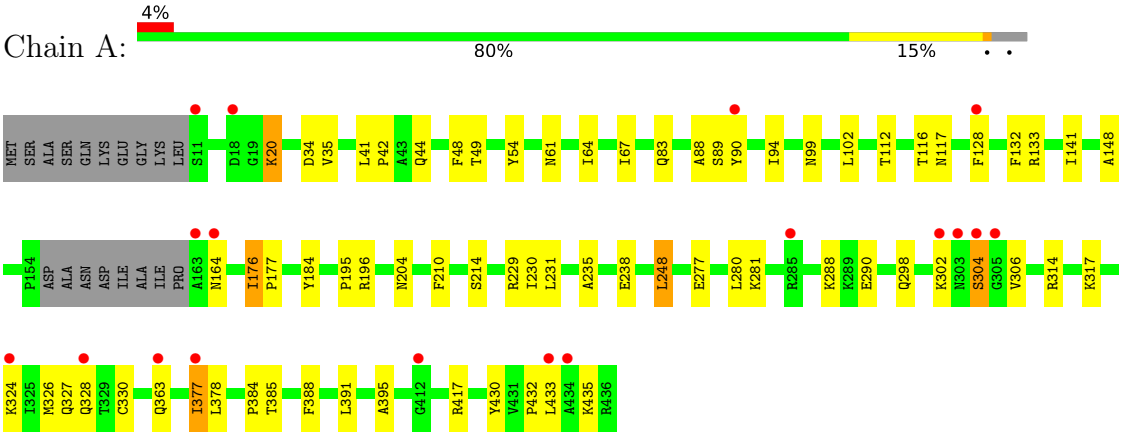
- Molecule 5 is water.

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

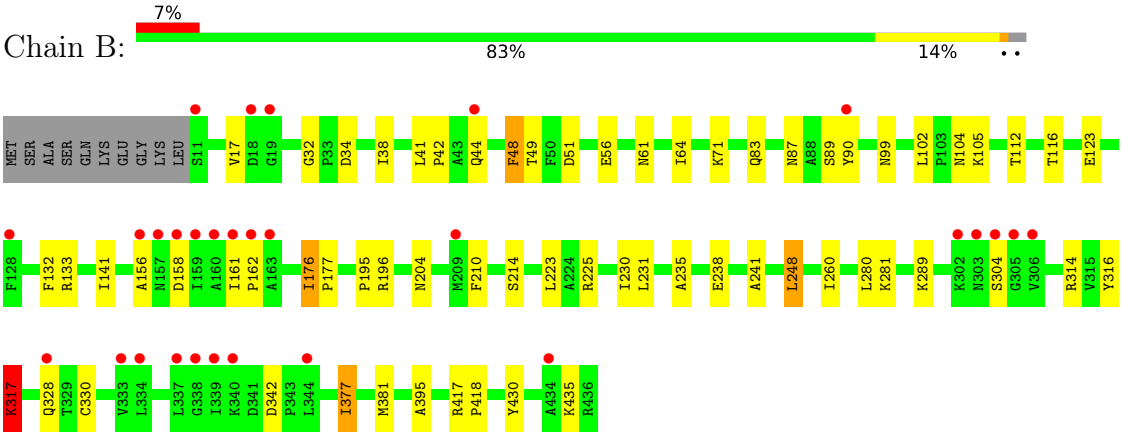
3 Residue-property plots (i)

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.

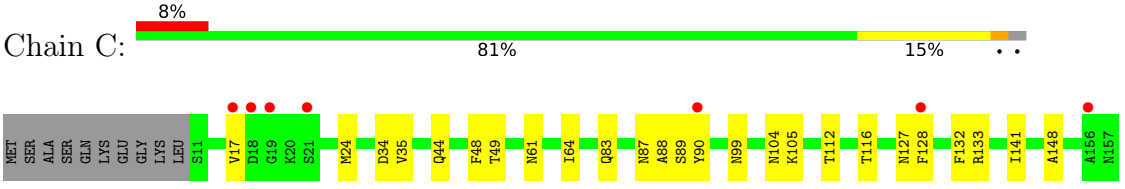
• Molecule 1: Citrate synthase

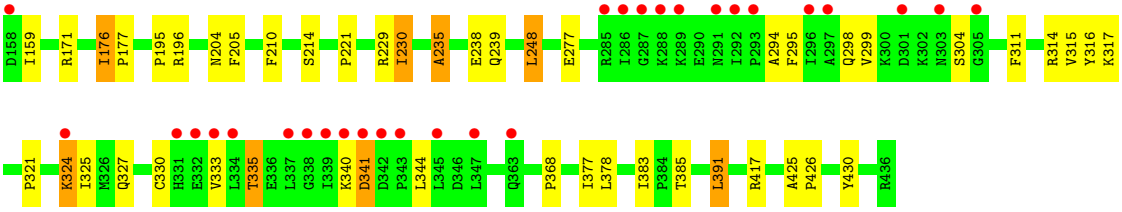


• Molecule 1: Citrate synthase

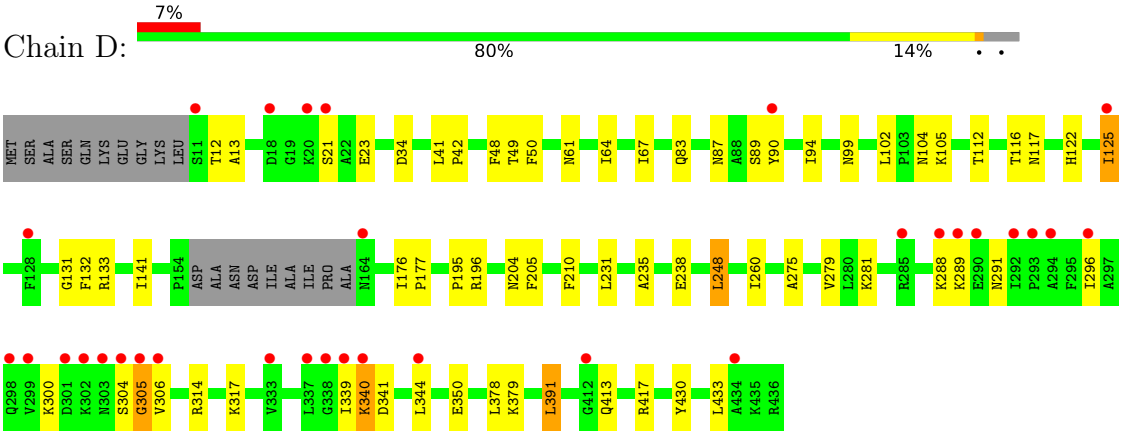


• Molecule 1: Citrate synthase

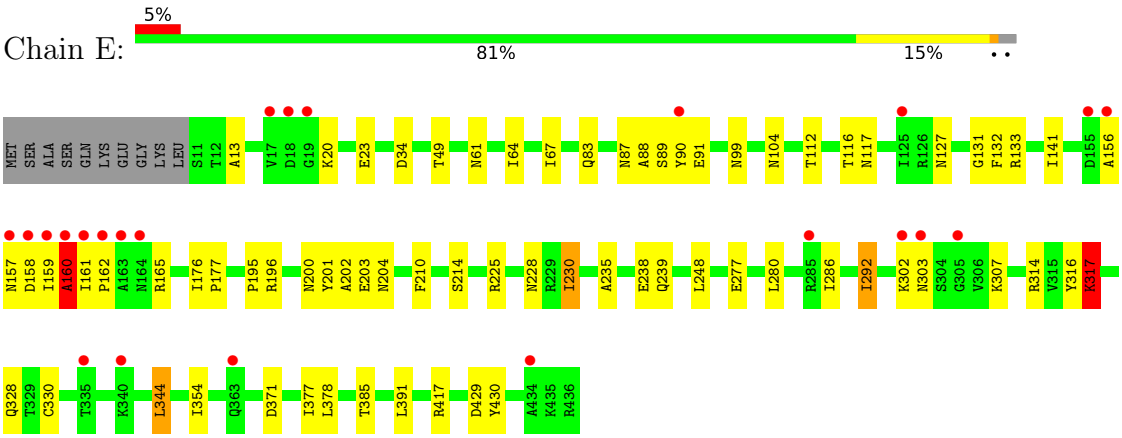




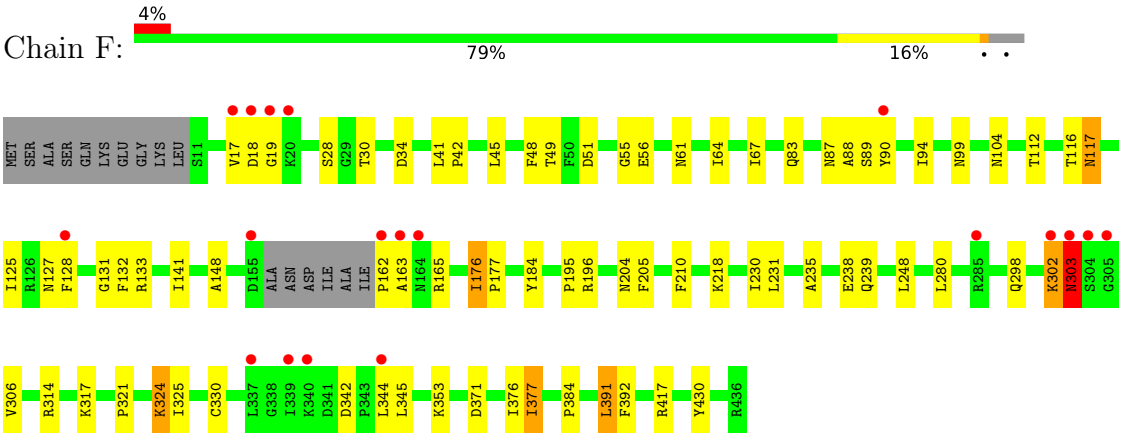
• Molecule 1: Citrate synthase



• Molecule 1: Citrate synthase



• Molecule 1: Citrate synthase



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 0.195 , 0.231	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 , 55.9	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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.52	1/3332 (0.0%)	1.00	20/4517 (0.4%)
1	B	0.51	1/3388 (0.0%)	1.04	27/4596 (0.6%)
1	C	0.52	2/3391 (0.1%)	1.02	22/4601 (0.5%)
1	D	0.54	1/3327 (0.0%)	1.03	23/4510 (0.5%)
1	E	0.54	1/3391 (0.0%)	1.03	24/4601 (0.5%)
1	F	0.51	1/3348 (0.0%)	1.02	25/4539 (0.6%)
All	All	0.52	7/20177 (0.0%)	1.02	141/27364 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	339	ILE	CA-CB	-6.55	1.46	1.54
1	C	176	ILE	CA-CB	6.05	1.58	1.53
1	E	292	ILE	CA-CB	5.68	1.57	1.54
1	F	176	ILE	CA-CB	5.56	1.57	1.53
1	A	176	ILE	CA-CB	5.47	1.57	1.53
1	C	335	THR	CA-CB	5.30	1.61	1.53
1	B	176	ILE	CA-CB	5.11	1.57	1.53

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	161	ILE	N-CA-C	12.96	120.85	107.76
1	F	163	ALA	N-CA-C	-10.90	99.38	112.89
1	B	304	SER	N-CA-C	8.70	120.84	111.36
1	D	87	ASN	N-CA-C	8.36	124.17	113.88
1	F	64	ILE	N-CA-C	8.30	118.29	110.74
1	E	302	LYS	N-CA-C	8.23	121.29	111.33
1	E	64	ILE	N-CA-C	8.08	118.02	110.42
1	B	64	ILE	N-CA-C	8.08	118.01	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ILE	N-CA-C	7.98	117.92	110.42
1	C	210	PHE	N-CA-C	7.97	123.18	113.38
1	E	87	ASN	N-CA-C	7.97	123.13	113.41
1	D	317	LYS	N-CA-C	-7.91	100.75	110.88
1	A	61	ASN	N-CA-C	-7.79	97.63	110.17
1	F	89	SER	N-CA-C	-7.69	99.14	110.52
1	E	157	ASN	N-CA-C	-7.65	104.08	113.19
1	D	64	ILE	N-CA-C	7.64	117.60	110.42
1	B	235	ALA	N-CA-C	7.61	119.21	111.07
1	D	89	SER	N-CA-C	-7.60	99.27	110.52
1	D	133	ARG	N-CA-C	-7.60	100.29	110.55
1	B	210	PHE	N-CA-C	7.59	123.59	113.72
1	E	317	LYS	N-CA-C	-7.58	101.18	110.88
1	D	49	THR	N-CA-C	-7.57	99.62	110.59
1	A	133	ARG	N-CA-C	-7.54	100.37	110.55
1	C	133	ARG	N-CA-C	-7.52	100.40	110.55
1	D	210	PHE	N-CA-C	7.48	123.44	113.72
1	D	304	SER	N-CA-C	7.45	122.84	112.93
1	B	87	ASN	N-CA-C	7.44	123.03	113.88
1	F	317	LYS	N-CA-C	-7.42	101.38	110.88
1	E	133	ARG	N-CA-C	-7.33	100.65	110.55
1	D	61	ASN	N-CA-C	-7.30	97.79	109.76
1	D	339	ILE	CA-C-N	7.28	130.25	120.65
1	D	339	ILE	C-N-CA	7.28	130.25	120.65
1	E	49	THR	N-CA-C	-7.25	100.07	110.59
1	B	161	ILE	N-CA-C	7.20	114.82	108.63
1	F	99	ASN	N-CA-C	7.19	122.34	113.50
1	F	87	ASN	N-CA-C	7.16	122.69	113.88
1	B	133	ARG	N-CA-C	-7.16	100.89	110.55
1	F	61	ASN	N-CA-C	-7.13	98.69	110.17
1	B	49	THR	N-CA-C	-7.13	100.26	110.59
1	A	49	THR	N-CA-C	-7.12	100.26	110.59
1	C	317	LYS	N-CA-C	-7.10	101.79	110.88
1	B	317	LYS	N-CA-C	-7.08	101.81	110.88
1	B	104	ASN	N-CA-C	-7.05	100.62	110.35
1	C	87	ASN	N-CA-C	7.02	122.52	113.88
1	A	317	LYS	N-CA-C	-7.01	101.91	110.88
1	F	133	ARG	N-CA-C	-7.01	101.09	110.55
1	A	210	PHE	N-CA-C	7.00	122.81	113.72
1	C	304	SER	N-CA-C	6.95	120.98	112.23
1	D	339	ILE	N-CA-CB	6.83	118.78	111.00
1	A	89	SER	N-CA-C	-6.82	100.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	413	GLN	N-CA-C	-6.80	100.22	110.28
1	A	235	ALA	N-CA-C	6.78	118.33	111.07
1	F	49	THR	N-CA-C	-6.78	100.76	110.59
1	B	89	SER	N-CA-C	-6.75	100.53	110.52
1	C	99	ASN	N-CA-C	6.71	121.59	113.41
1	F	210	PHE	N-CA-C	6.70	122.42	113.72
1	C	49	THR	N-CA-C	-6.68	100.91	110.59
1	B	61	ASN	N-CA-C	-6.67	99.42	110.17
1	C	61	ASN	N-CA-C	-6.64	99.47	110.17
1	E	235	ALA	N-CA-C	6.63	118.17	111.07
1	E	88	ALA	N-CA-C	6.62	120.31	110.52
1	C	341	ASP	N-CA-C	6.54	119.39	108.20
1	E	286	ILE	N-CA-C	-6.50	103.99	110.62
1	A	99	ASN	N-CA-C	6.47	121.46	113.50
1	E	99	ASN	N-CA-C	6.47	121.30	113.41
1	F	19	GLY	N-CA-C	-6.47	105.38	115.67
1	C	89	SER	N-CA-C	-6.47	100.04	110.32
1	E	160	ALA	N-CA-C	6.42	124.48	110.80
1	E	210	PHE	N-CA-C	6.39	121.86	113.30
1	E	61	ASN	N-CA-C	-6.32	99.99	110.17
1	D	305	GLY	N-CA-C	-6.29	106.55	115.43
1	C	64	ILE	N-CA-C	6.21	116.39	110.74
1	F	235	ALA	N-CA-C	6.20	118.55	111.11
1	B	99	ASN	N-CA-C	6.19	120.96	113.41
1	E	89	SER	N-CA-C	-6.19	101.36	110.52
1	D	306	VAL	N-CA-C	6.10	117.09	108.36
1	A	214	SER	N-CA-C	6.09	120.71	113.28
1	D	34	ASP	N-CA-C	-6.08	102.69	110.53
1	D	104	ASN	N-CA-C	-6.05	102.72	110.53
1	F	377	ILE	CB-CA-C	-6.04	104.23	111.97
1	B	342	ASP	CA-C-N	6.01	126.17	119.32
1	B	342	ASP	C-N-CA	6.01	126.17	119.32
1	E	161	ILE	CA-C-N	5.93	127.26	119.84
1	E	161	ILE	C-N-CA	5.93	127.26	119.84
1	A	88	ALA	N-CA-C	5.88	119.22	110.52
1	A	34	ASP	N-CA-C	-5.83	102.84	110.53
1	F	306	VAL	N-CA-C	5.83	116.58	109.30
1	D	235	ALA	N-CA-C	5.81	118.08	111.11
1	E	34	ASP	N-CA-C	-5.75	102.78	110.55
1	B	377	ILE	CB-CA-C	-5.71	104.54	112.02
1	B	34	ASP	N-CA-C	-5.70	102.86	110.55
1	E	239	GLN	N-CA-C	5.70	120.01	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	235	ALA	N-CA-C	5.69	117.94	111.11
1	F	55	GLY	N-CA-C	5.68	121.26	113.99
1	F	34	ASP	N-CA-C	-5.68	102.89	110.55
1	A	48	PHE	N-CA-C	-5.66	101.15	109.81
1	B	162	PRO	N-CA-CB	5.63	109.53	103.33
1	C	333	VAL	N-CA-C	5.61	115.80	110.42
1	F	239	GLN	N-CA-C	5.60	119.88	111.81
1	F	88	ALA	N-CA-C	5.58	118.08	110.55
1	E	104	ASN	N-CA-C	-5.57	102.67	110.35
1	F	67	ILE	CB-CA-C	-5.55	102.23	110.33
1	A	44	GLN	N-CA-C	5.54	117.12	111.14
1	F	342	ASP	CA-C-N	5.52	125.62	119.32
1	F	342	ASP	C-N-CA	5.52	125.62	119.32
1	C	426	PRO	N-CA-C	-5.48	103.50	111.33
1	C	88	ALA	N-CA-C	5.47	118.62	110.52
1	A	20	LYS	N-CA-C	5.47	119.01	110.32
1	F	30	THR	N-CA-C	-5.45	105.42	111.36
1	C	34	ASP	N-CA-C	-5.44	103.20	110.55
1	A	102	LEU	N-CA-C	-5.41	102.96	109.83
1	A	304	SER	N-CA-C	5.40	119.98	112.90
1	D	99	ASN	N-CA-C	5.39	120.13	113.50
1	C	214	SER	N-CA-C	5.37	119.83	113.28
1	F	48	PHE	N-CA-C	-5.36	101.61	109.81
1	C	239	GLN	N-CA-C	5.33	119.49	111.81
1	E	67	ILE	CB-CA-C	-5.29	102.60	110.33
1	A	377	ILE	CB-CA-C	-5.29	105.09	112.02
1	C	104	ASN	N-CA-C	-5.28	102.18	110.36
1	B	241	ALA	N-CA-C	5.26	116.70	111.07
1	A	164	ASN	N-CA-C	5.25	117.88	108.17
1	E	13	ALA	N-CA-C	-5.24	101.39	109.52
1	C	425	ALA	N-CA-C	5.21	116.26	109.64
1	D	48	PHE	N-CA-C	-5.21	101.84	109.81
1	D	67	ILE	CB-CA-C	-5.17	102.78	110.33
1	E	214	SER	N-CA-C	5.17	119.59	113.28
1	C	315	VAL	N-CA-C	5.16	116.58	111.67
1	F	392	PHE	N-CA-C	-5.16	105.55	111.07
1	D	340	LYS	N-CA-C	5.16	116.59	110.97
1	C	48	PHE	N-CA-C	-5.15	101.93	109.81
1	B	123	GLU	N-CA-C	5.09	118.26	111.75
1	B	38	ILE	CB-CA-C	-5.08	106.35	112.19
1	F	104	ASN	N-CA-C	-5.08	103.34	110.35
1	B	214	SER	N-CA-C	5.07	119.46	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	32	GLY	CA-C-N	5.04	125.31	119.92
1	B	32	GLY	C-N-CA	5.04	125.31	119.92
1	D	102	LEU	N-CA-C	-5.03	103.44	109.83
1	A	67	ILE	CB-CA-C	-5.02	103.00	110.33
1	B	48	PHE	N-CA-C	-5.01	102.14	109.81
1	B	105	LYS	N-CA-C	5.01	116.74	111.28
1	B	102	LEU	N-CA-C	-5.00	103.73	109.93

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	55	1
1	B	3313	0	3319	39	0
1	C	3315	0	3325	51	0
1	D	3253	0	3266	49	0
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	1
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	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	286	3

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 (286) 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
1:D:90:TYR:HE1	1:D:231:LEU:C	1.81	0.89
1:A:90:TYR:HE1	1:A:231:LEU:C	1.80	0.89
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:E:90:TYR:CE2	1:E:202:ALA:HB2	2.11	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:D:90:TYR:CE1	1:D:231:LEU:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:PHE:HE2	1:C:391:LEU:HD13	1.50	0.77
1:E:90:TYR:OH	1:E:200:ASN:CG	2.28	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: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:A:90:TYR:CE1	1:A:231:LEU:C	2.65	0.74
1:C:324:LYS:HG2	1:C:325:ILE:N	2.02	0.73
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:90:TYR:HH	1:E:200:ASN:CG	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CE1	1:E:91:GLU:CD	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:314:ARG:HG2	1:F:417:ARG:HB3	1.95	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:316:TYR:C	1:B:317:LYS:HD2	2.40	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:E:391:LEU:C	1:E:391:LEU:HD23	2.39	0.46
1:E:156:ALA:C	1:E:158:ASP:H	2.21	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
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:156:ALA:C	1:E:158:ASP:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:35:VAL:HG12	1:B:48:PHE:HB2	2.01	0.42
1:A:304:SER:C	1:A:306:VAL:H	2.28	0.42
1:C:324:LYS:HG2	1:C:325:ILE:H	1.82	0.42
1:D:12:THR:OG1	1:D:23:GLU:OE1	2.36	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: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:A:391:LEU:C	1:A:391:LEU:HD23	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:24:MET:HE1	1:C:44:GLN:NE2	2.36	0.41
1:C:159:ILE:HD12	1:C:159:ILE:C	2.45	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

All (3) 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
1:A:20:LYS:NZ	3:A:5047:SO4:O4[3_544]	2.01	0.19
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	413/436 (95%)	403 (98%)	10 (2%)	0	100	100
1	E	424/436 (97%)	413 (97%)	10 (2%)	1 (0%)	43	31
1	F	416/436 (95%)	406 (98%)	8 (2%)	2 (0%)	24	13
All	All	2515/2616 (96%)	2461 (98%)	51 (2%)	3 (0%)	48	35

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%)	336 (99%)	4 (1%)	63	55
1	B	345/354 (98%)	337 (98%)	8 (2%)	44	30
1	C	346/354 (98%)	338 (98%)	8 (2%)	44	30
1	D	340/354 (96%)	331 (97%)	9 (3%)	40	25
1	E	346/354 (98%)	339 (98%)	7 (2%)	48	36
1	F	342/354 (97%)	335 (98%)	7 (2%)	48	36
All	All	2059/2124 (97%)	2016 (98%)	43 (2%)	47	33

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	238	GLU
1	A	248	LEU
1	A	328	GLN
1	B	17	VAL

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Mol	Chain	Res	Type
1	B	238	GLU
1	B	248	LEU
1	B	260	ILE
1	B	280	LEU
1	B	289	LYS
1	B	317	LYS
1	B	328	GLN
1	C	230	ILE
1	C	238	GLU
1	C	248	LEU
1	C	324	LYS
1	C	340	LYS
1	C	341	ASP
1	C	344	LEU
1	C	391	LEU
1	D	21	SER
1	D	117	ASN
1	D	125	ILE
1	D	238	GLU
1	D	248	LEU
1	D	260	ILE
1	D	344	LEU
1	D	391	LEU
1	D	433	LEU
1	E	117	ASN
1	E	230	ILE
1	E	238	GLU
1	E	248	LEU
1	E	303	ASN
1	E	317	LYS
1	E	344	LEU
1	F	28	SER
1	F	117	ASN
1	F	238	GLU
1	F	248	LEU
1	F	303	ASN
1	F	324	LYS
1	F	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	83	GLN
1	A	204	ASN
1	A	363	GLN
1	B	83	GLN
1	B	117	ASN
1	B	164	ASN
1	B	204	ASN
1	B	239	GLN
1	B	328	GLN
1	C	44	GLN
1	C	83	GLN
1	C	204	ASN
1	C	298	GLN
1	D	83	GLN
1	D	188	GLN
1	D	204	ASN
1	D	291	ASN
1	D	327	GLN
1	E	83	GLN
1	E	204	ASN
1	E	303	ASN
1	F	83	GLN
1	F	188	GLN
1	F	204	ASN
1	F	298	GLN
1	F	303	ASN
1	F	327	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	B	5016	-	4,4,4	0.70	0	6,6,6	0.05	0
4	CMX	A	5001	-	51,53,53	1.17	4 (7%)	74,79,79	1.43	8 (10%)
4	CMX	F	5006	-	51,53,53	1.18	4 (7%)	74,79,79	1.43	8 (10%)
3	SO4	B	5045	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	C	5041	-	4,4,4	0.70	0	6,6,6	0.19	0
3	SO4	B	5053	-	4,4,4	0.71	0	6,6,6	0.05	0
3	SO4	E	5050	-	4,4,4	0.70	0	6,6,6	0.08	0
3	SO4	A	5029	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	E	5023	-	4,4,4	0.69	0	6,6,6	0.10	0
3	SO4	A	5014	-	4,4,4	0.69	0	6,6,6	0.05	0
3	SO4	C	5019	-	4,4,4	0.70	0	6,6,6	0.09	0
2	OAA	E	5011	-	8,8,8	1.23	0	8,10,10	1.35	1 (12%)
3	SO4	A	5015	-	4,4,4	0.69	0	6,6,6	0.05	0
3	SO4	E	5024	-	4,4,4	0.70	0	6,6,6	0.10	0
2	OAA	C	5009	-	8,8,8	1.24	0	8,10,10	1.39	1 (12%)
3	SO4	C	5027	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	A	5035	-	4,4,4	0.70	0	6,6,6	0.08	0
3	SO4	D	5028	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	D	5032	-	4,4,4	0.70	0	6,6,6	0.09	0
3	SO4	B	5036	-	4,4,4	0.70	0	6,6,6	0.10	0
3	SO4	E	5043	-	4,4,4	0.72	0	6,6,6	0.10	0
3	SO4	A	5052	-	4,4,4	0.71	0	6,6,6	0.06	0
3	SO4	D	5018	-	4,4,4	0.70	0	6,6,6	0.10	0
3	SO4	C	5046	-	4,4,4	0.70	0	6,6,6	0.07	0
4	CMX	C	5003	-	51,53,53	1.18	4 (7%)	74,79,79	1.42	8 (10%)
3	SO4	F	5044	-	4,4,4	0.72	0	6,6,6	0.13	0
4	CMX	D	5004	-	51,53,53	1.18	4 (7%)	74,79,79	1.42	9 (12%)
3	SO4	B	5017	-	4,4,4	0.70	0	6,6,6	0.13	0
3	SO4	A	5047	-	4,4,4	0.70	0	6,6,6	0.17	0
3	SO4	F	5022	-	4,4,4	0.70	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OAA	B	5008	-	8,8,8	1.22	0	8,10,10	1.53	1 (12%)
3	SO4	B	5039	-	4,4,4	0.70	0	6,6,6	0.06	0
2	OAA	D	5010	-	8,8,8	1.23	0	8,10,10	1.52	1 (12%)
3	SO4	E	5033	-	4,4,4	0.70	0	6,6,6	0.09	0
3	SO4	F	5051	-	4,4,4	0.70	0	6,6,6	0.09	0
4	CMX	E	5005	-	51,53,53	1.19	5 (9%)	74,79,79	1.41	10 (13%)
3	SO4	B	5013	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	E	5037	-	4,4,4	0.70	0	6,6,6	0.09	0
4	CMX	B	5002	-	51,53,53	1.18	4 (7%)	74,79,79	1.40	8 (10%)
3	SO4	C	5031	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	D	5021	-	4,4,4	0.70	0	6,6,6	0.09	0
2	OAA	A	5007	-	8,8,8	1.22	0	8,10,10	1.41	1 (12%)
3	SO4	E	5025	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	F	5026	-	4,4,4	0.70	0	6,6,6	0.09	0
3	SO4	D	5049	-	4,4,4	0.70	0	6,6,6	0.06	0
3	SO4	D	5042	-	4,4,4	0.70	0	6,6,6	0.10	0
3	SO4	F	5034	-	4,4,4	0.70	0	6,6,6	0.06	0
2	OAA	F	5012	-	8,8,8	1.22	0	8,10,10	1.56	1 (12%)
3	SO4	C	5020	-	4,4,4	0.71	0	6,6,6	0.10	0
3	SO4	F	5038	-	4,4,4	0.69	0	6,6,6	0.09	0
3	SO4	B	5030	-	4,4,4	0.70	0	6,6,6	0.10	0
3	SO4	A	5040	-	4,4,4	0.71	0	6,6,6	0.06	0
3	SO4	B	5048	-	4,4,4	0.70	0	6,6,6	0.05	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	E	5011	-	-	1/8/8/8	-
2	OAA	B	5008	-	-	0/8/8/8	-
2	OAA	D	5010	-	-	0/8/8/8	-
4	CMX	F	5006	-	-	6/51/67/67	0/3/3/3
2	OAA	C	5009	-	-	0/8/8/8	-
4	CMX	E	5005	-	-	6/51/67/67	0/3/3/3
2	OAA	F	5012	-	-	0/8/8/8	-
4	CMX	C	5003	-	-	5/51/67/67	0/3/3/3
4	CMX	D	5004	-	-	6/51/67/67	0/3/3/3
4	CMX	B	5002	-	-	7/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CMX	A	5001	-	-	6/51/67/67	0/3/3/3
2	OAA	A	5007	-	-	0/8/8/8	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5006	CMX	C5A-N7A	-3.16	1.33	1.39
4	E	5005	CMX	C5A-N7A	-3.16	1.33	1.39
4	A	5001	CMX	C5A-N7A	-3.15	1.33	1.39
4	D	5004	CMX	C5A-N7A	-3.13	1.33	1.39
4	B	5002	CMX	C5A-N7A	-3.07	1.33	1.39
4	C	5003	CMX	C5A-N7A	-3.04	1.33	1.39
4	B	5002	CMX	P2A-O4A	3.04	1.61	1.50
4	C	5003	CMX	P2A-O4A	3.03	1.61	1.50
4	A	5001	CMX	P1A-O1A	3.02	1.61	1.50
4	E	5005	CMX	P1A-O1A	3.02	1.61	1.50
4	D	5004	CMX	P2A-O4A	3.01	1.61	1.50
4	E	5005	CMX	P2A-O4A	3.01	1.61	1.50
4	C	5003	CMX	P1A-O1A	3.01	1.61	1.50
4	B	5002	CMX	P1A-O1A	3.00	1.61	1.50
4	D	5004	CMX	P1A-O1A	3.00	1.61	1.50
4	F	5006	CMX	P2A-O4A	2.99	1.61	1.50
4	F	5006	CMX	P1A-O1A	2.99	1.61	1.50
4	A	5001	CMX	P2A-O4A	2.96	1.61	1.50
4	F	5006	CMX	C8A-N9A	-2.33	1.33	1.37
4	D	5004	CMX	C8A-N9A	-2.30	1.33	1.37
4	C	5003	CMX	C8A-N9A	-2.28	1.33	1.37
4	B	5002	CMX	C8A-N9A	-2.28	1.33	1.37
4	A	5001	CMX	C8A-N9A	-2.27	1.33	1.37
4	E	5005	CMX	C8A-N9A	-2.26	1.33	1.37
4	E	5005	CMX	C4A-N9A	-2.03	1.33	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5001	CMX	C5A-C4A-N3A	-5.36	119.33	126.72
4	F	5006	CMX	C5A-C4A-N3A	-5.25	119.49	126.72
4	D	5004	CMX	C5A-C4A-N3A	-5.24	119.50	126.72
4	C	5003	CMX	C5A-C4A-N3A	-5.24	119.50	126.72
4	E	5005	CMX	C5A-C4A-N3A	-5.17	119.60	126.72
4	B	5002	CMX	C5A-C4A-N3A	-5.09	119.71	126.72
4	F	5006	CMX	N3A-C2A-N1A	-4.60	121.62	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5003	CMX	N3A-C2A-N1A	-4.55	121.70	128.58
4	B	5002	CMX	N3A-C2A-N1A	-4.52	121.75	128.58
4	D	5004	CMX	N3A-C2A-N1A	-4.47	121.81	128.58
4	A	5001	CMX	N3A-C2A-N1A	-4.46	121.83	128.58
4	E	5005	CMX	N3A-C2A-N1A	-4.43	121.88	128.58
4	A	5001	CMX	N3A-C4A-N9A	3.90	133.81	127.17
4	F	5006	CMX	N3A-C4A-N9A	3.86	133.74	127.17
4	C	5003	CMX	N3A-C4A-N9A	3.82	133.66	127.17
4	B	5002	CMX	N3A-C4A-N9A	3.82	133.66	127.17
4	D	5004	CMX	N3A-C4A-N9A	3.80	133.63	127.17
4	E	5005	CMX	N3A-C4A-N9A	3.75	133.54	127.17
2	F	5012	OAA	O4-C4-C3	-3.64	117.29	121.81
4	A	5001	CMX	C2A-N3A-C4A	3.58	120.58	111.83
4	F	5006	CMX	C2A-N3A-C4A	3.57	120.56	111.83
4	D	5004	CMX	C2A-N3A-C4A	3.50	120.38	111.83
4	C	5003	CMX	C2A-N3A-C4A	3.49	120.36	111.83
2	B	5008	OAA	O4-C4-C3	-3.49	117.47	121.81
2	D	5010	OAA	O4-C4-C3	-3.47	117.50	121.81
4	B	5002	CMX	C2A-N3A-C4A	3.46	120.28	111.83
4	E	5005	CMX	C2A-N3A-C4A	3.41	120.16	111.83
4	F	5006	CMX	N9A-C8A-N7A	-3.18	109.43	113.94
4	A	5001	CMX	N9A-C8A-N7A	-3.17	109.43	113.94
2	A	5007	OAA	O4-C4-C3	-3.14	117.91	121.81
4	D	5004	CMX	N9A-C8A-N7A	-3.12	109.50	113.94
2	C	5009	OAA	O4-C4-C3	-3.11	117.94	121.81
4	E	5005	CMX	N9A-C8A-N7A	-3.11	109.52	113.94
4	C	5003	CMX	N9A-C8A-N7A	-3.09	109.55	113.94
4	B	5002	CMX	N9A-C8A-N7A	-3.05	109.61	113.94
2	E	5011	OAA	O4-C4-C3	-2.91	118.19	121.81
4	F	5006	CMX	C5A-N7A-C8A	2.89	108.00	103.45
4	A	5001	CMX	C5A-N7A-C8A	2.85	107.93	103.45
4	C	5003	CMX	C5A-N7A-C8A	2.82	107.88	103.45
4	D	5004	CMX	C5A-N7A-C8A	2.81	107.87	103.45
4	E	5005	CMX	C5A-N7A-C8A	2.75	107.77	103.45
4	C	5003	CMX	C4A-C5A-N7A	-2.69	107.51	110.58
4	B	5002	CMX	C5A-N7A-C8A	2.68	107.66	103.45
4	D	5004	CMX	C4A-C5A-N7A	-2.65	107.55	110.58
4	A	5001	CMX	C4A-C5A-N7A	-2.64	107.56	110.58
4	F	5006	CMX	C4A-C5A-N7A	-2.63	107.58	110.58
4	E	5005	CMX	C4A-C5A-N7A	-2.53	107.68	110.58
4	B	5002	CMX	C4A-N9A-C8A	2.45	108.31	105.74
4	B	5002	CMX	C4A-C5A-N7A	-2.44	107.79	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5006	CMX	C4A-N9A-C8A	2.37	108.22	105.74
4	C	5003	CMX	C4A-N9A-C8A	2.36	108.21	105.74
4	A	5001	CMX	C4A-N9A-C8A	2.35	108.21	105.74
4	D	5004	CMX	C4A-N9A-C8A	2.34	108.19	105.74
4	E	5005	CMX	C4A-N9A-C8A	2.31	108.16	105.74
4	D	5004	CMX	O21-C2-C1	-2.04	116.61	123.09
4	E	5005	CMX	O21-C2-C1	-2.02	116.70	123.09
4	E	5005	CMX	O6A-CCP-CBP	-2.02	107.31	110.55

There are no chirality outliers.

All (37) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	F	5006	CMX	C2P-C1-C2-O22
4	A	5001	CMX	C2P-C1-C2-O21
4	F	5006	CMX	C2P-C1-C2-O21
4	C	5003	CMX	C2P-C1-C2-O21
4	B	5002	CMX	P1A-O3A-P2A-O5A
4	D	5004	CMX	P1A-O3A-P2A-O5A
2	E	5011	OAA	C1-C2-C3-C4
4	B	5002	CMX	P1A-O3A-P2A-O4A

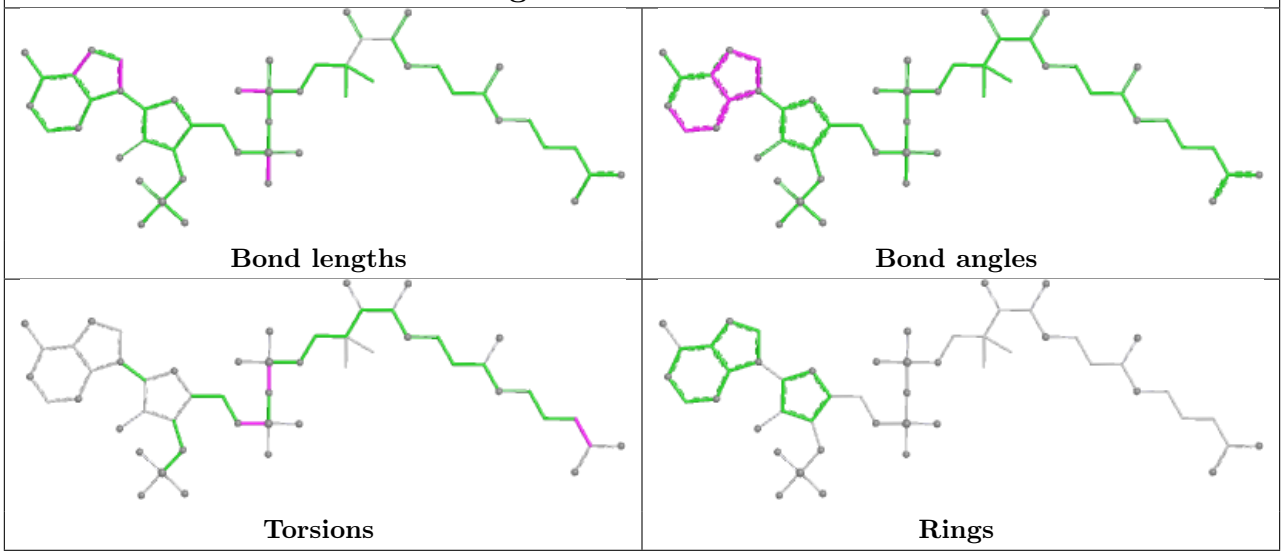
There are no ring outliers.

10 monomers are involved in 13 short contacts:

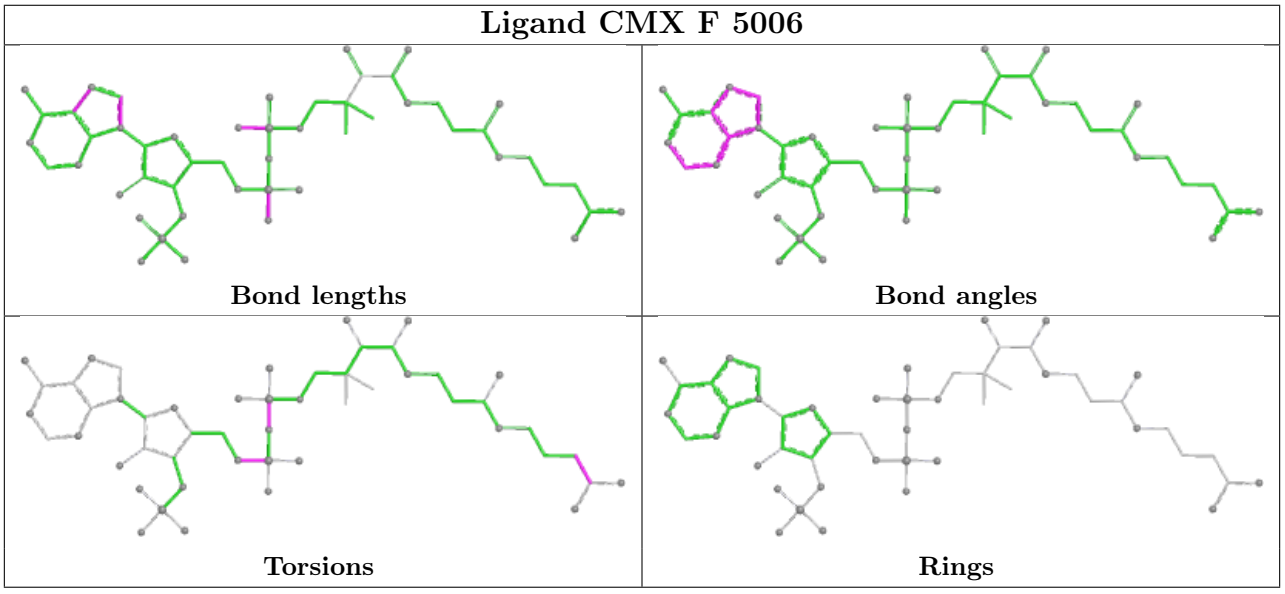
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	5006	CMX	1	0
3	B	5045	SO4	1	0
3	C	5041	SO4	3	0
3	E	5050	SO4	1	0
3	C	5046	SO4	1	0
4	C	5003	CMX	2	0
3	A	5047	SO4	0	1
4	E	5005	CMX	1	0
3	F	5038	SO4	1	0
3	B	5048	SO4	1	0

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.

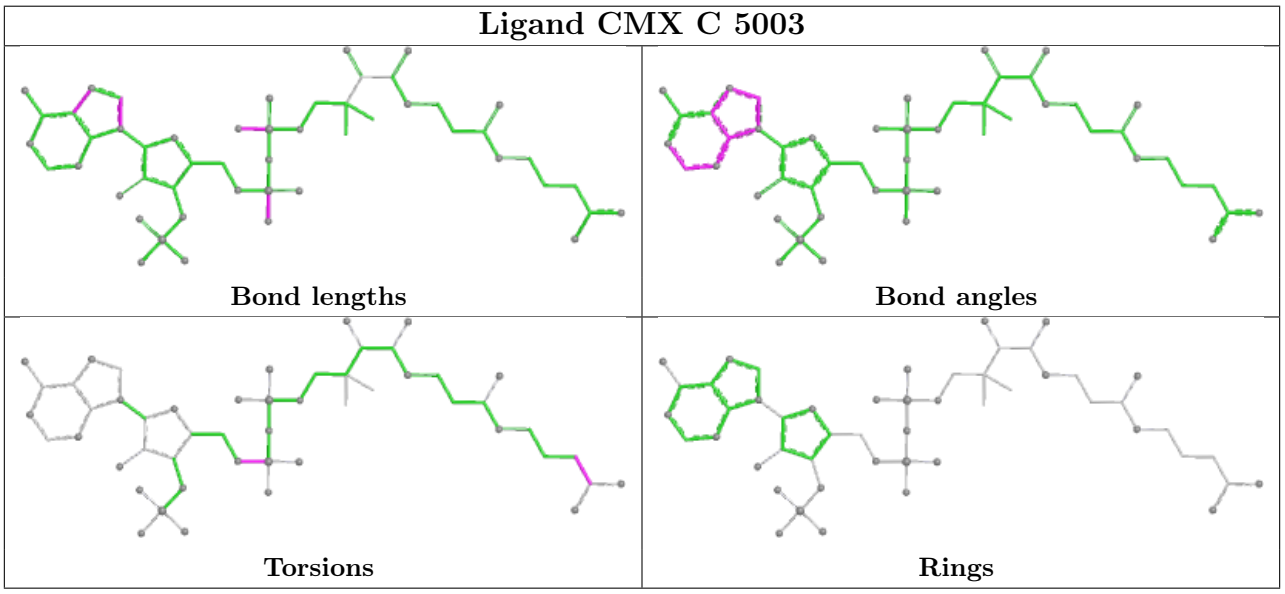
Ligand CMX A 5001



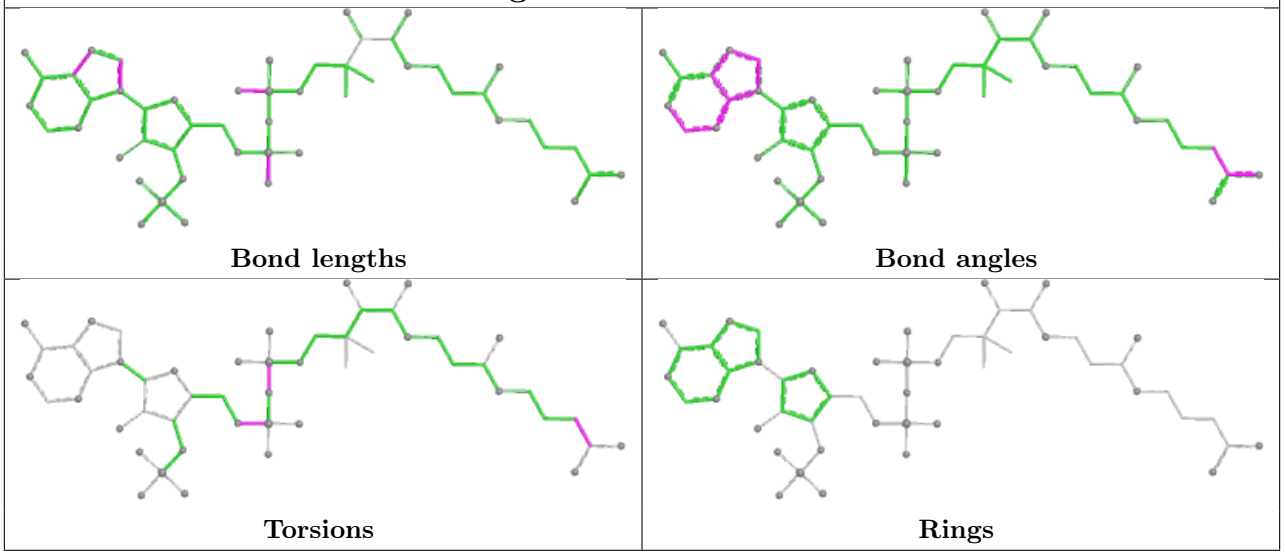
Ligand CMX F 5006



Ligand CMX C 5003



Ligand CMX D 5004



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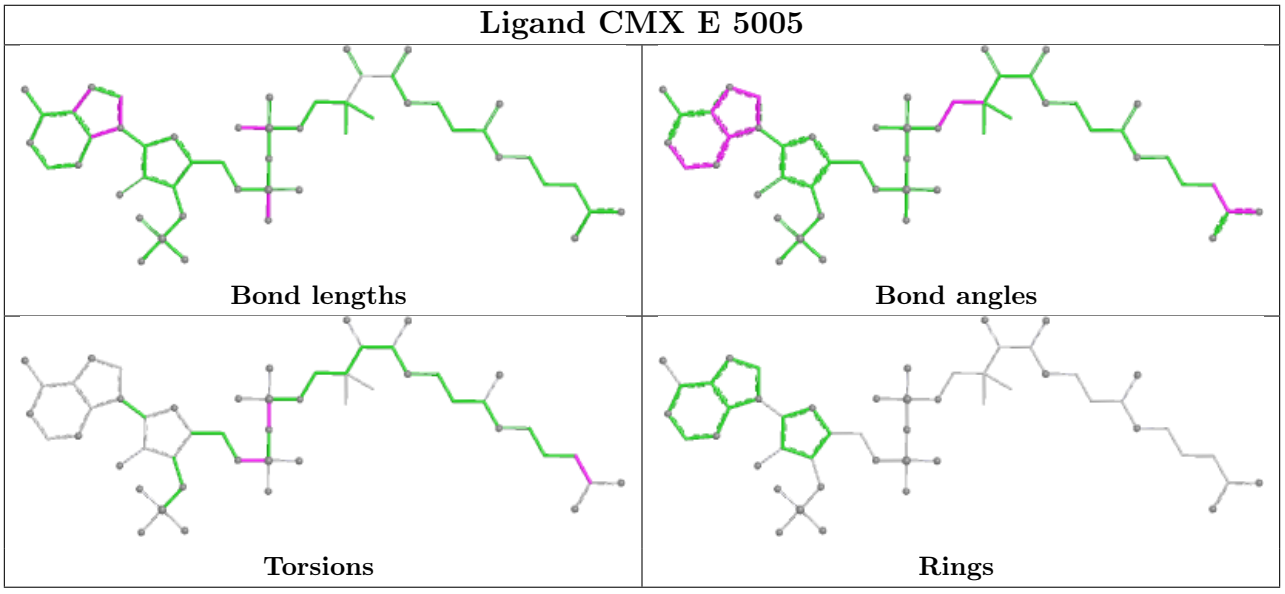
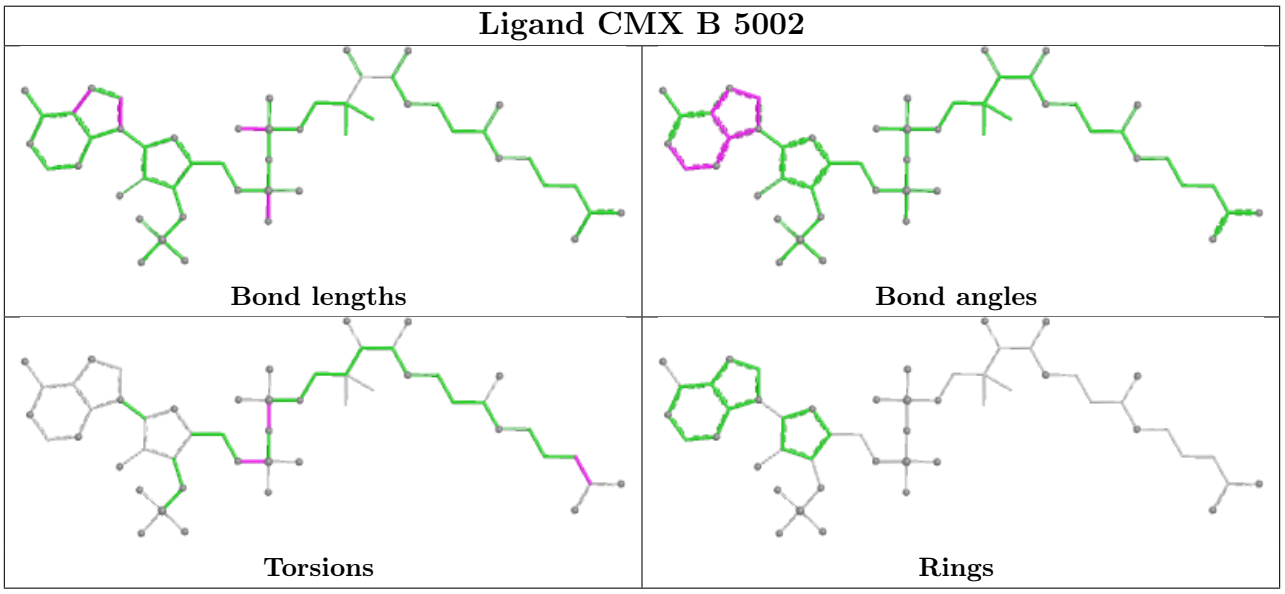


Ligand CMX B 5002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	418/436 (95%)	0.05	18 (4%)	40	43	15, 22, 39, 57	0
1	B	426/436 (97%)	0.21	29 (6%)	23	25	16, 23, 45, 59	0
1	C	426/436 (97%)	0.28	36 (8%)	16	17	16, 23, 47, 60	0
1	D	417/436 (95%)	0.30	32 (7%)	19	20	16, 24, 49, 66	0
1	E	426/436 (97%)	0.21	23 (5%)	31	34	15, 22, 46, 63	0
1	F	420/436 (96%)	0.14	19 (4%)	38	41	15, 23, 43, 58	0
All	All	2533/2616 (96%)	0.20	157 (6%)	26	29	15, 23, 46, 66	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	159	ILE	10.2
1	E	90	TYR	9.9
1	D	90	TYR	9.6
1	A	90	TYR	9.1
1	F	90	TYR	8.5
1	B	90	TYR	7.1
1	C	90	TYR	6.2
1	E	158	ASP	5.6
1	F	18	ASP	5.6
1	E	156	ALA	5.3
1	B	156	ALA	5.1
1	C	341	ASP	5.0
1	B	159	ILE	4.9
1	E	157	ASN	4.7
1	A	433	LEU	4.7
1	B	158	ASP	4.6
1	F	162	PRO	4.5
1	A	18	ASP	4.4
1	E	305	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	303	ASN	4.3
1	A	163	ALA	4.3
1	C	339	ILE	4.2
1	C	342	ASP	4.2
1	F	303	ASN	4.2
1	D	303	ASN	4.1
1	B	161	ILE	4.0
1	B	157	ASN	3.9
1	B	160	ALA	3.8
1	A	128	PHE	3.8
1	F	155	ASP	3.7
1	C	292	ILE	3.7
1	E	161	ILE	3.6
1	E	18	ASP	3.6
1	D	340	LYS	3.4
1	E	160	ALA	3.4
1	E	162	PRO	3.4
1	E	163	ALA	3.4
1	B	11	SER	3.3
1	E	303	ASN	3.3
1	D	339	ILE	3.3
1	A	302	LYS	3.3
1	C	128	PHE	3.3
1	C	287	GLY	3.3
1	C	340	LYS	3.2
1	F	163	ALA	3.2
1	D	304	SER	3.2
1	B	305	GLY	3.1
1	D	412	GLY	3.1
1	B	344	LEU	3.1
1	C	343	PRO	3.1
1	C	337	LEU	3.0
1	C	305	GLY	3.0
1	B	337	LEU	3.0
1	C	18	ASP	3.0
1	D	305	GLY	2.9
1	F	164	ASN	2.9
1	C	289	LYS	2.9
1	F	304	SER	2.8
1	F	302	LYS	2.8
1	B	18	ASP	2.8
1	F	128	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	19	GLY	2.8
1	A	377	ILE	2.8
1	C	17	VAL	2.8
1	C	331	HIS	2.8
1	B	162	PRO	2.8
1	F	305	GLY	2.7
1	A	304	SER	2.7
1	D	434	ALA	2.7
1	B	19	GLY	2.7
1	E	155	ASP	2.7
1	C	334	LEU	2.7
1	A	164	ASN	2.7
1	B	163	ALA	2.7
1	B	338	GLY	2.7
1	C	338	GLY	2.7
1	B	209	MET	2.6
1	C	301	ASP	2.6
1	C	285	ARG	2.6
1	B	339	ILE	2.6
1	C	286	ILE	2.6
1	A	305	GLY	2.6
1	B	333	VAL	2.6
1	F	344	LEU	2.6
1	D	125	ILE	2.6
1	D	296	ILE	2.6
1	A	412	GLY	2.6
1	C	158	ASP	2.6
1	D	290	GLU	2.6
1	C	291	ASN	2.6
1	E	125	ILE	2.5
1	C	297	ALA	2.5
1	D	164	ASN	2.5
1	D	128	PHE	2.5
1	C	333	VAL	2.5
1	D	285	ARG	2.5
1	A	303	ASN	2.4
1	C	296	ILE	2.4
1	E	17	VAL	2.4
1	C	347	LEU	2.4
1	F	339	ILE	2.4
1	A	434	ALA	2.4
1	A	363	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	19	GLY	2.4
1	A	11	SER	2.4
1	D	20	LYS	2.4
1	D	301	ASP	2.4
1	B	434	ALA	2.4
1	C	19	GLY	2.4
1	D	11	SER	2.4
1	C	324	LYS	2.4
1	D	289	LYS	2.4
1	E	335	THR	2.3
1	C	303	ASN	2.3
1	D	18	ASP	2.3
1	D	344	LEU	2.3
1	E	363	GLN	2.3
1	E	285	ARG	2.3
1	B	306	VAL	2.3
1	D	306	VAL	2.3
1	A	328	GLN	2.3
1	D	298	GLN	2.2
1	C	288	LYS	2.2
1	C	293	PRO	2.2
1	F	340	LYS	2.2
1	D	337	LEU	2.2
1	D	294	ALA	2.2
1	D	288	LYS	2.2
1	D	302	LYS	2.2
1	F	20	LYS	2.2
1	F	285	ARG	2.2
1	C	21	SER	2.2
1	D	293	PRO	2.2
1	C	156	ALA	2.2
1	E	434	ALA	2.2
1	A	324	LYS	2.2
1	E	302	LYS	2.2
1	D	299	VAL	2.1
1	B	340	LYS	2.1
1	D	292	ILE	2.1
1	C	332	GLU	2.1
1	B	334	LEU	2.1
1	B	304	SER	2.1
1	B	302	LYS	2.1
1	E	340	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	VAL	2.1
1	B	328	GLN	2.1
1	C	345	LEU	2.1
1	B	128	PHE	2.0
1	E	164	ASN	2.0
1	D	333	VAL	2.0
1	F	337	LEU	2.0
1	A	285	ARG	2.0
1	D	21	SER	2.0
1	B	44	GLN	2.0
1	C	363	GLN	2.0
1	D	338	GLY	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 oligosaccharides 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	C	5041	5/5	0.38	0.21	61,62,63,64	0
3	SO4	B	5045	5/5	0.51	0.17	58,58,59,62	0
3	SO4	E	5043	5/5	0.51	0.19	51,54,58,59	0
3	SO4	A	5052	5/5	0.52	0.18	57,58,60,61	0
3	SO4	A	5047	5/5	0.59	0.18	54,56,59,60	0
3	SO4	B	5039	5/5	0.60	0.17	53,54,57,58	0
3	SO4	A	5040	5/5	0.61	0.15	54,54,57,57	0
3	SO4	F	5044	5/5	0.62	0.17	56,57,58,59	0
3	SO4	D	5042	5/5	0.63	0.15	55,56,57,57	0
3	SO4	D	5049	5/5	0.64	0.18	72,73,74,75	0
3	SO4	E	5037	5/5	0.64	0.18	55,58,59,59	0

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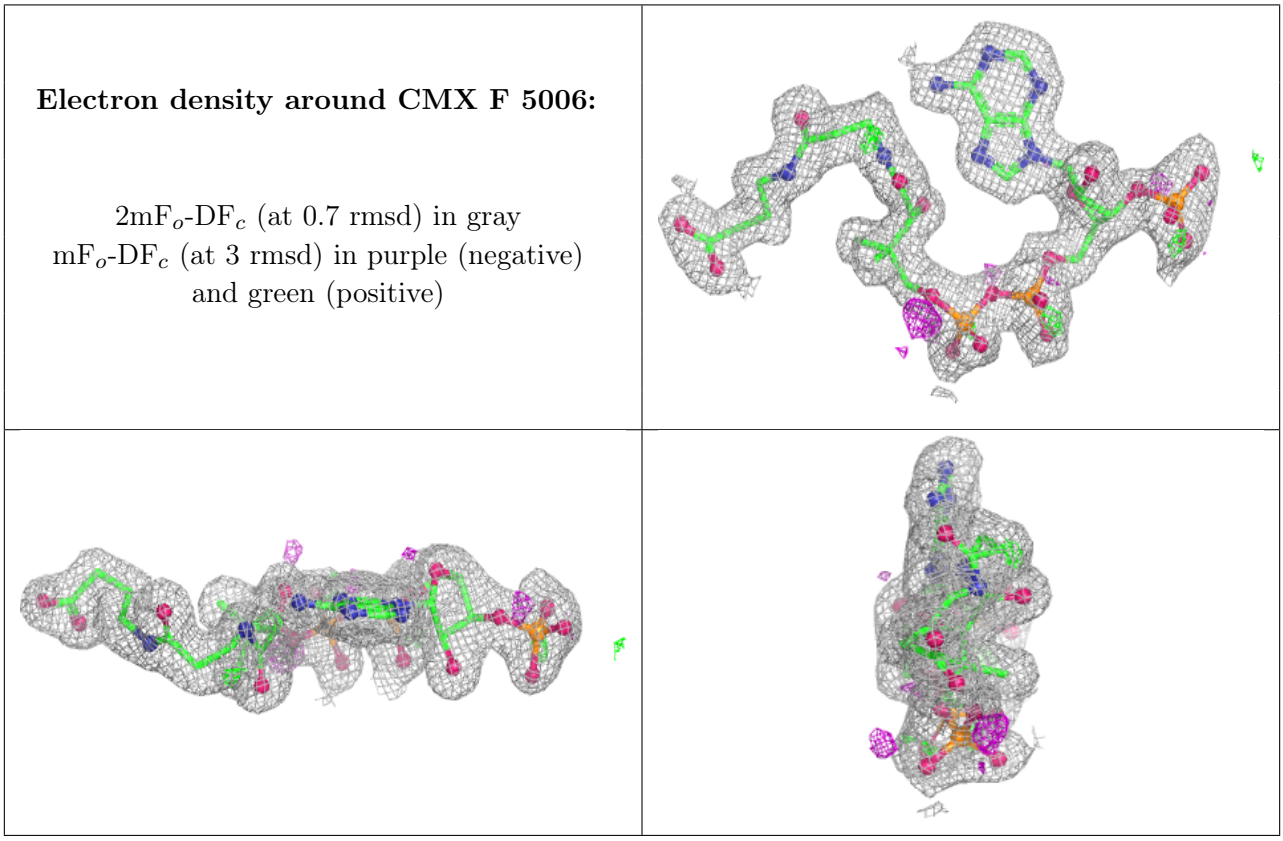
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	5048	5/5	0.67	0.15	58,60,62,62	0
3	SO4	B	5053	5/5	0.67	0.14	55,57,59,59	0
3	SO4	F	5051	5/5	0.67	0.15	50,53,55,56	0
3	SO4	E	5050	5/5	0.69	0.15	59,59,60,60	0
3	SO4	F	5038	5/5	0.72	0.14	61,61,62,64	0
3	SO4	C	5046	5/5	0.74	0.14	62,63,64,65	0
3	SO4	A	5035	5/5	0.75	0.14	59,60,60,63	0
3	SO4	B	5036	5/5	0.75	0.14	52,55,56,56	0
3	SO4	C	5027	5/5	0.79	0.14	69,70,71,71	0
3	SO4	C	5031	5/5	0.82	0.14	63,65,66,66	0
3	SO4	A	5029	5/5	0.84	0.13	52,52,54,55	0
3	SO4	F	5034	5/5	0.88	0.11	51,52,53,54	0
3	SO4	B	5030	5/5	0.88	0.11	43,43,46,48	0
3	SO4	D	5032	5/5	0.90	0.10	45,47,49,50	0
3	SO4	D	5028	5/5	0.90	0.10	58,59,59,60	0
3	SO4	E	5033	5/5	0.91	0.10	46,47,47,50	0
3	SO4	B	5017	5/5	0.93	0.12	36,39,40,41	0
4	CMX	F	5006	51/51	0.93	0.08	18,22,37,40	0
4	CMX	C	5003	51/51	0.94	0.08	18,25,39,42	0
4	CMX	E	5005	51/51	0.94	0.08	17,22,38,41	0
4	CMX	B	5002	51/51	0.94	0.08	19,26,41,43	0
4	CMX	D	5004	51/51	0.95	0.08	20,25,43,48	0
2	OAA	F	5012	9/9	0.95	0.07	16,18,22,23	0
4	CMX	A	5001	51/51	0.95	0.07	16,23,41,42	0
2	OAA	A	5007	9/9	0.96	0.06	19,20,24,24	0
3	SO4	D	5021	5/5	0.96	0.07	26,30,32,34	0
2	OAA	B	5008	9/9	0.96	0.06	17,20,22,23	0
2	OAA	C	5009	9/9	0.96	0.05	19,20,22,23	0
2	OAA	D	5010	9/9	0.96	0.06	20,21,24,26	0
3	SO4	B	5016	5/5	0.97	0.06	22,23,24,30	0
3	SO4	A	5014	5/5	0.97	0.06	25,28,32,33	0
3	SO4	E	5023	5/5	0.97	0.06	23,27,29,29	0
3	SO4	F	5026	5/5	0.97	0.07	25,29,31,32	0
3	SO4	E	5024	5/5	0.97	0.10	42,43,44,46	0
3	SO4	E	5025	5/5	0.97	0.09	24,26,29,31	0
2	OAA	E	5011	9/9	0.97	0.05	16,18,23,23	0
3	SO4	C	5020	5/5	0.98	0.07	27,30,31,33	0
3	SO4	A	5015	5/5	0.98	0.08	26,27,29,29	0
3	SO4	D	5018	5/5	0.98	0.08	28,28,31,31	0
3	SO4	F	5022	5/5	0.98	0.08	23,23,25,29	0
3	SO4	C	5019	5/5	0.98	0.05	26,26,30,30	0
3	SO4	B	5013	5/5	0.99	0.05	24,25,26,30	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.

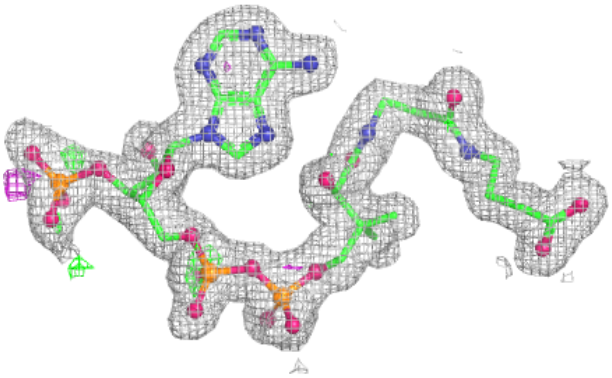
Electron density around CMX F 5006:

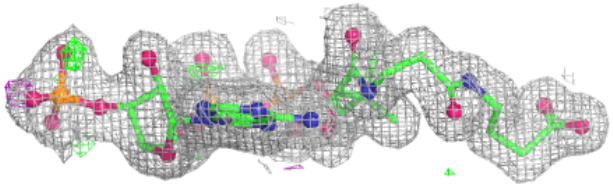
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

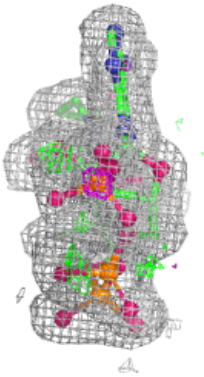


Electron density around CMX C 5003:

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

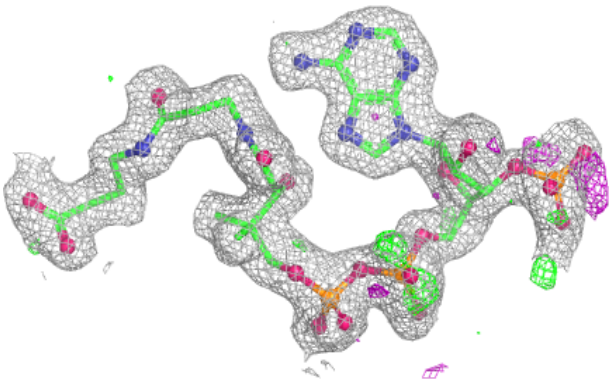


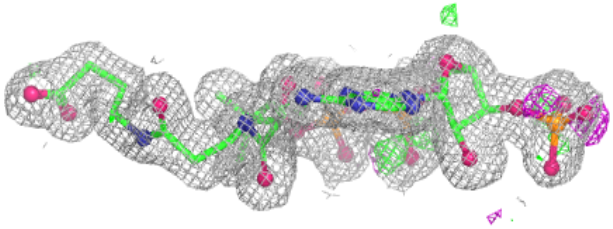


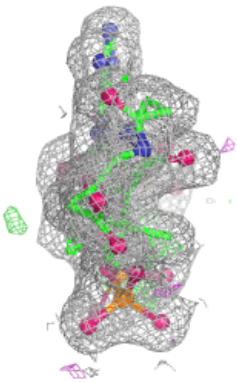


Electron density around CMX E 5005:

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

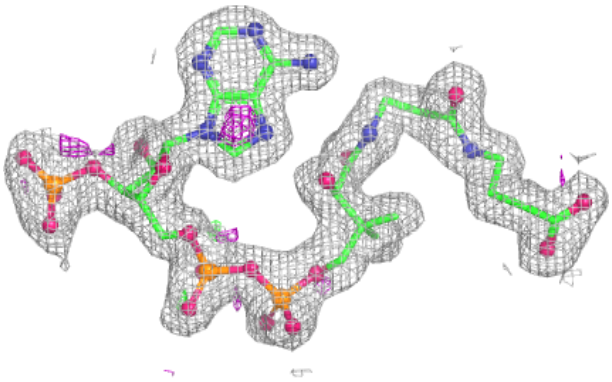


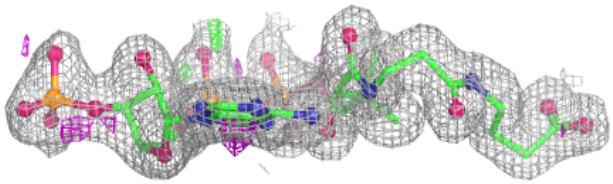


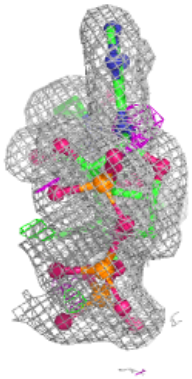


Electron density around CMX B 5002:

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

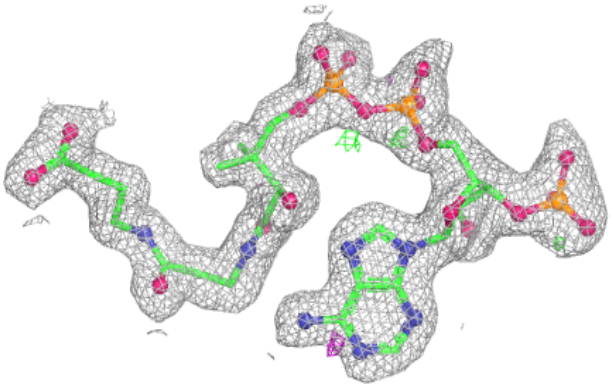


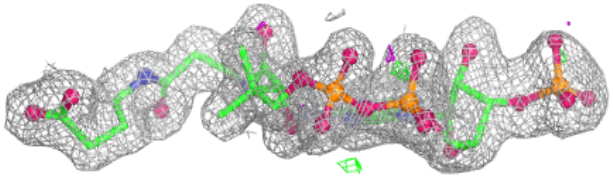


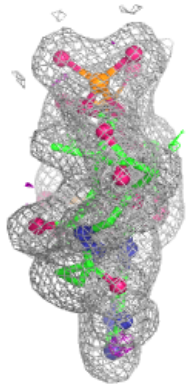


Electron density around CMX D 5004:

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

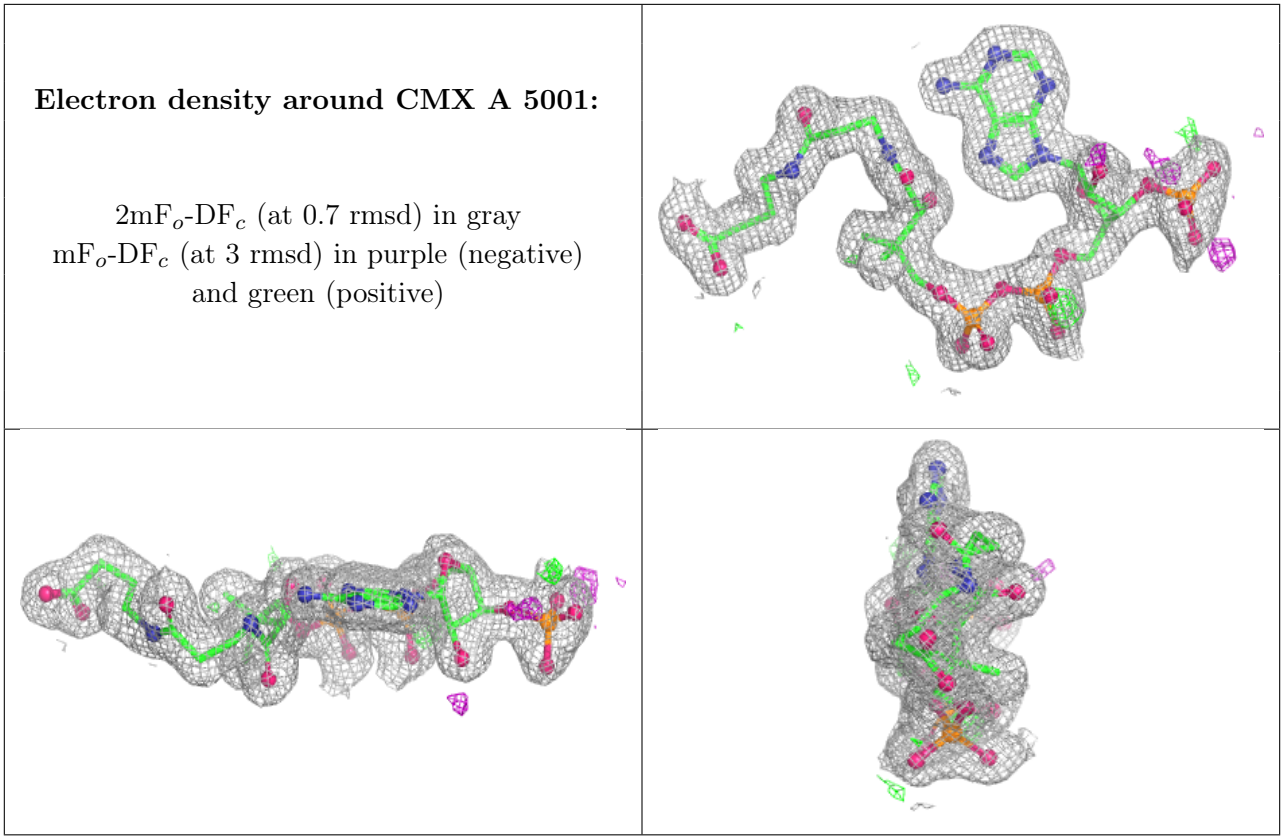






Electron density around CMX A 5001:

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



6.5 Other polymers (i)

There are no such residues in this entry.