Full wwPDB X-ray Structure Validation Report (i)

Jun 9, 2025 – 02:11 PM JST

PDB ID	:	8ZVL / pdb_00008zvl
Title	:	human citrate synthases complexed with oxaloacetate
Authors	:	Yang, L.Y.; Fang, Y.J.
Deposited on	:	2024-06-11
Resolution	:	2.05 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:

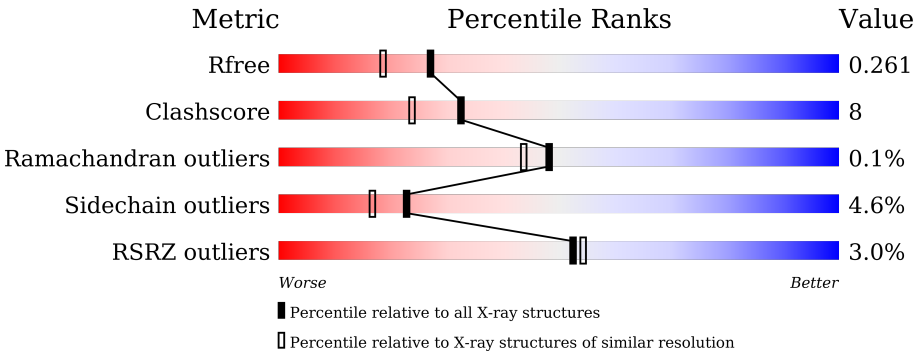
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	435	79% 19%
1	B	435	83% 15%
1	C	435	7% 78% 20%
1	D	435	3% 80% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OAA	D	501	-	-	X	-

2 Entry composition

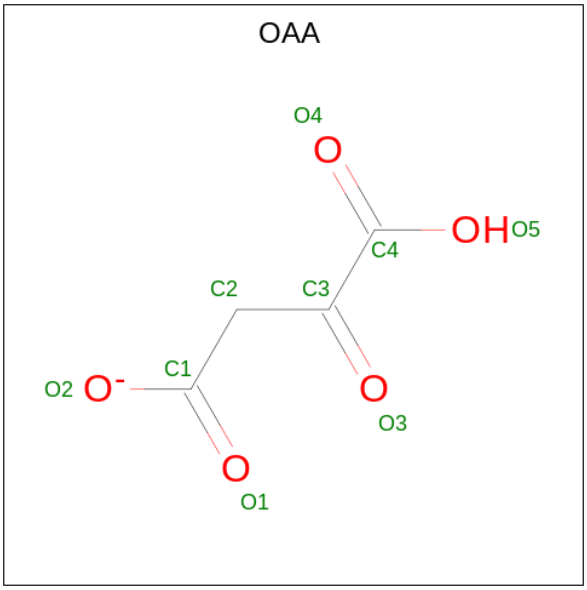
There are 3 unique types of molecules in this entry. The entry contains 14280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3420	2188	586	629	17			
1	D	435	Total	C	N	O	S	0	0	0
			3431	2194	590	630	17			
1	B	434	Total	C	N	O	S	0	1	0
			3424	2190	587	630	17			
1	C	435	Total	C	N	O	S	0	0	0
			3423	2188	588	630	17			

- Molecule 2 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 3 is water.

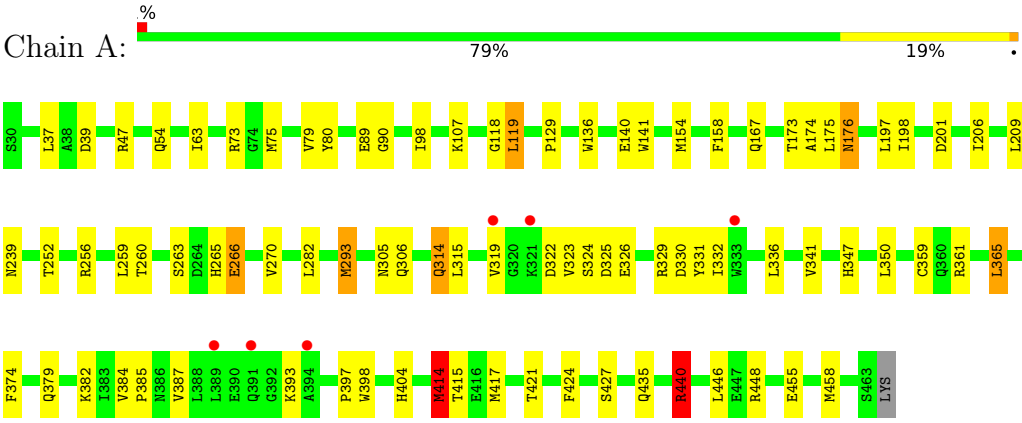
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0
3	D	150	Total O 150 150	0	0
3	B	147	Total O 147 147	0	0
3	C	107	Total O 107 107	0	0

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.

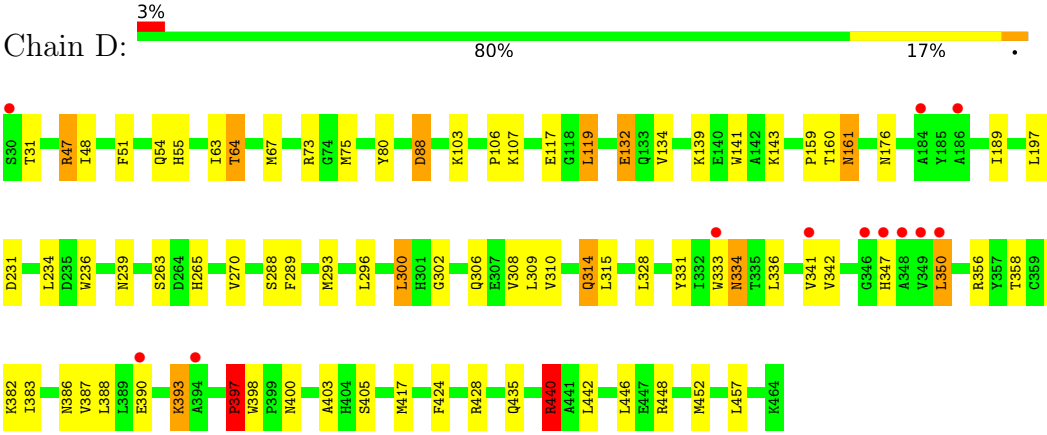
• Molecule 1: Citrate synthase, mitochondrial

Chain A:



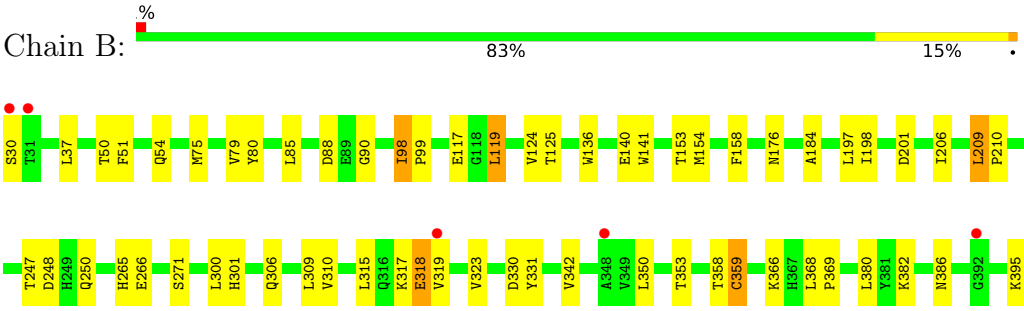
• Molecule 1: Citrate synthase, mitochondrial

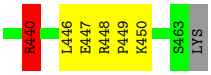
Chain D:



• Molecule 1: Citrate synthase, mitochondrial

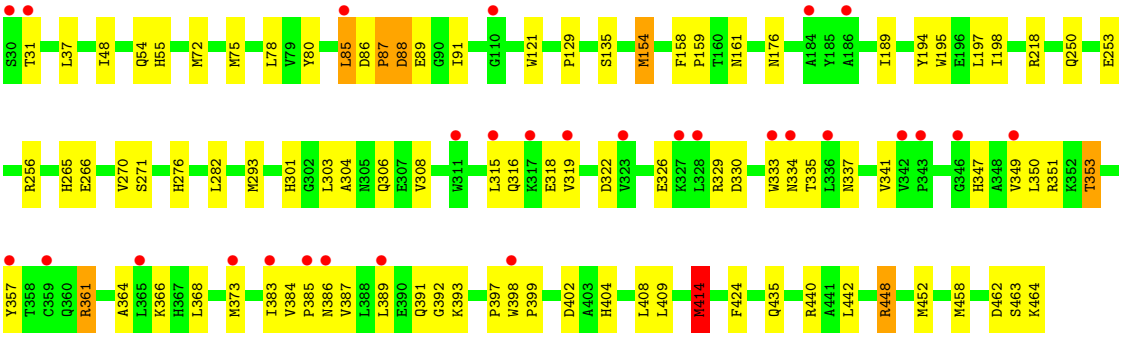
Chain B:





• Molecule 1: Citrate synthase, mitochondrial

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.60Å 78.01Å 103.12Å 70.75° 81.37° 74.74°	Depositor
Resolution (Å)	32.68 – 2.05 32.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.4 (32.68-2.05) 96.4 (32.68-2.05)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.194 , 0.258 0.199 , 0.261	Depositor DCC
R_{free} test set	4896 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14280	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9106e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: OAA

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	0.67	0/3508	1.22	10/4762 (0.2%)
1	B	0.69	1/3512 (0.0%)	1.21	17/4767 (0.4%)
1	C	0.70	2/3508 (0.1%)	1.20	9/4763 (0.2%)
1	D	0.67	0/3516	1.20	16/4771 (0.3%)
All	All	0.68	3/14044 (0.0%)	1.21	52/19063 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	2
1	D	0	3
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	GLU	C-N	12.18	1.50	1.33
1	C	318	GLU	C-N	8.55	1.45	1.33
1	C	364	ALA	C-N	5.64	1.41	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	414	MET	CG-SD-CE	9.29	121.34	100.90
1	D	397	PRO	N-CA-CB	-7.80	95.06	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	306	GLN	N-CA-CB	7.48	121.23	110.16
1	B	359	CYS	CB-CA-C	-6.92	99.74	110.81
1	A	379	GLN	CB-CA-C	-6.89	99.34	110.79
1	D	314	GLN	N-CA-CB	-6.88	100.01	110.12
1	D	358	THR	CA-CB-OG1	-6.79	99.42	109.60
1	B	318	GLU	CA-C-N	-6.72	109.88	121.97
1	B	318	GLU	C-N-CA	-6.72	109.88	121.97
1	B	358	THR	CA-CB-OG1	-6.67	99.59	109.60
1	B	201	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	440	ARG	CG-CD-NE	-6.39	97.95	112.00
1	A	424	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	88	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	153	THR	CA-CB-OG1	-6.30	100.15	109.60
1	C	330	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	117	GLU	CB-CA-C	-6.27	100.78	110.81
1	B	366	LYS	N-CA-CB	-6.05	101.25	110.26
1	C	87	PRO	N-CA-C	-6.00	101.79	111.14
1	B	247	THR	CA-CB-OG1	-5.96	100.66	109.60
1	D	314	GLN	CB-CA-C	5.93	120.64	110.79
1	D	440	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	D	390	GLU	N-CA-CB	5.79	118.62	110.12
1	D	236	TRP	N-CA-CB	-5.77	101.64	110.12
1	B	248	ASP	CA-CB-CG	5.73	118.33	112.60
1	D	64	THR	CA-CB-OG1	-5.72	101.01	109.60
1	B	353	THR	OG1-CB-CG2	-5.72	97.85	109.30
1	A	421	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	440	ARG	CG-CD-NE	-5.69	99.48	112.00
1	B	50	THR	CA-CB-OG1	-5.67	101.10	109.60
1	C	353	THR	CA-CB-OG1	-5.67	101.10	109.60
1	C	462	ASP	N-CA-C	-5.57	104.60	111.40
1	D	159	PRO	CA-C-N	5.54	128.26	120.28
1	D	159	PRO	C-N-CA	5.54	128.26	120.28
1	A	415	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	37	LEU	N-CA-CB	-5.43	102.12	110.16
1	A	39	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	160	THR	CA-CB-OG1	-5.37	101.54	109.60
1	A	414	MET	CG-SD-CE	5.36	112.69	100.90
1	C	402	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	37	LEU	N-CA-CB	-5.27	102.36	110.16
1	A	293	MET	CG-SD-CE	5.26	112.47	100.90
1	C	424	PHE	CA-CB-CG	5.26	119.06	113.80
1	D	88	ASP	CA-CB-CG	5.17	117.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	31	THR	CA-CB-OG1	-5.15	101.88	109.60
1	D	107	LYS	N-CA-CB	-5.15	102.86	111.20
1	D	457	LEU	N-CA-CB	-5.12	102.06	110.40
1	A	201	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	117	GLU	N-CA-CB	5.05	117.47	109.94
1	D	218	ARG	CB-CA-C	-5.05	102.27	110.85
1	B	125	THR	CA-CB-OG1	-5.04	102.04	109.60
1	B	342	VAL	CA-C-O	5.03	121.94	119.12

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ARG	Sidechain
1	A	440	ARG	Sidechain
1	A	47	ARG	Sidechain
1	B	440	ARG	Sidechain
1	B	448	ARG	Sidechain
1	C	361	ARG	Sidechain
1	C	448	ARG	Sidechain
1	D	440	ARG	Sidechain
1	D	448	ARG	Sidechain
1	D	47	ARG	Sidechain

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	3420	0	3398	64	0
1	B	3424	0	3404	54	0
1	C	3423	0	3395	60	0
1	D	3431	0	3417	55	0
2	A	9	0	2	2	0
2	B	9	0	2	0	0
2	D	9	0	2	5	0
3	A	151	0	0	16	0
3	B	147	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	107	0	0	6	0
3	D	150	0	0	3	0
All	All	14280	0	13620	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (212) 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:119:LEU:HD13	3:A:812:HOH:O	1.56	1.04
1:C:329:ARG:NH1	3:C:502:HOH:O	2.07	0.86
1:A:119:LEU:CG	3:A:812:HOH:O	2.23	0.85
1:D:309:LEU:HB3	1:D:417:MET:HE3	1.58	0.85
1:A:107:LYS:HE3	3:A:746:HOH:O	1.77	0.83
1:B:309:LEU:HB3	1:B:417:MET:HE3	1.60	0.83
1:C:154:MET:HE3	1:C:158:PHE:HZ	1.43	0.82
1:B:319:VAL:HG23	1:B:323:VAL:HB	1.60	0.81
1:C:154:MET:HE3	1:C:158:PHE:CZ	2.17	0.79
1:A:265:HIS:O	1:A:266:GLU:HB2	1.83	0.77
1:C:85:LEU:HD21	1:C:265:HIS:CE1	2.19	0.77
1:B:98:ILE:HG21	1:B:359:CYS:SG	2.26	0.76
1:A:119:LEU:HB3	3:A:812:HOH:O	1.85	0.75
1:C:326:GLU:OE2	3:C:501:HOH:O	2.04	0.73
1:A:119:LEU:CD1	3:A:812:HOH:O	2.20	0.73
1:A:119:LEU:CB	3:A:812:HOH:O	2.34	0.73
1:B:306:GLN:HG3	1:B:417:MET:HE2	1.71	0.72
1:C:329:ARG:NE	3:C:501:HOH:O	2.22	0.72
1:B:309:LEU:HB3	1:B:417:MET:CE	2.21	0.70
1:A:446:LEU:HD11	1:D:270:VAL:HG21	1.74	0.69
1:A:54:GLN:NE2	3:A:701:HOH:O	2.23	0.69
1:A:119:LEU:HD22	3:A:812:HOH:O	1.90	0.69
1:D:356:ARG:NH1	2:D:501:OAA:O5	2.24	0.69
1:D:334:ASN:HB3	3:D:728:HOH:O	1.93	0.68
1:D:231:ASP:H	1:D:239:ASN:HD21	1.41	0.68
1:D:288:SER:OG	3:D:601:HOH:O	2.12	0.68
1:D:288:SER:N	3:D:601:HOH:O	2.27	0.68
1:C:80:TYR:CE2	1:C:435:GLN:HG2	2.29	0.68
1:C:87:PRO:O	1:C:88:ASP:HB2	1.92	0.67
1:B:319:VAL:HG21	1:B:323:VAL:HG21	1.75	0.67
1:D:119:LEU:HD21	1:D:263:SER:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HD13	1:D:197:LEU:HD11	1.77	0.66
1:B:447:GLU:CD	1:C:72:MET:HE2	2.19	0.66
1:B:231:ASP:H	1:B:239:ASN:HD21	1.40	0.66
1:C:85:LEU:HD22	1:C:91:ILE:HD13	1.77	0.66
1:A:98:ILE:HG21	1:A:359:CYS:SG	2.36	0.65
1:B:310:VAL:HG23	1:B:417:MET:HE1	1.79	0.65
1:D:309:LEU:HB3	1:D:417:MET:CE	2.26	0.64
1:B:447:GLU:CG	1:C:72:MET:HE2	2.26	0.64
1:A:158:PHE:CD2	1:A:167:GLN:HG2	2.33	0.64
1:C:250:GLN:HG2	3:C:594:HOH:O	1.98	0.64
1:B:300:LEU:CD1	1:C:282:LEU:HD12	2.27	0.64
1:C:86:ASP:HB3	1:C:89:GLU:HB2	1.79	0.64
1:A:154:MET:HE1	1:A:174:ALA:HB3	1.79	0.63
1:D:161:ASN:H	1:D:161:ASN:HD22	1.45	0.62
1:B:319:VAL:HG21	1:B:323:VAL:CG2	2.29	0.62
1:A:315:LEU:HD13	1:A:331:TYR:CE1	2.33	0.62
1:A:314:GLN:HG3	3:A:709:HOH:O	2.00	0.62
1:A:293:MET:HE2	1:A:293:MET:HA	1.80	0.62
1:A:231:ASP:H	1:A:239:ASN:HD21	1.49	0.61
1:D:336:LEU:HD11	1:D:342:VAL:HG23	1.82	0.61
1:C:253:GLU:OE2	1:C:256:ARG:NH1	2.34	0.60
1:D:64:THR:HG23	1:D:67:MET:HE3	1.83	0.60
1:C:78:LEU:HD11	1:C:276:HIS:CD2	2.36	0.60
1:A:154:MET:HE1	1:A:174:ALA:CB	2.32	0.60
1:D:424:PHE:HZ	2:D:501:OAA:O4	1.84	0.60
1:A:265:HIS:O	1:A:266:GLU:CB	2.50	0.60
1:B:300:LEU:HD13	1:C:282:LEU:HD12	1.82	0.60
1:A:175:LEU:HD22	3:A:708:HOH:O	2.02	0.59
1:B:30:SER:OG	3:B:601:HOH:O	2.17	0.59
1:B:319:VAL:CG2	1:B:323:VAL:HB	2.32	0.58
1:C:80:TYR:CD2	1:C:435:GLN:HG2	2.38	0.58
1:C:189:ILE:HD13	1:C:197:LEU:HD11	1.85	0.58
1:A:54:GLN:HB2	3:A:756:HOH:O	2.02	0.58
1:B:271:SER:OG	1:B:301:HIS:HE1	1.87	0.57
1:B:231:ASP:H	1:B:239:ASN:ND2	2.03	0.56
1:B:98:ILE:CG2	1:B:359:CYS:SG	2.94	0.56
1:A:458:MET:HE2	1:D:51:PHE:HB2	1.86	0.56
1:B:449:PRO:HD3	1:C:72:MET:HE3	1.87	0.56
1:B:90:GLY:HA2	1:B:350:LEU:HD21	1.88	0.56
1:A:265:HIS:HD2	2:A:601:OAA:O2	1.89	0.56
1:A:80:TYR:CE2	1:A:435:GLN:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ILE:HG13	1:C:440:ARG:HG3	1.88	0.55
1:A:365:LEU:HD13	1:A:374:PHE:HZ	1.71	0.54
1:B:98:ILE:HB	1:B:99:PRO:HD3	1.88	0.54
1:A:119:LEU:CD2	3:A:812:HOH:O	2.45	0.54
1:B:51:PHE:HB2	1:C:458:MET:HE2	1.90	0.53
1:D:306:GLN:O	1:D:417:MET:HE1	2.09	0.53
1:B:75:MET:HE3	1:C:75:MET:CE	2.39	0.53
1:D:80:TYR:CE2	1:D:435:GLN:HG2	2.43	0.53
1:D:198:ILE:HG13	1:D:440:ARG:HG3	1.90	0.52
1:B:136:TRP:CH2	1:B:140:GLU:HG3	2.44	0.52
1:D:231:ASP:H	1:D:239:ASN:ND2	2.07	0.52
1:C:54:GLN:HG3	1:C:55:HIS:CD2	2.45	0.52
1:C:85:LEU:HD21	1:C:265:HIS:NE2	2.25	0.52
1:A:347:HIS:HE1	2:A:601:OAA:O3	1.93	0.52
1:A:446:LEU:HD11	1:D:270:VAL:CG2	2.39	0.52
1:B:75:MET:HE3	1:C:75:MET:HE1	1.92	0.52
1:D:428:ARG:HH22	2:D:501:OAA:C4	2.22	0.52
1:D:308:VAL:HG11	1:D:403:ALA:HA	1.90	0.52
1:D:328:LEU:HD23	1:D:383:ILE:HD12	1.92	0.52
1:B:140:GLU:HG2	3:B:670:HOH:O	2.10	0.51
1:B:368:LEU:N	1:B:369:PRO:CD	2.73	0.51
1:B:265:HIS:O	1:B:266:GLU:HB2	2.11	0.51
1:A:98:ILE:CG2	1:A:359:CYS:SG	2.99	0.51
1:D:106:PRO:HG2	1:D:134:VAL:HG21	1.93	0.51
1:C:384:VAL:N	1:C:385:PRO:HD2	2.26	0.50
1:D:231:ASP:HB3	1:D:234:LEU:HD12	1.93	0.50
1:D:333:TRP:CE2	1:D:387:VAL:HG13	2.47	0.50
1:D:347:HIS:CE1	1:D:398:TRP:HB2	2.47	0.50
1:A:306:GLN:HG3	1:A:417:MET:HB3	1.93	0.50
1:D:80:TYR:CD2	1:D:435:GLN:HG2	2.46	0.50
1:B:317:LYS:NZ	3:B:607:HOH:O	2.45	0.50
1:A:322:ASP:O	1:A:323:VAL:C	2.55	0.50
1:C:265:HIS:O	1:C:266:GLU:HB2	2.12	0.50
1:D:119:LEU:HD21	1:D:263:SER:OG	2.12	0.50
1:D:424:PHE:CZ	2:D:501:OAA:O4	2.65	0.49
1:C:361:ARG:HA	1:C:404:HIS:NE2	2.27	0.49
1:A:231:ASP:H	1:A:239:ASN:ND2	2.09	0.49
1:A:332:ILE:HG22	1:A:387:VAL:HG11	1.93	0.49
1:C:383:ILE:O	1:C:387:VAL:HG23	2.12	0.49
1:B:154:MET:HE2	1:B:158:PHE:HZ	1.76	0.49
1:B:184:ALA:HB3	1:B:197:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:THR:OG1	1:D:67:MET:HG3	2.13	0.49
1:B:318:GLU:O	1:B:319:VAL:CG1	2.61	0.49
1:C:389:LEU:O	1:C:392:GLY:N	2.46	0.48
1:A:361:ARG:HA	1:A:404:HIS:CE1	2.48	0.48
1:B:330:ASP:HB2	3:B:725:HOH:O	2.12	0.48
1:C:347:HIS:HD2	1:C:350:LEU:H	1.59	0.48
1:B:300:LEU:HD11	1:C:282:LEU:HD12	1.96	0.48
1:A:373:MET:HG2	3:A:815:HOH:O	2.13	0.48
1:C:463:SER:O	1:C:464:LYS:HB2	2.13	0.48
1:B:306:GLN:O	1:B:417:MET:HE1	2.14	0.47
1:D:289:PHE:CE1	1:D:293:MET:HE3	2.50	0.47
1:C:304:ALA:O	1:C:308:VAL:HG23	2.15	0.47
1:C:48:ILE:HD12	1:C:442:LEU:HD22	1.96	0.47
1:C:87:PRO:O	1:C:88:ASP:CB	2.61	0.47
1:D:310:VAL:HG23	1:D:417:MET:HE1	1.96	0.47
1:D:440:ARG:HD3	1:D:440:ARG:HA	1.64	0.47
1:B:119:LEU:O	1:B:119:LEU:HG	2.10	0.47
1:C:293:MET:HA	1:C:293:MET:HE2	1.96	0.47
1:C:31:THR:HA	3:C:535:HOH:O	2.14	0.47
1:C:271:SER:H	1:C:301:HIS:CE1	2.33	0.47
1:A:270:VAL:HG21	1:D:446:LEU:HD11	1.97	0.47
1:B:446:LEU:HD11	1:C:270:VAL:HG21	1.96	0.47
1:A:80:TYR:CD2	1:A:435:GLN:HG2	2.49	0.47
1:B:80:TYR:CD2	1:B:435:GLN:HG2	2.50	0.47
1:C:85:LEU:HD21	1:C:265:HIS:CD2	2.50	0.47
1:A:455:GLU:HG3	3:A:817:HOH:O	2.15	0.47
1:B:80:TYR:CE2	1:B:435:GLN:HG2	2.50	0.46
1:D:315:LEU:HD13	1:D:331:TYR:CE1	2.51	0.46
1:A:365:LEU:HD13	1:A:374:PHE:CZ	2.49	0.46
1:A:259:LEU:HD23	1:A:427:SER:HB2	1.97	0.46
1:A:63:ILE:HD11	1:D:75:MET:HG3	1.98	0.45
1:D:393:LYS:HD3	1:D:393:LYS:HA	1.53	0.45
1:A:252:THR:HG22	1:A:256:ARG:CZ	2.46	0.45
1:D:132:GLU:OE1	1:D:132:GLU:N	2.50	0.45
1:C:357:TYR:C	1:C:357:TYR:CD1	2.94	0.45
1:B:221:TYR:CG	1:B:416:GLU:HG2	2.51	0.45
1:C:86:ASP:CB	1:C:89:GLU:HB2	2.46	0.45
1:C:389:LEU:HD13	1:C:397:PRO:HG3	1.98	0.45
1:B:306:GLN:HA	1:B:417:MET:CE	2.47	0.45
1:B:221:TYR:CD1	1:B:416:GLU:HG2	2.52	0.44
1:A:136:TRP:CH2	1:A:140:GLU:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PRO:HB2	1:C:161:ASN:OD1	2.17	0.44
1:A:384:VAL:N	1:A:385:PRO:CD	2.81	0.44
1:A:458:MET:HE1	1:D:47:ARG:HG2	2.00	0.43
1:B:450:LYS:NZ	1:C:85:LEU:O	2.50	0.43
1:C:384:VAL:N	1:C:385:PRO:CD	2.81	0.43
1:A:325:ASP:O	1:A:329:ARG:HB2	2.18	0.43
1:A:265:HIS:HE1	3:A:764:HOH:O	2.02	0.43
1:B:37:LEU:HD13	1:B:124:VAL:CG1	2.48	0.43
1:B:85:LEU:N	1:B:266:GLU:HG3	2.34	0.43
1:A:282:LEU:HD12	1:D:300:LEU:HD13	2.00	0.43
1:D:48:ILE:CD1	1:D:442:LEU:HD13	2.49	0.43
1:B:184:ALA:CB	1:B:197:LEU:HD13	2.48	0.43
1:D:347:HIS:ND1	1:D:398:TRP:HB2	2.34	0.43
1:B:315:LEU:HD13	1:B:331:TYR:CE1	2.54	0.43
1:A:119:LEU:CD1	1:A:260:THR:O	2.66	0.43
1:A:90:GLY:HA2	1:A:350:LEU:HD21	2.01	0.42
1:A:397:PRO:HG2	1:A:398:TRP:CD1	2.54	0.42
1:D:350:LEU:HD13	1:D:350:LEU:HA	1.91	0.42
1:D:117:GLU:HG3	1:D:141:TRP:CZ3	2.54	0.42
1:B:79:VAL:HA	1:C:452:MET:O	2.19	0.42
1:B:231:ASP:OD1	1:B:231:ASP:C	2.62	0.42
1:B:198:ILE:HG13	1:B:440:ARG:HG3	2.02	0.42
1:C:409:LEU:HB3	1:C:414:MET:HG2	2.00	0.42
1:C:316:GLN:NE2	1:C:373:MET:SD	2.93	0.42
1:B:154:MET:HE2	1:B:158:PHE:CZ	2.55	0.42
1:B:209:LEU:N	1:B:210:PRO:CD	2.82	0.42
1:A:119:LEU:HD12	1:A:260:THR:O	2.20	0.42
1:A:198:ILE:HG13	1:A:440:ARG:HG3	2.02	0.42
1:D:296:LEU:O	1:D:302:GLY:HA3	2.20	0.42
1:C:398:TRP:HB3	1:C:399:PRO:HD2	2.02	0.42
1:A:141:TRP:CZ2	1:A:206:ILE:HG21	2.55	0.41
1:B:54:GLN:HB2	3:B:622:HOH:O	2.19	0.41
1:C:85:LEU:HD21	1:C:265:HIS:CG	2.55	0.41
1:A:173:THR:O	1:A:176:ASN:HB3	2.20	0.41
1:D:54:GLN:HG2	1:D:55:HIS:CD2	2.56	0.41
1:C:347:HIS:CD2	1:C:350:LEU:H	2.37	0.41
1:D:306:GLN:O	1:D:417:MET:CE	2.69	0.41
1:D:397:PRO:HD2	1:D:398:TRP:CD1	2.56	0.41
1:D:397:PRO:HD2	1:D:398:TRP:NE1	2.36	0.41
1:D:265:HIS:ND1	2:D:501:OAA:H22	2.35	0.41
1:A:305:ASN:OD1	1:A:305:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:CD1	1:A:263:SER:OG	2.69	0.41
1:C:189:ILE:CD1	1:C:197:LEU:HD11	2.51	0.41
1:A:371:ASP:HA	1:A:372:PRO:HD3	1.97	0.41
1:A:75:MET:HG3	1:D:63:ILE:HD11	2.03	0.40
1:A:197:LEU:HD13	3:A:786:HOH:O	2.21	0.40
1:A:324:SER:OG	1:A:326:GLU:HG3	2.21	0.40
1:C:85:LEU:HD22	1:C:91:ILE:CD1	2.47	0.40
1:B:141:TRP:CZ2	1:B:206:ILE:HG21	2.56	0.40
1:C:194:TYR:O	1:C:195:TRP:C	2.64	0.40
1:C:218:ARG:CZ	3:C:515:HOH:O	2.69	0.40
1:A:414:MET:O	1:A:414:MET:HG3	2.20	0.40
1:A:79:VAL:HA	1:D:452:MET:O	2.22	0.40
1:A:118:GLY:HA2	1:A:129:PRO:HG3	2.03	0.40
1:D:360:GLN:HE22	1:D:405:SER:HA	1.87	0.40
1:D:388:LEU:HB2	1:D:397:PRO:HB2	2.03	0.40
1:C:121:TRP:CG	1:C:129:PRO:HB3	2.57	0.40
1:C:333:TRP:O	1:C:337:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/435 (100%)	420 (97%)	13 (3%)	0	100	100
1	B	433/435 (100%)	426 (98%)	7 (2%)	0	100	100
1	C	433/435 (100%)	421 (97%)	11 (2%)	1 (0%)	44	38
1	D	433/435 (100%)	419 (97%)	14 (3%)	0	100	100
All	All	1732/1740 (100%)	1686 (97%)	45 (3%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	ASP

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	368/370 (100%)	351 (95%)	17 (5%)	23 17
1	B	369/370 (100%)	360 (98%)	9 (2%)	44 40
1	C	368/370 (100%)	346 (94%)	22 (6%)	16 9
1	D	370/370 (100%)	350 (95%)	20 (5%)	18 11
All	All	1475/1480 (100%)	1407 (95%)	68 (5%)	23 17

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	A	89	GLU
1	A	119	LEU
1	A	176	ASN
1	A	209	LEU
1	A	266	GLU
1	A	314	GLN
1	A	319	VAL
1	A	330	ASP
1	A	336	LEU
1	A	341	VAL
1	A	365	LEU
1	A	368	LEU
1	A	382	LYS
1	A	393	LYS
1	A	414	MET
1	A	448	ARG
1	D	73	ARG
1	D	88	ASP
1	D	103	LYS
1	D	119	LEU

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Mol	Chain	Res	Type
1	D	132	GLU
1	D	139	LYS
1	D	143	LYS
1	D	161	ASN
1	D	176	ASN
1	D	300	LEU
1	D	314	GLN
1	D	334	ASN
1	D	341	VAL
1	D	350	LEU
1	D	368	LEU
1	D	382	LYS
1	D	386	ASN
1	D	393	LYS
1	D	397	PRO
1	D	400	ASN
1	B	98	ILE
1	B	119	LEU
1	B	176	ASN
1	B	209	LEU
1	B	250	GLN
1	B	380	LEU
1	B	382	LYS
1	B	386	ASN
1	B	395	LYS
1	C	85	LEU
1	C	135	SER
1	C	154	MET
1	C	176	ASN
1	C	303	LEU
1	C	315	LEU
1	C	319	VAL
1	C	322	ASP
1	C	334	ASN
1	C	335	THR
1	C	341	VAL
1	C	349	VAL
1	C	351	ARG
1	C	353	THR
1	C	366	LYS
1	C	368	LEU
1	C	386	ASN

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Mol	Chain	Res	Type
1	C	391	GLN
1	C	393	LYS
1	C	408	LEU
1	C	414	MET
1	C	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	55	HIS
1	A	239	ASN
1	A	249	HIS
1	A	262	HIS
1	A	265	HIS
1	A	301	HIS
1	A	314	GLN
1	A	347	HIS
1	A	360	GLN
1	A	367	HIS
1	A	404	HIS
1	D	150	HIS
1	D	161	ASN
1	D	180	ASN
1	D	239	ASN
1	D	250	GLN
1	D	360	GLN
1	D	379	GLN
1	B	54	GLN
1	B	176	ASN
1	B	239	ASN
1	B	265	HIS
1	B	301	HIS
1	B	360	GLN
1	B	391	GLN
1	B	418	ASN
1	C	102	GLN
1	C	250	GLN
1	C	301	HIS
1	C	316	GLN
1	C	334	ASN
1	C	347	HIS

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Mol	Chain	Res	Type
1	C	370	ASN
1	C	379	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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OAA	B	501	-	8,8,8	4.20	3 (37%)	9,10,10	2.18	4 (44%)
2	OAA	D	501	-	8,8,8	6.72	2 (25%)	9,10,10	1.50	1 (11%)
2	OAA	A	601	-	8,8,8	4.47	2 (25%)	9,10,10	2.13	3 (33%)

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	B	501	-	-	1/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OAA	D	501	-	-	5/8/8/8	-
2	OAA	A	601	-	-	1/8/8/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	OAA	C3-C4	-18.64	1.28	1.53
2	A	601	OAA	C3-C4	-12.23	1.37	1.53
2	B	501	OAA	C3-C4	-11.20	1.38	1.53
2	B	501	OAA	C2-C1	3.02	1.55	1.51
2	D	501	OAA	O5-C4	-2.99	1.21	1.30
2	A	601	OAA	O5-C4	-2.12	1.24	1.30
2	B	501	OAA	O5-C4	-2.10	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	OAA	C2-C3-C4	3.68	124.07	117.85
2	A	601	OAA	O3-C3-C2	-3.56	115.43	120.58
2	A	601	OAA	C2-C3-C4	3.55	123.85	117.85
2	B	501	OAA	O3-C3-C2	-3.40	115.66	120.58
2	B	501	OAA	O5-C4-C3	2.64	121.20	113.97
2	A	601	OAA	O5-C4-C3	2.48	120.75	113.97
2	D	501	OAA	O4-C4-C3	-2.33	118.60	121.72
2	B	501	OAA	O5-C4-O4	-2.09	118.83	123.61

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	OAA	C2-C3-C4-O5
2	D	501	OAA	C1-C2-C3-O3
2	D	501	OAA	C2-C3-C4-O4
2	D	501	OAA	O3-C3-C4-O5
2	A	601	OAA	O1-C1-C2-C3
2	D	501	OAA	O1-C1-C2-C3
2	B	501	OAA	O1-C1-C2-C3

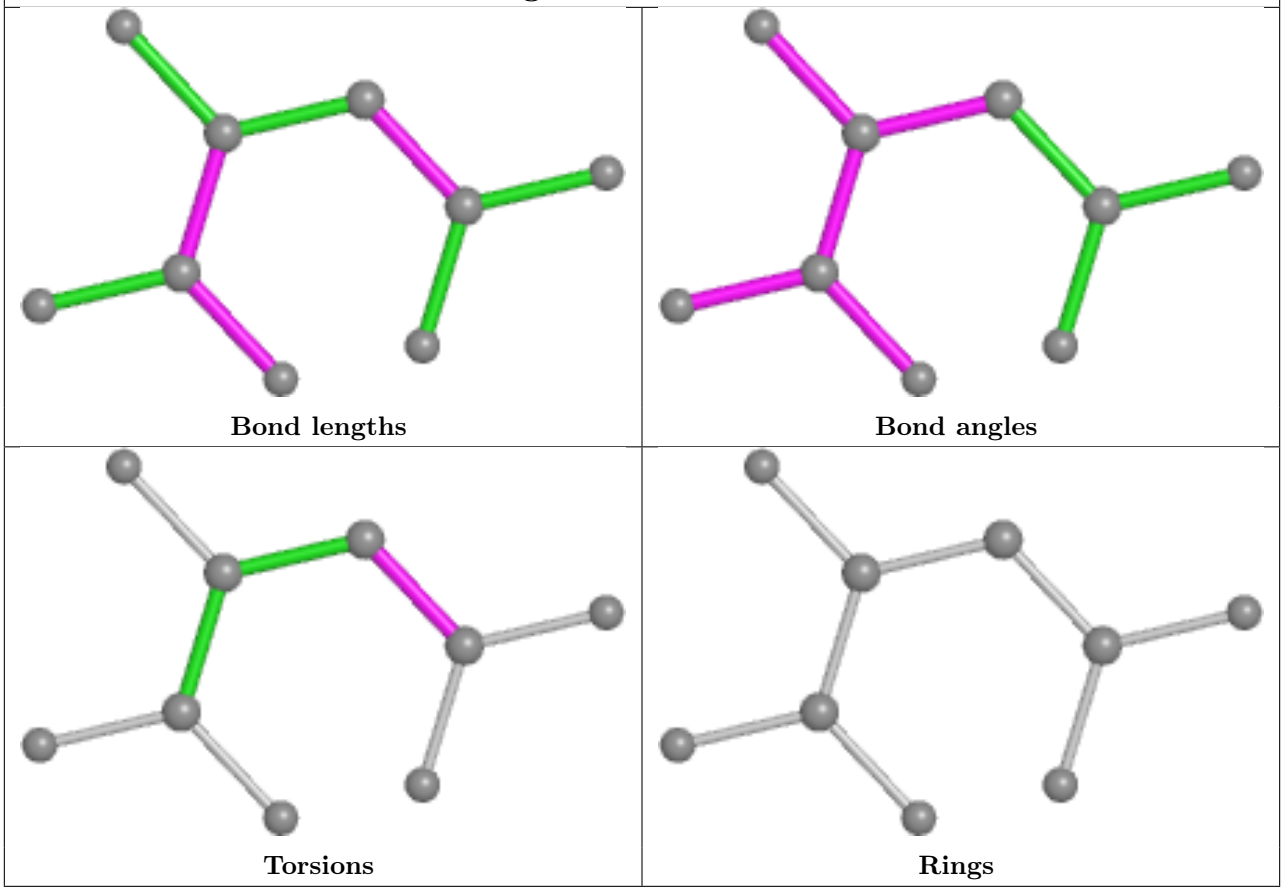
There are no ring outliers.

2 monomers are involved in 7 short contacts:

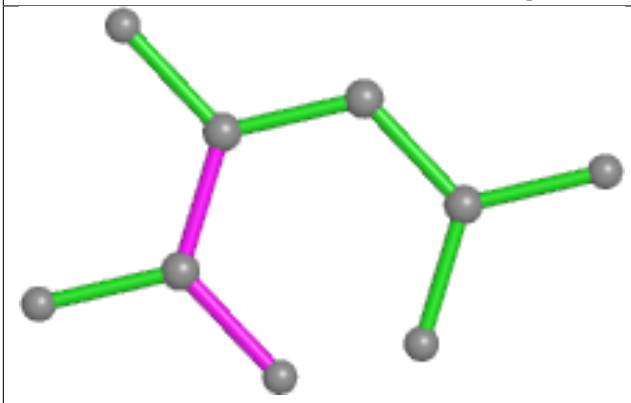
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	OAA	5	0
2	A	601	OAA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

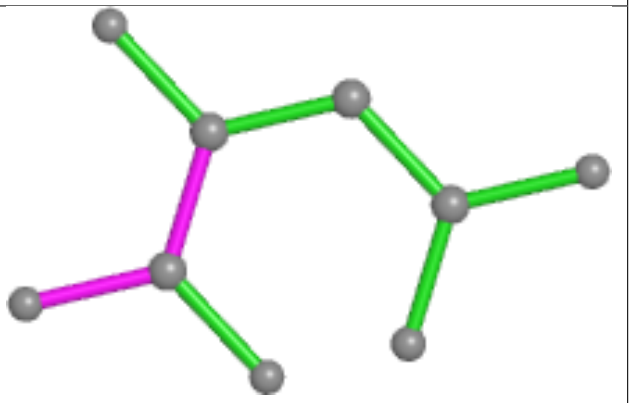
Ligand OAA B 501



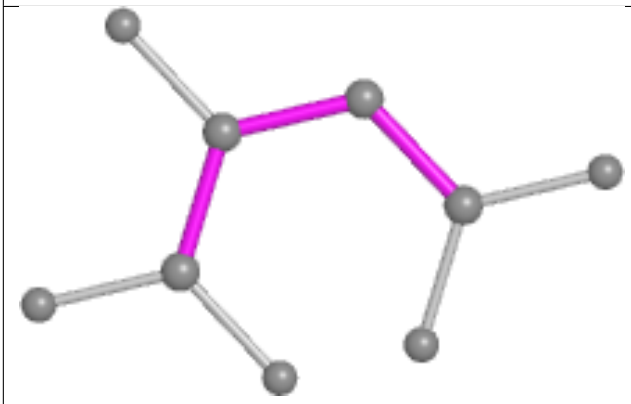
Ligand OAA D 501



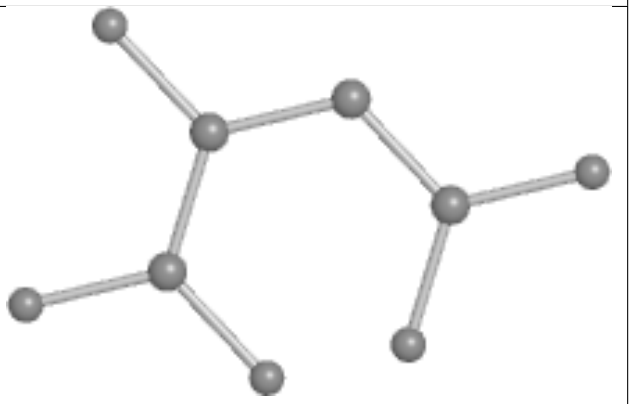
Bond lengths



Bond angles

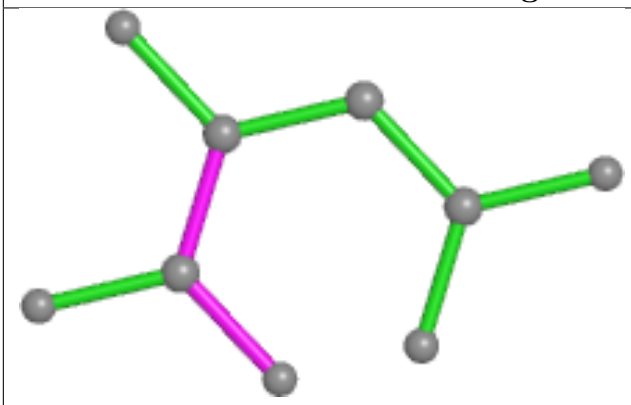


Torsions

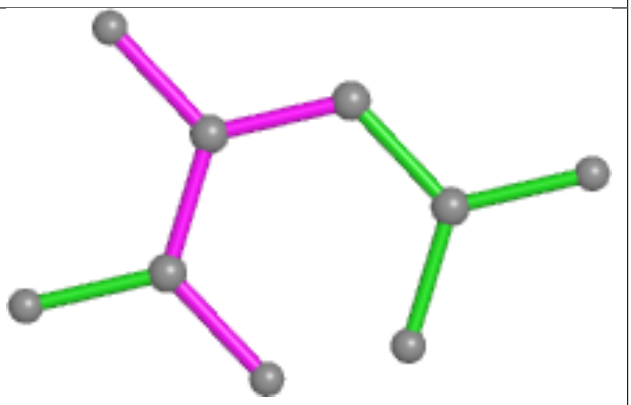


Rings

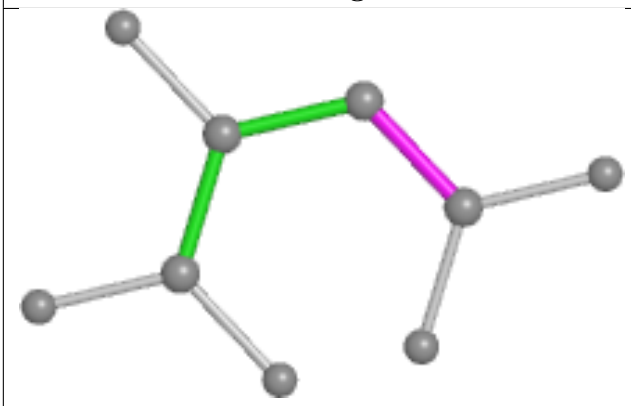
Ligand OAA A 601



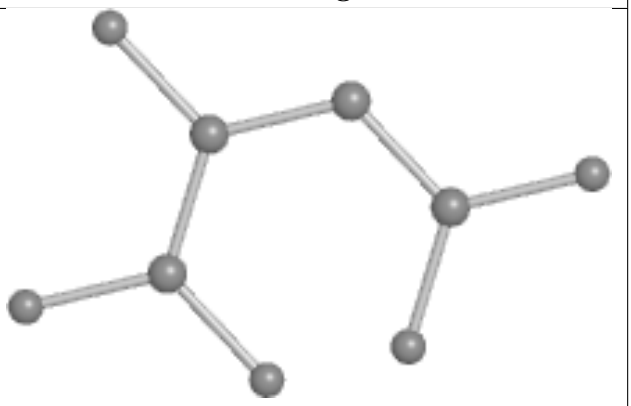
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	434/435 (99%)	-0.03	6 (1%)	73	75	22, 38, 72, 107	1 (0%)
1	B	434/435 (99%)	-0.11	5 (1%)	76	79	21, 36, 66, 92	1 (0%)
1	C	435/435 (100%)	0.22	29 (6%)	25	27	22, 41, 87, 116	0
1	D	435/435 (100%)	-0.02	12 (2%)	55	57	22, 37, 77, 172	0
All	All	1738/1740 (99%)	0.01	52 (2%)	52	54	21, 38, 77, 172	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	THR	5.6
1	C	85	LEU	5.1
1	C	319	VAL	5.0
1	C	31	THR	4.5
1	D	349	VAL	4.3
1	D	350	LEU	4.2
1	C	346	GLY	3.9
1	D	348	ALA	3.7
1	C	323	VAL	3.4
1	C	30	SER	3.3
1	B	30	SER	3.2
1	D	184	ALA	3.2
1	C	386	ASN	3.1
1	C	315	LEU	3.1
1	D	30	SER	3.1
1	A	391	GLN	3.0
1	A	319	VAL	2.9
1	C	336	LEU	2.7
1	D	347	HIS	2.7
1	B	392	GLY	2.7
1	A	389	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	357	TYR	2.6
1	C	398	TRP	2.6
1	C	373	MET	2.6
1	D	394	ALA	2.5
1	D	390	GLU	2.5
1	C	389	LEU	2.5
1	C	184	ALA	2.5
1	B	319	VAL	2.5
1	C	317	LYS	2.4
1	D	346	GLY	2.4
1	C	365	LEU	2.4
1	C	333	TRP	2.3
1	C	311	TRP	2.3
1	C	349	VAL	2.3
1	C	385	PRO	2.2
1	C	110	GLY	2.2
1	D	333	TRP	2.2
1	C	328	LEU	2.2
1	A	333	TRP	2.2
1	D	186	ALA	2.2
1	B	348	ALA	2.2
1	A	321	LYS	2.2
1	C	359	CYS	2.2
1	C	334	ASN	2.2
1	C	186	ALA	2.1
1	C	343	PRO	2.1
1	A	394	ALA	2.0
1	C	327	LYS	2.0
1	C	342	VAL	2.0
1	C	383	ILE	2.0
1	D	341	VAL	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

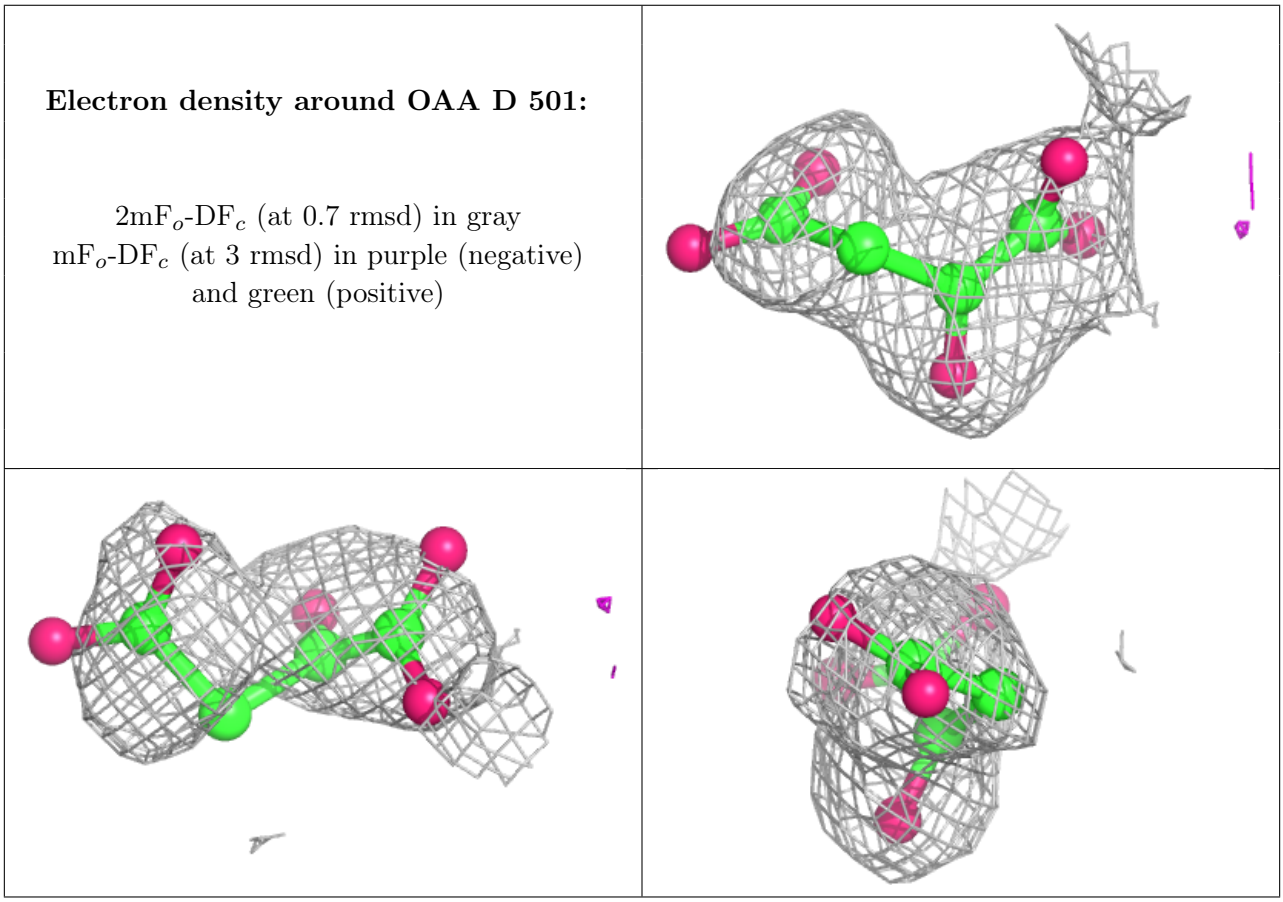
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OAA	D	501	9/9	0.82	0.11	38,69,78,87	0
2	OAA	A	601	9/9	0.92	0.07	32,36,41,42	0
2	OAA	B	501	9/9	0.92	0.07	32,34,40,41	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.

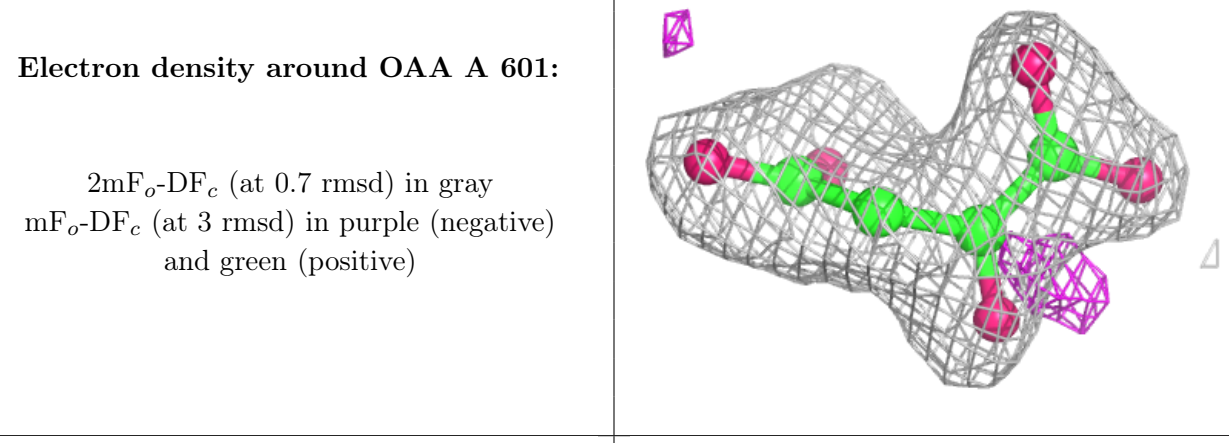
Electron density around OAA D 501:

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



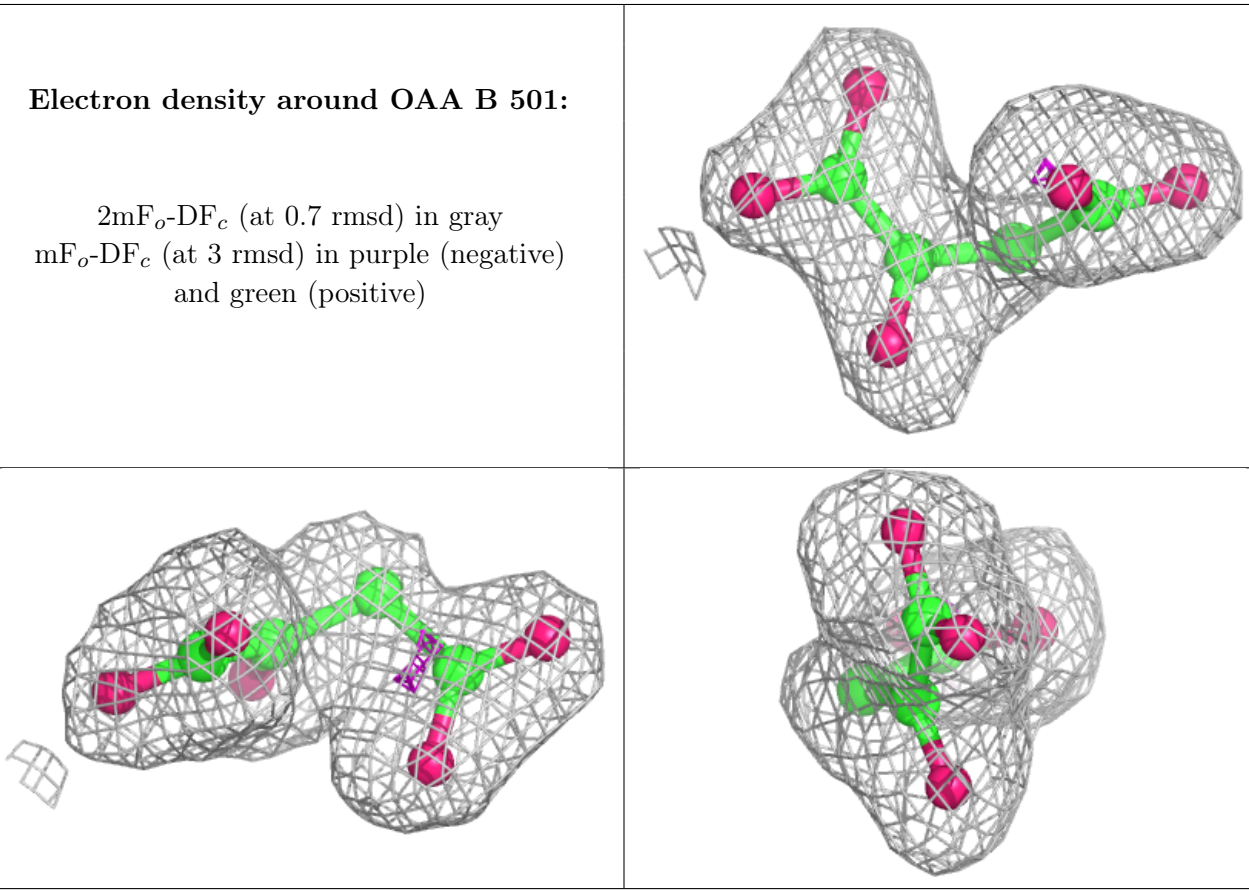
Electron density around OAA A 601:

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



Electron density around OAA B 501:

$2mF_o$-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.