Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:04 am BST

PDB ID	:	5J9W
Title	:	Crystal structure of the NuA4 core complex
Authors	:	Chen, Z.C.; Xu, P.
Deposited on	:	2016-04-11
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

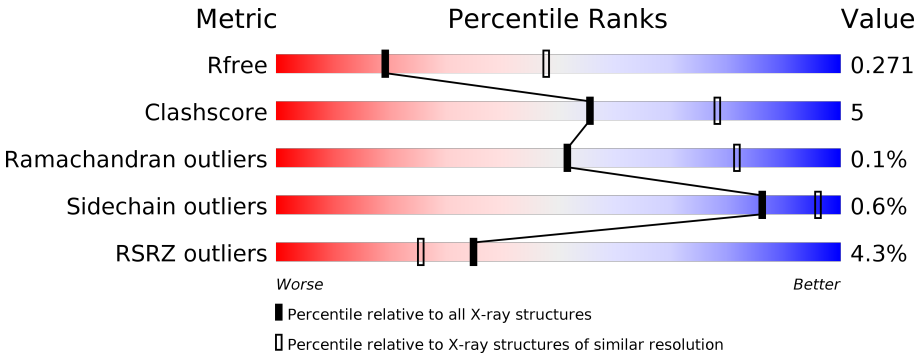
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	305	80% 11% 9%
1	E	305	3% 76% 15% 9%
1	I	305	5% 79% 12% 9%
2	B	113	4% 59% 6% 35%
2	F	113	4% 56% • 40%
2	J	113	3% 54% 8% 38%

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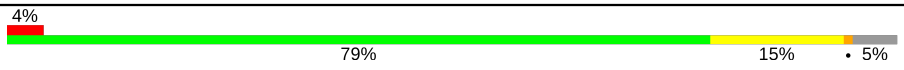
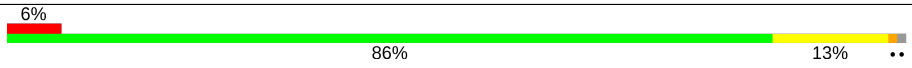
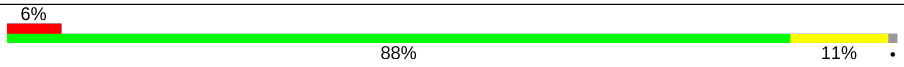
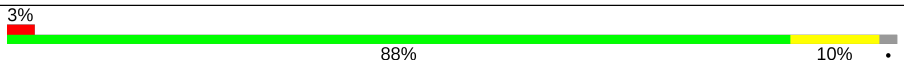
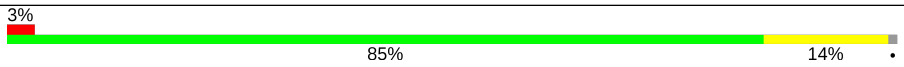
Mol	Chain	Length	Quality of chain
3	C	280	
3	G	280	
3	K	280	
4	D	120	
4	H	120	
4	L	120	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18691 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 Histone acetyltransferase ESA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	A	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	I	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	338	GLN	GLU	engineered mutation	UNP Q08649
A	338	GLN	GLU	engineered mutation	UNP Q08649
I	338	GLN	GLU	engineered mutation	UNP Q08649

- Molecule 2 is a protein called Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	68	Total	C	N	O		0	0	0
			570	355	96	119				
2	B	74	Total	C	N	O	S	0	0	0
			619	385	103	130	1			
2	J	70	Total	C	N	O		0	0	0
			587	367	99	121				

- Molecule 3 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	275	Total	C	N	O	S	0	0	0
			2307	1449	408	441	9			
3	C	267	Total	C	N	O	S	0	0	0
			2241	1410	392	430	9			

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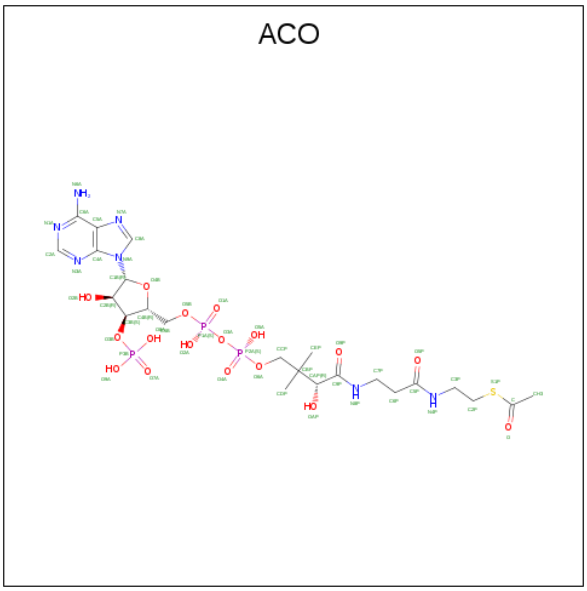
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	277	Total	C	N	O	S	0	0	0
			2321	1458	410	444	9			

- Molecule 4 is a protein called Chromatin modification-related protein YNG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	118	Total	C	N	O	S	0	0	0
			955	603	163	186	3			
4	D	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			
4	L	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			

- Molecule 5 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



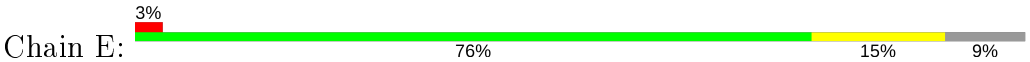
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

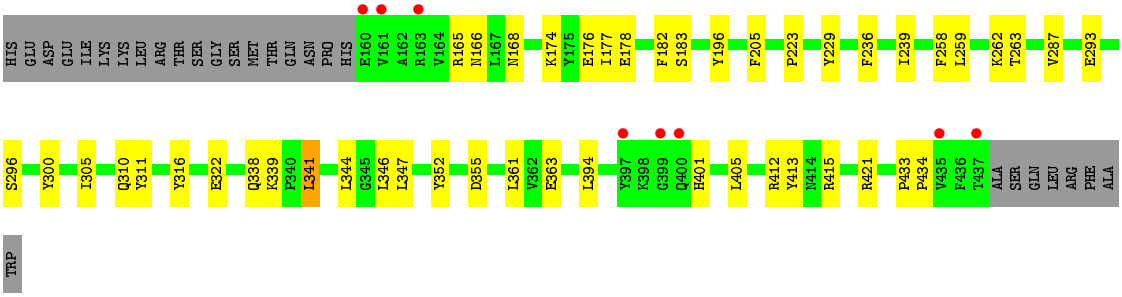
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Histone acetyltransferase ESA1

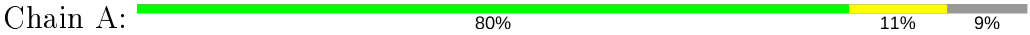
Chain E:

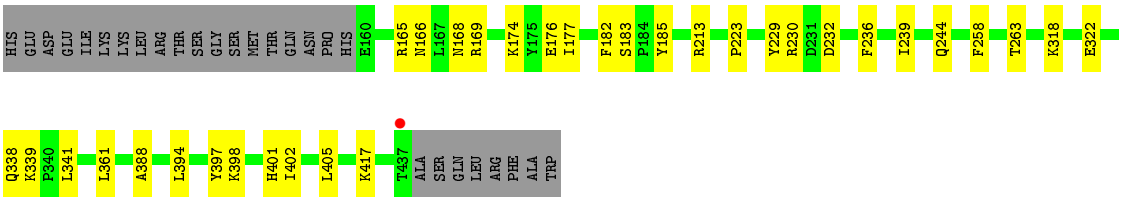




- Molecule 1: Histone acetyltransferase ESA1

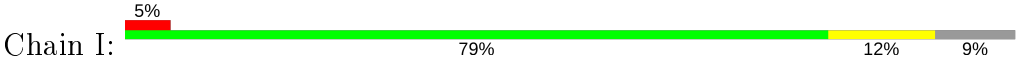
Chain A:

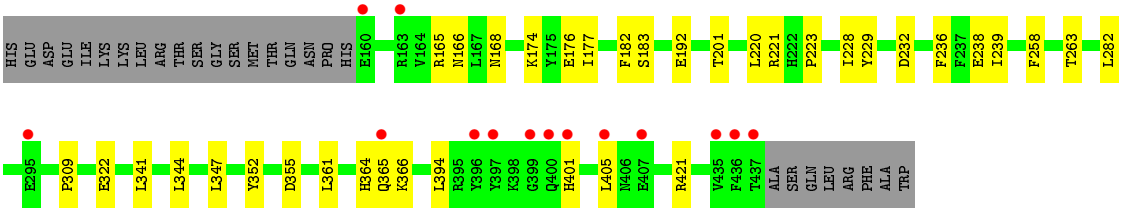




- Molecule 1: Histone acetyltransferase ESA1

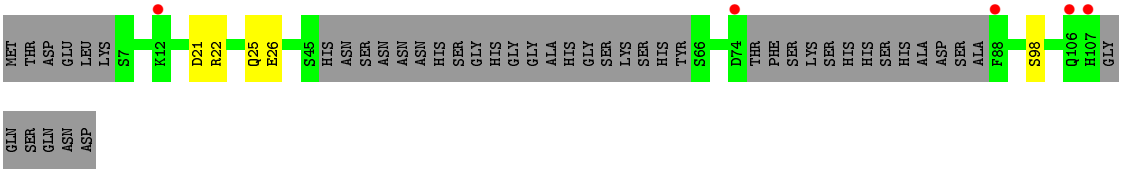
Chain I:



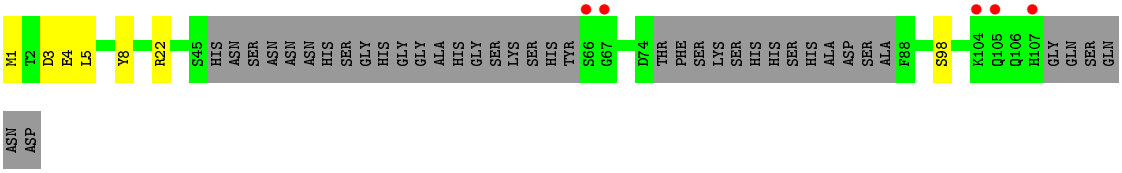


- Molecule 2: Chromatin modification-related protein EAF6

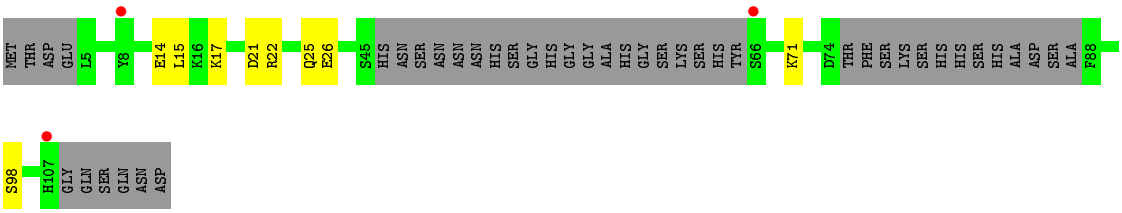
Chain F:



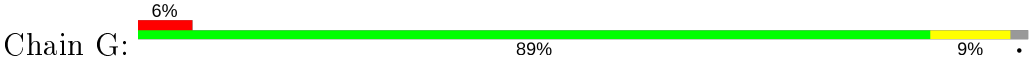
• Molecule 2: Chromatin modification-related protein EAF6

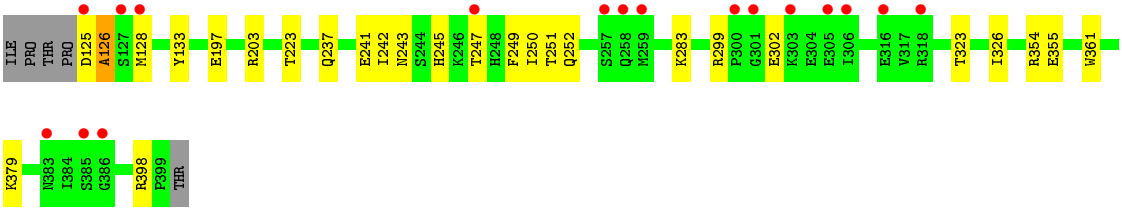


• Molecule 2: Chromatin modification-related protein EAF6

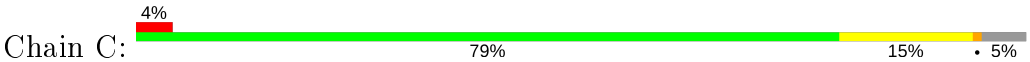


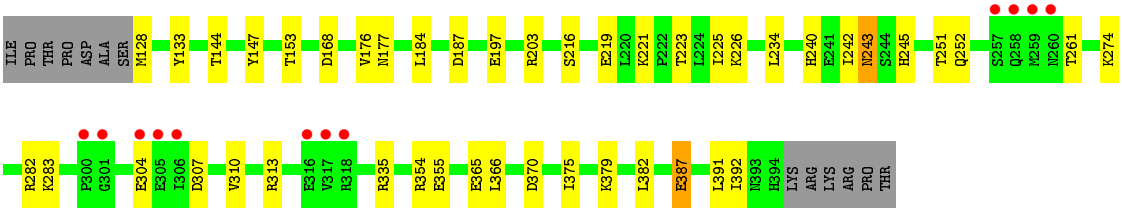
• Molecule 3: Enhancer of polycomb-like protein 1





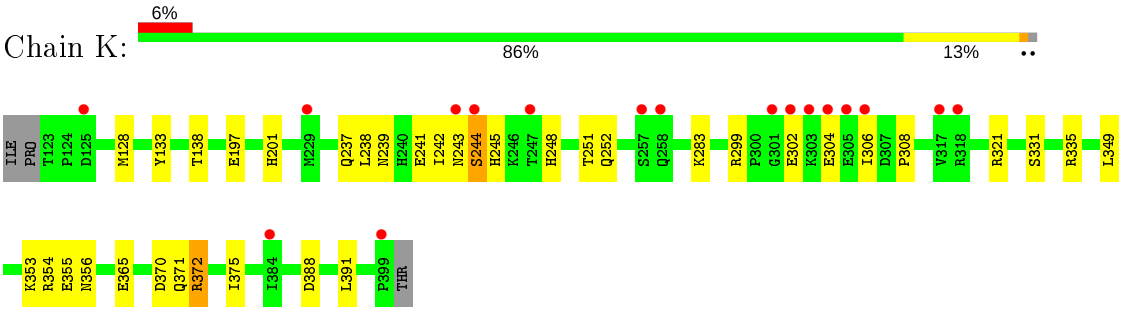
• Molecule 3: Enhancer of polycomb-like protein 1





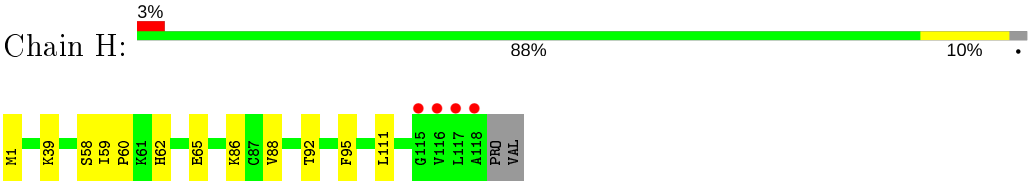
• Molecule 3: Enhancer of polycomb-like protein 1

Chain K:



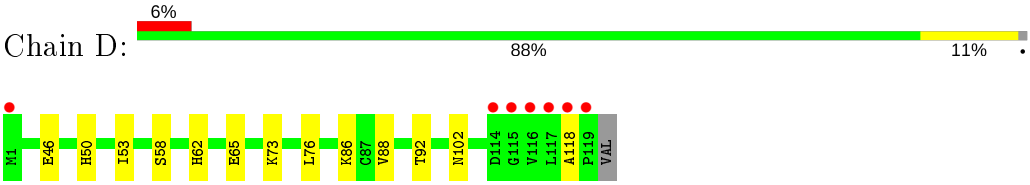
- Molecule 4: Chromatin modification-related protein YNG2

Chain H:



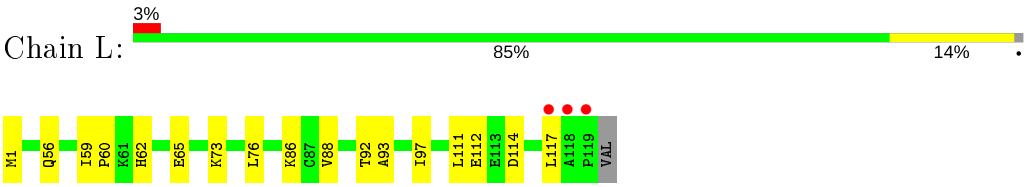
- Molecule 4: Chromatin modification-related protein YNG2

Chain D:



- Molecule 4: Chromatin modification-related protein YNG2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.26Å 138.57Å 167.87Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.6 (29.88-2.80) 75.8 (29.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.227 , 0.271 0.227 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.9	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	0.89	EDS
Total number of atoms	18691	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: ACO, ALY

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	0.26	0/2403	0.46	0/3246
1	E	0.28	0/2403	0.45	0/3246
1	I	0.27	0/2403	0.43	0/3246
2	B	0.26	0/626	0.42	0/834
2	F	0.25	0/577	0.37	0/769
2	J	0.25	0/594	0.40	0/791
3	C	0.26	0/2287	0.45	0/3080
3	G	0.27	0/2354	0.42	0/3168
3	K	0.29	0/2369	0.43	0/3190
4	D	0.25	0/974	0.38	0/1307
4	H	0.25	0/966	0.37	0/1295
4	L	0.25	0/974	0.38	0/1307
All	All	0.27	0/18930	0.43	0/25479

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	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLN	Peptide
2	B	4	GLU	Peptide

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	2355	0	2343	23	0
1	E	2355	0	2343	36	0
1	I	2355	0	2343	25	0
2	B	619	0	584	5	0
2	F	570	0	531	4	0
2	J	587	0	555	9	0
3	C	2241	0	2182	40	0
3	G	2307	0	2255	29	0
3	K	2321	0	2269	32	0
4	D	962	0	994	15	0
4	H	955	0	987	14	0
4	L	962	0	994	16	0
5	E	51	0	34	5	0
5	I	51	0	34	3	0
All	All	18691	0	18448	188	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 5.

All (188) 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:E:178:GLU:HB3	3:G:125:ASP:HB3	1.59	0.82
1:E:176:GLU:HB3	3:G:128:MET:HB2	1.62	0.80
1:E:341:LEU:HD23	1:E:346:LEU:HA	1.63	0.79
4:L:62:HIS:HB3	4:L:65:GLU:HB2	1.65	0.79
1:I:165:ARG:NH2	1:I:168:ASN:O	2.18	0.75
3:C:379:LYS:NZ	4:D:58:SER:OG	2.20	0.75
1:E:412:ARG:HG2	1:E:415:ARG:HH21	1.55	0.72
1:I:364:HIS:CE1	1:I:366:LYS:HB2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ASN:ND2	1:I:183:SER:O	2.24	0.69
3:G:251:THR:HB	4:H:92:THR:HG22	1.75	0.68
1:A:397:TYR:HB3	1:A:402:ILE:HD13	1.75	0.68
3:K:299:ARG:NE	3:K:302:GLU:OE2	2.26	0.68
3:K:251:THR:HB	4:L:92:THR:HG22	1.75	0.67
1:A:361:LEU:HB3	1:A:405:LEU:HD21	1.77	0.65
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.80	0.64
1:A:398:LYS:H	4:L:114:ASP:HA	1.63	0.64
3:G:197:GLU:OE2	3:G:283:LYS:NZ	2.31	0.63
3:C:391:LEU:HD21	4:D:53:ILE:HB	1.81	0.62
1:I:394:LEU:HD11	1:I:401:HIS:HB3	1.80	0.62
1:A:165:ARG:NH2	1:A:168:ASN:O	2.28	0.62
3:K:197:GLU:OE2	3:K:283:LYS:NZ	2.32	0.62
1:I:344:LEU:HG	5:I:500:ACO:H133	1.83	0.61
3:C:197:GLU:OE2	3:C:283:LYS:NZ	2.33	0.61
1:I:361:LEU:HB3	1:I:405:LEU:HD21	1.83	0.60
1:E:300:TYR:OH	1:E:339:LYS:HD2	2.03	0.59
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.85	0.59
2:F:98:SER:HB2	3:G:354:ARG:HH22	1.68	0.59
1:E:165:ARG:NH2	1:E:168:ASN:O	2.30	0.58
1:I:355:ASP:OD2	1:I:421:ARG:NH1	2.37	0.58
4:L:1:MET:HB3	4:L:111:LEU:HD23	1.86	0.58
2:J:98:SER:HB2	3:K:354:ARG:HH22	1.68	0.57
2:B:22:ARG:NH1	3:C:365:GLU:OE2	2.36	0.57
1:E:394:LEU:HD11	1:E:401:HIS:HB3	1.86	0.57
3:C:370:ASP:OD2	4:D:73:LYS:NZ	2.38	0.56
3:G:299:ARG:NH2	3:G:302:GLU:HG3	2.20	0.56
3:C:252:GLN:H	4:D:92:THR:HG22	1.71	0.56
3:C:240:HIS:HB2	3:C:245:HIS:HE1	1.70	0.56
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.88	0.55
3:C:240:HIS:HB2	3:C:245:HIS:CE1	2.42	0.55
1:E:176:GLU:O	3:G:126:ALA:HA	2.06	0.55
1:I:176:GLU:HB3	3:K:128:MET:HB2	1.88	0.55
1:A:174:LYS:HB3	3:C:133:TYR:CG	2.42	0.55
3:G:379:LYS:NZ	4:H:58:SER:OG	2.34	0.55
3:G:237:GLN:NE2	3:G:241:GLU:OE2	2.39	0.55
4:H:1:MET:HB3	4:H:111:LEU:HD23	1.88	0.55
1:E:363:GLU:OE2	1:E:413:TYR:OH	2.16	0.54
1:E:361:LEU:HB3	1:E:405:LEU:HD21	1.89	0.54
2:J:15:LEU:HD11	3:K:372:ARG:HD2	1.88	0.54
3:K:237:GLN:NE2	3:K:241:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ILE:HD12	1:E:258:PHE:HZ	1.72	0.54
4:D:88:VAL:O	4:D:92:THR:HG23	2.08	0.54
3:K:335:ARG:NH2	4:L:112:GLU:OE2	2.41	0.53
3:C:392:ILE:O	3:C:392:ILE:HG23	2.09	0.53
2:B:98:SER:HB2	3:C:354:ARG:HH22	1.73	0.53
3:C:392:ILE:HG22	4:D:50:HIS:CD2	2.44	0.53
3:G:242:ILE:O	3:G:243:ASN:HB2	2.08	0.53
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.91	0.53
1:E:177:ILE:HG22	3:G:126:ALA:HB2	1.91	0.52
1:A:230:ARG:NH2	3:C:144:THR:O	2.42	0.52
1:E:177:ILE:HA	3:G:125:ASP:O	2.10	0.52
1:I:168:ASN:ND2	1:I:192:GLU:O	2.42	0.52
4:L:56:GLN:HB3	4:L:60:PRO:HG2	1.92	0.52
1:A:394:LEU:HD11	1:A:401:HIS:HB3	1.92	0.52
3:C:366:LEU:HD12	4:D:76:LEU:HG	1.92	0.52
1:E:166:ASN:HB2	1:E:182:PHE:HA	1.91	0.51
3:G:252:GLN:H	4:H:92:THR:HG22	1.75	0.51
3:K:242:ILE:HB	3:K:244:SER:HB3	1.92	0.51
1:E:322:GLU:HG2	1:E:352:TYR:HE1	1.75	0.51
1:I:347:LEU:HD12	5:I:500:ACO:H1B	1.92	0.51
1:A:213:ARG:NH2	3:C:187:ASP:OD2	2.42	0.51
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.92	0.51
3:K:370:ASP:OD2	4:L:73:LYS:NZ	2.44	0.51
3:C:375:ILE:O	3:C:379:LYS:HG3	2.11	0.50
2:B:5:LEU:HD23	3:C:382:LEU:HD13	1.92	0.50
3:C:251:THR:HB	4:D:92:THR:HG22	1.93	0.50
1:I:201:THR:HG22	1:I:220:LEU:HD23	1.93	0.50
2:J:14:GLU:HA	2:J:17:LYS:HD3	1.93	0.49
3:K:239:ASN:HD21	3:K:248:HIS:HA	1.77	0.49
3:G:379:LYS:HZ2	4:H:58:SER:HG	1.60	0.49
1:I:341:LEU:HG	5:I:500:ACO:HH33	1.94	0.49
3:C:335:ARG:NH2	4:D:118:ALA:O	2.45	0.49
3:K:197:GLU:HG3	3:K:201:HIS:CE1	2.47	0.49
2:J:15:LEU:HD13	3:K:375:ILE:HD12	1.95	0.48
1:E:223:PRO:HB3	1:E:239:ILE:HD11	1.96	0.48
3:K:304:GLU:HG3	3:K:306:ILE:H	1.78	0.48
1:E:177:ILE:HG22	3:G:126:ALA:CB	2.44	0.48
1:E:300:TYR:CE2	1:E:338:GLN:HG3	2.49	0.48
3:K:331:SER:HB3	4:L:117:LEU:HD13	1.96	0.47
3:K:355:GLU:OE2	4:L:86:LYS:HE2	2.14	0.47
1:E:412:ARG:HG2	1:E:415:ARG:NH2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:242:ILE:O	3:K:243:ASN:HB2	2.15	0.47
2:J:15:LEU:HD12	3:K:371:GLN:HB3	1.95	0.47
3:C:307:ASP:HB3	3:C:310:VAL:HG23	1.95	0.47
3:C:379:LYS:HE2	3:C:379:LYS:HB3	1.61	0.47
1:A:166:ASN:ND2	1:A:183:SER:O	2.45	0.47
1:A:232:ASP:N	1:A:232:ASP:OD1	2.47	0.47
3:C:252:GLN:H	4:D:92:THR:CG2	2.27	0.47
2:F:26:GLU:HB3	3:G:398:ARG:NH1	2.30	0.47
3:K:197:GLU:HG3	3:K:201:HIS:HE1	1.78	0.47
2:F:22:ARG:O	2:F:26:GLU:HG3	2.14	0.46
3:G:249:PHE:HE2	4:H:95:PHE:HB2	1.80	0.46
3:G:252:GLN:H	4:H:92:THR:CG2	2.28	0.46
4:H:88:VAL:O	4:H:92:THR:HG23	2.16	0.46
1:A:223:PRO:HB3	1:A:239:ILE:HD11	1.98	0.46
3:G:361:TRP:CZ3	4:H:39:LYS:HE3	2.50	0.46
3:K:252:GLN:H	4:L:92:THR:CG2	2.28	0.46
3:K:252:GLN:H	4:L:92:THR:HG22	1.80	0.46
1:E:355:ASP:OD2	1:E:421:ARG:NH1	2.49	0.46
1:E:421:ARG:NH2	5:E:500:ACO:O9A	2.47	0.46
1:I:322:GLU:HG2	1:I:352:TYR:HE1	1.79	0.46
1:I:365:GLN:C	1:I:366:LYS:HG3	2.36	0.46
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.48	0.46
1:A:339:LYS:O	1:A:341:LEU:N	2.49	0.45
3:G:323:THR:HG23	3:G:326:ILE:H	1.80	0.45
4:L:88:VAL:O	4:L:92:THR:HG23	2.16	0.45
3:C:216:SER:HB3	3:C:219:GLU:HG3	1.98	0.45
1:E:344:LEU:HD23	5:E:500:ACO:HN8	1.80	0.45
1:E:347:LEU:HD12	5:E:500:ACO:H1B	1.98	0.45
3:K:238:LEU:O	3:K:242:ILE:HG13	2.16	0.45
1:I:174:LYS:HB3	3:K:133:TYR:CG	2.52	0.45
1:I:182:PHE:CE2	3:K:308:PRO:HB2	2.51	0.45
1:E:344:LEU:HG	5:E:500:ACO:H133	1.99	0.45
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.52	0.44
3:C:387:GLU:HG2	4:D:58:SER:OG	2.17	0.44
4:D:46:GLU:HG2	4:D:50:HIS:NE2	2.32	0.44
3:K:304:GLU:HA	3:K:304:GLU:OE1	2.17	0.44
1:I:232:ASP:N	1:I:232:ASP:OD1	2.50	0.44
1:E:305:ILE:HG23	5:E:500:ACO:H31	2.00	0.44
1:E:166:ASN:ND2	1:E:183:SER:O	2.49	0.44
1:E:310:GLN:HB3	3:G:126:ALA:HB1	2.00	0.44
3:C:391:LEU:HA	3:C:391:LEU:HD23	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:321:ARG:NH2	4:L:1:MET:O	2.51	0.43
1:A:169:ARG:NE	1:A:176:GLU:OE2	2.50	0.43
3:G:299:ARG:HH21	3:G:302:GLU:HG3	1.82	0.43
1:E:310:GLN:HG2	1:E:311:TYR:CD2	2.54	0.43
1:A:230:ARG:HB3	3:C:147:TYR:CE1	2.54	0.43
3:G:379:LYS:NZ	4:H:58:SER:HG	2.16	0.43
1:A:166:ASN:HB2	1:A:182:PHE:HA	2.01	0.43
1:A:177:ILE:HD12	1:A:258:PHE:HZ	1.83	0.43
1:A:388:ALA:HB1	1:A:394:LEU:HB2	2.00	0.43
1:I:166:ASN:HB2	1:I:182:PHE:HA	2.01	0.43
2:J:22:ARG:NH1	3:K:365:GLU:OE1	2.48	0.43
3:C:221:LYS:O	3:C:225:ILE:HG12	2.19	0.43
2:B:8:TYR:HE1	3:C:379:LYS:HG2	1.83	0.43
3:C:379:LYS:HZ1	3:C:387:GLU:HG3	1.84	0.43
1:I:258:PHE:CE1	1:I:309:PRO:HG2	2.53	0.43
1:A:244:GLN:OE1	3:C:153:THR:HA	2.19	0.43
3:C:176:VAL:HG22	3:C:274:LYS:HE3	2.01	0.43
2:B:8:TYR:CE1	3:C:379:LYS:HG2	2.54	0.42
1:A:177:ILE:HD12	1:A:258:PHE:CZ	2.54	0.42
3:C:304:GLU:CD	3:C:313:ARG:HH12	2.22	0.42
4:L:76:LEU:HA	4:L:76:LEU:HD12	1.91	0.42
3:C:355:GLU:OE2	4:D:86:LYS:HE2	2.20	0.42
1:I:228:ILE:HD13	1:I:238:GLU:HB2	2.01	0.42
3:K:349:LEU:HG	3:K:353:LYS:HE2	2.00	0.42
3:K:244:SER:HB2	3:K:356:ASN:ND2	2.34	0.42
2:F:21:ASP:O	2:F:25:GLN:HG2	2.19	0.42
3:G:355:GLU:OE2	4:H:86:LYS:HE2	2.18	0.42
1:A:183:SER:O	1:A:185:TYR:N	2.51	0.42
1:A:417:LYS:HA	1:A:417:LYS:HD2	1.86	0.42
3:C:177:ASN:ND2	3:C:184:LEU:O	2.48	0.42
3:K:388:ASP:HA	3:K:391:LEU:HD23	2.02	0.42
3:C:203:ARG:HD2	3:C:223:THR:OG1	2.19	0.42
1:E:293:GLU:HB2	1:E:296:SER:HB2	2.02	0.41
3:G:250:ILE:HG23	4:H:88:VAL:HG22	2.02	0.41
3:G:302:GLU:OE1	3:G:302:GLU:HA	2.20	0.41
3:C:242:ILE:HG22	3:C:243:ASN:HD22	1.85	0.41
1:E:311:TYR:HB3	1:E:316:TYR:CD2	2.55	0.41
2:J:22:ARG:O	2:J:26:GLU:HG3	2.21	0.41
2:J:71:LYS:HD3	2:J:71:LYS:HA	1.84	0.41
1:I:221:ARG:NH2	3:K:138:THR:O	2.45	0.41
4:L:93:ALA:O	4:L:97:ILE:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:PRO:HB3	1:I:239:ILE:HD11	2.03	0.41
1:A:318:LYS:HE2	1:A:322:GLU:OE2	2.21	0.41
1:I:177:ILE:HD12	1:I:258:PHE:HZ	1.86	0.41
3:C:226:LYS:H	3:C:226:LYS:HG3	1.68	0.41
4:H:59:ILE:HB	4:H:60:PRO:HD3	2.03	0.41
1:I:221:ARG:HD3	1:I:282:LEU:O	2.21	0.41
2:J:21:ASP:O	2:J:25:GLN:HG2	2.21	0.40
1:E:196:TYR:HB2	1:E:205:PHE:HB2	2.02	0.40
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.98	0.40
3:G:203:ARG:HD2	3:G:223:THR:OG1	2.22	0.40
3:C:234:LEU:HD13	4:D:102:ASN:ND2	2.35	0.40
1:E:259:LEU:HD12	1:E:262:ALY:HG2	2.03	0.40
3:G:243:ASN:HA	3:G:245:HIS:CE1	2.56	0.40
3:K:372:ARG:HG3	3:K:391:LEU:HD13	2.02	0.40
1:E:287:VAL:HA	1:E:311:TYR:CD2	2.55	0.40
4:L:59:ILE:HB	4:L:60:PRO:HD3	2.04	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	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
1	E	275/305 (90%)	265 (96%)	10 (4%)	0	100	100
1	I	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
2	B	68/113 (60%)	65 (96%)	3 (4%)	0	100	100
2	F	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
2	J	64/113 (57%)	62 (97%)	2 (3%)	0	100	100
3	C	265/280 (95%)	255 (96%)	9 (3%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	273/280 (98%)	262 (96%)	10 (4%)	1 (0%)	34 66
3	K	275/280 (98%)	264 (96%)	11 (4%)	0	100 100
4	D	117/120 (98%)	117 (100%)	0	0	100 100
4	H	116/120 (97%)	116 (100%)	0	0	100 100
4	L	117/120 (98%)	116 (99%)	1 (1%)	0	100 100
All	All	2182/2454 (89%)	2110 (97%)	70 (3%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	126	ALA
3	C	243	ASN

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	259/283 (92%)	258 (100%)	1 (0%)	91 97
1	E	259/283 (92%)	257 (99%)	2 (1%)	81 94
1	I	259/283 (92%)	258 (100%)	1 (0%)	91 97
2	B	69/100 (69%)	67 (97%)	2 (3%)	42 76
2	F	63/100 (63%)	63 (100%)	0	100 100
2	J	65/100 (65%)	65 (100%)	0	100 100
3	C	253/265 (96%)	250 (99%)	3 (1%)	71 92
3	G	260/265 (98%)	259 (100%)	1 (0%)	91 97
3	K	262/265 (99%)	259 (99%)	3 (1%)	73 92
4	D	110/111 (99%)	110 (100%)	0	100 100
4	H	109/111 (98%)	109 (100%)	0	100 100
4	L	110/111 (99%)	110 (100%)	0	100 100
All	All	2078/2277 (91%)	2065 (99%)	13 (1%)	86 96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	263	THR
1	E	341	LEU
3	G	247	THR
1	A	263	THR
2	B	1	MET
2	B	3	ASP
3	C	128	MET
3	C	261	THR
3	C	387	GLU
1	I	263	THR
3	K	244	SER
3	K	245	HIS
3	K	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	201	HIS
3	K	239	ASN
3	K	266	GLN
3	K	356	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	ALY	A	262	1	10,11,12	1.03	0	7,12,14	0.97	1 (14%)
1	ALY	E	262	1	10,11,12	1.00	0	7,12,14	1.03	0
1	ALY	I	262	1	10,11,12	1.01	0	7,12,14	0.96	1 (14%)

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
1	ALY	A	262	1	-	4/9/10/12	-
1	ALY	E	262	1	-	4/9/10/12	-
1	ALY	I	262	1	-	5/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	ALY	CD-CG-CB	-2.08	106.28	113.62
1	I	262	ALY	CD-CG-CB	-2.02	106.48	113.62

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	262	ALY	N-CA-CB-CG
1	A	262	ALY	C-CA-CB-CG
1	E	262	ALY	N-CA-CB-CG
1	E	262	ALY	C-CA-CB-CG
1	I	262	ALY	N-CA-CB-CG
1	I	262	ALY	C-CA-CB-CG
1	I	262	ALY	O-C-CA-CB
1	A	262	ALY	CG-CD-CE-NZ
1	E	262	ALY	CA-CB-CG-CD
1	E	262	ALY	CG-CD-CE-NZ
1	I	262	ALY	CG-CD-CE-NZ
1	A	262	ALY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	I	262	ALY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	262	ALY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
5	ACO	E	500	-	45,53,53	2.03	9 (20%)	56,79,79	1.30	4 (7%)
5	ACO	I	500	-	45,53,53	2.02	10 (22%)	56,79,79	1.46	9 (16%)

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
5	ACO	E	500	-	-	9/47/67/67	0/3/3/3
5	ACO	I	500	-	-	9/47/67/67	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	500	ACO	C5P-N4P	6.63	1.48	1.33
5	I	500	ACO	C5P-N4P	6.54	1.48	1.33
5	I	500	ACO	C2B-C1B	-5.42	1.45	1.53
5	E	500	ACO	C2B-C1B	-5.31	1.45	1.53
5	E	500	ACO	C9P-N8P	4.60	1.43	1.33
5	I	500	ACO	C9P-N8P	4.51	1.43	1.33
5	E	500	ACO	O4B-C1B	4.32	1.47	1.41
5	I	500	ACO	O4B-C1B	4.22	1.47	1.41
5	I	500	ACO	C2B-C3B	-4.20	1.43	1.52
5	E	500	ACO	C2B-C3B	-4.17	1.43	1.52
5	I	500	ACO	C6A-N6A	2.82	1.44	1.34
5	E	500	ACO	C6A-N6A	2.82	1.44	1.34
5	E	500	ACO	C2A-N3A	2.57	1.36	1.32
5	I	500	ACO	C2A-N3A	2.50	1.36	1.32
5	E	500	ACO	C3B-C4B	-2.38	1.46	1.52
5	I	500	ACO	C3B-C4B	-2.37	1.46	1.52
5	E	500	ACO	CEP-CBP	-2.32	1.48	1.53
5	I	500	ACO	CEP-CBP	-2.30	1.48	1.53
5	I	500	ACO	C5B-C4B	-2.07	1.45	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	500	ACO	N3A-C2A-N1A	-5.51	120.06	128.68
5	I	500	ACO	N3A-C2A-N1A	-5.50	120.08	128.68
5	I	500	ACO	P2A-O3A-P1A	-3.66	120.27	132.83
5	E	500	ACO	P2A-O3A-P1A	-3.56	120.60	132.83
5	I	500	ACO	CEP-CBP-CAP	2.69	113.49	108.82
5	I	500	ACO	C3B-C2B-C1B	2.42	105.26	99.89
5	E	500	ACO	C3B-C2B-C1B	2.41	105.24	99.89
5	I	500	ACO	C6P-C5P-N4P	2.34	120.35	116.42
5	I	500	ACO	C4A-C5A-N7A	-2.10	107.21	109.40
5	I	500	ACO	C7P-N8P-C9P	-2.10	118.84	122.59
5	I	500	ACO	O9P-C9P-N8P	-2.10	118.48	122.99
5	E	500	ACO	C4A-C5A-N7A	-2.09	107.22	109.40
5	I	500	ACO	C3P-N4P-C5P	-2.09	118.97	122.84

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	500	ACO	C3B-O3B-P3B-O9A

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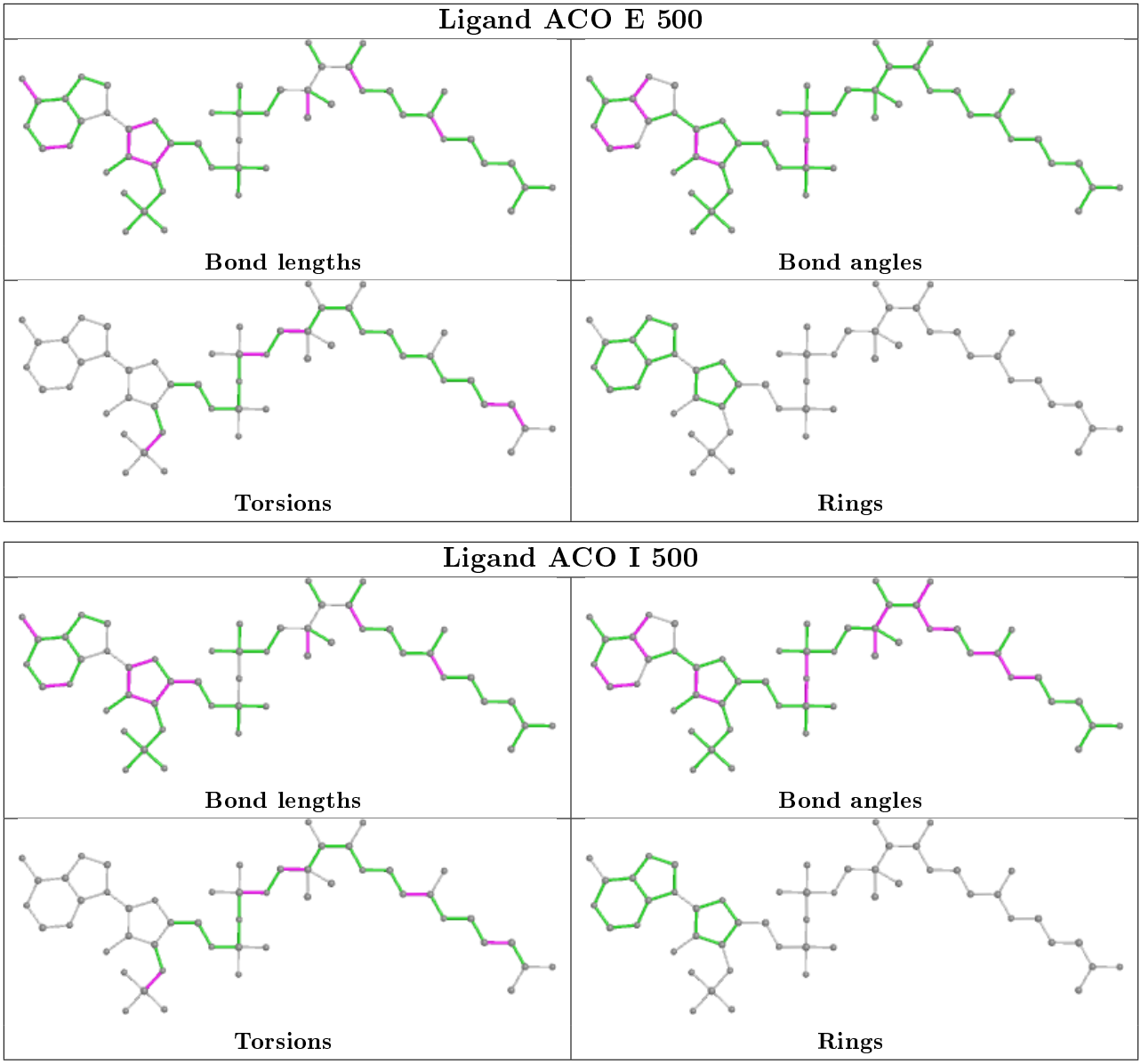
Mol	Chain	Res	Type	Atoms
5	E	500	ACO	CCP-O6A-P2A-O3A
5	E	500	ACO	CCP-O6A-P2A-O4A
5	E	500	ACO	C3P-C2P-S1P-C
5	E	500	ACO	O-C-S1P-C2P
5	E	500	ACO	CH3-C-S1P-C2P
5	I	500	ACO	CCP-O6A-P2A-O3A
5	I	500	ACO	CCP-O6A-P2A-O4A
5	I	500	ACO	C3P-C2P-S1P-C
5	E	500	ACO	CDP-CBP-CCP-O6A
5	E	500	ACO	CAP-CBP-CCP-O6A
5	I	500	ACO	CAP-CBP-CCP-O6A
5	I	500	ACO	CDP-CBP-CCP-O6A
5	E	500	ACO	CEP-CBP-CCP-O6A
5	I	500	ACO	CEP-CBP-CCP-O6A
5	I	500	ACO	O5P-C5P-C6P-C7P
5	I	500	ACO	C3B-O3B-P3B-O8A
5	I	500	ACO	N4P-C5P-C6P-C7P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	500	ACO	5	0
5	I	500	ACO	3	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	277/305 (90%)	-0.35	1 (0%)	92	91	21, 40, 73, 96	0
1	E	277/305 (90%)	-0.08	8 (2%)	51	41	26, 52, 91, 111	0
1	I	277/305 (90%)	0.05	14 (5%)	28	19	29, 56, 110, 141	0
2	B	74/113 (65%)	0.11	5 (6%)	17	10	33, 52, 91, 129	0
2	F	68/113 (60%)	0.18	5 (7%)	14	8	32, 63, 105, 124	0
2	J	70/113 (61%)	0.20	3 (4%)	35	25	37, 57, 96, 104	0
3	C	267/280 (95%)	-0.01	12 (4%)	33	23	20, 56, 98, 130	0
3	G	275/280 (98%)	-0.02	17 (6%)	20	13	26, 55, 99, 116	0
3	K	277/280 (98%)	0.05	17 (6%)	21	13	32, 61, 100, 132	0
4	D	119/120 (99%)	-0.21	7 (5%)	22	14	23, 41, 100, 130	0
4	H	118/120 (98%)	-0.09	4 (3%)	45	35	34, 55, 92, 112	0
4	L	119/120 (99%)	-0.12	3 (2%)	57	47	26, 52, 100, 107	0
All	All	2218/2454 (90%)	-0.05	96 (4%)	35	25	20, 53, 99, 141	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	107	HIS	6.3
3	C	259	MET	6.0
4	D	118	ALA	5.0
3	C	258	GLN	4.9
2	J	107	HIS	4.5
2	B	66	SER	4.4
4	D	115	GLY	4.4
3	K	306	ILE	4.4
3	C	306	ILE	4.3
1	I	160	GLU	4.2
3	C	317	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
4	D	119	PRO	4.2
2	F	107	HIS	4.1
4	L	119	PRO	4.1
3	G	385	SER	4.1
1	I	397	TYR	4.0
4	H	118	ALA	3.9
3	G	305	GLU	3.9
4	D	114	ASP	3.9
3	G	257	SER	3.8
3	G	306	ILE	3.8
1	E	163	ARG	3.6
1	I	295	GLU	3.5
2	J	66	SER	3.5
1	I	437	THR	3.4
3	G	383	ASN	3.4
3	K	304	GLU	3.4
4	H	115	GLY	3.4
1	E	437	THR	3.4
3	C	305	GLU	3.3
1	E	435	VAL	3.3
1	I	435	VAL	3.3
4	L	118	ALA	3.3
4	D	117	LEU	3.2
1	I	365	GLN	3.2
3	K	303	LYS	3.2
3	K	317	VAL	3.1
1	I	163	ARG	3.1
3	K	305	GLU	3.1
1	E	397	TYR	3.1
1	E	160	GLU	3.1
3	G	258	GLN	3.1
2	B	105	GLN	3.0
3	K	247	THR	3.0
4	H	116	VAL	3.0
3	G	318	ARG	3.0
3	C	301	GLY	3.0
1	E	399	GLY	2.9
4	D	1	MET	2.9
3	G	386	GLY	2.8
2	J	8	TYR	2.8
1	I	399	GLY	2.8
3	G	300	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	88	PHE	2.7
3	C	304	GLU	2.7
3	G	247	THR	2.6
4	H	117	LEU	2.6
1	A	437	THR	2.6
3	C	318	ARG	2.6
3	G	303	LYS	2.5
3	K	399	PRO	2.5
1	I	407	GLU	2.5
3	G	316	GLU	2.5
4	D	116	VAL	2.5
3	G	127	SER	2.5
3	K	302	GLU	2.4
3	G	125	ASP	2.4
1	I	401	HIS	2.4
3	C	316	GLU	2.4
1	I	400	GLN	2.3
4	L	117	LEU	2.3
3	K	243	ASN	2.3
3	K	257	SER	2.3
1	I	396	TYR	2.3
2	B	104	LYS	2.3
3	C	260	ASN	2.2
3	G	301	GLY	2.2
2	F	106	GLN	2.2
3	K	229	MET	2.2
3	K	384	ILE	2.2
1	E	400	GLN	2.2
2	F	12	LYS	2.2
1	I	436	PHE	2.2
3	K	125	ASP	2.2
3	G	259	MET	2.2
1	E	161	VAL	2.1
3	C	300	PRO	2.1
1	I	405	LEU	2.1
3	K	244	SER	2.1
2	B	67	GLY	2.1
3	K	301	GLY	2.1
3	G	128	MET	2.0
3	K	258	GLN	2.0
2	F	74	ASP	2.0
3	C	257	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	K	318	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	ALY	I	262	12/13	0.94	0.20	35,46,54,56	0
1	ALY	A	262	12/13	0.96	0.16	23,36,42,51	0
1	ALY	E	262	12/13	0.97	0.15	29,38,51,57	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

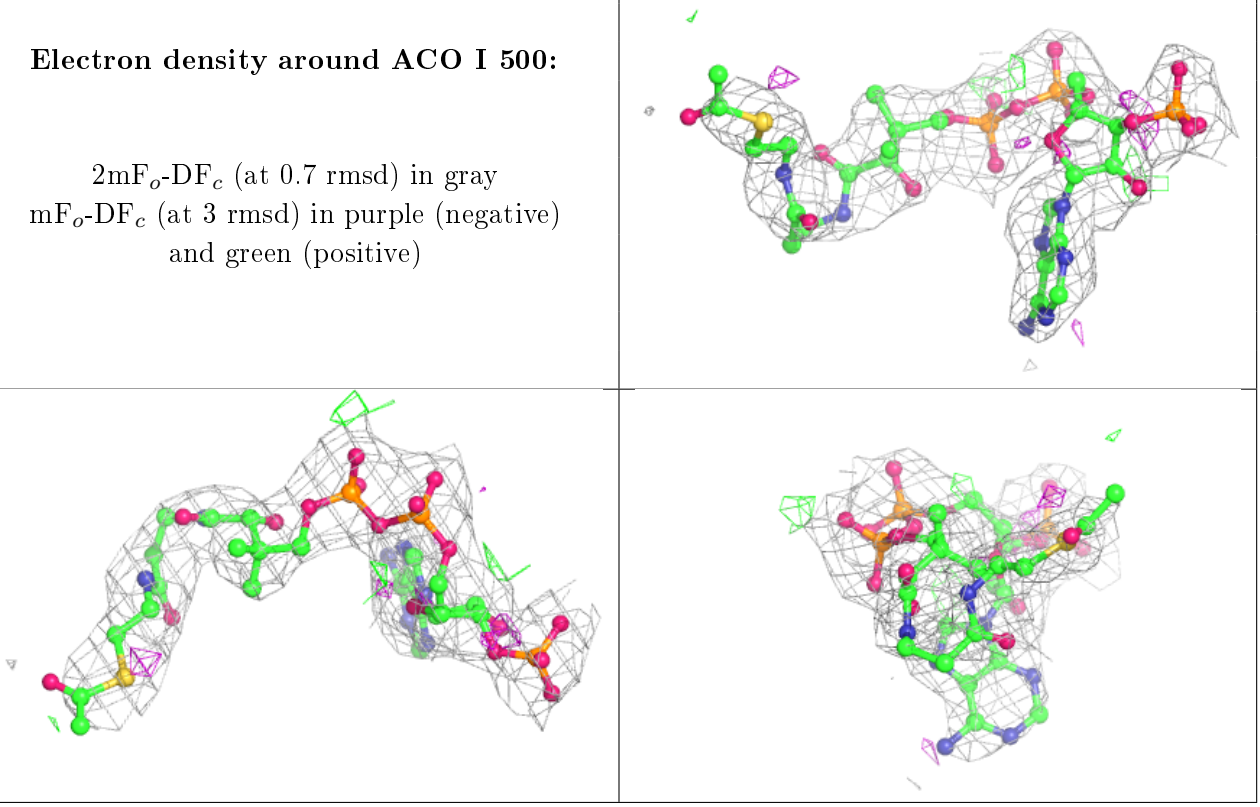
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACO	I	500	51/51	0.90	0.22	42,78,105,112	0
5	ACO	E	500	51/51	0.93	0.17	38,69,95,98	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.

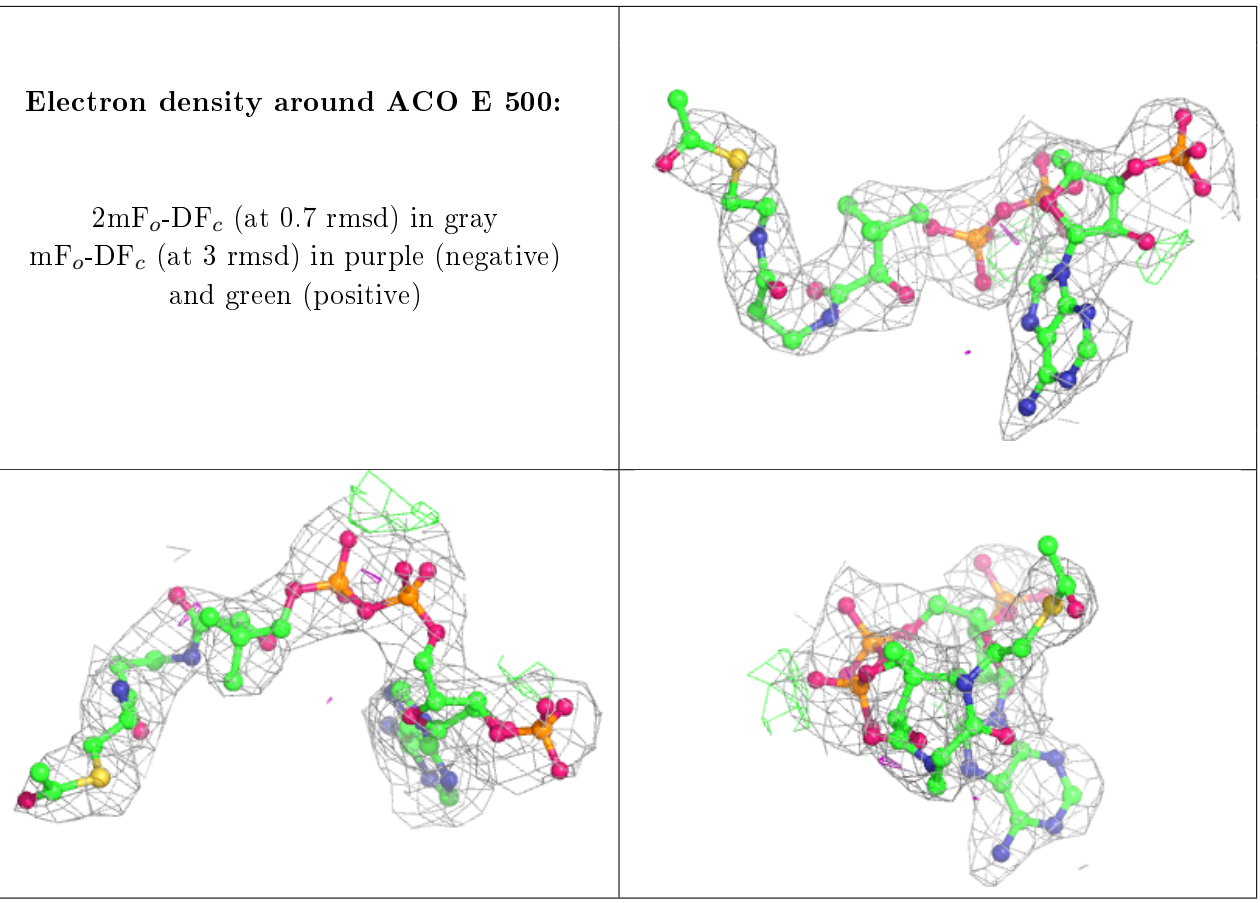
Electron density around ACO I 500:

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



Electron density around ACO E 500:

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



6.5 Other polymers (i)

There are no such residues in this entry.