



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 4KVO / pdb_00004kvo
Title : The NatA (Naa10p/Naa15p) amino-terminal acetyltransferase complex bound to AcCoA
Authors : Liszczak, G.P.; Marmorstein, R.Q.
Deposited on : 2013-05-22
Resolution : 3.15 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

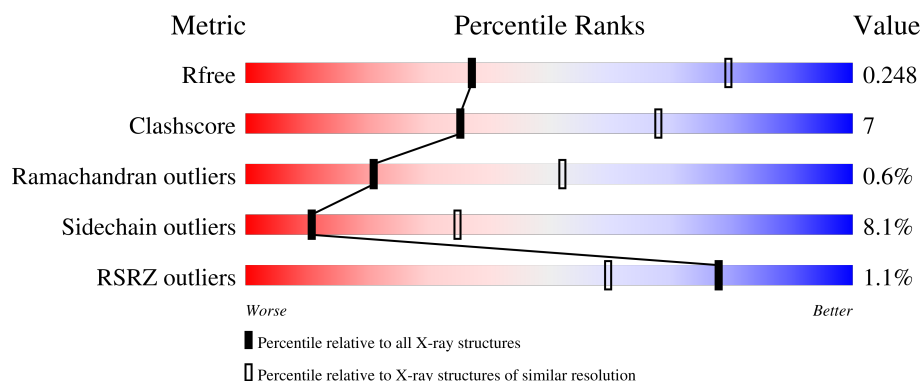
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

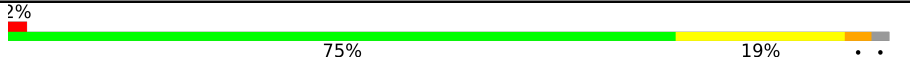
The reported resolution of this entry is 3.15 Å.

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.



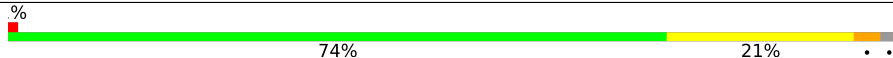
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. 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	731	
1	B	731	
1	C	731	
1	D	731	
2	E	156	

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Mol	Chain	Length	Quality of chain
2	F	156	
2	G	156	
2	H	156	

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
4	CL	A	802	-	-	X	-
4	CL	A	808	-	-	X	-
4	CL	D	803	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28430 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 N-terminal acetyltransferase A complex subunit nat1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	1	0
			5764	3679	968	1099	18			
1	B	722	Total	C	N	O	S	0	1	0
			5777	3686	971	1102	18			
1	C	717	Total	C	N	O	S	0	1	0
			5753	3671	968	1096	18			
1	D	717	Total	C	N	O	S	0	1	0
			5761	3678	969	1096	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	ALA	-	expression tag	UNP O74985
A	731	ALA	-	expression tag	UNP O74985
B	730	ALA	-	expression tag	UNP O74985
B	731	ALA	-	expression tag	UNP O74985
C	730	ALA	-	expression tag	UNP O74985
C	731	ALA	-	expression tag	UNP O74985
D	730	ALA	-	expression tag	UNP O74985
D	731	ALA	-	expression tag	UNP O74985

- Molecule 2 is a protein called N-terminal acetyltransferase A complex catalytic subunit ard1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			
2	F	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			
2	G	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			
2	H	153	Total	C	N	O	S	0	1	0
			1247	790	221	225	11			

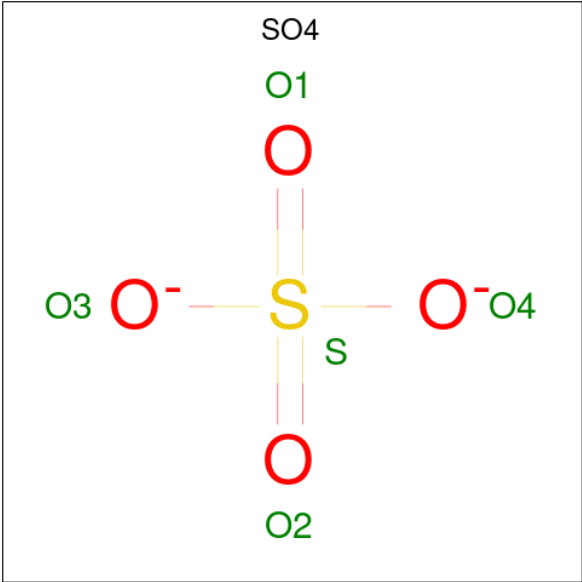
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	2	Total 2	Na 2	0	0
3	G	1	Total 1	Na 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

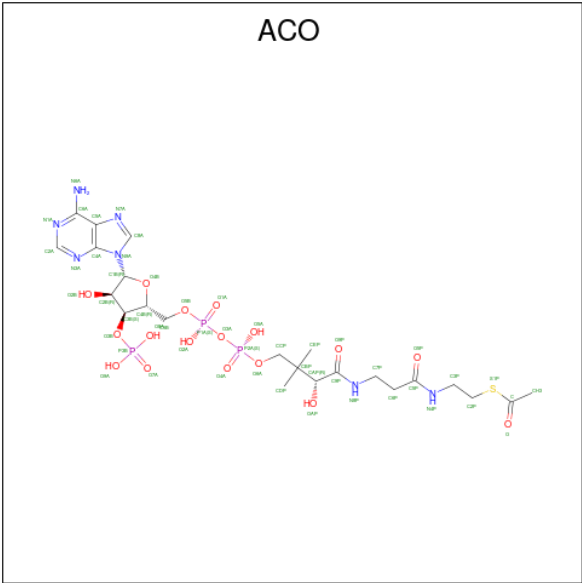
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	Cl 10	0	0
4	B	14	Total 14	Cl 14	0	0
4	C	15	Total 15	Cl 15	0	0
4	D	10	Total 10	Cl 10	0	0
4	E	7	Total 7	Cl 7	0	0
4	F	2	Total 2	Cl 2	0	0
4	G	2	Total 2	Cl 2	0	0
4	H	3	Total 3	Cl 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	G	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
6	H	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

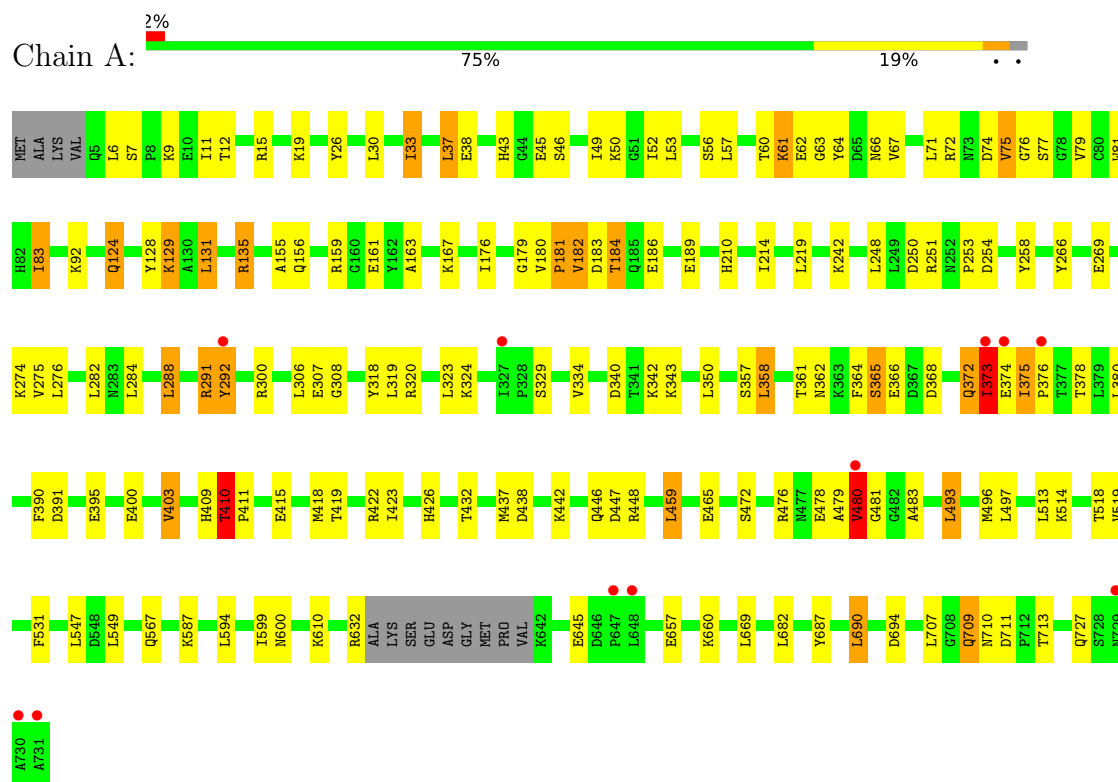
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	22	Total	O	0	0
			22	22		
7	B	22	Total	O	0	0
			22	22		
7	C	25	Total	O	0	0
			25	25		
7	D	11	Total	O	0	0
			11	11		
7	E	4	Total	O	0	0
			4	4		
7	F	6	Total	O	0	0
			6	6		
7	G	5	Total	O	0	0
			5	5		
7	H	10	Total	O	0	0
			10	10		

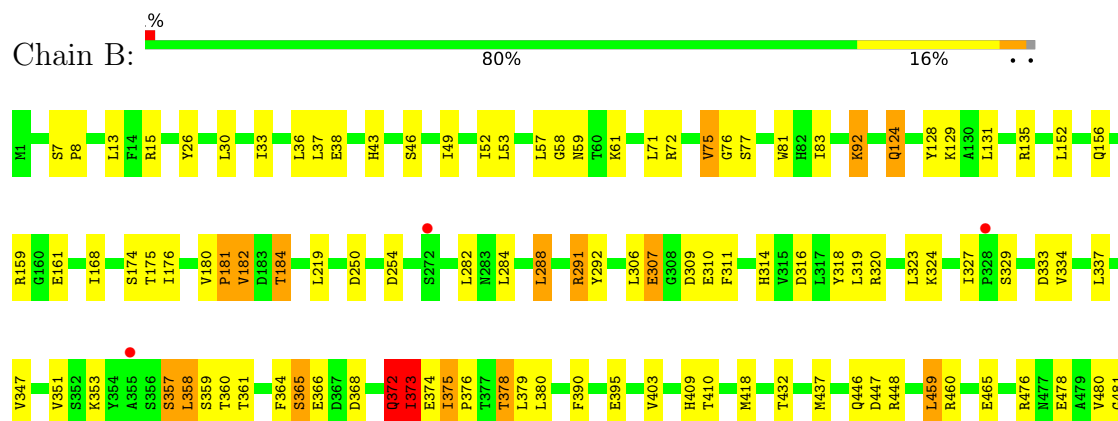
3 Residue-property plots

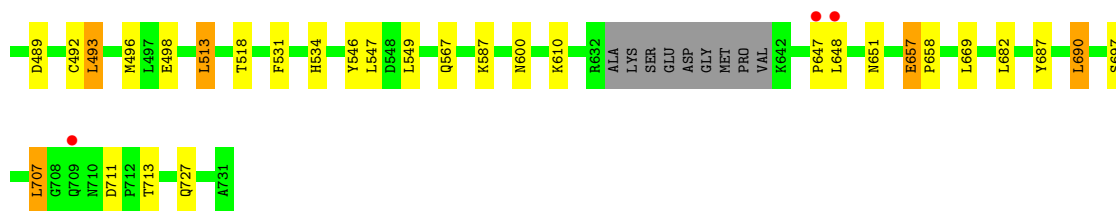
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-terminal acetyltransferase A complex subunit nat1

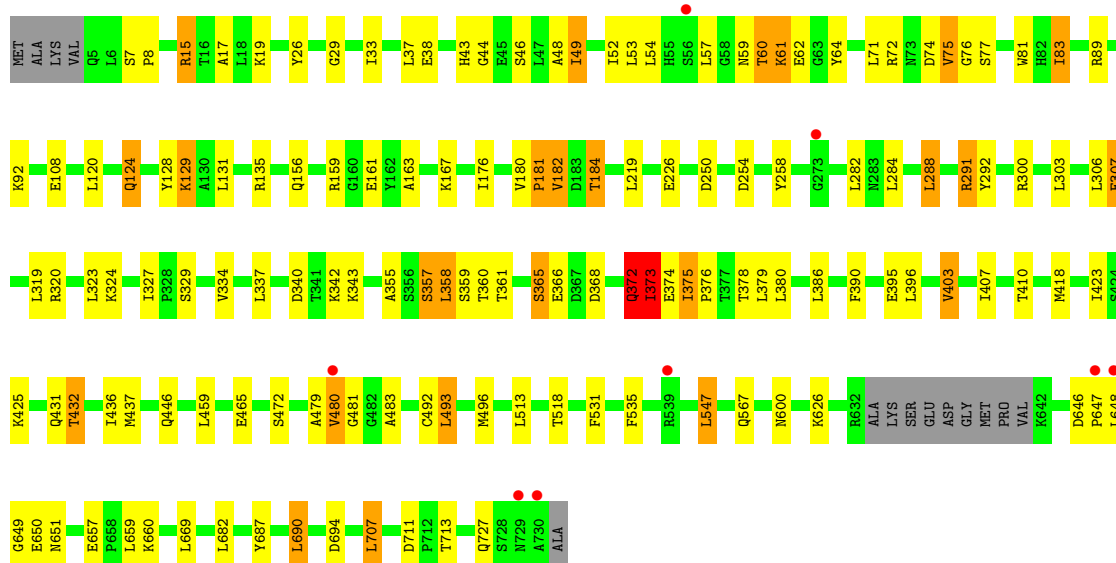
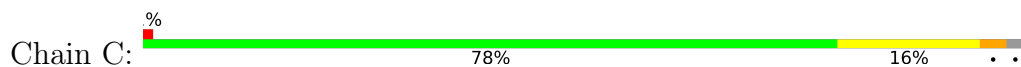


- Molecule 1: N-terminal acetyltransferase A complex subunit nat1

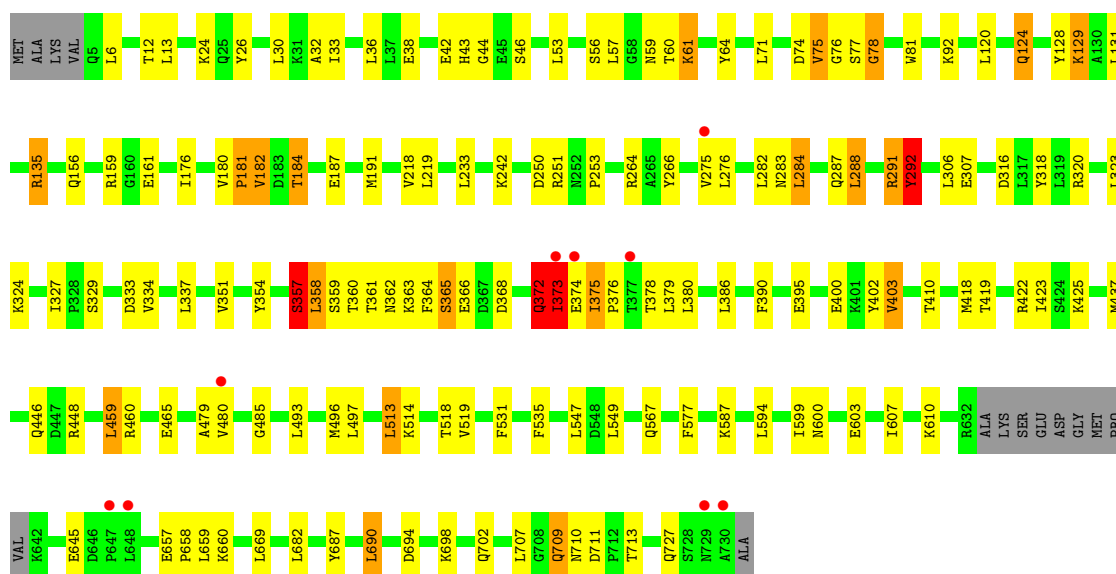
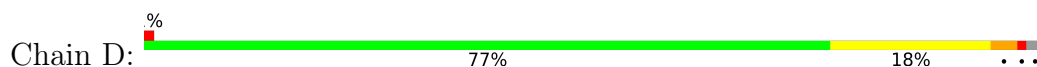




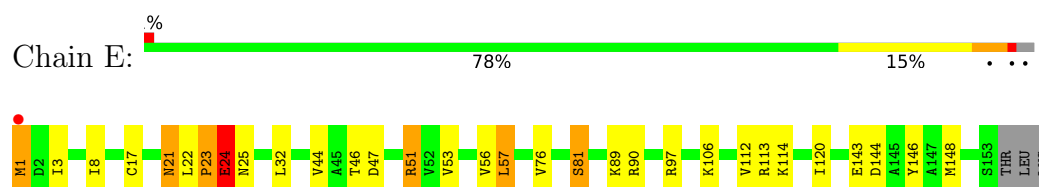
• Molecule 1: N-terminal acetyltransferase A complex subunit nat1



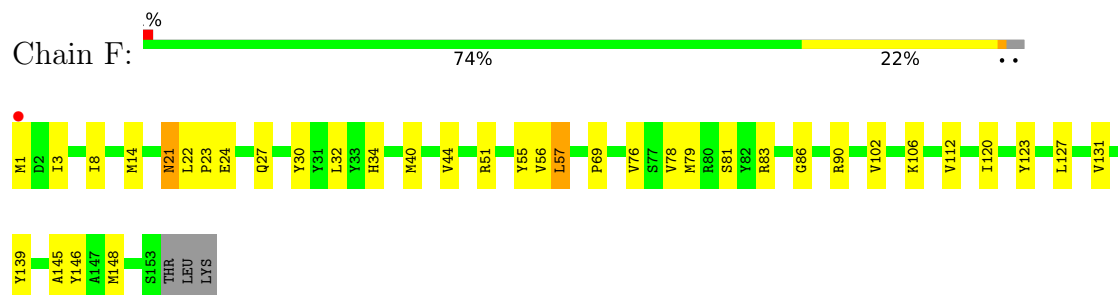
• Molecule 1: N-terminal acetyltransferase A complex subunit nat1



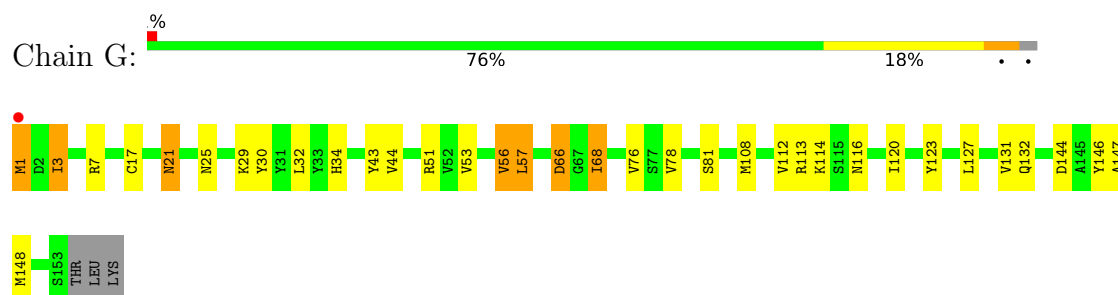
• Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



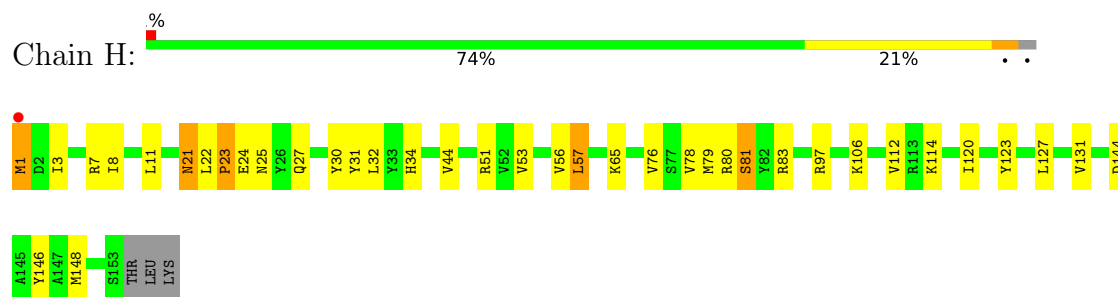
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.74Å 119.69Å 132.02Å 80.28° 76.85° 70.65°	Depositor
Resolution (Å)	49.05 – 3.15 49.05 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.05-3.15) 91.8 (49.05-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.217 , 0.246 0.220 , 0.248	Depositor DCC
R_{free} test set	3816 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, SO4, CL, NA

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	0.30	0/5878	0.75	8/7929 (0.1%)
1	B	0.30	0/5891	0.75	8/7948 (0.1%)
1	C	0.29	0/5867	0.73	8/7915 (0.1%)
1	D	0.30	0/5876	0.75	8/7927 (0.1%)
2	E	0.32	0/1277	0.82	4/1722 (0.2%)
2	F	0.28	0/1277	0.72	0/1722
2	G	0.28	0/1277	0.72	0/1722
2	H	0.32	0/1277	0.81	4/1722 (0.2%)
All	All	0.30	0/28620	0.75	40/38607 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	8.64	118.68	110.30
2	E	23	PRO	CA-C-N	8.47	136.95	121.70
2	E	23	PRO	C-N-CA	8.47	136.95	121.70
2	E	23	PRO	CA-C-O	-8.39	107.03	118.78
1	B	75	VAL	N-CA-C	7.99	118.54	110.23
1	D	75	VAL	N-CA-C	7.69	118.23	110.23
1	C	75	VAL	N-CA-C	7.49	118.22	110.36
2	H	23	PRO	CA-C-N	7.36	134.95	121.70
2	H	23	PRO	C-N-CA	7.36	134.95	121.70
2	H	23	PRO	N-CA-C	7.30	127.16	114.75
2	E	23	PRO	N-CA-C	7.15	126.90	114.75
2	H	23	PRO	CA-C-O	-6.89	109.14	118.78
1	D	365	SER	CB-CA-C	-5.73	109.95	116.54
1	A	365	SER	CB-CA-C	-5.61	110.09	116.54
1	D	372	GLN	N-CA-C	5.60	116.29	108.00
1	B	372	GLN	N-CA-C	5.57	116.25	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	TYR	CA-C-N	5.56	125.27	119.82
1	B	292	TYR	C-N-CA	5.56	125.27	119.82
1	C	365	SER	CB-CA-C	-5.54	110.17	116.54
1	B	365	SER	CB-CA-C	-5.54	110.17	116.54
1	A	410	THR	CA-C-N	5.43	125.52	119.87
1	A	410	THR	C-N-CA	5.43	125.52	119.87
1	C	292	TYR	CA-C-N	5.35	125.07	119.82
1	C	292	TYR	C-N-CA	5.35	125.07	119.82
1	A	480	VAL	N-CA-C	5.28	120.32	109.34
1	D	181	PRO	CA-C-O	-5.18	115.35	121.67
1	C	357	SER	CA-C-N	5.12	130.91	121.70
1	C	357	SER	C-N-CA	5.12	130.91	121.70
1	A	7	SER	CA-C-N	5.11	124.42	118.85
1	A	7	SER	C-N-CA	5.11	124.42	118.85
1	D	357	SER	CA-C-N	5.08	130.85	121.70
1	D	357	SER	C-N-CA	5.08	130.85	121.70
1	B	357	SER	CA-C-N	5.06	130.81	121.70
1	B	357	SER	C-N-CA	5.06	130.81	121.70
1	C	181	PRO	CA-C-O	-5.06	115.50	121.67
1	C	372	GLN	N-CA-C	5.05	115.47	108.00
1	D	292	TYR	CA-C-N	5.04	126.14	119.84
1	D	292	TYR	C-N-CA	5.04	126.14	119.84
1	A	181	PRO	CA-C-O	-5.02	115.55	121.67
1	B	181	PRO	CA-C-O	-5.01	115.55	121.67

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	5764	0	5685	101	0
1	B	5777	0	5697	71	0
1	C	5753	0	5675	80	0
1	D	5761	0	5686	92	1
2	E	1247	0	1233	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1247	0	1233	20	0
2	G	1247	0	1233	16	0
2	H	1247	0	1233	27	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
4	A	10	0	0	5	0
4	B	14	0	0	1	0
4	C	15	0	0	3	0
4	D	10	0	0	5	0
4	E	7	0	0	2	0
4	F	2	0	0	0	0
4	G	2	0	0	1	0
4	H	3	0	0	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	E	51	0	34	0	0
6	F	51	0	34	1	0
6	G	51	0	34	1	0
6	H	51	0	34	1	1
7	A	22	0	0	2	0
7	B	22	0	0	2	0
7	C	25	0	0	1	0
7	D	11	0	0	0	0
7	E	4	0	0	0	0
7	F	6	0	0	0	0
7	G	5	0	0	0	0
7	H	10	0	0	1	0
All	All	28430	0	27811	413	1

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 (413) 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:C:89:ARG:NH1	4:C:801:CL:CL	2.25	1.06
1:A:320:ARG:NH1	1:A:368:ASP:OD2	2.02	0.93
1:C:342:LYS:NZ	4:C:815:CL:CL	2.39	0.92
1:D:320:ARG:NH1	1:D:368:ASP:OD2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:NH1	1:C:368:ASP:OD2	2.10	0.83
1:B:320:ARG:NH1	1:B:368:ASP:OD2	2.13	0.81
2:H:80:ARG:NH1	7:H:310:HOH:O	2.08	0.79
1:D:26:TYR:HB3	1:D:53:LEU:HD22	1.66	0.78
1:D:250:ASP:OD2	1:D:291:ARG:NH1	2.16	0.78
1:A:250:ASP:OD2	1:A:291:ARG:NH1	2.19	0.76
1:D:479:ALA:HB1	1:D:480:VAL:HA	1.69	0.75
1:A:135:ARG:NH1	4:A:802:CL:CL	2.56	0.75
1:A:448:ARG:HH11	2:E:23:PRO:HA	1.52	0.72
1:D:358:LEU:HD12	1:D:379:LEU:HG	1.70	0.72
2:H:21:ASN:HD22	2:H:83:ARG:HH21	1.38	0.71
1:D:135:ARG:NH1	4:D:803:CL:CL	2.58	0.71
1:B:567:GLN:HG3	1:B:682:LEU:HD11	1.73	0.70
1:A:422:ARG:NH2	4:A:809:CL:CL	2.61	0.70
2:E:17:CYS:O	2:E:21:ASN:ND2	2.23	0.70
1:A:709:GLN:HG2	1:A:710:ASN:N	2.07	0.68
1:B:175:THR:OG1	7:B:902:HOH:O	2.11	0.68
2:F:21:ASN:HD21	2:F:79:MET:HA	1.58	0.68
1:D:253:PRO:HG3	1:D:292:TYR:HE2	1.59	0.67
1:A:308:GLY:N	4:A:808:CL:CL	2.62	0.67
1:D:567:GLN:HG3	1:D:682:LEU:HD11	1.76	0.67
1:C:358:LEU:HD12	1:C:379:LEU:HG	1.77	0.67
1:A:253:PRO:HG3	1:A:292:TYR:HE2	1.60	0.66
1:B:358:LEU:HD12	1:B:379:LEU:HG	1.78	0.66
1:C:567:GLN:HG3	1:C:682:LEU:HD11	1.78	0.65
1:C:26:TYR:HB2	1:C:57:LEU:HD23	1.79	0.65
1:B:447:ASP:OD1	7:B:907:HOH:O	2.14	0.65
1:D:184:THR:HG23	1:D:219:LEU:HD11	1.77	0.65
1:D:709:GLN:HG2	1:D:710:ASN:N	2.12	0.65
2:H:23:PRO:N	2:H:24:GLU:HB2	2.12	0.65
1:D:128:TYR:HB3	1:D:159:ARG:HG2	1.79	0.64
2:G:17:CYS:O	2:G:21:ASN:ND2	2.30	0.64
1:A:26:TYR:HB2	1:A:57:LEU:HD23	1.79	0.64
1:A:567:GLN:HG3	1:A:682:LEU:HD11	1.78	0.64
1:A:43:HIS:ND1	1:A:46:SER:OG	2.32	0.63
1:A:62:GLU:O	1:A:66:ASN:ND2	2.30	0.63
1:C:48:ALA:HB1	1:C:83:ILE:HG21	1.81	0.63
1:D:329:SER:OG	2:H:81:SER:O	2.17	0.63
1:A:340:ASP:OD2	1:A:343:LYS:HG3	1.99	0.62
1:A:184:THR:HG23	1:A:219:LEU:HD11	1.81	0.62
1:C:156:GLN:HG3	1:C:161:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:H	1:D:129:LYS:HZ2	1.46	0.62
1:D:129:LYS:HZ2	1:D:129:LYS:N	1.98	0.61
1:C:425:LYS:NZ	4:C:809:CL:CL	2.69	0.61
1:D:324:LYS:HG2	1:D:375:ILE:HD13	1.82	0.61
1:C:250:ASP:OD2	1:C:291:ARG:NH1	2.32	0.61
1:B:26:TYR:HB2	1:B:57:LEU:HD23	1.83	0.60
1:D:156:GLN:HG3	1:D:161:GLU:HB2	1.83	0.60
1:A:128:TYR:HB3	1:A:159:ARG:HG2	1.83	0.60
2:H:21:ASN:N	2:H:21:ASN:OD1	2.35	0.60
2:H:21:ASN:HD21	2:H:79:MET:HA	1.66	0.60
1:B:496:MET:HE2	1:B:518:THR:HG21	1.84	0.59
2:F:21:ASN:N	2:F:21:ASN:OD1	2.36	0.59
1:D:251:ARG:NH1	2:H:97:ARG:NH1	2.51	0.59
2:G:114:LYS:HE2	2:G:144:ASP:HB2	1.83	0.59
1:B:489:ASP:O	2:F:27:GLN:NE2	2.36	0.58
1:B:156:GLN:HG3	1:B:161:GLU:HB2	1.85	0.58
1:B:250:ASP:OD2	1:B:291:ARG:NH1	2.37	0.58
1:A:448:ARG:NH1	2:E:23:PRO:HA	2.17	0.58
1:C:373:ILE:HG22	1:C:374:GLU:H	1.68	0.58
2:E:46:THR:HG21	4:E:206:CL:CL	2.40	0.58
1:A:251:ARG:NH1	2:E:97:ARG:NH1	2.52	0.57
1:A:324:LYS:HG2	1:A:375:ILE:HD13	1.86	0.57
1:B:373:ILE:HG22	1:B:374:GLU:H	1.69	0.57
1:A:124:GLN:HG3	1:A:531:PHE:CD1	2.40	0.57
1:D:124:GLN:HG3	1:D:531:PHE:CD1	2.40	0.57
1:A:373:ILE:HG22	1:A:374:GLU:H	1.69	0.57
1:D:687:TYR:HA	1:D:690:LEU:HB2	1.87	0.57
2:H:23:PRO:CD	2:H:24:GLU:HB2	2.34	0.57
1:A:79:VAL:O	1:A:83:ILE:HG22	2.05	0.57
1:B:13:LEU:HB2	1:B:36:LEU:HD11	1.87	0.56
1:B:327:ILE:HG22	1:B:329:SER:H	1.70	0.56
1:C:479:ALA:HB1	1:C:480:VAL:HA	1.86	0.56
2:H:78:VAL:HG23	6:H:201:ACO:H142	1.87	0.56
1:B:124:GLN:HG3	1:B:531:PHE:CD1	2.40	0.56
1:D:373:ILE:HG22	1:D:374:GLU:H	1.69	0.56
1:A:37:LEU:HD21	1:A:46:SER:HB3	1.86	0.56
1:A:269:GLU:HG3	1:A:274:LYS:HA	1.88	0.56
1:C:124:GLN:HG3	1:C:531:PHE:CD1	2.41	0.56
1:C:327:ILE:HG22	1:C:329:SER:H	1.71	0.56
1:C:43:HIS:ND1	1:C:46:SER:OG	2.37	0.55
1:C:33:ILE:HG22	1:C:37:LEU:HG	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:HG3	1:A:161:GLU:HB2	1.88	0.55
1:C:687:TYR:HA	1:C:690:LEU:HB2	1.88	0.55
1:D:587:LYS:NZ	1:D:610:LYS:NZ	2.53	0.55
1:C:37:LEU:HD21	1:C:46:SER:HB3	1.89	0.55
1:C:128:TYR:HB3	1:C:159:ARG:HG2	1.88	0.55
2:E:22:LEU:HB3	2:E:24:GLU:HB3	1.88	0.55
1:C:129:LYS:NZ	1:C:129:LYS:H	2.05	0.55
1:D:422:ARG:NH2	4:D:807:CL:CL	2.77	0.55
2:E:89:LYS:HD2	4:E:210:CL:CL	2.44	0.55
1:C:324:LYS:HG2	1:C:375:ILE:HD13	1.89	0.54
2:E:23:PRO:HD2	2:E:24:GLU:HB2	1.88	0.54
2:F:23:PRO:HD2	2:F:24:GLU:OE2	2.07	0.54
2:F:69:PRO:HD2	2:F:106:LYS:HD2	1.87	0.54
1:B:324:LYS:HG2	1:B:375:ILE:HD13	1.89	0.54
1:D:77:SER:OG	1:D:78:GLY:N	2.40	0.54
2:H:23:PRO:HD2	2:H:24:GLU:HB2	1.89	0.54
1:B:309:ASP:C	1:B:311:PHE:H	2.16	0.53
1:D:657:GLU:N	1:D:657:GLU:OE2	2.40	0.53
2:F:21:ASN:HD22	2:F:83:ARG:HH21	1.56	0.53
1:A:320:ARG:NH1	1:A:364:PHE:HB2	2.23	0.53
1:D:448:ARG:HH12	2:H:25:ASN:HD21	1.56	0.53
1:C:319:LEU:HD21	1:C:334:VAL:HG21	1.91	0.53
1:C:650:GLU:OE1	7:C:915:HOH:O	2.19	0.53
1:B:282:LEU:HD21	1:B:306:LEU:HD21	1.91	0.53
1:B:307:GLU:N	1:B:307:GLU:OE2	2.42	0.53
1:B:476:ARG:HG2	1:B:478:GLU:HG2	1.91	0.52
1:D:496:MET:HE2	1:D:518:THR:HG21	1.92	0.52
2:F:40:MET:HG3	2:F:102:VAL:HG21	1.90	0.52
1:A:129[A]:LYS:NZ	1:A:129[A]:LYS:H	2.07	0.52
1:C:52:ILE:HB	1:C:83:ILE:HD11	1.91	0.52
1:A:390:PHE:HB3	1:A:395:GLU:HB2	1.90	0.52
1:C:282:LEU:HD21	1:C:306:LEU:HD21	1.90	0.52
1:C:659:LEU:HD13	1:C:690:LEU:HD22	1.92	0.52
2:E:112:VAL:HG23	2:E:146:TYR:HB2	1.92	0.52
1:C:75:VAL:N	1:C:76:GLY:HA3	2.25	0.52
1:D:61:LYS:HD3	1:D:64:TYR:HB2	1.92	0.51
1:C:418:MET:HG2	1:C:437:MET:HE1	1.92	0.51
1:D:448:ARG:HH12	2:H:25:ASN:ND2	2.09	0.51
1:D:549:LEU:HA	2:H:8:ILE:HG21	1.92	0.51
1:D:75:VAL:N	1:D:76:GLY:HA3	2.24	0.51
1:C:184:THR:HG23	1:C:219:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:HG13	1:B:37:LEU:HG	1.92	0.51
1:C:496:MET:HE2	1:C:518:THR:HG21	1.92	0.51
1:D:497:LEU:HD13	1:D:519:VAL:HG21	1.92	0.51
1:A:282:LEU:HD21	1:A:306:LEU:HD21	1.93	0.51
1:A:71:LEU:HD11	1:A:81:TRP:CE2	2.46	0.51
1:A:124:GLN:HG3	1:A:531:PHE:HD1	1.75	0.51
1:A:447:ASP:OD1	7:A:914:HOH:O	2.19	0.51
1:D:124:GLN:HG3	1:D:531:PHE:HD1	1.73	0.51
1:A:496:MET:HE2	1:A:518:THR:HG21	1.93	0.51
1:B:181:PRO:HA	1:B:182:VAL:HG22	1.92	0.51
1:C:300:ARG:HG2	2:G:1[A]:MET:HE1	1.93	0.51
1:D:120:LEU:HD11	1:D:535:PHE:HB2	1.93	0.51
2:E:114:LYS:HE2	2:E:144:ASP:HB2	1.92	0.50
1:A:128:TYR:H	1:A:129[A]:LYS:NZ	2.10	0.50
1:C:181:PRO:HA	1:C:182:VAL:HG22	1.92	0.50
2:E:23:PRO:CD	2:E:24:GLU:HB2	2.41	0.50
2:G:78:VAL:HG23	6:G:201:ACO:H142	1.94	0.50
1:A:37:LEU:CD2	1:A:46:SER:HB3	2.41	0.50
1:C:54:LEU:HD13	1:C:62:GLU:HG3	1.94	0.50
1:A:181:PRO:HA	1:A:182:VAL:HG22	1.93	0.50
1:B:254:ASP:OD2	2:F:90:ARG:HD3	2.12	0.50
1:A:128:TYR:N	1:A:129[A]:LYS:NZ	2.60	0.50
1:C:334:VAL:HG13	1:C:337:LEU:HD12	1.93	0.50
1:A:129[A]:LYS:H	1:A:129[A]:LYS:HZ3	1.59	0.50
1:A:242:LYS:HE3	1:A:266:TYR:CZ	2.47	0.50
2:G:29:LYS:HG2	4:G:203:CL:CL	2.49	0.50
1:C:647:PRO:HB3	1:C:651:ASN:HB2	1.92	0.49
1:D:711:ASP:OD2	1:D:713:THR:OG1	2.30	0.49
1:D:282:LEU:HD21	1:D:306:LEU:HD21	1.94	0.49
1:D:13:LEU:HD22	1:D:32:ALA:HB1	1.94	0.49
2:F:21:ASN:ND2	2:F:78:VAL:O	2.45	0.49
2:H:30:TYR:CZ	2:H:34:HIS:HE1	2.31	0.49
1:A:33:ILE:HG23	1:A:37:LEU:HG	1.95	0.49
1:B:128:TYR:HB3	1:B:159:ARG:HG2	1.93	0.49
1:D:135:ARG:HD2	4:D:803:CL:CL	2.50	0.49
1:C:59:ASN:HB3	1:C:60:THR:HG22	1.95	0.48
1:C:44:GLY:HA3	1:C:74:ASP:HB2	1.95	0.48
1:D:233:LEU:HD13	1:D:264:ARG:HD3	1.95	0.48
1:A:687:TYR:HA	1:A:690:LEU:HB2	1.95	0.48
1:A:342:LYS:NZ	4:A:808:CL:CL	2.69	0.48
1:B:184:THR:HG23	1:B:219:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PRO:HA	1:D:182:VAL:HG22	1.95	0.48
1:A:497:LEU:HD13	1:A:519:VAL:HG21	1.96	0.48
1:A:275:VAL:HA	1:A:276:LEU:HA	1.45	0.48
1:C:340:ASP:OD2	1:C:343:LYS:HG3	2.14	0.47
1:D:275:VAL:HA	1:D:276:LEU:HA	1.48	0.47
1:D:316:ASP:OD2	1:D:354:TYR:OH	2.27	0.47
2:F:123:TYR:HA	2:F:127:LEU:HB2	1.94	0.47
1:B:92:LYS:NZ	4:B:802:CL:CL	2.82	0.47
1:B:534:HIS:ND1	1:B:546:TYR:OH	2.47	0.47
1:A:549:LEU:HA	2:E:8:ILE:HG21	1.97	0.47
1:C:124:GLN:HG3	1:C:531:PHE:HD1	1.79	0.47
1:C:372:GLN:HB3	1:C:373:ILE:H	1.51	0.47
1:D:362:ASN:HB2	1:D:374:GLU:OE1	2.13	0.47
2:H:123:TYR:HA	2:H:127:LEU:HB2	1.96	0.47
1:D:357:SER:OG	1:D:363:LYS:O	2.30	0.47
1:A:26:TYR:CZ	1:A:56:SER:HB3	2.50	0.47
1:B:372:GLN:HB3	1:B:373:ILE:H	1.50	0.47
1:A:472:SER:HA	1:A:483:ALA:HB2	1.97	0.47
1:D:71:LEU:HD11	1:D:81:TRP:CE2	2.50	0.47
1:B:310:GLU:O	1:B:314:HIS:ND1	2.48	0.47
1:C:71:LEU:HD11	1:C:81:TRP:CE2	2.49	0.46
1:D:180:VAL:O	1:D:182:VAL:HG22	2.15	0.46
2:G:131:VAL:HG22	2:G:148:MET:HE3	1.97	0.46
1:B:334:VAL:HG13	1:B:337:LEU:HD12	1.97	0.46
1:C:472:SER:HA	1:C:483:ALA:HB2	1.97	0.46
1:D:13:LEU:HD12	1:D:36:LEU:HD11	1.98	0.46
1:D:218:VAL:HG23	4:D:805:CL:CL	2.52	0.46
1:B:291:ARG:HE	1:B:291:ARG:HB2	1.48	0.46
2:F:30:TYR:CZ	2:F:34:HIS:HE1	2.32	0.46
1:A:587:LYS:NZ	1:A:610:LYS:NZ	2.64	0.46
1:A:438:ASP:OD2	1:A:442:LYS:HE3	2.15	0.46
2:H:57:LEU:HD23	2:H:57:LEU:HA	1.82	0.46
1:B:75:VAL:N	1:B:76:GLY:HA3	2.31	0.46
1:B:288:LEU:O	1:B:291:ARG:HB3	2.14	0.46
1:C:626:LYS:HD3	1:C:646:ASP:HA	1.97	0.46
1:D:284:LEU:HD22	1:D:288:LEU:HD22	1.97	0.46
2:G:30:TYR:CZ	2:G:34:HIS:HE1	2.33	0.46
1:A:75:VAL:N	1:A:76:GLY:HA3	2.29	0.46
1:A:415:GLU:HG3	1:A:418:MET:HE2	1.96	0.46
1:D:365:SER:OG	1:D:366:GLU:N	2.48	0.46
1:D:587:LYS:HZ1	1:D:610:LYS:NZ	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:TYR:HA	2:G:127:LEU:HB2	1.97	0.46
1:A:74:ASP:CG	1:A:77:SER:HB3	2.40	0.46
1:A:319:LEU:HD12	1:A:350:LEU:HD23	1.98	0.46
1:A:594:LEU:HD23	1:A:599:ILE:HD11	1.98	0.46
1:B:71:LEU:HD11	1:B:81:TRP:CE2	2.51	0.46
1:B:418:MET:HG2	1:B:437:MET:HE1	1.98	0.46
1:C:15:ARG:O	1:C:19:LYS:HG2	2.16	0.46
1:D:480:VAL:O	1:D:485:GLY:HA3	2.15	0.46
1:D:603:GLU:O	1:D:607:ILE:HG12	2.16	0.46
2:F:14:MET:HE3	2:F:55:TYR:HB2	1.96	0.46
1:A:179:GLY:HA3	1:A:180:VAL:HA	1.69	0.45
1:C:61:LYS:HD3	1:C:64:TYR:HB2	1.96	0.45
1:D:320:ARG:NH1	1:D:364:PHE:HB2	2.31	0.45
1:C:120:LEU:HD11	1:C:535:PHE:HB2	1.98	0.45
1:A:52:ILE:HB	1:A:83:ILE:HG13	1.99	0.45
1:C:128:TYR:N	1:C:129:LYS:NZ	2.65	0.45
1:D:129:LYS:H	1:D:129:LYS:NZ	2.14	0.45
1:D:372:GLN:HB3	1:D:373:ILE:H	1.51	0.45
2:E:57:LEU:HD23	2:E:57:LEU:HA	1.83	0.45
1:A:45:GLU:O	1:A:49:ILE:HG13	2.17	0.45
1:A:372:GLN:HB3	1:A:373:ILE:H	1.51	0.45
1:B:43:HIS:HD1	1:B:46:SER:HG	1.64	0.45
1:A:251:ARG:NH1	2:E:97:ARG:HH12	2.15	0.45
1:A:479:ALA:HA	1:A:632:ARG:HE	1.82	0.45
1:A:694:ASP:OD1	1:A:694:ASP:N	2.50	0.45
1:A:391:ASP:OD1	1:A:426:HIS:ND1	2.46	0.45
1:B:707:LEU:O	1:B:711:ASP:HB2	2.16	0.45
1:D:187:GLU:OE2	1:D:191:MET:HE2	2.18	0.44
2:F:131:VAL:HG22	2:F:148:MET:HE3	1.98	0.44
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.88	0.44
1:D:359:SER:OG	1:D:360:THR:N	2.51	0.44
1:D:418:MET:HG2	1:D:437:MET:HE1	1.99	0.44
1:B:58:GLY:HA2	1:B:59:ASN:O	2.16	0.44
2:E:47:ASP:OD2	2:E:51:ARG:HG3	2.17	0.44
1:B:448:ARG:HH11	2:F:23:PRO:HA	1.82	0.44
1:A:254:ASP:OD2	2:E:90:ARG:HD3	2.17	0.44
1:A:711:ASP:OD2	1:A:713:THR:OG1	2.31	0.44
1:B:7:SER:HA	1:B:8:PRO:HD3	1.83	0.44
1:B:460:ARG:NH2	1:B:498:GLU:OE1	2.51	0.44
1:C:291:ARG:HE	1:C:291:ARG:HB2	1.53	0.44
1:D:318:TYR:OH	1:D:333:ASP:OD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:LEU:O	1:C:711:ASP:HB2	2.18	0.44
1:D:26:TYR:HB2	1:D:57:LEU:HD23	2.00	0.44
1:B:319:LEU:HD21	1:B:334:VAL:HG21	1.99	0.44
1:D:698:LYS:O	1:D:702:GLN:HG3	2.18	0.44
1:B:181:PRO:HA	1:B:182:VAL:CG2	2.48	0.44
1:C:163:ALA:O	1:C:167:LYS:HG2	2.17	0.44
2:H:114:LYS:HE2	2:H:144:ASP:HB2	2.00	0.44
1:B:459:LEU:HD12	1:B:459:LEU:HA	1.85	0.43
1:D:44:GLY:HA3	1:D:74:ASP:HB2	2.00	0.43
2:H:21:ASN:HD22	2:H:83:ARG:NH2	2.11	0.43
1:A:61:LYS:HD3	1:A:64:TYR:HB2	1.99	0.43
1:C:181:PRO:HA	1:C:182:VAL:CG2	2.48	0.43
1:B:318:TYR:OH	1:B:333:ASP:OD2	2.26	0.43
1:B:437:MET:HE3	1:B:437:MET:HA	2.00	0.43
1:C:180:VAL:O	1:C:182:VAL:HG22	2.17	0.43
1:D:59:ASN:HA	1:D:60:THR:HA	1.84	0.43
1:D:587:LYS:NZ	1:D:610:LYS:HZ2	2.16	0.43
1:A:365:SER:OG	1:A:366:GLU:N	2.51	0.43
1:A:437:MET:HA	1:A:437:MET:HE3	2.00	0.43
1:D:43:HIS:HD1	1:D:46:SER:HG	1.66	0.43
1:D:242:LYS:HE3	1:D:266:TYR:CZ	2.53	0.43
1:D:437:MET:HE3	1:D:437:MET:HA	2.00	0.43
2:E:148:MET:HE2	2:E:148:MET:HB3	1.95	0.43
1:A:329:SER:OG	2:E:81:SER:O	2.28	0.43
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.88	0.43
1:D:577:PHE:CD1	1:D:659:LEU:HD21	2.53	0.43
1:A:448:ARG:NH1	2:E:22:LEU:O	2.49	0.43
1:B:647:PRO:HB3	1:B:651:ASN:HB2	1.99	0.43
1:D:288:LEU:O	1:D:291:ARG:HB3	2.18	0.43
1:A:180:VAL:O	1:A:182:VAL:HG22	2.19	0.43
1:A:181:PRO:HA	1:A:182:VAL:CG2	2.49	0.43
1:C:359:SER:OG	1:C:360:THR:N	2.52	0.43
1:B:359:SER:OG	1:B:360:THR:N	2.52	0.43
2:H:112:VAL:HG23	2:H:146:TYR:HB2	2.01	0.43
1:A:33:ILE:HG21	1:A:50:LYS:HB2	2.01	0.43
1:A:288:LEU:O	1:A:291:ARG:HB3	2.19	0.43
1:B:316:ASP:CG	1:B:320:ARG:HE	2.26	0.43
1:B:358:LEU:HD13	1:B:358:LEU:HA	1.83	0.43
1:B:657:GLU:HA	1:B:658:PRO:HD2	1.88	0.43
2:H:148:MET:HE2	2:H:148:MET:HB3	1.94	0.43
1:C:288:LEU:O	1:C:291:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ASN:O	1:D:287:GLN:HG2	2.19	0.43
1:A:709:GLN:HG2	1:A:710:ASN:H	1.82	0.42
1:B:549:LEU:HA	2:F:8:ILE:HG21	2.00	0.42
1:C:128:TYR:H	1:C:129:LYS:NZ	2.17	0.42
1:A:358:LEU:HD13	1:A:362:ASN:HA	2.00	0.42
1:D:358:LEU:HD13	1:D:358:LEU:HA	1.82	0.42
2:G:68:ILE:H	2:G:68:ILE:HG13	1.43	0.42
1:A:9:LYS:O	1:A:12:THR:HG22	2.19	0.42
1:A:189:GLU:OE1	7:A:902:HOH:O	2.21	0.42
1:B:648:LEU:HD13	1:B:648:LEU:HA	1.93	0.42
2:F:112:VAL:HG23	2:F:146:TYR:HB2	2.00	0.42
2:G:113:ARG:HG3	2:G:116:ASN:HB2	2.01	0.42
2:G:43:TYR:H	2:G:56:VAL:HG13	1.84	0.42
1:B:180:VAL:O	1:B:182:VAL:HG22	2.18	0.42
1:B:365:SER:OG	1:B:366:GLU:N	2.51	0.42
1:D:514:LYS:NZ	1:D:645:GLU:OE1	2.47	0.42
1:D:660:LYS:HB2	1:D:660:LYS:HE2	1.92	0.42
2:E:23:PRO:N	2:E:24:GLU:HB2	2.34	0.42
1:A:15:ARG:O	1:A:19:LYS:HG3	2.20	0.42
1:A:418:MET:HG2	1:A:437:MET:HE1	2.01	0.42
1:B:347:VAL:O	1:B:351:VAL:HG22	2.19	0.42
1:C:493:LEU:HD12	1:C:493:LEU:HA	1.79	0.42
1:C:547:LEU:HD12	1:C:547:LEU:HA	1.91	0.42
1:D:694:ASP:OD1	1:D:694:ASP:N	2.49	0.42
2:F:86:GLY:N	6:F:201:ACO:O1A	2.53	0.42
2:G:57:LEU:HD23	2:G:57:LEU:HA	1.88	0.42
1:A:390:PHE:CD1	1:A:395:GLU:HG3	2.54	0.42
1:A:410:THR:HA	1:A:411:PRO:HD2	1.94	0.42
1:C:29:GLY:O	1:C:33:ILE:HG13	2.20	0.42
1:C:254:ASP:HB2	2:G:3:ILE:HG12	2.00	0.42
1:D:74:ASP:CG	1:D:77:SER:HB3	2.45	0.42
2:H:131:VAL:HG22	2:H:148:MET:HE3	2.02	0.42
1:C:226:GLU:OE2	1:C:258:TYR:OH	2.33	0.42
1:D:129:LYS:HZ3	1:D:129:LYS:HB2	1.85	0.42
2:G:112:VAL:HG23	2:G:146:TYR:HB2	2.01	0.42
1:A:300:ARG:HD3	1:A:318:TYR:CZ	2.54	0.42
1:B:390:PHE:HB3	1:B:395:GLU:HB2	2.02	0.42
1:C:355:ALA:HB2	1:C:386:LEU:HD11	2.02	0.42
1:C:365:SER:OG	1:C:366:GLU:N	2.51	0.42
1:D:351:VAL:HG23	1:D:386:LEU:HD21	2.02	0.42
2:G:66:ASP:OD2	2:G:66:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:O	1:A:67:VAL:HG23	2.20	0.41
1:B:492:CYS:O	1:B:496:MET:HG2	2.19	0.41
1:D:386:LEU:HD13	1:D:402:TYR:CZ	2.55	0.41
1:D:459:LEU:HD12	1:D:459:LEU:HA	1.82	0.41
1:D:657:GLU:HA	1:D:658:PRO:HD2	1.93	0.41
2:H:79:MET:O	2:H:83:ARG:HG3	2.20	0.41
1:A:163:ALA:O	1:A:167:LYS:HG2	2.20	0.41
1:A:319:LEU:HD21	1:A:334:VAL:HG21	2.01	0.41
1:B:124:GLN:HG3	1:B:531:PHE:HD1	1.84	0.41
2:H:65:LYS:H	2:H:65:LYS:HG2	1.66	0.41
1:A:291:ARG:HE	1:A:291:ARG:HB2	1.46	0.41
1:C:17:ALA:HB1	1:C:33:ILE:HD11	2.02	0.41
1:C:49:ILE:O	1:C:53:LEU:HD13	2.20	0.41
1:C:307:GLU:OE2	1:C:307:GLU:O	2.39	0.41
1:D:327:ILE:HG22	1:D:329:SER:H	1.84	0.41
1:D:334:VAL:HG13	1:D:337:LEU:HD12	2.02	0.41
1:D:390:PHE:HB3	1:D:395:GLU:HB2	2.01	0.41
2:E:47:ASP:OD1	2:E:51:ARG:HG3	2.21	0.41
1:C:358:LEU:HD13	1:C:358:LEU:HA	1.84	0.41
1:A:183:ASP:HB3	1:A:186:GLU:H	1.85	0.41
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.94	0.41
2:E:1[A]:MET:HB3	2:E:1[A]:MET:HE3	1.87	0.41
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.85	0.41
1:C:492:CYS:O	1:C:496:MET:HG2	2.20	0.41
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.87	0.41
2:F:22:LEU:HA	2:F:23:PRO:HD3	1.82	0.41
1:A:248:LEU:HB3	1:A:258:TYR:CE1	2.55	0.41
1:C:648:LEU:HD13	1:C:648:LEU:HA	1.92	0.41
2:E:113:ARG:HB2	2:E:143:GLU:OE1	2.20	0.41
1:B:320:ARG:NH1	1:B:364:PHE:HB2	2.35	0.41
2:H:22:LEU:HA	2:H:23:PRO:HD3	1.73	0.41
1:A:11:ILE:O	1:A:15:ARG:HG3	2.21	0.41
1:A:155:ALA:O	1:A:159:ARG:HG3	2.20	0.41
1:A:210:HIS:CE1	1:A:214:ILE:HD13	2.55	0.41
1:A:514:LYS:NZ	1:A:645:GLU:OE1	2.45	0.41
1:B:375:ILE:HD12	1:B:378:THR:HG21	2.03	0.41
1:B:478:GLU:HG2	1:B:478:GLU:H	1.73	0.41
1:B:493:LEU:HD12	1:B:493:LEU:HA	1.81	0.41
1:B:687:TYR:HA	1:B:690:LEU:HB2	2.03	0.41
1:B:711:ASP:OD2	1:B:713:THR:OG1	2.37	0.41
1:C:396:LEU:HD22	1:C:423:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:ASP:OD2	1:C:713:THR:OG1	2.36	0.41
1:D:181:PRO:HA	1:D:182:VAL:CG2	2.51	0.41
1:D:291:ARG:HE	1:D:291:ARG:HB2	1.49	0.41
2:F:139:TYR:CE2	2:F:145:ALA:HB2	2.56	0.41
2:H:1[A]:MET:HB3	2:H:1[A]:MET:HE3	1.86	0.41
2:H:11:LEU:HD22	2:H:31:TYR:HB3	2.02	0.41
1:A:131:LEU:HD11	4:A:802:CL:CL	2.58	0.41
1:A:251:ARG:CZ	2:E:97:ARG:NH1	2.84	0.41
1:B:152:LEU:HG	1:B:168:ILE:HD13	2.03	0.41
1:B:353:LYS:HB3	1:B:353:LYS:HE2	1.87	0.41
1:C:437:MET:HE3	1:C:437:MET:HA	2.03	0.41
1:C:694:ASP:OD1	1:C:694:ASP:N	2.52	0.41
1:D:26:TYR:CZ	1:D:56:SER:HB3	2.56	0.41
2:H:34:HIS:CD2	2:H:57:LEU:HD22	2.56	0.41
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.86	0.40
2:E:22:LEU:HA	2:E:23:PRO:HD3	1.81	0.40
2:G:132:GLN:N	2:G:147:ALA:O	2.49	0.40
1:C:59:ASN:HA	1:C:60:THR:HA	1.92	0.40
1:C:390:PHE:HB3	1:C:395:GLU:HB2	2.03	0.40
1:D:306:LEU:HD23	1:D:306:LEU:HA	1.96	0.40
1:D:425:LYS:NZ	4:D:808:CL:CL	2.91	0.40
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.86	0.40
1:D:594:LEU:HD23	1:D:599:ILE:HD11	2.02	0.40
2:F:57:LEU:HD23	2:F:57:LEU:HA	1.87	0.40
1:A:242:LYS:HE3	1:A:266:TYR:OH	2.22	0.40
1:A:419:THR:O	1:A:423:ILE:HG13	2.21	0.40
1:A:476:ARG:NH2	1:A:478:GLU:OE1	2.51	0.40
1:C:7:SER:HA	1:C:8:PRO:HD3	1.90	0.40
1:C:300:ARG:O	1:C:303:LEU:HB2	2.20	0.40
1:C:403:VAL:O	1:C:407:ILE:HG13	2.22	0.40
1:C:432:THR:O	1:C:436:ILE:HG13	2.21	0.40
1:C:647:PRO:C	1:C:649:GLY:H	2.29	0.40
1:D:400:GLU:HA	1:D:403:VAL:HG23	2.03	0.40
1:A:251:ARG:CZ	2:E:97:ARG:HH11	2.34	0.40
1:B:513:LEU:HD12	1:B:513:LEU:HA	1.86	0.40
1:B:587:LYS:NZ	1:B:610:LYS:NZ	2.69	0.40
1:A:400:GLU:HA	1:A:403:VAL:HG23	2.04	0.40
1:B:52:ILE:HB	1:B:83:ILE:HG23	2.03	0.40
1:D:419:THR:O	1:D:423:ILE:HG13	2.21	0.40

All (1) 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)
1:D:42:GLU:OE1	6:H:201:ACO:O2B[1_655]	2.16	0.04

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	715/731 (98%)	686 (96%)	23 (3%)	6 (1%)	16	46
1	B	719/731 (98%)	688 (96%)	26 (4%)	5 (1%)	18	49
1	C	714/731 (98%)	683 (96%)	26 (4%)	5 (1%)	18	49
1	D	714/731 (98%)	684 (96%)	25 (4%)	5 (1%)	18	49
2	E	151/156 (97%)	148 (98%)	2 (1%)	1 (1%)	18	49
2	F	151/156 (97%)	149 (99%)	2 (1%)	0	100	100
2	G	151/156 (97%)	149 (99%)	2 (1%)	0	100	100
2	H	151/156 (97%)	148 (98%)	3 (2%)	0	100	100
All	All	3466/3548 (98%)	3335 (96%)	109 (3%)	22 (1%)	21	52

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	ILE
1	A	480	VAL
1	B	373	ILE
1	C	373	ILE
1	D	373	ILE
2	E	24	GLU
1	A	182	VAL
1	A	481	GLY
1	B	182	VAL
1	B	481	GLY
1	C	77	SER
1	C	182	VAL

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Mol	Chain	Res	Type
1	C	481	GLY
1	D	182	VAL
1	B	77	SER
1	D	6	LEU
1	A	6	LEU
1	A	376	PRO
1	D	78	GLY
1	D	376	PRO
1	B	376	PRO
1	C	376	PRO

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	610/638 (96%)	560 (92%)	50 (8%)	10	34
1	B	610/638 (96%)	563 (92%)	47 (8%)	12	37
1	C	609/638 (96%)	563 (92%)	46 (8%)	12	37
1	D	610/638 (96%)	568 (93%)	42 (7%)	14	40
2	E	133/135 (98%)	117 (88%)	16 (12%)	5	20
2	F	133/135 (98%)	121 (91%)	12 (9%)	9	30
2	G	133/135 (98%)	115 (86%)	18 (14%)	4	16
2	H	133/135 (98%)	117 (88%)	16 (12%)	5	20
All	All	2971/3092 (96%)	2724 (92%)	247 (8%)	11	34

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	ILE
1	A	37	LEU
1	A	38	GLU
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	60	THR
1	A	61	LYS
1	A	72	ARG
1	A	83	ILE
1	A	92	LYS
1	A	124	GLN
1	A	129[A]	LYS
1	A	129[B]	LYS
1	A	131	LEU
1	A	135	ARG
1	A	176	ILE
1	A	184	THR
1	A	284	LEU
1	A	288	LEU
1	A	291	ARG
1	A	292	TYR
1	A	307	GLU
1	A	323	LEU
1	A	357	SER
1	A	358	LEU
1	A	361	THR
1	A	372	GLN
1	A	373	ILE
1	A	375	ILE
1	A	378	THR
1	A	380	LEU
1	A	403	VAL
1	A	409	HIS
1	A	410	THR
1	A	432	THR
1	A	446	GLN
1	A	459	LEU
1	A	465	GLU
1	A	480	VAL
1	A	493	LEU
1	A	513	LEU
1	A	547	LEU
1	A	600	ASN
1	A	657	GLU
1	A	660	LYS
1	A	669	LEU
1	A	690	LEU

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Mol	Chain	Res	Type
1	A	707	LEU
1	A	709	GLN
1	A	727	GLN
1	B	15	ARG
1	B	30	LEU
1	B	38	GLU
1	B	49	ILE
1	B	53	LEU
1	B	61	LYS
1	B	72	ARG
1	B	92	LYS
1	B	124	GLN
1	B	129[A]	LYS
1	B	129[B]	LYS
1	B	131	LEU
1	B	135	ARG
1	B	174	SER
1	B	176	ILE
1	B	184	THR
1	B	284	LEU
1	B	288	LEU
1	B	291	ARG
1	B	307	GLU
1	B	323	LEU
1	B	357	SER
1	B	358	LEU
1	B	361	THR
1	B	372	GLN
1	B	373	ILE
1	B	375	ILE
1	B	378	THR
1	B	380	LEU
1	B	403	VAL
1	B	409	HIS
1	B	410	THR
1	B	432	THR
1	B	446	GLN
1	B	459	LEU
1	B	465	GLU
1	B	480	VAL
1	B	493	LEU
1	B	513	LEU

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Mol	Chain	Res	Type
1	B	547	LEU
1	B	600	ASN
1	B	657	GLU
1	B	669	LEU
1	B	690	LEU
1	B	697	SER
1	B	707	LEU
1	B	727	GLN
1	C	15	ARG
1	C	38	GLU
1	C	49	ILE
1	C	60	THR
1	C	61	LYS
1	C	72	ARG
1	C	83	ILE
1	C	92	LYS
1	C	108	GLU
1	C	124	GLN
1	C	129	LYS
1	C	131	LEU
1	C	135	ARG
1	C	176	ILE
1	C	184	THR
1	C	284	LEU
1	C	288	LEU
1	C	291	ARG
1	C	307	GLU
1	C	323	LEU
1	C	357	SER
1	C	358	LEU
1	C	361	THR
1	C	372	GLN
1	C	373	ILE
1	C	375	ILE
1	C	378	THR
1	C	380	LEU
1	C	403	VAL
1	C	410	THR
1	C	431	GLN
1	C	432	THR
1	C	446	GLN
1	C	459	LEU

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Mol	Chain	Res	Type
1	C	465	GLU
1	C	480	VAL
1	C	493	LEU
1	C	513	LEU
1	C	547	LEU
1	C	600	ASN
1	C	657	GLU
1	C	660	LYS
1	C	669	LEU
1	C	690	LEU
1	C	707	LEU
1	C	727	GLN
1	D	12	THR
1	D	24	LYS
1	D	30	LEU
1	D	33	ILE
1	D	38	GLU
1	D	61	LYS
1	D	92	LYS
1	D	124	GLN
1	D	129	LYS
1	D	131	LEU
1	D	135	ARG
1	D	176	ILE
1	D	184	THR
1	D	284	LEU
1	D	288	LEU
1	D	291	ARG
1	D	292	TYR
1	D	307	GLU
1	D	323	LEU
1	D	357	SER
1	D	358	LEU
1	D	361	THR
1	D	372	GLN
1	D	373	ILE
1	D	375	ILE
1	D	378	THR
1	D	380	LEU
1	D	403	VAL
1	D	410	THR
1	D	446	GLN

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Mol	Chain	Res	Type
1	D	459	LEU
1	D	460	ARG
1	D	465	GLU
1	D	493	LEU
1	D	513	LEU
1	D	547	LEU
1	D	600	ASN
1	D	669	LEU
1	D	690	LEU
1	D	707	LEU
1	D	709	GLN
1	D	727	GLN
2	E	1[A]	MET
2	E	1[B]	MET
2	E	3	ILE
2	E	21	ASN
2	E	24	GLU
2	E	25	ASN
2	E	32	LEU
2	E	44	VAL
2	E	51	ARG
2	E	53	VAL
2	E	56	VAL
2	E	57	LEU
2	E	76	VAL
2	E	81	SER
2	E	106	LYS
2	E	120	ILE
2	F	1[A]	MET
2	F	1[B]	MET
2	F	3	ILE
2	F	21	ASN
2	F	32	LEU
2	F	44	VAL
2	F	51	ARG
2	F	56	VAL
2	F	57	LEU
2	F	76	VAL
2	F	81	SER
2	F	120	ILE
2	G	1[A]	MET
2	G	1[B]	MET

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Mol	Chain	Res	Type
2	G	3	ILE
2	G	7	ARG
2	G	21	ASN
2	G	25	ASN
2	G	32	LEU
2	G	44	VAL
2	G	51	ARG
2	G	53	VAL
2	G	56	VAL
2	G	57	LEU
2	G	66	ASP
2	G	68	ILE
2	G	76	VAL
2	G	81	SER
2	G	108	MET
2	G	120	ILE
2	H	1[A]	MET
2	H	1[B]	MET
2	H	3	ILE
2	H	7	ARG
2	H	21	ASN
2	H	27	GLN
2	H	32	LEU
2	H	44	VAL
2	H	51	ARG
2	H	53	VAL
2	H	56	VAL
2	H	57	LEU
2	H	76	VAL
2	H	81	SER
2	H	106	LYS
2	H	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	263	GLN
1	A	392	HIS
1	A	439	HIS
1	A	464	ASN
1	A	506	GLN

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Mol	Chain	Res	Type
1	A	600	ASN
1	B	195	ASN
1	B	263	GLN
1	B	451	ASN
1	B	464	ASN
1	B	506	GLN
1	B	600	ASN
1	B	676	ASN
1	C	66	ASN
1	C	96	GLN
1	C	195	ASN
1	C	210	HIS
1	C	256	HIS
1	C	263	GLN
1	C	431	GLN
1	C	702	GLN
1	D	96	GLN
1	D	111	ASN
1	D	263	GLN
1	D	388	GLN
1	D	439	HIS
1	D	600	ASN
1	D	709	GLN
2	E	21	ASN
2	F	21	ASN
2	G	21	ASN
2	H	21	ASN
2	H	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 74 ligands modelled in this entry, 68 are monoatomic - leaving 6 for Mogul analysis.

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
6	ACO	F	201	-	51,53,53	1.85	10 (19%)	73,79,79	1.73	16 (21%)
6	ACO	H	201	-	51,53,53	1.85	9 (17%)	73,79,79	1.77	16 (21%)
6	ACO	E	201	-	51,53,53	1.85	10 (19%)	73,79,79	1.77	16 (21%)
5	SO4	D	812	-	4,4,4	0.25	0	6,6,6	0.09	0
5	SO4	A	812	-	4,4,4	0.25	0	6,6,6	0.08	0
6	ACO	G	201	-	51,53,53	1.84	9 (17%)	73,79,79	1.76	17 (23%)

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
6	ACO	H	201	-	-	12/51/67/67	0/3/3/3
6	ACO	F	201	-	-	12/51/67/67	0/3/3/3
6	ACO	E	201	-	-	12/51/67/67	0/3/3/3
6	ACO	G	201	-	-	10/51/67/67	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	201	ACO	C9P-N8P	6.42	1.48	1.33
6	G	201	ACO	C9P-N8P	6.42	1.48	1.33
6	F	201	ACO	C9P-N8P	6.41	1.48	1.33
6	E	201	ACO	C9P-N8P	6.34	1.48	1.33
6	F	201	ACO	C5P-N4P	5.24	1.45	1.33
6	H	201	ACO	C5P-N4P	5.23	1.45	1.33
6	E	201	ACO	C5P-N4P	5.22	1.45	1.33
6	G	201	ACO	C5P-N4P	5.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	ACO	C2B-C3B	-4.07	1.44	1.53
6	G	201	ACO	C2B-C3B	-3.97	1.44	1.53
6	E	201	ACO	C2B-C3B	-3.89	1.44	1.53
6	H	201	ACO	C2B-C3B	-3.75	1.44	1.53
6	E	201	ACO	O-C	3.50	1.38	1.21
6	F	201	ACO	O-C	3.47	1.38	1.21
6	G	201	ACO	O-C	3.46	1.38	1.21
6	H	201	ACO	O-C	3.45	1.38	1.21
6	H	201	ACO	P1A-O3A	2.84	1.62	1.59
6	F	201	ACO	P1A-O3A	2.81	1.62	1.59
6	E	201	ACO	P1A-O3A	2.79	1.62	1.59
6	E	201	ACO	C3B-C4B	-2.72	1.45	1.52
6	E	201	ACO	P2A-O3A	2.68	1.62	1.59
6	G	201	ACO	C3B-C4B	-2.68	1.46	1.52
6	H	201	ACO	P2A-O3A	2.65	1.62	1.59
6	F	201	ACO	C3B-C4B	-2.64	1.46	1.52
6	H	201	ACO	C3B-C4B	-2.64	1.46	1.52
6	G	201	ACO	P1A-O3A	2.60	1.62	1.59
6	E	201	ACO	OAP-CAP	-2.58	1.37	1.42
6	F	201	ACO	OAP-CAP	-2.58	1.37	1.42
6	G	201	ACO	OAP-CAP	-2.50	1.37	1.42
6	G	201	ACO	C6A-N6A	2.50	1.40	1.34
6	H	201	ACO	C6A-N6A	2.50	1.40	1.34
6	H	201	ACO	OAP-CAP	-2.49	1.37	1.42
6	E	201	ACO	C6A-N6A	2.48	1.40	1.34
6	F	201	ACO	C6A-N6A	2.47	1.40	1.34
6	G	201	ACO	P2A-O3A	2.32	1.62	1.59
6	F	201	ACO	P2A-O3A	2.30	1.62	1.59
6	E	201	ACO	C5A-N7A	-2.01	1.35	1.39
6	F	201	ACO	C5A-N7A	-2.00	1.35	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	201	ACO	C5A-C4A-N3A	-5.22	119.53	126.72
6	H	201	ACO	C5A-C4A-N3A	-5.16	119.61	126.72
6	G	201	ACO	C5A-C4A-N3A	-5.13	119.66	126.72
6	F	201	ACO	C5A-C4A-N3A	-5.12	119.67	126.72
6	F	201	ACO	N3A-C2A-N1A	-4.41	121.91	128.58
6	G	201	ACO	N3A-C2A-N1A	-4.39	121.94	128.58
6	H	201	ACO	O6A-CCP-CBP	4.36	117.55	110.55
6	E	201	ACO	N3A-C2A-N1A	-4.31	122.06	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	201	ACO	N3A-C2A-N1A	-4.30	122.07	128.58
6	G	201	ACO	O6A-CCP-CBP	4.25	117.38	110.55
6	F	201	ACO	O6A-CCP-CBP	4.20	117.31	110.55
6	E	201	ACO	O6A-CCP-CBP	4.09	117.13	110.55
6	E	201	ACO	N3A-C4A-N9A	3.87	133.75	127.17
6	H	201	ACO	N3A-C4A-N9A	3.86	133.74	127.17
6	G	201	ACO	N3A-C4A-N9A	3.83	133.68	127.17
6	F	201	ACO	N3A-C4A-N9A	3.80	133.63	127.17
6	H	201	ACO	O-C-S1P	-3.75	107.50	122.65
6	G	201	ACO	O-C-S1P	-3.69	107.73	122.65
6	F	201	ACO	O-C-S1P	-3.57	108.22	122.65
6	E	201	ACO	O-C-S1P	-3.56	108.26	122.65
6	G	201	ACO	C7P-C6P-C5P	3.53	118.27	112.39
6	F	201	ACO	C2A-N3A-C4A	3.51	120.40	111.83
6	E	201	ACO	C2A-N3A-C4A	3.49	120.35	111.83
6	G	201	ACO	C2A-N3A-C4A	3.48	120.34	111.83
6	H	201	ACO	C2A-N3A-C4A	3.46	120.28	111.83
6	E	201	ACO	C7P-C6P-C5P	3.40	118.06	112.39
6	H	201	ACO	C3B-C2B-C1B	3.32	107.19	99.89
6	E	201	ACO	C3B-C2B-C1B	3.29	107.13	99.89
6	F	201	ACO	N9A-C8A-N7A	-3.29	109.27	113.94
6	E	201	ACO	O-C-CH3	-3.27	110.48	123.12
6	G	201	ACO	O-C-CH3	-3.24	110.56	123.12
6	G	201	ACO	N9A-C8A-N7A	-3.19	109.41	113.94
6	H	201	ACO	N9A-C8A-N7A	-3.18	109.42	113.94
6	F	201	ACO	O-C-CH3	-3.18	110.81	123.12
6	H	201	ACO	O-C-CH3	-3.18	110.83	123.12
6	E	201	ACO	N9A-C8A-N7A	-3.14	109.48	113.94
6	F	201	ACO	C7P-C6P-C5P	2.92	117.26	112.39
6	H	201	ACO	C7P-C6P-C5P	2.91	117.24	112.39
6	F	201	ACO	C5A-N7A-C8A	2.86	107.94	103.45
6	G	201	ACO	C5A-N7A-C8A	2.81	107.86	103.45
6	F	201	ACO	C2P-C3P-N4P	2.81	118.27	112.41
6	E	201	ACO	C5A-N7A-C8A	2.80	107.85	103.45
6	H	201	ACO	C5A-N7A-C8A	2.78	107.82	103.45
6	G	201	ACO	O5B-C5B-C4B	2.73	118.30	108.99
6	E	201	ACO	C2P-C3P-N4P	2.73	118.12	112.41
6	H	201	ACO	C2P-C3P-N4P	2.68	118.01	112.41
6	F	201	ACO	C4A-N9A-C8A	2.64	108.51	105.74
6	F	201	ACO	C4A-C5A-N7A	-2.62	107.58	110.58
6	G	201	ACO	C2P-C3P-N4P	2.60	117.85	112.41
6	F	201	ACO	O5B-C5B-C4B	2.60	117.83	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	201	ACO	C4A-N9A-C8A	2.59	108.45	105.74
6	E	201	ACO	C4A-C5A-N7A	-2.58	107.63	110.58
6	G	201	ACO	C4A-C5A-N7A	-2.58	107.63	110.58
6	G	201	ACO	C3B-C2B-C1B	2.58	105.56	99.89
6	H	201	ACO	C4A-C5A-N7A	-2.57	107.64	110.58
6	G	201	ACO	C4A-N9A-C8A	2.57	108.44	105.74
6	E	201	ACO	O5B-C5B-C4B	2.51	117.54	108.99
6	E	201	ACO	C4A-N9A-C8A	2.46	108.32	105.74
6	H	201	ACO	O5B-C5B-C4B	2.30	116.81	108.99
6	H	201	ACO	C6P-C5P-N4P	2.18	120.32	116.34
6	E	201	ACO	C6P-C5P-N4P	2.18	120.31	116.34
6	F	201	ACO	C6P-C7P-N8P	2.13	116.54	112.00
6	F	201	ACO	C6P-C5P-N4P	2.10	120.17	116.34
6	G	201	ACO	C6P-C7P-N8P	2.06	116.39	112.00
6	G	201	ACO	C6P-C5P-N4P	2.04	120.07	116.34

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	201	ACO	C5B-O5B-P1A-O1A
6	E	201	ACO	C5P-C6P-C7P-N8P
6	E	201	ACO	O-C-S1P-C2P
6	F	201	ACO	O4B-C4B-C5B-O5B
6	F	201	ACO	C5B-O5B-P1A-O1A
6	F	201	ACO	CDP-CBP-CCP-O6A
6	F	201	ACO	CEP-CBP-CCP-O6A
6	F	201	ACO	CAP-CBP-CCP-O6A
6	F	201	ACO	C5P-C6P-C7P-N8P
6	F	201	ACO	CH3-C-S1P-C2P
6	G	201	ACO	C5P-C6P-C7P-N8P
6	G	201	ACO	O-C-S1P-C2P
6	H	201	ACO	C5B-O5B-P1A-O1A
6	H	201	ACO	C5B-O5B-P1A-O3A
6	H	201	ACO	C5P-C6P-C7P-N8P
6	H	201	ACO	O-C-S1P-C2P
6	H	201	ACO	CH3-C-S1P-C2P
6	H	201	ACO	C3B-C4B-C5B-O5B
6	F	201	ACO	C3B-C4B-C5B-O5B
6	H	201	ACO	O4B-C4B-C5B-O5B
6	E	201	ACO	S1P-C2P-C3P-N4P
6	G	201	ACO	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
6	E	201	ACO	C3B-C4B-C5B-O5B
6	E	201	ACO	O4B-C4B-C5B-O5B
6	G	201	ACO	C3B-C4B-C5B-O5B
6	F	201	ACO	S1P-C2P-C3P-N4P
6	G	201	ACO	O4B-C4B-C5B-O5B
6	G	201	ACO	CDP-CBP-CCP-O6A
6	G	201	ACO	CEP-CBP-CCP-O6A
6	H	201	ACO	CDP-CBP-CCP-O6A
6	H	201	ACO	CEP-CBP-CCP-O6A
6	E	201	ACO	C3P-C2P-S1P-C
6	E	201	ACO	C5B-O5B-P1A-O2A
6	E	201	ACO	C5B-O5B-P1A-O3A
6	F	201	ACO	C5B-O5B-P1A-O3A
6	G	201	ACO	C5B-O5B-P1A-O2A
6	H	201	ACO	C5B-O5B-P1A-O2A
6	H	201	ACO	S1P-C2P-C3P-N4P
6	F	201	ACO	C3B-O3B-P3B-O7A
6	E	201	ACO	P1A-O3A-P2A-O4A
6	G	201	ACO	P1A-O3A-P2A-O5A
6	E	201	ACO	C3B-O3B-P3B-O8A
6	F	201	ACO	C3B-O3B-P3B-O9A
6	G	201	ACO	N8P-C9P-CAP-OAP
6	E	201	ACO	P1A-O3A-P2A-O5A
6	H	201	ACO	P1A-O3A-P2A-O5A

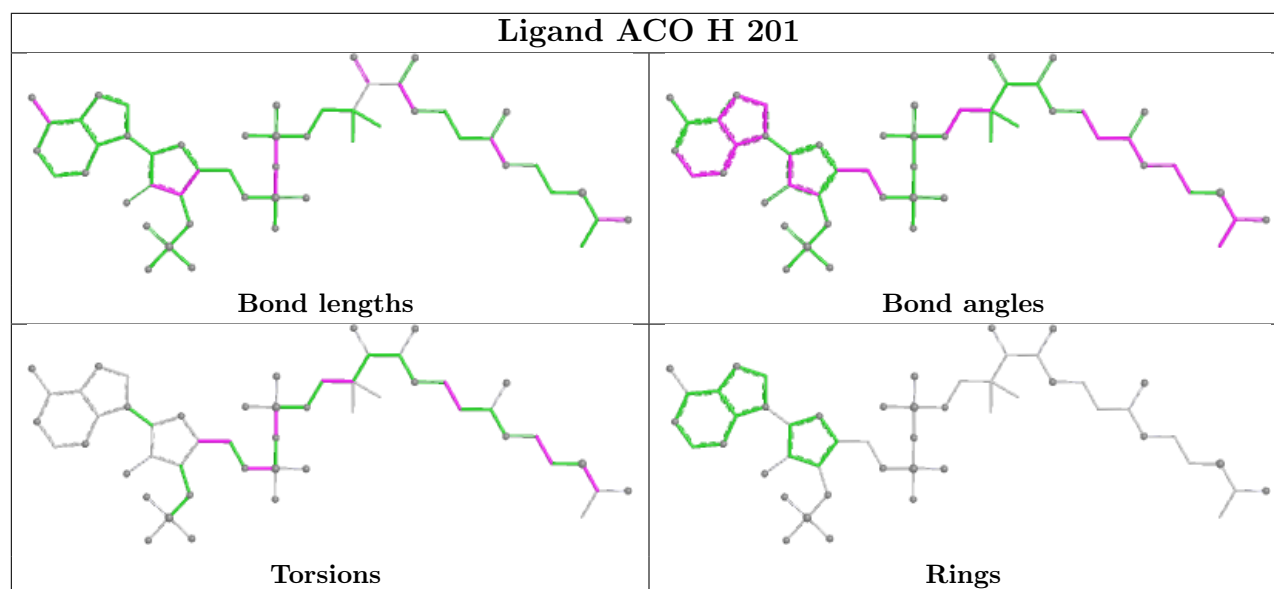
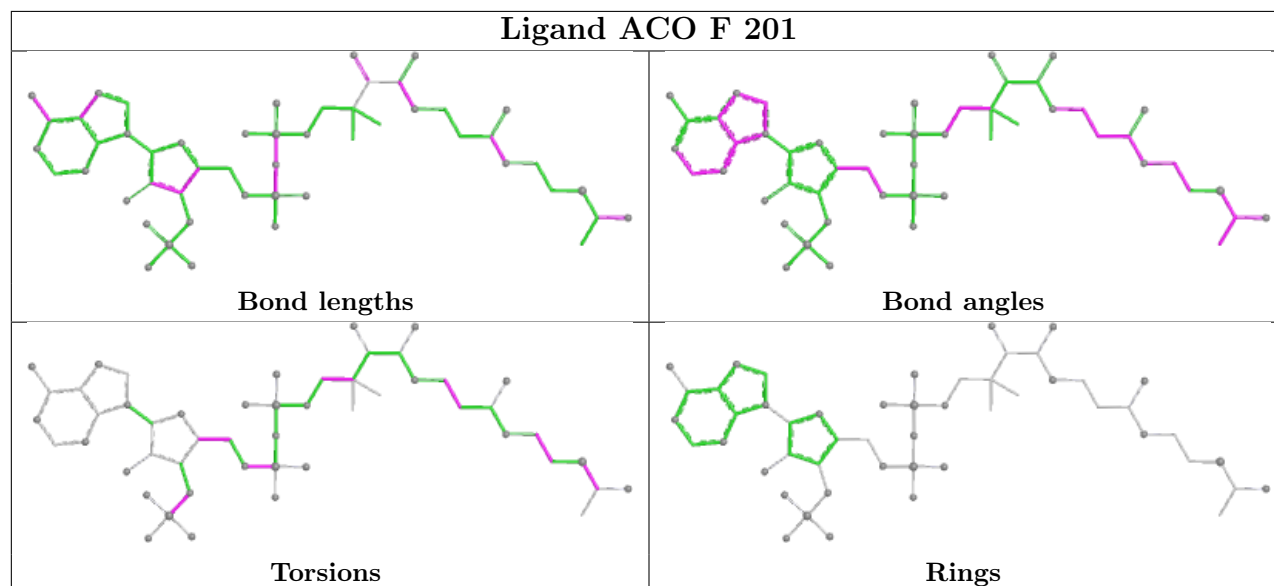
There are no ring outliers.

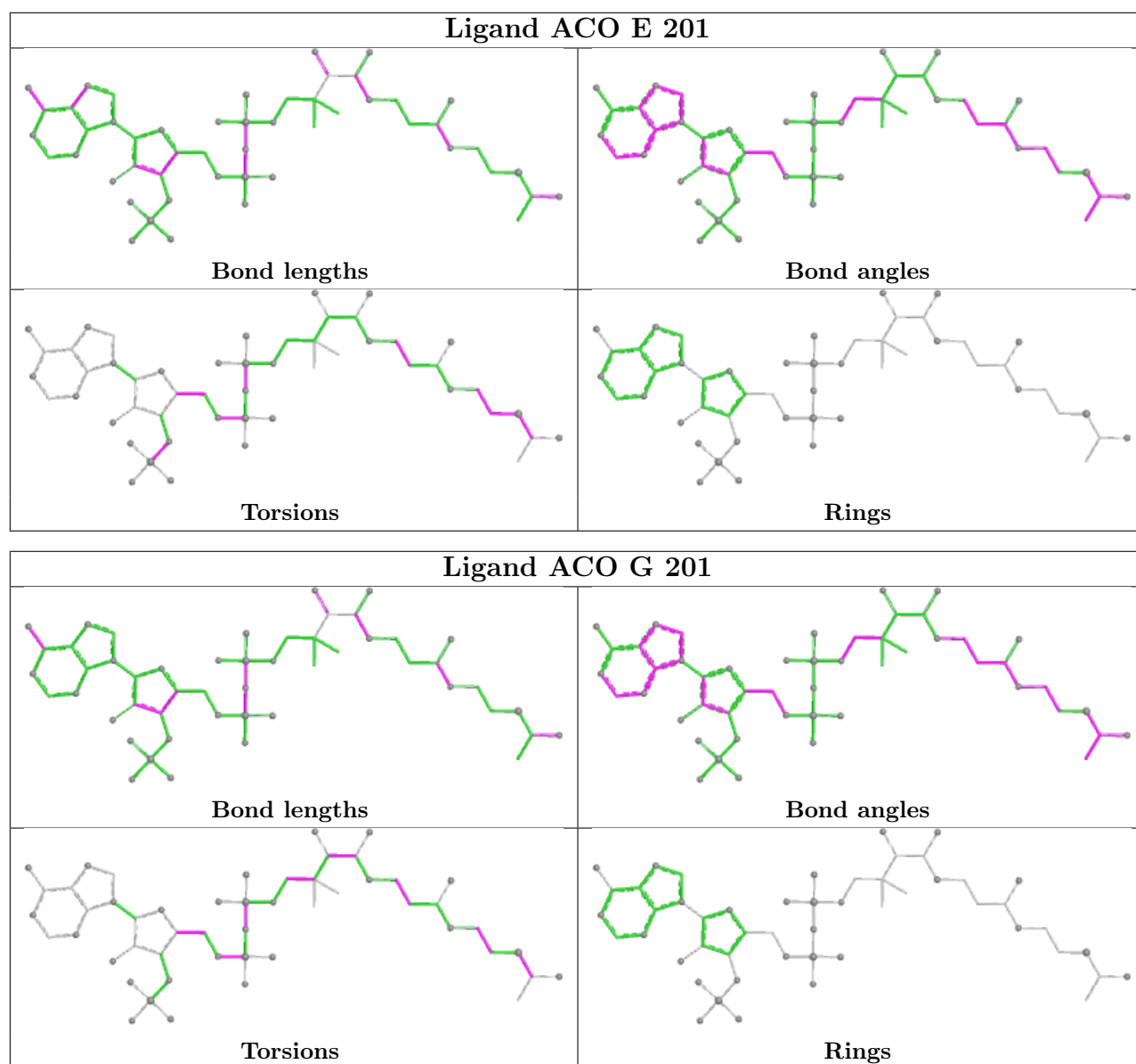
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	201	ACO	1	0
6	H	201	ACO	1	1
6	G	201	ACO	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 than 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 [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	718/731 (98%)	-0.18	11 (1%)	72 52	35, 68, 149, 217	1 (0%)
1	B	722/731 (98%)	-0.07	6 (0%)	82 66	36, 90, 170, 249	1 (0%)
1	C	717/731 (98%)	-0.10	8 (1%)	78 60	27, 84, 160, 213	1 (0%)
1	D	717/731 (98%)	-0.15	9 (1%)	75 55	26, 73, 158, 203	1 (0%)
2	E	153/156 (98%)	-0.37	1 (0%)	84 69	32, 57, 101, 149	1 (0%)
2	F	153/156 (98%)	-0.09	1 (0%)	84 69	36, 79, 146, 169	1 (0%)
2	G	153/156 (98%)	-0.02	1 (0%)	84 69	35, 84, 156, 185	1 (0%)
2	H	153/156 (98%)	-0.25	1 (0%)	84 69	36, 59, 135, 172	1 (0%)
All	All	3486/3548 (98%)	-0.14	38 (1%)	78 60	26, 76, 159, 249	8 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1[A]	MET	6.9
1	D	730	ALA	5.7
2	H	1[A]	MET	5.3
2	G	1[A]	MET	4.4
1	D	647	PRO	3.6
1	B	647	PRO	3.4
1	A	731	ALA	3.3
2	E	1[A]	MET	3.2
1	A	647	PRO	3.2
1	A	730	ALA	3.2
1	C	647	PRO	3.1
1	D	729	ASN	3.1
1	D	648	LEU	2.9
1	C	729	ASN	2.9
1	D	373	ILE	2.9
1	C	539[A]	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	730	ALA	2.7
1	D	480	VAL	2.7
1	A	373	ILE	2.7
1	A	648	LEU	2.6
1	B	272	SER	2.5
1	D	374	GLU	2.5
1	A	729	ASN	2.5
1	D	377	THR	2.4
1	D	275	VAL	2.4
1	B	355	ALA	2.3
1	B	709	GLN	2.3
1	A	374	GLU	2.2
1	B	648	LEU	2.2
1	C	648	LEU	2.2
1	A	292	TYR	2.2
1	A	327	ILE	2.2
1	A	480	VAL	2.1
1	B	328	PRO	2.1
1	A	376	PRO	2.1
1	C	480	VAL	2.0
1	C	56	SER	2.0
1	C	273	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
4	CL	E	206	1/1	0.49	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	C	813	1/1	0.60	0.13	86,86,86,86	0
4	CL	A	805	1/1	0.67	0.10	122,122,122,122	0
4	CL	D	811	1/1	0.76	0.07	78,78,78,78	0
4	CL	B	804	1/1	0.76	0.10	92,92,92,92	0
4	CL	E	207	1/1	0.77	0.21	100,100,100,100	0
4	CL	D	808	1/1	0.78	0.17	97,97,97,97	0
4	CL	A	808	1/1	0.78	0.11	85,85,85,85	0
4	CL	B	809	1/1	0.79	0.15	78,78,78,78	0
4	CL	H	203	1/1	0.79	0.18	121,121,121,121	0
4	CL	E	210	1/1	0.80	0.10	73,73,73,73	0
4	CL	C	805	1/1	0.80	0.10	62,62,62,62	0
6	ACO	F	201	51/51	0.81	0.13	89,154,252,337	0
4	CL	C	809	1/1	0.82	0.19	89,89,89,89	0
6	ACO	H	201	51/51	0.82	0.14	77,128,209,268	0
6	ACO	G	201	51/51	0.83	0.14	117,151,232,233	0
4	CL	C	802	1/1	0.83	0.12	77,77,77,77	0
4	CL	A	807	1/1	0.84	0.10	104,104,104,104	0
4	CL	C	812	1/1	0.84	0.10	78,78,78,78	0
4	CL	F	203	1/1	0.85	0.31	80,80,80,80	0
4	CL	B	802	1/1	0.85	0.11	87,87,87,87	0
4	CL	B	803	1/1	0.85	0.10	83,83,83,83	0
4	CL	B	814	1/1	0.85	0.08	76,76,76,76	0
4	CL	D	810	1/1	0.85	0.17	61,61,61,61	0
4	CL	B	812	1/1	0.86	0.14	103,103,103,103	0
4	CL	E	205	1/1	0.86	0.09	76,76,76,76	0
4	CL	B	808	1/1	0.87	0.15	59,59,59,59	0
4	CL	D	803	1/1	0.87	0.19	94,94,94,94	0
4	CL	E	209	1/1	0.87	0.08	91,91,91,91	0
4	CL	B	806	1/1	0.88	0.11	91,91,91,91	0
4	CL	C	810	1/1	0.88	0.21	83,83,83,83	0
3	NA	E	203	1/1	0.89	0.17	39,39,39,39	0
4	CL	C	815	1/1	0.89	0.08	133,133,133,133	0
4	CL	C	803	1/1	0.89	0.25	111,111,111,111	0
4	CL	G	203	1/1	0.89	0.23	77,77,77,77	0
4	CL	C	801	1/1	0.90	0.24	117,117,117,117	0
3	NA	A	801	1/1	0.90	0.22	38,38,38,38	0
4	CL	A	811	1/1	0.90	0.06	74,74,74,74	0
4	CL	B	810	1/1	0.90	0.25	98,98,98,98	0
4	CL	D	809	1/1	0.90	0.14	88,88,88,88	0
4	CL	C	806	1/1	0.90	0.07	77,77,77,77	0
4	CL	B	805	1/1	0.90	0.10	73,73,73,73	0
4	CL	B	813	1/1	0.90	0.06	80,80,80,80	0

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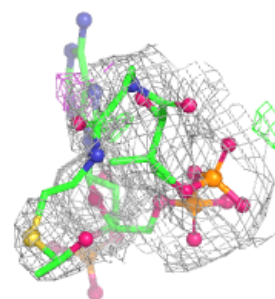
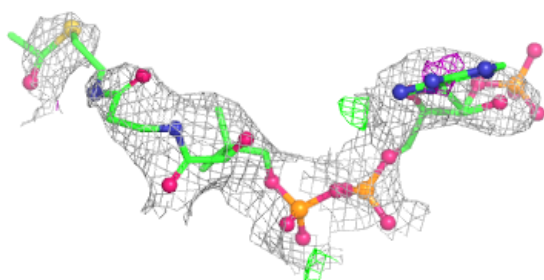
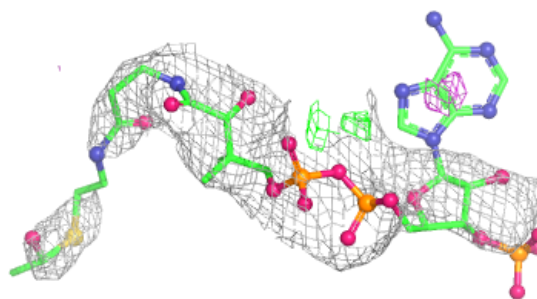
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	802	1/1	0.90	0.14	108,108,108,108	0
3	NA	G	202	1/1	0.91	0.10	65,65,65,65	0
4	CL	E	208	1/1	0.91	0.11	65,65,65,65	0
5	SO4	D	812	5/5	0.91	0.11	66,66,68,69	0
6	ACO	E	201	51/51	0.91	0.12	30,100,183,184	0
4	CL	A	810	1/1	0.91	0.18	72,72,72,72	0
4	CL	B	807	1/1	0.91	0.16	64,64,64,64	0
4	CL	B	811	1/1	0.91	0.17	81,81,81,81	0
5	SO4	A	812	5/5	0.92	0.10	61,62,63,65	0
4	CL	C	808	1/1	0.92	0.15	57,57,57,57	0
4	CL	G	204	1/1	0.93	0.15	72,72,72,72	0
4	CL	C	811	1/1	0.93	0.09	43,43,43,43	0
4	CL	D	805	1/1	0.93	0.17	87,87,87,87	0
4	CL	D	806	1/1	0.93	0.12	99,99,99,99	0
3	NA	D	801	1/1	0.94	0.07	60,60,60,60	0
4	CL	A	809	1/1	0.94	0.10	55,55,55,55	0
4	CL	C	807	1/1	0.94	0.09	61,61,61,61	0
4	CL	H	204	1/1	0.95	0.11	59,59,59,59	0
3	NA	E	202	1/1	0.95	0.15	72,72,72,72	0
4	CL	D	804	1/1	0.95	0.06	100,100,100,100	0
4	CL	C	804	1/1	0.95	0.12	82,82,82,82	0
4	CL	A	804	1/1	0.95	0.13	62,62,62,62	0
4	CL	C	814	1/1	0.95	0.09	77,77,77,77	0
4	CL	B	801	1/1	0.95	0.15	65,65,65,65	0
4	CL	A	803	1/1	0.96	0.06	59,59,59,59	0
4	CL	D	802	1/1	0.96	0.10	70,70,70,70	0
4	CL	D	807	1/1	0.96	0.04	47,47,47,47	0
4	CL	H	202	1/1	0.97	0.11	44,44,44,44	0
4	CL	E	204	1/1	0.97	0.12	47,47,47,47	0
4	CL	A	806	1/1	0.97	0.05	77,77,77,77	0
4	CL	F	202	1/1	0.98	0.10	43,43,43,43	0

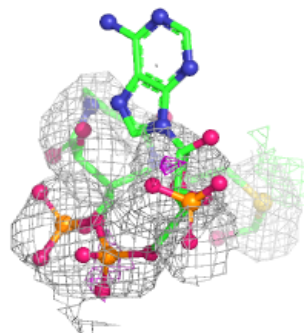
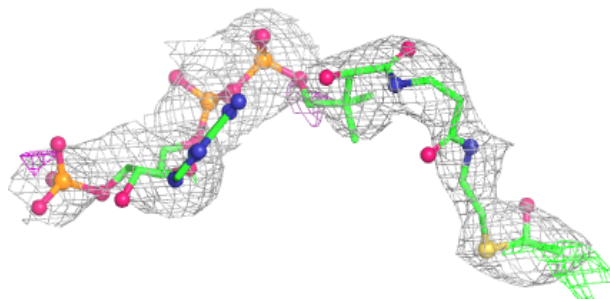
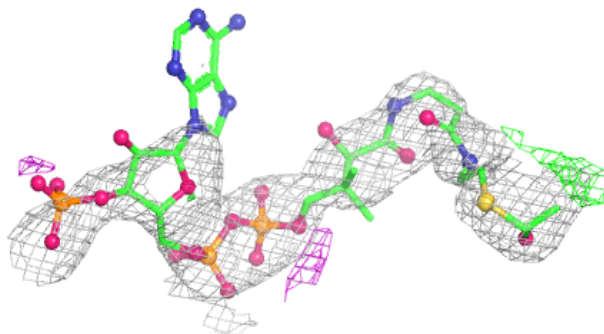
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO F 201:

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

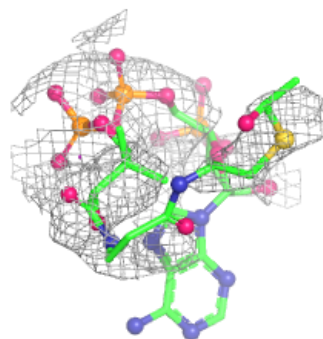
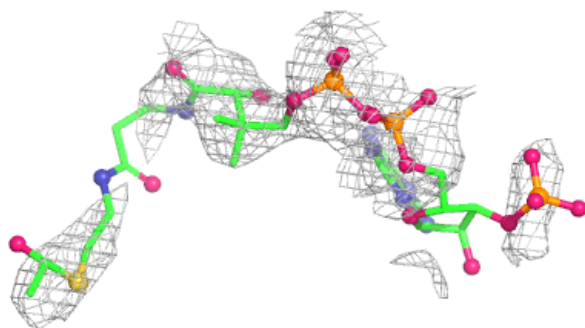
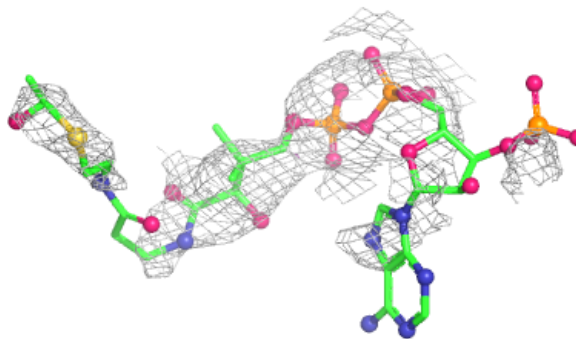
**Electron density around ACO H 201:**

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

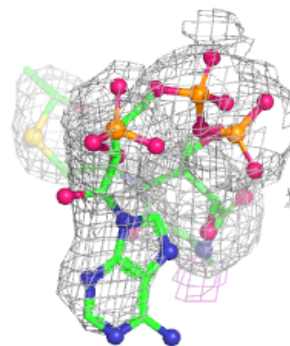
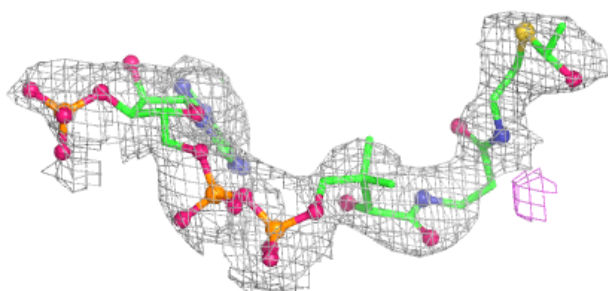
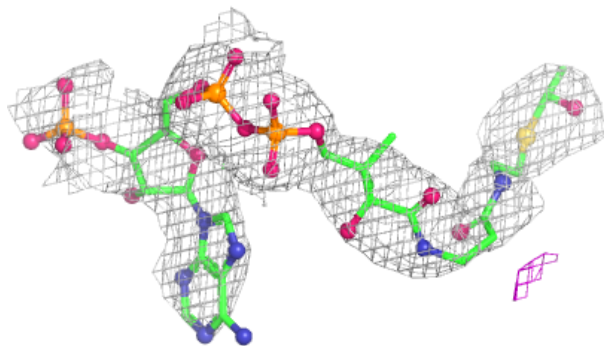


Electron density around ACO G 201:

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

**Electron density around ACO E 201:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.