



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 09:05 PM EST

PDB ID : 4KVO  
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](mailto: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>.

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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 : 2.36  
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) : 2.36

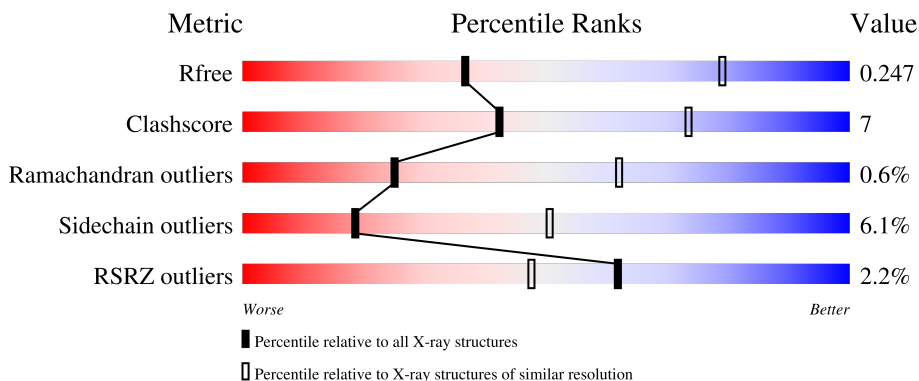
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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  $\geq 3$ , 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	 2% 77% 19% ..
1	B	731	 2% 82% 15% ..
1	C	731	 3% 79% 16% ..
1	D	731	 2% 79% 17% ..
2	E	156	 % 83% 12% ...

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Mol	Chain	Length	Quality of chain
2	F	156	 3% 78% 18% . .
2	G	156	 2% 79% 15% . .
2	H	156	 2% 79% 16% . .

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	B	810	-	-	-	X
4	CL	C	803	-	-	-	X
4	CL	C	809	-	-	-	X
4	CL	D	803	-	-	X	-
4	CL	E	207	-	-	-	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
			Total	C	N	O	S			
1	A	718	Total 5764	C 3679	N 968	O 1099	S 18	0	1	0
1	B	722	Total 5777	C 3686	N 971	O 1102	S 18	0	1	0
1	C	717	Total 5753	C 3671	N 968	O 1096	S 18	0	1	0
1	D	717	Total 5761	C 3678	N 969	O 1096	S 18	0	1	0

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
			Total	C	N	O	S			
2	E	153	Total 1247	C 790	N 221	O 225	S 11	0	1	0
2	F	153	Total 1247	C 790	N 221	O 225	S 11	0	1	0
2	G	153	Total 1247	C 790	N 221	O 225	S 11	0	1	0
2	H	153	Total 1247	C 790	N 221	O 225	S 11	0	1	0

- Molecule 3 is SODIUM ION (three-letter code: 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 (three-letter code: CL) (formula: Cl).

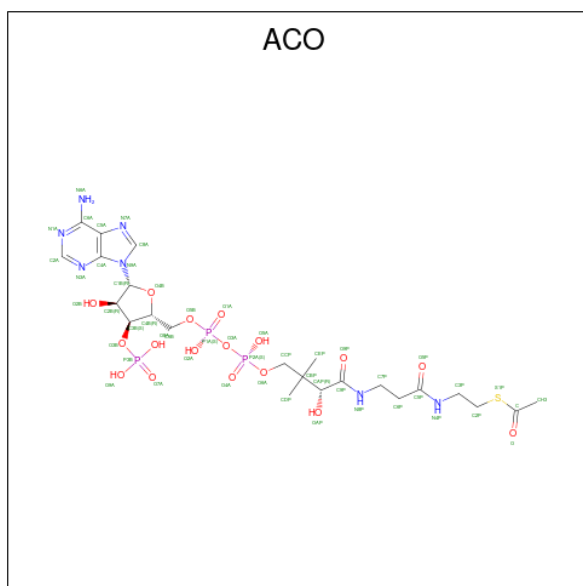
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	Cl 10	0	0
4	B	14	Total 14	Cl 14	0	0
4	C	15	Total 15	Cl 15	0	0
4	D	10	Total 10	Cl 10	0	0
4	E	7	Total 7	Cl 7	0	0
4	F	2	Total 2	Cl 2	0	0
4	G	2	Total 2	Cl 2	0	0
4	H	3	Total 3	Cl 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



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

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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		

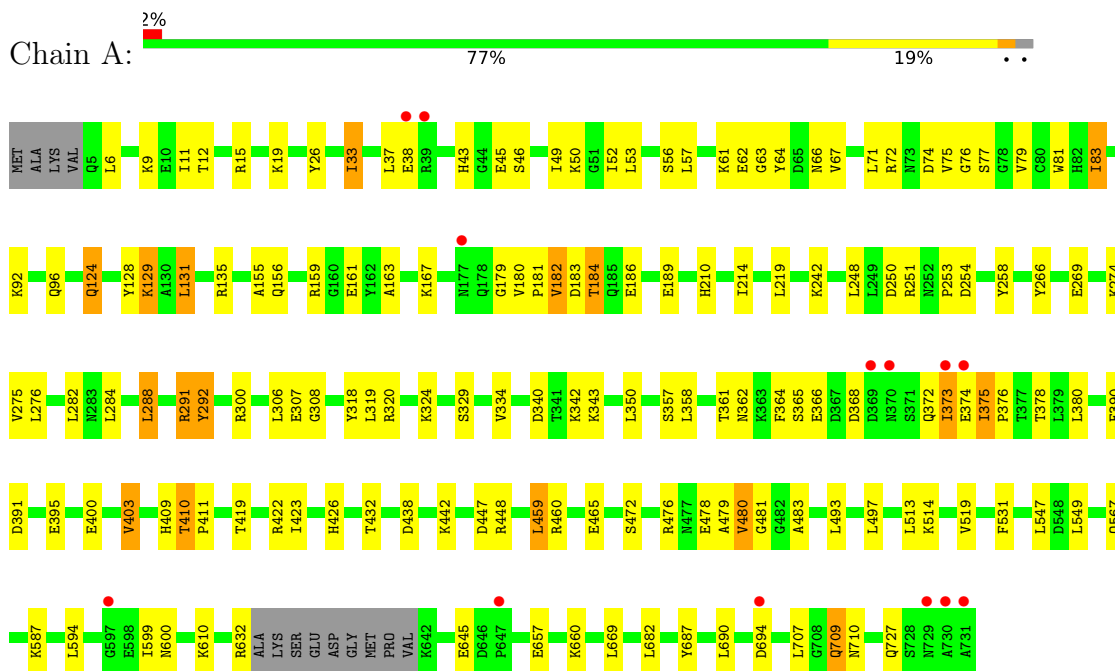
- Molecule 7 is water.

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		

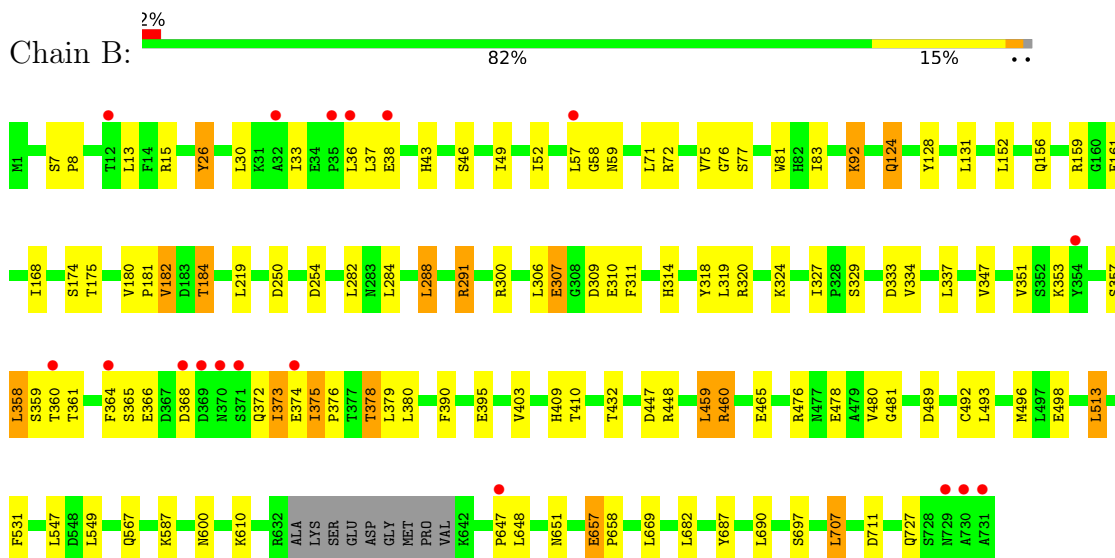
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

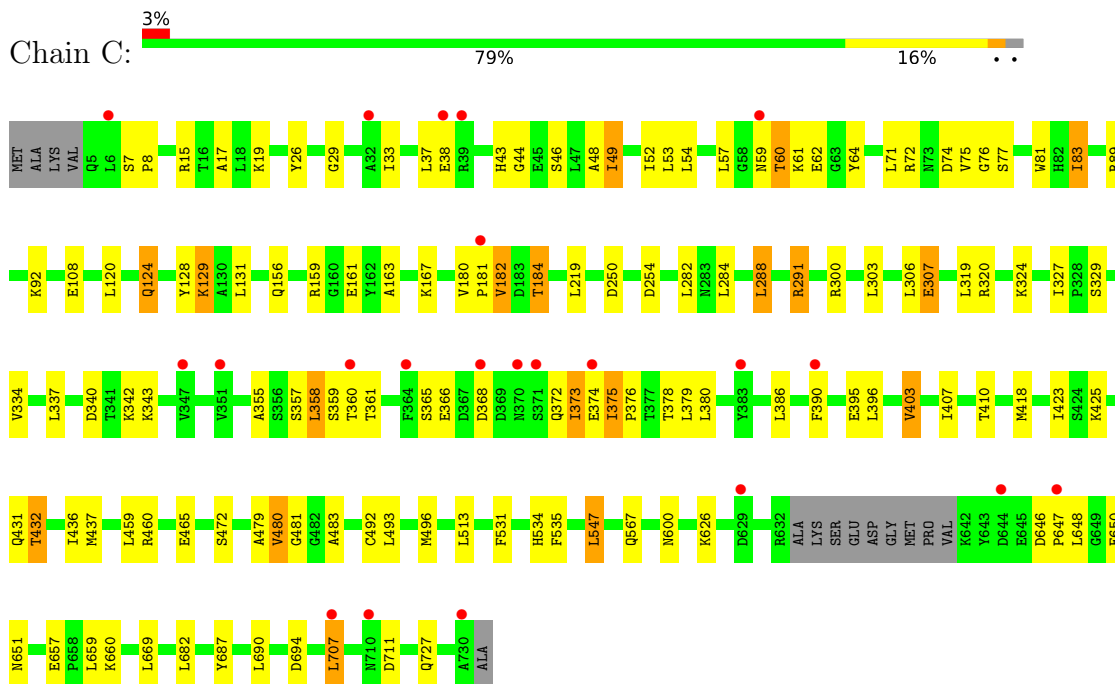


- Molecule 1: N-terminal acetyltransferase A complex subunit nat1

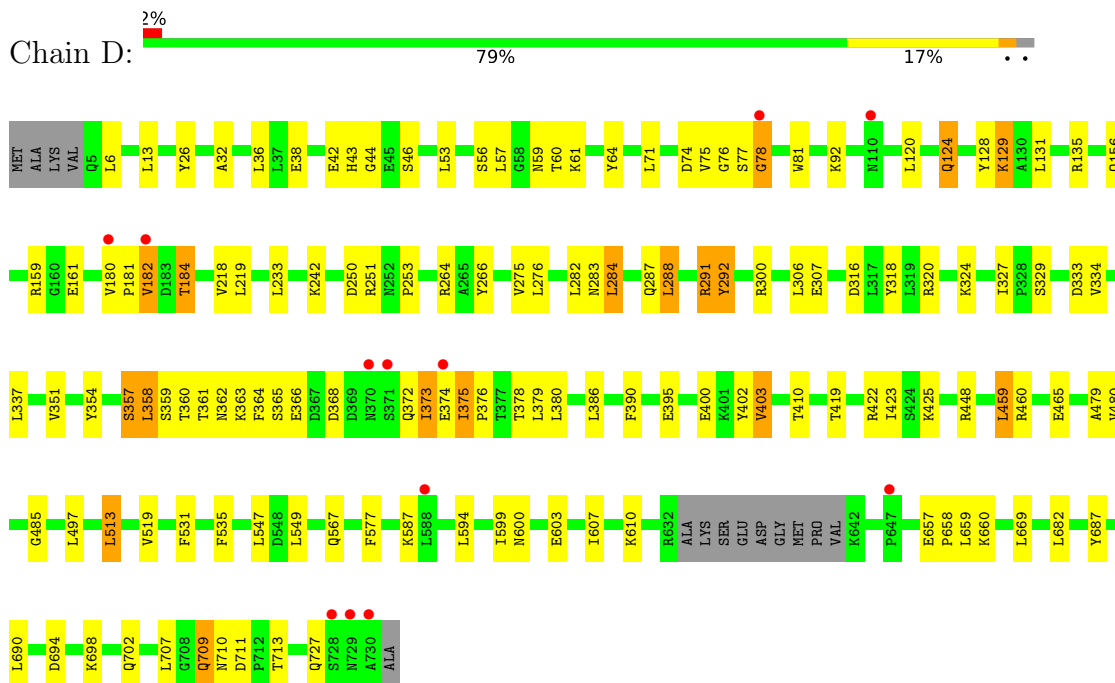




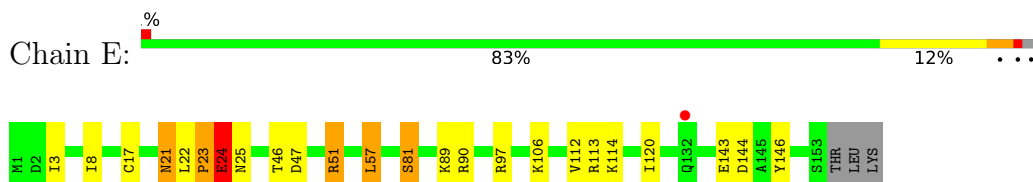
- Molecule 1: N-terminal acetyltransferase A complex subunit nat1



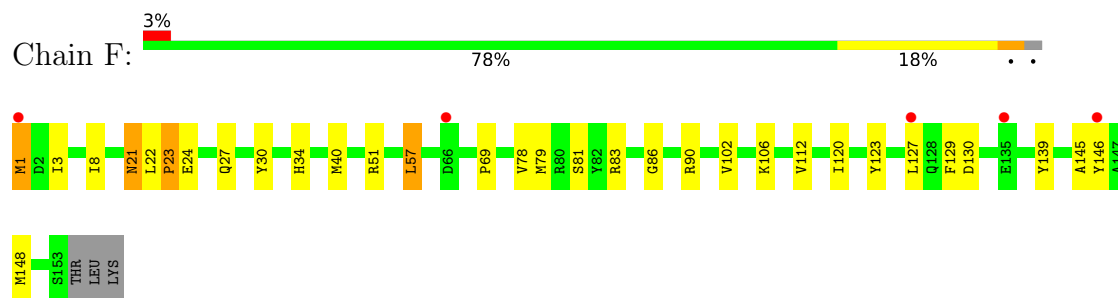
- Molecule 1: N-terminal acetyltransferase A complex subunit nat1



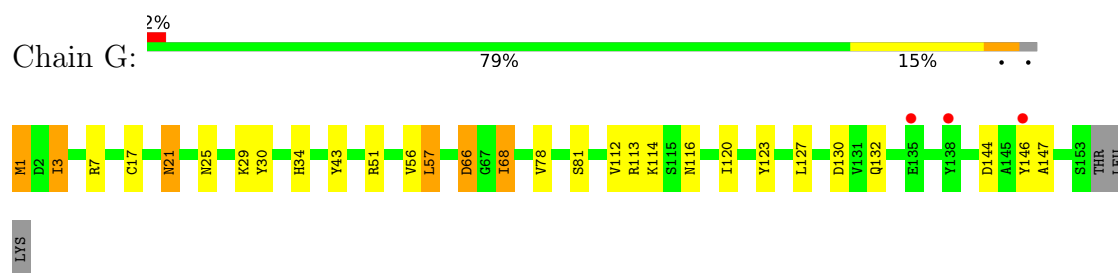
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



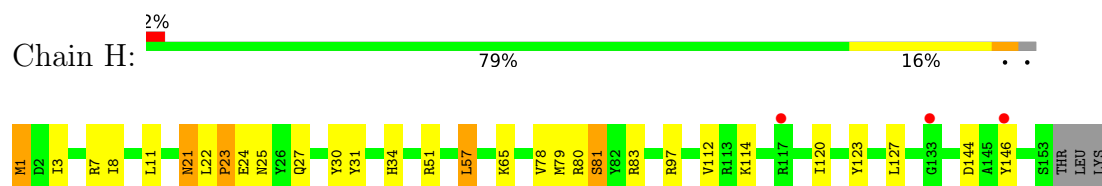
- Molecule 2: N-terminal acetyltransferase A complex catalytic subunit ard1



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 91.9 (49.05-3.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.217 , 0.246 0.217 , 0.247	Depositor DCC
$R_{free}$ test set	3802 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.5	Xtrriage
Anisotropy	0.603	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NA, CL, ACO

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	0.23	0/5878	0.41	0/7929
1	B	0.22	0/5891	0.41	0/7948
1	C	0.22	0/5867	0.41	0/7915
1	D	0.23	0/5876	0.42	0/7927
2	E	0.24	0/1277	0.52	4/1722 (0.2%)
2	F	0.22	0/1277	0.41	0/1722
2	G	0.22	0/1277	0.40	0/1722
2	H	0.25	0/1277	0.50	3/1722 (0.2%)
All	All	0.23	0/28620	0.42	7/38607 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	23	PRO	CA-C-N	6.96	132.52	117.20
2	E	23	PRO	C-N-CA	6.10	136.95	121.70
2	H	23	PRO	CA-C-N	6.10	130.62	117.20
2	H	23	PRO	N-CA-C	5.79	127.16	112.10
2	E	23	PRO	N-CA-C	5.69	126.90	112.10
2	E	23	PRO	CA-C-O	-5.49	107.03	120.20
2	H	23	PRO	C-N-CA	5.30	134.95	121.70

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	96	0
1	B	5777	0	5697	66	0
1	C	5753	0	5675	76	0
1	D	5761	0	5686	87	1
2	E	1247	0	1233	25	0
2	F	1247	0	1233	20	0
2	G	1247	0	1233	15	0
2	H	1247	0	1233	25	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	387	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 (387) 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
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	0.69
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:C:300:ARG:HG2	2:G:1[A]:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:D:129:LYS:H	1:D:129:LYS:HZ2	1.49	0.58
1:D:329:SER:OG	2:H:81:SER:O	2.17	0.57
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:D:129:LYS:HZ2	1:D:129:LYS:N	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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: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:B:181:PRO:HA	1:B:182:VAL:HG22	1.92	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: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: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:B:309:ASP:C	1:B:311:PHE:H	2.16	0.49
1:D:129:LYS:HZ3	1:D:129:LYS:HB2	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:365:SER:OG	1:D:366:GLU:N	2.48	0.46
2:G:123:TYR:HA	2:G:127:LEU:HB2	1.97	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: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
1:A:179:GLY:HA3	1:A:180:VAL:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:HD3	1:C:64:TYR:HB2	1.96	0.45
1:D:300:ARG:HG2	2:H:1[A]:MET:HE1	1.97	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:D:43:HIS:HD1	1:D: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:B:300:ARG:HG2	2:F:1[A]:MET:HE1	1.98	0.44
2:F:129:PHE:HB3	2:F:148:MET:HE2	1.99	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:242:LYS:HE3	1:D:266:TYR:CZ	2.53	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:D:587:LYS:HZ1	1:D:610:LYS:NZ	2.15	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: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
1:B:92:LYS:NZ	4:B:802:CL:CL	2.82	0.43
1:C:288:LEU:O	1:C:291:ARG:HB3	2.18	0.43
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:660:LYS:HB2	1:D:660:LYS:HE2	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:418:MET:HG2	1:C:437:MET:HE1	2.02	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
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
1:A:63:GLY:O	1:A:67:VAL:HG23	2.20	0.41
1:A:74:ASP:CG	1:A:77:SER:HB3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.94	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
1:D:711:ASP:OD2	1:D:713:THR:OG1	2.30	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:129[A]:LYS:H	1:A:129[A]:LYS:HZ3	1.68	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:C:124:GLN:HG2	1:C:534:HIS:HE2	1.85	0.41
1:C:396:LEU:HD22	1:C:423:ILE:HG23	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	19	55
1	B	719/731 (98%)	688 (96%)	26 (4%)	5 (1%)	22	59
1	C	714/731 (98%)	683 (96%)	26 (4%)	5 (1%)	22	59
1	D	714/731 (98%)	684 (96%)	25 (4%)	5 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	151/156 (97%)	148 (98%)	2 (1%)	1 (1%)	22	59
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%)	25	62

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
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%)	571 (94%)	39 (6%)	17	49
1	B	610/638 (96%)	573 (94%)	37 (6%)	18	50
1	C	609/638 (96%)	572 (94%)	37 (6%)	18	50
1	D	610/638 (96%)	581 (95%)	29 (5%)	25	59
2	E	133/135 (98%)	124 (93%)	9 (7%)	16	46
2	F	133/135 (98%)	123 (92%)	10 (8%)	13	42
2	G	133/135 (98%)	120 (90%)	13 (10%)	8	28
2	H	133/135 (98%)	123 (92%)	10 (8%)	13	42
All	All	2971/3092 (96%)	2787 (94%)	184 (6%)	18	50

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	38	GLU
1	A	53	LEU
1	A	72	ARG
1	A	83	ILE
1	A	92	LYS
1	A	96	GLN
1	A	124	GLN
1	A	129[A]	LYS
1	A	129[B]	LYS
1	A	131	LEU
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	357	SER
1	A	361	THR
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	459	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	460	ARG
1	A	465	GLU
1	A	480	VAL
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	707	LEU
1	A	709	GLN
1	A	727	GLN
1	B	15	ARG
1	B	26	TYR
1	B	30	LEU
1	B	38	GLU
1	B	49	ILE
1	B	72	ARG
1	B	92	LYS
1	B	124	GLN
1	B	131	LEU
1	B	174	SER
1	B	184	THR
1	B	284	LEU
1	B	288	LEU
1	B	291	ARG
1	B	307	GLU
1	B	357	SER
1	B	358	LEU
1	B	361	THR
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	459	LEU
1	B	460	ARG
1	B	465	GLU
1	B	480	VAL
1	B	513	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	547	LEU
1	B	600	ASN
1	B	657	GLU
1	B	669	LEU
1	B	697	SER
1	B	707	LEU
1	B	727	GLN
1	C	38	GLU
1	C	49	ILE
1	C	60	THR
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	184	THR
1	C	284	LEU
1	C	288	LEU
1	C	291	ARG
1	C	307	GLU
1	C	357	SER
1	C	358	LEU
1	C	361	THR
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	459	LEU
1	C	460	ARG
1	C	465	GLU
1	C	480	VAL
1	C	513	LEU
1	C	547	LEU
1	C	600	ASN
1	C	657	GLU
1	C	660	LYS
1	C	669	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	707	LEU
1	C	727	GLN
1	D	38	GLU
1	D	92	LYS
1	D	124	GLN
1	D	129	LYS
1	D	131	LEU
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	357	SER
1	D	358	LEU
1	D	361	THR
1	D	375	ILE
1	D	378	THR
1	D	380	LEU
1	D	403	VAL
1	D	410	THR
1	D	459	LEU
1	D	460	ARG
1	D	465	GLU
1	D	513	LEU
1	D	547	LEU
1	D	600	ASN
1	D	669	LEU
1	D	707	LEU
1	D	709	GLN
1	D	727	GLN
2	E	3	ILE
2	E	21	ASN
2	E	24	GLU
2	E	25	ASN
2	E	51	ARG
2	E	57	LEU
2	E	81	SER
2	E	106	LYS
2	E	120	ILE
2	F	1[A]	MET
2	F	1[B]	MET

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Mol	Chain	Res	Type
2	F	3	ILE
2	F	21	ASN
2	F	23	PRO
2	F	51	ARG
2	F	57	LEU
2	F	81	SER
2	F	120	ILE
2	F	130	ASP
2	G	1[A]	MET
2	G	1[B]	MET
2	G	3	ILE
2	G	7	ARG
2	G	21	ASN
2	G	25	ASN
2	G	51	ARG
2	G	57	LEU
2	G	66	ASP
2	G	68	ILE
2	G	81	SER
2	G	120	ILE
2	G	130	ASP
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	51	ARG
2	H	57	LEU
2	H	81	SER
2	H	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	431	GLN
1	D	392	HIS
2	E	21	ASN
2	F	21	ASN
2	G	21	ASN
2	H	21	ASN
2	H	25	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
5	SO4	D	812	-	4,4,4	0.15	0	6,6,6	0.09	0
6	ACO	F	201	-	45,53,53	1.93	7 (15%)	56,79,79	1.55	11 (19%)
5	SO4	A	812	-	4,4,4	0.15	0	6,6,6	0.06	0
6	ACO	H	201	-	45,53,53	1.91	7 (15%)	56,79,79	1.58	11 (19%)
6	ACO	G	201	-	45,53,53	1.92	7 (15%)	56,79,79	1.57	11 (19%)
6	ACO	E	201	-	45,53,53	1.91	7 (15%)	56,79,79	1.57	10 (17%)

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	E	201	-	-	10/47/67/67	0/3/3/3
6	ACO	H	201	-	-	12/47/67/67	0/3/3/3
6	ACO	F	201	-	-	12/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ACO	G	201	-	-	13/47/67/67	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	201	ACO	C9P-N8P	6.90	1.48	1.33
6	G	201	ACO	C9P-N8P	6.90	1.48	1.33
6	F	201	ACO	C9P-N8P	6.88	1.48	1.33
6	E	201	ACO	C9P-N8P	6.81	1.48	1.33
6	F	201	ACO	C5P-N4P	5.47	1.45	1.33
6	H	201	ACO	C5P-N4P	5.45	1.45	1.33
6	E	201	ACO	C5P-N4P	5.45	1.45	1.33
6	G	201	ACO	C5P-N4P	5.42	1.45	1.33
6	F	201	ACO	C2B-C3B	-3.97	1.44	1.52
6	G	201	ACO	C2B-C3B	-3.87	1.44	1.52
6	E	201	ACO	C2B-C3B	-3.80	1.44	1.52
6	E	201	ACO	O-C	3.76	1.38	1.20
6	F	201	ACO	O-C	3.73	1.38	1.20
6	G	201	ACO	O-C	3.72	1.38	1.20
6	H	201	ACO	O-C	3.70	1.38	1.20
6	H	201	ACO	C2B-C3B	-3.66	1.44	1.52
6	F	201	ACO	C2B-C1B	-3.27	1.48	1.53
6	G	201	ACO	C2B-C1B	-2.95	1.49	1.53
6	H	201	ACO	C2B-C1B	-2.89	1.49	1.53
6	E	201	ACO	C2B-C1B	-2.88	1.49	1.53
6	E	201	ACO	C3B-C4B	-2.60	1.45	1.52
6	G	201	ACO	C3B-C4B	-2.57	1.46	1.52
6	F	201	ACO	C3B-C4B	-2.53	1.46	1.52
6	H	201	ACO	C3B-C4B	-2.53	1.46	1.52
6	E	201	ACO	OAP-CAP	-2.48	1.37	1.42
6	F	201	ACO	OAP-CAP	-2.47	1.37	1.42
6	G	201	ACO	OAP-CAP	-2.40	1.37	1.42
6	H	201	ACO	OAP-CAP	-2.39	1.37	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	201	ACO	O6A-CCP-CBP	4.36	117.55	110.55
6	F	201	ACO	N3A-C2A-N1A	-4.33	121.91	128.68
6	G	201	ACO	N3A-C2A-N1A	-4.31	121.94	128.68
6	G	201	ACO	O6A-CCP-CBP	4.25	117.38	110.55
6	E	201	ACO	N3A-C2A-N1A	-4.24	122.06	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	201	ACO	N3A-C2A-N1A	-4.23	122.07	128.68
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	F	201	ACO	P2A-O3A-P1A	-3.80	119.79	132.83
6	G	201	ACO	C7P-C6P-C5P	3.55	118.27	112.36
6	E	201	ACO	C7P-C6P-C5P	3.43	118.06	112.36
6	G	201	ACO	P2A-O3A-P1A	-3.42	121.08	132.83
6	H	201	ACO	O-C-S1P	-3.40	107.50	122.60
6	H	201	ACO	P2A-O3A-P1A	-3.40	121.16	132.83
6	G	201	ACO	O-C-S1P	-3.35	107.73	122.60
6	H	201	ACO	C3B-C2B-C1B	3.29	107.19	99.89
6	E	201	ACO	C3B-C2B-C1B	3.27	107.13	99.89
6	F	201	ACO	O-C-S1P	-3.24	108.22	122.60
6	E	201	ACO	O-C-S1P	-3.23	108.26	122.60
6	E	201	ACO	P2A-O3A-P1A	-3.14	122.06	132.83
6	E	201	ACO	O-C-CH3	-3.07	110.48	123.07
6	G	201	ACO	O-C-CH3	-3.05	110.56	123.07
6	F	201	ACO	O-C-CH3	-2.99	110.81	123.07
6	H	201	ACO	O-C-CH3	-2.98	110.83	123.07
6	F	201	ACO	C7P-C6P-C5P	2.94	117.26	112.36
6	H	201	ACO	C7P-C6P-C5P	2.93	117.24	112.36
6	F	201	ACO	C2P-C3P-N4P	2.79	118.27	112.42
6	E	201	ACO	C2P-C3P-N4P	2.71	118.12	112.42
6	G	201	ACO	O5B-C5B-C4B	2.71	118.30	108.99
6	H	201	ACO	C2P-C3P-N4P	2.66	118.01	112.42
6	G	201	ACO	C2P-C3P-N4P	2.59	117.85	112.42
6	F	201	ACO	O5B-C5B-C4B	2.57	117.83	108.99
6	G	201	ACO	C3B-C2B-C1B	2.56	105.56	99.89
6	E	201	ACO	O5B-C5B-C4B	2.48	117.54	108.99
6	H	201	ACO	C6P-C5P-N4P	2.32	120.32	116.42
6	E	201	ACO	C6P-C5P-N4P	2.31	120.31	116.42
6	F	201	ACO	C6P-C7P-N8P	2.30	116.54	111.90
6	H	201	ACO	O5B-C5B-C4B	2.27	116.81	108.99
6	G	201	ACO	C6P-C7P-N8P	2.23	116.39	111.90
6	F	201	ACO	C6P-C5P-N4P	2.23	120.17	116.42
6	G	201	ACO	C6P-C5P-N4P	2.17	120.07	116.42
6	F	201	ACO	O4B-C1B-C2B	-2.04	103.94	106.93
6	H	201	ACO	C6P-C7P-N8P	2.01	115.95	111.90

There are no chirality outliers.

All (47) 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	C3B-O3B-P3B-O7A
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	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	C5P-C6P-C7P-N8P
6	H	201	ACO	O-C-S1P-C2P
6	H	201	ACO	CH3-C-S1P-C2P
6	F	201	ACO	C3B-C4B-C5B-O5B
6	H	201	ACO	C3B-C4B-C5B-O5B
6	H	201	ACO	O4B-C4B-C5B-O5B
6	F	201	ACO	CEP-CBP-CCP-O6A
6	E	201	ACO	S1P-C2P-C3P-N4P
6	G	201	ACO	S1P-C2P-C3P-N4P
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	E	201	ACO	C5B-O5B-P1A-O3A
6	G	201	ACO	C5B-O5B-P1A-O3A
6	H	201	ACO	C5B-O5B-P1A-O3A
6	E	201	ACO	C5B-O5B-P1A-O2A
6	G	201	ACO	C5B-O5B-P1A-O2A
6	H	201	ACO	C5B-O5B-P1A-O2A
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	H	201	ACO	S1P-C2P-C3P-N4P
6	E	201	ACO	P1A-O3A-P2A-O4A
6	G	201	ACO	O9P-C9P-CAP-OAP
6	E	201	ACO	C3B-O3B-P3B-O7A
6	G	201	ACO	C3B-O3B-P3B-O7A
6	G	201	ACO	N8P-C9P-CAP-OAP

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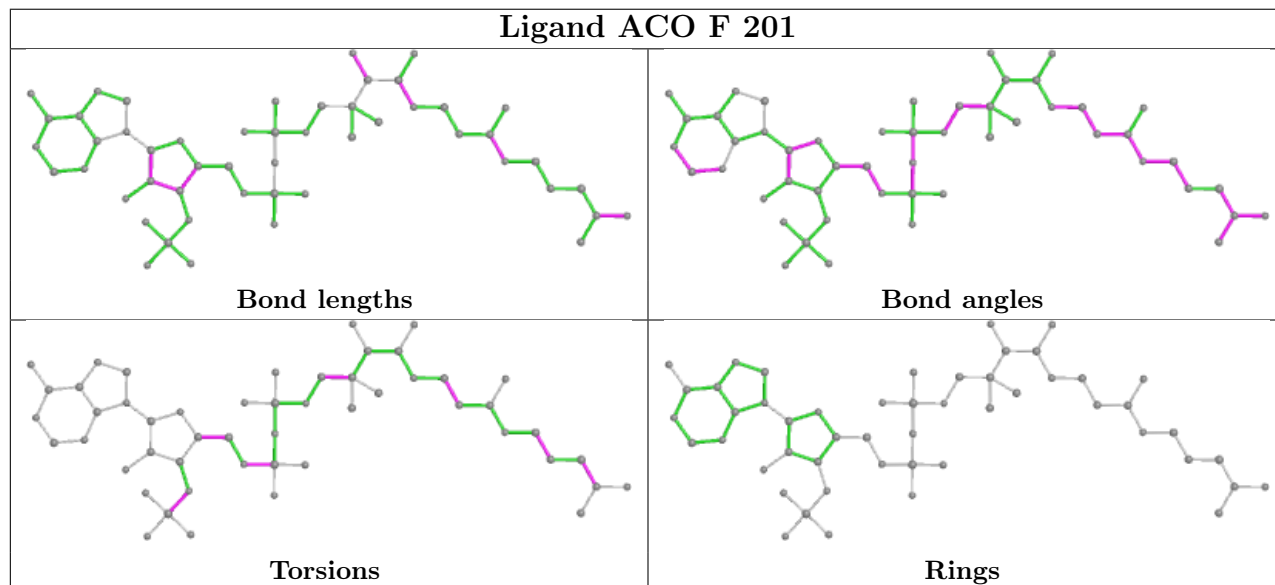
Mol	Chain	Res	Type	Atoms
6	H	201	ACO	C3B-O3B-P3B-O7A
6	F	201	ACO	C3B-O3B-P3B-O9A
6	F	201	ACO	C5B-O5B-P1A-O3A
6	G	201	ACO	P1A-O3A-P2A-O5A

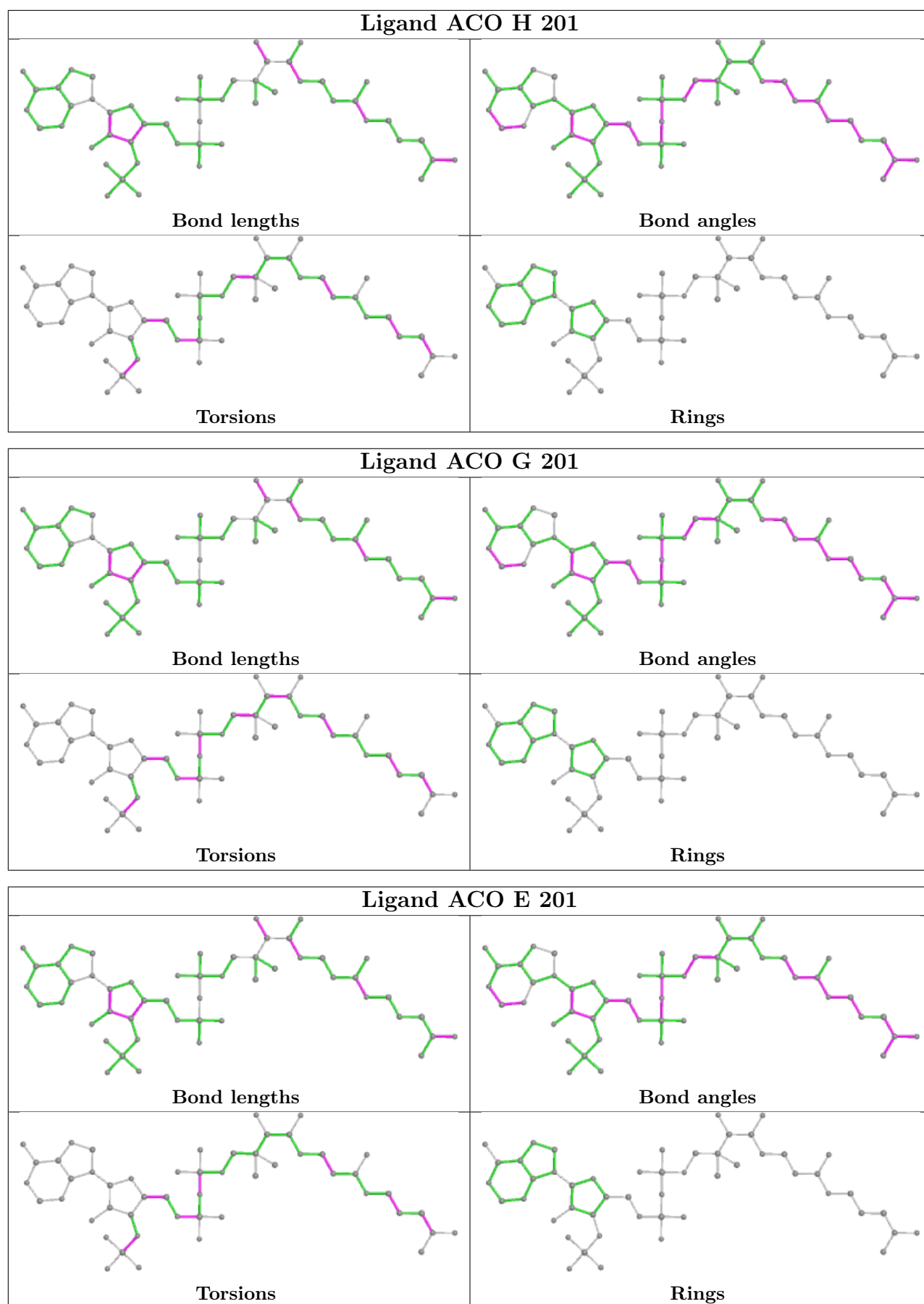
There are no ring outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	718/731 (98%)	-0.20	13 (1%) 68 55	38, 69, 149, 217	0
1	B	722/731 (98%)	-0.02	18 (2%) 57 42	37, 90, 170, 249	0
1	C	717/731 (98%)	-0.08	22 (3%) 49 32	30, 84, 160, 213	0
1	D	717/731 (98%)	-0.15	12 (1%) 70 57	40, 73, 158, 203	0
2	E	153/156 (98%)	-0.25	1 (0%) 87 81	38, 57, 101, 149	0
2	F	153/156 (98%)	-0.04	5 (3%) 46 29	36, 80, 146, 169	0
2	G	153/156 (98%)	0.08	3 (1%) 65 50	35, 86, 156, 185	0
2	H	153/156 (98%)	-0.11	3 (1%) 65 50	36, 60, 135, 172	0
All	All	3486/3548 (98%)	-0.11	77 (2%) 62 47	30, 76, 159, 249	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	ALA	11.3
1	B	730	ALA	10.7
1	C	730	ALA	10.2
1	D	729	ASN	9.8
1	B	368	ASP	5.3
1	B	729	ASN	5.2
1	B	360	THR	5.1
1	D	374	GLU	5.1
1	C	370	ASN	4.7
1	B	57	LEU	4.6
1	A	729	ASN	4.4
1	C	181	PRO	4.2
1	C	644	ASP	4.0
1	C	707	LEU	4.0
1	A	730	ALA	3.9
2	F	66	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	39	ARG	3.6
1	B	374	GLU	3.4
1	C	59	ASN	3.4
1	A	38	GLU	3.3
1	C	710	ASN	3.3
1	D	730	ALA	3.3
1	C	38	GLU	3.2
1	B	32	ALA	3.2
1	D	728	SER	3.2
1	A	369	ASP	3.1
1	D	371	SER	3.1
1	C	374	GLU	3.1
2	G	135	GLU	3.1
1	A	370	ASN	2.9
1	B	12	THR	2.9
1	B	370	ASN	2.8
1	B	36	LEU	2.8
2	F	146	TYR	2.8
2	G	138	TYR	2.8
1	B	364	PHE	2.7
1	C	368	ASP	2.7
1	A	177	ASN	2.6
1	A	39	ARG	2.6
1	D	370	ASN	2.6
1	C	383	TYR	2.6
1	A	373	ILE	2.6
2	F	127	LEU	2.5
1	A	597	GLY	2.5
1	C	32	ALA	2.5
1	B	369	ASP	2.5
2	H	133	GLY	2.4
1	C	647	PRO	2.4
1	C	360	THR	2.4
1	D	78	GLY	2.4
1	D	180	VAL	2.4
2	G	146	TYR	2.3
1	A	647	PRO	2.3
1	A	694	ASP	2.3
1	A	731	ALA	2.3
1	C	364	PHE	2.3
1	D	647	PRO	2.2
1	C	347	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	146	TYR	2.2
1	C	390	PHE	2.2
1	A	374	GLU	2.2
1	B	371	SER	2.2
1	B	354	TYR	2.1
1	C	629	ASP	2.1
1	C	351	VAL	2.1
1	D	588	LEU	2.1
1	D	182	VAL	2.1
2	F	135	GLU	2.1
2	H	117	ARG	2.1
1	C	6	LEU	2.1
1	C	371	SER	2.0
1	D	110	ASN	2.0
1	B	35	PRO	2.0
1	B	647	PRO	2.0
2	E	132	GLN	2.0
1	B	38	GLU	2.0
2	F	1[A]	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CL	D	808	1/1	-0.13	0.36	97,97,97,97	0
4	CL	A	805	1/1	0.27	0.19	122,122,122,122	0
4	CL	D	809	1/1	0.31	0.35	88,88,88,88	0
4	CL	E	206	1/1	0.38	0.28	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	E	207	1/1	0.51	0.52	100,100,100,100	0
4	CL	B	802	1/1	0.54	0.18	87,87,87,87	0
4	CL	H	203	1/1	0.56	0.21	121,121,121,121	0
4	CL	C	813	1/1	0.59	0.14	86,86,86,86	0
4	CL	B	810	1/1	0.59	0.54	98,98,98,98	0
4	CL	C	803	1/1	0.64	1.92	111,111,111,111	0
4	CL	A	807	1/1	0.65	0.29	104,104,104,104	0
4	CL	B	806	1/1	0.69	0.26	91,91,91,91	0
4	CL	C	812	1/1	0.74	0.21	78,78,78,78	0
3	NA	G	202	1/1	0.77	0.09	65,65,65,65	0
4	CL	C	814	1/1	0.78	0.19	77,77,77,77	0
4	CL	C	809	1/1	0.79	0.41	89,89,89,89	0
4	CL	D	806	1/1	0.80	0.19	99,99,99,99	0
4	CL	B	803	1/1	0.80	0.32	83,83,83,83	0
4	CL	E	209	1/1	0.80	0.16	91,91,91,91	0
4	CL	C	805	1/1	0.80	0.15	62,62,62,62	0
4	CL	D	804	1/1	0.81	0.14	100,100,100,100	0
4	CL	C	815	1/1	0.81	0.33	133,133,133,133	0
4	CL	C	810	1/1	0.83	0.37	83,83,83,83	0
4	CL	D	810	1/1	0.83	0.20	61,61,61,61	0
4	CL	B	813	1/1	0.83	0.14	80,80,80,80	0
6	ACO	F	201	51/51	0.83	0.31	89,154,252,337	0
6	ACO	G	201	51/51	0.83	0.31	117,151,232,233	0
4	CL	D	811	1/1	0.84	0.15	78,78,78,78	0
6	ACO	H	201	51/51	0.84	0.32	77,128,209,268	0
4	CL	B	814	1/1	0.85	0.10	76,76,76,76	0
4	CL	A	802	1/1	0.85	0.70	108,108,108,108	0
4	CL	F	203	1/1	0.85	0.44	80,80,80,80	0
4	CL	G	204	1/1	0.85	0.27	72,72,72,72	0
4	CL	C	801	1/1	0.86	0.89	117,117,117,117	0
4	CL	E	210	1/1	0.86	0.20	73,73,73,73	0
4	CL	D	803	1/1	0.87	0.49	94,94,94,94	0
4	CL	E	205	1/1	0.87	0.15	76,76,76,76	0
4	CL	A	809	1/1	0.87	0.29	55,55,55,55	0
3	NA	E	203	1/1	0.87	0.47	39,39,39,39	0
4	CL	B	812	1/1	0.88	0.16	103,103,103,103	0
4	CL	C	808	1/1	0.88	0.23	57,57,57,57	0
4	CL	C	806	1/1	0.90	0.19	77,77,77,77	0
4	CL	A	810	1/1	0.90	0.33	72,72,72,72	0
4	CL	B	811	1/1	0.91	0.32	81,81,81,81	0
4	CL	A	811	1/1	0.91	0.09	74,74,74,74	0
4	CL	C	811	1/1	0.91	0.16	43,43,43,43	0

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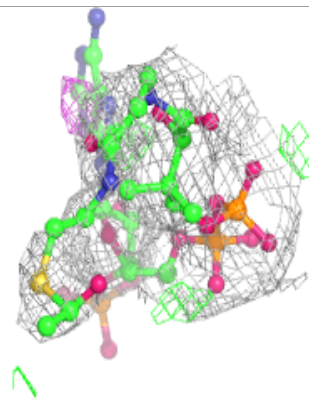
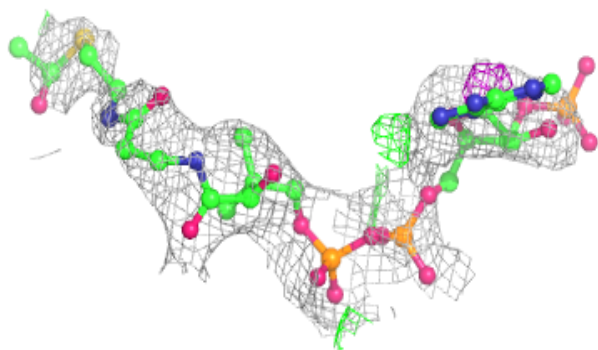
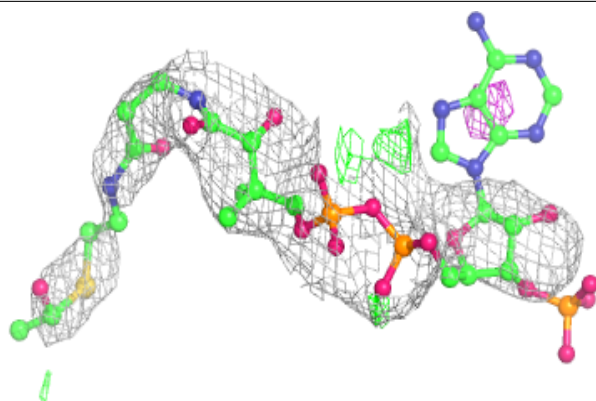
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	804	1/1	0.91	0.12	92,92,92,92	0
4	CL	G	203	1/1	0.91	0.42	77,77,77,77	0
4	CL	B	805	1/1	0.92	0.15	73,73,73,73	0
4	CL	A	808	1/1	0.92	0.27	85,85,85,85	0
4	CL	C	802	1/1	0.92	0.22	77,77,77,77	0
4	CL	E	204	1/1	0.93	0.25	47,47,47,47	0
4	CL	E	208	1/1	0.93	0.25	65,65,65,65	0
6	ACO	E	201	51/51	0.93	0.23	30,100,183,184	0
4	CL	C	804	1/1	0.94	0.24	82,82,82,82	0
4	CL	C	807	1/1	0.94	0.15	61,61,61,61	0
3	NA	E	202	1/1	0.95	0.33	72,72,72,72	0
4	CL	A	803	1/1	0.95	0.13	59,59,59,59	0
4	CL	D	807	1/1	0.95	0.14	47,47,47,47	0
4	CL	H	204	1/1	0.95	0.25	59,59,59,59	0
4	CL	A	806	1/1	0.96	0.15	77,77,77,77	0
4	CL	D	805	1/1	0.96	0.34	87,87,87,87	0
5	SO4	D	812	5/5	0.96	0.12	66,66,68,69	0
3	NA	A	801	1/1	0.96	0.25	38,38,38,38	0
4	CL	B	807	1/1	0.96	0.26	64,64,64,64	0
4	CL	B	809	1/1	0.96	0.32	78,78,78,78	0
4	CL	B	801	1/1	0.96	0.18	65,65,65,65	0
4	CL	B	808	1/1	0.97	0.20	59,59,59,59	0
3	NA	D	801	1/1	0.97	0.21	60,60,60,60	0
4	CL	A	804	1/1	0.97	0.15	62,62,62,62	0
5	SO4	A	812	5/5	0.98	0.12	61,62,63,65	0
4	CL	D	802	1/1	0.98	0.12	70,70,70,70	0
4	CL	F	202	1/1	0.99	0.26	43,43,43,43	0
4	CL	H	202	1/1	0.99	0.26	44,44,44,44	0

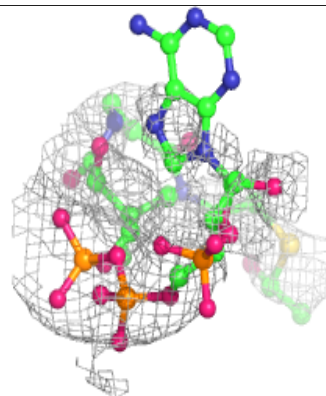
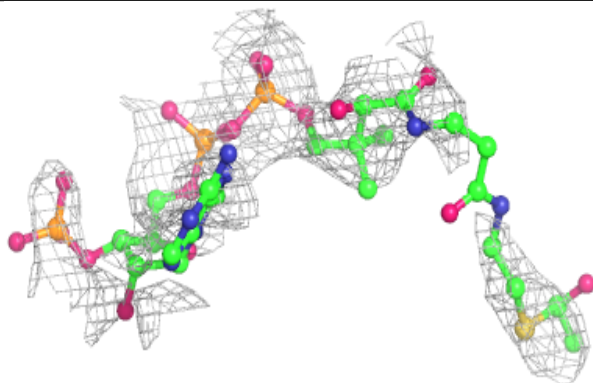
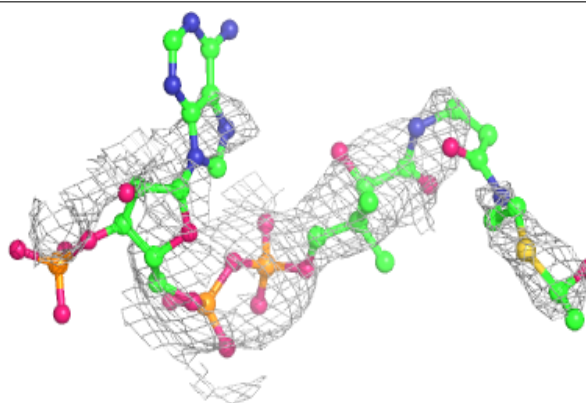
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

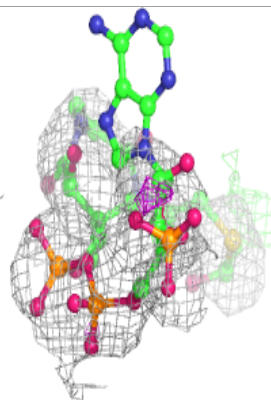
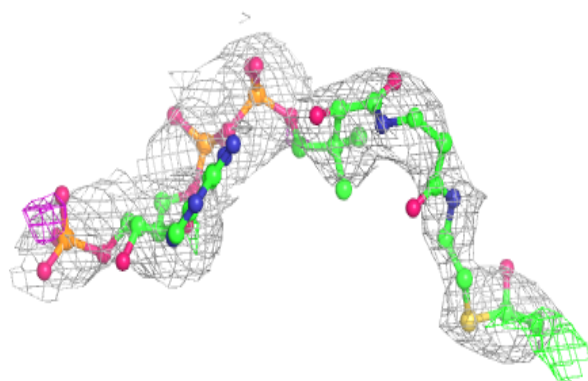
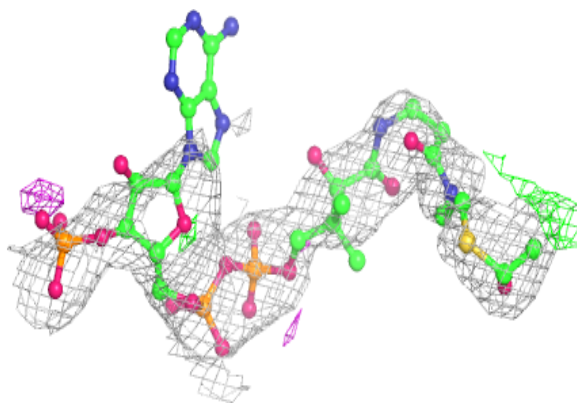
**Electron density around ACO G 201:**

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

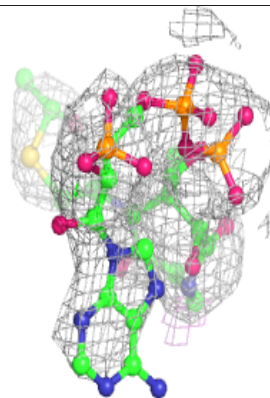
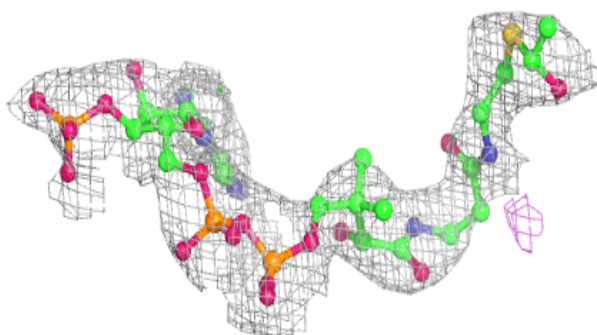
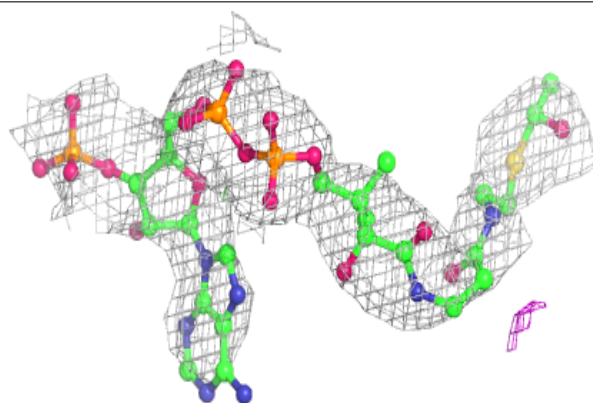


**Electron density around ACO H 201:**

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

**Electron density around ACO 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 [i](#)

There are no such residues in this entry.