



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 10:06 PM EDT

PDB ID : 3KVU
Title : Structural basis of the activity and substrate specificity of the fluoroacetyl-CoA
FLK - T42S mutant in complex with Acetyl-CoA
Authors : Dias, M.V.B.; Huang, F.; Chirgadze, D.Y.; Tosin, M.; Spitter, D.; Valentine,
E.F.; Leadlay, P.F.; Spencer, J.B.; Blundell, T.L.
Deposited on : 2009-11-30
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

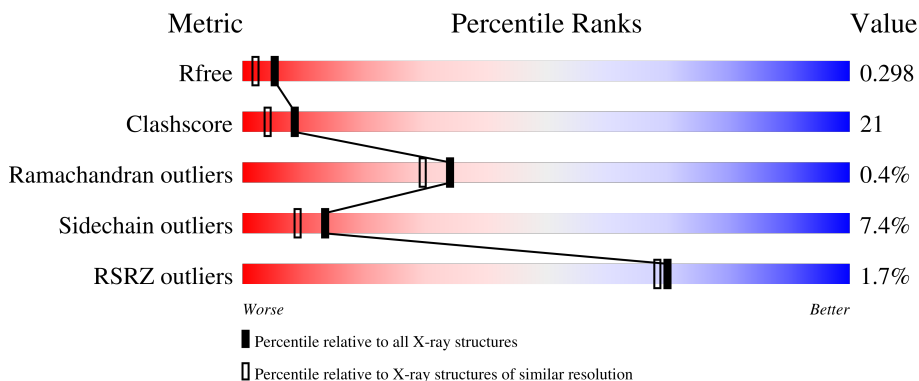
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	139	 2% 58% 32% 6% 2%
1	B	139	 2% 64% 25% 6% 2%
1	C	139	 64% 25% 6% 2%
1	D	139	 2% 68% 20% 6% 2%

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
2	ACO	B	200	X	-	-	-
2	ACO	D	202	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4539 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.

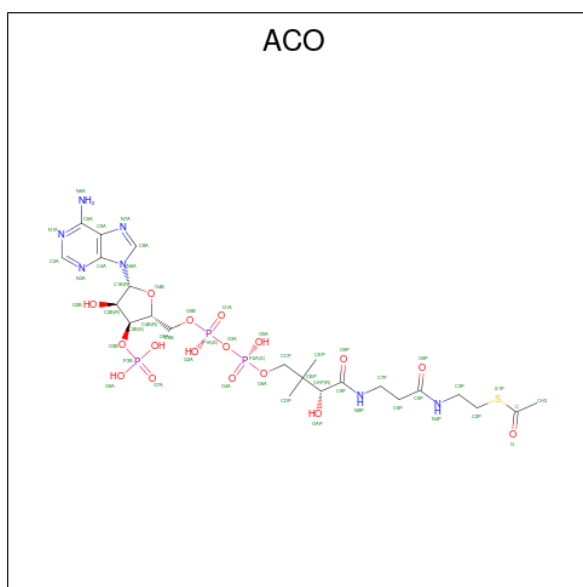
- Molecule 1 is a protein called Fluoroacetyl-CoA thioesterase FIK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1017	647	179	185	6	0	0	0
1	B	133	1027	652	182	187	6	0	0	0
1	C	133	1023	650	182	185	6	0	0	0
1	D	133	1027	652	182	187	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	THR	engineered mutation	UNP Q1EMV2
B	42	SER	THR	engineered mutation	UNP Q1EMV2
C	42	SER	THR	engineered mutation	UNP Q1EMV2
D	42	SER	THR	engineered mutation	UNP Q1EMV2

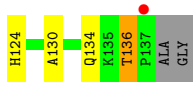
- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	16	9	2	4	1	0	0
2	B	1	51	23	7	17	3	1	0
2	D	1	21	13	2	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	70	Total	O	0	0
			70	70		
3	C	113	Total	O	0	0
			113	113		
3	D	100	Total	O	0	0
			100	100		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.98Å 55.97Å 96.41Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	31.91 – 2.00 31.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.91-2.00) 100.0 (31.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.75 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.295 0.217 , 0.298	Depositor DCC
R_{free} test set	1631 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1967e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.25	2/1046 (0.2%)	1.13	4/1425 (0.3%)
1	B	1.29	5/1056 (0.5%)	1.08	2/1437 (0.1%)
1	C	1.55	13/1052 (1.2%)	1.20	5/1432 (0.3%)
1	D	1.39	3/1056 (0.3%)	1.22	6/1437 (0.4%)
All	All	1.37	23/4210 (0.5%)	1.16	17/5731 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	GLU	CD-OE1	11.44	1.38	1.25
1	C	126	GLU	CG-CD	9.87	1.66	1.51
1	C	126	GLU	CD-OE2	8.68	1.35	1.25
1	D	71	ALA	CA-CB	7.29	1.67	1.52
1	C	35	GLU	CG-CD	6.98	1.62	1.51
1	C	71	ALA	CA-CB	6.72	1.66	1.52
1	C	102	TRP	CB-CG	6.34	1.61	1.50
1	B	35	GLU	CG-CD	6.33	1.61	1.51
1	A	93	ARG	CG-CD	6.30	1.67	1.51
1	C	133	ARG	CG-CD	6.09	1.67	1.51
1	C	126	GLU	CB-CG	6.02	1.63	1.52
1	B	35	GLU	CB-CG	5.40	1.62	1.52
1	B	74	VAL	CB-CG2	-5.39	1.41	1.52
1	C	105	SER	CA-CB	-5.34	1.45	1.52
1	C	50	GLU	CD-OE1	5.34	1.31	1.25
1	D	35	GLU	CG-CD	5.29	1.59	1.51
1	B	50	GLU	CB-CG	-5.24	1.42	1.52
1	C	112	GLU	CB-CG	5.19	1.62	1.52
1	D	102	TRP	CG-CD1	5.16	1.44	1.36
1	C	44	PHE	CE2-CZ	5.15	1.47	1.37
1	C	54	VAL	CB-CG1	5.14	1.63	1.52
1	A	119	GLU	CG-CD	-5.11	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ARG	CG-CD	5.11	1.64	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	C	5	MET	CG-SD-CE	-7.88	87.58	100.20
1	C	93	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	93	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	55	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	99	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	93	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	10	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	10	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	89	THR	N-CA-CB	-5.94	99.01	110.30
1	C	48	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	D	26	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	D	68	LEU	CA-CB-CG	-5.37	102.94	115.30
1	C	120	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	99	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	93	ARG	CG-CD-NE	5.13	122.57	111.80
1	B	120	ARG	NE-CZ-NH2	5.06	122.83	120.30

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	1017	0	985	53	0
1	B	1027	0	1000	40	1
1	C	1023	0	996	37	0
1	D	1027	0	1000	38	2
2	A	16	0	13	6	0
2	B	51	0	34	16	1
2	D	21	0	23	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	74	0	0	4	2
3	B	70	0	0	2	2
3	C	113	0	0	5	4
3	D	100	0	0	6	1
All	All	4539	0	4051	170	7

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 21.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HE2	2:B:200:ACO:H2B	1.25	1.07
1:A:131:LYS:CE	2:B:200:ACO:H2B	1.84	1.06
1:A:32:GLU:OE2	1:B:55:ARG:NH1	1.89	1.05
1:A:55:ARG:HH11	1:A:55:ARG:CG	1.72	1.01
1:C:133:ARG:HD3	3:C:407:HOH:O	1.60	0.99
1:D:5:MET:N	3:D:350:HOH:O	1.94	0.98
1:A:7:VAL:HG12	1:A:93:ARG:NH2	1.79	0.98
1:B:10:ARG:HD2	3:B:140:HOH:O	1.63	0.98
1:B:98:ARG:HH11	1:B:98:ARG:HG2	1.26	0.98
1:D:99:ARG:HG3	3:D:363:HOH:O	1.64	0.95
1:C:69:GLY:H	2:D:202:ACO:HH33	1.35	0.89
2:B:200:ACO:H21	2:B:200:ACO:O5P	1.73	0.88
1:D:98:ARG:HG2	1:D:98:ARG:HH11	1.36	0.88
2:A:201:ACO:CH3	1:B:50:GLU:OE1	2.23	0.87
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.37	0.86
1:A:7:VAL:CG1	1:A:93:ARG:NH2	2.39	0.85
1:A:91:GLU:OE2	1:A:93:ARG:NH1	2.09	0.84
2:B:200:ACO:CEP	2:B:200:ACO:O9P	2.25	0.84
2:B:200:ACO:O9P	2:B:200:ACO:H142	1.77	0.84
2:B:200:ACO:H143	2:B:200:ACO:O1A	1.78	0.84
1:C:107:HIS:HD2	1:C:109:GLY:H	1.25	0.83
1:C:133:ARG:CD	3:C:407:HOH:O	2.23	0.83
1:C:133:ARG:HG2	1:C:133:ARG:HH11	1.41	0.83
1:D:118:HIS:HE1	1:D:120:ARG:HH11	1.26	0.82
1:D:107:HIS:HD2	1:D:109:GLY:H	1.25	0.82
1:C:118:HIS:HE1	1:C:120:ARG:HH11	1.27	0.80
2:A:201:ACO:HH31	1:B:50:GLU:OE1	1.81	0.80
1:D:112:GLU:HB2	3:D:397:HOH:O	1.81	0.80
1:A:131:LYS:HE2	2:B:200:ACO:C2B	2.11	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ALA:HA	1:C:133:ARG:HD2	1.64	0.78
1:A:118:HIS:HE1	1:A:120:ARG:HH11	1.33	0.76
1:C:98:ARG:HG2	1:C:98:ARG:NH2	2.02	0.74
1:C:107:HIS:CD2	1:C:109:GLY:H	2.04	0.74
1:A:8:GLY:HA2	3:A:143:HOH:O	1.87	0.74
1:D:103:ARG:NH1	3:D:229:HOH:O	2.20	0.74
1:A:46:VAL:O	1:A:50:GLU:HG3	1.87	0.73
1:A:55:ARG:HH11	1:A:55:ARG:HG3	1.53	0.72
1:B:98:ARG:HG2	1:B:98:ARG:NH1	2.03	0.72
1:A:51:TRP:HE1	1:A:55:ARG:HH12	1.39	0.71
2:A:201:ACO:HH32	1:B:50:GLU:OE1	1.88	0.70
1:B:50:GLU:HG2	1:B:118:HIS:CE1	2.26	0.70
1:A:13:HIS:HA	3:A:147:HOH:O	1.91	0.70
1:D:118:HIS:CE1	1:D:120:ARG:HH11	2.10	0.69
1:C:81:PRO:HG2	1:D:136:THR:HG23	1.75	0.69
1:A:131:LYS:HE3	2:B:200:ACO:H2B	1.72	0.69
1:C:98:ARG:HG2	1:C:98:ARG:HH21	1.56	0.69
1:B:89:THR:HG22	1:B:105:SER:HB2	1.74	0.68
1:C:129:ASN:O	1:C:133:ARG:HG3	1.93	0.68
1:D:107:HIS:HD2	1:D:109:GLY:N	1.92	0.68
1:A:69:GLY:H	2:B:200:ACO:HH32	1.59	0.67
2:A:201:ACO:HH31	1:B:50:GLU:CD	2.15	0.67
1:A:129:ASN:HA	1:A:132:VAL:HG12	1.79	0.65
1:C:118:HIS:CE1	1:C:120:ARG:HH11	2.13	0.64
1:A:55:ARG:HG2	1:A:55:ARG:NH1	2.03	0.63
1:D:13:HIS:HD2	1:D:55:ARG:HH11	1.46	0.63
1:C:107:HIS:HD2	1:C:109:GLY:N	1.97	0.62
1:B:98:ARG:HH11	1:B:98:ARG:CG	2.08	0.62
1:C:10:ARG:NH1	3:C:309:HOH:O	2.28	0.62
1:A:13:HIS:CE1	3:A:152:HOH:O	2.52	0.62
1:D:76:HIS:ND1	2:D:202:ACO:H22	2.16	0.61
1:C:14:ASP:OD2	1:C:87:THR:HG23	2.02	0.60
1:C:100:LEU:HD12	1:C:100:LEU:N	2.15	0.60
1:B:84:LEU:N	1:B:84:LEU:HD12	2.16	0.60
1:A:107:HIS:HD2	1:A:112:GLU:CD	2.05	0.59
2:B:200:ACO:O9P	2:B:200:ACO:H141	2.01	0.59
1:D:93:ARG:CD	1:D:103:ARG:HB2	2.32	0.59
1:A:92:LEU:HD21	1:A:95:VAL:CG2	2.33	0.59
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.13	0.59
1:A:118:HIS:CE1	1:A:120:ARG:HH11	2.19	0.58
1:D:93:ARG:HD3	1:D:103:ARG:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD21	1:B:37:PRO:HG2	1.87	0.57
1:D:6:ARG:HD3	1:D:9:GLU:HB3	1.87	0.56
1:D:107:HIS:CD2	1:D:109:GLY:H	2.15	0.56
1:A:107:HIS:ND1	1:A:109:GLY:N	2.48	0.56
1:A:137:PRO:HD3	1:B:84:LEU:HD11	1.87	0.56
1:C:112:GLU:HG2	3:C:381:HOH:O	2.05	0.56
1:C:133:ARG:CG	3:C:407:HOH:O	2.50	0.56
1:D:98:ARG:HG2	1:D:98:ARG:NH1	2.15	0.55
1:A:51:TRP:HE1	1:A:55:ARG:NH1	2.02	0.55
1:C:69:GLY:N	2:D:202:ACO:HH33	2.16	0.55
1:A:7:VAL:HG12	1:A:93:ARG:HH22	1.68	0.55
1:B:107:HIS:HD2	1:B:109:GLY:H	1.53	0.55
1:B:71:ALA:O	1:B:118:HIS:HD2	1.89	0.55
1:C:98:ARG:HH21	1:C:98:ARG:CG	2.19	0.54
1:C:131:LYS:NZ	1:C:134:GLN:HE22	2.06	0.54
1:D:71:ALA:O	1:D:118:HIS:HD2	1.91	0.54
1:D:6:ARG:CD	1:D:9:GLU:HB3	2.38	0.54
1:A:55:ARG:CG	1:A:55:ARG:NH1	2.45	0.53
1:D:76:HIS:CE1	2:D:202:ACO:H22	2.44	0.53
1:C:133:ARG:HH11	1:C:133:ARG:CG	2.17	0.53
2:B:200:ACO:O5P	2:B:200:ACO:C2P	2.50	0.52
1:B:101:SER:HB3	1:B:119:GLU:HG3	1.91	0.52
1:B:118:HIS:HE1	1:B:120:ARG:HH11	1.58	0.52
1:A:53:CYS:O	1:A:57:MET:HG2	2.10	0.52
1:B:90:ALA:HA	1:B:103:ARG:O	2.09	0.51
1:C:107:HIS:CD2	1:C:109:GLY:N	2.76	0.51
1:A:81:PRO:HD2	1:A:84:LEU:HD12	1.92	0.51
2:A:201:ACO:HH31	1:B:50:GLU:OE2	2.09	0.51
1:D:6:ARG:HD3	1:D:6:ARG:O	2.11	0.51
1:D:13:HIS:CD2	1:D:55:ARG:HH11	2.28	0.51
1:D:99:ARG:NE	3:D:344:HOH:O	2.43	0.51
1:A:127:LYS:HB2	1:A:127:LYS:HZ3	1.76	0.50
1:C:5:MET:HE3	1:C:9:GLU:HG2	1.92	0.50
1:A:8:GLY:CA	3:A:143:HOH:O	2.52	0.50
1:D:18:PRO:HD2	1:D:21:LYS:HG2	1.93	0.50
1:D:72:ILE:O	1:D:72:ILE:HG23	2.11	0.50
1:B:98:ARG:HH21	1:B:124:HIS:CE1	2.28	0.50
1:A:7:VAL:CG1	1:A:93:ARG:HH21	2.24	0.50
1:A:11:PHE:HB2	1:A:56:ALA:HB2	1.93	0.49
1:A:23:VAL:HA	1:A:41:ALA:HB2	1.95	0.49
1:D:89:THR:HG22	1:D:105:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HG23	1:C:72:ILE:O	2.11	0.49
1:A:84:LEU:HD23	1:B:137:PRO:HG3	1.95	0.48
1:B:76:HIS:CE1	2:B:200:ACO:H31	2.47	0.48
1:A:80:THR:OG1	1:A:113:ILE:HG21	2.14	0.48
1:B:6:ARG:O	1:B:7:VAL:C	2.51	0.48
1:A:107:HIS:CD2	1:A:112:GLU:OE2	2.68	0.47
1:A:135:LYS:HG2	1:A:135:LYS:O	2.13	0.47
1:C:124:HIS:HB2	1:C:127:LYS:HZ2	1.79	0.47
1:D:93:ARG:HD2	1:D:103:ARG:HB2	1.96	0.47
1:B:39:VAL:HG23	2:B:200:ACO:H32	1.95	0.47
1:C:133:ARG:HG2	1:C:133:ARG:NH1	2.22	0.47
1:A:49:MET:HB3	1:A:104:VAL:HG11	1.96	0.46
1:A:51:TRP:NE1	1:A:55:ARG:NH1	2.62	0.46
1:B:93:ARG:HG2	1:B:101:SER:O	2.15	0.46
1:B:101:SER:HB3	1:B:119:GLU:CD	2.36	0.46
1:A:45:MET:O	1:A:49:MET:HG3	2.15	0.46
1:C:11:PHE:CZ	1:C:55:ARG:HG2	2.51	0.46
1:C:73:CYS:HA	1:D:73:CYS:HA	1.97	0.46
1:A:5:MET:HG2	1:A:60:TYR:CG	2.51	0.46
1:D:73:CYS:O	1:D:116:GLY:HA3	2.16	0.46
1:B:79:ALA:HB2	2:B:200:ACO:H61	1.98	0.45
1:D:130:ALA:O	1:D:134:GLN:HG3	2.17	0.45
1:A:10:ARG:HD2	1:A:89:THR:CG2	2.47	0.45
1:D:98:ARG:CG	1:D:98:ARG:NH1	2.78	0.45
1:A:107:HIS:HD2	1:A:112:GLU:OE2	2.00	0.45
1:C:71:ALA:O	1:C:118:HIS:HD2	1.99	0.44
1:D:18:PRO:HD2	1:D:21:LYS:CG	2.48	0.44
1:A:30:SER:HB2	1:B:51:TRP:CE2	2.52	0.44
1:B:81:PRO:HG2	1:B:84:LEU:HD13	2.00	0.44
1:B:67:SER:HA	1:B:121:ALA:O	2.17	0.44
1:C:23:VAL:HA	1:C:41:ALA:HB2	1.98	0.44
1:B:7:VAL:HG22	1:B:94:SER:HA	1.99	0.44
1:A:76:HIS:O	2:A:201:ACO:H62	2.17	0.44
1:A:22:THR:HA	1:A:39:VAL:O	2.18	0.43
2:B:200:ACO:O9P	2:B:200:ACO:C6P	2.66	0.43
1:D:98:ARG:HH22	1:D:124:HIS:HE1	1.65	0.43
1:B:71:ALA:HB3	1:B:119:GLU:HB2	2.01	0.43
1:C:67:SER:HA	1:C:121:ALA:O	2.19	0.43
1:B:89:THR:O	1:B:104:VAL:HA	2.18	0.43
2:B:200:ACO:H31	3:B:365:HOH:O	2.19	0.43
1:C:127:LYS:HE3	1:C:127:LYS:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:O	1:B:6:ARG:HG3	2.18	0.42
1:D:68:LEU:HA	1:D:68:LEU:HD23	1.46	0.42
1:C:131:LYS:NZ	1:C:134:GLN:NE2	2.67	0.42
1:B:68:LEU:HD11	1:B:128:PHE:CE1	2.54	0.42
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.91	0.42
1:B:22:THR:HA	1:B:39:VAL:O	2.20	0.42
1:D:10:ARG:HA	1:D:90:ALA:O	2.20	0.41
1:A:5:MET:SD	1:A:57:MET:HB3	2.60	0.41
1:A:118:HIS:CE1	1:A:120:ARG:HG2	2.54	0.41
1:B:94:SER:OG	1:B:101:SER:OG	2.36	0.41
1:B:46:VAL:HG13	1:B:72:ILE:HG12	2.03	0.41
1:D:22:THR:OG1	1:D:25:HIS:HD2	2.03	0.41
1:C:20:HIS:H	1:C:20:HIS:CD2	2.38	0.41
2:D:202:ACO:O9P	2:D:202:ACO:C6P	2.69	0.41
1:A:30:SER:HA	1:A:31:PRO:HD3	1.85	0.41
1:B:10:ARG:HG2	1:B:91:GLU:HB2	2.02	0.41
1:C:133:ARG:CG	1:C:133:ARG:NH1	2.84	0.40
1:D:112:GLU:HG2	3:D:353:HOH:O	2.19	0.40

All (7) 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:99:ARG:NH2	3:C:422:HOH:O[2_646]	1.53	0.67
2:B:200:ACO:O7A	3:C:292:HOH:O[2_645]	1.93	0.27
3:A:157:HOH:O	3:A:188:HOH:O[2_555]	1.94	0.26
1:B:38:GLU:OE1	3:B:373:HOH:O[2_555]	1.97	0.23
3:A:143:HOH:O	3:B:202:HOH:O[1_655]	2.13	0.07
3:C:260:HOH:O	3:D:298:HOH:O[2_656]	2.13	0.07
1:D:6:ARG:NH2	3:C:276:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/139 (94%)	122 (93%)	8 (6%)	1 (1%)	19	13
1	B	131/139 (94%)	128 (98%)	2 (2%)	1 (1%)	19	13
1	C	131/139 (94%)	129 (98%)	2 (2%)	0	100	100
1	D	131/139 (94%)	131 (100%)	0	0	100	100
All	All	524/556 (94%)	510 (97%)	12 (2%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	VAL
1	A	23	VAL

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	107/113 (95%)	100 (94%)	7 (6%)	17	12
1	B	109/113 (96%)	101 (93%)	8 (7%)	14	9
1	C	108/113 (96%)	100 (93%)	8 (7%)	13	9
1	D	109/113 (96%)	100 (92%)	9 (8%)	11	7
All	All	433/452 (96%)	401 (93%)	32 (7%)	13	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	55	ARG
1	A	99	ARG
1	A	101	SER
1	A	104	VAL
1	A	115	SER
1	A	127	LYS

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Mol	Chain	Res	Type
1	B	23	VAL
1	B	38	GLU
1	B	55	ARG
1	B	89	THR
1	B	96	GLU
1	B	98	ARG
1	B	119	GLU
1	B	131	LYS
1	C	18	PRO
1	C	93	ARG
1	C	98	ARG
1	C	99	ARG
1	C	103	ARG
1	C	115	SER
1	C	127	LYS
1	C	133	ARG
1	D	6	ARG
1	D	29	GLU
1	D	89	THR
1	D	98	ARG
1	D	101	SER
1	D	103	ARG
1	D	112	GLU
1	D	119	GLU
1	D	136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	118	HIS
1	B	107	HIS
1	B	118	HIS
1	C	107	HIS
1	C	118	HIS
1	C	134	GLN
1	D	13	HIS
1	D	25	HIS
1	D	107	HIS
1	D	118	HIS
1	D	124	HIS

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACO	B	200	-	45,53,53	1.16	4 (8%)	56,79,79	3.48	18 (32%)
2	ACO	D	202	-	18,20,53	0.95	0	23,26,79	2.99	7 (30%)
2	ACO	A	201	-	15,15,53	0.97	1 (6%)	16,17,79	3.29	9 (56%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	B	200	-	2/2/12/14	26/47/67/67	0/3/3/3
2	ACO	D	202	-	1/1/5/14	15/26/26/67	-
2	ACO	A	201	-	-	5/14/15/67	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	ACO	C2A-N3A	2.91	1.36	1.32
2	B	200	ACO	C5A-C4A	2.81	1.48	1.40
2	B	200	ACO	P3B-O3B	2.33	1.63	1.59
2	B	200	ACO	O4B-C1B	2.25	1.44	1.41
2	A	201	ACO	C-S1P	-2.06	1.63	1.75

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	ACO	CDP-CBP-CAP	-15.71	81.57	108.82
2	B	200	ACO	CEP-CBP-CAP	-10.03	91.43	108.82
2	D	202	ACO	C6P-C5P-N4P	8.55	130.81	116.42
2	B	200	ACO	CDP-CBP-CCP	7.30	120.14	108.23
2	B	200	ACO	CEP-CBP-CCP	7.04	119.72	108.23
2	A	201	ACO	O5P-C5P-N4P	-6.80	110.18	123.01
2	D	202	ACO	O5P-C5P-N4P	-6.59	110.57	123.01
2	B	200	ACO	CAP-C9P-N8P	-5.95	104.74	116.58
2	A	201	ACO	C3P-N4P-C5P	-5.69	112.28	122.84
2	B	200	ACO	CEP-CBP-CDP	5.15	119.66	109.17
2	D	202	ACO	C3P-N4P-C5P	-5.08	113.40	122.84
2	B	200	ACO	C6P-C7P-N8P	-4.99	101.83	111.90
2	A	201	ACO	C7P-N8P-C9P	4.49	131.17	122.84
2	A	201	ACO	C2P-C3P-N4P	-4.42	103.14	112.42
2	A	201	ACO	C6P-C5P-N4P	4.28	123.63	116.42
2	B	200	ACO	C7P-C6P-C5P	-4.13	105.48	112.36
2	D	202	ACO	C7P-C6P-C5P	-4.09	105.54	112.36
2	B	200	ACO	OAP-CAP-CBP	3.53	118.56	110.25
2	A	201	ACO	OAP-CAP-C9P	3.41	118.84	111.62
2	B	200	ACO	N3A-C2A-N1A	-3.33	123.47	128.68
2	D	202	ACO	CDP-CBP-CAP	3.25	114.46	108.82
2	B	200	ACO	C4A-C5A-N7A	-3.23	106.03	109.40
2	A	201	ACO	C6P-C7P-N8P	-3.04	105.75	111.90
2	D	202	ACO	C2P-C3P-N4P	-2.97	106.18	112.42
2	B	200	ACO	O5P-C5P-C6P	-2.80	116.89	122.02
2	B	200	ACO	O9P-C9P-CAP	2.74	129.43	121.06
2	B	200	ACO	C7P-N8P-C9P	2.71	127.42	122.59
2	B	200	ACO	O3B-P3B-O7A	-2.58	99.41	109.39
2	D	202	ACO	OAP-CAP-C9P	-2.53	97.24	109.42
2	B	200	ACO	O5B-C5B-C4B	2.39	117.22	108.99
2	B	200	ACO	O4B-C1B-C2B	-2.34	103.51	106.93
2	A	201	ACO	C2P-S1P-C	-2.32	89.47	101.68
2	A	201	ACO	O5P-C5P-C6P	2.28	126.18	122.02
2	B	200	ACO	C2P-C3P-N4P	-2.27	107.65	112.42

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	200	ACO	C4B
2	B	200	ACO	CAP
2	D	202	ACO	CAP

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	ACO	O9P-C9P-CAP-OAP
2	A	201	ACO	S1P-C2P-C3P-N4P
2	A	201	ACO	O-C-S1P-C2P
2	A	201	ACO	CH3-C-S1P-C2P
2	B	200	ACO	C4B-C5B-O5B-P1A
2	B	200	ACO	C5B-O5B-P1A-O1A
2	B	200	ACO	CEP-CBP-CCP-O6A
2	B	200	ACO	CAP-CBP-CCP-O6A
2	B	200	ACO	OAP-CAP-CBP-CCP
2	B	200	ACO	C9P-CAP-CBP-CCP
2	B	200	ACO	OAP-CAP-CBP-CDP
2	B	200	ACO	C9P-CAP-CBP-CDP
2	B	200	ACO	OAP-CAP-CBP-CEP
2	B	200	ACO	C9P-CAP-CBP-CEP
2	B	200	ACO	O9P-C9P-CAP-OAP
2	B	200	ACO	N8P-C9P-CAP-OAP
2	B	200	ACO	C5P-C6P-C7P-N8P
2	B	200	ACO	C2P-C3P-N4P-C5P
2	B	200	ACO	S1P-C2P-C3P-N4P
2	B	200	ACO	C3P-C2P-S1P-C
2	B	200	ACO	O-C-S1P-C2P
2	B	200	ACO	CH3-C-S1P-C2P
2	D	202	ACO	OAP-CAP-CBP-CCP
2	D	202	ACO	C9P-CAP-CBP-CCP
2	D	202	ACO	OAP-CAP-CBP-CDP
2	D	202	ACO	C9P-CAP-CBP-CDP
2	D	202	ACO	OAP-CAP-CBP-CEP
2	D	202	ACO	C9P-CAP-CBP-CEP
2	D	202	ACO	C5P-C6P-C7P-N8P
2	D	202	ACO	S1P-C2P-C3P-N4P
2	D	202	ACO	C3P-C2P-S1P-C
2	D	202	ACO	O-C-S1P-C2P
2	D	202	ACO	CH3-C-S1P-C2P
2	B	200	ACO	C6P-C7P-N8P-C9P
2	D	202	ACO	C6P-C7P-N8P-C9P

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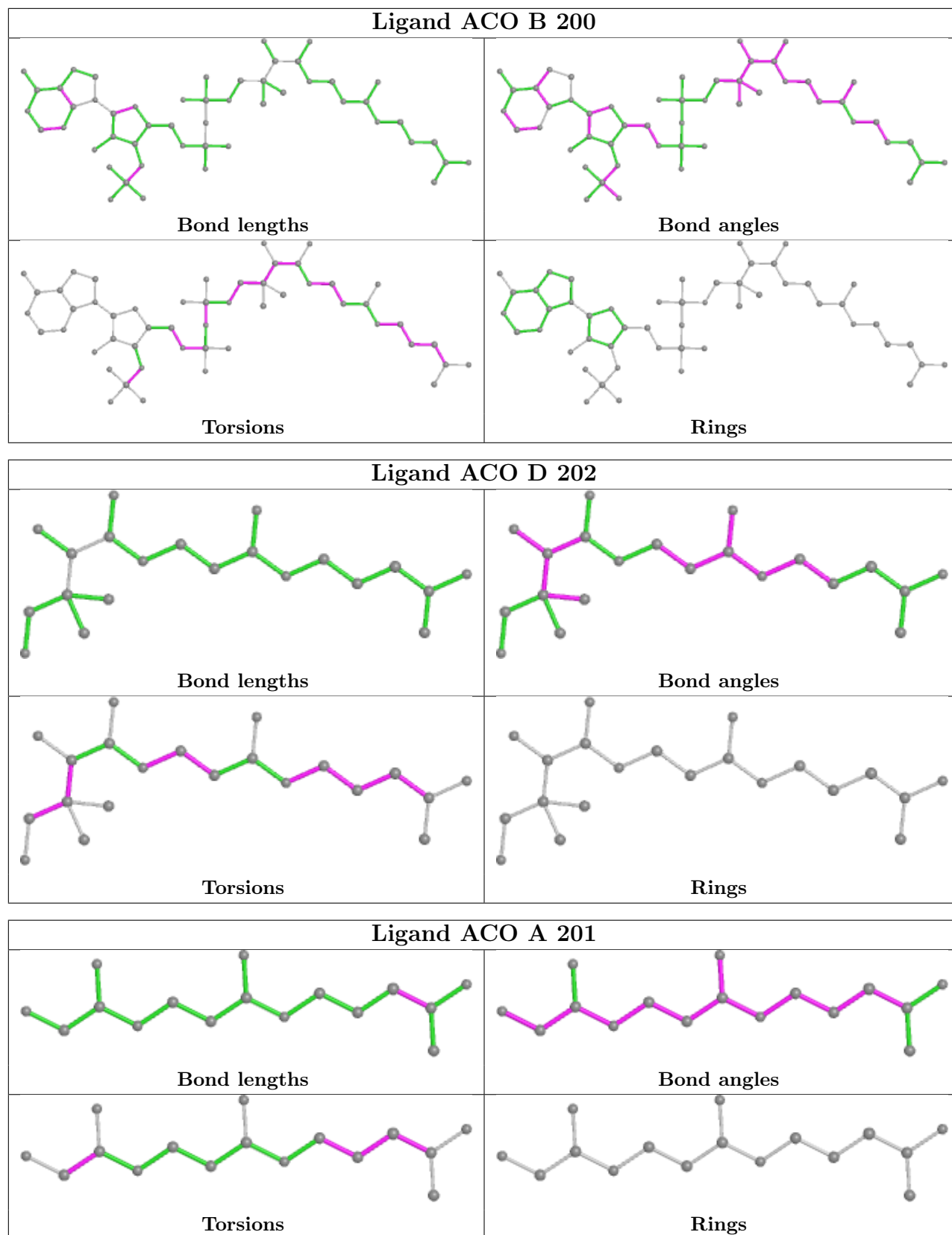
Mol	Chain	Res	Type	Atoms
2	D	202	ACO	CAP-CBP-CCP-O6A
2	B	200	ACO	C5B-O5B-P1A-O3A
2	B	200	ACO	C5B-O5B-P1A-O2A
2	D	202	ACO	C2P-C3P-N4P-C5P
2	D	202	ACO	CEP-CBP-CCP-O6A
2	B	200	ACO	O9P-C9P-CAP-CBP
2	B	200	ACO	N8P-C9P-CAP-CBP
2	A	201	ACO	C3P-C2P-S1P-C
2	B	200	ACO	P1A-O3A-P2A-O6A
2	B	200	ACO	C3B-O3B-P3B-O9A
2	B	200	ACO	CBP-CCP-O6A-P2A

There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	ACO	16	1
2	D	202	ACO	5	0
2	A	201	ACO	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	133/139 (95%)	0.09	3 (2%) 60 59	18, 27, 36, 41	2 (1%)
1	B	133/139 (95%)	0.27	3 (2%) 60 59	15, 28, 38, 51	4 (3%)
1	C	133/139 (95%)	-0.37	0 100 100	4, 15, 28, 34	1 (0%)
1	D	133/139 (95%)	-0.32	3 (2%) 60 59	3, 16, 31, 51	4 (3%)
All	All	532/556 (95%)	-0.08	9 (1%) 70 68	3, 22, 35, 51	11 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	PRO	4.5
1	B	105	SER	4.3
1	D	105	SER	2.9
1	A	12	THR	2.7
1	D	107	HIS	2.5
1	B	107	HIS	2.3
1	B	103	ARG	2.2
1	A	93	ARG	2.0
1	A	83	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](#)

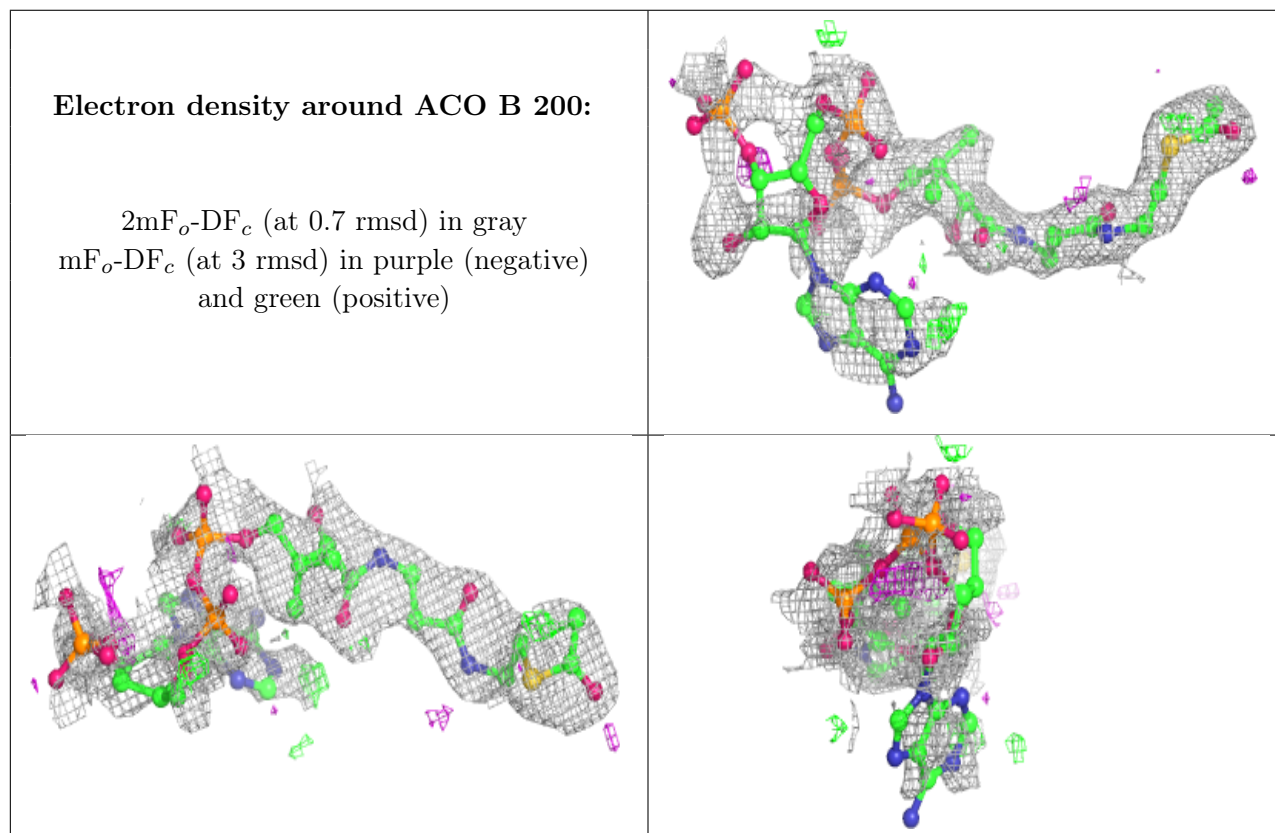
There are no monosaccharides in this entry.

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, 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.

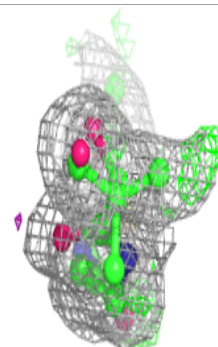
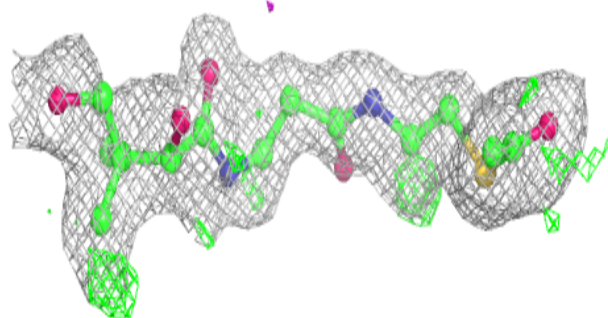
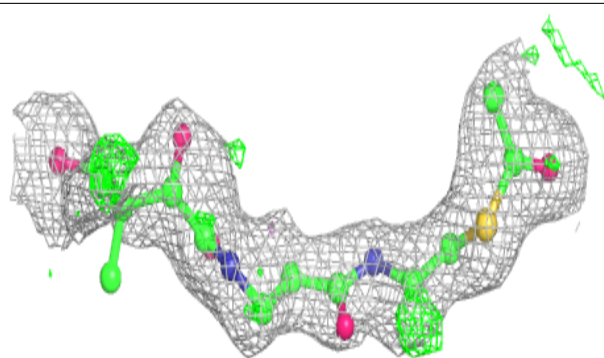
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACO	B	200	51/51	0.74	0.25	32,87,114,115	0
2	ACO	D	202	21/51	0.79	0.18	25,34,45,48	0
2	ACO	A	201	16/51	0.84	0.17	33,46,53,54	0

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.

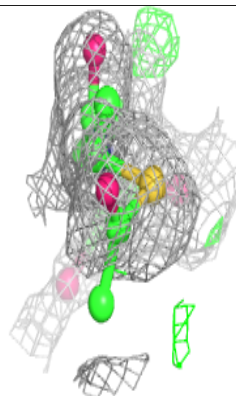
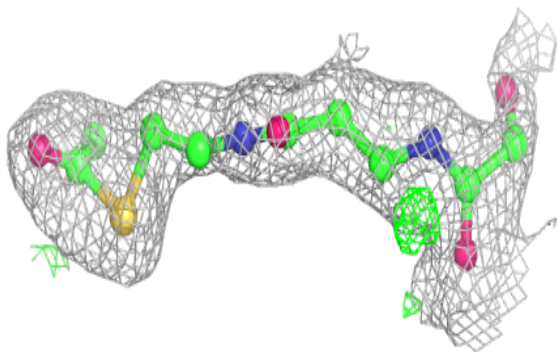
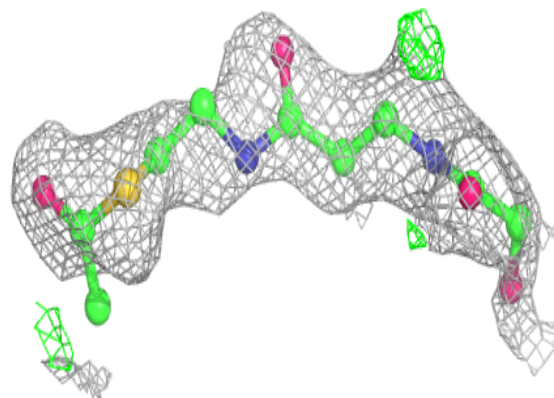


Electron density around ACO D 202:

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

**Electron density around ACO A 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.