



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:40 pm GMT

PDB ID : 3EQ6
Title : Crystal structure of human acyl-CoA synthetase medium-chain family member 2A (L64P mutation) in a ternary complex with products
Authors : Pilka, E.S.; Kochan, G.; Yue, W.W.; Bhatia, C.; Von delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2008-09-30
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

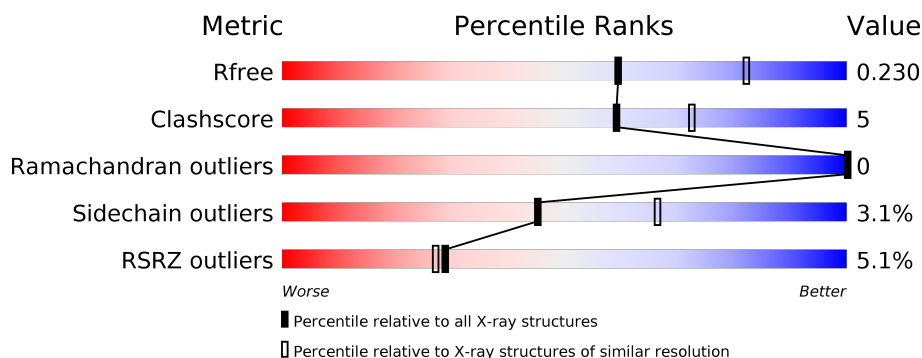
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	570	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	570	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>

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
3	BCO	A	911	X	-	-	-
3	BCO	B	912	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8852 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 Acyl-coenzyme A synthetase ACSM2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	8	4	0
			4153	2651	702	773	27			
1	B	533	Total	C	N	O	S	0	0	0
			4100	2619	687	767	27			

There are 50 discrepancies between the modelled and reference sequences:

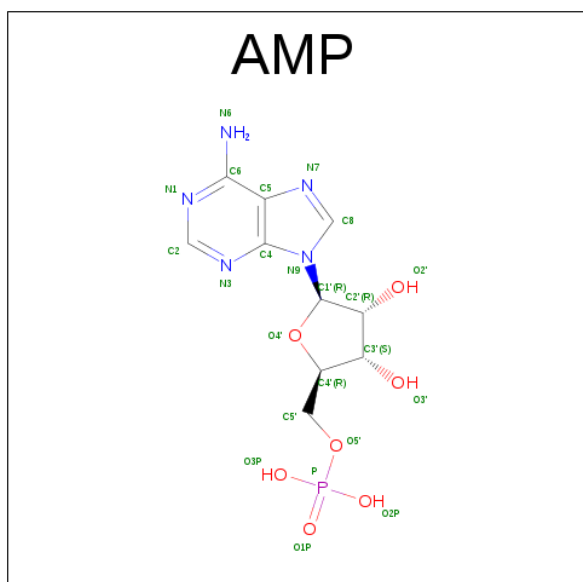
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	EXPRESSION TAG	UNP Q08AH3
A	9	GLY	-	EXPRESSION TAG	UNP Q08AH3
A	10	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	11	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	12	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	13	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	14	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	15	HIS	-	EXPRESSION TAG	UNP Q08AH3
A	16	SER	-	EXPRESSION TAG	UNP Q08AH3
A	17	SER	-	EXPRESSION TAG	UNP Q08AH3
A	18	GLY	-	EXPRESSION TAG	UNP Q08AH3
A	19	VAL	-	EXPRESSION TAG	UNP Q08AH3
A	20	ASP	-	EXPRESSION TAG	UNP Q08AH3
A	21	LEU	-	EXPRESSION TAG	UNP Q08AH3
A	22	GLY	-	EXPRESSION TAG	UNP Q08AH3
A	23	THR	-	EXPRESSION TAG	UNP Q08AH3
A	24	GLU	-	EXPRESSION TAG	UNP Q08AH3
A	25	ASN	-	EXPRESSION TAG	UNP Q08AH3
A	26	LEU	-	EXPRESSION TAG	UNP Q08AH3
A	27	TYR	-	EXPRESSION TAG	UNP Q08AH3
A	28	PHE	-	EXPRESSION TAG	UNP Q08AH3
A	29	GLN	-	EXPRESSION TAG	UNP Q08AH3
A	30	SER	-	EXPRESSION TAG	UNP Q08AH3
A	31	MET	-	EXPRESSION TAG	UNP Q08AH3
A	64	PRO	LEU	ENGINEERED MUTATION	UNP Q08AH3

Continued on next page...

Continued from previous page...

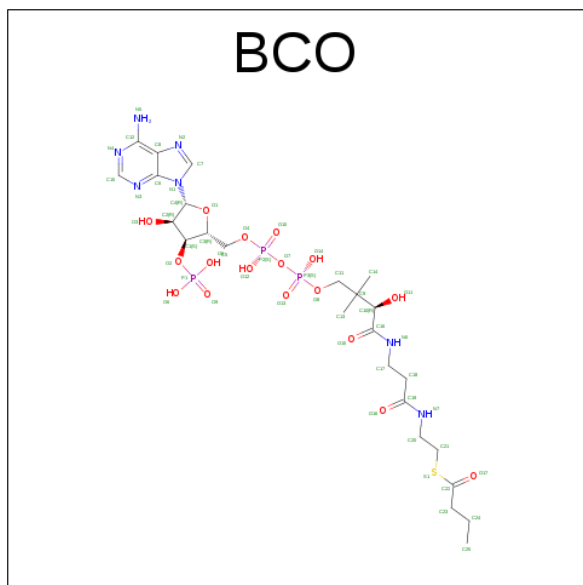
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	EXPRESSION TAG	UNP Q08AH3
B	9	GLY	-	EXPRESSION TAG	UNP Q08AH3
B	10	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	11	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	12	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	13	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	14	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	15	HIS	-	EXPRESSION TAG	UNP Q08AH3
B	16	SER	-	EXPRESSION TAG	UNP Q08AH3
B	17	SER	-	EXPRESSION TAG	UNP Q08AH3
B	18	GLY	-	EXPRESSION TAG	UNP Q08AH3
B	19	VAL	-	EXPRESSION TAG	UNP Q08AH3
B	20	ASP	-	EXPRESSION TAG	UNP Q08AH3
B	21	LEU	-	EXPRESSION TAG	UNP Q08AH3
B	22	GLY	-	EXPRESSION TAG	UNP Q08AH3
B	23	THR	-	EXPRESSION TAG	UNP Q08AH3
B	24	GLU	-	EXPRESSION TAG	UNP Q08AH3
B	25	ASN	-	EXPRESSION TAG	UNP Q08AH3
B	26	LEU	-	EXPRESSION TAG	UNP Q08AH3
B	27	TYR	-	EXPRESSION TAG	UNP Q08AH3
B	28	PHE	-	EXPRESSION TAG	UNP Q08AH3
B	29	GLN	-	EXPRESSION TAG	UNP Q08AH3
B	30	SER	-	EXPRESSION TAG	UNP Q08AH3
B	31	MET	-	EXPRESSION TAG	UNP Q08AH3
B	64	PRO	LEU	ENGINEERED MUTATION	UNP Q08AH3

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is BUTYRYL COENZYME A (three-letter code: BCO) (formula: $C_{25}H_{42}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 53	C 25	N 7	O 17	P 3	S 1	0	0
3	B	1	Total 53	C 25	N 7	O 17	P 3	S 1	0	0

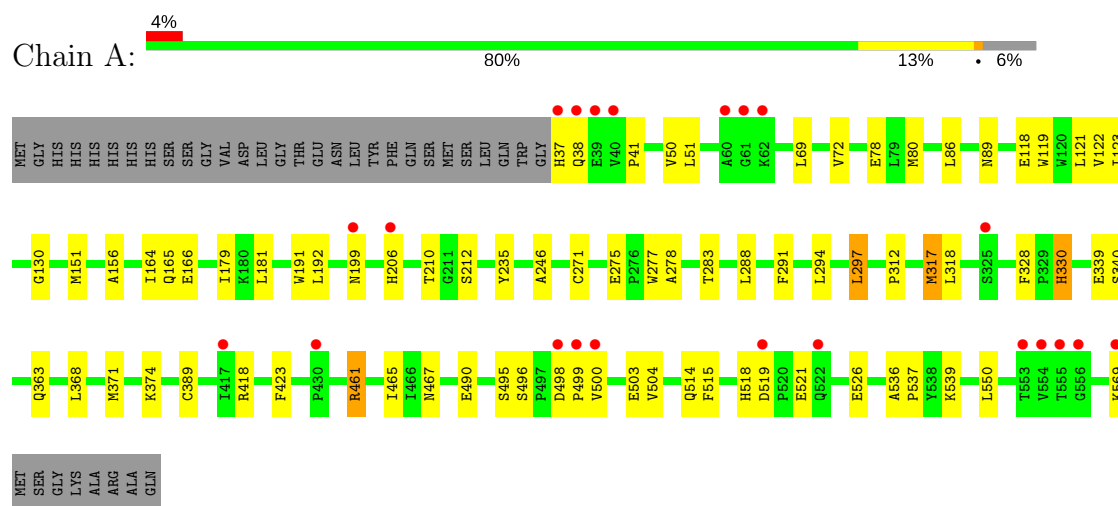
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	152	Total	O	0	0
			152	152		

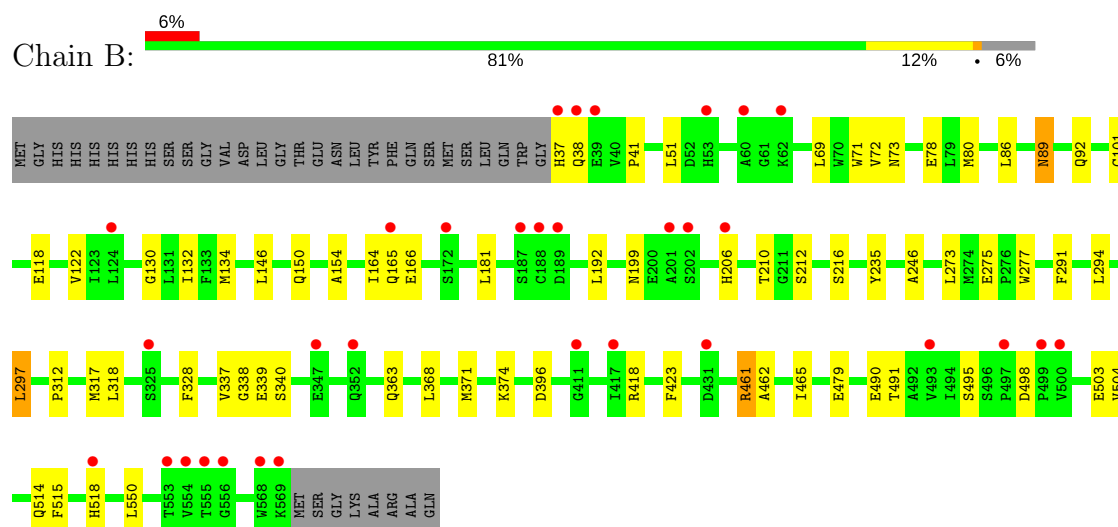
3 Residue-property plots

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

• Molecule 1: Acyl-coenzyme A synthetase ACSM2A



• Molecule 1: Acyl-coenzyme A synthetase ACSM2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 98.04Å 116.66Å 90.00° 94.12° 90.00°	Depositor
Resolution (Å)	21.73 – 2.40 21.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.73-2.40) 99.4 (21.56-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.187 , 0.236 0.188 , 0.230	Depositor DCC
R_{free} test set	2531 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: AMP, BCO

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	0.82	2/4261 (0.0%)	0.78	1/5789 (0.0%)
1	B	0.72	1/4197 (0.0%)	0.73	0/5709
All	All	0.77	3/8458 (0.0%)	0.75	1/11498 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	CYS	CB-SG	-5.38	1.73	1.81
1	A	271	CYS	CB-SG	-5.13	1.73	1.81
1	A	467	ASN	CB-CG	5.12	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	MET	CG-SD-CE	6.75	111.00	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4153	0	4122	47	0
1	B	4100	0	4030	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	12	1	0
2	B	23	0	12	1	0
3	A	53	0	40	2	0
3	B	53	0	40	0	0
4	A	295	0	0	3	0
4	B	152	0	0	2	0
All	All	8852	0	8256	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (89) 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:B:297:LEU:HD13	1:B:318:LEU:HD22	1.75	0.69
1:A:328:PHE:HA	1:A:330[A]:HIS:CE1	2.30	0.66
1:A:515:PHE:HA	1:A:518:HIS:CD2	2.31	0.66
1:A:297:LEU:HD13	1:A:318:LEU:HD22	1.79	0.65
1:B:515:PHE:HA	1:B:518:HIS:CD2	2.32	0.65
1:A:181:LEU:HD23	1:A:192:LEU:HB2	1.80	0.64
3:A:911:BCO:O15	3:A:911:BCO:H18	1.97	0.63
1:A:515:PHE:HA	1:A:518:HIS:HD2	1.64	0.61
1:A:389:CYS:N	4:A:1151:HOH:O	2.28	0.61
1:B:515:PHE:HA	1:B:518:HIS:HD2	1.64	0.60
1:A:38:GLN:HG2	1:A:418:ARG:O	2.02	0.60
1:B:181:LEU:HD23	1:B:192:LEU:HB2	1.83	0.60
1:A:72:VAL:HG12	1:A:78:GLU:HG2	1.84	0.58
1:B:38:GLN:HG2	1:B:418:ARG:O	2.03	0.57
1:A:51:LEU:HD11	1:A:86:LEU:HD23	1.87	0.56
1:B:291:PHE:CE2	1:B:317:MET:HE1	2.40	0.56
1:B:490:GLU:HG2	1:B:550:LEU:HD12	1.86	0.56
1:A:490:GLU:HG2	1:A:550:LEU:HD12	1.87	0.56
1:A:206:HIS:HB3	4:A:1266:HOH:O	2.05	0.56
1:B:498:ASP:HB2	1:B:504:VAL:HG13	1.89	0.55
1:A:291:PHE:CE2	1:A:317:MET:HE1	2.43	0.53
1:A:498:ASP:HB2	1:A:504:VAL:HG13	1.91	0.53
3:A:911:BCO:O15	3:A:911:BCO:C13	2.57	0.52
1:B:312:PRO:HD2	1:B:339:GLU:HB2	1.92	0.51
1:B:206:HIS:CD2	4:B:1298:HOH:O	2.64	0.50
1:A:164:ILE:HG23	1:A:165:GLN:N	2.27	0.50
1:A:41:PRO:O	1:A:212:SER:OG	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLU:O	1:B:122:VAL:HG23	2.12	0.49
1:A:37:HIS:O	1:A:418:ARG:N	2.41	0.49
1:B:41:PRO:O	1:B:212:SER:OG	2.17	0.48
1:B:479:GLU:HG2	1:B:491:THR:HG23	1.95	0.48
1:A:515:PHE:CA	1:A:518:HIS:HD2	2.26	0.48
1:B:515:PHE:CA	1:B:518:HIS:HD2	2.26	0.48
1:B:273:LEU:C	1:B:273:LEU:HD23	2.34	0.48
1:A:514[B]:GLN:HG3	1:A:515:PHE:CD2	2.48	0.48
1:B:132:ILE:HA	1:B:216:SER:O	2.14	0.48
1:A:495:SER:HB2	1:A:503:GLU:CG	2.44	0.47
1:A:291:PHE:CD2	1:A:317:MET:CE	2.98	0.47
1:B:461:ARG:HA	1:B:461:ARG:HD2	1.78	0.47
1:A:495:SER:HB2	1:A:503:GLU:HG3	1.96	0.47
1:A:118:GLU:O	1:A:122:VAL:HG23	2.15	0.46
1:B:461:ARG:NH2	1:B:465:ILE:HD12	2.30	0.46
1:B:164:ILE:HG23	1:B:165:GLN:N	2.31	0.46
1:A:496:SER:O	1:A:503:GLU:HA	2.16	0.46
1:A:461:ARG:HD2	1:A:461:ARG:HA	1.84	0.46
1:B:146:LEU:HD11	1:B:150:GLN:NE2	2.31	0.45
1:B:71:TRP:CH2	1:B:73:ASN:HB3	2.52	0.45
1:A:50:VAL:HG11	1:A:278:ALA:HA	1.98	0.45
1:B:396:ASP:C	1:B:396:ASP:OD1	2.55	0.45
1:B:462:ALA:HB1	4:B:1137:HOH:O	2.15	0.45
1:B:69:LEU:O	1:B:80:MET:HA	2.16	0.45
1:A:363:GLN:CB	2:A:901:AMP:H5'1	2.47	0.45
1:A:519:ASP:OD2	1:A:521:GLU:N	2.50	0.44
1:B:515:PHE:CD1	1:B:518:HIS:CD2	3.05	0.44
1:A:312:PRO:HD2	1:A:339:GLU:HB2	1.99	0.44
1:B:246:ALA:HA	1:B:275:GLU:OE1	2.18	0.44
1:B:291:PHE:CD2	1:B:317:MET:CE	3.00	0.44
1:B:495:SER:HB2	1:B:503:GLU:CG	2.47	0.43
1:B:337:VAL:HG22	1:B:338:GLY:N	2.33	0.43
1:B:72:VAL:HG12	1:B:78:GLU:HG2	2.00	0.43
1:B:37:HIS:O	1:B:418:ARG:N	2.42	0.43
1:A:291:PHE:CD2	1:A:317:MET:HE1	2.53	0.43
1:A:210:THR:HG21	1:A:235:TYR:CZ	2.54	0.43
1:A:461:ARG:NH2	1:A:465:ILE:HD12	2.34	0.42
1:B:134:MET:HE1	1:B:154:ALA:HB2	2.00	0.42
1:B:210:THR:HG21	1:B:235:TYR:CZ	2.54	0.42
1:B:291:PHE:CD2	1:B:317:MET:HE1	2.54	0.42
1:A:69:LEU:O	1:A:80:MET:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HD2	1:A:317:MET:HE3	1.82	0.42
1:A:526:GLU:OE1	4:A:1304:HOH:O	2.22	0.42
1:B:51:LEU:HD11	1:B:86:LEU:HD23	2.01	0.42
1:A:164:ILE:HD11	1:A:191:TRP:CD1	2.55	0.42
1:A:536:ALA:O	1:A:539:LYS:HG2	2.19	0.42
1:B:130:GLY:HA2	1:B:235:TYR:OH	2.19	0.42
1:A:130:GLY:HA2	1:A:235:TYR:OH	2.20	0.42
1:A:536:ALA:HA	1:A:537:PRO:HD3	1.90	0.42
1:B:514:GLN:HG2	1:B:515:PHE:CD2	2.55	0.41
1:B:86:LEU:HD21	1:B:277:TRP:CH2	2.55	0.41
1:A:151:MET:HE3	1:A:151:MET:HB3	1.95	0.41
1:A:156:ALA:HA	1:A:179:ILE:O	2.21	0.41
1:A:291:PHE:CD2	1:A:317:MET:HE3	2.55	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.85	0.41
1:A:86:LEU:HD21	1:A:277:TRP:CH2	2.56	0.41
1:A:119:TRP:O	1:A:123:ILE:HG12	2.20	0.40
1:A:499:PRO:HG2	1:A:500:VAL:HG23	2.03	0.40
1:B:363:GLN:CB	2:B:902:AMP:H5'1	2.51	0.40
1:A:246:ALA:HA	1:A:275:GLU:OE1	2.21	0.40
1:B:89:ASN:O	1:B:92:GLN:HB2	2.21	0.40
1:A:50:VAL:CG1	1:A:278:ALA:HA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	535/570 (94%)	526 (98%)	9 (2%)	0	100	100
1	B	531/570 (93%)	520 (98%)	11 (2%)	0	100	100
All	All	1066/1140 (94%)	1046 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	450/485 (93%)	434 (96%)	16 (4%)	40	60
1	B	437/485 (90%)	425 (97%)	12 (3%)	50	71
All	All	887/970 (91%)	859 (97%)	28 (3%)	45	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	166	GLU
1	A	199	ASN
1	A	283	THR
1	A	288	LEU
1	A	294	LEU
1	A	297	LEU
1	A	330[A]	HIS
1	A	330[B]	HIS
1	A	340	SER
1	A	368	LEU
1	A	371	MET
1	A	374	LYS
1	A	423	PHE
1	A	461	ARG
1	A	569	LYS
1	B	89	ASN
1	B	166	GLU
1	B	199	ASN
1	B	294	LEU
1	B	297	LEU
1	B	328	PHE
1	B	340	SER
1	B	368	LEU
1	B	371	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	LYS
1	B	423	PHE
1	B	461	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	HIS
1	A	522	GLN
1	B	518	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	AMP	A	901	-	22,25,25	1.19	2 (9%)	24,38,38	1.70	5 (20%)
3	BCO	A	911	-	48,55,55	2.28	8 (16%)	55,81,81	2.47	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AMP	B	902	-	22,25,25	1.19	3 (13%)	24,38,38	1.91	4 (16%)
3	BCO	B	912	-	48,55,55	2.21	7 (14%)	55,81,81	2.38	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	901	-	-	0/6/26/26	0/3/3/3
3	BCO	A	911	-	1/1/12/14	0/50/70/70	0/3/3/3
2	AMP	B	902	-	-	0/6/26/26	0/3/3/3
3	BCO	B	912	-	1/1/12/14	0/50/70/70	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	912	BCO	C22-S1	-5.62	1.64	1.76
3	A	911	BCO	C22-S1	-5.20	1.65	1.76
2	B	902	AMP	C2-N3	2.08	1.35	1.32
2	B	902	AMP	O4'-C1'	2.10	1.44	1.41
3	B	912	BCO	C15-N3	2.12	1.35	1.32
3	A	911	BCO	O17-C22	2.25	1.24	1.21
3	A	911	BCO	O1-C4	2.26	1.44	1.41
3	B	912	BCO	P1-O9	2.45	1.59	1.50
2	A	901	AMP	C2-N3	2.59	1.36	1.32
3	A	911	BCO	P1-O9	2.73	1.60	1.50
2	B	902	AMP	C5-C4	3.26	1.47	1.40
2	A	901	AMP	C5-C4	3.42	1.48	1.40
3	B	912	BCO	P1-O5	5.69	1.78	1.54
3	A	911	BCO	P1-O5	5.77	1.78	1.54
3	B	912	BCO	P1-O6	5.81	1.78	1.54
3	A	911	BCO	P1-O6	5.86	1.78	1.54
3	B	912	BCO	P2-O10	7.11	1.77	1.50
3	A	911	BCO	P3-O13	7.13	1.77	1.50
3	B	912	BCO	P3-O13	7.48	1.79	1.50
3	A	911	BCO	P2-O10	7.67	1.79	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	911	BCO	N3-C15-N4	-9.62	120.48	128.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	912	BCO	N3-C15-N4	-7.93	121.95	128.86
3	B	912	BCO	O17-C22-S1	-7.64	114.84	122.84
2	B	902	AMP	N3-C2-N1	-7.06	122.71	128.86
3	B	912	BCO	C17-C18-C19	-6.64	101.54	112.22
3	A	911	BCO	O17-C22-S1	-6.44	116.09	122.84
3	A	911	BCO	C17-C18-C19	-5.85	102.82	112.22
2	A	901	AMP	N3-C2-N1	-5.71	123.89	128.86
3	B	912	BCO	O16-C19-C18	-4.63	113.31	122.01
3	A	911	BCO	C14-C9-C10	-4.20	101.54	108.82
3	B	912	BCO	C10-C16-N6	-3.12	110.09	116.58
3	A	911	BCO	C13-C9-C11	-3.02	103.93	108.37
3	A	911	BCO	O16-C19-C18	-2.64	117.06	122.01
3	A	911	BCO	C17-N6-C16	-2.51	117.90	122.59
2	A	901	AMP	C4-C5-N7	-2.51	106.98	109.41
2	A	901	AMP	C1'-N9-C4	-2.23	122.78	126.64
2	B	902	AMP	O5'-P-O1P	-2.06	100.69	106.47
3	A	911	BCO	C18-C17-N6	2.09	116.20	111.87
2	B	902	AMP	C2-N1-C6	2.22	122.66	118.77
3	B	912	BCO	C20-N7-C19	2.23	127.13	122.84
2	A	901	AMP	N6-C6-N1	2.24	123.20	118.77
3	B	912	BCO	O16-C19-N7	2.27	127.32	122.97
2	A	901	AMP	C2-N1-C6	2.28	122.76	118.77
2	B	902	AMP	N6-C6-N1	2.61	123.95	118.77
3	B	912	BCO	C13-C9-C10	2.97	113.96	108.82
3	A	911	BCO	C13-C9-C10	4.49	116.61	108.82
3	A	911	BCO	C14-C9-C11	5.02	115.73	108.37
3	A	911	BCO	C23-C22-S1	5.54	118.86	113.28
3	B	912	BCO	C23-C22-S1	7.26	120.60	113.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	912	BCO	C10
3	A	911	BCO	C10

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AMP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	911	BCO	2	0
2	B	902	AMP	1	0

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	533/570 (93%)	-0.04	22 (4%) 38 36	8, 17, 39, 71	0
1	B	533/570 (93%)	0.12	32 (6%) 23 21	8, 18, 38, 71	1 (0%)
All	All	1066/1140 (93%)	0.04	54 (5%) 29 27	8, 18, 39, 71	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	HIS	6.1
1	A	39	GLU	5.8
1	A	37	HIS	5.6
1	A	500	VAL	5.5
1	B	39	GLU	5.4
1	A	38	GLN	5.2
1	A	553	THR	4.5
1	B	189	ASP	4.5
1	B	553	THR	4.3
1	B	325	SER	4.2
1	B	187	SER	4.0
1	B	555	THR	3.9
1	A	556	GLY	3.9
1	B	569	LYS	3.8
1	B	60	ALA	3.7
1	B	556	GLY	3.7
1	A	569	LYS	3.6
1	B	188	CYS	3.5
1	A	554	VAL	3.5
1	A	555	THR	3.3
1	B	352	GLN	3.3
1	B	499	PRO	3.2
1	B	554	VAL	3.2
1	B	568	TRP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	417	ILE	3.0
1	A	61	GLY	3.0
1	A	40	VAL	2.9
1	B	202	SER	2.9
1	B	206	HIS	2.9
1	A	206	HIS	2.9
1	A	60	ALA	2.8
1	A	417	ILE	2.8
1	B	53	HIS	2.8
1	B	62	LYS	2.8
1	B	201	ALA	2.8
1	B	165	GLN	2.8
1	B	497	PRO	2.7
1	B	500	VAL	2.6
1	B	38	GLN	2.5
1	B	124	LEU	2.4
1	A	199	ASN	2.4
1	A	499	PRO	2.4
1	B	411	GLY	2.4
1	A	430	PRO	2.3
1	B	493	VAL	2.3
1	A	522	GLN	2.3
1	B	347	GLU	2.2
1	B	518	HIS	2.2
1	A	498	ASP	2.2
1	A	62	LYS	2.1
1	B	431	ASP	2.1
1	A	325	SER	2.0
1	A	519	ASP	2.0
1	B	172	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	BCO	B	912	53/53	0.86	0.22	1.99	25,47,70,75	0
3	BCO	A	911	53/53	0.87	0.22	1.92	17,48,92,105	0
2	AMP	B	902	23/23	0.94	0.13	-0.04	25,34,55,67	0
2	AMP	A	901	23/23	0.96	0.12	-0.65	13,21,40,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.