



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2020 – 10:47 AM EST

PDB ID : 6L2G
Title : Crystal structure of Aspergillus fumigatus mitochondrial acetyl-CoA acetyltransferase
Authors : Zhang, Y.; Wei, W.; Raimi, O.G.; Ferenbach, A.T.; Fang, W.
Deposited on : 2019-10-03
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

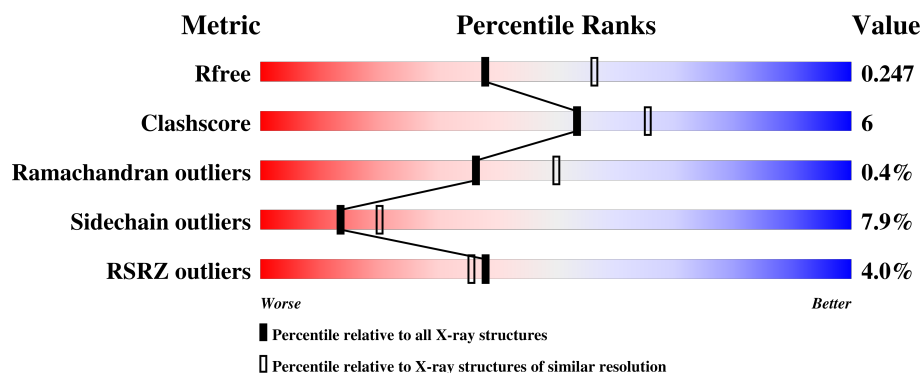
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	111664	4090 (2.44-2.40)
Clashscore	122126	4587 (2.44-2.40)
Ramachandran outliers	120053	4522 (2.44-2.40)
Sidechain outliers	120020	4523 (2.44-2.40)
RSRZ outliers	108989	3987 (2.44-2.40)

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	397	<div> <div>3%</div> <div>83% 16% .</div> </div>
1	B	397	<div> <div>6%</div> <div>84% 14% .</div> </div>
1	C	397	<div> <div>%</div> <div>85% 14% .</div> </div>
1	D	397	<div> <div>6%</div> <div>82% 16% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11908 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 Acetyl-CoA-acetyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			2944	1852	515	565	12			
1	B	397	Total	C	N	O	S	0	0	0
			2944	1852	515	565	12			
1	C	397	Total	C	N	O	S	0	0	0
			2944	1852	515	565	12			
1	D	397	Total	C	N	O	S	0	0	0
			2944	1852	515	565	12			

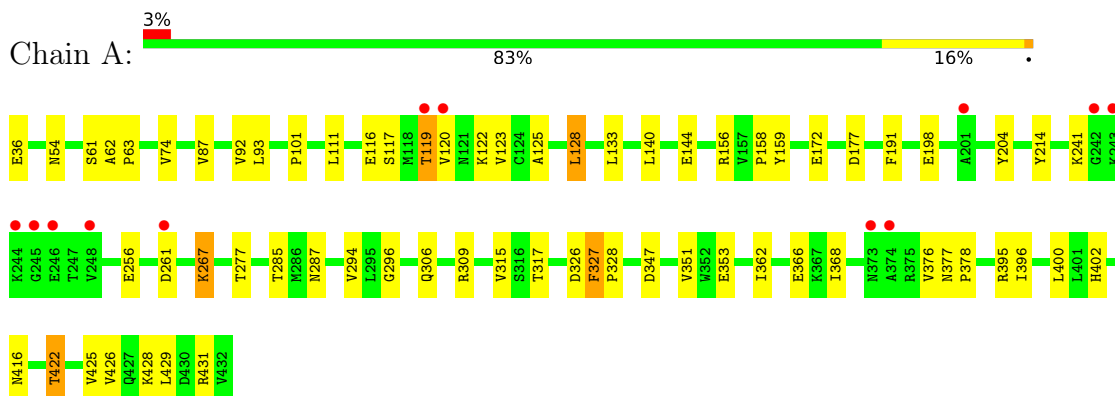
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	44	Total	O	0	0
			44	44		
2	C	35	Total	O	0	0
			35	35		
2	D	18	Total	O	0	0
			18	18		

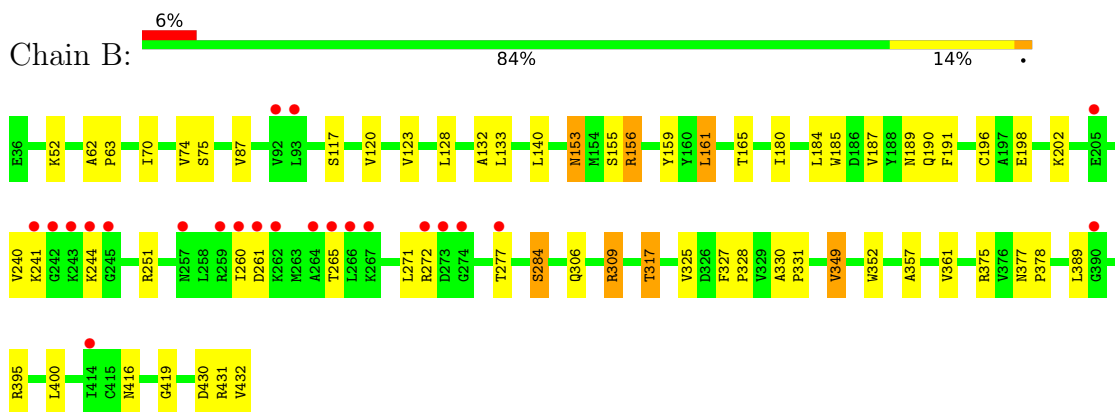
3 Residue-property plots

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.

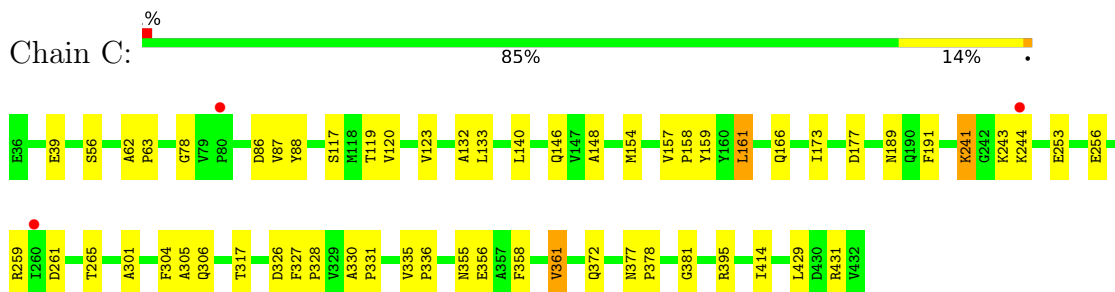
- Molecule 1: Acetyl-CoA-acetyltransferase, putative



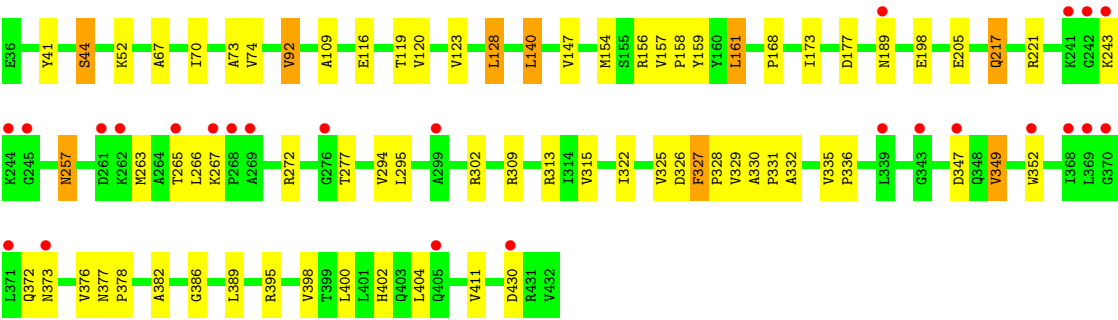
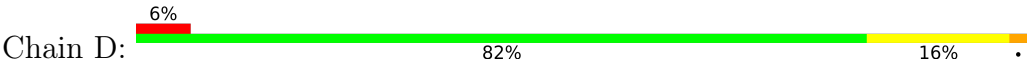
- Molecule 1: Acetyl-CoA-acetyltransferase, putative



- Molecule 1: Acetyl-CoA-acetyltransferase, putative



- Molecule 1: Acetyl-CoA-acetyltransferase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.51Å 174.78Å 179.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 2.41 48.84 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.84-2.41) 97.0 (48.84-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.200 , 0.252 0.204 , 0.247	Depositor DCC
R_{free} test set	2100 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11908	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCY

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	0.70	0/2980	0.86	0/4036
1	B	0.70	0/2980	0.87	1/4036 (0.0%)
1	C	0.68	0/2980	0.86	0/4036
1	D	0.69	0/2980	0.84	0/4036
All	All	0.69	0/11920	0.86	1/16144 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	ARG	NE-CZ-NH1	-5.17	117.72	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	2944	0	2980	37	0
1	B	2944	0	2980	34	0
1	C	2944	0	2980	34	0
1	D	2944	0	2980	41	0
2	A	35	0	0	0	0
2	B	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	35	0	0	0	0
2	D	18	0	0	0	0
All	All	11908	0	11920	137	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 6.

All (137) 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:D:44:SER:OG	1:D:73:ALA:O	1.76	1.02
1:A:198:GLU:OE1	1:A:277:THR:HG22	1.70	0.91
1:C:241:LYS:H	1:C:241:LYS:HE2	1.39	0.87
1:C:241:LYS:H	1:C:241:LYS:CE	1.92	0.81
1:B:153:ASN:HD21	1:B:155:SER:HB2	1.59	0.66
1:C:78:GLY:O	1:C:304:PHE:HB3	1.96	0.66
1:A:125:ALA:HB1	1:A:422:THR:HG23	1.77	0.66
1:D:335:VAL:CG2	1:D:336:PRO:HD3	2.28	0.64
1:C:306:GLN:OE1	1:C:431:ARG:CB	2.47	0.62
1:D:44:SER:CB	1:D:73:ALA:O	2.47	0.62
1:D:198:GLU:OE1	1:D:277:THR:HG22	2.00	0.62
1:D:189:ASN:OD1	1:D:325:VAL:HG13	2.00	0.62
1:B:198:GLU:OE1	1:B:277:THR:HG22	2.02	0.60
1:B:62:ALA:HB3	1:B:63:PRO:HD3	1.84	0.60
1:C:306:GLN:OE1	1:C:431:ARG:HB2	2.01	0.59
1:A:122:LYS:HZ2	1:A:422:THR:HG22	1.68	0.58
1:A:92:VAL:HG22	1:A:93:LEU:HG	1.84	0.58
1:A:159:TYR:CE2	1:D:173:ILE:HG12	2.38	0.58
1:B:309:ARG:HH21	1:B:309:ARG:HG2	1.68	0.58
1:B:309:ARG:HG2	1:B:309:ARG:NH2	2.17	0.57
1:B:327:PHE:N	1:B:328:PRO:CD	2.68	0.57
1:B:349:VAL:CG2	1:B:352:TRP:CE2	2.88	0.56
1:B:306:GLN:OE1	1:B:431:ARG:HB2	2.06	0.55
1:C:140:LEU:HD21	1:D:140:LEU:HD13	1.87	0.55
1:B:284:SER:OG	1:B:357:ALA:O	2.23	0.55
1:D:349:VAL:HG21	1:D:352:TRP:CE2	2.43	0.54
1:C:241:LYS:N	1:C:241:LYS:HE2	2.14	0.54
1:C:306:GLN:OE1	1:C:431:ARG:CA	2.56	0.54
1:D:349:VAL:CG2	1:D:352:TRP:CE2	2.91	0.53
1:B:306:GLN:OE1	1:B:431:ARG:CB	2.56	0.53
1:D:322:ILE:HD11	1:D:326:ASP:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:TYR:CE1	1:D:313:ARG:HB2	2.43	0.53
1:C:358:PHE:O	1:C:361:VAL:HG12	2.09	0.53
1:A:315:VAL:CG2	1:A:425:VAL:HG12	2.38	0.52
1:C:306:GLN:OE1	1:C:431:ARG:HA	2.09	0.52
1:D:335:VAL:HG22	1:D:336:PRO:HD3	1.90	0.52
1:D:257:ASN:HD22	1:D:257:ASN:N	2.07	0.52
1:B:196:CYS:HB3	1:B:325:VAL:O	2.09	0.52
1:D:44:SER:HB2	1:D:294:VAL:HB	1.92	0.52
1:A:306:GLN:OE1	1:A:431:ARG:HB2	2.10	0.51
1:B:327:PHE:CG	1:B:328:PRO:HD3	2.46	0.51
1:C:326:ASP:C	1:C:328:PRO:HD2	2.31	0.51
1:B:306:GLN:O	1:B:430:ASP:O	2.29	0.51
1:B:153:ASN:ND2	1:B:156:ARG:HG3	2.25	0.51
1:C:154:MET:HA	1:C:157:VAL:HG13	1.91	0.50
1:B:187:VAL:O	1:B:190:GLN:NE2	2.36	0.50
1:C:330:ALA:N	1:C:331:PRO:CD	2.73	0.50
1:A:377:ASN:N	1:A:378:PRO:HD3	2.27	0.50
1:B:153:ASN:CG	1:B:156:ARG:HG3	2.31	0.50
1:D:335:VAL:HG23	1:D:336:PRO:HD3	1.93	0.50
1:C:158:PRO:O	1:C:177:ASP:O	2.29	0.50
1:D:327:PHE:N	1:D:328:PRO:CD	2.75	0.50
1:B:153:ASN:C	1:B:153:ASN:HD22	2.15	0.50
1:D:382:ALA:HA	1:D:386:GLY:O	2.12	0.49
1:A:366:GLU:OE1	1:A:376:VAL:HG21	2.13	0.49
1:D:309:ARG:NH1	1:D:402:HIS:O	2.42	0.49
1:A:36:GLU:OE2	1:A:36:GLU:N	2.46	0.48
1:A:204:TYR:CE2	1:A:368:ILE:HD11	2.48	0.48
1:A:101:PRO:HD2	1:A:119:THR:HG21	1.95	0.48
1:A:353:GLU:CG	1:A:396:ILE:HB	2.43	0.48
1:C:132:ALA:HB2	1:C:317:THR:HG21	1.95	0.48
1:C:159:TYR:HB2	1:D:161:LEU:HB3	1.96	0.48
1:C:56:SER:OG	1:C:253:GLU:OE1	2.29	0.47
1:A:309:ARG:NH1	1:A:402:HIS:O	2.44	0.47
1:D:41:TYR:HE1	1:D:313:ARG:HB2	1.79	0.47
1:A:122:LYS:NZ	1:A:422:THR:HG22	2.30	0.47
1:B:70:ILE:O	1:B:74:VAL:HG13	2.15	0.47
1:D:41:TYR:CD1	1:D:313:ARG:HA	2.49	0.47
1:D:158:PRO:O	1:D:177:ASP:O	2.32	0.46
1:B:87:VAL:O	1:B:117:SER:HA	2.15	0.46
1:A:306:GLN:OE1	1:A:431:ARG:CB	2.64	0.46
1:A:54:ASN:CG	1:B:165:THR:HG21	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:NH1	2:B:501:HOH:O	2.49	0.46
1:B:330:ALA:N	1:B:331:PRO:CD	2.79	0.46
1:D:395:ARG:O	1:D:398:VAL:HG22	2.16	0.46
1:B:349:VAL:HG21	1:B:352:TRP:CE2	2.50	0.45
1:A:158:PRO:O	1:A:177:ASP:O	2.33	0.45
1:C:154:MET:HA	1:C:157:VAL:CG1	2.46	0.45
1:D:349:VAL:CG2	1:D:352:TRP:NE1	2.79	0.45
1:C:301:ALA:O	1:C:305:ALA:N	2.32	0.45
1:A:326:ASP:C	1:A:328:PRO:HD2	2.36	0.45
1:A:327:PHE:N	1:A:328:PRO:CD	2.79	0.45
1:C:161:LEU:HB3	1:D:159:TYR:HB2	1.99	0.45
1:D:41:TYR:HD1	1:D:313:ARG:HA	1.82	0.45
1:B:328:PRO:HB3	1:B:361:VAL:HG22	1.99	0.44
1:D:330:ALA:N	1:D:331:PRO:CD	2.81	0.44
1:D:329:VAL:O	1:D:332:ALA:HB3	2.18	0.44
1:A:159:TYR:HB2	1:B:161:LEU:HB3	1.99	0.44
1:A:315:VAL:HG22	1:A:425:VAL:HG12	1.99	0.44
1:A:74:VAL:HA	1:A:294:VAL:HG21	2.00	0.44
1:C:377:ASN:N	1:C:378:PRO:HD3	2.33	0.44
1:D:217:GLN:OE1	1:D:221:ARG:NH1	2.51	0.44
1:D:377:ASN:N	1:D:378:PRO:HD3	2.32	0.44
1:C:88:TYR:O	1:C:148:ALA:HA	2.18	0.43
1:A:140:LEU:HD21	1:B:140:LEU:HG	2.00	0.43
1:C:86:ASP:HB2	1:C:146:GLN:NE2	2.33	0.43
1:C:166:GLN:OE1	1:D:156:ARG:HA	2.19	0.43
1:C:159:TYR:HA	1:C:177:ASP:O	2.18	0.43
1:D:294:VAL:C	1:D:295:LEU:HD23	2.39	0.43
1:D:67:ALA:HA	1:D:109:ALA:HB2	2.01	0.43
1:C:327:PHE:CG	1:C:328:PRO:HD3	2.54	0.43
1:D:376:VAL:O	1:D:376:VAL:HG23	2.19	0.43
1:B:159:TYR:CE2	1:C:173:ILE:HG12	2.54	0.43
1:B:309:ARG:HH21	1:B:309:ARG:CG	2.28	0.42
1:A:62:ALA:N	1:A:63:PRO:CD	2.82	0.42
1:D:128:LEU:HA	1:D:128:LEU:HD23	1.80	0.42
1:D:400:LEU:HD21	1:D:404:LEU:HD11	2.00	0.42
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.87	0.42
1:C:356:GLU:CD	1:C:381:GLY:HA3	2.40	0.42
1:A:172:GLU:H	1:A:172:GLU:CD	2.22	0.42
1:C:86:ASP:HB2	1:C:146:GLN:HE22	1.85	0.42
1:A:285:THR:OG1	1:A:287:ASN:OD1	2.27	0.42
1:C:62:ALA:HB3	1:C:63:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:O	1:A:117:SER:HA	2.20	0.42
1:A:61:SER:HA	1:A:156:ARG:HD2	2.02	0.42
1:A:315:VAL:CG2	1:A:425:VAL:CG1	2.97	0.42
1:A:353:GLU:HG3	1:A:396:ILE:HB	2.02	0.41
1:C:327:PHE:N	1:C:328:PRO:CD	2.83	0.41
1:C:355:ASN:HB2	1:C:414:ILE:HD12	2.02	0.41
1:A:327:PHE:CG	1:A:328:PRO:HD3	2.56	0.41
1:D:140:LEU:HA	1:D:140:LEU:HD12	1.93	0.41
1:B:349:VAL:HG22	1:B:352:TRP:CE2	2.55	0.41
1:B:377:ASN:N	1:B:378:PRO:HD3	2.35	0.41
1:B:180:ILE:O	1:B:185:TRP:HB2	2.21	0.41
1:A:144:GLU:O	1:A:296:GLY:HA2	2.20	0.41
1:C:335:VAL:HB	1:C:336:PRO:HD3	2.01	0.41
1:D:168:PRO:HD2	1:D:173:ILE:HD12	2.03	0.41
1:B:284:SER:OG	1:B:357:ALA:HA	2.21	0.41
1:D:92:VAL:CG1	1:D:389:LEU:HB3	2.51	0.41
1:C:87:VAL:O	1:C:117:SER:HA	2.20	0.41
1:B:327:PHE:CB	1:B:419:GLY:HA2	2.51	0.40
1:A:214:TYR:CZ	1:A:362:ILE:HG21	2.56	0.40
1:B:132:ALA:HB2	1:B:317:THR:HG21	2.03	0.40
1:D:70:ILE:O	1:D:74:VAL:HG13	2.22	0.40
1:A:267:LYS:H	1:A:267:LYS:HG3	1.77	0.40
1:A:327:PHE:CD1	1:A:327:PHE:C	2.95	0.40
1:D:154:MET:HA	1:D:157:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	394/397 (99%)	375 (95%)	18 (5%)	1 (0%)	43 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	394/397 (99%)	377 (96%)	15 (4%)	2 (0%)	31	43
1	C	394/397 (99%)	370 (94%)	23 (6%)	1 (0%)	43	57
1	D	394/397 (99%)	370 (94%)	22 (6%)	2 (0%)	31	43
All	All	1576/1588 (99%)	1492 (95%)	78 (5%)	6 (0%)	36	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	B	123	VAL
1	B	241	LYS
1	C	123	VAL
1	D	123	VAL
1	D	205	GLU

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	299/299 (100%)	277 (93%)	22 (7%)	15	23
1	B	299/299 (100%)	271 (91%)	28 (9%)	9	13
1	C	299/299 (100%)	281 (94%)	18 (6%)	21	32
1	D	299/299 (100%)	272 (91%)	27 (9%)	10	15
All	All	1196/1196 (100%)	1101 (92%)	95 (8%)	13	20

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	A	116	GLU
1	A	119	THR
1	A	120	VAL
1	A	128	LEU

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	191	PHE
1	A	241	LYS
1	A	256	GLU
1	A	261	ASP
1	A	267	LYS
1	A	317	THR
1	A	327	PHE
1	A	347	ASP
1	A	351	VAL
1	A	395	ARG
1	A	400	LEU
1	A	416	ASN
1	A	422	THR
1	A	426	VAL
1	A	428	LYS
1	A	429	LEU
1	B	52	LYS
1	B	75	SER
1	B	120	VAL
1	B	128	LEU
1	B	133	LEU
1	B	153	ASN
1	B	156	ARG
1	B	161	LEU
1	B	184	LEU
1	B	189	ASN
1	B	191	PHE
1	B	202	LYS
1	B	240	VAL
1	B	244	LYS
1	B	260	ILE
1	B	261	ASP
1	B	265	THR
1	B	271	LEU
1	B	272	ARG
1	B	284	SER
1	B	309	ARG
1	B	317	THR
1	B	349	VAL
1	B	389	LEU
1	B	395	ARG

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Mol	Chain	Res	Type
1	B	400	LEU
1	B	416	ASN
1	B	432	VAL
1	C	39	GLU
1	C	119	THR
1	C	120	VAL
1	C	133	LEU
1	C	161	LEU
1	C	189	ASN
1	C	191	PHE
1	C	241	LYS
1	C	243	LYS
1	C	244	LYS
1	C	256	GLU
1	C	259	ARG
1	C	261	ASP
1	C	265	THR
1	C	361	VAL
1	C	372	GLN
1	C	395	ARG
1	C	429	LEU
1	D	44	SER
1	D	52	LYS
1	D	92	VAL
1	D	116	GLU
1	D	119	THR
1	D	120	VAL
1	D	128	LEU
1	D	140	LEU
1	D	147	VAL
1	D	161	LEU
1	D	217	GLN
1	D	243	LYS
1	D	257	ASN
1	D	263	MET
1	D	265	THR
1	D	266	LEU
1	D	267	LYS
1	D	272	ARG
1	D	302	ARG
1	D	315	VAL
1	D	327	PHE

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Mol	Chain	Res	Type
1	D	347	ASP
1	D	349	VAL
1	D	372	GLN
1	D	373	ASN
1	D	411	VAL
1	D	430	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	257	ASN
1	B	153	ASN
1	B	211	GLN
1	B	213	GLN
1	B	257	ASN
1	C	137	ASN
1	C	146	GLN
1	C	211	GLN
1	C	355	ASN
1	C	427	GLN
1	D	257	ASN
1	D	355	ASN
1	D	373	ASN
1	D	416	ASN
1	D	427	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SCY	A	124	1	8,8,9	1.00	1 (12%)	4,9,11	1.20	1 (25%)
1	SCY	B	124	1	8,8,9	0.94	1 (12%)	4,9,11	0.88	0
1	SCY	C	124	1	8,8,9	0.95	1 (12%)	4,9,11	1.43	1 (25%)
1	SCY	D	124	1	8,8,9	1.04	1 (12%)	4,9,11	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	A	124	1	-	3/5/7/9	-
1	SCY	B	124	1	-	3/5/7/9	-
1	SCY	C	124	1	-	3/5/7/9	-
1	SCY	D	124	1	-	3/5/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	124	SCY	CA-C	2.74	1.53	1.50
1	A	124	SCY	CA-C	2.60	1.53	1.50
1	C	124	SCY	CA-C	2.43	1.53	1.50
1	B	124	SCY	CA-C	2.35	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	SCY	O-C-CA	-2.82	117.43	124.98
1	A	124	SCY	O-C-CA	-2.27	118.89	124.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	124	SCY	CA-CB-SG-CD
1	D	124	SCY	OCD-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	D	124	SCY	CE-CD-SG-CB
1	C	124	SCY	CA-CB-SG-CD
1	C	124	SCY	OCD-CD-SG-CB
1	C	124	SCY	CE-CD-SG-CB
1	B	124	SCY	CA-CB-SG-CD
1	B	124	SCY	OCD-CD-SG-CB
1	B	124	SCY	CE-CD-SG-CB
1	A	124	SCY	OCD-CD-SG-CB
1	A	124	SCY	CE-CD-SG-CB
1	A	124	SCY	CA-CB-SG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	396/397 (99%)	-0.06	12 (3%)	50	47	38, 58, 86, 144	0
1	B	396/397 (99%)	0.16	23 (5%)	23	21	40, 56, 97, 142	0
1	C	396/397 (99%)	-0.06	3 (0%)	86	84	43, 61, 91, 138	0
1	D	396/397 (99%)	0.28	25 (6%)	20	17	43, 81, 116, 160	0
All	All	1584/1588 (99%)	0.08	63 (3%)	38	36	38, 62, 102, 160	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	LYS	6.5
1	A	244	LYS	6.2
1	D	371	LEU	5.5
1	D	244	LYS	5.2
1	B	242	GLY	5.1
1	D	343	GLY	4.8
1	D	243	LYS	4.8
1	A	242	GLY	4.4
1	B	244	LYS	4.2
1	D	370	GLY	4.1
1	D	265	THR	4.1
1	D	269	ALA	3.6
1	B	265	THR	3.6
1	B	259	ARG	3.6
1	D	267	LYS	3.6
1	D	245	GLY	3.6
1	B	262	LYS	3.5
1	D	369	LEU	3.4
1	D	368	ILE	3.4
1	B	245	GLY	3.4
1	D	276	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	347	ASP	3.3
1	A	243	LYS	3.2
1	B	274	GLY	3.1
1	D	242	GLY	3.1
1	B	92	VAL	3.1
1	B	266	LEU	3.1
1	D	261	ASP	2.9
1	D	352	TRP	2.9
1	A	245	GLY	2.8
1	B	241	LYS	2.8
1	D	241	LYS	2.7
1	C	80	PRO	2.7
1	D	373	ASN	2.6
1	A	201	ALA	2.6
1	A	374	ALA	2.6
1	B	260	ILE	2.6
1	B	273	ASP	2.5
1	B	261	ASP	2.5
1	D	268	PRO	2.5
1	C	244	LYS	2.5
1	B	267	LYS	2.4
1	B	272	ARG	2.4
1	D	430	ASP	2.4
1	A	119	THR	2.3
1	A	373	ASN	2.3
1	D	339	LEU	2.2
1	D	189	ASN	2.2
1	D	262	LYS	2.2
1	C	260	ILE	2.2
1	B	264	ALA	2.2
1	A	248	VAL	2.2
1	D	405	GLN	2.1
1	A	261	ASP	2.1
1	B	414	ILE	2.1
1	A	246	GLU	2.1
1	B	93	LEU	2.1
1	D	299	ALA	2.1
1	B	277	THR	2.1
1	B	257	ASN	2.1
1	A	120	VAL	2.0
1	B	205	GLU	2.0
1	B	390	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
1	SCY	C	124	9/10	0.89	0.25	49,57,86,95	0
1	SCY	D	124	9/10	0.95	0.13	61,74,94,95	0
1	SCY	B	124	9/10	0.95	0.34	43,46,72,74	0
1	SCY	A	124	9/10	0.96	0.17	40,44,67,71	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.