



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:07 PM GMT

PDB ID : 5AHS
Title : 3-Sulfinopropionyl-Coenzyme A (3SP-CoA) desulfonase from *Advenella mimgardefordensis* DPN7T: holo crystal structure with the substrate analog succinyl-CoA
Authors : Cianci, M.; Schuermann, M.; Meijers, R.; Schneider, T.R.; Steinbuechel, A.
Deposited on : 2015-02-06
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

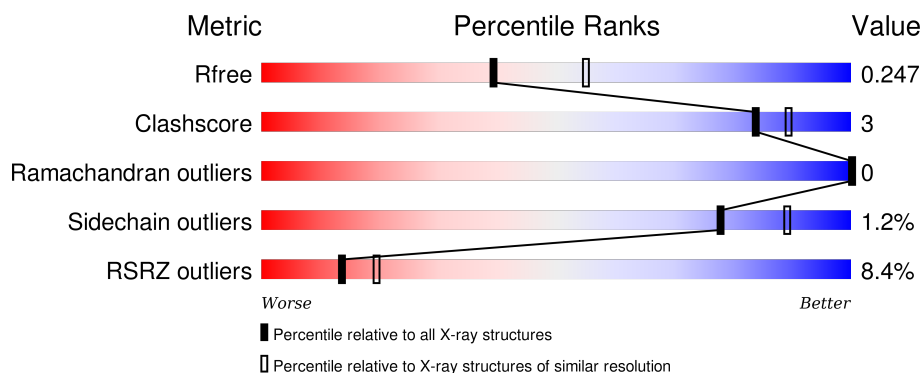
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	401	<div> <div>3%</div> <div>92%</div> <div>6%</div> </div>
1	B	401	<div> <div>4%</div> <div>91%</div> <div>6%</div> </div>
1	C	401	<div> <div>5%</div> <div>89%</div> <div>8%</div> </div>
1	D	401	<div> <div>4%</div> <div>92%</div> <div>•</div> </div>
1	E	401	<div> <div>13%</div> <div>89%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	401	

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	COA	A	411	-	-	-	X
3	COA	B	411	-	-	-	X
3	COA	D	411	-	-	-	X
3	COA	E	411	-	-	-	X
4	SIN	C	412	-	-	-	X

2 Entry composition [i](#)

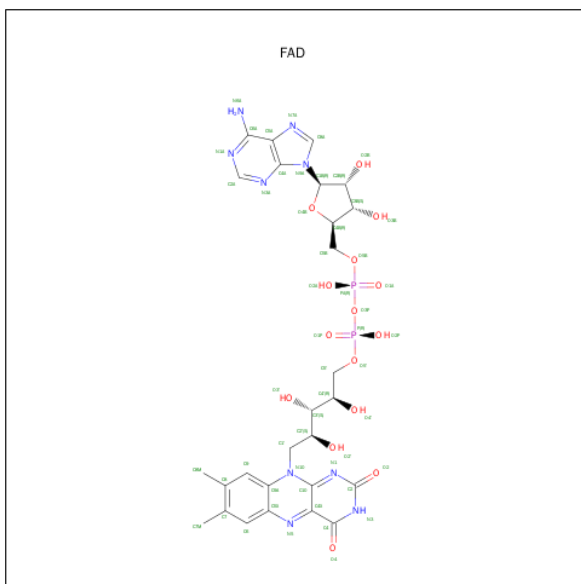
There are 6 unique types of molecules in this entry. The entry contains 19886 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-COA DEHYDROGENASE.

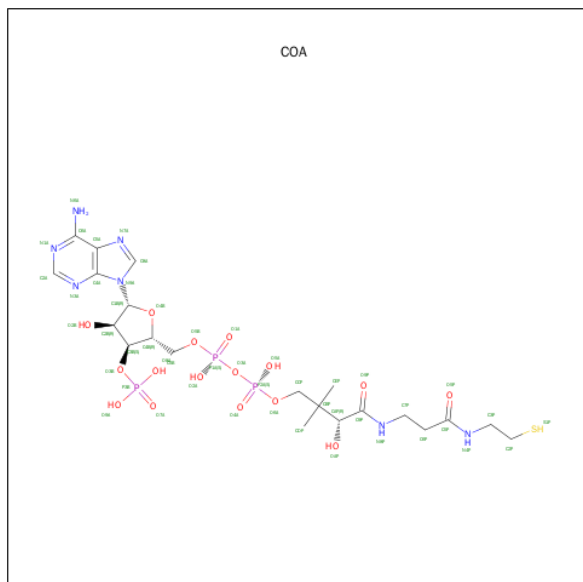
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			2980	1871	527	563	19			
1	B	391	Total	C	N	O	S	0	1	0
			2983	1872	528	564	19			
1	C	391	Total	C	N	O	S	0	0	0
			2974	1867	526	562	19			
1	D	390	Total	C	N	O	S	0	0	0
			2962	1858	525	560	19			
1	E	391	Total	C	N	O	S	0	0	0
			2974	1867	526	562	19			
1	F	391	Total	C	N	O	S	0	1	0
			2980	1871	527	563	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



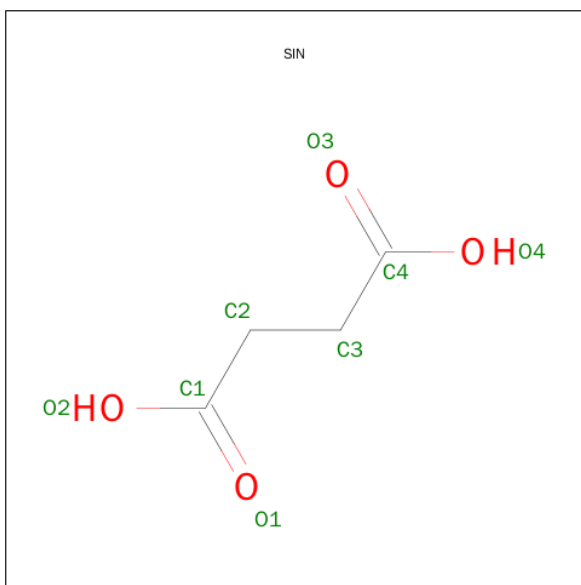
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

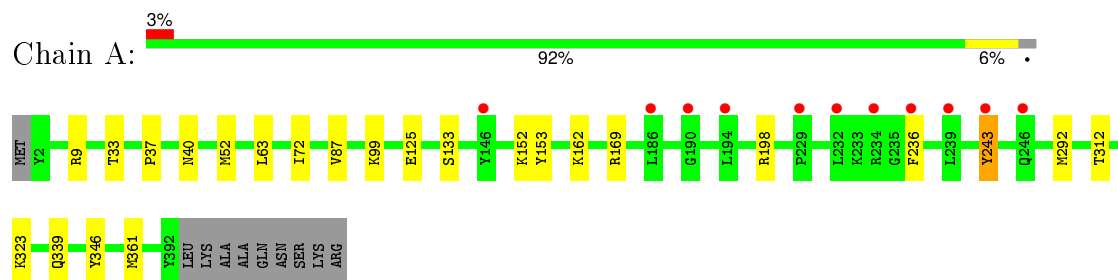
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total 327	O 327	0	0
6	B	271	Total 271	O 271	0	0
6	C	236	Total 236	O 236	0	0
6	D	220	Total 220	O 220	0	0
6	E	203	Total 203	O 203	0	0
6	F	205	Total 205	O 205	0	0

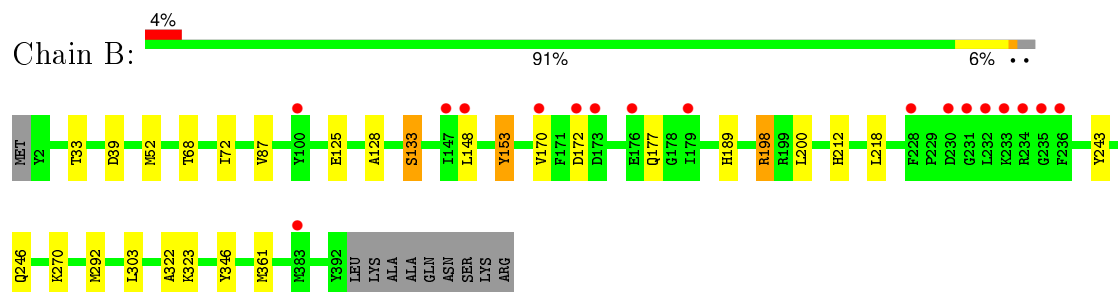
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

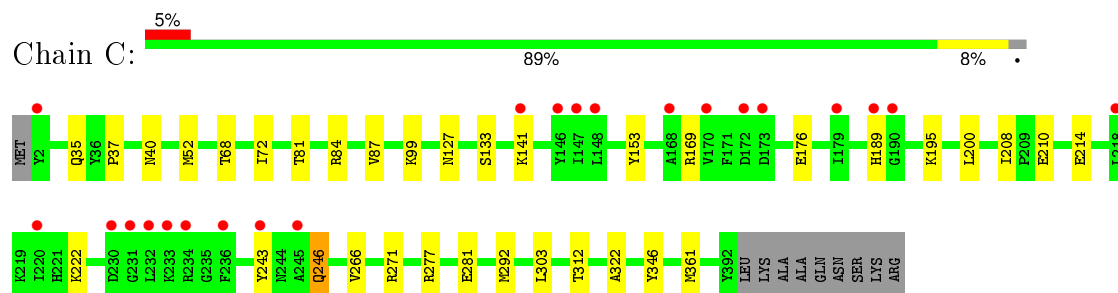
• Molecule 1: ACYL-COA DEHYDROGENASE



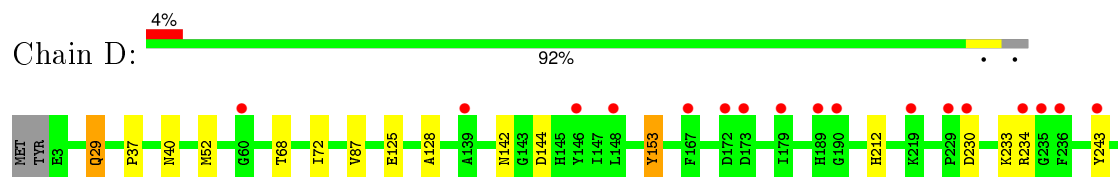
• Molecule 1: ACYL-COA DEHYDROGENASE



• Molecule 1: ACYL-COA DEHYDROGENASE

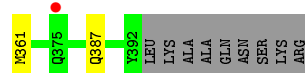
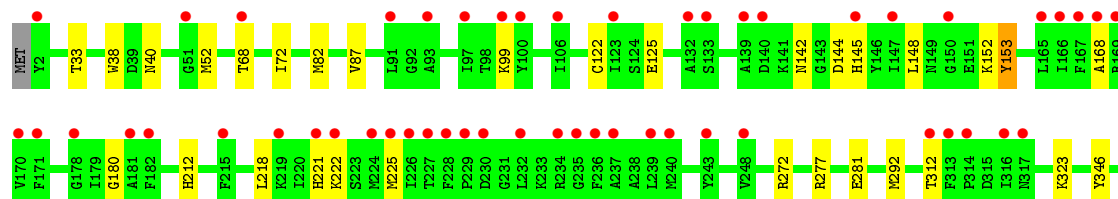
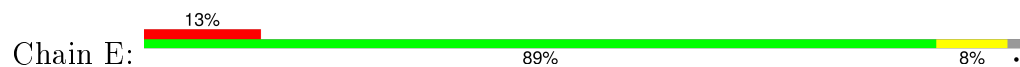


• Molecule 1: ACYL-COA DEHYDROGENASE

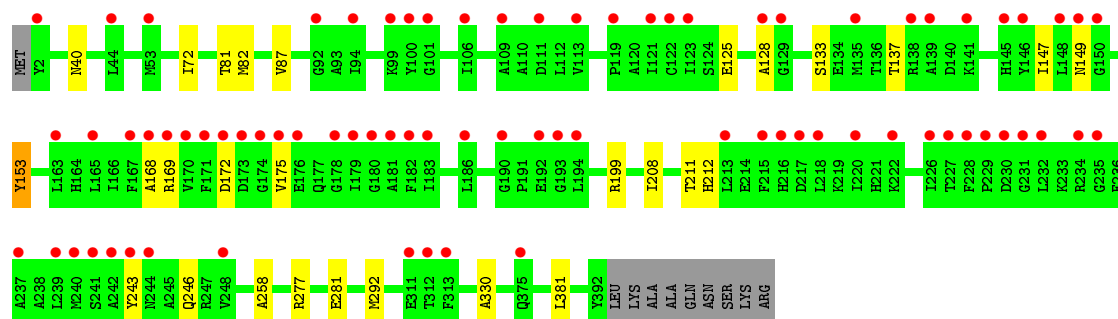
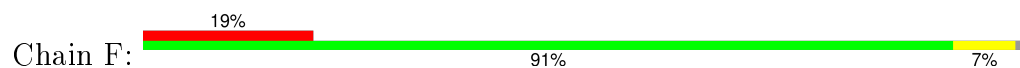




• Molecule 1: ACYL-COA DEHYDROGENASE



• Molecule 1: ACYL-COA DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.07 Å 233.49 Å 121.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.75 – 2.30 116.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (116.75-2.30) 99.8 (116.75-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.244 0.207 , 0.247	Depositor DCC
R_{free} test set	6352 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 126414 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19886	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, SO4, FAD, SIN

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	0.21	0/3034	0.36	0/4095
1	B	0.21	0/3034	0.36	0/4095
1	C	0.21	0/3025	0.36	0/4083
1	D	0.21	0/3012	0.36	0/4065
1	E	0.21	0/3025	0.35	0/4083
1	F	0.21	0/3034	0.35	0/4095
All	All	0.21	0/18164	0.36	0/24516

There are no bond length outliers.

There are no bond angle outliers.

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	2980	0	2971	18	0
1	B	2983	0	2970	19	0
1	C	2974	0	2963	22	0
1	D	2962	0	2954	13	0
1	E	2974	0	2963	24	0
1	F	2980	0	2971	14	0
2	A	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	2	0
2	E	53	0	31	1	0
2	F	53	0	31	3	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
3	D	48	0	32	3	0
3	E	48	0	32	1	0
3	F	48	0	32	2	0
4	C	8	0	4	3	0
5	C	5	0	0	0	0
6	A	327	0	0	6	0
6	B	271	0	0	4	0
6	C	236	0	0	6	0
6	D	220	0	0	4	0
6	E	203	0	0	7	0
6	F	205	0	0	1	0
All	All	19886	0	18142	109	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 3.

All (109) 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:E:122:CYS:SG	6:E:2084:HOH:O	2.44	0.75
1:B:243:TYR:OH	3:B:411:COA:S1P	2.48	0.69
1:E:180:GLY:O	6:E:2105:HOH:O	2.11	0.69
1:A:198:ARG:NH1	6:A:2172:HOH:O	2.29	0.66
1:D:354:ARG:NH1	6:D:2067:HOH:O	2.29	0.66
1:C:271:ARG:NH1	6:C:2160:HOH:O	2.31	0.63
1:A:133:SER:O	1:A:169:ARG:NH2	2.32	0.62
1:B:170:VAL:HG23	1:B:177:GLN:HB2	1.83	0.60
1:A:99:LYS:NZ	6:A:2126:HOH:O	2.34	0.60
4:C:412:SIN:O3	6:C:2188:HOH:O	2.17	0.60
1:A:9:ARG:NH2	6:A:2012:HOH:O	2.31	0.59
1:C:346:TYR:CZ	1:E:361:MET:HB3	2.38	0.59
1:C:246:GLN:NE2	6:C:2151:HOH:O	2.29	0.59
1:B:33:THR:HG22	1:E:33:THR:HG22	1.85	0.59
1:A:236:PHE:O	6:A:2216:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LYS:NZ	1:D:144:ASP:OD2	2.36	0.57
6:C:2162:HOH:O	1:E:387:GLN:O	2.17	0.57
2:A:410:FAD:O2'	3:A:411:COA:S1P	2.61	0.57
1:C:133:SER:O	1:C:169:ARG:NH2	2.38	0.56
1:D:52:MET:HE3	1:D:68:THR:HG22	1.88	0.56
1:F:72:ILE:HD13	1:F:87:VAL:HG22	1.88	0.56
1:C:361:MET:HB3	1:E:346:TYR:CZ	2.41	0.56
1:D:323:LYS:NZ	6:D:2178:HOH:O	2.38	0.56
1:E:142:ASN:ND2	6:E:2097:HOH:O	2.39	0.56
1:A:33:THR:HG22	1:E:38:TRP:HB3	1.87	0.55
1:F:243:TYR:OH	3:F:411:COA:S1P	2.55	0.55
1:C:52:MET:HE3	1:C:68:THR:HG22	1.90	0.54
1:A:361:MET:HB3	1:B:346:TYR:CZ	2.43	0.54
1:F:125:GLU:HB2	1:F:128:ALA:HB3	1.89	0.54
1:C:72:ILE:HD13	1:C:87:VAL:HG22	1.90	0.53
1:D:72:ILE:HD13	1:D:87:VAL:HG22	1.90	0.53
2:E:410:FAD:O2'	3:E:411:COA:S1P	2.66	0.53
2:F:410:FAD:O2A	6:F:2192:HOH:O	2.19	0.53
1:E:72:ILE:HD13	1:E:87:VAL:HG22	1.91	0.53
1:F:137:THR:HG23	1:F:168:ALA:HA	1.90	0.52
1:B:72:ILE:HD13	1:B:87:VAL:HG22	1.91	0.52
1:A:346:TYR:CZ	1:B:361:MET:HB3	2.45	0.52
1:B:125:GLU:HB2	1:B:128:ALA:HB3	1.92	0.51
2:D:410:FAD:HO2'	3:D:411:COA:HS1	1.50	0.51
2:D:410:FAD:O2'	3:D:411:COA:S1P	2.64	0.51
1:A:162:LYS:NZ	6:A:2180:HOH:O	2.42	0.50
2:F:410:FAD:O2'	3:F:411:COA:S1P	2.67	0.50
1:D:230:ASP:HB2	1:D:234:ARG:HH21	1.76	0.50
1:F:277:ARG:HD2	1:F:281:GLU:HB2	1.94	0.49
1:E:168:ALA:N	6:E:2105:HOH:O	2.31	0.49
1:C:81:THR:HG23	1:C:208:ILE:HG13	1.95	0.49
1:E:168:ALA:O	6:E:2105:HOH:O	2.20	0.48
1:C:84:ARG:HE	4:C:412:SIN:C1	2.27	0.48
1:C:127:ASN:HA	1:E:272:ARG:HH12	1.78	0.48
1:B:148:LEU:HB2	1:B:218:LEU:HB3	1.96	0.47
1:A:52:MET:HB3	1:A:63:LEU:HD12	1.96	0.47
1:C:277:ARG:HD2	1:C:281:GLU:HB2	1.96	0.47
1:A:323:LYS:NZ	6:A:2271:HOH:O	2.47	0.47
1:E:292:MET:HE3	1:E:292:MET:HB2	1.74	0.46
1:B:323:LYS:NZ	6:B:2226:HOH:O	2.47	0.46
1:D:37:PRO:HB2	1:D:40:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:GLY:N	6:E:2105:HOH:O	2.49	0.46
1:D:153:TYR:HA	1:D:212:HIS:HA	1.98	0.46
1:E:52:MET:HE3	1:E:68:THR:HG22	1.98	0.46
1:D:142:ASN:ND2	6:D:2110:HOH:O	2.49	0.45
1:C:141:LYS:NZ	6:C:2102:HOH:O	2.48	0.45
1:B:198:ARG:NH1	6:B:2157:HOH:O	2.49	0.45
1:D:243:TYR:OH	3:D:411:COA:S1P	2.56	0.45
1:E:144:ASP:HA	1:E:222:LYS:NZ	2.32	0.45
1:B:52:MET:HE3	1:B:68:THR:HG22	1.99	0.45
1:B:246[A]:GLN:NE2	6:B:2171:HOH:O	2.48	0.44
1:E:40:ASN:HB3	1:E:82:MET:SD	2.57	0.44
1:E:323:LYS:NZ	6:E:2163:HOH:O	2.51	0.44
1:F:81:THR:HG23	1:F:208:ILE:HG13	2.00	0.44
1:D:125:GLU:HB2	1:D:128:ALA:HB3	1.99	0.44
1:A:37:PRO:HB2	1:A:40:ASN:HB2	2.00	0.43
1:C:37:PRO:HB2	1:C:40:ASN:HB2	1.99	0.43
1:E:148:LEU:HB2	1:E:218:LEU:HB3	2.01	0.43
1:F:292:MET:HE3	1:F:292:MET:HB2	1.84	0.43
1:E:277:ARG:HD2	1:E:281:GLU:HB2	2.00	0.43
1:C:292:MET:HE3	1:C:292:MET:HB2	1.82	0.43
1:E:153:TYR:HA	1:E:212:HIS:HA	2.01	0.43
1:E:125:GLU:HG2	1:E:152:LYS:HD3	2.01	0.43
1:C:84:ARG:HH21	4:C:412:SIN:H32	1.83	0.43
1:A:339:GLN:O	2:B:410:FAD:O3B	2.30	0.43
1:A:243:TYR:OH	3:A:411:COA:S1P	2.59	0.43
1:B:153:TYR:HA	1:B:212:HIS:HA	2.01	0.43
1:C:169:ARG:NH1	1:C:176:GLU:OE2	2.48	0.42
2:F:410:FAD:O5'	2:F:410:FAD:O3'	2.36	0.42
1:C:303:LEU:HD23	1:C:322:ALA:HB1	1.99	0.42
1:F:258:ALA:HB2	1:F:330:ALA:HA	2.01	0.42
1:B:292:MET:HE3	1:B:292:MET:HB2	1.83	0.42
1:F:40:ASN:HB3	1:F:82:MET:SD	2.60	0.42
1:A:125:GLU:HG2	1:A:152:LYS:HD3	2.01	0.42
1:F:153:TYR:HA	1:F:212:HIS:HA	2.01	0.42
1:C:195:LYS:HB3	1:C:214:GLU:HB2	2.02	0.42
1:A:292:MET:HE3	1:A:292:MET:HB2	1.89	0.42
1:D:233:LYS:NZ	6:D:2122:HOH:O	2.52	0.42
1:C:99:LYS:HD3	1:C:312:THR:HG21	2.02	0.41
1:D:29:GLN:HA	1:D:29:GLN:HE21	1.85	0.41
1:E:145:HIS:CD2	1:E:221:HIS:HD2	2.38	0.41
1:C:200:LEU:N	1:C:210:GLU:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HD3	1:A:312:THR:HG21	2.03	0.41
1:A:72:ILE:HD13	1:A:87:VAL:HG22	2.01	0.41
1:F:199:ARG:HA	1:F:211:THR:HG22	2.03	0.41
1:B:133:SER:OG	6:B:2138:HOH:O	2.21	0.41
1:F:172:ASP:O	1:F:175:VAL:HG12	2.20	0.40
1:F:133:SER:O	1:F:169:ARG:NH2	2.55	0.40
1:B:303:LEU:HD23	1:B:322:ALA:HB1	2.03	0.40
1:E:99:LYS:HD3	1:E:312:THR:HG21	2.02	0.40
1:B:200:LEU:HD21	1:B:212:HIS:HE1	1.85	0.40
1:C:35:GLN:NE2	6:C:2029:HOH:O	2.41	0.40
1:C:266:VAL:HG13	1:F:381:LEU:HD23	2.03	0.40
1:B:39:ASP:N	1:B:39:ASP:OD1	2.55	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	390/401 (97%)	382 (98%)	8 (2%)	0	100	100
1	B	390/401 (97%)	380 (97%)	10 (3%)	0	100	100
1	C	389/401 (97%)	381 (98%)	8 (2%)	0	100	100
1	D	388/401 (97%)	380 (98%)	8 (2%)	0	100	100
1	E	389/401 (97%)	381 (98%)	8 (2%)	0	100	100
1	F	390/401 (97%)	377 (97%)	13 (3%)	0	100	100
All	All	2336/2406 (97%)	2281 (98%)	55 (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	304/311 (98%)	302 (99%)	2 (1%)	88	95
1	B	304/311 (98%)	299 (98%)	5 (2%)	70	84
1	C	303/311 (97%)	298 (98%)	5 (2%)	68	83
1	D	302/311 (97%)	299 (99%)	3 (1%)	82	91
1	E	303/311 (97%)	301 (99%)	2 (1%)	88	95
1	F	304/311 (98%)	299 (98%)	5 (2%)	70	84
All	All	1820/1866 (98%)	1798 (99%)	22 (1%)	78	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	TYR
1	A	243	TYR
1	B	133	SER
1	B	153	TYR
1	B	172	ASP
1	B	189	HIS
1	B	198	ARG
1	C	153	TYR
1	C	189	HIS
1	C	222	LYS
1	C	243	TYR
1	C	246	GLN
1	D	29	GLN
1	D	153	TYR
1	D	312	THR
1	E	153	TYR
1	E	225	MET
1	F	147	ILE
1	F	149	ASN
1	F	153	TYR
1	F	246[A]	GLN
1	F	246[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	D	29	GLN
1	D	212	HIS
1	D	295	GLN
1	D	355	HIS
1	D	370	GLN
1	E	212	HIS
1	F	177	GLN
1	F	212	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](#)

13 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	FAD	A	410	-	48,58,58	1.33	6 (12%)	54,89,89	2.06	11 (20%)
3	COA	A	411	-	40,50,50	0.80	1 (2%)	50,75,75	1.51	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	410	-	48,58,58	1.35	6 (12%)	54,89,89	2.07	10 (18%)
3	COA	B	411	-	40,50,50	0.79	1 (2%)	50,75,75	1.51	3 (6%)
5	SO4	C	1393	-	4,4,4	0.29	0	6,6,6	0.79	0
2	FAD	C	410	-	48,58,58	1.33	5 (10%)	54,89,89	2.12	11 (20%)
4	SIN	C	412	-	1,7,7	0.15	0	2,8,8	2.29	2 (100%)
2	FAD	D	410	-	48,58,58	1.34	6 (12%)	54,89,89	2.08	11 (20%)
3	COA	D	411	-	40,50,50	0.80	1 (2%)	50,75,75	1.53	4 (8%)
2	FAD	E	410	-	48,58,58	1.36	6 (12%)	54,89,89	2.10	11 (20%)
3	COA	E	411	-	40,50,50	0.80	1 (2%)	50,75,75	1.53	4 (8%)
2	FAD	F	410	-	48,58,58	1.35	6 (12%)	54,89,89	2.14	11 (20%)
3	COA	F	411	-	40,50,50	0.80	1 (2%)	50,75,75	1.45	4 (8%)

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	FAD	A	410	-	-	0/30/50/50	0/6/6/6
3	COA	A	411	-	-	0/44/64/64	0/3/3/3
2	FAD	B	410	-	-	0/30/50/50	0/6/6/6
3	COA	B	411	-	-	0/44/64/64	0/3/3/3
5	SO4	C	1393	-	-	0/0/0/0	0/0/0/0
2	FAD	C	410	-	-	0/30/50/50	0/6/6/6
4	SIN	C	412	-	-	0/1/5/5	0/0/0/0
2	FAD	D	410	-	-	0/30/50/50	0/6/6/6
3	COA	D	411	-	-	0/44/64/64	0/3/3/3
2	FAD	E	410	-	-	0/30/50/50	0/6/6/6
3	COA	E	411	-	-	0/44/64/64	0/3/3/3
2	FAD	F	410	-	-	0/30/50/50	0/6/6/6
3	COA	F	411	-	-	0/44/64/64	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	FAD	C9A-N10	2.02	1.41	1.38
2	F	410	FAD	C9A-N10	2.07	1.41	1.38
2	D	410	FAD	C9A-N10	2.10	1.41	1.38
2	E	410	FAD	C9A-N10	2.11	1.41	1.38
2	B	410	FAD	C9A-N10	2.15	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	410	FAD	C8-C7	2.97	1.48	1.41
2	D	410	FAD	C8-C7	2.97	1.49	1.41
2	B	410	FAD	C8-C7	2.99	1.49	1.41
2	C	410	FAD	C5A-C4A	3.00	1.47	1.40
2	A	410	FAD	C8-C7	3.00	1.49	1.41
2	E	410	FAD	C8-C7	3.01	1.49	1.41
2	F	410	FAD	C8-C7	3.03	1.49	1.41
2	A	410	FAD	C5A-C4A	3.05	1.47	1.40
3	D	411	COA	C5A-C4A	3.06	1.47	1.40
2	E	410	FAD	C5A-C4A	3.06	1.47	1.40
3	F	411	COA	C5A-C4A	3.06	1.47	1.40
2	F	410	FAD	C5A-C4A	3.07	1.47	1.40
2	B	410	FAD	C5A-C4A	3.07	1.47	1.40
3	B	411	COA	C5A-C4A	3.08	1.47	1.40
2	D	410	FAD	C5A-C4A	3.09	1.47	1.40
3	E	411	COA	C5A-C4A	3.10	1.47	1.40
3	A	411	COA	C5A-C4A	3.10	1.47	1.40
2	C	410	FAD	C9A-C5X	3.41	1.49	1.42
2	D	410	FAD	C9A-C5X	3.43	1.49	1.42
2	B	410	FAD	C9A-C5X	3.43	1.49	1.42
2	F	410	FAD	C9A-C5X	3.46	1.49	1.42
2	E	410	FAD	C9A-C5X	3.46	1.49	1.42
2	A	410	FAD	C9A-C5X	3.46	1.49	1.42
2	A	410	FAD	C4-C4X	3.61	1.48	1.41
2	C	410	FAD	C4-C4X	3.64	1.48	1.41
2	D	410	FAD	C4-C4X	3.68	1.48	1.41
2	B	410	FAD	C4-C4X	3.77	1.48	1.41
2	F	410	FAD	C4-C4X	3.82	1.48	1.41
2	A	410	FAD	C4X-C10	3.83	1.48	1.41
2	E	410	FAD	C4-C4X	3.83	1.48	1.41
2	B	410	FAD	C4X-C10	3.90	1.48	1.41
2	C	410	FAD	C4X-C10	3.91	1.48	1.41
2	E	410	FAD	C4X-C10	3.94	1.48	1.41
2	D	410	FAD	C4X-C10	3.97	1.48	1.41
2	F	410	FAD	C4X-C10	4.00	1.48	1.41

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	411	COA	N3A-C2A-N1A	-6.91	123.61	128.89
3	B	411	COA	N3A-C2A-N1A	-6.90	123.61	128.89
2	B	410	FAD	N3A-C2A-N1A	-6.86	123.64	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	410	FAD	N3A-C2A-N1A	-6.86	123.64	128.89
3	A	411	COA	N3A-C2A-N1A	-6.85	123.65	128.89
2	F	410	FAD	N3A-C2A-N1A	-6.85	123.65	128.89
2	E	410	FAD	N3A-C2A-N1A	-6.83	123.66	128.89
3	D	411	COA	N3A-C2A-N1A	-6.83	123.67	128.89
3	E	411	COA	N3A-C2A-N1A	-6.80	123.69	128.89
2	D	410	FAD	N3A-C2A-N1A	-6.79	123.70	128.89
2	A	410	FAD	N3A-C2A-N1A	-6.74	123.73	128.89
2	F	410	FAD	C4-C4X-C10	-5.38	116.50	119.94
2	C	410	FAD	C4-C4X-C10	-5.08	116.69	119.94
2	E	410	FAD	C4-C4X-C10	-4.85	116.84	119.94
2	B	410	FAD	C4-C4X-C10	-4.77	116.89	119.94
2	A	410	FAD	C4-C4X-C10	-4.72	116.92	119.94
2	D	410	FAD	C4-C4X-C10	-4.71	116.93	119.94
3	B	411	COA	P2A-O3A-P1A	-4.63	119.72	132.73
3	D	411	COA	P2A-O3A-P1A	-4.53	120.01	132.73
3	A	411	COA	P2A-O3A-P1A	-4.39	120.39	132.73
2	E	410	FAD	P-O3P-PA	-4.06	121.33	132.73
2	F	410	FAD	P-O3P-PA	-3.94	121.67	132.73
2	C	410	FAD	C4X-C4-N3	-3.79	118.40	123.59
2	A	410	FAD	C4X-C4-N3	-3.78	118.42	123.59
2	B	410	FAD	C4X-C4-N3	-3.76	118.45	123.59
2	E	410	FAD	C4X-C4-N3	-3.75	118.46	123.59
2	D	410	FAD	C4X-C4-N3	-3.74	118.47	123.59
2	F	410	FAD	C4X-C4-N3	-3.70	118.53	123.59
2	D	410	FAD	P-O3P-PA	-3.70	122.35	132.73
2	C	410	FAD	P-O3P-PA	-3.67	122.42	132.73
3	E	411	COA	P2A-O3A-P1A	-3.59	122.64	132.73
2	A	410	FAD	P-O3P-PA	-3.43	123.09	132.73
2	B	410	FAD	P-O3P-PA	-3.41	123.16	132.73
3	E	411	COA	C4A-C5A-N7A	-3.19	106.55	109.48
3	F	411	COA	C4A-C5A-N7A	-3.18	106.56	109.48
2	A	410	FAD	C4A-C5A-N7A	-3.14	106.59	109.48
3	B	411	COA	C4A-C5A-N7A	-3.14	106.59	109.48
2	B	410	FAD	C4A-C5A-N7A	-3.13	106.60	109.48
2	D	410	FAD	C4A-C5A-N7A	-3.08	106.65	109.48
3	A	411	COA	C4A-C5A-N7A	-3.07	106.65	109.48
2	F	410	FAD	C4A-C5A-N7A	-3.05	106.67	109.48
2	C	410	FAD	C4A-C5A-N7A	-3.02	106.70	109.48
2	E	410	FAD	C4A-C5A-N7A	-3.02	106.70	109.48
3	D	411	COA	C4A-C5A-N7A	-2.98	106.74	109.48
2	E	410	FAD	C2B-C1B-N9A	-2.72	110.14	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	410	FAD	C2B-C1B-N9A	-2.70	110.17	114.29
2	F	410	FAD	C2B-C1B-N9A	-2.56	110.38	114.29
2	C	410	FAD	C2B-C1B-N9A	-2.49	110.48	114.29
4	C	412	SIN	C2-C3-C4	-2.37	108.40	112.75
2	B	410	FAD	C2B-C1B-N9A	-2.31	110.76	114.29
3	F	411	COA	P2A-O3A-P1A	-2.27	126.36	132.73
4	C	412	SIN	C3-C2-C1	-2.20	108.72	112.75
3	F	411	COA	C2B-C1B-N9A	-2.18	110.97	114.29
2	A	410	FAD	C2B-C1B-N9A	-2.16	111.00	114.29
3	E	411	COA	O6A-CCP-CBP	-2.11	107.16	110.55
3	D	411	COA	C7P-C6P-C5P	-2.05	108.94	112.31
2	D	410	FAD	C1'-N10-C9A	2.14	121.26	118.86
2	E	410	FAD	C1'-N10-C9A	2.16	121.29	118.86
2	E	410	FAD	C5X-C9A-N10	2.18	119.28	117.62
2	B	410	FAD	C1'-N10-C9A	2.24	121.38	118.86
2	A	410	FAD	C5X-C9A-N10	2.26	119.34	117.62
2	C	410	FAD	C5X-C9A-N10	2.28	119.35	117.62
2	F	410	FAD	C5X-C9A-N10	2.29	119.36	117.62
2	F	410	FAD	C1'-N10-C9A	2.31	121.45	118.86
2	C	410	FAD	C1'-N10-C9A	2.37	121.53	118.86
2	D	410	FAD	C5X-C9A-N10	2.43	119.47	117.62
2	A	410	FAD	C4-C4X-N5	2.45	121.69	118.72
2	D	410	FAD	C4-C4X-N5	2.48	121.73	118.72
2	A	410	FAD	C1'-N10-C9A	2.52	121.69	118.86
2	B	410	FAD	C4-C4X-N5	2.66	121.95	118.72
2	E	410	FAD	C4-C4X-N5	2.70	121.99	118.72
2	C	410	FAD	C4-C4X-N5	2.77	122.08	118.72
2	F	410	FAD	C4-C4X-N5	3.06	122.44	118.72
2	A	410	FAD	C4X-N5-C5X	3.40	120.67	116.76
2	C	410	FAD	C4X-N5-C5X	3.48	120.77	116.76
2	D	410	FAD	C4X-N5-C5X	3.52	120.81	116.76
2	B	410	FAD	C4X-N5-C5X	3.58	120.88	116.76
2	F	410	FAD	C4X-N5-C5X	3.59	120.90	116.76
2	E	410	FAD	C4X-N5-C5X	3.67	120.99	116.76
2	D	410	FAD	C4-N3-C2	7.91	122.08	115.25
2	A	410	FAD	C4-N3-C2	7.95	122.12	115.25
2	C	410	FAD	C4-N3-C2	8.01	122.17	115.25
2	E	410	FAD	C4-N3-C2	8.03	122.19	115.25
2	B	410	FAD	C4-N3-C2	8.07	122.22	115.25
2	F	410	FAD	C4-N3-C2	8.12	122.26	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	410	FAD	1	0
3	A	411	COA	2	0
2	B	410	FAD	1	0
3	B	411	COA	1	0
4	C	412	SIN	3	0
2	D	410	FAD	2	0
3	D	411	COA	3	0
2	E	410	FAD	1	0
3	E	411	COA	1	0
2	F	410	FAD	3	0
3	F	411	COA	2	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	391/401 (97%)	0.19	11 (2%) 56 66	29, 43, 68, 98	0
1	B	391/401 (97%)	0.34	17 (4%) 39 48	27, 45, 84, 112	0
1	C	391/401 (97%)	0.39	22 (5%) 28 36	31, 50, 81, 104	0
1	D	390/401 (97%)	0.20	17 (4%) 38 47	34, 53, 77, 106	0
1	E	391/401 (97%)	0.82	53 (13%) 4 6	30, 53, 89, 112	0
1	F	391/401 (97%)	1.00	78 (19%) 1 2	30, 58, 101, 119	0
All	All	2345/2406 (97%)	0.49	198 (8%) 14 19	27, 50, 89, 119	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	171	PHE	9.0
1	F	170	VAL	7.8
1	F	100	TYR	7.4
1	E	239	LEU	7.2
1	E	226	ILE	7.2
1	C	236	PHE	7.1
1	F	182	PHE	6.3
1	C	190	GLY	6.3
1	B	232	LEU	6.3
1	B	231	GLY	6.2
1	E	236	PHE	6.1
1	F	226	ILE	6.0
1	B	233	LYS	5.9
1	E	97	ILE	5.9
1	F	178	GLY	5.9
1	C	2	TYR	5.9
1	E	227	THR	5.7
1	F	228	PHE	5.6
1	C	233	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	150	GLY	5.2
1	E	178	GLY	5.1
1	F	215	PHE	5.1
1	E	232	LEU	4.9
1	E	181	ALA	4.8
1	F	175	VAL	4.8
1	E	224	MET	4.8
1	C	230	ASP	4.7
1	C	147	ILE	4.6
1	F	168	ALA	4.6
1	F	313	PHE	4.5
1	F	146	TYR	4.5
1	A	236	PHE	4.5
1	E	100	TYR	4.5
1	F	311	GLU	4.4
1	F	240	MET	4.3
1	E	228	PHE	4.3
1	F	169	ARG	4.3
1	C	231	GLY	4.3
1	B	230	ASP	4.3
1	F	220	ILE	4.2
1	C	243	TYR	4.1
1	F	109	ALA	4.1
1	D	167	PHE	3.9
1	F	111	ASP	3.9
1	F	179	ILE	3.9
1	A	190	GLY	3.9
1	F	192	GLU	3.8
1	A	234	ARG	3.8
1	F	227	THR	3.8
1	F	217	ASP	3.8
1	F	139	ALA	3.7
1	F	181	ALA	3.7
1	B	228	PHE	3.7
1	F	190	GLY	3.7
1	C	148	LEU	3.7
1	F	172	ASP	3.7
1	E	314	PRO	3.7
1	F	148	LEU	3.7
1	F	173	ASP	3.7
1	E	51	GLY	3.7
1	E	182	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	3.6
1	B	179	ILE	3.6
1	E	235	GLY	3.5
1	E	167	PHE	3.5
1	E	139	ALA	3.5
1	F	235	GLY	3.5
1	E	222	LYS	3.5
1	C	234	ARG	3.4
1	F	113	VAL	3.4
1	F	218	LEU	3.4
1	E	234	ARG	3.4
1	E	132	ALA	3.4
1	E	169	ARG	3.3
1	C	189	HIS	3.3
1	E	313	PHE	3.3
1	A	243	TYR	3.3
1	D	60	GLY	3.3
1	F	194	LEU	3.3
1	F	141	LYS	3.3
1	C	218	LEU	3.3
1	D	172	ASP	3.2
1	B	236	PHE	3.2
1	F	123	ILE	3.2
1	F	94	ILE	3.2
1	E	68	THR	3.2
1	E	93	ALA	3.1
1	F	239	LEU	3.1
1	F	243	TYR	3.1
1	B	170	VAL	3.1
1	F	193	GLY	3.1
1	F	138	ARG	3.1
1	E	133	SER	3.0
1	E	171	PHE	3.0
1	D	179	ILE	3.0
1	C	220	ILE	3.0
1	F	183	ILE	3.0
1	E	229	PRO	3.0
1	F	2	TYR	2.9
1	F	101	GLY	2.9
1	A	194	LEU	2.9
1	D	189	HIS	2.8
1	E	312	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	146	TYR	2.8
1	E	317	ASN	2.8
1	D	234	ARG	2.8
1	E	2	TYR	2.8
1	E	166	ILE	2.8
1	F	165	LEU	2.8
1	F	174	GLY	2.8
1	B	234	ARG	2.8
1	C	170	VAL	2.8
1	E	240	MET	2.8
1	B	176	GLU	2.8
1	B	173	ASP	2.7
1	F	92	GLY	2.7
1	F	229	PRO	2.7
1	E	219	LYS	2.7
1	F	242	ALA	2.7
1	F	241	SER	2.7
1	F	244	ASN	2.7
1	B	148	LEU	2.7
1	F	163	LEU	2.7
1	E	168	ALA	2.7
1	E	243	TYR	2.7
1	F	230	ASP	2.7
1	D	190	GLY	2.6
1	E	221	HIS	2.6
1	F	99	LYS	2.6
1	F	149	ASN	2.6
1	E	230	ASP	2.6
1	F	106	ILE	2.6
1	E	165	LEU	2.6
1	F	232	LEU	2.6
1	F	53	MET	2.6
1	D	230	ASP	2.5
1	B	383	MET	2.5
1	E	375	GLN	2.5
1	F	121	ILE	2.5
1	F	180	GLY	2.4
1	E	147	ILE	2.4
1	F	237	ALA	2.4
1	D	146	TYR	2.4
1	C	141	LYS	2.4
1	C	179	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	139	ALA	2.4
1	C	245	ALA	2.4
1	F	234	ARG	2.4
1	F	231	GLY	2.3
1	C	232	LEU	2.3
1	E	91	LEU	2.3
1	F	145	HIS	2.3
1	F	122	CYS	2.3
1	B	147	ILE	2.3
1	A	229	PRO	2.3
1	F	312	THR	2.3
1	A	246[A]	GLN	2.3
1	E	145	HIS	2.3
1	E	150	GLY	2.3
1	D	236	PHE	2.3
1	F	167	PHE	2.3
1	A	232	LEU	2.2
1	F	128	ALA	2.2
1	E	248	VAL	2.2
1	C	168	ALA	2.2
1	E	316	ILE	2.2
1	C	172	ASP	2.2
1	D	235	GLY	2.2
1	E	225	MET	2.2
1	E	106	ILE	2.2
1	E	123	ILE	2.2
1	A	146	TYR	2.2
1	D	243	TYR	2.2
1	D	219	LYS	2.1
1	F	222	LYS	2.1
1	F	375	GLN	2.1
1	A	186	LEU	2.1
1	F	129	GLY	2.1
1	E	170	VAL	2.1
1	F	176	GLU	2.1
1	A	239	LEU	2.1
1	D	148	LEU	2.1
1	D	229	PRO	2.1
1	F	119	PRO	2.1
1	D	173	ASP	2.1
1	E	99	LYS	2.1
1	E	215	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	135	MET	2.1
1	E	237	ALA	2.0
1	B	235	GLY	2.0
1	B	172	ASP	2.0
1	E	140	ASP	2.0
1	F	213	LEU	2.0
1	F	216	HIS	2.0
1	F	248	VAL	2.0
1	F	44	LEU	2.0
1	F	186	LEU	2.0
1	B	100	TYR	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 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	COA	A	411	48/48	0.67	0.48	4.83	41,56,69,76	48
3	COA	D	411	48/48	0.77	0.34	3.94	43,60,75,77	48
4	SIN	C	412	8/8	0.91	0.35	3.61	39,60,75,98	0
3	COA	B	411	48/48	0.81	0.33	3.58	48,60,72,77	48
3	COA	E	411	48/48	0.75	0.41	2.95	58,66,75,91	48
3	COA	F	411	48/48	0.82	0.26	0.66	61,71,79,115	48
2	FAD	D	410	53/53	0.97	0.15	0.42	31,40,54,62	0
2	FAD	A	410	53/53	0.97	0.15	0.26	26,33,47,51	0
2	FAD	B	410	53/53	0.96	0.14	0.19	29,42,52,57	0
2	FAD	C	410	53/53	0.97	0.15	0.13	28,39,52,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	E	410	53/53	0.94	0.16	0.05	35,53,64,68	0
2	FAD	F	410	53/53	0.95	0.14	-0.43	50,61,77,84	0
5	SO4	C	1393	5/5	0.80	0.28	-	83,88,102,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.