



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:55 am GMT

PDB ID : 2UUU
Title : ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE IN P212121
Authors : Razeto, A.; Mattioli, F.; Carpanelli, E.; Aliverti, A.; Pandini, V.; Coda, A.; Mattevi, A.
Deposited on : 2007-03-07
Resolution : 1.95 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

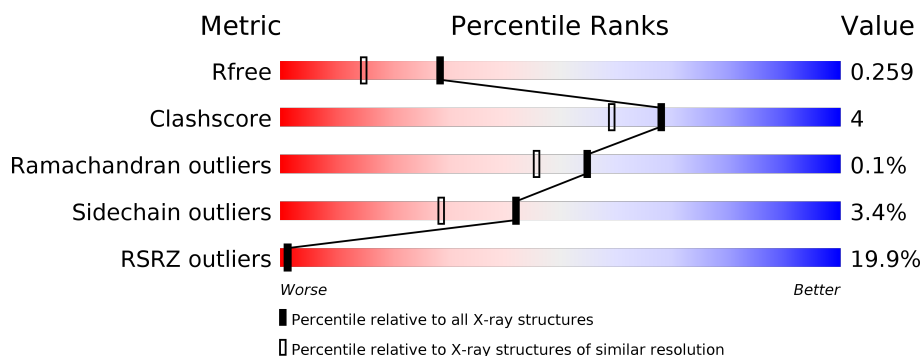
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	584	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	584	<div> <div>19%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	C	584	<div> <div>19%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
1	D	584	<div> <div>22%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>8%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PL3	A	1588	-	-	-	X
3	PL3	B	1588	-	-	-	X
3	PL3	C	1587	-	-	-	X
3	PL3	D	1587	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19178 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.

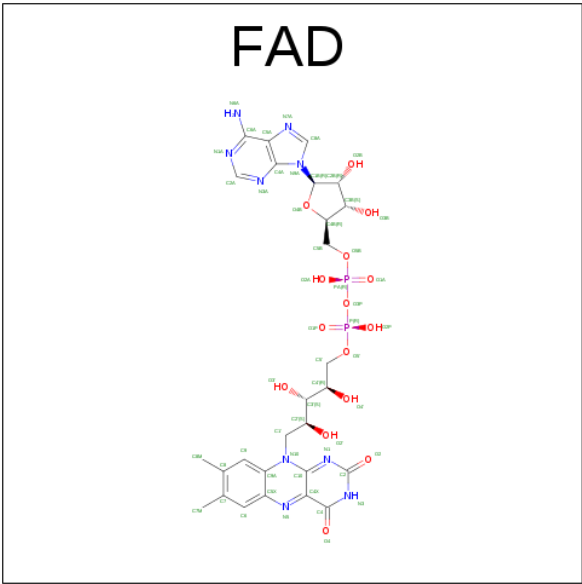
- Molecule 1 is a protein called ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	3	0
			4408	2839	751	798	20			
1	B	540	Total	C	N	O	S	0	1	0
			4329	2788	739	783	19			
1	C	541	Total	C	N	O	S	0	0	0
			4323	2784	735	786	18			
1	D	537	Total	C	N	O	S	0	0	0
			4288	2763	730	776	19			

There are 20 discrepancies between the modelled and reference sequences:

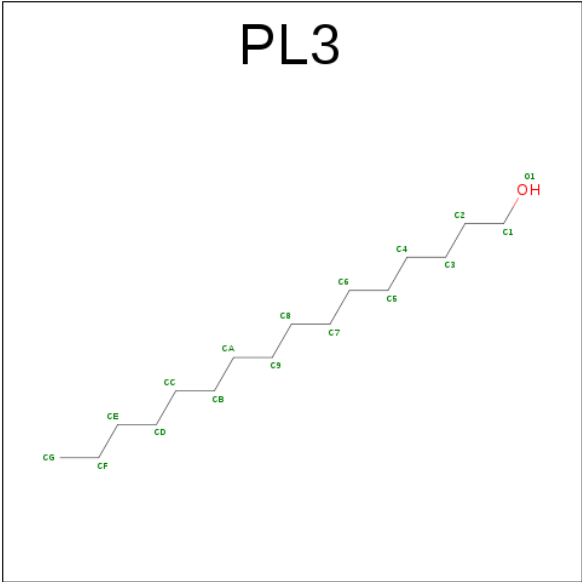
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP O96759
A	-4	ALA	-	EXPRESSION TAG	UNP O96759
A	-3	MET	-	EXPRESSION TAG	UNP O96759
A	-2	GLY	-	EXPRESSION TAG	UNP O96759
A	-1	SER	-	EXPRESSION TAG	UNP O96759
B	-5	GLY	-	EXPRESSION TAG	UNP O96759
B	-4	ALA	-	EXPRESSION TAG	UNP O96759
B	-3	MET	-	EXPRESSION TAG	UNP O96759
B	-2	GLY	-	EXPRESSION TAG	UNP O96759
B	-1	SER	-	EXPRESSION TAG	UNP O96759
C	-5	GLY	-	EXPRESSION TAG	UNP O96759
C	-4	ALA	-	EXPRESSION TAG	UNP O96759
C	-3	MET	-	EXPRESSION TAG	UNP O96759
C	-2	GLY	-	EXPRESSION TAG	UNP O96759
C	-1	SER	-	EXPRESSION TAG	UNP O96759
D	-5	GLY	-	EXPRESSION TAG	UNP O96759
D	-4	ALA	-	EXPRESSION TAG	UNP O96759
D	-3	MET	-	EXPRESSION TAG	UNP O96759
D	-2	GLY	-	EXPRESSION TAG	UNP O96759
D	-1	SER	-	EXPRESSION TAG	UNP O96759

- 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		

- Molecule 3 is HEXADECAN-1-OL (three-letter code: PL3) (formula: $C_{16}H_{34}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		
3	C	1	Total	C	O	0	0
			17	16	1		
3	D	1	Total	C	O	0	0
			17	16	1		

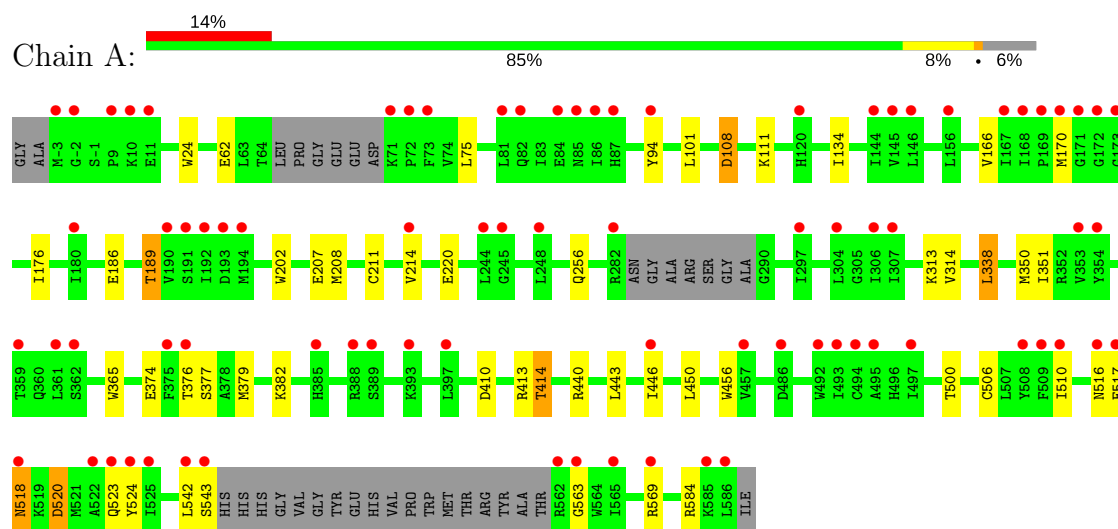
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	484	Total	O	0	0
			484	484		
4	B	385	Total	O	0	0
			385	385		
4	C	333	Total	O	0	0
			333	333		
4	D	348	Total	O	0	0
			348	348		

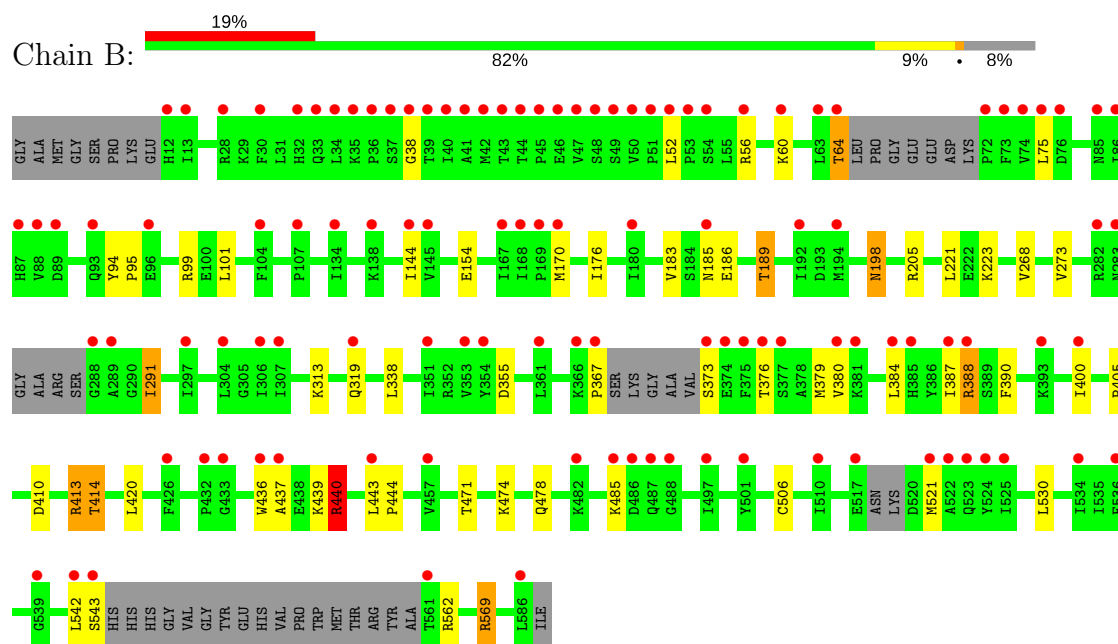
3 Residue-property plots [i](#)

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

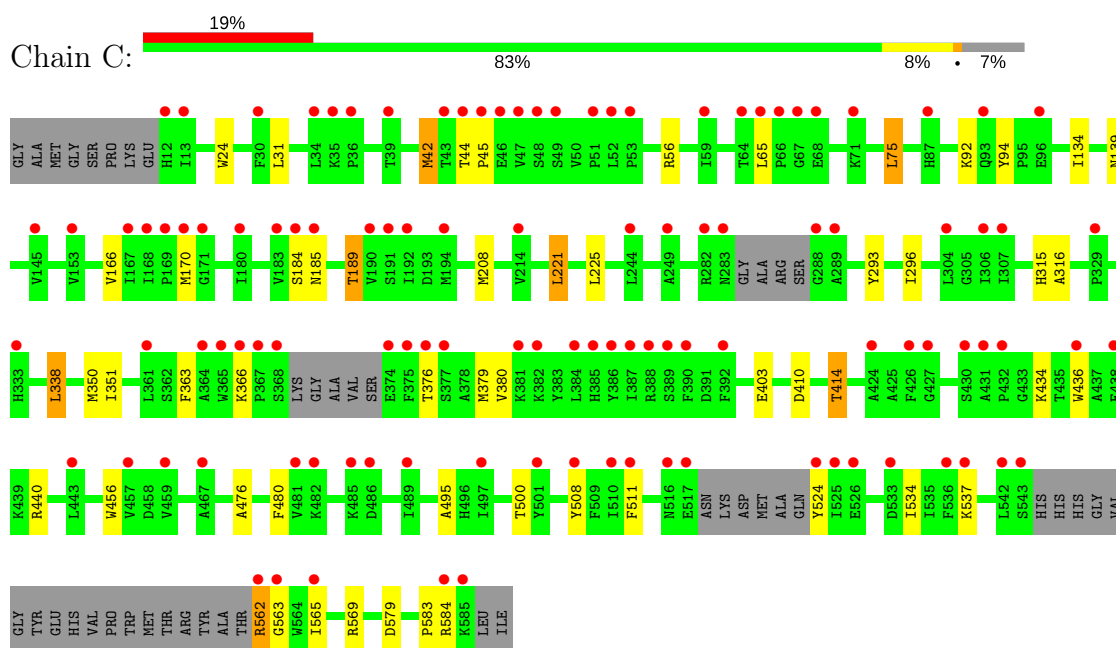
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



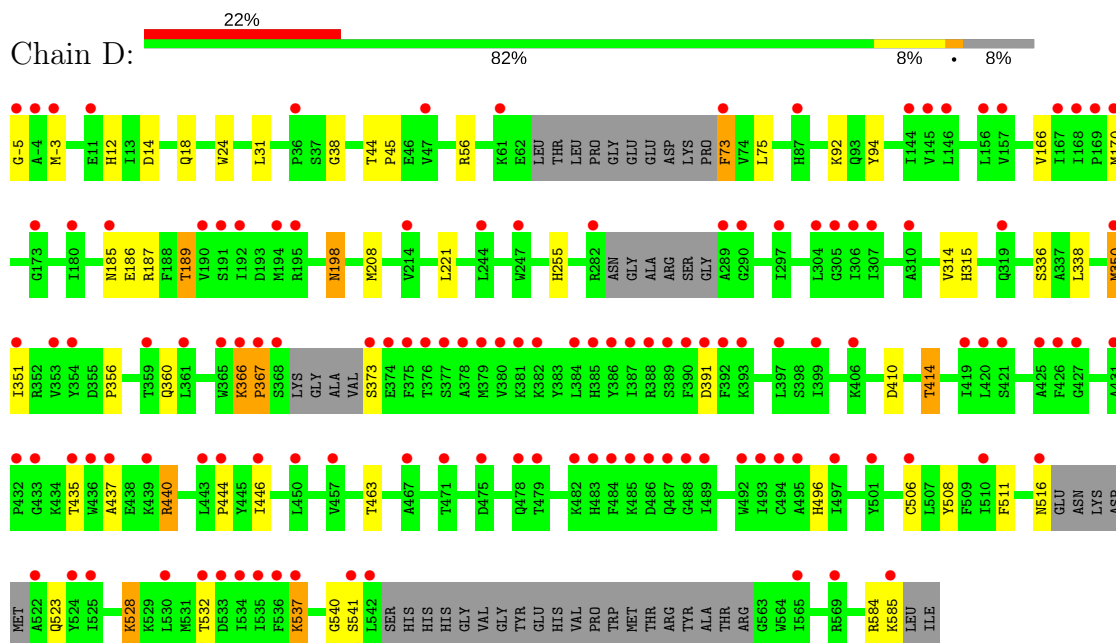
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.50Å 108.91Å 216.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 1.95 29.93 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-1.95) 99.8 (29.93-1.95)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.244 0.220 , 0.259	Depositor DCC
R_{free} test set	8931 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19178	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% 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: PL3, FAD

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	0.80	1/4527 (0.0%)	0.71	2/6127 (0.0%)
1	B	0.72	0/4439	0.71	4/6008 (0.1%)
1	C	0.65	0/4431	0.65	0/6000
1	D	0.69	0/4395	0.67	0/5948
All	All	0.72	1/17792 (0.0%)	0.68	6/24083 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	VAL	CB-CG1	5.50	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	413	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	413	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	413	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	413	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	355	ASP	CB-CG-OD1	5.11	122.89	118.30

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	4408	0	4422	40	0
1	B	4329	0	4327	41	0
1	C	4323	0	4311	33	0
1	D	4288	0	4283	40	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	17	0	33	4	0
3	B	17	0	33	2	0
3	C	17	0	33	0	0
3	D	17	0	33	0	0
4	A	484	0	0	9	0
4	B	385	0	0	9	0
4	C	333	0	0	5	0
4	D	348	0	0	11	0
All	All	19178	0	17599	156	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 4.

All (156) 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:220:GLU:HG2	4:A:2203:HOH:O	1.49	1.13
1:C:92:LYS:HE3	1:C:185:ASN:O	1.48	1.11
1:A:208:MET:CE	1:A:314:VAL:HG23	1.88	1.03
1:B:373:SER:HA	1:B:376:THR:HG22	1.49	0.94
1:B:410:ASP:O	1:B:414:THR:HG23	1.69	0.92
1:C:139:ASN:HB2	4:C:2128:HOH:O	1.72	0.86
1:D:92:LYS:HE2	1:D:185:ASN:O	1.80	0.81
1:B:373:SER:HA	1:B:376:THR:CG2	2.13	0.79
1:B:379:MET:SD	1:B:436:TRP:CZ2	2.77	0.78
1:A:256:GLN:HE21	1:A:350:MET:HE3	1.47	0.78
1:A:410:ASP:O	1:A:414:THR:HG23	1.84	0.78
1:D:437:ALA:O	1:D:440:ARG:HD3	1.82	0.77
1:A:208:MET:HE2	1:A:314:VAL:HG23	1.67	0.75
1:C:338:LEU:HG	1:C:500:THR:HG21	1.68	0.75
1:B:379:MET:SD	1:B:436:TRP:CH2	2.78	0.75
1:B:388:ARG:HD3	4:B:2280:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ASP:O	1:D:414:THR:HG22	1.87	0.74
1:D:-5:GLY:N	4:D:2004:HOH:O	2.20	0.73
1:B:542:LEU:O	1:B:543:SER:HB2	1.89	0.72
1:A:256:GLN:HE21	1:A:350:MET:CE	2.02	0.72
1:B:223:LYS:HE2	4:B:2169:HOH:O	1.91	0.70
1:A:542:LEU:HD23	4:A:2406:HOH:O	1.90	0.70
1:B:569:ARG:NH2	4:B:2368:HOH:O	2.23	0.70
1:B:319:GLN:HG2	1:B:405:PRO:HA	1.74	0.69
1:C:92:LYS:CE	1:C:185:ASN:O	2.36	0.68
1:A:176:ILE:HG21	3:A:1588:PL3:H1C1	1.77	0.67
1:A:189:THR:HG21	4:A:2195:HOH:O	1.95	0.67
1:B:373:SER:CA	1:B:376:THR:HG22	2.25	0.66
1:D:496:HIS:CE1	1:D:508:TYR:CD1	2.85	0.64
1:C:562:ARG:HD2	1:C:565:ILE:HG13	1.79	0.64
1:D:166:VAL:HB	1:D:189:THR:HB	1.79	0.64
1:A:256:GLN:NE2	1:A:350:MET:CE	2.60	0.63
1:B:474:LYS:HE2	1:B:478:GLN:HE22	1.63	0.63
1:D:185:ASN:HB3	4:D:2119:HOH:O	1.98	0.62
1:D:516:ASN:H	1:D:523:GLN:HE22	1.46	0.62
1:C:410:ASP:O	1:C:414:THR:HG23	2.00	0.62
1:A:208:MET:HE3	1:A:314:VAL:HG23	1.78	0.61
1:B:189:THR:HG21	4:B:2142:HOH:O	1.99	0.61
1:C:166:VAL:HB	1:C:189:THR:HB	1.81	0.61
1:A:256:GLN:NE2	1:A:350:MET:HE3	2.16	0.60
1:C:208:MET:HE2	1:C:316:ALA:N	2.17	0.60
1:D:221:LEU:HD22	4:D:2185:HOH:O	2.02	0.60
1:D:463:THR:O	1:D:540:GLY:HA2	2.03	0.59
1:B:291:ILE:N	1:B:291:ILE:HD13	2.19	0.58
1:C:569:ARG:HD2	4:C:2320:HOH:O	2.03	0.58
1:D:208:MET:HE3	1:D:314:VAL:HG23	1.86	0.57
1:D:73:PHE:HA	4:D:2050:HOH:O	2.04	0.57
1:A:443:LEU:O	1:A:446:ILE:HG22	2.05	0.57
1:D:-3:MET:HE2	4:D:2005:HOH:O	2.04	0.57
1:A:510:ILE:HG21	3:A:1588:PL3:HAC1	1.87	0.57
1:C:379:MET:SD	1:C:436:TRP:CZ2	2.98	0.57
1:A:108:ASP:O	1:A:111:LYS:HE2	2.05	0.56
1:D:44:THR:HB	1:D:45:PRO:HD2	1.87	0.56
1:B:198:ASN:HD22	1:B:198:ASN:H	1.54	0.55
1:B:38:GLY:O	1:B:56:ARG:HD2	2.06	0.55
1:D:189:THR:HG21	4:D:2154:HOH:O	2.06	0.54
1:C:24:TRP:CZ3	2:C:1586:FAD:HM83	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LEU:HD23	1:D:221:LEU:C	2.28	0.54
1:B:380:VAL:O	1:B:384:LEU:HG	2.08	0.53
1:A:256:GLN:NE2	1:A:350:MET:HE1	2.24	0.52
1:A:365:TRP:HD1	1:A:365:TRP:O	1.92	0.52
1:B:60:LYS:O	1:B:64:THR:HB	2.09	0.52
1:C:579:ASP:O	1:C:583:PRO:HG3	2.10	0.52
3:A:1588:PL3:O1	4:A:2484:HOH:O	2.19	0.51
1:C:221:LEU:HD22	1:C:225:LEU:CD1	2.41	0.51
1:D:373:SER:HA	4:D:2276:HOH:O	2.11	0.51
1:C:366:LYS:HD3	1:C:380:VAL:HG21	1.93	0.51
1:D:186:GLU:HG2	4:D:2153:HOH:O	2.10	0.51
1:A:518:ASN:OD1	1:A:518:ASN:N	2.43	0.51
1:B:471:THR:HG23	4:B:2332:HOH:O	2.12	0.50
1:D:198:ASN:H	1:D:198:ASN:HD22	1.60	0.50
1:B:474:LYS:HE2	1:B:478:GLN:NE2	2.25	0.50
1:B:183:VAL:HG13	4:B:2141:HOH:O	2.11	0.50
1:D:511:PHE:HZ	1:D:528:LYS:HE2	1.76	0.50
1:C:476:ALA:CB	1:C:534:ILE:HD12	2.42	0.49
1:A:414:THR:HG21	4:A:2168:HOH:O	2.13	0.49
1:A:376:THR:HA	1:A:379:MET:HE2	1.94	0.49
1:B:176:ILE:HG21	3:B:1588:PL3:H2C1	1.94	0.49
1:B:439:LYS:HD2	4:B:2274:HOH:O	2.11	0.49
1:B:95:PRO:HB2	1:B:99[B]:ARG:HH12	1.78	0.49
1:B:387:ILE:HA	1:B:390:PHE:O	2.12	0.49
1:A:24:TRP:CZ3	2:A:1587:FAD:HM83	2.47	0.49
1:C:403:GLU:OE2	1:C:434:LYS:HE3	2.12	0.49
1:C:184:SER:HB3	4:C:2132:HOH:O	2.11	0.49
1:C:456:TRP:CG	1:C:524:TYR:HE2	2.30	0.49
1:A:207:GLU:O	1:A:313:LYS:NZ	2.43	0.48
1:C:44:THR:HB	1:C:45:PRO:HD2	1.96	0.48
1:A:365:TRP:CD1	1:A:365:TRP:O	2.67	0.48
1:A:456:TRP:CD1	1:A:524:TYR:HE2	2.31	0.48
1:B:443:LEU:N	1:B:444:PRO:HD2	2.28	0.48
1:C:208:MET:HE2	1:C:315:HIS:C	2.34	0.48
1:D:187:ARG:O	1:D:189:THR:HG22	2.14	0.47
1:D:356:PRO:O	1:D:360:GLN:HG3	2.13	0.47
1:A:506:CYS:HB2	4:A:2441:HOH:O	2.13	0.47
1:D:12:HIS:HE1	1:D:14:ASP:OD1	1.96	0.47
1:C:563:GLY:HA2	4:C:2317:HOH:O	2.14	0.47
1:A:166:VAL:HB	1:A:189:THR:HB	1.96	0.47
1:B:410:ASP:OD1	1:B:413:ARG:NH2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ALA:HA	1:C:508:TYR:O	2.15	0.47
1:D:92:LYS:CE	1:D:185:ASN:O	2.56	0.46
1:D:366:LYS:O	1:D:366:LYS:HG2	2.14	0.46
1:A:62:GLU:OE1	1:A:62:GLU:HA	2.16	0.45
1:B:410:ASP:O	1:B:414:THR:CG2	2.54	0.45
1:D:537:LYS:O	1:D:537:LYS:HG2	2.17	0.45
1:C:476:ALA:HA	1:C:534:ILE:HD12	1.99	0.45
1:B:205:ARG:HD2	4:B:2154:HOH:O	2.15	0.45
1:D:255:HIS:HB3	1:D:350:MET:CE	2.46	0.45
1:B:52:LEU:HD23	1:B:367:PRO:HA	1.98	0.45
3:B:1588:PL3:H1C1	3:B:1588:PL3:H4C2	1.57	0.45
1:B:198:ASN:HD22	1:B:198:ASN:N	2.12	0.44
1:C:134:ILE:HG23	4:C:2096:HOH:O	2.17	0.44
1:A:374:GLU:HB3	4:A:2343:HOH:O	2.17	0.44
1:C:350:MET:HG2	1:C:351:ILE:N	2.33	0.44
1:C:363:PHE:HD1	1:C:380:VAL:HG22	1.83	0.44
1:A:517:GLU:O	1:A:517:GLU:HG3	2.18	0.44
1:B:439:LYS:HD3	1:B:439:LYS:C	2.39	0.43
1:D:444:PRO:HG3	2:D:1586:FAD:HM73	2.00	0.43
1:D:208:MET:HE1	1:D:315:HIS:C	2.38	0.43
1:D:366:LYS:HA	1:D:367:PRO:HD3	1.74	0.43
1:C:410:ASP:O	1:C:414:THR:CG2	2.66	0.43
1:D:506:CYS:HB2	4:D:2320:HOH:O	2.18	0.43
1:A:520:ASP:O	1:A:523:GLN:HG2	2.19	0.43
1:D:350:MET:HG3	1:D:351:ILE:N	2.34	0.43
1:A:563:GLY:HA2	4:A:2466:HOH:O	2.18	0.43
1:A:134:ILE:HG23	4:A:2141:HOH:O	2.17	0.43
1:A:450:LEU:HD11	3:A:1588:PL3:HDC2	2.01	0.43
1:B:183:VAL:O	1:B:183:VAL:CG1	2.68	0.42
1:B:268:VAL:CG2	1:B:313:LYS:HG3	2.49	0.42
1:C:31:LEU:CD2	1:C:42:MET:HE3	2.49	0.42
1:A:338:LEU:HD12	1:A:351:ILE:HD13	2.01	0.42
1:B:221:LEU:C	1:B:221:LEU:HD23	2.39	0.42
1:B:154:GLU:HA	1:B:273:VAL:HG11	2.01	0.42
1:C:456:TRP:CD1	1:C:524:TYR:HE2	2.38	0.42
1:D:24:TRP:CG	1:D:444:PRO:HB2	2.54	0.42
1:D:31:LEU:HD12	1:D:446:ILE:HA	2.02	0.42
1:A:338:LEU:HG	1:A:500:THR:HG21	2.01	0.42
1:B:291:ILE:N	1:B:291:ILE:CD1	2.83	0.42
1:D:463:THR:OG1	1:D:541:SER:HB3	2.20	0.42
1:A:542:LEU:O	1:A:543:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:TYR:HD2	1:C:296:ILE:HD12	1.84	0.41
1:D:511:PHE:HZ	1:D:528:LYS:CE	2.32	0.41
1:A:516:ASN:ND2	1:A:518:ASN:OD1	2.54	0.41
1:B:437:ALA:O	1:B:440:ARG:HD3	2.20	0.41
1:D:24:TRP:CZ3	2:D:1586:FAD:HM83	2.56	0.41
1:C:480:PHE:CZ	1:C:511:PHE:HB2	2.55	0.41
1:A:108:ASP:C	1:A:108:ASP:OD1	2.58	0.41
1:A:202:TRP:CE2	1:A:211:CYS:HB2	2.56	0.41
1:C:56:ARG:NH1	1:C:75:LEU:HD22	2.36	0.41
1:D:38:GLY:O	1:D:56:ARG:NH1	2.53	0.41
1:A:376:THR:HA	1:A:379:MET:CE	2.51	0.41
1:B:400:ILE:HD12	1:B:420:LEU:HD11	2.03	0.41
1:D:18:GLN:HG2	4:D:2022:HOH:O	2.21	0.41
1:D:391:ASP:HB2	4:D:2278:HOH:O	2.21	0.41
1:C:534:ILE:O	1:C:537:LYS:HB3	2.22	0.40
1:B:144:ILE:N	1:B:144:ILE:HD12	2.37	0.40
1:B:506:CYS:CB	4:B:2325:HOH:O	2.70	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	545/584 (93%)	538 (99%)	7 (1%)	0	100	100
1	B	529/584 (91%)	518 (98%)	10 (2%)	1 (0%)	51	41
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	38	25
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	55	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	537	LYS
1	B	562	ARG
1	D	367	PRO

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	484/507 (96%)	467 (96%)	17 (4%)	41	27
1	B	474/507 (94%)	456 (96%)	18 (4%)	38	24
1	C	472/507 (93%)	459 (97%)	13 (3%)	49	37
1	D	468/507 (92%)	451 (96%)	17 (4%)	40	26
All	All	1898/2028 (94%)	1833 (97%)	65 (3%)	42	29

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	94	TYR
1	A	101	LEU
1	A	108	ASP
1	A	170	MET
1	A	186	GLU
1	A	189	THR
1	A	338	LEU
1	A	377	SER
1	A	382[A]	LYS
1	A	382[B]	LYS
1	A	414	THR
1	A	440	ARG
1	A	518	ASN
1	A	520	ASP
1	A	569	ARG
1	A	584	ARG
1	B	64	THR
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	94	TYR
1	B	101	LEU
1	B	170	MET
1	B	185	ASN
1	B	186	GLU
1	B	189	THR
1	B	198	ASN
1	B	291	ILE
1	B	338	LEU
1	B	388	ARG
1	B	414	THR
1	B	440	ARG
1	B	485	LYS
1	B	521	MET
1	B	530	LEU
1	B	569	ARG
1	C	42	MET
1	C	65	LEU
1	C	75	LEU
1	C	94	TYR
1	C	170	MET
1	C	189	THR
1	C	221	LEU
1	C	338	LEU
1	C	376	THR
1	C	414	THR
1	C	440	ARG
1	C	562	ARG
1	C	584	ARG
1	D	73	PHE
1	D	75	LEU
1	D	94	TYR
1	D	170	MET
1	D	189	THR
1	D	198	ASN
1	D	336	SER
1	D	338	LEU
1	D	350	MET
1	D	366	LYS
1	D	414	THR
1	D	435	THR
1	D	440	ARG

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Mol	Chain	Res	Type
1	D	528	LYS
1	D	532	THR
1	D	584	ARG
1	D	585	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	93	GLN
1	A	228	GLN
1	A	256	GLN
1	A	315	HIS
1	A	499	HIS
1	B	12	HIS
1	B	33	GLN
1	B	198	ASN
1	B	256	GLN
1	B	283	ASN
1	B	315	HIS
1	B	394	ASN
1	B	478	GLN
1	B	499	HIS
1	C	12	HIS
1	C	82	GLN
1	C	87	HIS
1	C	224	GLN
1	C	283	ASN
1	C	487	GLN
1	D	12	HIS
1	D	85	ASN
1	D	198	ASN
1	D	315	HIS
1	D	394	ASN
1	D	487	GLN
1	D	523	GLN

5.3.3 RNA ⓘ

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](#)

8 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	1587	-	51,58,58	1.67	7 (13%)	54,89,89	2.14	10 (18%)
3	PL3	A	1588	-	16,16,16	0.89	1 (6%)	15,15,15	0.83	0
2	FAD	B	1587	-	51,58,58	1.54	7 (13%)	54,89,89	2.52	14 (25%)
3	PL3	B	1588	-	16,16,16	0.96	1 (6%)	15,15,15	0.72	0
2	FAD	C	1586	-	51,58,58	1.55	7 (13%)	54,89,89	2.01	7 (12%)
3	PL3	C	1587	-	16,16,16	0.92	1 (6%)	15,15,15	0.86	0
2	FAD	D	1586	-	51,58,58	1.55	9 (17%)	54,89,89	2.42	9 (16%)
3	PL3	D	1587	-	16,16,16	0.91	1 (6%)	15,15,15	0.73	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
2	FAD	A	1587	-	-	0/28/50/50	0/6/6/6
3	PL3	A	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1587	-	-	0/28/50/50	0/6/6/6
3	PL3	B	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1586	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PL3	C	1587	-	-	0/14/14/14	0/0/0/0
2	FAD	D	1586	-	-	0/28/50/50	0/6/6/6
3	PL3	D	1587	-	-	0/14/14/14	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1588	PL3	O1-C1	-3.71	1.22	1.42
3	C	1587	PL3	O1-C1	-3.56	1.23	1.42
3	D	1587	PL3	O1-C1	-3.55	1.23	1.42
3	A	1588	PL3	O1-C1	-3.52	1.23	1.42
2	C	1586	FAD	C6-C5X	-2.36	1.38	1.41
2	D	1586	FAD	O4B-C1B	2.00	1.44	1.41
2	C	1586	FAD	C5'-C4'	2.06	1.54	1.51
2	A	1587	FAD	C9-C8	2.09	1.43	1.37
2	B	1587	FAD	C1'-N10	2.43	1.50	1.48
2	B	1587	FAD	C2A-N1A	2.59	1.38	1.33
2	B	1587	FAD	C10-N1	2.62	1.36	1.33
2	D	1586	FAD	C10-N1	2.69	1.37	1.33
2	D	1586	FAD	C5X-N5	2.70	1.39	1.35
2	D	1586	FAD	C5'-C4'	2.71	1.55	1.51
2	D	1586	FAD	C4-N3	2.79	1.38	1.33
2	D	1586	FAD	C2A-N3A	2.82	1.36	1.32
2	B	1587	FAD	C9A-N10	2.84	1.42	1.38
2	A	1587	FAD	C4-N3	2.85	1.38	1.33
2	C	1586	FAD	C4-N3	2.91	1.38	1.33
2	B	1587	FAD	C4-N3	3.10	1.38	1.33
2	C	1586	FAD	C2A-N3A	3.20	1.37	1.32
2	A	1587	FAD	C9A-N10	3.22	1.43	1.38
2	D	1586	FAD	C2A-N1A	3.31	1.40	1.33
2	A	1587	FAD	C5X-N5	3.39	1.40	1.35
2	C	1586	FAD	C10-N1	3.79	1.38	1.33
2	D	1586	FAD	C4X-N5	4.02	1.39	1.33
2	B	1587	FAD	C4X-N5	4.12	1.39	1.33
2	A	1587	FAD	C2A-N3A	4.42	1.39	1.32
2	C	1586	FAD	C4X-N5	4.54	1.39	1.33
2	A	1587	FAD	C4X-N5	5.02	1.40	1.33
2	D	1586	FAD	C1'-N10	5.03	1.53	1.48
2	B	1587	FAD	C2A-N3A	5.48	1.41	1.32
2	A	1587	FAD	C10-N1	5.52	1.41	1.33
2	C	1586	FAD	C1'-N10	5.85	1.54	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-12.02	118.39	128.86
2	D	1586	FAD	N3A-C2A-N1A	-11.95	118.45	128.86
2	C	1586	FAD	N3A-C2A-N1A	-10.83	119.43	128.86
2	A	1587	FAD	N3A-C2A-N1A	-10.42	119.78	128.86
2	B	1587	FAD	C4X-C4-N3	-3.76	118.13	123.48
2	D	1586	FAD	C4X-C4-N3	-3.69	118.23	123.48
2	B	1587	FAD	O4'-C4'-C5'	-3.44	102.33	110.00
2	A	1587	FAD	C4X-C4-N3	-2.41	120.05	123.48
2	B	1587	FAD	C1B-N9A-C4A	-2.37	122.55	126.64
2	B	1587	FAD	C8M-C8-C9	-2.34	114.46	120.34
2	A	1587	FAD	C4A-C5A-N7A	-2.33	107.16	109.41
2	A	1587	FAD	C1B-N9A-C4A	-2.24	122.76	126.64
2	B	1587	FAD	C4A-C5A-N7A	-2.11	107.37	109.41
2	C	1586	FAD	C4X-C4-N3	-2.09	120.50	123.48
2	A	1587	FAD	C4-C4X-C10	-2.02	118.33	119.96
2	A	1587	FAD	C1'-N10-C9A	2.08	120.25	118.35
2	C	1586	FAD	C5X-C9A-N10	2.17	119.27	117.66
2	C	1586	FAD	C1'-N10-C9A	2.34	120.49	118.35
2	A	1587	FAD	C2A-N1A-C6A	2.44	123.03	118.77
2	A	1587	FAD	C1'-N10-C10	2.51	121.08	118.50
2	D	1586	FAD	C4-C4X-N5	2.57	121.50	118.68
2	D	1586	FAD	C2A-N1A-C6A	2.60	123.32	118.77
2	B	1587	FAD	C4-C4X-N5	2.65	121.59	118.68
2	B	1587	FAD	C2A-N1A-C6A	2.78	123.64	118.77
2	B	1587	FAD	C1'-N10-C9A	2.93	121.03	118.35
2	D	1586	FAD	O2P-P-O5'	2.97	122.18	108.14
2	B	1587	FAD	C4X-C10-N10	3.06	122.64	120.52
2	C	1586	FAD	C4-C4X-N5	3.06	122.04	118.68
2	A	1587	FAD	C5X-C9A-N10	3.29	120.10	117.66
2	B	1587	FAD	C1'-N10-C10	3.29	121.88	118.50
2	D	1586	FAD	C5X-C9A-N10	3.66	120.37	117.66
2	B	1587	FAD	C4X-N5-C5X	3.67	120.64	116.76
2	C	1586	FAD	C4X-N5-C5X	3.75	120.72	116.76
2	D	1586	FAD	C1'-N10-C9A	3.75	121.78	118.35
2	D	1586	FAD	C4X-N5-C5X	4.07	121.06	116.76
2	B	1587	FAD	C5X-C9A-N10	4.65	121.11	117.66
2	C	1586	FAD	C4-N3-C2	5.21	119.72	115.16
2	B	1587	FAD	C4-N3-C2	6.56	120.89	115.16
2	A	1587	FAD	C4-N3-C2	6.68	121.00	115.16
2	D	1586	FAD	C4-N3-C2	7.89	122.06	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1587	FAD	1	0
3	A	1588	PL3	4	0
3	B	1588	PL3	2	0
2	C	1586	FAD	1	0
2	D	1586	FAD	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 [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	550/584 (94%)	0.84	80 (14%) 3 4	8, 20, 36, 58	0
1	B	540/584 (92%)	1.09	113 (20%) 1 1	8, 21, 43, 66	0
1	C	541/584 (92%)	1.16	111 (20%) 1 1	13, 27, 46, 56	0
1	D	537/584 (91%)	1.26	127 (23%) 1 0	12, 26, 59, 81	0
All	All	2168/2336 (92%)	1.08	431 (19%) 1 1	8, 22, 47, 81	0

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	PHE	11.6
1	D	377	SER	9.9
1	D	376	THR	9.9
1	B	522	ALA	9.2
1	D	432	PRO	9.0
1	A	586	LEU	7.9
1	C	375	PHE	7.9
1	A	525	ILE	7.8
1	B	437	ALA	7.7
1	D	436	TRP	7.6
1	C	368	SER	7.4
1	C	436	TRP	7.2
1	D	373	SER	6.8
1	A	-3	MET	6.7
1	C	65	LEU	6.6
1	C	388	ARG	6.6
1	C	384	LEU	6.5
1	D	374	GLU	6.4
1	D	379	MET	6.4
1	B	38	GLY	6.3
1	D	289	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	282	ARG	6.3
1	C	367	PRO	6.3
1	B	436	TRP	6.1
1	C	185	ASN	6.1
1	A	9	PRO	6.1
1	D	388	ARG	6.1
1	D	484	PHE	6.0
1	C	525	ILE	5.8
1	D	536	PHE	5.8
1	B	73	PHE	5.7
1	D	73	PHE	5.7
1	C	431	ALA	5.7
1	B	47	VAL	5.7
1	A	11	GLU	5.6
1	D	368	SER	5.6
1	C	66	PRO	5.6
1	C	390	PHE	5.6
1	B	50	VAL	5.6
1	C	542	LEU	5.6
1	D	525	ILE	5.5
1	A	192	ILE	5.5
1	B	288	GLY	5.4
1	B	37	SER	5.4
1	C	289	ALA	5.4
1	B	561	THR	5.4
1	D	381	LYS	5.4
1	B	34	LEU	5.3
1	B	543	SER	5.3
1	B	367	PRO	5.3
1	B	542	LEU	5.2
1	C	387	ILE	5.2
1	A	562	ARG	5.1
1	D	367	PRO	5.1
1	B	72	PRO	5.1
1	C	192	ILE	5.0
1	B	388	ARG	5.0
1	C	365	TRP	4.9
1	B	432	PRO	4.9
1	D	431	ALA	4.9
1	C	283	ASN	4.9
1	C	385	HIS	4.8
1	C	288	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	387	ILE	4.8
1	C	392	PHE	4.8
1	B	306	ILE	4.7
1	D	437	ALA	4.7
1	D	192	ILE	4.7
1	B	36	PRO	4.7
1	A	306	ILE	4.7
1	A	510	ILE	4.6
1	A	71	LYS	4.6
1	D	366	LYS	4.6
1	A	72	PRO	4.6
1	D	145	VAL	4.6
1	A	10	LYS	4.6
1	D	384	LEU	4.5
1	C	307	ILE	4.5
1	C	432	PRO	4.5
1	B	192	ILE	4.5
1	C	562	ARG	4.4
1	C	68	GLU	4.4
1	B	384	LEU	4.4
1	A	168	ILE	4.3
1	A	307	ILE	4.3
1	D	306	ILE	4.3
1	B	63	LEU	4.3
1	C	510	ILE	4.3
1	A	543	SER	4.3
1	D	535	ILE	4.2
1	A	457	VAL	4.2
1	D	282	ARG	4.2
1	B	185	ASN	4.1
1	D	386	TYR	4.1
1	A	194	MET	4.1
1	D	488	GLY	4.1
1	C	48	SER	4.1
1	C	386	TYR	4.1
1	B	87	HIS	4.1
1	D	483	HIS	4.0
1	D	475	ASP	4.0
1	B	488	GLY	4.0
1	D	537	LYS	4.0
1	A	146	LEU	4.0
1	D	501	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	565	ILE	4.0
1	A	169	PRO	4.0
1	B	373	SER	4.0
1	C	43	THR	3.9
1	D	426	PHE	3.9
1	B	380	VAL	3.9
1	C	485	LYS	3.9
1	A	375	PHE	3.9
1	C	382	LYS	3.9
1	B	385	HIS	3.8
1	B	45	PRO	3.8
1	C	482	LYS	3.8
1	C	374	GLU	3.8
1	A	145	VAL	3.8
1	C	381	LYS	3.8
1	B	64	THR	3.7
1	D	-5	GLY	3.7
1	B	46	GLU	3.7
1	C	34	LEU	3.7
1	C	67	GLY	3.7
1	B	289	ALA	3.7
1	D	-4	ALA	3.7
1	B	366	LYS	3.7
1	B	376	THR	3.7
1	C	376	THR	3.7
1	C	516	ASN	3.7
1	D	457	VAL	3.7
1	D	478	GLN	3.7
1	B	39	THR	3.6
1	C	59	ILE	3.6
1	C	306	ILE	3.6
1	C	169	PRO	3.6
1	A	522	ALA	3.6
1	B	381	LYS	3.6
1	C	12	HIS	3.6
1	C	366	LYS	3.6
1	C	537	LYS	3.6
1	A	388	ARG	3.6
1	B	74	VAL	3.6
1	D	492	TRP	3.6
1	D	486	ASP	3.6
1	A	144	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	565	ILE	3.6
1	B	56	ARG	3.6
1	B	75	LEU	3.6
1	B	487	GLN	3.6
1	B	486	ASP	3.6
1	D	61	LYS	3.5
1	D	169	PRO	3.5
1	C	214	VAL	3.5
1	A	180	ILE	3.5
1	B	167	ILE	3.5
1	D	494	CYS	3.5
1	C	36	PRO	3.5
1	B	12	HIS	3.5
1	C	426	PHE	3.5
1	B	521	MET	3.4
1	B	510	ILE	3.4
1	B	525	ILE	3.4
1	D	489	ILE	3.4
1	B	48	SER	3.4
1	D	354	TYR	3.4
1	A	73	PHE	3.4
1	B	51	PRO	3.4
1	C	53	PRO	3.4
1	B	523	GLN	3.4
1	D	378	ALA	3.4
1	D	144	ILE	3.4
1	D	350	MET	3.4
1	B	457	VAL	3.3
1	C	190	VAL	3.3
1	C	45	PRO	3.3
1	D	482	LYS	3.3
1	B	33	GLN	3.3
1	B	375	PHE	3.3
1	C	329	PRO	3.3
1	D	244	LEU	3.3
1	B	586	LEU	3.3
1	D	542	LEU	3.3
1	A	86	ILE	3.2
1	A	167	ILE	3.2
1	B	297	ILE	3.2
1	B	377	SER	3.2
1	C	536	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	170	MET	3.2
1	D	446	ILE	3.2
1	A	-2	GLY	3.2
1	C	443	LEU	3.2
1	D	524	TYR	3.2
1	D	393	LYS	3.2
1	A	85	ASN	3.2
1	B	517	GLU	3.1
1	D	433	GLY	3.1
1	D	487	GLN	3.1
1	B	86	ILE	3.1
1	D	565	ILE	3.1
1	B	194	MET	3.1
1	C	424	ALA	3.1
1	A	563	GLY	3.1
1	A	569	ARG	3.1
1	D	380	VAL	3.1
1	C	526	GLU	3.1
1	B	145	VAL	3.1
1	D	450	LEU	3.1
1	A	494	CYS	3.1
1	C	64	THR	3.0
1	D	443	LEU	3.0
1	B	307	ILE	3.0
1	D	497	ILE	3.0
1	C	501	TYR	3.0
1	C	457	VAL	3.0
1	A	282	ARG	3.0
1	A	397	LEU	3.0
1	B	13	ILE	3.0
1	B	49	SER	3.0
1	A	385	HIS	3.0
1	C	71	LYS	3.0
1	D	214	VAL	3.0
1	B	485	LYS	3.0
1	B	169	PRO	3.0
1	C	333	HIS	3.0
1	D	157	VAL	3.0
1	D	156	LEU	2.9
1	D	365	TRP	2.9
1	B	42	MET	2.9
1	D	194	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	82	GLN	2.9
1	A	244	LEU	2.9
1	B	144	ILE	2.9
1	D	351	ILE	2.9
1	B	44	THR	2.9
1	B	353	VAL	2.9
1	C	168	ILE	2.9
1	A	354	TYR	2.9
1	A	376	THR	2.9
1	C	481	VAL	2.9
1	D	36	PRO	2.9
1	B	40	ILE	2.9
1	C	194	MET	2.9
1	A	523	GLN	2.9
1	A	156	LEU	2.9
1	C	167	ILE	2.9
1	C	497	ILE	2.9
1	B	536	PHE	2.9
1	D	522	ALA	2.9
1	B	35	LYS	2.8
1	B	539	GLY	2.8
1	D	467	ALA	2.8
1	D	353	VAL	2.8
1	A	492	TRP	2.8
1	B	52	LEU	2.8
1	A	84	GLU	2.8
1	D	506	CYS	2.8
1	D	585	LYS	2.8
1	B	361	LEU	2.8
1	B	497	ILE	2.8
1	D	87	HIS	2.8
1	D	297	ILE	2.8
1	B	32	HIS	2.8
1	B	426	PHE	2.8
1	D	11	GLU	2.8
1	B	433	GLY	2.7
1	D	-3	MET	2.7
1	A	353	VAL	2.7
1	C	183	VAL	2.7
1	D	361	LEU	2.7
1	D	406	LYS	2.7
1	B	134	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	76	ASP	2.7
1	B	28	ARG	2.7
1	C	170	MET	2.7
1	A	486	ASP	2.7
1	D	479	THR	2.7
1	B	354	TYR	2.7
1	C	585	LYS	2.7
1	C	47	VAL	2.7
1	C	153	VAL	2.7
1	C	508	TYR	2.7
1	A	248	LEU	2.7
1	A	361	LEU	2.7
1	D	397	LEU	2.7
1	D	530	LEU	2.7
1	B	107	PRO	2.7
1	B	374	GLU	2.7
1	C	377	SER	2.7
1	B	60	LYS	2.6
1	B	393	LYS	2.6
1	D	307	ILE	2.6
1	A	191	SER	2.6
1	C	389	SER	2.6
1	B	88	VAL	2.6
1	C	361	LEU	2.6
1	A	193	ASP	2.6
1	A	585	LYS	2.6
1	B	170	MET	2.6
1	D	510	ILE	2.6
1	D	390	PHE	2.5
1	A	94	TYR	2.5
1	A	171	GLY	2.5
1	A	172	GLY	2.5
1	B	168	ILE	2.5
1	C	13	ILE	2.5
1	C	489	ILE	2.5
1	C	364	ALA	2.5
1	D	439	LYS	2.5
1	A	359	THR	2.5
1	C	145	VAL	2.5
1	B	30	PHE	2.5
1	A	524	TYR	2.5
1	D	304	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	54	SER	2.5
1	C	430	SER	2.5
1	C	486	ASP	2.5
1	D	534	ILE	2.5
1	C	543	SER	2.5
1	C	51	PRO	2.5
1	D	167	ILE	2.5
1	D	180	ILE	2.5
1	A	173	GLY	2.5
1	C	180	ILE	2.4
1	D	391	ASP	2.4
1	C	96	GLU	2.4
1	C	244	LEU	2.4
1	A	518	ASN	2.4
1	D	359	THR	2.4
1	D	471	THR	2.4
1	D	382	LYS	2.4
1	D	185	ASN	2.4
1	A	362	SER	2.4
1	A	389	SER	2.4
1	B	482	LYS	2.4
1	C	184	SER	2.4
1	A	297	ILE	2.4
1	A	190	VAL	2.4
1	A	508	TYR	2.4
1	D	310	ALA	2.4
1	D	541	SER	2.4
1	D	533	ASP	2.4
1	D	168	ILE	2.4
1	D	305	GLY	2.4
1	B	319	GLN	2.4
1	A	542	LEU	2.4
1	B	41	ALA	2.4
1	B	43	THR	2.4
1	C	171	GLY	2.4
1	B	89	ASP	2.3
1	A	120	HIS	2.3
1	C	533	ASP	2.3
1	C	44	THR	2.3
1	C	30	PHE	2.3
1	D	485	LYS	2.3
1	C	191	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	493	ILE	2.3
1	B	93	GLN	2.3
1	B	304	LEU	2.3
1	D	420	LEU	2.3
1	B	501	TYR	2.3
1	C	524	TYR	2.3
1	B	104	PHE	2.3
1	C	511	PHE	2.3
1	C	459	VAL	2.3
1	D	399	ILE	2.3
1	C	49	SER	2.3
1	D	389	SER	2.3
1	D	392	PHE	2.3
1	A	495	ALA	2.3
1	D	495	ALA	2.3
1	B	283	ASN	2.3
1	D	290	GLY	2.2
1	D	170	MET	2.2
1	C	249	ALA	2.2
1	D	190	VAL	2.2
1	B	534	ILE	2.2
1	B	282	ARG	2.2
1	C	427	GLY	2.2
1	C	563	GLY	2.2
1	C	584	ARG	2.2
1	A	497	ILE	2.2
1	A	517	GLU	2.2
1	C	93	GLN	2.2
1	D	191	SER	2.2
1	D	421	SER	2.2
1	A	214	VAL	2.2
1	D	173	GLY	2.2
1	B	180	ILE	2.2
1	B	387	ILE	2.2
1	D	419	ILE	2.2
1	B	85	ASN	2.2
1	B	443	LEU	2.2
1	C	517	GLU	2.2
1	B	524	TYR	2.2
1	D	47	VAL	2.2
1	B	400	ILE	2.1
1	B	96	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	435	THR	2.1
1	C	35	LYS	2.1
1	D	516	ASN	2.1
1	C	467	ALA	2.1
1	D	385	HIS	2.1
1	A	393	LYS	2.1
1	A	81	LEU	2.1
1	A	304	LEU	2.1
1	C	304	LEU	2.1
1	B	53	PRO	2.1
1	A	245	GLY	2.1
1	D	247	TRP	2.1
1	D	427	GLY	2.1
1	D	493	ILE	2.1
1	C	52	LEU	2.1
1	B	138	LYS	2.1
1	D	425	ALA	2.1
1	D	146	LEU	2.1
1	D	444	PRO	2.1
1	C	39	THR	2.0
1	A	509	PHE	2.0
1	B	351	ILE	2.0
1	D	319	GLN	2.0
1	A	516	ASN	2.0
1	A	87	HIS	2.0
1	D	195	ARG	2.0
1	D	569	ARG	2.0
1	A	446	ILE	2.0
1	C	87	HIS	2.0
1	D	532	THR	2.0
1	C	46	GLU	2.0
1	C	438	GLU	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	PL3	D	1587	17/17	0.81	0.48	5.65	45,47,49,49	0
3	PL3	C	1587	17/17	0.78	0.41	4.18	34,36,42,43	0
3	PL3	B	1588	17/17	0.83	0.38	4.06	34,39,42,43	0
3	PL3	A	1588	17/17	0.77	0.37	3.45	31,33,37,39	0
2	FAD	B	1587	53/53	0.97	0.12	-0.54	6,12,13,15	0
2	FAD	C	1586	53/53	0.96	0.14	-0.66	6,11,15,16	0
2	FAD	A	1587	53/53	0.96	0.12	-0.91	3,8,10,11	0
2	FAD	D	1586	53/53	0.96	0.13	-1.04	7,11,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.