



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:48 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 (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

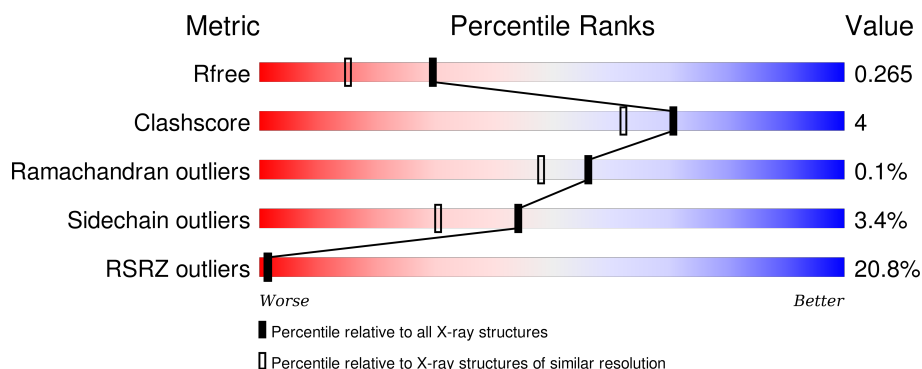
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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>85%</div> <div>8%</div> <div>6%</div> </div>
1	B	584	<div> <div>20%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	C	584	<div> <div>20%</div> <div>83%</div> <div>8%</div> <div>7%</div> </div>
1	D	584	<div> <div>22%</div> <div>82%</div> <div>8%</div> <div>8%</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.

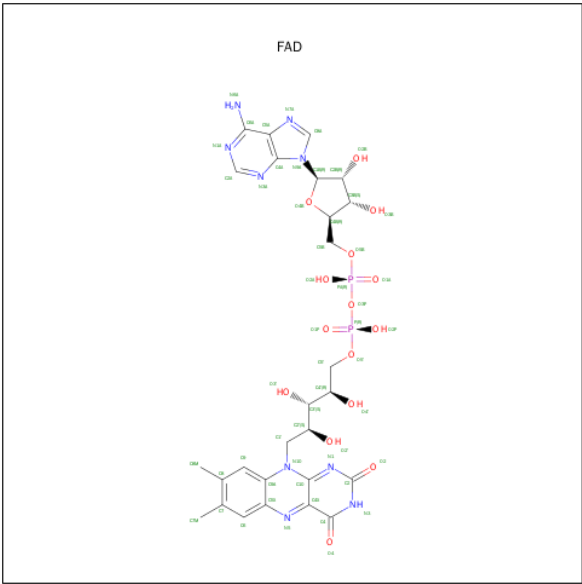
- Molecule 1 is a protein called ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE.

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:

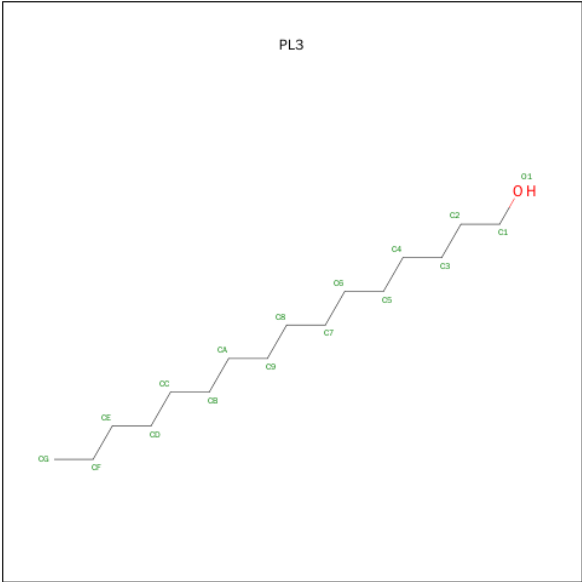
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP O96759
A	-4	ALA	-	EXPRESSION TAG	UNP O96759
A	-3	MET	-	EXPRESSION TAG	UNP O96759
A	-2	GLY	-	EXPRESSION TAG	UNP O96759
A	-1	SER	-	EXPRESSION TAG	UNP O96759
B	-5	GLY	-	EXPRESSION TAG	UNP O96759
B	-4	ALA	-	EXPRESSION TAG	UNP O96759
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: C₂₇H₃₃N₉O₁₅P₂).



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: C₁₆H₃₄O).



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		

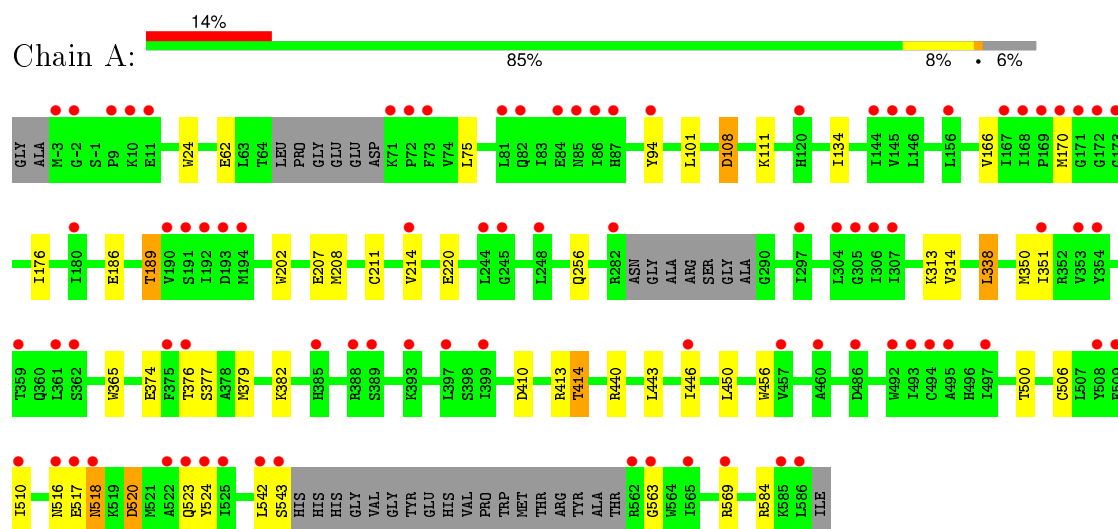
- Molecule 4 is water.

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		

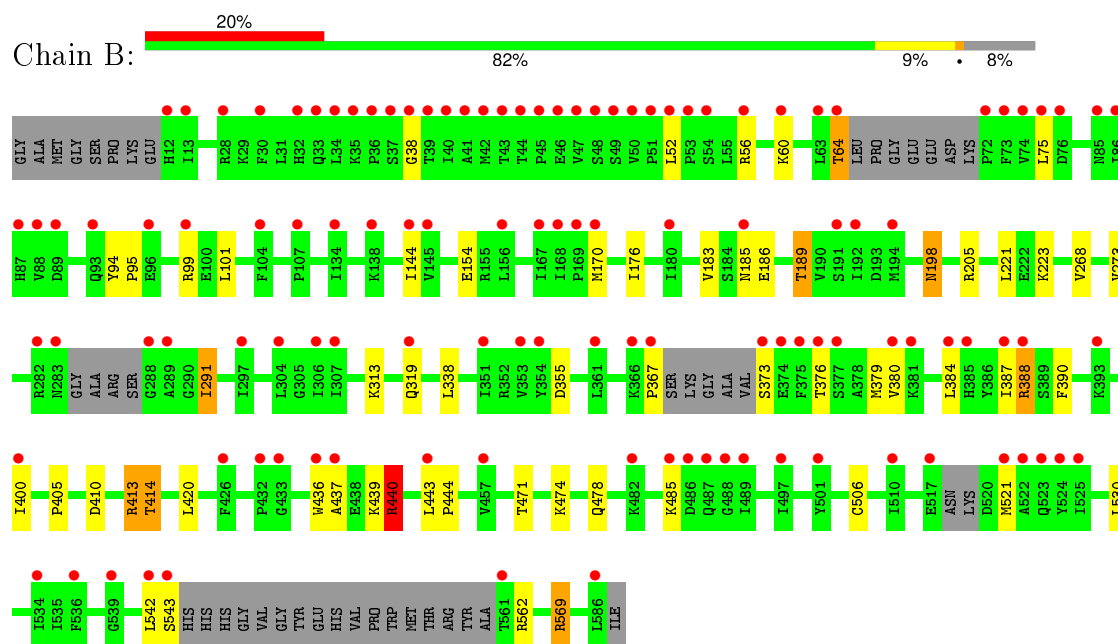
3 Residue-property plots

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.

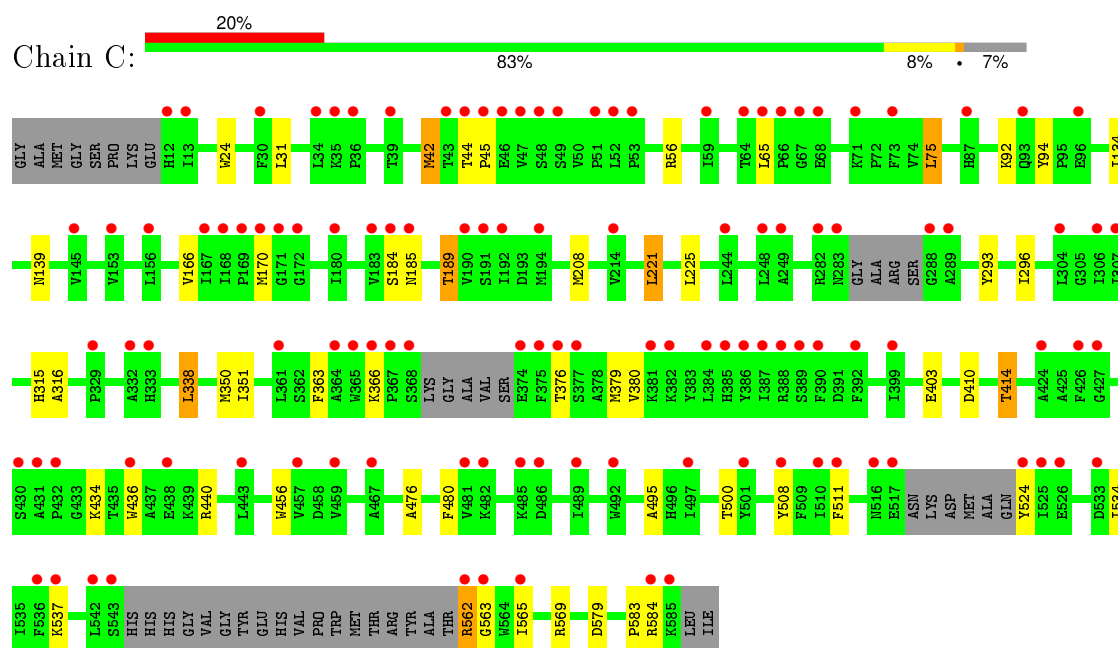
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



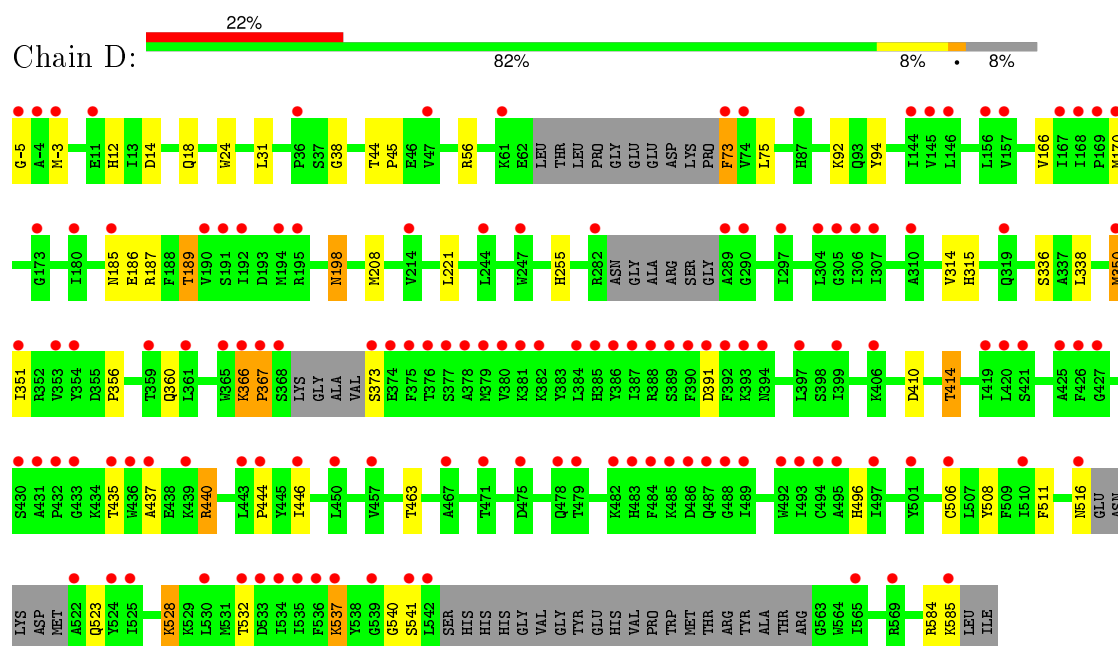
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



• 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 0.223 , 0.265	Depositor DCC
R_{free} test set	8930 reflections (5.29%)	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
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 177635 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:73:PHE:HA	4:D:2050:HOH:O	2.04	0.57
1:D:208:MET:HE3	1:D:314:VAL:HG23	1.86	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:D:221:LEU:HD23	1:D:221:LEU:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:TRP:CZ3	2:C:1586:FAD:HM83	2.42	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:D:373:SER:HA	4:D:2276:HOH:O	2.11	0.51
1:C:221:LEU:HD22	1:C:225:LEU:CD1	2.41	0.51
1:D:186:GLU:HG2	4:D:2153:HOH:O	2.10	0.51
1:C:366:LYS:HD3	1:C:380:VAL:HG21	1.93	0.51
1:A:518:ASN:OD1	1:A:518:ASN:N	2.43	0.51
1:D:198:ASN:H	1:D:198:ASN:HD22	1.60	0.50
1:B:471:THR:HG23	4:B:2332:HOH:O	2.12	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:95:PRO:HB2	1:B:99[B]:ARG:HH12	1.78	0.49
1:B:439:LYS:HD2	4:B:2274:HOH:O	2.11	0.49
1:B:176:ILE:HG21	3:B:1588:PL3:H2C1	1.94	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:C:44:THR:HB	1:C:45:PRO:HD2	1.96	0.48
1:A:207:GLU:O	1:A:313:LYS:NZ	2.43	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:C:208:MET:HE2	1:C:315:HIS:C	2.34	0.48
1:B:443:LEU:N	1:B:444:PRO:HD2	2.28	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: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:A:62:GLU:OE1	1:A:62:GLU:HA	2.16	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:363:PHE:HD1	1:C:380:VAL:HG22	1.83	0.44
1:C:350:MET:HG2	1:C:351:ILE:N	2.33	0.44
1:A:517:GLU:O	1:A:517:GLU:HG3	2.18	0.44
1:D:208:MET:HE1	1:D:315:HIS:C	2.38	0.43
1:B:439:LYS:HD3	1:B:439:LYS:C	2.39	0.43
1:D:366:LYS:HA	1:D:367:PRO:HD3	1.74	0.43
1:D:444:PRO:HG3	2:D:1586:FAD:HM73	2.00	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:D:350:MET:HG3	1:D:351:ILE:N	2.34	0.43
1:A:520:ASP:O	1:A:523:GLN:HG2	2.19	0.43
1:A:563:GLY:HA2	4:A:2466:HOH:O	2.18	0.43
1:A:450:LEU:HD11	3:A:1588:PL3:HDC2	2.01	0.43
1:A:134:ILE:HG23	4:A:2141:HOH:O	2.17	0.43
1:B:183:VAL:O	1:B:183:VAL:CG1	2.68	0.42
1:C:31:LEU:CD2	1:C:42:MET:HE3	2.49	0.42
1:B:268:VAL:CG2	1:B:313:LYS:HG3	2.49	0.42
1:B:221:LEU:C	1:B:221:LEU:HD23	2.39	0.42
1:A:338:LEU:HD12	1:A:351:ILE:HD13	2.01	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:D:463:THR:OG1	1:D:541:SER:HB3	2.20	0.42
1:B:291:ILE:N	1:B:291:ILE:CD1	2.83	0.42
1:A:338:LEU:HG	1:A:500:THR:HG21	2.01	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:D:511:PHE:HZ	1:D:528:LYS:CE	2.32	0.41
1:C:293:TYR:HD2	1:C:296:ILE:HD12	1.84	0.41
1:A:516:ASN:ND2	1:A:518:ASN:OD1	2.54	0.41
1:D:24:TRP:CZ3	2:D:1586:FAD:HM83	2.56	0.41
1:B:437:ALA:O	1:B:440:ARG:HD3	2.20	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: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:202:TRP:CE2	1:A:211:CYS:HB2	2.56	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:391:ASP:HB2	4:D:2278:HOH:O	2.21	0.41
1:D:18:GLN:HG2	4:D:2022: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%)	52	43
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	39	27
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	56	48

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%)	43	29
1	B	474/507 (94%)	456 (96%)	18 (4%)	40	25
1	C	472/507 (93%)	459 (97%)	13 (3%)	51	39
1	D	468/507 (92%)	451 (96%)	17 (4%)	42	28
All	All	1898/2028 (94%)	1833 (97%)	65 (3%)	44	30

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	48,58,58	1.52	8 (16%)	54,89,89	2.29	11 (20%)
3	PL3	A	1588	-	16,16,16	0.87	1 (6%)	15,15,15	0.84	0
2	FAD	B	1587	-	48,58,58	1.47	6 (12%)	54,89,89	2.66	14 (25%)
3	PL3	B	1588	-	16,16,16	0.93	1 (6%)	15,15,15	0.73	0
2	FAD	C	1586	-	48,58,58	1.49	6 (12%)	54,89,89	2.19	8 (14%)
3	PL3	C	1587	-	16,16,16	0.90	1 (6%)	15,15,15	0.87	0
2	FAD	D	1586	-	48,58,58	1.50	8 (16%)	54,89,89	2.58	10 (18%)
3	PL3	D	1587	-	16,16,16	0.89	1 (6%)	15,15,15	0.74	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	-	-	0/30/50/50	0/6/6/6
3	PL3	A	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1587	-	-	0/30/50/50	0/6/6/6
3	PL3	B	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1586	-	-	0/30/50/50	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	-	-	0/30/50/50	0/6/6/6
3	PL3	D	1587	-	-	0/14/14/14	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1588	PL3	O1-C1	-3.61	1.22	1.42
3	C	1587	PL3	O1-C1	-3.47	1.23	1.42
3	D	1587	PL3	O1-C1	-3.46	1.23	1.42
3	A	1588	PL3	O1-C1	-3.43	1.23	1.42
2	C	1586	FAD	C6-C5X	-2.28	1.38	1.41
2	A	1587	FAD	C9A-C5X	-2.05	1.38	1.42
2	A	1587	FAD	C9-C8	2.01	1.43	1.37
2	C	1586	FAD	C5'-C4'	2.07	1.54	1.51
2	D	1586	FAD	O4B-C1B	2.23	1.44	1.41
2	B	1587	FAD	C1'-N10	2.36	1.50	1.48
2	B	1587	FAD	C2A-N1A	2.56	1.38	1.33
2	D	1586	FAD	C5X-N5	2.59	1.39	1.35
2	D	1586	FAD	C2A-N3A	2.66	1.36	1.32
2	B	1587	FAD	C9A-N10	2.68	1.42	1.38
2	D	1586	FAD	C4-N3	2.69	1.38	1.33
2	D	1586	FAD	C5'-C4'	2.71	1.55	1.51
2	A	1587	FAD	C4-N3	2.75	1.38	1.33
2	C	1586	FAD	C4-N3	2.81	1.38	1.33
2	B	1587	FAD	C4-N3	3.00	1.38	1.33
2	C	1586	FAD	C2A-N3A	3.00	1.37	1.32
2	A	1587	FAD	C9A-N10	3.04	1.43	1.38
2	A	1587	FAD	C10-N1	3.23	1.41	1.35
2	A	1587	FAD	C5X-N5	3.24	1.40	1.35
2	D	1586	FAD	C2A-N1A	3.28	1.40	1.33
2	D	1586	FAD	C4X-N5	3.68	1.39	1.33
2	B	1587	FAD	C4X-N5	3.77	1.39	1.33
2	A	1587	FAD	C2A-N3A	4.15	1.39	1.32
2	C	1586	FAD	C4X-N5	4.16	1.39	1.33
2	A	1587	FAD	C4X-N5	4.60	1.40	1.33
2	D	1586	FAD	C1'-N10	4.91	1.53	1.48
2	B	1587	FAD	C2A-N3A	5.15	1.41	1.32
2	C	1586	FAD	C1'-N10	5.71	1.54	1.48

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-13.72	118.39	128.89
2	D	1586	FAD	N3A-C2A-N1A	-13.64	118.45	128.89
2	C	1586	FAD	N3A-C2A-N1A	-12.36	119.43	128.89
2	A	1587	FAD	N3A-C2A-N1A	-11.90	119.78	128.89
2	B	1587	FAD	C4X-C4-N3	-3.99	118.13	123.59
2	D	1586	FAD	C4X-C4-N3	-3.92	118.23	123.59
2	B	1587	FAD	O4'-C4'-C5'	-3.61	102.33	110.19
2	B	1587	FAD	C1B-N9A-C4A	-2.91	122.55	126.94
2	A	1587	FAD	C1B-N9A-C4A	-2.77	122.76	126.94
2	D	1586	FAD	O3P-P-O5'	-2.74	95.68	102.94
2	A	1587	FAD	C4X-C4-N3	-2.58	120.05	123.59
2	C	1586	FAD	P-O3P-PA	-2.53	125.62	132.73
2	A	1587	FAD	C4A-C5A-N7A	-2.52	107.16	109.48
2	A	1587	FAD	C4-C4X-C10	-2.51	118.33	119.94
2	B	1587	FAD	O4B-C1B-N9A	-2.41	103.06	108.10
2	A	1587	FAD	O4B-C1B-N9A	-2.37	103.14	108.10
2	C	1586	FAD	C1B-N9A-C4A	-2.34	123.41	126.94
2	B	1587	FAD	C4A-C5A-N7A	-2.29	107.37	109.48
2	C	1586	FAD	C4X-C4-N3	-2.26	120.50	123.59
2	B	1587	FAD	C8M-C8-C9	-2.14	114.46	120.28
2	A	1587	FAD	O4'-C4'-C5'	-2.00	105.83	110.19
2	B	1587	FAD	O2P-P-O3P	2.07	114.49	105.09
2	C	1586	FAD	C5X-C9A-N10	2.17	119.27	117.62
2	A	1587	FAD	P-O3P-PA	2.23	139.00	132.73
2	D	1586	FAD	C4-C4X-N5	2.29	121.50	118.72
2	B	1587	FAD	C4-C4X-N5	2.36	121.59	118.72
2	A	1587	FAD	C2A-N1A-C6A	2.39	123.03	118.77
2	D	1586	FAD	C2A-N1A-C6A	2.55	123.32	118.77
2	D	1586	FAD	C1'-N10-C9A	2.60	121.78	118.86
2	D	1586	FAD	O2P-P-O5'	2.72	122.18	108.46
2	B	1587	FAD	C2A-N1A-C6A	2.72	123.64	118.77
2	C	1586	FAD	C4-C4X-N5	2.73	122.04	118.72
2	A	1587	FAD	C5X-C9A-N10	3.27	120.10	117.62
2	B	1587	FAD	C4X-N5-C5X	3.37	120.64	116.76
2	C	1586	FAD	C4X-N5-C5X	3.44	120.72	116.76
2	B	1587	FAD	C4X-C10-N10	3.60	122.64	120.52
2	D	1586	FAD	C5X-C9A-N10	3.62	120.37	117.62
2	D	1586	FAD	C4X-N5-C5X	3.73	121.06	116.76
2	B	1587	FAD	C5X-C9A-N10	4.60	121.11	117.62
2	C	1586	FAD	C4-N3-C2	5.17	119.72	115.25
2	B	1587	FAD	C4-N3-C2	6.53	120.89	115.25
2	A	1587	FAD	C4-N3-C2	6.66	121.00	115.25
2	D	1586	FAD	C4-N3-C2	7.88	122.06	115.25

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 ⓘ

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	550/584 (94%)	0.88	84 (15%) 3 4	8, 20, 36, 58	0
1	B	540/584 (92%)	1.14	117 (21%) 1 1	8, 21, 43, 66	0
1	C	541/584 (92%)	1.21	118 (21%) 1 1	13, 27, 46, 56	0
1	D	537/584 (91%)	1.31	131 (24%) 1 1	12, 26, 59, 81	0
All	All	2168/2336 (92%)	1.13	450 (20%) 1 1	8, 22, 47, 81	0

All (450) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	PHE	11.8
1	D	377	SER	10.1
1	D	376	THR	10.0
1	B	522	ALA	9.4
1	D	432	PRO	9.1
1	A	586	LEU	8.1
1	C	375	PHE	8.0
1	A	525	ILE	8.0
1	B	437	ALA	7.9
1	D	436	TRP	7.7
1	C	368	SER	7.5
1	C	436	TRP	7.3
1	D	373	SER	6.9
1	A	-3	MET	6.7
1	C	65	LEU	6.7
1	C	384	LEU	6.6
1	C	388	ARG	6.6
1	D	374	GLU	6.5
1	D	289	ALA	6.5
1	D	379	MET	6.4
1	B	38	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	367	PRO	6.4
1	C	282	ARG	6.3
1	B	436	TRP	6.2
1	A	9	PRO	6.2
1	C	185	ASN	6.2
1	D	388	ARG	6.2
1	D	484	PHE	6.1
1	C	525	ILE	5.9
1	D	536	PHE	5.9
1	B	47	VAL	5.9
1	C	431	ALA	5.9
1	D	73	PHE	5.9
1	B	73	PHE	5.8
1	B	50	VAL	5.8
1	C	390	PHE	5.7
1	D	368	SER	5.7
1	C	66	PRO	5.7
1	C	542	LEU	5.7
1	A	11	GLU	5.7
1	D	525	ILE	5.7
1	A	192	ILE	5.7
1	B	288	GLY	5.5
1	B	37	SER	5.5
1	C	289	ALA	5.5
1	B	34	LEU	5.5
1	B	561	THR	5.4
1	B	543	SER	5.4
1	D	381	LYS	5.4
1	B	367	PRO	5.4
1	B	542	LEU	5.3
1	C	387	ILE	5.3
1	D	367	PRO	5.2
1	B	72	PRO	5.2
1	A	562	ARG	5.2
1	C	192	ILE	5.2
1	C	365	TRP	5.0
1	D	431	ALA	5.0
1	B	432	PRO	5.0
1	B	388	ARG	5.0
1	C	283	ASN	5.0
1	D	387	ILE	4.9
1	C	288	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	385	HIS	4.9
1	B	306	ILE	4.9
1	C	392	PHE	4.9
1	D	192	ILE	4.8
1	D	437	ALA	4.8
1	A	306	ILE	4.8
1	B	36	PRO	4.8
1	A	510	ILE	4.8
1	D	145	VAL	4.7
1	A	72	PRO	4.7
1	A	71	LYS	4.7
1	D	384	LEU	4.7
1	D	366	LYS	4.6
1	C	307	ILE	4.6
1	A	10	LYS	4.6
1	B	192	ILE	4.6
1	C	432	PRO	4.6
1	A	168	ILE	4.5
1	A	307	ILE	4.5
1	B	384	LEU	4.5
1	C	562	ARG	4.5
1	C	68	GLU	4.4
1	D	306	ILE	4.4
1	B	63	LEU	4.4
1	C	510	ILE	4.4
1	A	543	SER	4.4
1	A	457	VAL	4.3
1	D	535	ILE	4.3
1	D	282	ARG	4.2
1	C	48	SER	4.2
1	B	185	ASN	4.2
1	D	488	GLY	4.2
1	D	386	TYR	4.2
1	C	386	TYR	4.1
1	A	194	MET	4.1
1	B	87	HIS	4.1
1	D	475	ASP	4.1
1	A	146	LEU	4.1
1	D	483	HIS	4.1
1	B	488	GLY	4.1
1	C	565	ILE	4.1
1	D	537	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	4.1
1	D	426	PHE	4.1
1	D	501	TYR	4.0
1	A	169	PRO	4.0
1	B	373	SER	4.0
1	C	43	THR	4.0
1	A	375	PHE	4.0
1	C	485	LYS	3.9
1	C	382	LYS	3.9
1	B	385	HIS	3.9
1	A	145	VAL	3.9
1	B	45	PRO	3.9
1	C	374	GLU	3.9
1	C	482	LYS	3.8
1	C	34	LEU	3.8
1	B	64	THR	3.8
1	C	67	GLY	3.8
1	D	-5	GLY	3.8
1	B	289	ALA	3.8
1	C	381	LYS	3.8
1	D	-4	ALA	3.8
1	B	46	GLU	3.8
1	D	457	VAL	3.8
1	C	376	THR	3.8
1	C	59	ILE	3.7
1	C	306	ILE	3.7
1	B	376	THR	3.7
1	A	522	ALA	3.7
1	C	516	ASN	3.7
1	B	366	LYS	3.7
1	B	74	VAL	3.7
1	D	478	GLN	3.7
1	C	169	PRO	3.7
1	A	144	ILE	3.7
1	A	565	ILE	3.7
1	B	39	THR	3.7
1	B	75	LEU	3.7
1	C	12	HIS	3.7
1	D	486	ASP	3.7
1	D	492	TRP	3.7
1	B	381	LYS	3.7
1	C	366	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	537	LYS	3.6
1	B	486	ASP	3.6
1	A	388	ARG	3.6
1	D	169	PRO	3.6
1	C	214	VAL	3.6
1	B	487	GLN	3.6
1	B	56	ARG	3.6
1	A	180	ILE	3.6
1	B	167	ILE	3.6
1	D	494	CYS	3.6
1	D	61	LYS	3.6
1	C	426	PHE	3.6
1	B	510	ILE	3.6
1	C	36	PRO	3.5
1	B	525	ILE	3.5
1	D	489	ILE	3.5
1	B	12	HIS	3.5
1	B	48	SER	3.5
1	A	73	PHE	3.5
1	D	144	ILE	3.5
1	B	51	PRO	3.5
1	D	354	TYR	3.5
1	B	457	VAL	3.5
1	B	521	MET	3.5
1	C	53	PRO	3.5
1	D	378	ALA	3.5
1	C	190	VAL	3.4
1	B	523	GLN	3.4
1	B	375	PHE	3.4
1	D	350	MET	3.4
1	C	45	PRO	3.4
1	D	244	LEU	3.4
1	D	542	LEU	3.4
1	C	329	PRO	3.4
1	D	482	LYS	3.4
1	B	33	GLN	3.3
1	A	86	ILE	3.3
1	A	167	ILE	3.3
1	B	297	ILE	3.3
1	B	586	LEU	3.3
1	C	536	PHE	3.3
1	B	377	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	446	ILE	3.3
1	C	443	LEU	3.3
1	B	86	ILE	3.3
1	A	-2	GLY	3.2
1	A	170	MET	3.2
1	D	433	GLY	3.2
1	D	524	TYR	3.2
1	D	565	ILE	3.2
1	A	85	ASN	3.2
1	D	380	VAL	3.2
1	D	393	LYS	3.2
1	B	517	GLU	3.2
1	C	424	ALA	3.2
1	D	487	GLN	3.2
1	B	145	VAL	3.2
1	A	563	GLY	3.2
1	D	450	LEU	3.2
1	B	194	MET	3.1
1	D	443	LEU	3.1
1	A	494	CYS	3.1
1	C	457	VAL	3.1
1	A	569	ARG	3.1
1	B	13	ILE	3.1
1	B	307	ILE	3.1
1	C	526	GLU	3.1
1	D	497	ILE	3.1
1	C	64	THR	3.1
1	A	397	LEU	3.1
1	D	214	VAL	3.1
1	B	49	SER	3.1
1	C	501	TYR	3.1
1	D	157	VAL	3.1
1	A	385	HIS	3.0
1	A	244	LEU	3.0
1	D	156	LEU	3.0
1	D	351	ILE	3.0
1	B	169	PRO	3.0
1	B	353	VAL	3.0
1	C	71	LYS	3.0
1	B	144	ILE	3.0
1	C	333	HIS	3.0
1	C	481	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	ARG	3.0
1	D	365	TRP	3.0
1	B	485	LYS	3.0
1	C	168	ILE	3.0
1	D	194	MET	3.0
1	B	40	ILE	3.0
1	A	82	GLN	3.0
1	A	354	TYR	3.0
1	B	42	MET	3.0
1	B	44	THR	3.0
1	A	156	LEU	3.0
1	C	167	ILE	3.0
1	C	497	ILE	3.0
1	A	376	THR	2.9
1	B	536	PHE	2.9
1	D	36	PRO	2.9
1	D	522	ALA	2.9
1	B	52	LEU	2.9
1	D	353	VAL	2.9
1	D	467	ALA	2.9
1	A	523	GLN	2.9
1	B	361	LEU	2.9
1	B	539	GLY	2.9
1	C	194	MET	2.9
1	B	497	ILE	2.9
1	A	492	TRP	2.9
1	D	506	CYS	2.9
1	B	35	LYS	2.9
1	A	84	GLU	2.9
1	D	297	ILE	2.9
1	A	353	VAL	2.9
1	B	426	PHE	2.8
1	D	87	HIS	2.8
1	C	183	VAL	2.8
1	B	32	HIS	2.8
1	B	433	GLY	2.8
1	D	361	LEU	2.8
1	B	134	ILE	2.8
1	D	585	LYS	2.8
1	D	11	GLU	2.8
1	B	76	ASP	2.8
1	A	361	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	-3	MET	2.8
1	D	307	ILE	2.8
1	C	47	VAL	2.8
1	C	153	VAL	2.8
1	A	486	ASP	2.8
1	A	248	LEU	2.7
1	D	397	LEU	2.7
1	D	479	THR	2.7
1	D	530	LEU	2.7
1	B	88	VAL	2.7
1	D	406	LYS	2.7
1	B	354	TYR	2.7
1	C	377	SER	2.7
1	B	28	ARG	2.7
1	C	170	MET	2.7
1	A	191	SER	2.7
1	B	107	PRO	2.7
1	C	508	TYR	2.7
1	C	585	LYS	2.7
1	C	361	LEU	2.7
1	C	389	SER	2.7
1	B	374	GLU	2.7
1	B	60	LYS	2.7
1	B	393	LYS	2.7
1	A	193	ASP	2.7
1	B	168	ILE	2.6
1	D	510	ILE	2.6
1	D	390	PHE	2.6
1	C	13	ILE	2.6
1	C	145	VAL	2.6
1	C	489	ILE	2.6
1	D	304	LEU	2.6
1	C	364	ALA	2.6
1	A	171	GLY	2.6
1	A	172	GLY	2.6
1	A	94	TYR	2.6
1	A	585	LYS	2.6
1	B	30	PHE	2.6
1	B	170	MET	2.6
1	D	167	ILE	2.6
1	A	359	THR	2.6
1	D	180	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	534	ILE	2.6
1	B	54	SER	2.6
1	C	430	SER	2.6
1	A	524	TYR	2.6
1	C	486	ASP	2.6
1	D	439	LYS	2.5
1	C	180	ILE	2.5
1	C	543	SER	2.5
1	A	173	GLY	2.5
1	C	51	PRO	2.5
1	C	244	LEU	2.5
1	D	391	ASP	2.5
1	A	190	VAL	2.5
1	A	297	ILE	2.5
1	D	168	ILE	2.5
1	C	96	GLU	2.5
1	D	359	THR	2.5
1	A	518	ASN	2.5
1	A	362	SER	2.5
1	A	389	SER	2.5
1	C	184	SER	2.5
1	D	310	ALA	2.5
1	A	542	LEU	2.5
1	D	471	THR	2.5
1	D	185	ASN	2.4
1	D	382	LYS	2.4
1	D	541	SER	2.4
1	B	41	ALA	2.4
1	D	533	ASP	2.4
1	A	508	TYR	2.4
1	D	305	GLY	2.4
1	B	482	LYS	2.4
1	C	171	GLY	2.4
1	B	43	THR	2.4
1	B	319	GLN	2.4
1	B	89	ASP	2.4
1	C	533	ASP	2.4
1	C	30	PHE	2.4
1	C	459	VAL	2.4
1	A	493	ILE	2.4
1	A	120	HIS	2.4
1	C	44	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	304	LEU	2.4
1	D	420	LEU	2.4
1	B	104	PHE	2.4
1	C	511	PHE	2.4
1	C	191	SER	2.4
1	D	399	ILE	2.4
1	D	485	LYS	2.4
1	D	392	PHE	2.4
1	C	49	SER	2.4
1	B	93	GLN	2.3
1	B	501	TYR	2.3
1	C	524	TYR	2.3
1	A	495	ALA	2.3
1	C	249	ALA	2.3
1	D	495	ALA	2.3
1	D	389	SER	2.3
1	D	190	VAL	2.3
1	A	497	ILE	2.3
1	B	534	ILE	2.3
1	B	283	ASN	2.3
1	C	563	GLY	2.3
1	D	290	GLY	2.3
1	B	180	ILE	2.3
1	B	443	LEU	2.3
1	C	427	GLY	2.3
1	A	214	VAL	2.3
1	B	282	ARG	2.3
1	B	387	ILE	2.3
1	D	419	ILE	2.3
1	D	170	MET	2.3
1	D	191	SER	2.3
1	D	421	SER	2.3
1	D	173	GLY	2.3
1	C	93	GLN	2.3
1	A	517	GLU	2.2
1	C	584	ARG	2.2
1	D	47	VAL	2.2
1	B	85	ASN	2.2
1	B	400	ILE	2.2
1	C	517	GLU	2.2
1	B	524	TYR	2.2
1	A	304	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	435	THR	2.2
1	C	467	ALA	2.2
1	A	81	LEU	2.2
1	C	304	LEU	2.2
1	D	385	HIS	2.2
1	B	96	GLU	2.2
1	C	35	LYS	2.2
1	D	516	ASN	2.2
1	D	493	ILE	2.2
1	C	52	LEU	2.2
1	D	146	LEU	2.2
1	B	53	PRO	2.1
1	A	245	GLY	2.1
1	D	427	GLY	2.1
1	D	247	TRP	2.1
1	B	351	ILE	2.1
1	A	393	LYS	2.1
1	D	425	ALA	2.1
1	A	509	PHE	2.1
1	A	446	ILE	2.1
1	D	444	PRO	2.1
1	C	39	THR	2.1
1	A	351	ILE	2.1
1	B	138	LYS	2.1
1	A	87	HIS	2.1
1	D	532	THR	2.1
1	A	399	ILE	2.1
1	A	516	ASN	2.1
1	D	319	GLN	2.1
1	D	539	GLY	2.1
1	C	87	HIS	2.1
1	C	46	GLU	2.0
1	C	73	PHE	2.0
1	C	399	ILE	2.0
1	D	195	ARG	2.0
1	D	569	ARG	2.0
1	C	156	LEU	2.0
1	D	430	SER	2.0
1	C	438	GLU	2.0
1	A	460	ALA	2.0
1	B	156	LEU	2.0
1	C	248	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	492	TRP	2.0
1	B	99[A]	ARG	2.0
1	D	74	VAL	2.0
1	D	394	ASN	2.0
1	B	191	SER	2.0
1	C	332	ALA	2.0
1	A	305	GLY	2.0
1	C	172	GLY	2.0
1	B	489	ILE	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	5.67	45,47,49,49	0
3	PL3	C	1587	17/17	0.78	0.41	4.17	34,36,42,43	0
3	PL3	B	1588	17/17	0.83	0.38	4.02	34,39,42,43	0
3	PL3	A	1588	17/17	0.77	0.37	3.44	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	-0.90	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.