



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:15 AM GMT

PDB ID : 2UUU
Title : ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE 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 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/ValidationPDFNotes.html>

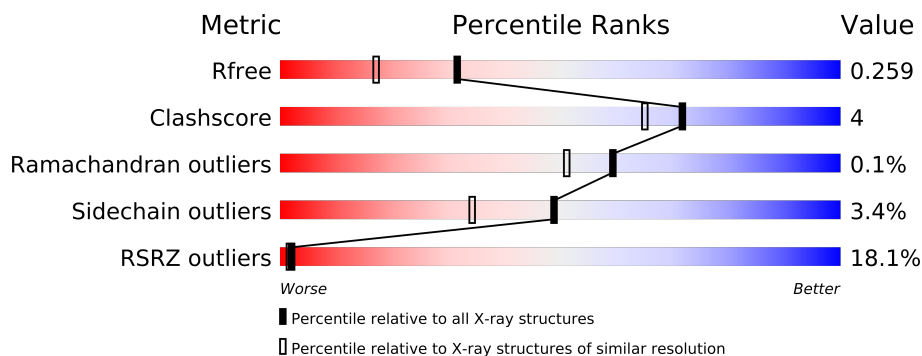
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	
1	C	584	
1	D	584	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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 hydrogen and 0 are deuterium.

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.

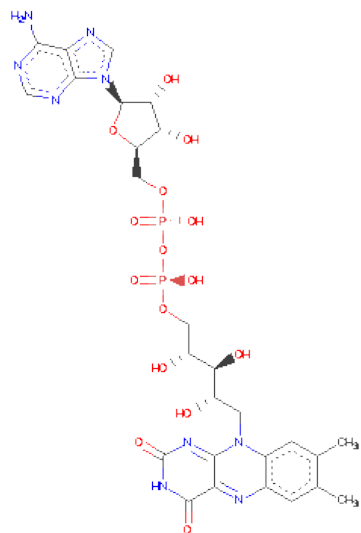
- Molecule 1 is a protein called ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE.

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:

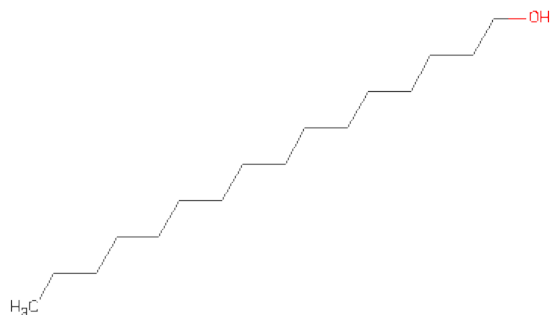
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP O96759
A	-4	ALA	-	EXPRESSION TAG	UNP O96759
A	-3	MET	-	EXPRESSION TAG	UNP O96759
A	-2	GLY	-	EXPRESSION TAG	UNP O96759
A	-1	SER	-	EXPRESSION TAG	UNP O96759
B	-5	GLY	-	EXPRESSION TAG	UNP O96759
B	-4	ALA	-	EXPRESSION TAG	UNP O96759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

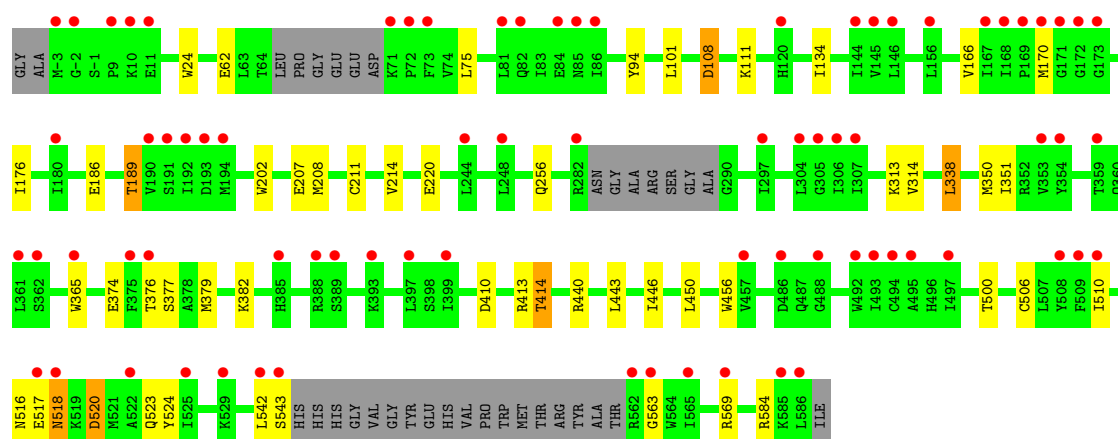
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	484	Total	O	0	0
			484	484		
4	B	385	Total	O	0	0
			385	385		
4	C	333	Total	O	0	0
			333	333		
4	D	348	Total	O	0	0
			348	348		

3 Residue-property plots

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.

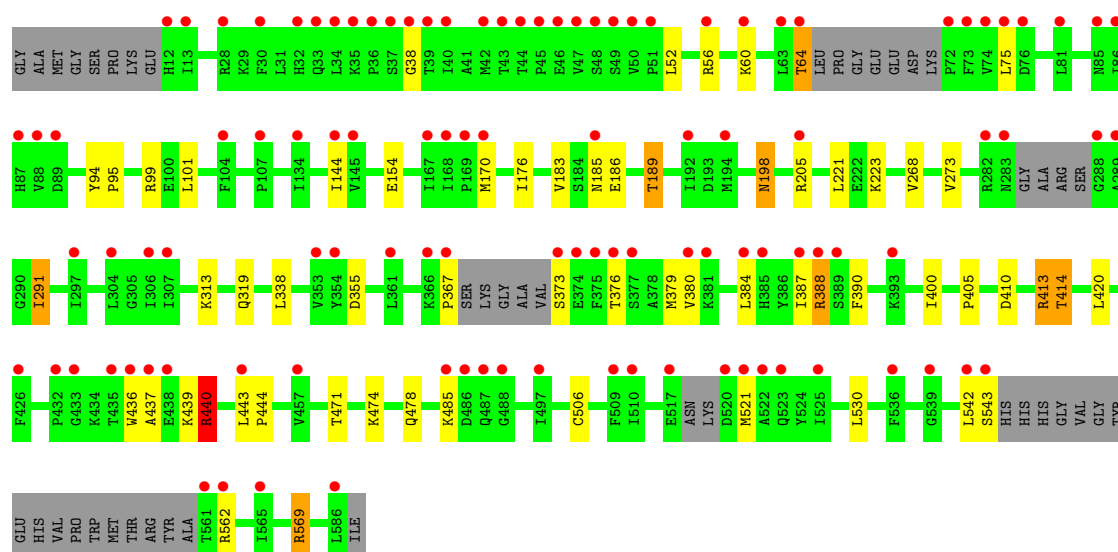
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain A: 



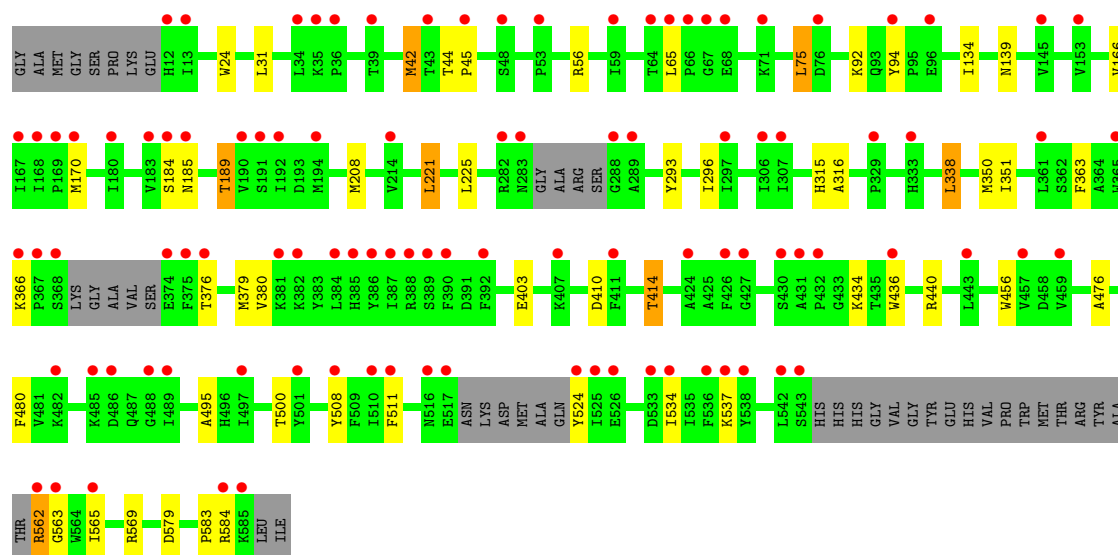
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain B: 



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain C: 



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)	0.36 , 41.6	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (156) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:C:24:TRP:CZ3	2:C:1586:FAD:HM83	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	56	46
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	43	30
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	59	51

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%)	48	32
1	B	474/507 (94%)	456 (96%)	18 (4%)	44	29
1	C	472/507 (93%)	459 (97%)	13 (3%)	56	43
1	D	468/507 (92%)	451 (96%)	17 (4%)	47	31
All	All	1898/2028 (94%)	1833 (97%)	65 (3%)	49	34

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
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

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Mol	Chain	Res	Type
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
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 chains 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	-	58,58,58	1.47	7 (12%)	85,89,89	2.01	15 (17%)
3	PL3	A	1588	-	16,16,16	0.87	1 (6%)	15,15,15	0.81	0
2	FAD	B	1587	-	58,58,58	1.46	5 (8%)	85,89,89	2.30	19 (22%)
3	PL3	B	1588	-	16,16,16	0.94	1 (6%)	15,15,15	0.71	0
2	FAD	C	1586	-	58,58,58	1.37	5 (8%)	85,89,89	1.82	10 (11%)
3	PL3	C	1587	-	16,16,16	0.91	1 (6%)	15,15,15	0.84	0
2	FAD	D	1586	-	58,58,58	1.40	7 (12%)	85,89,89	1.98	13 (15%)
3	PL3	D	1587	-	16,16,16	0.90	1 (6%)	15,15,15	0.72	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	-	-	0/34/50/50	0/1/6/6
3	PL3	A	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1587	-	-	0/34/50/50	0/1/6/6
3	PL3	B	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1586	-	-	0/34/50/50	0/1/6/6
3	PL3	C	1587	-	-	0/14/14/14	0/0/0/0
2	FAD	D	1586	-	-	0/34/50/50	0/1/6/6
3	PL3	D	1587	-	-	0/14/14/14	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1587	FAD	C1'-C2'	6.36	1.57	1.51
2	B	1587	FAD	C1'-C2'	6.33	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1586	FAD	C1'-N10	5.53	1.54	1.48
2	D	1586	FAD	C1'-N10	4.78	1.53	1.48
2	B	1587	FAD	C2A-N3A	4.62	1.41	1.32
2	C	1586	FAD	C1'-C2'	3.89	1.55	1.51
2	A	1587	FAD	C2A-N3A	3.72	1.39	1.32
3	B	1588	PL3	O1-C1	-3.63	1.22	1.42
2	D	1586	FAD	C1'-C2'	3.63	1.55	1.51
3	C	1587	PL3	O1-C1	-3.48	1.23	1.42
3	D	1587	PL3	O1-C1	-3.48	1.23	1.42
3	A	1588	PL3	O1-C1	-3.44	1.23	1.42
2	A	1587	FAD	C5X-N5	3.38	1.40	1.35
2	D	1586	FAD	C2A-N1A	3.16	1.40	1.33
2	A	1587	FAD	C10-N1	2.98	1.41	1.35
2	C	1586	FAD	C6-C5X	-2.89	1.38	1.41
2	A	1587	FAD	C9A-N10	2.80	1.43	1.38
2	D	1586	FAD	C5X-N5	2.70	1.39	1.35
2	C	1586	FAD	C2A-N3A	2.69	1.37	1.32
2	D	1586	FAD	C5'-C4'	2.60	1.55	1.51
2	C	1586	FAD	P-O3P	2.55	1.64	1.59
2	B	1587	FAD	C2A-N1A	2.46	1.38	1.33
2	B	1587	FAD	C9A-N10	2.46	1.42	1.38
2	B	1587	FAD	C1'-N10	2.42	1.50	1.48
2	D	1586	FAD	C2A-N3A	2.38	1.36	1.32
2	D	1586	FAD	P-O3P	2.21	1.63	1.59
2	A	1587	FAD	C4X-N5	2.11	1.40	1.36
2	A	1587	FAD	C9-C8	2.01	1.43	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-12.34	118.39	128.71
2	D	1586	FAD	N3A-C2A-N1A	-12.27	118.45	128.71
2	C	1586	FAD	N3A-C2A-N1A	-11.10	119.43	128.71
2	A	1587	FAD	N3A-C2A-N1A	-10.68	119.78	128.71
2	A	1587	FAD	C2'-C1'-N10	6.72	121.36	112.45
2	B	1587	FAD	O4B-C1B-N9A	-5.78	103.06	108.44
2	A	1587	FAD	O4B-C1B-N9A	-5.70	103.14	108.44
2	C	1586	FAD	C2-N1-C10	5.65	120.67	114.98
2	B	1587	FAD	C2'-C1'-N10	5.11	119.24	112.45
2	B	1587	FAD	C2-N1-C10	5.08	120.10	114.98
2	B	1587	FAD	C9A-N10-C10	-5.05	116.81	121.77
2	D	1586	FAD	C2-N1-C10	5.04	120.06	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	C5X-C9A-N10	4.38	121.11	116.80
2	B	1587	FAD	C4X-C10-N10	4.28	122.64	120.51
2	A	1587	FAD	C2-N1-C10	3.97	118.98	114.98
2	D	1586	FAD	C4X-N5-C5X	3.89	121.06	116.69
2	B	1587	FAD	O4'-C4'-C5'	-3.79	102.33	110.12
2	D	1586	FAD	C5X-C9A-N10	3.63	120.37	116.80
2	C	1586	FAD	C4X-N5-C5X	3.59	120.72	116.69
2	B	1587	FAD	C4X-N5-C5X	3.51	120.64	116.69
2	A	1587	FAD	C9A-N10-C10	-3.39	118.44	121.77
2	A	1587	FAD	C5X-C9A-N10	3.35	120.10	116.80
2	C	1586	FAD	C2'-C1'-N10	3.26	116.78	112.45
2	D	1586	FAD	N3A-C4A-N9A	3.18	131.18	125.43
2	B	1587	FAD	C4X-C10-N1	-3.07	119.67	122.73
2	D	1586	FAD	C1'-N10-C9A	2.99	121.78	118.87
2	C	1586	FAD	C4X-C10-N1	-2.90	119.83	122.73
2	C	1586	FAD	N3A-C4A-N9A	2.90	130.66	125.43
2	D	1586	FAD	C2'-C1'-N10	2.88	116.27	112.45
2	D	1586	FAD	C8A-N9A-C4A	2.79	109.03	106.90
2	C	1586	FAD	C4-N3-C2	-2.76	119.72	125.39
2	A	1587	FAD	C4A-C5A-N7A	-2.76	107.16	109.52
2	D	1586	FAD	O2P-P-O5'	2.71	122.18	108.51
2	B	1587	FAD	C2A-N1A-C6A	2.69	123.64	118.77
2	D	1586	FAD	C9A-N10-C10	-2.59	119.22	121.77
2	D	1586	FAD	C2A-N1A-C6A	2.52	123.32	118.77
2	B	1587	FAD	C5'-C4'-C3'	2.52	116.81	112.06
2	B	1587	FAD	C4A-C5A-N7A	-2.51	107.37	109.52
2	C	1586	FAD	C5X-C9A-N10	2.50	119.27	116.80
2	A	1587	FAD	P-O3P-PA	2.49	139.00	131.68
2	B	1587	FAD	C8M-C8-C9	-2.45	114.46	120.38
2	D	1586	FAD	C4X-C10-N1	-2.43	120.30	122.73
2	B	1587	FAD	C1B-N9A-C4A	-2.37	122.55	126.64
2	A	1587	FAD	C2A-N1A-C6A	2.36	123.03	118.77
2	D	1586	FAD	N7A-C8A-N9A	-2.32	107.79	114.36
2	B	1587	FAD	N3A-C4A-N9A	2.28	129.55	125.43
2	A	1587	FAD	O4B-C1B-C2B	-2.27	103.30	106.77
2	A	1587	FAD	C1B-N9A-C4A	-2.24	122.76	126.64
2	B	1587	FAD	C1'-N10-C9A	2.22	121.03	118.87
2	A	1587	FAD	N3A-C4A-N9A	2.22	129.44	125.43
2	B	1587	FAD	C4-N3-C2	-2.19	120.89	125.39
2	B	1587	FAD	P-O3P-PA	2.19	138.09	131.68
2	A	1587	FAD	C4-N3-C2	-2.14	121.00	125.39
2	A	1587	FAD	O4'-C4'-C5'	-2.09	105.83	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1586	FAD	P-O3P-PA	-2.07	125.62	131.68
2	A	1587	FAD	C8M-C8-C9	-2.06	115.41	120.38
2	C	1586	FAD	O4'-C4'-C5'	-2.05	105.91	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.81	77 (14%) 3 3	8, 20, 36, 58	0
1	B	540/584 (92%)	1.07	107 (19%) 2 1	8, 21, 43, 66	0
1	C	541/584 (92%)	1.12	101 (18%) 2 1	13, 27, 46, 56	0
1	D	537/584 (91%)	1.18	109 (20%) 1 1	12, 26, 59, 81	0
All	All	2168/2336 (92%)	1.04	394 (18%) 2 1	8, 22, 47, 81	0

All (394) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	377	SER	10.0
1	D	432	PRO	9.9
1	D	375	PHE	9.9
1	D	376	THR	9.5
1	B	522	ALA	8.9
1	D	436	TRP	7.5
1	C	65	LEU	7.4
1	C	375	PHE	7.3
1	A	586	LEU	7.1
1	B	437	ALA	7.0
1	D	373	SER	7.0
1	C	368	SER	6.7
1	C	388	ARG	6.5
1	C	436	TRP	6.5
1	C	390	PHE	6.3
1	C	185	ASN	6.2
1	C	282	ARG	6.2
1	B	38	GLY	6.1
1	A	11	GLU	6.0
1	B	288	GLY	6.0
1	A	-3	MET	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	289	ALA	5.9
1	C	66	PRO	5.9
1	D	388	ARG	5.9
1	B	34	LEU	5.8
1	B	542	LEU	5.8
1	D	484	PHE	5.8
1	D	374	GLU	5.7
1	A	9	PRO	5.6
1	D	536	PHE	5.5
1	B	47	VAL	5.5
1	B	388	ARG	5.4
1	B	384	LEU	5.4
1	A	525	ILE	5.4
1	C	283	ASN	5.4
1	A	192	ILE	5.3
1	B	436	TRP	5.3
1	D	289	ALA	5.3
1	C	384	LEU	5.3
1	C	68	GLU	5.3
1	C	387	ILE	5.3
1	C	525	ILE	5.2
1	D	431	ALA	5.2
1	C	367	PRO	5.2
1	C	542	LEU	5.2
1	D	73	PHE	5.1
1	B	561	THR	5.0
1	C	288	GLY	5.0
1	B	73	PHE	5.0
1	D	366	LYS	5.0
1	D	381	LYS	5.0
1	A	562	ARG	4.9
1	A	10	LYS	4.8
1	C	386	TYR	4.8
1	C	392	PHE	4.7
1	D	145	VAL	4.7
1	C	431	ALA	4.7
1	C	192	ILE	4.6
1	A	306	ILE	4.6
1	D	501	TYR	4.6
1	B	50	VAL	4.6
1	D	542	LEU	4.5
1	B	74	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	543	SER	4.5
1	A	71	LYS	4.5
1	B	36	PRO	4.5
1	B	72	PRO	4.5
1	A	72	PRO	4.5
1	B	37	SER	4.4
1	C	307	ILE	4.4
1	D	437	ALA	4.4
1	D	379	MET	4.4
1	C	365	TRP	4.4
1	B	86	ILE	4.4
1	B	432	PRO	4.3
1	D	192	ILE	4.3
1	C	67	GLY	4.3
1	A	510	ILE	4.3
1	D	535	ILE	4.3
1	D	-5	GLY	4.2
1	B	380	VAL	4.2
1	B	192	ILE	4.2
1	B	306	ILE	4.2
1	D	483	HIS	4.2
1	D	306	ILE	4.2
1	B	521	MET	4.1
1	C	385	HIS	4.1
1	B	64	THR	4.1
1	D	282	ARG	4.1
1	D	367	PRO	4.1
1	B	63	LEU	4.1
1	C	516	ASN	4.0
1	D	368	SER	4.0
1	C	510	ILE	4.0
1	D	169	PRO	4.0
1	A	543	SER	4.0
1	B	373	SER	3.9
1	D	525	ILE	3.9
1	A	307	ILE	3.9
1	A	168	ILE	3.9
1	C	562	ARG	3.9
1	D	387	ILE	3.9
1	B	45	PRO	3.8
1	D	426	PHE	3.8
1	B	75	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	486	ASP	3.8
1	B	33	GLN	3.8
1	B	46	GLU	3.8
1	C	426	PHE	3.8
1	B	367	PRO	3.7
1	B	376	THR	3.7
1	A	457	VAL	3.7
1	C	169	PRO	3.7
1	A	169	PRO	3.6
1	C	432	PRO	3.6
1	B	385	HIS	3.6
1	D	386	TYR	3.6
1	D	384	LEU	3.6
1	A	194	MET	3.6
1	B	289	ALA	3.5
1	D	144	ILE	3.5
1	B	48	SER	3.5
1	C	366	LYS	3.5
1	B	510	ILE	3.5
1	B	523	GLN	3.5
1	A	522	ALA	3.5
1	B	76	ASP	3.5
1	C	59	ILE	3.5
1	C	64	THR	3.5
1	C	48	SER	3.5
1	B	381	LYS	3.5
1	B	167	ILE	3.5
1	B	44	THR	3.4
1	D	-4	ALA	3.4
1	D	475	ASP	3.4
1	B	35	LYS	3.4
1	A	388	ARG	3.4
1	C	501	TYR	3.4
1	A	86	ILE	3.4
1	C	536	PHE	3.4
1	A	144	ILE	3.4
1	B	377	SER	3.4
1	B	387	ILE	3.4
1	B	56	ARG	3.4
1	C	53	PRO	3.4
1	D	530	LEU	3.4
1	A	375	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	488	GLY	3.4
1	C	381	LYS	3.4
1	D	537	LYS	3.4
1	D	457	VAL	3.3
1	C	306	ILE	3.3
1	C	482	LYS	3.3
1	A	354	TYR	3.3
1	A	-2	GLY	3.3
1	B	87	HIS	3.3
1	B	297	ILE	3.3
1	C	374	GLU	3.3
1	C	489	ILE	3.3
1	C	43	THR	3.3
1	B	12	HIS	3.3
1	A	569	ARG	3.2
1	A	82	GLN	3.2
1	D	478	GLN	3.2
1	A	585	LYS	3.2
1	C	12	HIS	3.2
1	C	36	PRO	3.2
1	D	467	ALA	3.2
1	C	329	PRO	3.2
1	C	537	LYS	3.2
1	C	190	VAL	3.2
1	B	539	GLY	3.2
1	C	13	ILE	3.2
1	B	39	THR	3.2
1	B	366	LYS	3.2
1	C	543	SER	3.2
1	A	180	ILE	3.2
1	B	51	PRO	3.2
1	A	73	PHE	3.1
1	B	375	PHE	3.1
1	B	517	GLU	3.1
1	A	146	LEU	3.1
1	A	397	LEU	3.1
1	C	485	LYS	3.1
1	D	61	LYS	3.1
1	C	526	GLU	3.1
1	B	60	LYS	3.1
1	D	487	GLN	3.1
1	D	541	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	351	ILE	3.1
1	A	145	VAL	3.1
1	B	393	LYS	3.1
1	B	169	PRO	3.1
1	A	85	ASN	3.1
1	C	214	VAL	3.0
1	D	390	PHE	3.0
1	D	443	LEU	3.0
1	D	354	TYR	3.0
1	D	494	CYS	3.0
1	B	134	ILE	3.0
1	B	525	ILE	3.0
1	A	542	LEU	3.0
1	C	34	LEU	3.0
1	C	457	VAL	3.0
1	D	489	ILE	3.0
1	C	71	LYS	3.0
1	D	433	GLY	3.0
1	B	353	VAL	2.9
1	B	457	VAL	2.9
1	B	433	GLY	2.9
1	B	536	PHE	2.9
1	C	382	LYS	2.9
1	D	446	ILE	2.9
1	D	482	LYS	2.9
1	C	376	THR	2.9
1	B	586	LEU	2.9
1	B	488	GLY	2.9
1	D	492	TRP	2.9
1	C	443	LEU	2.9
1	A	353	VAL	2.9
1	C	565	ILE	2.9
1	C	184	SER	2.9
1	B	185	ASN	2.9
1	D	378	ALA	2.8
1	C	497	ILE	2.8
1	D	-3	MET	2.8
1	B	28	ARG	2.8
1	B	361	LEU	2.8
1	C	361	LEU	2.8
1	C	524	TYR	2.8
1	D	350	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	374	GLU	2.8
1	D	297	ILE	2.8
1	D	565	ILE	2.8
1	D	87	HIS	2.8
1	A	282	ARG	2.8
1	D	393	LYS	2.8
1	B	487	GLN	2.8
1	C	508	TYR	2.7
1	A	84	GLU	2.7
1	D	167	ILE	2.7
1	B	520	ASP	2.7
1	D	185	ASN	2.7
1	A	170	MET	2.7
1	D	406	LYS	2.7
1	D	427	GLY	2.7
1	B	107	PRO	2.7
1	A	191	SER	2.7
1	A	167	ILE	2.7
1	B	144	ILE	2.7
1	D	497	ILE	2.7
1	A	385	HIS	2.7
1	C	39	THR	2.7
1	B	486	ASP	2.6
1	A	171	GLY	2.6
1	A	494	CYS	2.6
1	B	32	HIS	2.6
1	C	153	VAL	2.6
1	C	168	ILE	2.6
1	C	511	PHE	2.6
1	D	510	ILE	2.6
1	A	492	TRP	2.6
1	C	183	VAL	2.6
1	D	157	VAL	2.6
1	C	389	SER	2.6
1	A	297	ILE	2.6
1	A	565	ILE	2.6
1	B	168	ILE	2.6
1	A	376	THR	2.6
1	A	193	ASP	2.6
1	D	156	LEU	2.6
1	B	194	MET	2.6
1	B	485	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	534	ILE	2.6
1	D	439	LYS	2.6
1	A	518	ASN	2.6
1	A	362	SER	2.6
1	A	393	LYS	2.6
1	C	76	ASP	2.6
1	B	13	ILE	2.6
1	B	43	THR	2.6
1	B	49	SER	2.6
1	D	585	LYS	2.5
1	B	307	ILE	2.5
1	C	180	ILE	2.5
1	D	11	GLU	2.5
1	C	430	SER	2.5
1	A	359	THR	2.5
1	D	495	ALA	2.5
1	D	307	ILE	2.5
1	C	145	VAL	2.5
1	B	443	LEU	2.5
1	B	497	ILE	2.5
1	D	168	ILE	2.5
1	D	36	PRO	2.5
1	D	522	ALA	2.5
1	A	361	LEU	2.4
1	A	508	TYR	2.4
1	D	194	MET	2.4
1	D	524	TYR	2.4
1	A	172	GLY	2.4
1	A	173	GLY	2.4
1	D	244	LEU	2.4
1	D	506	CYS	2.4
1	D	444	PRO	2.4
1	A	486	ASP	2.4
1	B	354	TYR	2.4
1	C	486	ASP	2.4
1	D	305	GLY	2.4
1	A	156	LEU	2.4
1	A	190	VAL	2.4
1	C	563	GLY	2.4
1	D	214	VAL	2.4
1	B	42	MET	2.4
1	C	533	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	584	ARG	2.3
1	D	361	LEU	2.3
1	B	426	PHE	2.3
1	C	170	MET	2.3
1	C	167	ILE	2.3
1	D	485	LYS	2.3
1	D	450	LEU	2.3
1	C	191	SER	2.3
1	C	194	MET	2.3
1	D	74	VAL	2.3
1	D	190	VAL	2.3
1	D	471	THR	2.3
1	A	495	ALA	2.3
1	B	389	SER	2.3
1	C	96	GLU	2.3
1	B	40	ILE	2.3
1	D	534	ILE	2.3
1	C	333	HIS	2.3
1	D	304	LEU	2.3
1	B	283	ASN	2.3
1	B	145	VAL	2.3
1	D	353	VAL	2.3
1	A	120	HIS	2.3
1	C	45	PRO	2.3
1	C	424	ALA	2.3
1	C	427	GLY	2.3
1	A	304	LEU	2.3
1	C	517	GLU	2.3
1	D	319	GLN	2.3
1	D	365	TRP	2.2
1	C	538	TYR	2.2
1	B	30	PHE	2.2
1	A	563	GLY	2.2
1	C	585	LYS	2.2
1	A	244	LEU	2.2
1	A	488	GLY	2.2
1	A	517	GLU	2.2
1	B	81	LEU	2.2
1	C	35	LYS	2.2
1	B	88	VAL	2.2
1	A	248	LEU	2.2
1	A	497	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	MET	2.2
1	A	365	TRP	2.2
1	B	282	ARG	2.2
1	B	562	ARG	2.2
1	D	191	SER	2.2
1	A	399	ILE	2.1
1	C	94	TYR	2.1
1	A	509	PHE	2.1
1	B	304	LEU	2.1
1	A	529	LYS	2.1
1	B	565	ILE	2.1
1	D	399	ILE	2.1
1	D	493	ILE	2.1
1	D	533	ASP	2.1
1	D	435	THR	2.1
1	D	532	THR	2.1
1	A	81	LEU	2.1
1	B	104	PHE	2.1
1	C	411	PHE	2.1
1	D	397	LEU	2.1
1	C	488	GLY	2.1
1	B	85	ASN	2.1
1	B	438	GLU	2.1
1	C	297	ILE	2.1
1	A	389	SER	2.1
1	C	459	VAL	2.1
1	D	146	LEU	2.1
1	B	205	ARG	2.1
1	D	173	GLY	2.1
1	D	180	ILE	2.1
1	D	539	GLY	2.1
1	B	89	ASP	2.1
1	B	435	THR	2.0
1	A	305	GLY	2.0
1	A	493	ILE	2.0
1	C	407	LYS	2.0
1	B	509	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PL3	D	1587	17/17	0.45	5.01	45,47,49,49	0
3	PL3	C	1587	17/17	0.42	4.09	34,36,42,43	0
3	PL3	B	1588	17/17	0.40	4.07	34,39,42,43	0
3	PL3	A	1588	17/17	0.37	3.59	31,33,37,39	0
2	FAD	C	1586	53/53	0.14	-0.57	6,11,15,16	0
2	FAD	B	1587	53/53	0.12	-0.66	6,12,13,15	0
2	FAD	D	1586	53/53	0.14	-0.81	7,11,15,16	0
2	FAD	A	1587	53/53	0.13	-0.87	3,8,10,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.