



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:08 PM GMT

PDB ID : 4BC9
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATESYN-
THASE: WILD-TYPE, ADDUCT WITH CYANOETHYL
Authors : Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck,
A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2012-10-01
Resolution : 2.41 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>

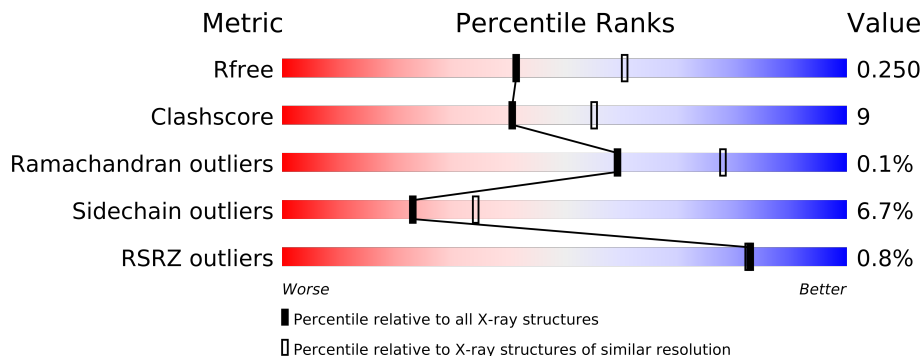
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	658	
1	B	658	
1	C	658	
1	D	658	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	CNV	B	998	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17839 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 ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	1	0
			4365	2773	754	813	25			
1	B	542	Total	C	N	O	S	0	0	0
			4259	2705	737	793	24			
1	C	552	Total	C	N	O	S	0	1	0
			4331	2745	750	812	24			
1	D	550	Total	C	N	O	S	0	1	0
			4321	2739	752	806	24			

- Molecule 2 is PROPANENITRILE (three-letter code: CNV) (formula: C₃H₅N).



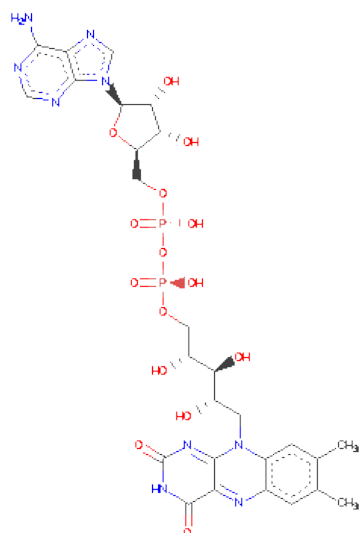
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			4	3	1		
2	B	1	Total	C	N	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			4	3	1		
2	D	1	Total	C	N	0	0
			4	3	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

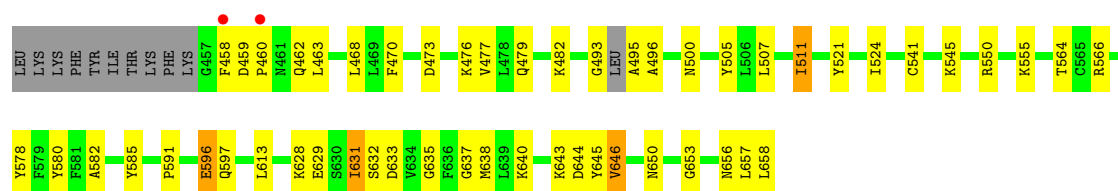
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

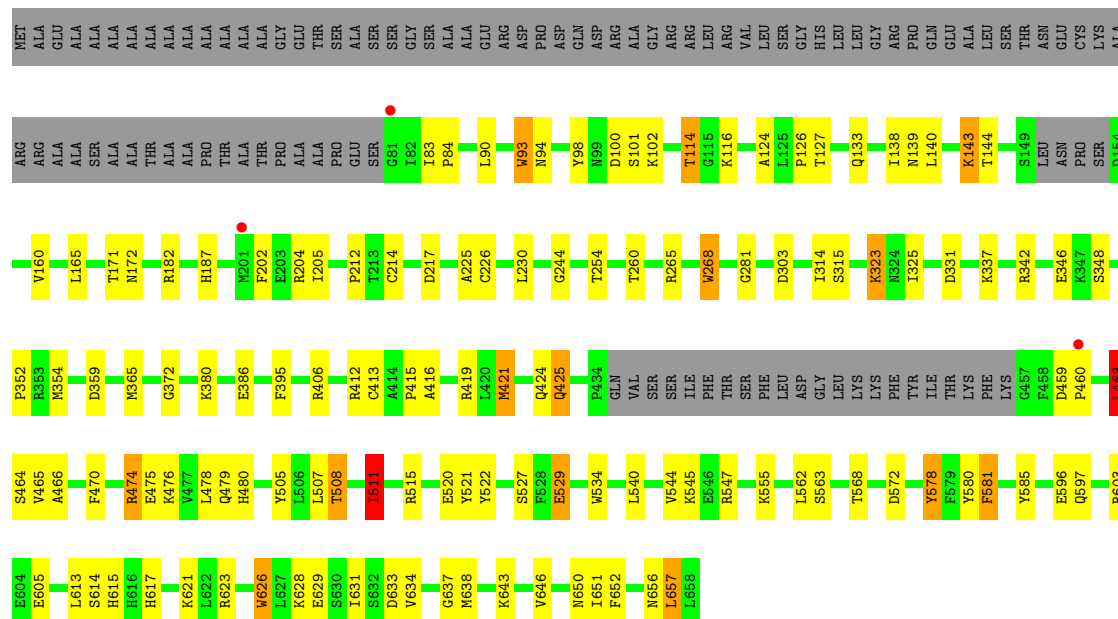
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	73	Total	O	0	0
			73	73		
5	C	91	Total	O	0	0
			91	91		
5	D	66	Total	O	0	0
			66	66		



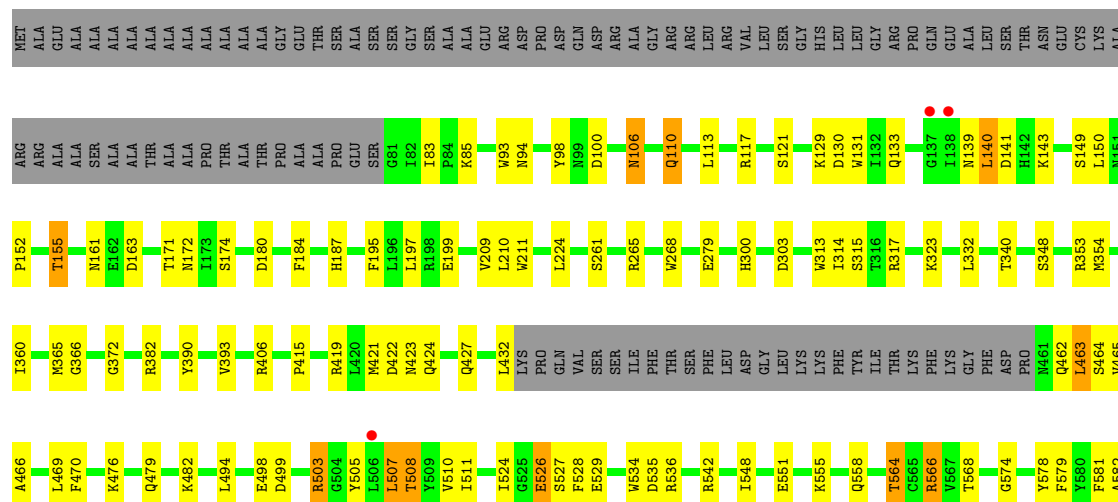
- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE, PEROXISOMAL

Chain C:



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE, PEROXISOMAL

Chain D:



F683	N584	S589	L592	Q597	R603	L613	Y619	G620	K621	K624	Q625	M626	L627	K628	E629	S630	I631	S632	D633	V634	G635	F636	G637	M638	L639	K640	S641	Y642	K643	D644	Y645	Y646	N650	L651	F652	G653	L657	L658
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.91Å 98.62Å 106.28Å 90.92° 89.84° 95.66°	Depositor
Resolution (Å)	54.06 – 2.41 54.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.6 (54.06-2.41) 97.7 (54.00-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.186 , 0.248 0.187 , 0.250	Depositor DCC
R_{free} test set	1014 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.7	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 92832 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17839	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: CNV, SO4, 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	0.73	2/4465 (0.0%)	0.82	2/6038 (0.0%)
1	B	0.75	5/4354 (0.1%)	0.82	2/5888 (0.0%)
1	C	0.73	4/4430 (0.1%)	0.82	4/5993 (0.1%)
1	D	0.73	6/4420 (0.1%)	0.79	1/5981 (0.0%)
All	All	0.74	17/17669 (0.1%)	0.81	9/23900 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	626	TRP	CD2-CE2	7.13	1.50	1.41
1	B	268	TRP	CD2-CE2	6.93	1.49	1.41
1	B	313	TRP	CD2-CE2	6.31	1.49	1.41
1	B	96	TRP	CD2-CE2	6.29	1.48	1.41
1	C	534	TRP	CD2-CE2	6.18	1.48	1.41
1	C	626	TRP	CD2-CE2	6.18	1.48	1.41
1	C	268	TRP	CD2-CE2	6.07	1.48	1.41
1	B	93	TRP	CD2-CE2	5.84	1.48	1.41
1	D	268	TRP	CD2-CE2	5.81	1.48	1.41
1	D	313	TRP	CD2-CE2	5.80	1.48	1.41
1	D	211	TRP	CD2-CE2	5.70	1.48	1.41
1	D	534	TRP	CD2-CE2	5.58	1.48	1.41
1	B	131	TRP	CD2-CE2	5.30	1.47	1.41
1	A	93	TRP	CD2-CE2	5.24	1.47	1.41
1	D	131	TRP	CD2-CE2	5.13	1.47	1.41
1	A	211	TRP	CD2-CE2	5.04	1.47	1.41
1	C	93	TRP	CD2-CE2	5.03	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	603	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	C	623	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	463	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	317	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	631	ILE	N-CA-C	-5.23	96.89	111.00
1	A	317	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	572	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	422	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	631	ILE	C-N-CA	-5.00	109.19	121.70

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	4365	0	4289	85	0
1	B	4259	0	4174	84	0
1	C	4331	0	4236	89	0
1	D	4321	0	4239	81	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
2	C	4	0	3	5	0
2	D	4	0	3	1	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	90	0	0	5	0
5	B	73	0	0	3	0
5	C	91	0	0	3	0
5	D	66	0	0	0	0
All	All	17839	0	17074	322	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 9.

All (322) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.77	1.03
1:D:503:ARG:HH11	1:D:503:ARG:HG3	1.23	1.01
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.82	0.97
1:C:144:THR:HG22	1:C:520:GLU:HA	1.48	0.94
1:C:505:TYR:O	1:C:508:THR:HG23	1.68	0.93
1:B:139:ASN:O	1:B:140:LEU:HB2	1.68	0.93
1:A:596:GLU:HB2	5:A:2084:HOH:O	1.69	0.91
1:C:419:ARG:HH22	1:C:508:THR:CG2	1.86	0.88
1:A:615:HIS:HD2	1:A:616:HIS:HD2	0.93	0.88
1:B:555:LYS:HE3	1:B:597:GLN:HE21	1.42	0.84
1:B:555:LYS:HE3	1:B:597:GLN:NE2	1.92	0.84
1:B:555:LYS:CE	1:B:597:GLN:HE21	1.91	0.83
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.79	0.82
1:A:439:ILE:HG12	1:D:535:ASP:HB2	1.63	0.80
1:C:628:LYS:O	1:C:631:ILE:O	2.01	0.78
1:C:144:THR:CG2	1:C:520:GLU:HA	2.13	0.78
1:A:187:HIS:HD2	1:A:188:GLY:O	1.68	0.77
1:B:596:GLU:HG2	1:B:597:GLN:N	1.99	0.76
1:C:419:ARG:HH22	1:C:508:THR:HG21	1.48	0.76
1:B:425:GLN:NE2	1:B:566:ARG:HD3	2.01	0.75
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.69	0.74
1:C:139:ASN:O	1:C:140:LEU:HB2	1.89	0.73
1:B:495:ALA:N	5:B:2054:HOH:O	2.21	0.73
1:B:100:ASP:O	1:B:114:THR:HG22	1.90	0.71
1:A:243:TYR:HE2	1:A:622:LEU:HD13	1.53	0.71
1:C:421:MET:HE2	1:C:465:VAL:HB	1.71	0.71
1:B:277:HIS:HD2	1:B:378:THR:OG1	1.73	0.70
1:D:603:ARG:HH11	1:D:603:ARG:HG2	1.57	0.69
1:C:421:MET:CE	1:C:465:VAL:HB	2.22	0.69
1:C:656:ASN:O	1:C:657:LEU:HB2	1.92	0.69
1:B:115:GLY:O	1:B:121:SER:HB3	1.93	0.68
1:D:507:LEU:O	1:D:511:ILE:HD12	1.92	0.68
1:C:419:ARG:HH22	1:C:508:THR:HG22	1.57	0.68
1:B:277:HIS:HE1	1:B:376:GLU:OE1	1.78	0.67
1:A:243:TYR:CE2	1:A:622:LEU:HD13	2.29	0.66
1:B:650:ASN:HD21	1:B:653:GLY:HA2	1.60	0.66
1:A:423:ASN:HD21	1:A:427:GLN:HE21	1.43	0.66
1:B:419:ARG:NH1	1:B:505:TYR:CE1	2.64	0.66
1:B:340:THR:HB	1:B:646:VAL:HG13	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:541:CYS:O	1:B:545:LYS:HG3	1.98	0.64
1:C:638:MET:HG2	1:D:642:VAL:HG13	1.78	0.64
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.79	0.63
1:B:507:LEU:O	1:B:511:ILE:HD12	1.99	0.63
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.69	0.63
1:B:192:HIS:CB	1:B:243:TYR:OH	2.48	0.62
1:C:421:MET:HB2	1:C:425:GLN:HB3	1.81	0.61
1:D:423:ASN:HD21	1:D:427:GLN:NE2	1.98	0.61
1:A:81:GLY:HA3	1:A:286:GLU:OE1	2.01	0.61
1:A:557:VAL:HA	1:A:588:ILE:HD11	1.83	0.60
1:C:133:GLN:HG2	1:C:138:ILE:O	2.01	0.60
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.84	0.60
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.84	0.60
1:B:473:ASP:HB2	1:B:476:LYS:HD3	1.84	0.60
1:B:94:ASN:HD22	1:B:94:ASN:H	1.48	0.59
1:B:251:GLU:OE2	1:B:253:ARG:NE	2.33	0.59
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.85	0.59
1:D:603:ARG:NH1	1:D:603:ARG:HG2	2.16	0.58
1:D:390:TYR:O	1:D:498:GLU:HG3	2.03	0.58
1:D:152:PRO:HA	1:D:155:THR:HG23	1.86	0.58
1:D:650:ASN:HD21	1:D:653:GLY:HA2	1.67	0.58
1:D:187:HIS:CE1	1:D:197:LEU:HD11	2.38	0.58
5:A:2051:HOH:O	1:B:632:SER:HB2	2.03	0.58
1:C:359:ASP:H	1:D:317[B]:ARG:NH2	2.02	0.57
1:A:251:GLU:OE2	1:A:253:ARG:HB2	2.05	0.57
1:C:93:TRP:CE2	1:C:94:ASN:HB3	2.40	0.57
1:A:419:ARG:O	1:A:466:ALA:HA	2.05	0.56
1:A:534:TRP:HH2	1:A:570:THR:HG22	1.70	0.56
1:A:230:LEU:HD22	1:A:254:THR:HB	1.87	0.56
1:A:82:ILE:HG12	1:A:264:ASN:ND2	2.21	0.56
1:D:419:ARG:O	1:D:466:ALA:HA	2.06	0.56
1:C:182:ARG:HB3	1:C:205:ILE:HD12	1.87	0.55
1:C:419:ARG:NH2	1:C:508:THR:CG2	2.65	0.55
1:C:421:MET:O	1:C:464:SER:HB2	2.07	0.55
1:C:613:LEU:HD21	1:C:626:TRP:HB2	1.89	0.55
1:C:143:LYS:HB3	1:C:521:TYR:CE1	2.42	0.55
1:A:505:TYR:O	1:A:508:THR:HG23	2.07	0.55
1:A:215:HIS:CD2	1:A:375:THR:OG1	2.56	0.54
1:B:286:GLU:OE2	1:B:289:ARG:NH2	2.38	0.54
1:B:171:THR:O	1:B:172:ASN:HB2	2.06	0.54
1:C:540:LEU:O	1:C:544:VAL:HG23	2.06	0.54
1:D:424:GLN:HB2	1:D:564:THR:CG2	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:419:ARG:NH2	1:C:508:THR:HG22	2.22	0.54
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.90	0.54
1:A:248:PRO:HG2	1:A:655:ARG:HG3	1.90	0.54
1:B:215:HIS:CE1	1:B:337:LYS:HD2	2.42	0.54
1:D:130:ASP:HA	1:D:133:GLN:HE21	1.73	0.53
1:D:422:ASP:OD1	1:D:564:THR:HG22	2.08	0.53
1:B:288:GLU:OE1	1:B:298:THR:HB	2.08	0.53
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.43	0.53
1:B:555:LYS:CE	1:B:597:GLN:NE2	2.61	0.53
1:B:640:LYS:HE3	1:B:644:ASP:OD2	2.08	0.53
1:D:421:MET:HE2	1:D:465:VAL:HB	1.90	0.53
1:A:192:HIS:CD2	1:A:592:LEU:CD1	2.92	0.52
1:A:630:SER:HA	1:B:348:SER:OG	2.08	0.52
1:D:603:ARG:CG	1:D:603:ARG:HH11	2.22	0.52
1:D:139:ASN:O	1:D:140:LEU:HB2	2.09	0.52
1:D:503:ARG:HH11	1:D:503:ARG:CG	2.08	0.52
1:D:93:TRP:HA	1:D:184:PHE:CE2	2.44	0.52
1:B:244:GLY:HA2	1:B:656:ASN:HD21	1.75	0.52
1:B:277:HIS:CD2	1:B:378:THR:OG1	2.57	0.52
1:D:340:THR:HB	1:D:646:VAL:HG13	1.90	0.52
1:D:113:LEU:HD23	1:D:121:SER:HA	1.92	0.52
1:C:413:CYS:O	1:C:480:HIS:NE2	2.37	0.52
1:C:547:ARG:NH1	1:C:605:GLU:OE1	2.37	0.52
1:C:631:ILE:HB	1:D:360:ILE:HD13	1.91	0.52
1:D:551:GLU:O	1:D:555:LYS:HD2	2.09	0.51
1:B:127:THR:O	1:B:127:THR:HG22	2.10	0.51
1:C:323:LYS:HD2	1:C:323:LYS:C	2.30	0.51
1:C:331:ASP:O	1:C:380:LYS:HE3	2.11	0.51
1:B:299:GLY:HA3	1:B:326:TYR:CG	2.45	0.51
1:C:101:SER:HA	1:C:114:THR:HG22	1.93	0.51
1:B:217:ASP:O	1:B:221:ILE:HG13	2.10	0.50
1:D:303:ASP:HB2	2:D:998:CNV:HAA1	1.94	0.50
1:C:337:LYS:HE2	1:C:346:GLU:OE2	2.11	0.50
1:A:628:LYS:O	1:A:631:ILE:O	2.30	0.50
1:C:226:CYS:SG	1:C:651:ILE:HD13	2.52	0.50
1:D:503:ARG:NH1	1:D:503:ARG:HG3	2.02	0.50
1:C:144:THR:HG22	1:C:520:GLU:CA	2.31	0.50
1:B:210:LEU:HD13	1:B:256:ILE:HG23	1.94	0.50
1:A:129:LYS:HG3	1:A:140:LEU:HD22	1.93	0.50
1:B:458:PHE:HB2	1:B:463:LEU:HD12	1.93	0.50
1:B:138:ILE:HD13	1:B:521:TYR:HB3	1.94	0.50
1:C:204:ARG:HD2	5:C:2016:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:ILE:O	1:B:365:MET:HA	2.11	0.49
1:A:425:GLN:OE1	1:A:566:ARG:HD3	2.11	0.49
1:A:423:ASN:HD21	1:A:427:GLN:NE2	2.06	0.49
1:C:100:ASP:O	1:C:114:THR:HG22	2.12	0.49
1:A:526:GLU:HB3	1:A:595:PHE:HZ	1.77	0.49
1:A:372:GLY:HA2	1:A:652:PHE:CZ	2.46	0.49
1:A:528:PHE:HZ	1:A:548:ILE:HD11	1.76	0.49
1:C:171:THR:O	1:C:172:ASN:HB2	2.11	0.49
2:B:998:CNV:CAC	3:B:999:FAD:C10	2.91	0.49
1:C:372:GLY:HA2	1:C:652:PHE:CZ	2.48	0.49
1:A:481:GLU:O	1:A:485:TYR:HD2	1.95	0.49
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.28	0.49
1:B:496:ALA:O	1:B:500:ASN:ND2	2.42	0.49
1:A:541:CYS:O	1:A:545:LYS:HG3	2.12	0.49
1:B:298:THR:CG2	1:B:300:HIS:H	2.26	0.49
1:B:585:TYR:CD1	1:B:591:PRO:HG3	2.48	0.49
1:B:277:HIS:CE1	1:B:376:GLU:OE1	2.63	0.48
1:A:167:GLU:OE2	1:A:228:TYR:OH	2.20	0.48
1:C:419:ARG:O	1:C:466:ALA:HA	2.13	0.48
1:A:194:ILE:O	1:A:198:ARG:HG3	2.14	0.48
1:D:634:VAL:O	1:D:638:MET:HG3	2.12	0.48
1:B:425:GLN:HE22	1:B:566:ARG:HD3	1.77	0.48
1:D:619:VAL:HB	1:D:657:LEU:HD23	1.95	0.48
1:C:412:ARG:CZ	1:D:382:ARG:HD3	2.43	0.48
1:C:160:VAL:HG22	1:C:254:THR:HG21	1.96	0.48
5:A:2055:HOH:O	1:B:317:ARG:NH2	2.47	0.48
1:D:503:ARG:O	1:D:507:LEU:HB2	2.13	0.48
1:D:98:TYR:CD2	1:D:117:ARG:HD3	2.49	0.48
1:C:214:CYS:O	1:C:217:ASP:HB2	2.14	0.47
1:A:539:ASP:OD1	1:A:542:ARG:NH2	2.47	0.47
1:D:93:TRP:CE2	1:D:94:ASN:HB3	2.49	0.47
1:A:432:LEU:HD13	1:A:507:LEU:HD21	1.95	0.47
1:C:348:SER:HB3	1:D:629:GLU:O	2.14	0.47
1:C:124:ALA:O	1:C:126:PRO:HD3	2.15	0.47
1:C:621:LYS:HG3	1:C:656:ASN:HD22	1.80	0.47
2:B:998:CNV:CAC	3:B:999:FAD:C9A	2.92	0.47
1:A:515:ARG:NH2	1:A:526:GLU:OE1	2.47	0.47
1:A:164:PHE:HB2	1:A:228:TYR:CD2	2.49	0.47
1:D:640:LYS:HE2	1:D:644:ASP:OD1	2.15	0.47
1:D:100:ASP:OD2	1:D:117:ARG:NH2	2.40	0.47
1:C:421:MET:HE1	1:C:465:VAL:HB	1.97	0.46
1:B:323:LYS:C	1:B:323:LYS:HD2	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:139:ASN:O	1:C:140:LEU:CB	2.62	0.46
1:A:319:SER:HA	1:A:328:ASN:HD22	1.80	0.46
1:D:555:LYS:HE2	1:D:597:GLN:HB2	1.97	0.46
1:C:585:TYR:O	1:C:585:TYR:CD1	2.68	0.46
1:A:88:GLN:CD	1:A:88:GLN:H	2.18	0.46
1:C:562:LEU:O	1:C:581:PHE:HA	2.15	0.46
1:A:160:VAL:HG11	1:A:165:LEU:HD13	1.97	0.46
1:B:209:VAL:C	1:B:210:LEU:HD12	2.35	0.46
1:A:421[A]:MET:HB2	1:A:425:GLN:HB3	1.96	0.46
1:C:545:LYS:HD2	1:C:563:SER:O	2.16	0.46
1:A:529:GLU:OE1	1:A:617:HIS:CG	2.69	0.46
5:C:2055:HOH:O	1:D:632:SER:HB2	2.15	0.46
1:C:83:ILE:HA	1:C:84:PRO:HD3	1.83	0.46
1:B:100:ASP:C	1:B:100:ASP:OD1	2.54	0.46
1:B:244:GLY:HA2	1:B:656:ASN:ND2	2.31	0.46
1:B:419:ARG:NH1	1:B:505:TYR:CD1	2.83	0.46
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.98	0.46
1:C:578:TYR:OH	2:C:998:CNV:NAB	2.49	0.46
1:A:133:GLN:HG2	1:D:536:ARG:NH2	2.30	0.46
1:B:94:ASN:HD22	1:B:94:ASN:N	2.11	0.46
1:C:507:LEU:O	1:C:511:ILE:HD12	2.16	0.46
1:C:527:SER:HB3	1:C:580:TYR:HD2	1.81	0.46
1:C:93:TRP:CD2	1:C:94:ASN:HB3	2.50	0.46
1:D:640:LYS:HA	1:D:640:LYS:HD2	1.77	0.46
1:C:415:PRO:HB3	1:C:470:PHE:CE1	2.50	0.45
1:D:300:HIS:HB2	1:D:332:LEU:CD1	2.46	0.45
1:B:204:ARG:NH2	1:B:253:ARG:O	2.49	0.45
1:A:192:HIS:CD2	1:A:592:LEU:HD11	2.51	0.45
1:A:417:SER:HB3	1:A:469:LEU:HB3	1.97	0.45
1:A:592:LEU:HB2	5:A:2083:HOH:O	2.15	0.45
1:D:650:ASN:O	1:D:650:ASN:ND2	2.49	0.45
1:D:628:LYS:HE2	1:D:636:PHE:CD1	2.52	0.45
1:C:260:THR:O	1:C:281:GLY:HA3	2.16	0.45
1:A:571:TYR:HA	4:A:1659:SO4:O3	2.17	0.45
1:D:83:ILE:HB	1:D:261:SER:HB2	1.98	0.45
1:B:258:LEU:HD23	1:B:258:LEU:C	2.37	0.45
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.45
1:C:421:MET:HB3	1:C:425:GLN:HG2	1.98	0.45
1:D:419:ARG:NH2	1:D:566:ARG:HH21	2.15	0.45
1:B:265:ARG:HG2	1:B:279:GLU:OE1	2.17	0.45
1:B:397:ASN:HA	1:B:462:GLN:O	2.17	0.45
1:B:194:ILE:O	1:B:198:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:GLY:O	1:B:357:GLY:HA2	2.17	0.44
1:B:116:LYS:HA	1:B:116:LYS:HD3	1.83	0.44
1:C:212:PRO:HB3	1:C:217:ASP:HB3	2.00	0.44
1:A:319:SER:HA	1:A:328:ASN:ND2	2.32	0.44
1:D:424:GLN:CB	1:D:564:THR:CG2	2.95	0.44
1:C:325:ILE:HD11	1:C:416:ALA:HB2	2.00	0.44
1:B:628:LYS:O	1:B:631:ILE:O	2.35	0.44
1:D:469:LEU:HD12	1:D:470:PHE:N	2.32	0.44
1:D:650:ASN:O	1:D:650:ASN:CG	2.55	0.44
1:A:386:GLU:HB2	1:A:472:GLY:O	2.18	0.44
1:B:493:GLY:C	5:B:2054:HOH:O	2.55	0.44
1:D:526:GLU:HG3	1:D:527:SER:N	2.33	0.44
1:A:545:LYS:HD2	1:A:563:SER:O	2.17	0.44
1:D:315:SER:O	1:D:366:GLY:HA2	2.18	0.43
1:C:314:ILE:HG23	1:C:365:MET:HG2	2.00	0.43
1:B:643:LYS:NZ	1:B:650:ASN:HD22	2.16	0.43
1:D:542:ARG:HE	1:D:542:ARG:HB3	1.51	0.43
1:D:195:PHE:CD1	1:D:592:LEU:HD11	2.53	0.43
1:B:564:THR:HG22	1:B:580:TYR:HB3	2.00	0.43
1:C:303:ASP:HB2	2:C:998:CNV:HAA1	2.00	0.43
1:A:138:ILE:CD1	1:A:140:LEU:HD12	2.49	0.43
1:A:191:LEU:HD12	1:A:595:PHE:CD2	2.54	0.43
1:B:470:PHE:HB3	1:B:477:VAL:HG13	2.01	0.43
1:D:621:LYS:HG2	1:D:624:LYS:HD2	2.01	0.43
1:C:165:LEU:HD12	1:C:165:LEU:HA	1.90	0.43
1:D:187:HIS:CD2	1:D:197:LEU:HD11	2.53	0.43
1:B:323:LYS:HD2	1:B:324:ASN:N	2.34	0.43
1:D:415:PRO:HB3	1:D:470:PHE:CE2	2.54	0.43
1:A:284:GLY:HA2	1:A:313:TRP:HH2	1.84	0.43
1:D:171:THR:O	1:D:172:ASN:HB2	2.18	0.43
1:C:225:ALA:HA	1:C:230:LEU:HD12	2.00	0.43
1:A:94:ASN:HA	1:A:197:LEU:HD13	2.00	0.43
1:C:629:GLU:O	1:D:348:SER:HB3	2.19	0.43
1:D:463:LEU:O	1:D:463:LEU:HD23	2.19	0.43
1:C:419:ARG:NH2	1:C:508:THR:HG21	2.25	0.43
1:C:100:ASP:O	1:C:114:THR:CG2	2.66	0.43
1:A:185:ARG:HG2	1:A:235:ILE:HD13	2.00	0.43
1:A:482:LYS:NZ	1:A:486:ASP:OD2	2.49	0.43
1:C:90:LEU:HD23	1:C:98:TYR:HE1	1.84	0.43
1:B:524:ILE:O	1:B:582:ALA:HA	2.18	0.42
1:C:395:PHE:O	1:C:463:LEU:HB2	2.19	0.42
1:A:265:ARG:HD2	1:A:279:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:424:GLN:CB	1:D:564:THR:HG23	2.49	0.42
1:C:265:ARG:HD3	5:C:2019:HOH:O	2.19	0.42
1:C:474:ARG:NH1	1:C:478:LEU:HD11	2.33	0.42
1:C:555:LYS:HZ2	1:C:597:GLN:HB3	1.84	0.42
1:B:555:LYS:HE2	1:B:597:GLN:HB2	1.99	0.42
1:A:138:ILE:HD12	1:A:140:LEU:HD12	1.99	0.42
1:A:390:TYR:CE2	1:A:469:LEU:HD13	2.55	0.42
1:C:529:GLU:OE1	1:C:615:HIS:N	2.33	0.42
1:A:299:GLY:HA3	1:A:326:TYR:CD2	2.54	0.42
1:A:613:LEU:HD11	1:A:623:ARG:HB3	2.00	0.42
1:D:93:TRP:NE1	1:D:94:ASN:ND2	2.68	0.42
1:B:629:GLU:HG3	5:B:2068:HOH:O	2.18	0.42
1:C:522:TYR:HA	1:C:585:TYR:CE2	2.54	0.42
1:A:527:SER:HB3	1:A:580:TYR:HD2	1.85	0.42
1:A:645:TYR:CZ	1:B:637:GLY:HA3	2.55	0.42
1:B:555:LYS:HE2	1:B:597:GLN:CB	2.50	0.42
1:D:527:SER:HA	1:D:579:PHE:O	2.20	0.42
1:D:106:ASN:HD21	1:D:110:GLN:H	1.68	0.42
1:A:171:THR:O	1:A:172:ASN:HB2	2.20	0.42
1:A:555:LYS:HE2	1:A:597:GLN:HB3	2.01	0.42
1:B:459:ASP:C	1:B:459:ASP:OD1	2.59	0.42
1:B:418:ILE:HG13	1:B:468:LEU:CD2	2.50	0.41
1:C:637:GLY:HA3	1:D:645:TYR:CZ	2.55	0.41
1:B:229:ASN:O	1:B:253:ARG:HD2	2.20	0.41
1:D:528:PHE:HZ	1:D:548:ILE:HD11	1.85	0.41
1:A:119:PRO:CG	1:A:506:LEU:HD22	2.50	0.41
1:B:628:LYS:HD3	1:B:633:ASP:OD1	2.20	0.41
1:B:193:GLU:HG3	1:B:243:TYR:CE2	2.56	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.74	0.41
1:C:303:ASP:OD2	2:C:998:CNV:HAA1	2.21	0.41
1:A:524:ILE:HG21	1:A:524:ILE:HD13	1.79	0.41
1:D:499:ASP:HB3	1:D:503:ARG:NH2	2.35	0.41
1:D:421:MET:O	1:D:464:SER:HB2	2.20	0.41
1:C:585:TYR:O	1:C:585:TYR:HD1	2.03	0.41
1:A:637:GLY:HA3	1:B:645:TYR:CZ	2.55	0.41
1:A:571:TYR:OH	1:A:615:HIS:CE1	2.70	0.41
1:A:164:PHE:HB2	1:A:228:TYR:CG	2.56	0.41
1:C:615:HIS:O	1:D:353:ARG:NH1	2.52	0.41
1:B:268:TRP:CZ2	1:B:277:HIS:HB2	2.56	0.41
1:C:212:PRO:CB	1:C:217:ASP:HB3	2.50	0.41
1:D:463:LEU:HD23	1:D:463:LEU:C	2.41	0.41
1:A:524:ILE:O	1:A:582:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:459:ASP:HA	1:C:460:PRO:HD3	1.91	0.41
1:D:555:LYS:HE3	1:D:597:GLN:OE1	2.21	0.41
1:A:372:GLY:HA2	1:A:652:PHE:CE1	2.56	0.41
1:C:643:LYS:NZ	1:C:650:ASN:HD22	2.19	0.41
1:A:243:TYR:HA	5:A:2018:HOH:O	2.21	0.41
1:A:479:GLN:HE22	1:B:479:GLN:HE22	1.69	0.41
1:A:438:SER:O	1:A:441:THR:HG22	2.21	0.41
1:A:187:HIS:CD2	1:A:188:GLY:O	2.59	0.40
1:A:555:LYS:HE2	1:A:597:GLN:CB	2.51	0.40
1:B:155:THR:HG21	1:B:179:ALA:HB1	2.03	0.40
1:B:298:THR:HG22	1:B:300:HIS:H	1.84	0.40
1:C:578:TYR:OH	2:C:998:CNV:CAC	2.70	0.40
1:A:459:ASP:HA	1:A:460:PRO:HD3	1.95	0.40
3:A:999:FAD:N1	3:A:999:FAD:H3'	2.36	0.40
1:D:265:ARG:HB2	1:D:279:GLU:OE1	2.22	0.40
1:C:479:GLN:OE1	1:D:479:GLN:NE2	2.54	0.40
1:D:524:ILE:O	1:D:582:ALA:HA	2.21	0.40
1:A:281:GLY:O	1:A:309:THR:HG22	2.21	0.40
1:D:393:VAL:O	1:D:465:VAL:HG13	2.22	0.40
1:C:617:HIS:NE2	2:C:998:CNV:NAB	2.69	0.40
1:D:505:TYR:O	1:D:508:THR:OG1	2.33	0.40
1:C:352:PRO:HG3	1:D:574:GLY:C	2.42	0.40
1:B:332:LEU:HB3	1:B:379:ILE:HG23	2.03	0.40
1:C:244:GLY:HA2	1:C:656:ASN:HD21	1.86	0.40
1:C:540:LEU:HD23	1:C:540:LEU:C	2.42	0.40
1:C:342:ARG:HG3	1:D:634:VAL:HG22	2.03	0.40
1:D:372:GLY:HA2	1:D:652:PHE:CZ	2.57	0.40
1:C:187:HIS:HB3	1:C:202:PHE:CZ	2.56	0.40
1:B:187:HIS:HB3	1:B:202:PHE:CZ	2.56	0.40
1:D:161:ASN:OD1	1:D:163:ASP:N	2.54	0.40
1:D:209:VAL:C	1:D:210:LEU:HD12	2.42	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	550/658 (84%)	527 (96%)	23 (4%)	0	100	100
1	B	534/658 (81%)	509 (95%)	24 (4%)	1 (0%)	56	74
1	C	547/658 (83%)	527 (96%)	19 (4%)	1 (0%)	56	74
1	D	547/658 (83%)	529 (97%)	17 (3%)	1 (0%)	56	74
All	All	2178/2632 (83%)	2092 (96%)	83 (4%)	3 (0%)	59	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	558	GLN
1	B	460	PRO
1	C	511	ILE

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	469/545 (86%)	439 (94%)	30 (6%)	25	37
1	B	456/545 (84%)	431 (94%)	25 (6%)	30	45
1	C	464/545 (85%)	435 (94%)	29 (6%)	25	38
1	D	463/545 (85%)	423 (91%)	40 (9%)	15	22
All	All	1852/2180 (85%)	1728 (93%)	124 (7%)	23	34

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	102	LYS
1	A	116	LYS
1	A	138	ILE
1	A	140	LEU
1	A	174	SER
1	A	191	LEU
1	A	195	PHE
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	354	MET
1	A	406	ARG
1	A	419	ARG
1	A	439	ILE
1	A	441	THR
1	A	462	GLN
1	A	468	LEU
1	A	476	LYS
1	A	508	THR
1	A	510	VAL
1	A	511	ILE
1	A	515	ARG
1	A	516	ASP
1	A	535	ASP
1	A	550	ARG
1	A	578	TYR
1	A	588	ILE
1	A	592	LEU
1	A	631	ILE
1	A	646	VAL
1	A	657	LEU
1	B	90	LEU
1	B	94	ASN
1	B	102	LYS
1	B	105	LEU
1	B	174	SER
1	B	191	LEU
1	B	195	PHE
1	B	198	ARG
1	B	201	MET
1	B	265	ARG
1	B	298	THR
1	B	323	LYS
1	B	334	VAL
1	B	386	GLU
1	B	426	PHE
1	B	427	GLN
1	B	482	LYS
1	B	511	ILE
1	B	550	ARG
1	B	578	TYR
1	B	596	GLU

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Mol	Chain	Res	Type
1	B	613	LEU
1	B	646	VAL
1	B	657	LEU
1	B	658	LEU
1	C	102	LYS
1	C	114	THR
1	C	116	LYS
1	C	127	THR
1	C	143	LYS
1	C	315	SER
1	C	323	LYS
1	C	354	MET
1	C	386	GLU
1	C	406	ARG
1	C	421	MET
1	C	424	GLN
1	C	425	GLN
1	C	463	LEU
1	C	474	ARG
1	C	475	GLU
1	C	476	LYS
1	C	508	THR
1	C	511	ILE
1	C	515	ARG
1	C	529	GLU
1	C	568	THR
1	C	578	TYR
1	C	581	PHE
1	C	596	GLU
1	C	614	SER
1	C	633	ASP
1	C	646	VAL
1	C	657	LEU
1	D	85	LYS
1	D	106	ASN
1	D	110	GLN
1	D	129	LYS
1	D	140	LEU
1	D	141	ASP
1	D	143	LYS
1	D	149	SER
1	D	150	LEU

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Mol	Chain	Res	Type
1	D	155	THR
1	D	174	SER
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	323	LYS
1	D	354	MET
1	D	406	ARG
1	D	432	LEU
1	D	462	GLN
1	D	463	LEU
1	D	476	LYS
1	D	482	LYS
1	D	494	LEU
1	D	503	ARG
1	D	507	LEU
1	D	508	THR
1	D	510	VAL
1	D	526	GLU
1	D	529	GLU
1	D	564	THR
1	D	566	ARG
1	D	568	THR
1	D	578	TYR
1	D	581	PHE
1	D	584	ASN
1	D	589	SER
1	D	603	ARG
1	D	613	LEU
1	D	630	SER
1	D	641	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	172	ASN
1	A	187	HIS
1	A	192	HIS
1	A	215	HIS
1	A	290	GLN
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	335	HIS
1	A	423	ASN
1	A	479	GLN
1	A	500	ASN
1	A	615	HIS
1	A	616	HIS
1	B	94	ASN
1	B	110	GLN
1	B	133	GLN
1	B	177	GLN
1	B	277	HIS
1	B	362	HIS
1	B	423	ASN
1	B	597	GLN
1	B	650	ASN
1	B	656	ASN
1	C	139	ASN
1	C	177	GLN
1	C	400	GLN
1	C	479	GLN
1	C	500	ASN
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	106	ASN
1	D	133	GLN
1	D	151	ASN
1	D	189	HIS
1	D	427	GLN
1	D	479	GLN
1	D	500	ASN
1	D	650	ASN
1	D	656	ASN

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 ⓘ

11 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$
4	SO4	A	1659	-	4,4,4	0.63	0	6,6,6	0.44	0
2	CNV	A	998	3	3,3,3	0.68	0	2,2,2	0.54	0
3	FAD	A	999	2	58,58,58	1.74	10 (17%)	85,89,89	2.11	19 (22%)
4	SO4	B	1659	-	4,4,4	0.87	0	6,6,6	0.43	0
2	CNV	B	998	3	3,3,3	1.45	1 (33%)	2,2,2	0.53	0
3	FAD	B	999	2	58,58,58	1.81	8 (13%)	85,89,89	1.96	17 (20%)
2	CNV	C	998	3	3,3,3	1.60	1 (33%)	2,2,2	0.50	0
3	FAD	C	999	2	58,58,58	1.51	9 (15%)	85,89,89	2.18	22 (25%)
4	SO4	D	1659	-	4,4,4	0.94	0	6,6,6	0.30	0
2	CNV	D	998	3	3,3,3	0.45	0	2,2,2	0.65	0
3	FAD	D	999	2	58,58,58	1.68	11 (18%)	85,89,89	2.04	16 (18%)

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
4	SO4	A	1659	-	-	0/0/0/0	0/0/0/0
2	CNV	A	998	3	-	0/1/1/1	0/0/0/0
3	FAD	A	999	2	-	0/34/50/50	0/1/6/6
4	SO4	B	1659	-	-	0/0/0/0	0/0/0/0
2	CNV	B	998	3	-	0/1/1/1	0/0/0/0
3	FAD	B	999	2	-	0/34/50/50	0/1/6/6
2	CNV	C	998	3	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	999	2	-	0/34/50/50	0/1/6/6
4	SO4	D	1659	-	-	0/0/0/0	0/0/0/0
2	CNV	D	998	3	-	0/1/1/1	0/0/0/0
3	FAD	D	999	2	-	0/34/50/50	0/1/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	FAD	C5X-N5	7.30	1.46	1.35
3	A	999	FAD	C5X-N5	6.14	1.44	1.35
3	D	999	FAD	C5X-N5	5.28	1.43	1.35
3	B	999	FAD	C4-C4X	5.05	1.49	1.41
3	B	999	FAD	C4X-C10	4.61	1.48	1.40
3	A	999	FAD	C4X-C10	4.53	1.48	1.40
3	A	999	FAD	C9A-N10	4.49	1.45	1.38
3	C	999	FAD	C4-C4X	4.19	1.48	1.41
3	D	999	FAD	C4-C4X	4.18	1.48	1.41
3	A	999	FAD	C9A-C5X	4.04	1.50	1.42
3	D	999	FAD	C9A-N10	4.03	1.44	1.38
3	C	999	FAD	C9A-N10	3.90	1.44	1.38
3	C	999	FAD	C5X-N5	3.86	1.41	1.35
3	A	999	FAD	C4A-N9A	-3.77	1.32	1.37
3	B	999	FAD	C9A-C5X	3.71	1.50	1.42
3	B	999	FAD	C4A-N9A	-3.67	1.32	1.37
3	A	999	FAD	C4-C4X	3.65	1.47	1.41
3	B	999	FAD	C5A-C4A	3.58	1.48	1.40
3	C	999	FAD	C4X-C10	3.52	1.47	1.40
3	D	999	FAD	C5A-C4A	3.48	1.48	1.40
3	A	999	FAD	C8-C7	3.45	1.50	1.40
3	B	999	FAD	C8-C7	3.30	1.50	1.40
3	D	999	FAD	C9A-C5X	3.25	1.49	1.42
3	D	999	FAD	C8-C7	3.19	1.50	1.40
3	D	999	FAD	C4X-C10	2.95	1.46	1.40
3	C	999	FAD	C8-C7	2.90	1.49	1.40
3	C	999	FAD	C5A-C4A	2.89	1.47	1.40
3	C	999	FAD	C1'-C2'	-2.78	1.48	1.51
3	C	999	FAD	C9A-C5X	2.73	1.48	1.42
2	C	998	CNV	CAC-NAB	2.71	1.25	1.14
3	D	999	FAD	C4X-N5	2.64	1.41	1.36
3	B	999	FAD	C9A-N10	2.56	1.42	1.38
3	A	999	FAD	C5A-C4A	2.35	1.45	1.40
2	B	998	CNV	CAC-NAB	2.35	1.24	1.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	FAD	O4-C4	2.23	1.28	1.24
3	D	999	FAD	PA-O3P	2.21	1.63	1.59
3	D	999	FAD	C4A-N9A	-2.11	1.34	1.37
3	A	999	FAD	O2-C2	2.06	1.27	1.23
3	A	999	FAD	C8A-N9A	-2.05	1.33	1.36
3	C	999	FAD	C4X-N5	-2.05	1.31	1.36

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	C2-N1-C10	8.47	123.52	114.98
3	D	999	FAD	C2-N1-C10	8.35	123.40	114.98
3	C	999	FAD	O4B-C1B-N9A	-8.02	100.98	108.44
3	A	999	FAD	C2-N1-C10	7.91	122.95	114.98
3	D	999	FAD	N3A-C2A-N1A	-7.29	122.61	128.71
3	C	999	FAD	C1'-N10-C9A	6.85	125.53	118.87
3	B	999	FAD	N3A-C2A-N1A	-6.65	123.15	128.71
3	A	999	FAD	O4B-C1B-N9A	-6.59	102.31	108.44
3	D	999	FAD	O4B-C1B-N9A	-5.96	102.89	108.44
3	A	999	FAD	N3A-C2A-N1A	-5.73	123.92	128.71
3	C	999	FAD	C2-N1-C10	5.48	120.50	114.98
3	C	999	FAD	C4X-N5-C5X	5.43	122.79	116.69
3	A	999	FAD	N3A-C4A-N9A	5.13	134.69	125.43
3	A	999	FAD	C8A-N9A-C4A	5.12	110.81	106.90
3	C	999	FAD	N3A-C2A-N1A	-4.99	124.54	128.71
3	B	999	FAD	C4X-C10-N1	-4.98	117.75	122.73
3	C	999	FAD	N3A-C4A-N9A	4.90	134.28	125.43
3	C	999	FAD	C4A-C5A-N7A	-4.87	105.35	109.52
3	D	999	FAD	N3A-C4A-N9A	4.66	133.84	125.43
3	B	999	FAD	N3A-C4A-N9A	4.53	133.61	125.43
3	D	999	FAD	C4X-C10-N1	-4.36	118.37	122.73
3	D	999	FAD	C1'-N10-C9A	4.32	123.08	118.87
3	A	999	FAD	C4X-N5-C5X	4.12	121.32	116.69
3	A	999	FAD	C5X-C9A-N10	4.03	120.77	116.80
3	B	999	FAD	O4B-C1B-N9A	-3.86	104.85	108.44
3	B	999	FAD	C4X-N5-C5X	3.80	120.96	116.69
3	A	999	FAD	C4X-C10-N1	-3.76	118.97	122.73
3	A	999	FAD	C1'-N10-C9A	3.75	122.52	118.87
3	C	999	FAD	C9A-N10-C10	-3.70	118.13	121.77
3	C	999	FAD	C4X-C10-N1	-3.67	119.06	122.73
3	B	999	FAD	C5X-C9A-N10	3.64	120.38	116.80
3	B	999	FAD	C1'-N10-C9A	3.57	122.35	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FAD	C9A-C5X-N5	-3.54	116.94	122.37
3	A	999	FAD	C4A-C5A-N7A	-3.39	106.62	109.52
3	D	999	FAD	C4X-N5-C5X	3.34	120.44	116.69
3	C	999	FAD	C5A-C4A-N3A	-3.22	118.68	125.70
3	B	999	FAD	C9A-N10-C10	-2.93	118.89	121.77
3	B	999	FAD	C9A-C5X-N5	-2.86	117.98	122.37
3	B	999	FAD	C8A-N9A-C4A	2.75	109.00	106.90
3	C	999	FAD	C8A-N9A-C4A	2.73	108.98	106.90
3	D	999	FAD	C2A-N1A-C6A	2.72	123.69	118.77
3	D	999	FAD	C8A-N9A-C4A	2.72	108.98	106.90
3	C	999	FAD	C9A-C5X-N5	-2.63	118.33	122.37
3	D	999	FAD	C5X-C9A-N10	2.62	119.38	116.80
3	A	999	FAD	C9A-N10-C10	-2.62	119.20	121.77
3	A	999	FAD	C5A-C4A-N3A	-2.61	120.02	125.70
3	C	999	FAD	O2'-C2'-C3'	2.60	115.53	109.05
3	C	999	FAD	O2'-C2'-C1'	-2.59	103.27	109.71
3	C	999	FAD	P-O3P-PA	-2.54	124.23	131.68
3	D	999	FAD	C1B-N9A-C4A	-2.54	122.25	126.64
3	A	999	FAD	P-O3P-PA	-2.52	124.30	131.68
3	A	999	FAD	C4X-C10-N10	-2.49	119.27	120.51
3	B	999	FAD	C5'-C4'-C3'	2.49	116.76	112.06
3	C	999	FAD	C5X-C9A-N10	2.47	119.23	116.80
3	D	999	FAD	P-O3P-PA	-2.44	124.52	131.68
3	D	999	FAD	O3'-C3'-C4'	2.41	114.82	108.74
3	C	999	FAD	C4B-O4B-C1B	2.39	112.34	109.75
3	B	999	FAD	C2A-N1A-C6A	2.38	123.08	118.77
3	A	999	FAD	C2'-C1'-N10	2.36	115.59	112.45
3	A	999	FAD	C6-C5X-N5	2.31	121.66	118.97
3	C	999	FAD	C2A-N3A-C4A	2.29	120.52	114.01
3	D	999	FAD	C9A-C5X-N5	-2.24	118.93	122.37
3	A	999	FAD	C2A-N3A-C4A	2.24	120.39	114.01
3	A	999	FAD	N1-C10-N10	2.19	121.74	115.97
3	B	999	FAD	O3B-C3B-C2B	-2.20	104.69	111.83
3	D	999	FAD	C5A-C4A-N3A	-2.15	121.02	125.70
3	B	999	FAD	C4B-O4B-C1B	2.13	112.06	109.75
3	C	999	FAD	C3B-C2B-C1B	2.12	104.22	100.91
3	D	999	FAD	N6A-C6A-N1A	2.11	123.50	119.36
3	C	999	FAD	C1'-N10-C10	-2.09	116.20	119.17
3	C	999	FAD	C8A-N7A-C5A	2.03	109.87	103.58
3	C	999	FAD	C1B-N9A-C4A	-2.01	123.17	126.64
3	B	999	FAD	N1-C10-N10	2.01	121.25	115.97
3	B	999	FAD	P-O3P-PA	-2.01	125.80	131.68

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	555/658 (84%)	-0.34	4 (0%) 84 84	17, 30, 58, 89	0
1	B	542/658 (82%)	-0.35	7 (1%) 74 73	15, 31, 60, 91	0
1	C	552/658 (83%)	-0.42	3 (0%) 88 88	16, 31, 59, 84	0
1	D	550/658 (83%)	-0.32	3 (0%) 88 88	16, 34, 61, 79	0
All	All	2199/2632 (83%)	-0.36	17 (0%) 83 82	15, 31, 60, 91	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	PRO	3.7
1	B	458	PHE	3.5
1	B	81	GLY	3.2
1	C	201	MET	2.6
1	C	81	GLY	2.5
1	A	83	ILE	2.5
1	D	137	GLY	2.3
1	A	172	ASN	2.3
1	B	201	MET	2.2
1	A	589	SER	2.1
1	B	155	THR	2.1
1	A	159	ILE	2.1
1	B	82	ILE	2.1
1	D	506	LEU	2.0
1	B	434	PRO	2.0
1	C	460	PRO	2.0
1	D	138	ILE	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
2	CNV	B	998	4/4	0.13	2.42	28,28,31,32	0
2	CNV	D	998	4/4	0.14	1.26	38,40,44,45	0
2	CNV	C	998	4/4	0.12	0.33	23,24,27,31	0
2	CNV	A	998	4/4	0.12	0.25	24,28,33,34	0
4	SO4	A	1659	5/5	0.14	0.19	50,51,62,63	0
4	SO4	B	1659	5/5	0.17	-0.04	53,57,61,63	0
3	FAD	A	999	53/53	0.11	-0.10	14,19,23,25	0
3	FAD	D	999	53/53	0.12	-0.11	15,22,26,27	0
3	FAD	C	999	53/53	0.11	-0.29	14,17,20,22	0
3	FAD	B	999	53/53	0.10	-0.33	16,21,27,30	0
4	SO4	D	1659	5/5	0.10	-0.85	40,46,53,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.