



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:07 PM GMT

PDB ID : 4BC7
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATESYN-
THASE: Arg419His mutant
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 : 2.40 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>

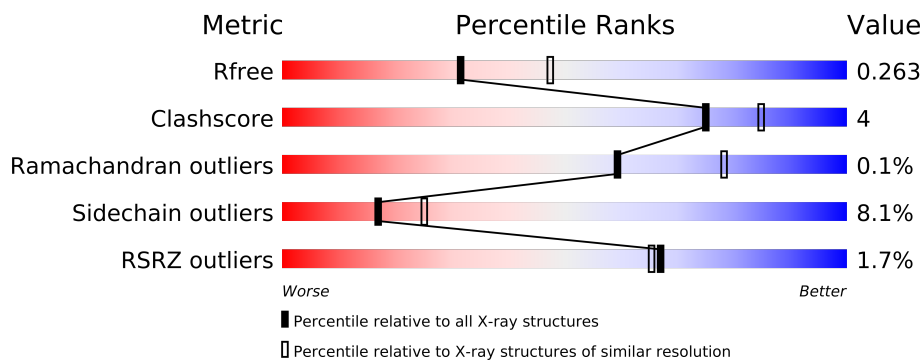
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17858 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.

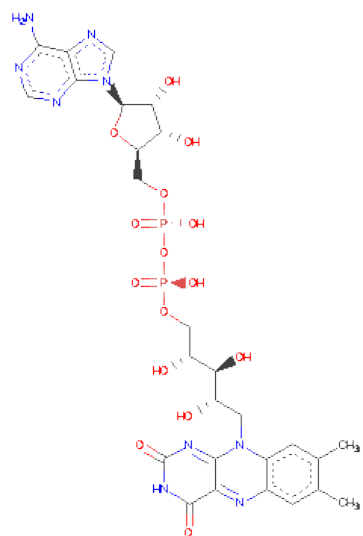
- Molecule 1 is a protein called ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	1	0
			4396	2791	761	820	24			
1	B	543	Total	C	N	O	S	0	0	0
			4300	2732	746	798	24			
1	C	557	Total	C	N	O	S	0	0	0
			4404	2793	765	822	24			
1	D	550	Total	C	N	O	S	0	0	0
			4349	2757	756	812	24			

There are 4 discrepancies between the modelled and reference sequences:

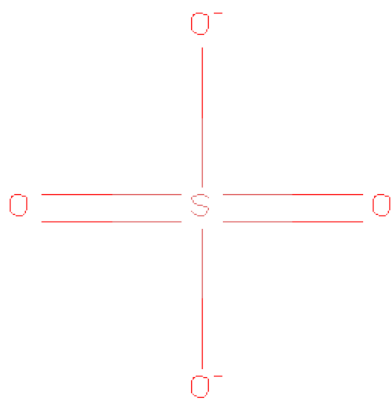
Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	ARG	ENGINEERED MUTATION	UNP P97275
B	419	HIS	ARG	ENGINEERED MUTATION	UNP P97275
C	419	HIS	ARG	ENGINEERED MUTATION	UNP P97275
D	419	HIS	ARG	ENGINEERED MUTATION	UNP P97275

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



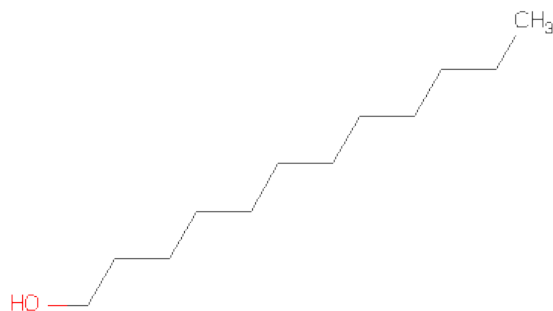
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1-DODECANOL (three-letter code: 1DO) (formula: C₁₂H₂₆O).

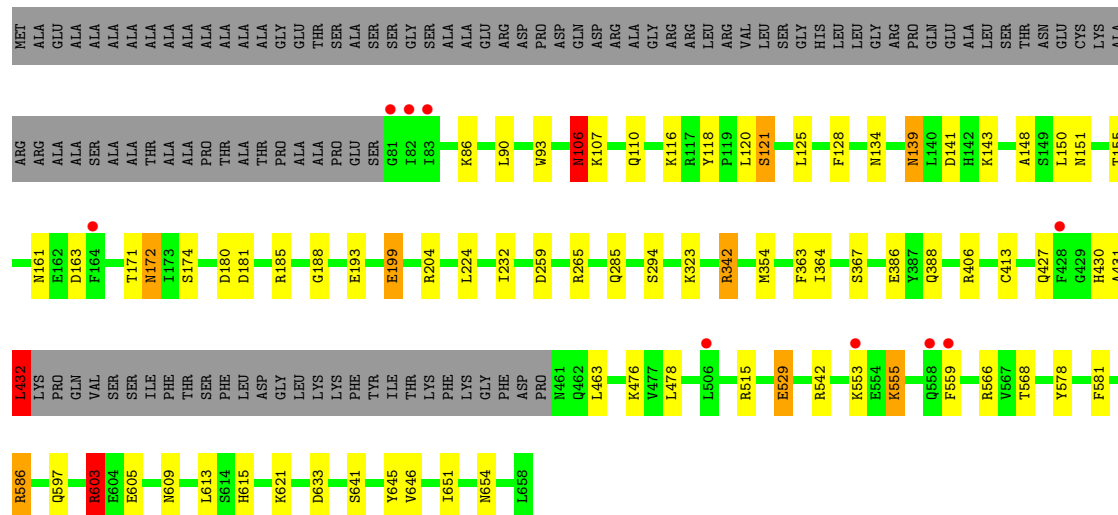


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	12	1		
4	C	1	Total	C	O	0	0
			13	12	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	36	Total	O	0	0
			36	36		
5	C	49	Total	O	0	0
			49	49		
5	D	30	Total	O	0	0
			30	30		

- Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.41Å 99.19Å 107.46Å 90.58° 91.88° 95.03°	Depositor
Resolution (Å)	54.17 – 2.40 54.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (54.17-2.40) 95.4 (54.17-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.270 0.211 , 0.263	Depositor DCC
R_{free} test set	1033 reflections (1.11%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 15.1	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 94187 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17858	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: 1DO, 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	1.22	57/4500 (1.3%)	1.05	25/6084 (0.4%)
1	B	0.94	11/4398 (0.3%)	0.95	20/5945 (0.3%)
1	C	0.90	8/4505 (0.2%)	0.89	10/6092 (0.2%)
1	D	0.85	6/4447 (0.1%)	0.85	12/6013 (0.2%)
All	All	0.99	82/17850 (0.5%)	0.94	67/24134 (0.3%)

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	PHE	CE2-CZ	-11.11	1.16	1.37
1	A	595	PHE	CE1-CZ	-11.02	1.16	1.37
1	D	265	ARG	CG-CD	-9.74	1.27	1.51
1	A	528	PHE	CG-CD2	-9.57	1.24	1.38
1	A	195	PHE	CE1-CZ	-9.52	1.19	1.37
1	A	528	PHE	CE1-CZ	-9.51	1.19	1.37
1	A	390	TYR	CE2-CZ	-9.31	1.26	1.38
1	A	195	PHE	CG-CD2	-9.31	1.24	1.38
1	A	595	PHE	CG-CD2	-9.30	1.24	1.38
1	A	559	PHE	CG-CD2	-9.20	1.25	1.38
1	A	167	GLU	CD-OE1	-9.14	1.15	1.25
1	B	334	VAL	CB-CG2	-9.12	1.33	1.52
1	A	636	PHE	CE2-CZ	-9.09	1.20	1.37
1	A	390	TYR	CG-CD1	-9.04	1.27	1.39
1	A	542	ARG	CZ-NH1	-8.94	1.21	1.33
1	B	629	GLU	CB-CG	-8.82	1.35	1.52
1	A	195	PHE	CG-CD1	-8.77	1.25	1.38
1	A	199	GLU	CD-OE1	-8.50	1.16	1.25
1	A	470	PHE	CE2-CZ	-8.42	1.21	1.37
1	A	636	PHE	CG-CD1	-8.39	1.26	1.38
1	A	195	PHE	CE2-CZ	-8.32	1.21	1.37
1	B	623	ARG	CZ-NH1	-8.27	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	PHE	CE1-CZ	-8.21	1.21	1.37
1	A	390	TYR	CE1-CZ	-8.17	1.27	1.38
1	A	184	PHE	CG-CD1	-8.15	1.26	1.38
1	A	390	TYR	CG-CD2	-8.15	1.28	1.39
1	A	559	PHE	CE1-CZ	-8.00	1.22	1.37
1	A	536	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	636	PHE	CE1-CZ	-7.73	1.22	1.37
1	A	470	PHE	CG-CD1	-7.65	1.27	1.38
1	A	363	PHE	CG-CD2	-7.54	1.27	1.38
1	A	203	GLU	CD-OE1	-7.50	1.17	1.25
1	A	526	GLU	CD-OE1	-7.49	1.17	1.25
1	A	184	PHE	CE1-CZ	-7.45	1.23	1.37
1	A	595	PHE	CE2-CZ	-7.41	1.23	1.37
1	B	559	PHE	CB-CG	-7.40	1.38	1.51
1	A	603	ARG	CZ-NH1	-7.39	1.23	1.33
1	B	334	VAL	CB-CG1	-7.32	1.37	1.52
1	A	167	GLU	CD-OE2	-7.32	1.17	1.25
1	A	470	PHE	CG-CD2	-7.12	1.28	1.38
1	A	529	GLU	CG-CD	-7.11	1.41	1.51
1	A	568	THR	CB-CG2	-6.94	1.29	1.52
1	D	199	GLU	CD-OE1	-6.82	1.18	1.25
1	A	515	ARG	CZ-NH2	-6.79	1.24	1.33
1	A	526	GLU	CD-OE2	-6.77	1.18	1.25
1	A	636	PHE	CG-CD2	-6.62	1.28	1.38
1	A	528	PHE	CG-CD1	-6.62	1.28	1.38
1	A	184	PHE	CG-CD2	-6.61	1.28	1.38
1	C	199	GLU	CD-OE1	-6.56	1.18	1.25
1	D	180	ASP	CB-CG	-6.49	1.38	1.51
1	A	342	ARG	CG-CD	-6.46	1.35	1.51
1	A	193	GLU	CD-OE2	-6.42	1.18	1.25
1	A	595	PHE	CG-CD1	-6.42	1.29	1.38
1	C	265	ARG	NE-CZ	-6.40	1.24	1.33
1	A	596	GLU	CD-OE1	-6.37	1.18	1.25
1	C	265	ARG	CG-CD	-6.30	1.36	1.51
1	B	559	PHE	CG-CD2	-6.14	1.29	1.38
1	A	193	GLU	CD-OE1	-6.08	1.19	1.25
1	B	529	GLU	CG-CD	-6.07	1.42	1.51
1	A	363	PHE	CE2-CZ	-6.03	1.25	1.37
1	A	541	CYS	CB-SG	-5.97	1.72	1.81
1	D	265	ARG	CD-NE	-5.95	1.36	1.46
1	B	363	PHE	CE2-CZ	-5.92	1.26	1.37
1	B	406	ARG	CG-CD	-5.91	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	471	GLU	CB-CG	-5.88	1.41	1.52
1	A	528	PHE	CE2-CZ	-5.86	1.26	1.37
1	A	515	ARG	CZ-NH1	-5.86	1.25	1.33
1	C	596	GLU	CD-OE1	-5.81	1.19	1.25
1	A	363	PHE	CE1-CZ	-5.72	1.26	1.37
1	A	566	ARG	CZ-NH1	-5.66	1.25	1.33
1	D	265	ARG	NE-CZ	-5.61	1.25	1.33
1	C	342	ARG	CG-CD	-5.40	1.38	1.51
1	D	413	CYS	CB-SG	-5.37	1.73	1.81
1	A	203	GLU	CD-OE2	-5.27	1.19	1.25
1	B	559	PHE	CD1-CE1	-5.27	1.28	1.39
1	C	162	GLU	CG-CD	-5.20	1.44	1.51
1	C	641	SER	CB-OG	-5.19	1.35	1.42
1	A	224	LEU	CG-CD1	-5.17	1.32	1.51
1	A	363	PHE	CG-CD1	-5.17	1.30	1.38
1	A	265	ARG	CZ-NH2	-5.06	1.26	1.33
1	A	224	LEU	CG-CD2	-5.05	1.33	1.51
1	B	567	VAL	CB-CG2	-5.02	1.42	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ARG	NE-CZ-NH2	15.53	128.06	120.30
1	B	623	ARG	NE-CZ-NH2	13.76	127.18	120.30
1	A	542	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	A	515	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	C	603	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	B	559	PHE	CB-CG-CD2	12.04	129.23	120.80
1	A	603	ARG	NE-CZ-NH2	11.69	126.14	120.30
1	A	566	ARG	NE-CZ-NH2	10.69	125.65	120.30
1	B	603	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	536	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	B	633	ASP	CB-CG-OD1	9.50	126.85	118.30
1	A	526	GLU	OE1-CD-OE2	-9.20	112.26	123.30
1	C	342	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	203	GLU	OE1-CD-OE2	-8.53	113.07	123.30
1	B	265	ARG	CG-CD-NE	-8.33	94.31	111.80
1	B	265	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	603	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	193	GLU	OE1-CD-OE2	-7.98	113.73	123.30
1	A	167	GLU	OE1-CD-OE2	-7.95	113.76	123.30
1	C	354	MET	CA-CB-CG	7.52	126.08	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	VAL	CG1-CB-CG2	-7.05	99.62	110.90
1	D	180	ASP	CB-CG-OD1	-7.05	111.95	118.30
1	D	515	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	C	250	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	542	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	515	ARG	CG-CD-NE	-6.77	97.59	111.80
1	A	265	ARG	CB-CG-CD	-6.68	94.23	111.60
1	D	180	ASP	CB-CG-OD2	6.58	124.22	118.30
1	C	86	LYS	CD-CE-NZ	6.54	126.74	111.70
1	D	603	ARG	CD-NE-CZ	6.51	132.72	123.60
1	C	515	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	191	LEU	CD1-CG-CD2	-6.40	91.30	110.50
1	B	406	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	180	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	638	MET	CG-SD-CE	6.36	110.37	100.20
1	D	633	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	595	PHE	CB-CG-CD1	6.05	125.03	120.80
1	B	406	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	421	MET	CG-SD-CE	5.96	109.73	100.20
1	D	603	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	566	ARG	CB-CG-CD	-5.87	96.35	111.60
1	D	204	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	559	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	A	250	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	342	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	B	623	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	D	90	LEU	CA-CB-CG	5.72	128.47	115.30
1	D	265	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	B	170	LYS	CD-CE-NZ	5.70	124.81	111.70
1	A	596	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	559	PHE	CB-CG-CD1	5.58	124.71	120.80
1	B	90	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	A	224	LEU	CD1-CG-CD2	-5.52	93.94	110.50
1	A	566	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	603	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	B	90	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	379	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	B	265	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	C	140	LEU	CA-CB-CG	5.28	127.43	115.30
1	B	536	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	265	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	C	463	LEU	CA-CB-CG	5.15	127.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	432	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	603	ARG	CD-NE-CZ	5.11	130.75	123.60
1	B	250	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	342	ARG	CA-CB-CG	-5.07	102.24	113.40
1	A	390	TYR	CD1-CE1-CZ	5.02	124.32	119.80

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	4396	0	0	14	0
1	B	4300	0	0	20	2
1	C	4404	0	0	15	2
1	D	4349	0	0	23	0
2	A	53	0	0	0	0
2	B	53	0	0	0	0
2	C	53	0	0	0	0
2	D	53	0	0	0	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	B	13	0	26	1	0
4	C	13	0	26	0	0
5	A	46	0	0	2	0
5	B	36	0	0	0	0
5	C	49	0	0	0	0
5	D	30	0	0	0	0
All	All	17858	0	52	71	2

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:507:LEU:O	1:B:511:ILE:CD1	1.65	1.44
1:B:621:LYS:NZ	1:B:654:ASN:O	1.80	1.13
1:B:511:ILE:N	1:B:511:ILE:CD1	2.26	0.97
1:C:139:ASN:CB	1:C:141:ASP:OD1	2.28	0.80
1:B:265:ARG:NH1	1:B:265:ARG:CA	2.47	0.78
1:D:86:LYS:NZ	1:D:181:ASP:OD2	2.16	0.77
1:D:529:GLU:OE2	1:D:615:HIS:N	2.18	0.76
1:B:507:LEU:C	1:B:511:ILE:CD1	2.54	0.76
1:C:100:ASP:O	1:C:114:THR:CG2	2.35	0.74
1:C:621:LYS:NZ	1:C:654:ASN:O	2.20	0.74
1:C:342:ARG:NE	1:C:645:TYR:O	2.21	0.74
1:B:192:HIS:CB	1:B:243:TYR:OH	2.39	0.70
1:D:93:TRP:NE1	1:D:148:ALA:O	2.26	0.69
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.81	0.68
1:B:527:SER:OG	4:B:888:IDO:H1C2	1.93	0.68
1:D:139:ASN:N	1:D:139:ASN:ND2	2.45	0.64
1:D:185:ARG:NE	1:D:259:ASP:OD2	2.31	0.63
1:B:133:GLN:OE1	1:B:139:ASN:O	2.17	0.62
1:B:507:LEU:O	1:B:511:ILE:CG1	2.45	0.62
1:C:586:ARG:CG	1:C:586:ARG:NH1	2.63	0.62
1:B:139:ASN:O	1:B:140:LEU:CB	2.48	0.61
1:A:265:ARG:NH1	1:A:265:ARG:CG	2.58	0.61
1:B:265:ARG:NH1	1:B:265:ARG:CG	2.53	0.60
1:D:86:LYS:NZ	1:D:181:ASP:CG	2.57	0.58
1:B:190:CYS:SG	1:B:241:VAL:O	2.61	0.58
1:C:142:HIS:CD2	1:C:586:ARG:NH2	2.73	0.57
1:D:430:HIS:O	1:D:432:LEU:N	2.38	0.57
1:D:605:GLU:O	1:D:609:ASN:ND2	2.39	0.55
1:C:192:HIS:CB	1:C:243:TYR:OH	2.55	0.55
1:A:82:ILE:CG1	1:A:264:ASN:ND2	2.70	0.55
1:D:586:ARG:NH1	1:D:586:ARG:CG	2.67	0.55
1:C:139:ASN:O	1:C:140:LEU:CB	2.56	0.53
1:D:86:LYS:NZ	1:D:181:ASP:OD1	2.42	0.52
1:B:192:HIS:ND1	1:B:592:LEU:CD1	2.72	0.52
1:A:571:TYR:OH	1:A:615:HIS:CE1	2.64	0.51
1:D:364:ILE:O	1:D:367:SER:OG	2.29	0.50
1:B:510:VAL:O	1:B:513:TYR:N	2.45	0.50
1:A:262:GLN:N	5:A:2005:HOH:O	2.45	0.49
1:D:529:GLU:O	1:D:603:ARG:NH2	2.46	0.49
1:D:555:LYS:NZ	1:D:597:GLN:NE2	2.60	0.49
1:D:342:ARG:NE	1:D:645:TYR:O	2.46	0.49
1:A:618:GLY:O	1:A:623:ARG:NH1	2.46	0.48
1:D:188:GLY:N	1:D:193:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:539:ASP:OD1	1:A:542:ARG:NH2	2.47	0.48
1:D:430:HIS:C	1:D:432:LEU:N	2.66	0.47
1:A:507:LEU:O	1:A:511:ILE:CG1	2.63	0.47
1:A:100:ASP:O	1:A:114:THR:OG1	2.33	0.46
1:C:92:LYS:NZ	1:C:101:SER:O	2.49	0.46
1:B:481:GLU:CG	1:B:485:TYR:CE2	2.99	0.46
1:A:250:ASP:OD1	1:A:250:ASP:N	2.48	0.46
1:C:185:ARG:NE	1:C:259:ASP:OD2	2.50	0.45
1:C:326:TYR:OH	1:C:471:GLU:OE2	2.35	0.45
1:C:232:ILE:N	1:C:651:ILE:O	2.49	0.45
1:A:215:HIS:CD2	1:A:375:THR:OG1	2.71	0.44
1:D:106:ASN:ND2	1:D:110:GLN:N	2.65	0.44
1:B:615:HIS:ND1	1:B:616:HIS:ND1	2.66	0.44
1:B:643:LYS:NZ	1:B:647:ASP:OD2	2.50	0.44
1:A:463:LEU:C	1:A:463:LEU:CD1	2.86	0.44
1:D:232:ILE:N	1:D:651:ILE:O	2.50	0.44
1:C:529:GLU:OE1	1:C:615:HIS:N	2.51	0.44
1:D:161:ASN:OD1	1:D:163:ASP:N	2.51	0.44
1:A:330:GLU:OE1	1:B:353:ARG:NH2	2.51	0.43
1:A:347:LYS:N	5:A:2024:HOH:O	2.52	0.43
1:D:171:THR:O	1:D:172:ASN:CB	2.67	0.43
1:C:419:HIS:CD2	1:C:566:ARG:NH2	2.87	0.42
1:D:621:LYS:NZ	1:D:654:ASN:O	2.52	0.42
1:C:499:ASP:N	1:C:499:ASP:OD1	2.53	0.41
1:D:118:TYR:O	1:D:121:SER:OG	2.38	0.41
1:D:363:PHE:N	1:D:363:PHE:CD1	2.89	0.40
1:B:481:GLU:O	1:B:485:TYR:CD2	2.74	0.40
1:B:277:HIS:CD2	1:B:378:THR:OG1	2.74	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:ASN:ND2	1:C:536:ARG:NH2[1_546]	2.04	0.16
1:B:265:ARG:CD	1:C:151:ASN:OD1[1_556]	2.13	0.07

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%)	539 (98%)	11 (2%)	0	100	100
1	B	537/658 (82%)	521 (97%)	16 (3%)	0	100	100
1	C	553/658 (84%)	536 (97%)	16 (3%)	1 (0%)	56	74
1	D	546/658 (83%)	524 (96%)	20 (4%)	2 (0%)	43	61
All	All	2186/2632 (83%)	2120 (97%)	63 (3%)	3 (0%)	59	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	431	ALA
1	C	140	LEU
1	D	106	ASN

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	477/545 (88%)	447 (94%)	30 (6%)	25	38
1	B	464/545 (85%)	427 (92%)	37 (8%)	17	26
1	C	477/545 (88%)	435 (91%)	42 (9%)	14	21
1	D	471/545 (86%)	428 (91%)	43 (9%)	14	20
All	All	1889/2180 (87%)	1737 (92%)	152 (8%)	17	26

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	90	LEU
1	A	120	LEU
1	A	141	ASP
1	A	144	THR
1	A	159	ILE

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Mol	Chain	Res	Type
1	A	174	SER
1	A	191	LEU
1	A	323	LYS
1	A	342	ARG
1	A	349	CYS
1	A	354	MET
1	A	406	ARG
1	A	434	PRO
1	A	439	ILE
1	A	463	LEU
1	A	476	LYS
1	A	502	GLN
1	A	526	GLU
1	A	529	GLU
1	A	559	PHE
1	A	566	ARG
1	A	584	ASN
1	A	586	ARG
1	A	588	ILE
1	A	592	LEU
1	A	596	GLU
1	A	599	GLU
1	A	630	SER
1	A	646	VAL
1	B	90	LEU
1	B	94	ASN
1	B	120	LEU
1	B	127	THR
1	B	140	LEU
1	B	170	LYS
1	B	195	PHE
1	B	199	GLU
1	B	265	ARG
1	B	298	THR
1	B	323	LYS
1	B	354	MET
1	B	406	ARG
1	B	428	PHE
1	B	433	LYS
1	B	435	GLN
1	B	463	LEU
1	B	475	GLU

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Mol	Chain	Res	Type
1	B	487	ILE
1	B	502	GLN
1	B	503	ARG
1	B	510	VAL
1	B	511	ILE
1	B	520	GLU
1	B	524	ILE
1	B	526	GLU
1	B	529	GLU
1	B	555	LYS
1	B	566	ARG
1	B	578	TYR
1	B	581	PHE
1	B	592	LEU
1	B	613	LEU
1	B	614	SER
1	B	628	LYS
1	B	633	ASP
1	B	646	VAL
1	C	90	LEU
1	C	105	LEU
1	C	114	THR
1	C	129	LYS
1	C	140	LEU
1	C	141	ASP
1	C	150	LEU
1	C	174	SER
1	C	199	GLU
1	C	224	LEU
1	C	265	ARG
1	C	271	GLU
1	C	323	LYS
1	C	342	ARG
1	C	349	CYS
1	C	354	MET
1	C	360	ILE
1	C	406	ARG
1	C	425	GLN
1	C	428	PHE
1	C	432	LEU
1	C	433	LYS
1	C	462	GLN

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Mol	Chain	Res	Type
1	C	463	LEU
1	C	490	LYS
1	C	499	ASP
1	C	508	THR
1	C	511	ILE
1	C	520	GLU
1	C	526	GLU
1	C	542	ARG
1	C	559	PHE
1	C	566	ARG
1	C	568	THR
1	C	578	TYR
1	C	584	ASN
1	C	586	ARG
1	C	588	ILE
1	C	596	GLU
1	C	613	LEU
1	C	633	ASP
1	C	641	SER
1	D	106	ASN
1	D	107	LYS
1	D	116	LYS
1	D	120	LEU
1	D	121	SER
1	D	125	LEU
1	D	128	PHE
1	D	134	ASN
1	D	139	ASN
1	D	141	ASP
1	D	143	LYS
1	D	150	LEU
1	D	151	ASN
1	D	155	THR
1	D	172	ASN
1	D	174	SER
1	D	199	GLU
1	D	224	LEU
1	D	285	GLN
1	D	294	SER
1	D	323	LYS
1	D	354	MET
1	D	386	GLU

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Mol	Chain	Res	Type
1	D	388	GLN
1	D	406	ARG
1	D	427	GLN
1	D	432	LEU
1	D	463	LEU
1	D	476	LYS
1	D	478	LEU
1	D	529	GLU
1	D	542	ARG
1	D	553	LYS
1	D	555	LYS
1	D	559	PHE
1	D	568	THR
1	D	578	TYR
1	D	581	PHE
1	D	586	ARG
1	D	603	ARG
1	D	613	LEU
1	D	641	SER
1	D	646	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\# Z > 2$
3	SO4	A	1659	-	4,4,4	0.24	0	6,6,6	0.27	0
2	FAD	A	999	-	58,58,58	1.12	5 (8%)	85,89,89	2.23	17 (20%)
4	1DO	B	888	-	12,12,12	0.73	0	11,11,11	0.40	0
2	FAD	B	999	-	58,58,58	1.37	7 (12%)	85,89,89	2.09	15 (17%)
4	1DO	C	888	-	12,12,12	0.70	0	11,11,11	0.50	0
2	FAD	C	999	-	58,58,58	1.33	8 (13%)	85,89,89	1.97	16 (18%)
3	SO4	D	1659	-	4,4,4	0.69	0	6,6,6	0.56	0
2	FAD	D	999	-	58,58,58	1.29	6 (10%)	85,89,89	1.98	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
3	SO4	A	1659	-	-	0/0/0/0	0/0/0/0
2	FAD	A	999	-	-	0/34/50/50	0/1/6/6
4	1DO	B	888	-	-	0/10/10/10	0/0/0/0
2	FAD	B	999	-	-	0/34/50/50	0/1/6/6
4	1DO	C	888	-	-	0/10/10/10	0/0/0/0
2	FAD	C	999	-	-	0/34/50/50	0/1/6/6
3	SO4	D	1659	-	-	0/0/0/0	0/0/0/0
2	FAD	D	999	-	-	0/34/50/50	0/1/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	999	FAD	C1'-N10	4.59	1.53	1.48
2	B	999	FAD	C1'-N10	4.58	1.53	1.48
2	B	999	FAD	C2A-N3A	3.91	1.39	1.32
2	C	999	FAD	C1'-N10	3.58	1.52	1.48
2	D	999	FAD	C8A-N9A	3.15	1.41	1.36
2	C	999	FAD	P-O3P	3.07	1.65	1.59
2	A	999	FAD	C4X-N5	2.99	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	FAD	C10-N1	2.87	1.40	1.35
2	C	999	FAD	C5X-N5	2.86	1.39	1.35
2	B	999	FAD	C2A-N1A	2.86	1.39	1.33
2	A	999	FAD	C2A-N3A	2.84	1.37	1.32
2	A	999	FAD	C5X-N5	2.78	1.39	1.35
2	C	999	FAD	C8A-N9A	2.76	1.40	1.36
2	C	999	FAD	C1'-C2'	2.66	1.54	1.51
2	C	999	FAD	PA-O3P	2.63	1.64	1.59
2	D	999	FAD	C2A-N3A	2.58	1.37	1.32
2	B	999	FAD	C5X-N5	2.49	1.39	1.35
2	D	999	FAD	C2A-N1A	2.40	1.38	1.33
2	D	999	FAD	C5X-N5	2.37	1.38	1.35
2	B	999	FAD	O4'-C4'	-2.35	1.38	1.43
2	B	999	FAD	C1'-C2'	2.33	1.53	1.51
2	C	999	FAD	C2A-N3A	2.31	1.36	1.32
2	D	999	FAD	C6-C5X	-2.29	1.39	1.41
2	C	999	FAD	C6-C5X	-2.18	1.39	1.41
2	A	999	FAD	C6-C5X	-2.16	1.39	1.41
2	A	999	FAD	C2A-N1A	2.05	1.38	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	N3A-C2A-N1A	-13.80	117.17	128.71
2	C	999	FAD	N3A-C2A-N1A	-11.25	119.31	128.71
2	D	999	FAD	N3A-C2A-N1A	-10.63	119.82	128.71
2	B	999	FAD	N3A-C2A-N1A	-8.15	121.89	128.71
2	B	999	FAD	O4B-C1B-N9A	-7.88	101.11	108.44
2	D	999	FAD	C2-N1-C10	6.92	121.95	114.98
2	B	999	FAD	C2-N1-C10	6.59	121.62	114.98
2	A	999	FAD	C2-N1-C10	6.01	121.03	114.98
2	C	999	FAD	C2-N1-C10	5.50	120.52	114.98
2	B	999	FAD	C1'-N10-C9A	4.93	123.67	118.87
2	B	999	FAD	N3A-C4A-N9A	4.05	132.75	125.43
2	B	999	FAD	C4X-C10-N1	-3.93	118.80	122.73
2	C	999	FAD	C4X-N5-C5X	3.90	121.07	116.69
2	C	999	FAD	N3A-C4A-N9A	3.89	132.45	125.43
2	A	999	FAD	C5X-C9A-N10	3.83	120.57	116.80
2	C	999	FAD	O4'-C4'-C5'	-3.82	102.27	110.12
2	D	999	FAD	C4X-C10-N1	-3.78	118.96	122.73
2	B	999	FAD	O4'-C4'-C5'	-3.73	102.45	110.12
2	A	999	FAD	C1B-N9A-C4A	-3.70	120.24	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C8A-N9A-C4A	3.70	109.72	106.90
2	D	999	FAD	C5'-C4'-C3'	3.58	118.81	112.06
2	D	999	FAD	C4X-N5-C5X	3.47	120.59	116.69
2	C	999	FAD	C1'-N10-C9A	3.39	122.17	118.87
2	D	999	FAD	C4-N3-C2	-3.26	118.69	125.39
2	B	999	FAD	C8A-N9A-C4A	3.21	109.35	106.90
2	A	999	FAD	N3A-C4A-N9A	3.17	131.15	125.43
2	C	999	FAD	C4X-C10-N1	-3.12	119.61	122.73
2	A	999	FAD	O3P-PA-O5B	-3.05	89.78	103.41
2	B	999	FAD	C5X-C9A-N10	3.04	119.80	116.80
2	D	999	FAD	C9A-N10-C10	-3.04	118.78	121.77
2	A	999	FAD	O2A-PA-O3P	3.00	119.35	105.14
2	D	999	FAD	C5X-C9A-N10	2.97	119.73	116.80
2	A	999	FAD	C4-N3-C2	-2.90	119.43	125.39
2	A	999	FAD	C2'-C1'-N10	2.80	116.17	112.45
2	C	999	FAD	O4B-C1B-N9A	-2.76	105.87	108.44
2	A	999	FAD	N7A-C8A-N9A	-2.71	106.68	114.36
2	B	999	FAD	C5'-C4'-C3'	2.70	117.15	112.06
2	D	999	FAD	O3'-C3'-C2'	-2.67	101.98	108.74
2	A	999	FAD	C9A-N10-C10	-2.64	119.17	121.77
2	C	999	FAD	C4-C4X-C10	2.63	121.19	116.95
2	D	999	FAD	O2A-PA-O3P	2.62	117.59	105.14
2	C	999	FAD	O3'-C3'-C2'	-2.62	102.12	108.74
2	B	999	FAD	C9A-N10-C10	-2.60	119.22	121.77
2	B	999	FAD	C4X-N5-C5X	2.56	119.56	116.69
2	C	999	FAD	C2A-N3A-C4A	2.54	121.23	114.01
2	C	999	FAD	C9A-N10-C10	-2.49	119.32	121.77
2	A	999	FAD	O2'-C2'-C1'	2.49	115.88	109.71
2	A	999	FAD	C2A-N3A-C4A	2.47	121.04	114.01
2	B	999	FAD	O2A-PA-O3P	2.45	116.78	105.14
2	A	999	FAD	O3B-C3B-C4B	-2.35	104.15	111.08
2	D	999	FAD	O4'-C4'-C3'	2.31	114.80	109.05
2	B	999	FAD	O3B-C3B-C4B	-2.29	104.33	111.08
2	C	999	FAD	C5X-C9A-N10	2.26	119.02	116.80
2	C	999	FAD	C5A-C4A-N3A	-2.22	120.87	125.70
2	A	999	FAD	C4X-C10-N1	-2.21	120.52	122.73
2	A	999	FAD	P-O3P-PA	-2.19	125.25	131.68
2	C	999	FAD	O3B-C3B-C4B	-2.19	104.64	111.08
2	D	999	FAD	C1'-N10-C9A	2.11	120.93	118.87
2	D	999	FAD	N3A-C4A-N9A	2.09	129.20	125.43
2	B	999	FAD	N7A-C8A-N9A	-2.07	108.50	114.36
2	D	999	FAD	O3'-C3'-C4'	2.07	113.97	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	999	FAD	O4'-C4'-C5'	-2.07	105.87	110.12
2	C	999	FAD	O2P-P-O3P	2.02	114.70	105.14
2	D	999	FAD	P-O3P-PA	-2.00	125.81	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%)	-0.25	13 (2%) 57 55	13, 33, 63, 83	0
1	B	543/658 (82%)	-0.20	11 (2%) 62 59	14, 35, 65, 85	0
1	C	557/658 (84%)	-0.32	5 (0%) 81 81	14, 33, 59, 72	0
1	D	550/658 (83%)	-0.16	9 (1%) 68 67	15, 39, 71, 84	0
All	All	2205/2632 (83%)	-0.23	38 (1%) 67 65	13, 35, 66, 85	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	ILE	5.5
1	A	82	ILE	4.3
1	B	197	LEU	4.1
1	D	83	ILE	4.0
1	C	81	GLY	3.9
1	D	82	ILE	3.8
1	A	437	SER	3.7
1	A	440	PHE	3.7
1	B	162	GLU	3.6
1	B	458	PHE	3.5
1	D	81	GLY	3.4
1	A	81	GLY	3.3
1	A	83	ILE	3.2
1	B	558	GLN	3.2
1	B	201	MET	3.2
1	C	83	ILE	3.2
1	B	180	ASP	3.1
1	D	558	GLN	3.0
1	A	438	SER	3.0
1	B	166	HIS	2.9
1	B	81	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	458	PHE	2.8
1	A	155	THR	2.7
1	A	439	ILE	2.7
1	A	197	LEU	2.7
1	B	93	TRP	2.7
1	D	559	PHE	2.6
1	B	460	PRO	2.6
1	D	164	PHE	2.6
1	C	432	LEU	2.3
1	C	457	GLY	2.2
1	A	441	THR	2.1
1	D	428	PHE	2.1
1	B	587	GLY	2.1
1	D	506	LEU	2.1
1	D	553	LYS	2.0
1	A	435	GLN	2.0
1	A	559	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
4	1DO	C	888	13/13	0.17	1.36	31,34,41,42	0
3	SO4	D	1659	5/5	0.12	1.24	48,49,51,53	0
4	1DO	B	888	13/13	0.17	0.88	29,33,36,37	0
2	FAD	A	999	53/53	0.11	-0.01	15,19,24,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	D	999	53/53	0.11	-0.11	15,22,26,27	0
2	FAD	B	999	53/53	0.10	-0.66	12,17,21,23	0
3	SO4	A	1659	5/5	0.13	-0.70	53,53,54,57	0
2	FAD	C	999	53/53	0.10	-0.75	6,11,16,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.