



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3M13
Title : Crystal Structure of the Lys265Arg PEG-crystallized mutant of monomeric sarcosine oxidase
Authors : Mathews, F.S.; Chen, Z.-W.; Jorns, M.S.
Deposited on : 2010-03-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

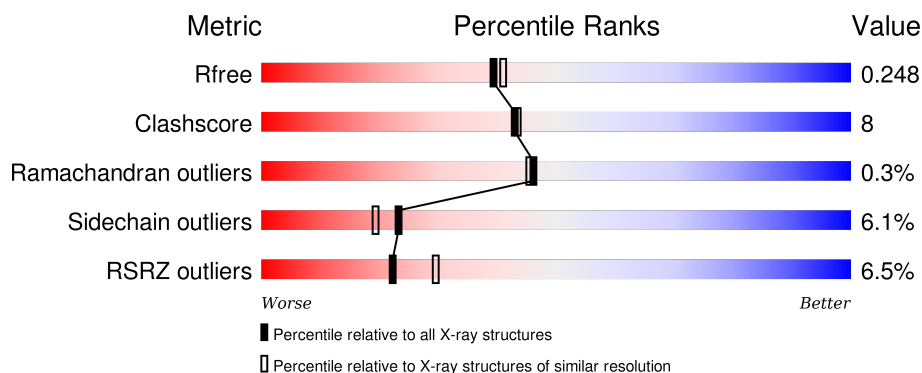
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	389	<div> <div>3%</div> <div>79%</div> <div>16%</div> <div>...</div> </div>
1	B	389	<div> <div>11%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	C	389	<div> <div>7%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	389	<div> <div>4%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	390	-	-	-	X
4	PO4	D	390	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Monomeric sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	B	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	C	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	D	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ARG	LYS	ENGINEERED	UNP P40859
B	265	ARG	LYS	ENGINEERED	UNP P40859
C	265	ARG	LYS	ENGINEERED	UNP P40859
D	265	ARG	LYS	ENGINEERED	UNP P40859

- 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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

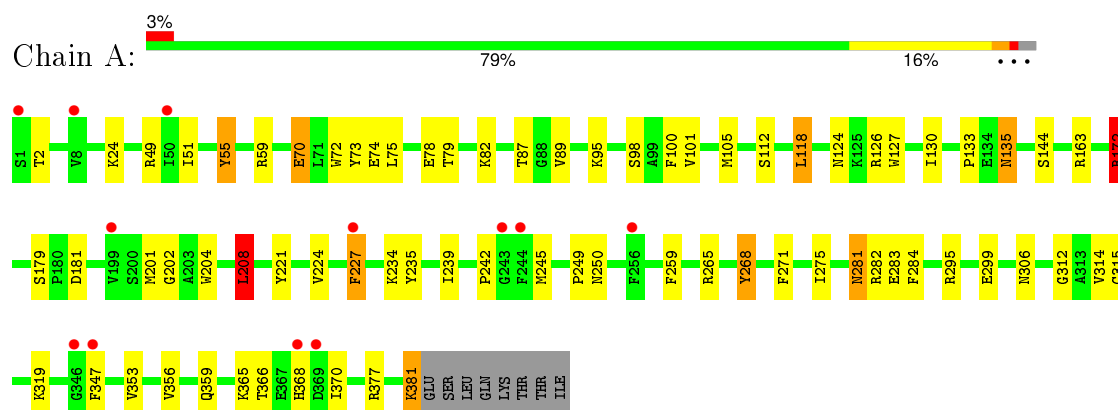
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	87	Total	O	0	0
			87	87		
5	C	77	Total	O	0	0
			77	77		
5	D	139	Total	O	0	0
			139	139		

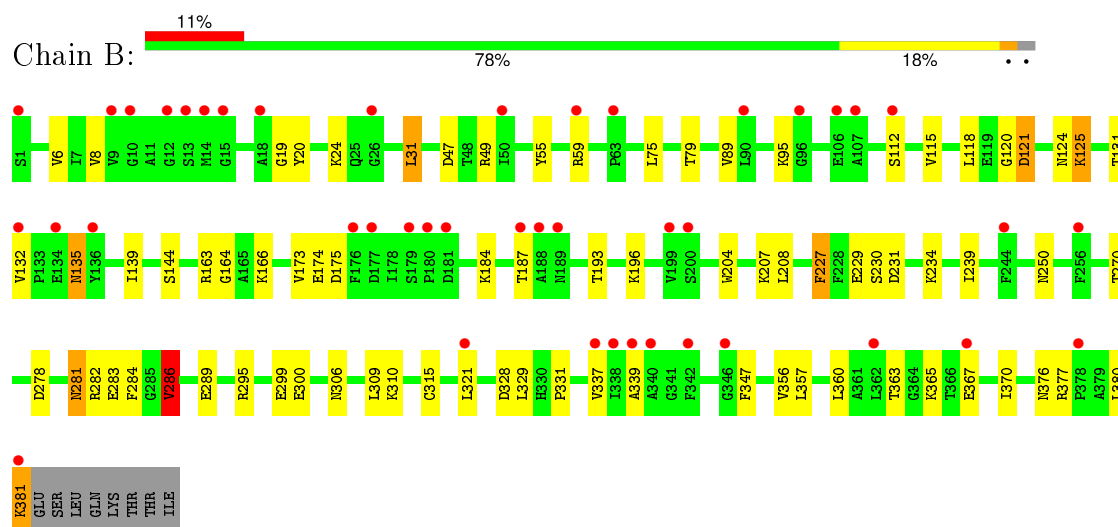
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

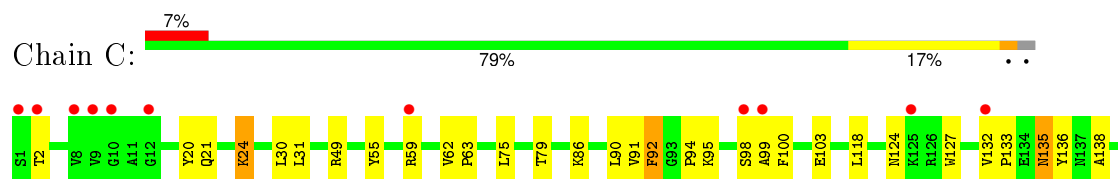
• Molecule 1: Monomeric sarcosine oxidase

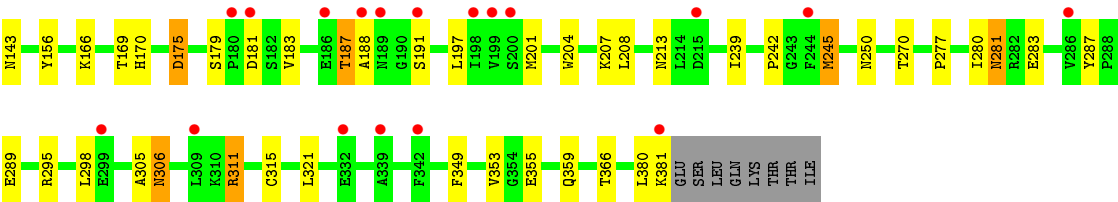


• Molecule 1: Monomeric sarcosine oxidase

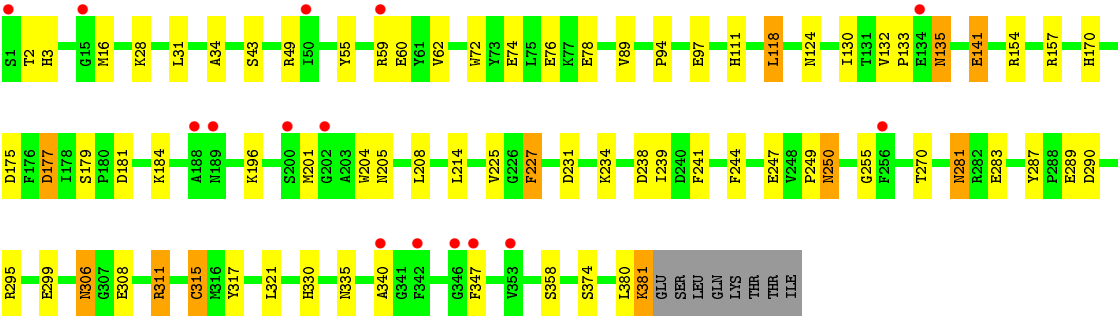
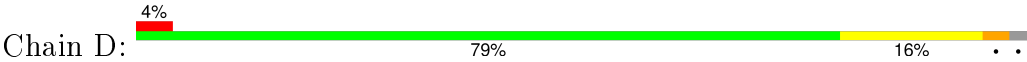


• Molecule 1: Monomeric sarcosine oxidase





● Molecule 1: Monomeric sarcosine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30 Å 69.30 Å 111.43 Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	29.20 – 2.10 29.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.20-2.10) 94.9 (29.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.187 , 0.248 0.186 , 0.248	Depositor DCC
R_{free} test set	4212 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83763 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12635	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 18.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FAD, CL

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	1.27	9/3053 (0.3%)	1.04	8/4135 (0.2%)
1	B	0.95	0/3053	0.92	6/4135 (0.1%)
1	C	1.00	0/3053	0.87	1/4135 (0.0%)
1	D	1.16	9/3053 (0.3%)	0.99	4/4135 (0.1%)
All	All	1.10	18/12212 (0.1%)	0.96	19/16540 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	TRP	CB-CG	7.62	1.64	1.50
1	A	259	PHE	CE2-CZ	7.01	1.50	1.37
1	D	89	VAL	CB-CG1	6.74	1.67	1.52
1	D	241	PHE	CE1-CZ	6.69	1.50	1.37
1	A	89	VAL	CB-CG1	6.58	1.66	1.52
1	A	353	VAL	CB-CG1	5.91	1.65	1.52
1	A	70	GLU	CG-CD	5.82	1.60	1.51
1	A	73	TYR	CD2-CE2	5.82	1.48	1.39
1	D	72	TRP	CB-CG	5.80	1.60	1.50
1	A	55	TYR	CE2-CZ	5.69	1.46	1.38
1	D	141	GLU	CB-CG	-5.60	1.41	1.52
1	D	60	GLU	CG-CD	5.55	1.60	1.51
1	A	268	TYR	CD1-CE1	5.49	1.47	1.39
1	D	340	ALA	CA-CB	5.46	1.64	1.52
1	D	317	TYR	CD1-CE1	5.40	1.47	1.39
1	D	225	VAL	CB-CG2	-5.37	1.41	1.52
1	A	235	TYR	CD1-CE1	5.22	1.47	1.39
1	D	43	SER	CB-OG	5.21	1.49	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	LEU	CA-CB-CG	8.51	134.86	115.30
1	B	286	VAL	CB-CA-C	-8.14	95.93	111.40
1	A	118	LEU	CA-CB-CG	7.57	132.71	115.30
1	B	286	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	A	126	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	172	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	172	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	282	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	B	282	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	D	238	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	289	GLU	CB-CA-C	-5.62	99.17	110.40
1	D	154	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	377	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	290	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	C	175	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	87	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	208	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	47	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	163	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2978	0	2881	51	0
1	B	2978	0	2881	47	0
1	C	2978	0	2881	54	0
1	D	2978	0	2881	42	0
2	A	53	0	31	9	0
2	B	53	0	31	7	0
2	C	53	0	31	7	0
2	D	53	0	31	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	5	0
5	A	194	0	0	3	1
5	B	87	0	0	2	0
5	C	77	0	0	6	0
5	D	139	0	0	1	0
All	All	12635	0	11648	194	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:CYS:SG	2:A:400:FAD:HM82	1.30	1.66
1:D:315:CYS:SG	2:D:400:FAD:HM82	1.38	1.60
1:B:315:CYS:SG	2:B:400:FAD:HM82	1.41	1.57
1:C:315:CYS:SG	2:C:400:FAD:HM82	1.52	1.49
1:A:315:CYS:SG	2:A:400:FAD:C8M	2.21	1.28
1:D:315:CYS:SG	2:D:400:FAD:C8M	2.31	1.18
1:B:315:CYS:SG	2:B:400:FAD:C8M	2.32	1.16
1:C:315:CYS:SG	2:C:400:FAD:C8M	2.42	1.07
1:A:381:LYS:HG3	5:A:530:HOH:O	1.70	0.89
1:B:124:ASN:HD21	1:B:132:VAL:HG22	1.37	0.89
1:C:381:LYS:HG3	5:C:406:HOH:O	1.72	0.88
1:A:95:LYS:HB3	1:A:95:LYS:HZ2	1.40	0.86
1:C:281:ASN:HD22	1:C:283:GLU:H	1.27	0.82
1:B:331:PRO:HB3	1:B:376:ASN:HD21	1.46	0.79
1:A:95:LYS:HB3	1:A:95:LYS:NZ	1.93	0.79
1:D:3:HIS:O	1:D:28:LYS:NZ	2.17	0.76
1:C:100:PHE:CZ	1:C:245:MET:HG2	2.22	0.74
1:B:173:VAL:HG22	1:B:187:THR:HG22	1.71	0.72
1:A:227:PHE:CE1	1:A:265:ARG:NE	2.56	0.72
1:C:281:ASN:ND2	1:C:283:GLU:H	1.86	0.72
1:A:135:ASN:HD22	1:A:135:ASN:H	1.38	0.70
1:A:295:ARG:O	1:A:299:GLU:HG2	1.92	0.70
1:B:315:CYS:CB	2:B:400:FAD:HM82	2.23	0.69
1:C:94:PRO:HD2	1:C:98:SER:HB2	1.76	0.68
1:A:133:PRO:HB2	1:A:135:ASN:ND2	2.09	0.68
1:A:315:CYS:CB	2:A:400:FAD:HM82	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ARG:HD3	1:C:306:ASN:HD21	1.60	0.67
1:B:295:ARG:HH11	1:B:306:ASN:ND2	1.92	0.66
1:C:315:CYS:CB	2:C:400:FAD:HM82	2.25	0.66
1:C:381:LYS:HB3	5:C:419:HOH:O	1.96	0.65
1:D:295:ARG:HH11	1:D:306:ASN:ND2	1.95	0.64
1:B:124:ASN:ND2	1:B:132:VAL:HG22	2.12	0.63
1:B:315:CYS:HB3	2:B:400:FAD:HM71	1.78	0.63
1:A:172:ARG:NH2	1:A:208:LEU:HD21	2.14	0.63
1:C:124:ASN:HD21	1:C:132:VAL:HG22	1.64	0.62
1:C:295:ARG:HH11	1:C:306:ASN:ND2	1.97	0.62
1:A:221:TYR:CE2	1:A:319:LYS:HD2	2.34	0.62
1:D:281:ASN:HD22	1:D:283:GLU:H	1.47	0.62
1:C:381:LYS:CG	5:C:419:HOH:O	2.48	0.61
1:D:62:VAL:HG21	1:D:111:HIS:CE1	2.35	0.61
1:C:95:LYS:HG3	1:C:135:ASN:O	2.00	0.61
1:C:315:CYS:HB3	2:C:400:FAD:HM71	1.82	0.61
1:D:141:GLU:HG3	4:D:390:PO4:O2	2.02	0.60
1:A:281:ASN:HD22	1:A:283:GLU:H	1.47	0.60
1:B:283:GLU:O	1:B:286:VAL:HG22	2.02	0.60
1:C:381:LYS:HG2	5:C:419:HOH:O	2.02	0.59
1:D:244:PHE:CZ	1:D:255:GLY:HA3	2.38	0.59
1:A:295:ARG:HH11	1:A:306:ASN:ND2	1.99	0.59
1:B:124:ASN:HD21	1:B:132:VAL:H	1.50	0.59
1:C:95:LYS:HB3	1:C:95:LYS:NZ	2.18	0.58
1:C:179:SER:HB3	1:C:181:ASP:OD1	2.03	0.58
1:A:227:PHE:HE1	1:A:265:ARG:HH21	1.51	0.57
1:D:231:ASP:OD1	1:D:234:LYS:HD2	2.04	0.57
1:C:95:LYS:HB3	1:C:95:LYS:HZ2	1.68	0.57
1:C:281:ASN:C	1:C:281:ASN:HD22	2.08	0.57
1:A:359:GLN:NE2	1:A:366:THR:OG1	2.38	0.56
1:B:8:VAL:HB	1:B:31:LEU:HD23	1.87	0.56
1:B:328:ASP:OD2	1:B:329:LEU:N	2.39	0.56
1:A:227:PHE:N	1:A:227:PHE:CD2	2.73	0.56
1:B:124:ASN:ND2	1:B:132:VAL:H	2.04	0.56
1:A:368:HIS:ND1	1:A:368:HIS:N	2.54	0.56
1:D:177:ASP:HB2	1:D:184:LYS:HZ2	1.71	0.55
1:D:133:PRO:HB2	1:D:135:ASN:ND2	2.21	0.55
1:C:381:LYS:CB	5:C:419:HOH:O	2.54	0.55
1:A:204:TRP:CE3	2:A:400:FAD:H8A	2.42	0.55
1:B:6:VAL:HG22	1:B:196:LYS:HB2	1.88	0.55
1:B:89:VAL:HG23	1:B:144:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:TYR:HB3	1:C:289:GLU:OE1	2.08	0.54
1:A:124:ASN:ND2	1:A:130:ILE:O	2.41	0.54
1:A:127:TRP:CD1	1:A:242:PRO:HD3	2.42	0.54
1:B:20:TYR:CZ	1:B:24:LYS:HD3	2.42	0.54
1:A:101:VAL:O	1:A:105:MET:HG3	2.08	0.53
1:C:21:GLN:HG3	1:C:355:GLU:HA	1.90	0.53
1:C:100:PHE:HZ	1:C:245:MET:HG2	1.70	0.53
1:B:75:LEU:O	1:B:79:THR:HG22	2.09	0.53
1:B:250:ASN:ND2	5:B:435:HOH:O	2.26	0.53
1:B:207:LYS:HG3	5:B:427:HOH:O	2.08	0.53
1:D:227:PHE:HD2	1:D:227:PHE:N	2.07	0.53
1:B:321:LEU:HD12	1:B:381:LYS:HB2	1.91	0.53
1:B:347:PHE:HB2	2:B:400:FAD:H2'	1.90	0.52
1:C:207:LYS:HD2	1:C:277:PRO:HG2	1.92	0.51
1:C:49:ARG:HD2	2:C:400:FAD:C4X	2.40	0.51
1:D:94:PRO:HB2	1:D:97:GLU:HB2	1.92	0.51
1:A:74:GLU:O	1:A:78:GLU:HG3	2.10	0.51
1:D:141:GLU:OE2	4:D:390:PO4:O2	2.29	0.51
1:D:227:PHE:N	1:D:227:PHE:CD2	2.79	0.51
1:D:234:LYS:HE2	5:D:507:HOH:O	2.09	0.51
1:D:311:ARG:HB2	1:D:311:ARG:HH11	1.76	0.51
1:B:295:ARG:HH11	1:B:306:ASN:HD21	1.59	0.50
1:A:315:CYS:SG	2:A:400:FAD:C8	2.98	0.50
1:A:234:LYS:HE2	5:A:544:HOH:O	2.11	0.50
1:C:381:LYS:HD2	1:C:381:LYS:N	2.26	0.50
1:B:363:THR:OG1	1:B:365:LYS:HG2	2.12	0.50
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.76	0.50
1:A:133:PRO:HB2	1:A:135:ASN:HD21	1.77	0.49
1:A:75:LEU:O	1:A:79:THR:HG22	2.12	0.49
1:B:229:GLU:OE1	1:B:310:LYS:HD2	2.12	0.49
1:C:90:LEU:HD11	1:C:138:ALA:HB1	1.95	0.49
1:D:74:GLU:O	1:D:78:GLU:HG3	2.13	0.49
1:D:250:ASN:O	1:D:250:ASN:OD1	2.30	0.49
1:B:299:GLU:HG2	1:B:300:GLU:N	2.26	0.49
1:C:91:VAL:HA	1:C:245:MET:O	2.13	0.48
1:C:62:VAL:HB	1:C:63:PRO:HD3	1.95	0.48
1:A:281:ASN:HD22	1:A:281:ASN:C	2.17	0.48
1:C:2:THR:HA	5:C:440:HOH:O	2.13	0.48
1:A:98:SER:OG	1:A:101:VAL:HG23	2.13	0.48
1:C:99:ALA:O	1:C:103:GLU:HB2	2.14	0.47
1:A:315:CYS:HB3	2:A:400:FAD:HM71	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLY:HA3	1:B:31:LEU:HD21	1.96	0.47
1:B:207:LYS:NZ	1:B:278:ASP:OD1	2.45	0.47
1:B:95:LYS:HG3	1:B:135:ASN:O	2.14	0.47
1:D:201:MET:H	1:D:205:ASN:HD21	1.63	0.47
1:A:227:PHE:N	1:A:227:PHE:HD2	2.11	0.47
1:C:183:VAL:HG21	1:C:197:LEU:HB2	1.97	0.47
1:A:100:PHE:CZ	1:A:245:MET:HG2	2.50	0.47
1:D:141:GLU:HG2	4:D:390:PO4:O1	2.16	0.46
1:A:239:ILE:HD12	1:A:239:ILE:HA	1.83	0.46
1:B:284:PHE:CE1	1:B:309:LEU:HD21	2.51	0.46
1:A:347:PHE:HB2	2:A:400:FAD:H2'	1.98	0.46
1:C:92:PHE:CD1	1:C:92:PHE:C	2.89	0.46
1:C:86:LYS:HD2	1:C:143:ASN:HA	1.97	0.46
1:D:34:ALA:O	1:D:170:HIS:HA	2.15	0.46
1:C:127:TRP:CD1	1:C:242:PRO:HD3	2.50	0.46
1:B:164:GLY:O	1:B:166:LYS:HD3	2.15	0.46
1:B:231:ASP:OD1	1:B:234:LYS:HG3	2.16	0.46
1:A:356:VAL:HG22	1:A:368:HIS:CE1	2.51	0.46
1:A:356:VAL:HG22	1:A:368:HIS:HE1	1.81	0.46
1:C:207:LYS:HB2	1:C:208:LEU:HD22	1.98	0.46
1:C:30:LEU:HA	1:C:166:LYS:O	2.16	0.46
1:B:95:LYS:HB3	1:B:95:LYS:HE3	1.60	0.45
1:D:124:ASN:ND2	1:D:130:ILE:O	2.50	0.45
1:B:356:VAL:HG11	1:B:370:ILE:HG21	1.97	0.45
1:D:287:TYR:HB3	1:D:289:GLU:OE2	2.15	0.45
1:A:24:LYS:NZ	5:A:415:HOH:O	2.49	0.45
1:D:49:ARG:HD2	2:D:400:FAD:C4X	2.46	0.45
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.71	0.45
1:C:359:GLN:HE21	1:C:366:THR:HA	1.82	0.45
1:A:281:ASN:ND2	1:A:283:GLU:H	2.12	0.45
1:C:321:LEU:HD12	1:C:381:LYS:HB2	1.99	0.44
1:C:201:MET:HE3	1:C:208:LEU:HB2	1.99	0.44
1:C:49:ARG:HD2	2:C:400:FAD:C10	2.47	0.44
1:C:239:ILE:HD12	1:C:239:ILE:HA	1.82	0.44
1:A:268:TYR:CE2	1:A:271:PHE:HB3	2.52	0.44
2:A:400:FAD:H1'1	2:A:400:FAD:H9	1.79	0.44
1:A:49:ARG:HD2	2:A:400:FAD:C4X	2.47	0.44
1:D:347:PHE:HB2	2:D:400:FAD:H2'	1.99	0.44
1:A:224:VAL:HG12	1:A:314:VAL:HG22	2.00	0.44
1:B:284:PHE:HE1	1:B:309:LEU:HD21	1.83	0.43
1:D:124:ASN:HD21	1:D:132:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG21	1:B:139:ILE:HD11	2.00	0.43
1:A:201:MET:O	1:A:202:GLY:C	2.56	0.43
1:A:172:ARG:HH21	1:A:208:LEU:HD21	1.83	0.43
1:C:311:ARG:HH11	1:C:311:ARG:HB3	1.82	0.43
1:A:172:ARG:NH2	1:A:208:LEU:CD2	2.81	0.43
1:C:20:TYR:CZ	1:C:24:LYS:HD2	2.54	0.43
1:B:204:TRP:CE3	2:B:400:FAD:H8A	2.54	0.43
1:D:133:PRO:HB2	1:D:135:ASN:HD22	1.84	0.43
1:C:298:LEU:HD22	1:C:305:ALA:HB3	2.01	0.43
1:C:349:PHE:O	1:C:353:VAL:HG23	2.19	0.43
1:D:295:ARG:O	1:D:299:GLU:HG2	2.18	0.42
1:D:94:PRO:HD3	1:D:247:GLU:O	2.19	0.42
1:D:124:ASN:HD21	1:D:132:VAL:H	1.66	0.42
1:A:275:ILE:HD12	1:A:275:ILE:C	2.38	0.42
1:A:51:ILE:O	1:A:144:SER:HB2	2.19	0.42
1:D:204:TRP:CE3	2:D:400:FAD:H8A	2.54	0.42
1:B:377:ARG:CZ	1:B:380:LEU:HD13	2.50	0.42
1:C:321:LEU:HA	1:C:321:LEU:HD23	1.89	0.42
1:B:239:ILE:HA	1:B:239:ILE:HD12	1.92	0.42
1:D:214:LEU:HD11	1:D:330:HIS:CD2	2.55	0.42
1:A:70:GLU:OE2	1:A:74:GLU:OE1	2.38	0.42
1:B:356:VAL:O	1:B:360:LEU:HG	2.20	0.41
1:A:82:LYS:NZ	1:D:76:GLU:OE2	2.39	0.41
1:D:16:MET:SD	1:D:157:ARG:HB2	2.60	0.41
1:B:49:ARG:HD2	2:B:400:FAD:C10	2.51	0.41
1:B:339:ALA:HB2	1:B:357:LEU:HD21	2.03	0.41
1:A:284:PHE:CG	1:A:312:GLY:HA3	2.56	0.41
1:C:204:TRP:CE3	2:C:400:FAD:H8A	2.55	0.41
1:D:321:LEU:HD12	1:D:381:LYS:HD3	2.00	0.41
1:D:141:GLU:HG3	4:D:390:PO4:P	2.61	0.41
1:C:133:PRO:HG2	1:C:136:TYR:CE1	2.56	0.41
1:A:250:ASN:O	1:A:268:TYR:OH	2.34	0.41
1:C:169:THR:O	1:C:170:HIS:C	2.58	0.41
1:D:315:CYS:SG	2:D:400:FAD:C8	3.06	0.41
1:C:75:LEU:O	1:C:79:THR:HG22	2.20	0.41
1:B:227:PHE:N	1:B:227:PHE:CD2	2.89	0.40
1:B:121:ASP:O	1:B:125:LYS:HB2	2.21	0.40
1:B:281:ASN:HD22	1:B:283:GLU:H	1.69	0.40
1:D:380:LEU:HD12	1:D:380:LEU:HA	1.87	0.40
1:D:196:LYS:HD3	1:D:335:ASN:HB2	2.03	0.40
1:C:91:VAL:HG13	1:C:100:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:LYS:HD2	1:D:381:LYS:HA	1.75	0.40
1:B:131:THR:O	1:B:131:THR:OG1	2.25	0.40
1:C:187:THR:OG1	1:C:188:ALA:N	2.55	0.40
1:D:141:GLU:CG	4:D:390:PO4:O2	2.69	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:392:HOH:O	5:A:521:HOH:O[2_656]	2.07	0.13

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	379/389 (97%)	368 (97%)	10 (3%)	1 (0%)	46	45
1	B	379/389 (97%)	358 (94%)	20 (5%)	1 (0%)	46	45
1	C	379/389 (97%)	362 (96%)	16 (4%)	1 (0%)	46	45
1	D	379/389 (97%)	363 (96%)	15 (4%)	1 (0%)	46	45
All	All	1516/1556 (97%)	1451 (96%)	61 (4%)	4 (0%)	46	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	250	ASN
1	B	120	GLY
1	A	370	ILE
1	C	280	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	318/326 (98%)	303 (95%)	15 (5%)	32	30
1	B	318/326 (98%)	297 (93%)	21 (7%)	21	17
1	C	318/326 (98%)	299 (94%)	19 (6%)	24	20
1	D	318/326 (98%)	295 (93%)	23 (7%)	18	14
All	All	1272/1304 (98%)	1194 (94%)	78 (6%)	23	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	55	TYR
1	A	59	ARG
1	A	112	SER
1	A	118	LEU
1	A	135	ASN
1	A	172	ARG
1	A	179	SER
1	A	181	ASP
1	A	208	LEU
1	A	227	PHE
1	A	249	PRO
1	A	281	ASN
1	A	365	LYS
1	A	381	LYS
1	B	31	LEU
1	B	55	TYR
1	B	59	ARG
1	B	112	SER
1	B	118	LEU
1	B	121	ASP
1	B	125	LYS
1	B	135	ASN
1	B	174	GLU

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Mol	Chain	Res	Type
1	B	175	ASP
1	B	184	LYS
1	B	193	THR
1	B	208	LEU
1	B	227	PHE
1	B	230	SER
1	B	270	THR
1	B	281	ASN
1	B	286	VAL
1	B	337	VAL
1	B	367	GLU
1	B	381	LYS
1	C	24	LYS
1	C	31	LEU
1	C	55	TYR
1	C	59	ARG
1	C	92	PHE
1	C	118	LEU
1	C	135	ASN
1	C	156	TYR
1	C	175	ASP
1	C	187	THR
1	C	191	SER
1	C	213	ASN
1	C	245	MET
1	C	250	ASN
1	C	270	THR
1	C	281	ASN
1	C	306	ASN
1	C	311	ARG
1	C	380	LEU
1	D	2	THR
1	D	31	LEU
1	D	55	TYR
1	D	59	ARG
1	D	118	LEU
1	D	135	ASN
1	D	175	ASP
1	D	177	ASP
1	D	179	SER
1	D	181	ASP
1	D	208	LEU

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Mol	Chain	Res	Type
1	D	227	PHE
1	D	239	ILE
1	D	249	PRO
1	D	270	THR
1	D	281	ASN
1	D	306	ASN
1	D	308	GLU
1	D	311	ARG
1	D	315	CYS
1	D	358	SER
1	D	374	SER
1	D	381	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	69	GLN
1	A	124	ASN
1	A	135	ASN
1	A	143	ASN
1	A	189	ASN
1	A	205	ASN
1	A	213	ASN
1	A	281	ASN
1	A	293	ASN
1	A	306	ASN
1	A	359	GLN
1	B	21	GLN
1	B	41	ASN
1	B	69	GLN
1	B	124	ASN
1	B	143	ASN
1	B	205	ASN
1	B	213	ASN
1	B	219	GLN
1	B	281	ASN
1	B	293	ASN
1	B	306	ASN
1	B	333	HIS
1	B	359	GLN
1	B	376	ASN

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Mol	Chain	Res	Type
1	C	21	GLN
1	C	69	GLN
1	C	124	ASN
1	C	135	ASN
1	C	189	ASN
1	C	205	ASN
1	C	219	GLN
1	C	250	ASN
1	C	281	ASN
1	C	293	ASN
1	C	306	ASN
1	C	359	GLN
1	D	69	GLN
1	D	124	ASN
1	D	135	ASN
1	D	143	ASN
1	D	205	ASN
1	D	223	GLN
1	D	281	ASN
1	D	306	ASN
1	D	359	GLN
1	D	368	HIS
1	D	376	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	400	-	48,58,58	1.56	8 (16%)	54,89,89	1.79	12 (22%)
4	PO4	B	390	-	4,4,4	0.52	0	6,6,6	0.26	0
2	FAD	B	400	-	48,58,58	1.45	8 (16%)	54,89,89	1.96	9 (16%)
2	FAD	C	400	-	48,58,58	1.34	6 (12%)	54,89,89	2.19	14 (25%)
4	PO4	D	390	-	4,4,4	0.44	0	6,6,6	0.33	0
2	FAD	D	400	-	48,58,58	1.47	8 (16%)	54,89,89	2.11	13 (24%)

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	400	-	-	0/30/50/50	0/6/6/6
4	PO4	B	390	-	-	0/0/0/0	0/0/0/0
2	FAD	B	400	-	-	0/30/50/50	0/6/6/6
2	FAD	C	400	-	-	0/30/50/50	0/6/6/6
4	PO4	D	390	-	-	0/0/0/0	0/0/0/0
2	FAD	D	400	-	-	0/30/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	FAD	C10-N10	-3.36	1.35	1.39
2	C	400	FAD	C9A-C5X	-3.11	1.36	1.42
2	D	400	FAD	C10-N10	-2.79	1.35	1.39
2	A	400	FAD	C10-N1	-2.20	1.32	1.35
2	D	400	FAD	PA-O1A	2.00	1.58	1.51
2	B	400	FAD	C10-N1	2.01	1.39	1.35
2	A	400	FAD	O2B-C2B	2.04	1.47	1.43
2	C	400	FAD	C4-C4X	2.20	1.45	1.41
2	C	400	FAD	C2A-N3A	2.21	1.36	1.32
2	D	400	FAD	C9A-N10	2.22	1.41	1.38
2	B	400	FAD	C2A-N3A	2.24	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	FAD	C2A-N3A	2.41	1.36	1.32
2	D	400	FAD	O2B-C2B	2.57	1.49	1.43
2	B	400	FAD	C4X-N5	2.62	1.37	1.33
2	A	400	FAD	O4B-C1B	2.67	1.44	1.41
2	B	400	FAD	C5'-C4'	2.77	1.55	1.51
2	D	400	FAD	C4X-N5	2.79	1.37	1.33
2	B	400	FAD	C4-C4X	2.79	1.46	1.41
2	B	400	FAD	C4A-N3A	3.04	1.40	1.35
2	C	400	FAD	C9A-N10	3.05	1.43	1.38
2	A	400	FAD	C4-C4X	3.09	1.47	1.41
2	A	400	FAD	C7M-C7	3.49	1.58	1.51
2	A	400	FAD	C4X-N5	3.57	1.38	1.33
2	D	400	FAD	C2A-N3A	3.66	1.38	1.32
2	B	400	FAD	C9A-N10	3.67	1.43	1.38
2	D	400	FAD	C4-C4X	3.83	1.48	1.41
2	C	400	FAD	O4-C4	3.88	1.34	1.24
2	D	400	FAD	O4-C4	4.07	1.34	1.24
2	A	400	FAD	O4-C4	4.33	1.35	1.24
2	B	400	FAD	O4-C4	4.64	1.35	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	FAD	N3A-C2A-N1A	-9.69	121.47	128.89
2	B	400	FAD	N3A-C2A-N1A	-7.64	123.05	128.89
2	A	400	FAD	N3A-C2A-N1A	-7.41	123.22	128.89
2	D	400	FAD	N3A-C2A-N1A	-7.08	123.47	128.89
2	C	400	FAD	C4X-C10-N10	-4.83	117.67	120.52
2	D	400	FAD	C4B-O4B-C1B	-4.80	104.45	109.72
2	D	400	FAD	C4-C4X-C10	-4.79	116.87	119.94
2	B	400	FAD	C4X-C10-N10	-4.66	117.77	120.52
2	B	400	FAD	C4X-C4-N3	-3.78	118.43	123.59
2	A	400	FAD	C4X-C4-N3	-3.24	119.15	123.59
2	D	400	FAD	P-O3P-PA	-3.18	123.80	132.73
2	C	400	FAD	C4-C4X-C10	-2.88	118.10	119.94
2	C	400	FAD	C4B-O4B-C1B	-2.80	106.64	109.72
2	C	400	FAD	C9A-C5X-N5	-2.67	118.41	122.36
2	C	400	FAD	C4X-C4-N3	-2.64	119.98	123.59
2	A	400	FAD	O5B-PA-O1A	-2.62	99.46	109.62
2	D	400	FAD	C4X-C4-N3	-2.61	120.03	123.59
2	C	400	FAD	O3P-PA-O5B	-2.50	96.29	102.94
2	C	400	FAD	C8M-C8-C9	-2.37	113.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	FAD	P-O3P-PA	-2.32	126.21	132.73
2	A	400	FAD	C1'-C2'-C3'	-2.28	103.29	109.82
2	C	400	FAD	O2'-C2'-C1'	-2.18	104.58	109.94
2	A	400	FAD	C8M-C8-C9	-2.18	114.35	120.28
2	D	400	FAD	O3B-C3B-C4B	-2.15	104.61	111.05
2	B	400	FAD	C9A-C5X-N5	-2.13	119.21	122.36
2	A	400	FAD	C4A-C5A-N7A	-2.08	107.56	109.48
2	D	400	FAD	C4X-C10-N10	-2.04	119.32	120.52
2	B	400	FAD	C1B-N9A-C4A	-2.00	123.92	126.94
2	A	400	FAD	C4-N3-C2	2.01	116.98	115.25
2	D	400	FAD	O2A-PA-O5B	2.13	119.22	108.46
2	C	400	FAD	C8M-C8-C7	2.14	125.43	120.73
2	C	400	FAD	N6A-C6A-N1A	2.15	123.82	119.20
2	D	400	FAD	C2B-C1B-N9A	2.21	117.67	114.29
2	B	400	FAD	C6-C5X-C9A	2.23	121.92	118.98
2	A	400	FAD	O2'-C2'-C3'	2.27	114.73	109.02
2	A	400	FAD	C4-C4X-N5	2.29	121.50	118.72
2	D	400	FAD	C1'-N10-C9A	2.38	121.54	118.86
2	D	400	FAD	O2P-P-O3P	2.41	116.02	105.09
2	A	400	FAD	C2B-C3B-C4B	2.47	107.69	102.61
2	A	400	FAD	C5X-C9A-N10	2.60	119.59	117.62
2	C	400	FAD	C4X-N5-C5X	2.99	120.21	116.76
2	C	400	FAD	C5X-C9A-N10	3.55	120.32	117.62
2	B	400	FAD	C4X-N5-C5X	4.00	121.36	116.76
2	A	400	FAD	C4X-N5-C5X	4.08	121.46	116.76
2	C	400	FAD	C4-N3-C2	4.70	119.31	115.25
2	D	400	FAD	C5X-C9A-N10	4.82	121.28	117.62
2	B	400	FAD	C4-N3-C2	5.82	120.28	115.25
2	D	400	FAD	C4-N3-C2	6.00	120.43	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	FAD	9	0
2	B	400	FAD	7	0
2	C	400	FAD	7	0
4	D	390	PO4	5	0
2	D	400	FAD	6	0

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	381/389 (97%)	0.04	12 (3%) 52 61	16, 27, 41, 61	0
1	B	381/389 (97%)	0.57	43 (11%) 7 9	26, 41, 65, 81	0
1	C	381/389 (97%)	0.44	29 (7%) 17 23	26, 42, 59, 68	0
1	D	381/389 (97%)	0.17	15 (3%) 43 52	17, 33, 47, 67	0
All	All	1524/1556 (97%)	0.31	99 (6%) 22 29	16, 36, 58, 81	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	SER	7.5
1	A	1	SER	6.8
1	B	1	SER	5.6
1	B	188	ALA	5.6
1	C	1	SER	5.3
1	B	180	PRO	5.1
1	B	187	THR	4.8
1	C	2	THR	4.7
1	B	26	GLY	4.5
1	D	188	ALA	4.2
1	B	338	ILE	4.1
1	B	199	VAL	3.9
1	C	9	VAL	3.7
1	C	198	ILE	3.7
1	B	106	GLU	3.7
1	B	321	LEU	3.6
1	B	59	ARG	3.6
1	C	8	VAL	3.6
1	C	199	VAL	3.4
1	B	15	GLY	3.4
1	B	50	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	362	LEU	3.4
1	C	181	ASP	3.3
1	C	132	VAL	3.2
1	B	189	ASN	3.2
1	D	189	ASN	3.1
1	C	191	SER	3.1
1	B	339	ALA	3.0
1	B	340	ALA	3.0
1	D	340	ALA	3.0
1	C	10	GLY	3.0
1	B	176	PHE	3.0
1	A	369	ASP	2.9
1	C	200	SER	2.9
1	B	367	GLU	2.9
1	A	50	ILE	2.8
1	B	10	GLY	2.8
1	D	59	ARG	2.8
1	B	342	PHE	2.8
1	B	112	SER	2.8
1	A	368	HIS	2.7
1	B	378	PRO	2.7
1	A	243	GLY	2.7
1	C	244	PHE	2.7
1	B	14	MET	2.7
1	B	381	LYS	2.6
1	B	181	ASP	2.6
1	B	179	SER	2.6
1	D	50	ILE	2.6
1	B	9	VAL	2.6
1	B	337	VAL	2.6
1	D	353	VAL	2.6
1	A	8	VAL	2.5
1	B	346	GLY	2.5
1	C	186	GLU	2.5
1	C	309	LEU	2.5
1	C	99	ALA	2.5
1	D	202	GLY	2.5
1	D	347	PHE	2.4
1	D	342	PHE	2.4
1	C	286	VAL	2.3
1	A	199	VAL	2.3
1	D	256	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	125	LYS	2.3
1	B	177	ASP	2.3
1	C	339	ALA	2.3
1	B	63	PRO	2.3
1	B	96	GLY	2.2
1	D	200	SER	2.2
1	B	244	PHE	2.2
1	C	342	PHE	2.2
1	A	346	GLY	2.2
1	B	12	GLY	2.2
1	C	332	GLU	2.2
1	C	180	PRO	2.2
1	D	346	GLY	2.2
1	A	256	PHE	2.2
1	B	200	SER	2.2
1	B	134	GLU	2.2
1	A	244	PHE	2.2
1	C	188	ALA	2.2
1	B	132	VAL	2.1
1	C	299	GLU	2.1
1	D	134	GLU	2.1
1	A	227	PHE	2.1
1	B	107	ALA	2.1
1	B	13	SER	2.1
1	A	347	PHE	2.1
1	C	98	SER	2.1
1	B	256	PHE	2.1
1	C	12	GLY	2.0
1	B	136	TYR	2.0
1	C	59	ARG	2.0
1	B	90	LEU	2.0
1	B	18	ALA	2.0
1	C	215	ASP	2.0
1	C	189	ASN	2.0
1	D	15	GLY	2.0
1	C	381	LYS	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PO4	B	390	5/5	0.94	0.19	2.98	55,62,63,64	0
3	CL	A	405	1/1	0.99	0.17	0.96	23,23,23,23	0
2	FAD	D	400	53/53	0.96	0.20	0.61	20,28,36,38	0
2	FAD	B	400	53/53	0.96	0.18	0.22	22,29,37,39	0
2	FAD	A	400	53/53	0.98	0.17	0.22	13,20,25,27	0
2	FAD	C	400	53/53	0.95	0.17	0.21	23,32,44,46	0
4	PO4	D	390	5/5	0.97	0.09	-0.35	38,44,45,46	0
3	CL	B	405	1/1	0.99	0.13	-0.44	35,35,35,35	0
3	CL	C	405	1/1	0.99	0.10	-0.68	31,31,31,31	0
3	CL	D	405	1/1	0.99	0.14	-0.81	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.