



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 AM GMT

PDB ID : 2E1M
Title : Crystal Structure of L-Glutamate Oxidase from Streptomyces sp. X-119-6
Authors : Sasaki, C.; Kashima, A.; Sakaguchi, C.; Mizuno, H.; Arima, J.; Kusakabe, H.;
Tamura, T.; Sugio, S.; Inagaki, K.
Deposited on : 2006-10-26
Resolution : 2.80 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

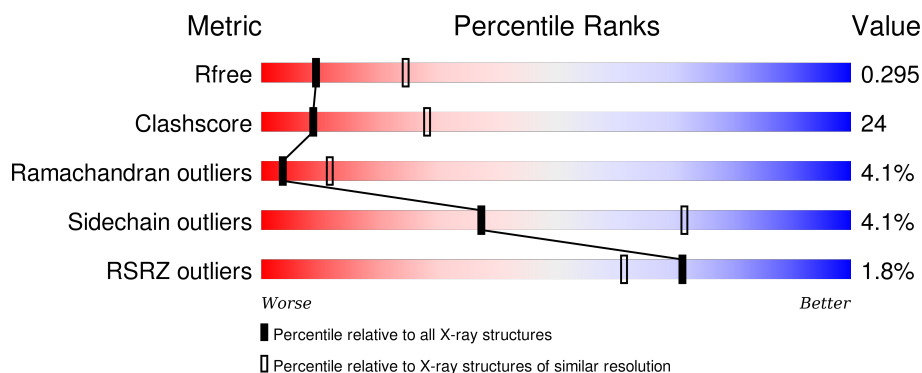
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	376	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>5%</div> <div>5%</div> </div> </div>
2	B	130	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>28%</div> <div>•</div> <div>31%</div> </div> </div>
3	C	181	<div> <div></div> <div> <div>54%</div> <div>25%</div> <div>•</div> <div>17%</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	A	902	-	-	-	X
4	PO4	A	903	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4807 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 L-glutamate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2818	1786	497	526	9			

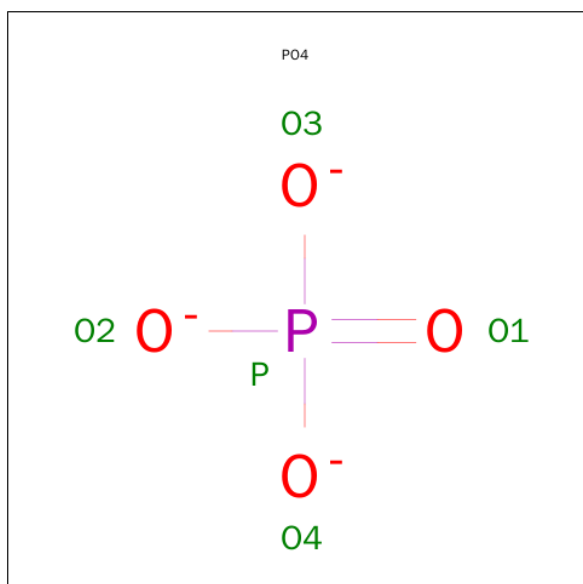
- Molecule 2 is a protein called L-glutamate oxidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	0	0	0
			751	488	124	139			

- Molecule 3 is a protein called L-glutamate oxidase.

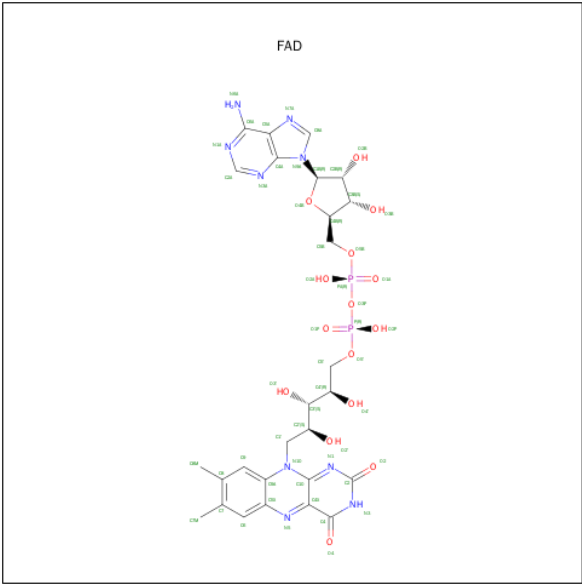
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	0
			1170	740	205	222	3			

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



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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

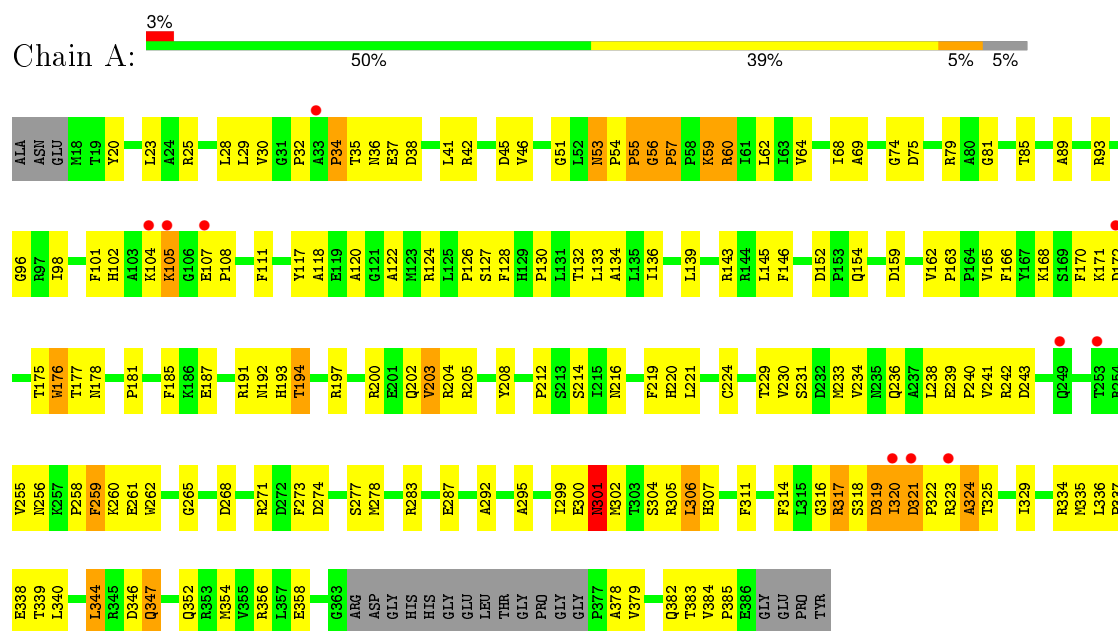


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O P	0	0
			53	27	9	15 2		

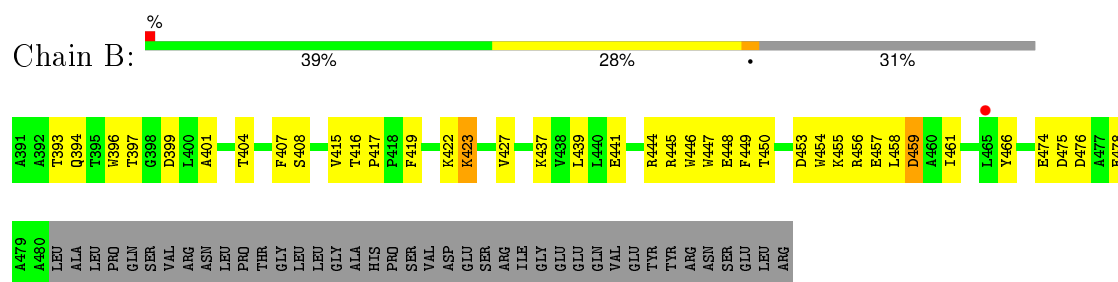
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

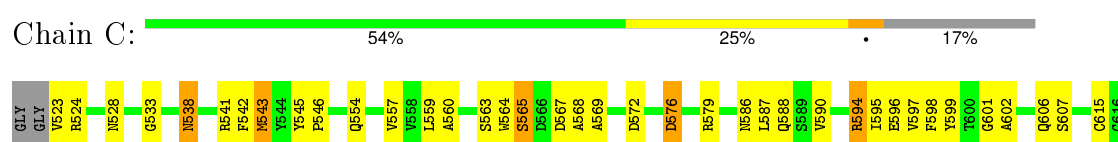
• Molecule 1: L-glutamate oxidase



• Molecule 2: L-glutamate oxidase



• Molecule 3: L-glutamate oxidase



E617 H624 T627 A628 F629 D632 V633 W634 E645 H646 K650 R651 A652 W653 R663 I666 A671 P672 V673 GLY ASP THR THR GLY VAL VAL THR ALA ALA ALA ALA ALA GLY ARG ARG ARG GLU PRO MET ANG ANS CYS GLN GLU ALA LEU THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.88Å 123.88Å 168.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.27 – 2.80 49.82 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.27-2.80) 99.9 (49.82-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.308 0.238 , 0.295	Depositor DCC
R_{free} test set	951 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24333 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4807	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 3.12% 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

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	0.38	0/2887	0.69	1/3918 (0.0%)
2	B	0.42	0/775	0.67	0/1057
3	C	0.41	0/1208	0.68	0/1655
All	All	0.39	0/4870	0.68	1/6630 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	277	SER	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2818	0	2770	167	0
2	B	751	0	714	41	0
3	C	1170	0	1079	52	0
4	A	15	0	0	4	0
5	A	53	0	31	7	0
All	All	4807	0	4594	221	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (221) 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:347:GLN:N	1:A:347:GLN:HE21	1.39	1.18
1:A:304:SER:HB2	3:C:565:SER:HB3	1.31	1.10
1:A:216:ASN:HB3	1:A:221:LEU:HD12	1.52	0.89
1:A:53:ASN:O	1:A:55:PRO:HD3	1.72	0.88
1:A:192:ASN:HB3	1:A:205:ARG:HB2	1.57	0.85
1:A:347:GLN:N	1:A:347:GLN:NE2	2.22	0.84
1:A:347:GLN:HE21	1:A:347:GLN:H	1.26	0.82
1:A:212:PRO:HB2	1:A:216:ASN:HD21	1.41	0.82
1:A:321:ASP:HB3	1:A:324:ALA:HB2	1.59	0.81
1:A:323:ARG:HH11	1:A:323:ARG:HB2	1.46	0.79
1:A:238:LEU:HB2	1:A:242:ARG:HH12	1.50	0.76
1:A:238:LEU:HB2	1:A:242:ARG:NH1	2.01	0.74
1:A:212:PRO:HB2	1:A:216:ASN:ND2	2.04	0.73
1:A:274:ASP:OD2	3:C:627:THR:HG23	1.89	0.72
1:A:321:ASP:CB	1:A:324:ALA:HB2	2.18	0.72
2:B:437:LYS:HG2	3:C:559:LEU:HD11	1.71	0.72
1:A:256:ASN:HB3	1:A:262:TRP:CD1	2.26	0.71
1:A:53:ASN:HB3	1:A:54:PRO:HD3	1.72	0.70
1:A:358:GLU:HG3	2:B:416:THR:HG23	1.73	0.69
1:A:347:GLN:H	1:A:347:GLN:NE2	1.89	0.67
5:A:801:FAD:H5'2	3:C:645:GLU:HB2	1.76	0.67
1:A:323:ARG:NH1	1:A:323:ARG:HB2	2.10	0.67
1:A:260:LYS:HE2	1:A:261:GLU:OE2	1.96	0.66
2:B:445:ARG:HG2	2:B:447:TRP:CZ2	2.29	0.66
1:A:30:VAL:HG22	1:A:170:PHE:CZ	2.31	0.66
1:A:221:LEU:HD21	1:A:292:ALA:HA	1.78	0.65
1:A:194:THR:OG1	1:A:205:ARG:HD2	1.97	0.65
3:C:634:VAL:HG11	3:C:663:ARG:NH2	2.11	0.65
1:A:352:GLN:NE2	1:A:383:THR:OG1	2.30	0.65
1:A:301:ASN:HD22	1:A:301:ASN:C	2.01	0.63
1:A:60:ARG:HH12	1:A:85:THR:CB	2.12	0.63
1:A:323:ARG:O	1:A:323:ARG:HG2	1.99	0.62
3:C:650:LYS:O	3:C:653:TRP:HB2	1.99	0.62
1:A:166:PHE:HE2	1:A:168:LYS:HG3	1.64	0.62
1:A:53:ASN:HB3	1:A:54:PRO:CD	2.30	0.62
1:A:120:ALA:HB1	3:C:606:GLN:HG2	1.81	0.61
1:A:122:ALA:HA	5:A:801:FAD:C4X	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:MET:HA	1:A:383:THR:HG22	1.82	0.61
1:A:384:VAL:HG13	1:A:385:PRO:HD2	1.82	0.61
1:A:166:PHE:CE2	1:A:168:LYS:HG3	2.36	0.61
1:A:229:THR:O	1:A:233:MET:HG3	2.01	0.61
1:A:134:ALA:HA	1:A:178:ASN:HD21	1.64	0.61
1:A:230:VAL:HG21	1:A:299:ILE:HB	1.82	0.60
3:C:533:GLY:HA2	3:C:545:TYR:CE1	2.36	0.60
1:A:46:VAL:O	1:A:51:GLY:HA2	2.02	0.60
1:A:242:ARG:HH21	1:A:317:ARG:HD2	1.66	0.60
1:A:192:ASN:HB3	1:A:205:ARG:CB	2.28	0.60
1:A:329:ILE:HG21	1:A:335:MET:HB2	1.84	0.60
1:A:356:ARG:HB3	1:A:382:GLN:HB3	1.84	0.60
1:A:283:ARG:O	1:A:287:GLU:HA	2.01	0.59
1:A:102:HIS:CE1	1:A:334:ARG:HD3	2.37	0.59
1:A:136:ILE:HG12	1:A:336:LEU:HD13	1.85	0.59
1:A:166:PHE:CD1	1:A:177:THR:HG22	2.37	0.59
1:A:136:ILE:CD1	1:A:329:ILE:HD11	2.32	0.58
1:A:300:GLU:O	1:A:302:MET:HG3	2.03	0.58
1:A:200:ARG:HD3	2:B:478:GLU:OE2	2.03	0.58
1:A:136:ILE:HD13	1:A:329:ILE:HD11	1.86	0.58
1:A:305:ARG:NE	3:C:564:TRP:CE3	2.72	0.58
1:A:316:GLY:O	1:A:317:ARG:C	2.42	0.57
1:A:122:ALA:HA	5:A:801:FAD:N5	2.18	0.57
1:A:154:GLN:HE21	1:A:154:GLN:HA	1.69	0.57
1:A:301:ASN:HB2	3:C:542:PHE:CE1	2.40	0.57
1:A:154:GLN:NE2	1:A:154:GLN:HA	2.20	0.57
1:A:36:ASN:O	1:A:171:LYS:HE2	2.04	0.57
1:A:53:ASN:CB	1:A:54:PRO:CD	2.83	0.56
1:A:133:LEU:HB3	1:A:165:VAL:HG22	1.88	0.56
2:B:408:SER:OG	3:C:615:CYS:HB2	2.05	0.56
2:B:474:GLU:CG	3:C:523:VAL:HA	2.35	0.55
1:A:301:ASN:H	3:C:542:PHE:HZ	1.54	0.55
1:A:203:VAL:HG23	1:A:204:ARG:O	2.07	0.55
1:A:111:PHE:HB3	2:B:441:GLU:CD	2.27	0.54
1:A:301:ASN:HB2	3:C:542:PHE:CZ	2.43	0.54
1:A:37:GLU:OE1	1:A:42:ARG:NH2	2.40	0.54
2:B:449:PHE:CZ	2:B:457:GLU:HG2	2.42	0.54
1:A:274:ASP:OD2	3:C:624:HIS:HA	2.07	0.54
3:C:563:SER:O	3:C:568:ALA:HB2	2.08	0.54
1:A:28:LEU:HD22	1:A:262:TRP:CZ2	2.42	0.54
1:A:197:ARG:HD3	3:C:590:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HH22	4:A:903:PO4:P	2.30	0.53
1:A:133:LEU:HB3	1:A:165:VAL:CG2	2.39	0.53
1:A:346:ASP:C	1:A:347:GLN:HE21	2.06	0.53
2:B:450:THR:H	2:B:453:ASP:HB2	1.73	0.53
3:C:579:ARG:HH12	3:C:607:SER:HB2	1.73	0.52
1:A:241:VAL:HG22	1:A:273:PHE:CZ	2.45	0.52
1:A:208:TYR:CD1	1:A:212:PRO:HA	2.44	0.52
1:A:305:ARG:O	1:A:307:HIS:N	2.43	0.52
2:B:454:TRP:CZ2	3:C:594:ARG:HD3	2.45	0.52
1:A:25:ARG:HH11	1:A:30:VAL:CG1	2.22	0.52
1:A:93:ARG:NH2	1:A:96:GLY:O	2.42	0.52
2:B:475:ASP:OD2	2:B:476:ASP:N	2.43	0.52
1:A:111:PHE:HB3	2:B:441:GLU:OE2	2.11	0.51
1:A:32:PRO:C	1:A:34:PRO:HD2	2.30	0.51
1:A:162:VAL:HG12	1:A:163:PRO:O	2.09	0.51
1:A:25:ARG:HH11	1:A:30:VAL:HG12	1.75	0.51
1:A:165:VAL:HG23	1:A:178:ASN:HD22	1.74	0.51
1:A:68:ILE:HG23	1:A:69:ALA:N	2.25	0.51
1:A:28:LEU:O	1:A:29:LEU:HB2	2.10	0.51
2:B:454:TRP:O	2:B:458:LEU:HB2	2.11	0.51
1:A:55:PRO:O	1:A:56:GLY:O	2.29	0.51
1:A:152:ASP:HA	1:A:191:ARG:HD2	1.93	0.51
1:A:57:PRO:HG2	1:A:59:LYS:NZ	2.26	0.50
2:B:474:GLU:OE2	3:C:524:ARG:N	2.35	0.50
1:A:93:ARG:NH1	4:A:901:PO4:O3	2.44	0.50
1:A:42:ARG:O	1:A:45:ASP:HB3	2.11	0.50
1:A:278:MET:HG2	1:A:302:MET:HE3	1.93	0.50
1:A:268:ASP:HA	1:A:271:ARG:NH1	2.26	0.50
1:A:314:PHE:O	1:A:317:ARG:HB2	2.11	0.50
1:A:145:LEU:HD21	1:A:187:GLU:HB3	1.93	0.50
1:A:46:VAL:HG21	3:C:666:ILE:HD11	1.93	0.49
1:A:334:ARG:HD2	1:A:338:GLU:OE2	2.12	0.49
2:B:423:LYS:NZ	3:C:632:ASP:O	2.37	0.49
1:A:334:ARG:HG3	1:A:335:MET:N	2.28	0.49
1:A:265:GLY:O	1:A:268:ASP:HB2	2.13	0.49
1:A:378:ALA:HB3	2:B:399:ASP:HA	1.94	0.49
1:A:127:SER:HB3	1:A:325:THR:H	1.78	0.49
1:A:197:ARG:NH2	2:B:478:GLU:OE2	2.45	0.49
3:C:646:HIS:HA	3:C:651:HIS:CD2	2.47	0.48
1:A:38:ASP:OD2	1:A:41:LEU:HG	2.13	0.48
3:C:524:ARG:HH11	3:C:524:ARG:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HH11	1:A:323:ARG:CB	2.20	0.48
1:A:128:PHE:C	1:A:130:PRO:HD3	2.33	0.48
1:A:320:ILE:O	1:A:322:PRO:HD3	2.14	0.48
1:A:302:MET:O	1:A:306:LEU:HD13	2.13	0.48
2:B:394:GLN:HG2	2:B:396:TRP:CH2	2.49	0.47
1:A:383:THR:HG1	2:B:396:TRP:HZ3	1.62	0.47
2:B:407:PHE:CD1	2:B:427:VAL:HG22	2.49	0.47
1:A:42:ARG:O	1:A:46:VAL:HG23	2.15	0.47
3:C:533:GLY:HA2	3:C:545:TYR:CD1	2.48	0.47
1:A:255:VAL:HG13	1:A:255:VAL:O	2.15	0.47
1:A:139:LEU:HD11	1:A:340:LEU:HD21	1.97	0.47
1:A:54:PRO:O	1:A:56:GLY:N	2.48	0.47
2:B:446:TRP:CE3	2:B:447:TRP:N	2.83	0.47
1:A:89:ALA:HB2	5:A:801:FAD:C2A	2.45	0.47
1:A:301:ASN:ND2	1:A:301:ASN:C	2.68	0.46
2:B:444:ARG:HA	3:C:554:GLN:O	2.15	0.46
3:C:538:ASN:OD1	3:C:586:ASN:HB3	2.16	0.46
1:A:384:VAL:CG1	1:A:385:PRO:HD2	2.45	0.46
1:A:268:ASP:HA	1:A:271:ARG:HH12	1.81	0.46
1:A:139:LEU:HD22	1:A:339:THR:HG22	1.98	0.46
1:A:166:PHE:CE2	1:A:168:LYS:HE2	2.51	0.46
1:A:268:ASP:OD1	1:A:271:ARG:NH1	2.45	0.46
1:A:319:ASP:O	1:A:321:ASP:N	2.48	0.46
1:A:334:ARG:O	1:A:337:PRO:HD2	2.16	0.46
1:A:175:THR:O	1:A:176:TRP:HB2	2.15	0.46
2:B:461:ILE:HD11	3:C:598:PHE:HE2	1.81	0.46
1:A:104:LYS:O	1:A:105:LYS:C	2.54	0.46
1:A:126:PRO:HB3	1:A:128:PHE:CE2	2.51	0.46
1:A:107:GLU:HB2	1:A:108:PRO:CD	2.46	0.46
1:A:132:THR:O	1:A:136:ILE:HG13	2.16	0.45
1:A:197:ARG:HH11	1:A:202:GLN:HB2	1.81	0.45
1:A:42:ARG:HD3	3:C:666:ILE:HD13	1.97	0.45
1:A:239:GLU:N	1:A:240:PRO:HD2	2.32	0.45
3:C:597:VAL:HG23	3:C:598:PHE:N	2.31	0.45
1:A:242:ARG:NH2	1:A:319:ASP:OD2	2.49	0.45
2:B:393:THR:OG1	2:B:394:GLN:N	2.49	0.45
1:A:166:PHE:HE2	1:A:168:LYS:HE2	1.82	0.45
1:A:35:THR:O	1:A:36:ASN:HB2	2.17	0.45
1:A:20:TYR:CZ	1:A:271:ARG:HG3	2.51	0.45
1:A:107:GLU:HB2	1:A:108:PRO:HD2	1.99	0.45
1:A:219:PHE:O	1:A:220:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LYS:HD3	2:B:422:LYS:HA	1.79	0.45
1:A:307:HIS:HA	4:A:903:PO4:O4	2.17	0.45
2:B:458:LEU:HD23	2:B:466:TYR:HA	2.00	0.44
1:A:379:VAL:O	2:B:397:THR:HA	2.16	0.44
1:A:378:ALA:HB3	2:B:399:ASP:O	2.16	0.44
1:A:62:LEU:O	2:B:401:ALA:HA	2.17	0.44
1:A:101:PHE:O	1:A:117:TYR:HB2	2.17	0.44
1:A:242:ARG:NH2	1:A:317:ARG:HD2	2.30	0.44
1:A:64:VAL:O	2:B:404:THR:OG1	2.29	0.44
1:A:274:ASP:CG	3:C:627:THR:HG23	2.38	0.44
1:A:231:SER:O	1:A:234:VAL:N	2.49	0.44
3:C:569:ALA:O	3:C:572:ASP:HB2	2.18	0.44
1:A:230:VAL:O	1:A:234:VAL:HG23	2.18	0.44
2:B:394:GLN:HB3	2:B:396:TRP:CZ3	2.53	0.43
1:A:197:ARG:HD2	1:A:202:GLN:OE1	2.18	0.43
1:A:240:PRO:O	1:A:243:ASP:HB2	2.18	0.43
1:A:314:PHE:O	1:A:317:ARG:CB	2.66	0.43
1:A:321:ASP:HB2	1:A:324:ALA:HB2	1.99	0.43
5:A:801:FAD:H5'2	3:C:645:GLU:CB	2.45	0.43
2:B:454:TRP:CH2	3:C:594:ARG:HD3	2.54	0.43
1:A:283:ARG:NH2	4:A:903:PO4:O2	2.51	0.43
1:A:317:ARG:HE	1:A:317:ARG:HB3	1.69	0.43
1:A:197:ARG:HG3	1:A:202:GLN:HB2	2.01	0.43
3:C:563:SER:HB2	3:C:567:ASP:CB	2.49	0.43
1:A:96:GLY:C	1:A:98:ILE:H	2.22	0.43
1:A:59:LYS:NZ	3:C:671:ALA:O	2.36	0.43
3:C:588:GLN:NE2	3:C:596:GLU:HB3	2.34	0.43
1:A:242:ARG:HE	1:A:317:ARG:HH11	1.66	0.43
5:A:801:FAD:HM83	3:C:617:GLU:HG3	2.01	0.43
2:B:461:ILE:HD11	3:C:598:PHE:CE2	2.53	0.43
1:A:258:PRO:O	1:A:259:PHE:C	2.56	0.43
1:A:23:LEU:HD11	3:C:627:THR:HA	2.01	0.43
1:A:118:ALA:HB1	2:B:439:LEU:HD22	2.01	0.42
1:A:74:GLY:O	1:A:344:LEU:HD21	2.19	0.42
1:A:75:ASP:HA	1:A:344:LEU:HD21	2.02	0.42
3:C:543:MET:HG2	3:C:560:ALA:O	2.19	0.42
2:B:416:THR:HA	2:B:417:PRO:C	2.37	0.41
1:A:295:ALA:O	1:A:299:ILE:HG12	2.20	0.41
3:C:599:TYR:CE2	3:C:601:GLY:HA2	2.55	0.41
2:B:455:LYS:O	2:B:459:ASP:HB2	2.20	0.41
3:C:546:PRO:HG3	3:C:557:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.85	0.41
3:C:671:ALA:HA	3:C:672:PRO:HD3	1.90	0.41
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.72	0.41
2:B:456:ARG:HG2	2:B:457:GLU:N	2.35	0.41
3:C:543:MET:CE	3:C:587:LEU:HD12	2.50	0.41
1:A:205:ARG:HG2	1:A:205:ARG:HH11	1.85	0.41
1:A:205:ARG:NH1	1:A:205:ARG:HG2	2.36	0.41
5:A:801:FAD:HM83	3:C:617:GLU:CG	2.51	0.41
3:C:543:MET:HE2	3:C:587:LEU:HD12	2.03	0.41
1:A:124:ARG:HD3	1:A:146:PHE:CE2	2.55	0.41
2:B:415:VAL:HG11	2:B:419:PHE:CE2	2.56	0.41
1:A:163:PRO:HD3	1:A:185:PHE:CG	2.56	0.41
1:A:38:ASP:HB3	1:A:41:LEU:HD12	2.03	0.41
3:C:588:GLN:HG3	3:C:595:ILE:HD11	2.03	0.40
2:B:441:GLU:OE2	3:C:602:ALA:HB3	2.21	0.40
2:B:448:GLU:O	3:C:528:ASN:ND2	2.54	0.40
2:B:474:GLU:OE2	3:C:523:VAL:HA	2.21	0.40
1:A:143:ARG:NH1	1:A:162:VAL:HG11	2.36	0.40
1:A:68:ILE:CG2	1:A:69:ALA:N	2.85	0.40
3:C:634:VAL:HG11	3:C:663:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	352/376 (94%)	297 (84%)	35 (10%)	20 (6%)	2	6
2	B	88/130 (68%)	80 (91%)	8 (9%)	0	100	100
3	C	149/181 (82%)	129 (87%)	16 (11%)	4 (3%)	6	21
All	All	589/687 (86%)	506 (86%)	59 (10%)	24 (4%)	3	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	172	ASP
1	A	259	PHE
1	A	306	LEU
1	A	320	ILE
1	A	56	GLY
1	A	301	ASN
1	A	319	ASP
1	A	34	PRO
1	A	214	SER
1	A	317	ARG
3	C	541	ARG
3	C	576	ASP
3	C	645	GLU
1	A	55	PRO
1	A	57	PRO
1	A	105	LYS
1	A	176	TRP
1	A	318	SER
1	A	324	ALA
1	A	344	LEU
3	C	565	SER
1	A	81	GLY
1	A	181	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/311 (96%)	286 (96%)	12 (4%)	38	73
2	B	76/111 (68%)	74 (97%)	2 (3%)	54	86
3	C	116/132 (88%)	110 (95%)	6 (5%)	29	62
All	All	490/554 (88%)	470 (96%)	20 (4%)	37	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	60	ARG
1	A	159	ASP
1	A	193	HIS
1	A	194	THR
1	A	203	VAL
1	A	224	CYS
1	A	236	GLN
1	A	301	ASN
1	A	311	PHE
1	A	321	ASP
1	A	347	GLN
2	B	423	LYS
2	B	459	ASP
3	C	538	ASN
3	C	543	MET
3	C	576	ASP
3	C	594	ARG
3	C	627	THR
3	C	629	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	50	ASN
1	A	154	GLN
1	A	158	GLN
1	A	178	ASN
1	A	216	ASN
1	A	236	GLN
1	A	301	ASN
1	A	347	GLN
1	A	352	GLN
1	A	382	GLN
2	B	471	GLN
3	C	586	ASN
3	C	630	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
5	FAD	A	801	-	48,58,58	2.45	17 (35%)	54,89,89	2.03	12 (22%)
4	PO4	A	901	-	4,4,4	1.70	0	6,6,6	0.28	0
4	PO4	A	902	-	4,4,4	1.56	0	6,6,6	0.28	0
4	PO4	A	903	-	4,4,4	1.69	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	801	-	-	0/30/50/50	0/6/6/6
4	PO4	A	901	-	-	0/0/0/0	0/0/0/0
4	PO4	A	902	-	-	0/0/0/0	0/0/0/0
4	PO4	A	903	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	FAD	PA-O2A	-4.04	1.37	1.54
5	A	801	FAD	P-O2P	-3.15	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	FAD	C10-N1	2.36	1.39	1.35
5	A	801	FAD	C9A-C5X	2.48	1.47	1.42
5	A	801	FAD	C2A-N1A	2.65	1.38	1.33
5	A	801	FAD	C2A-N3A	2.69	1.37	1.32
5	A	801	FAD	C1'-N10	2.81	1.51	1.48
5	A	801	FAD	C4X-N5	3.26	1.38	1.33
5	A	801	FAD	C5X-N5	3.27	1.40	1.35
5	A	801	FAD	C4A-N3A	3.28	1.40	1.35
5	A	801	FAD	O5'-C5'	3.36	1.58	1.44
5	A	801	FAD	C8-C7	3.56	1.50	1.41
5	A	801	FAD	C4-C4X	3.82	1.48	1.41
5	A	801	FAD	C4-N3	4.21	1.40	1.33
5	A	801	FAD	C4X-C10	5.09	1.50	1.41
5	A	801	FAD	O4B-C1B	5.88	1.48	1.41
5	A	801	FAD	C9A-N10	6.76	1.48	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	FAD	C4X-C4-N3	-4.75	117.10	123.59
5	A	801	FAD	C4-C4X-C10	-4.57	117.01	119.94
5	A	801	FAD	N3A-C2A-N1A	-4.47	125.47	128.89
5	A	801	FAD	O4B-C1B-N9A	-3.29	101.20	108.10
5	A	801	FAD	C4X-C10-N10	-2.79	118.88	120.52
5	A	801	FAD	O5'-P-O1P	-2.26	100.85	109.62
5	A	801	FAD	C4-C4X-N5	2.01	121.15	118.72
5	A	801	FAD	O4'-C4'-C3'	2.18	114.50	109.02
5	A	801	FAD	C2B-C1B-N9A	2.25	117.73	114.29
5	A	801	FAD	C2A-N1A-C6A	2.55	123.32	118.77
5	A	801	FAD	O3P-P-O5'	3.09	111.14	102.94
5	A	801	FAD	C4-N3-C2	8.10	122.25	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	FAD	7	0
4	A	901	PO4	1	0
4	A	903	PO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	356/376 (94%)	-0.06	10 (2%) 56 44	16, 36, 59, 77	0
2	B	90/130 (69%)	-0.06	1 (1%) 82 74	10, 29, 57, 59	0
3	C	151/181 (83%)	-0.20	0 100 100	8, 26, 50, 58	0
All	All	597/687 (86%)	-0.10	11 (1%) 71 61	8, 32, 57, 77	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ARG	2.9
1	A	320	ILE	2.7
1	A	107	GLU	2.7
1	A	104	LYS	2.7
1	A	253	THR	2.6
1	A	249	GLN	2.4
1	A	105	LYS	2.4
1	A	33	ALA	2.2
1	A	321	ASP	2.1
1	A	172	ASP	2.0
2	B	465	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PO4	A	902	5/5	0.79	0.22	2.62	61,62,63,63	0
5	FAD	A	801	53/53	0.96	0.19	0.10	8,20,30,32	0
4	PO4	A	901	5/5	0.96	0.17	-0.20	56,56,57,58	0
4	PO4	A	903	5/5	0.94	0.16	-0.61	67,67,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.