Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RGO
Title	:	Structure of Alpha-Glycerophosphate Oxidase from Streptococcus sp.: A Template for the Mitochondrial Alpha-Glycerophosphate Dehydrogenase
Authors	:	Colussi, T.; Boles, W.; Mallett, T.C.; Karplus, P.A.; Claiborne, A.
Deposited on	:	2007-10-04
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

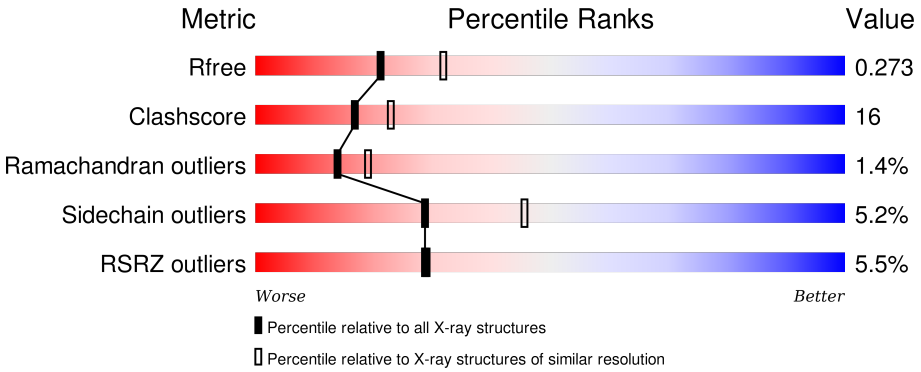
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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 <=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	607	2% 73% 16% • 8%
1	B	607	8% 50% 34% • 13%

2 Entry composition

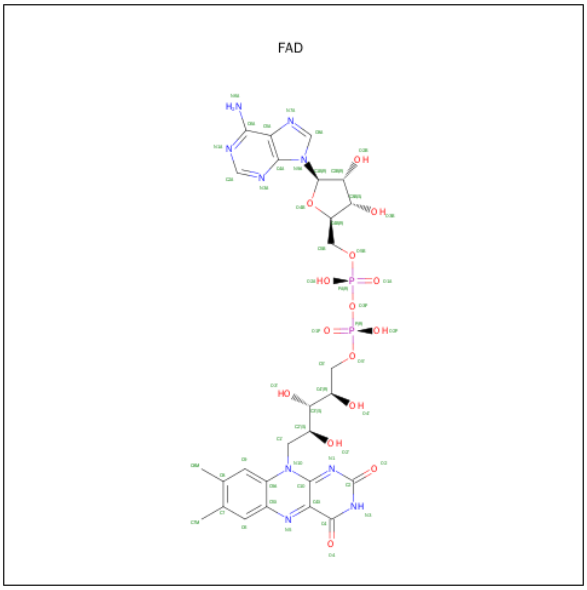
There are 3 unique types of molecules in this entry. The entry contains 8862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-Glycerophosphate Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4361	2759	733	858	11			
1	B	530	Total	C	N	O	S	0	0	0
			4163	2640	701	811	11			

- 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		

- Molecule 3 is water.

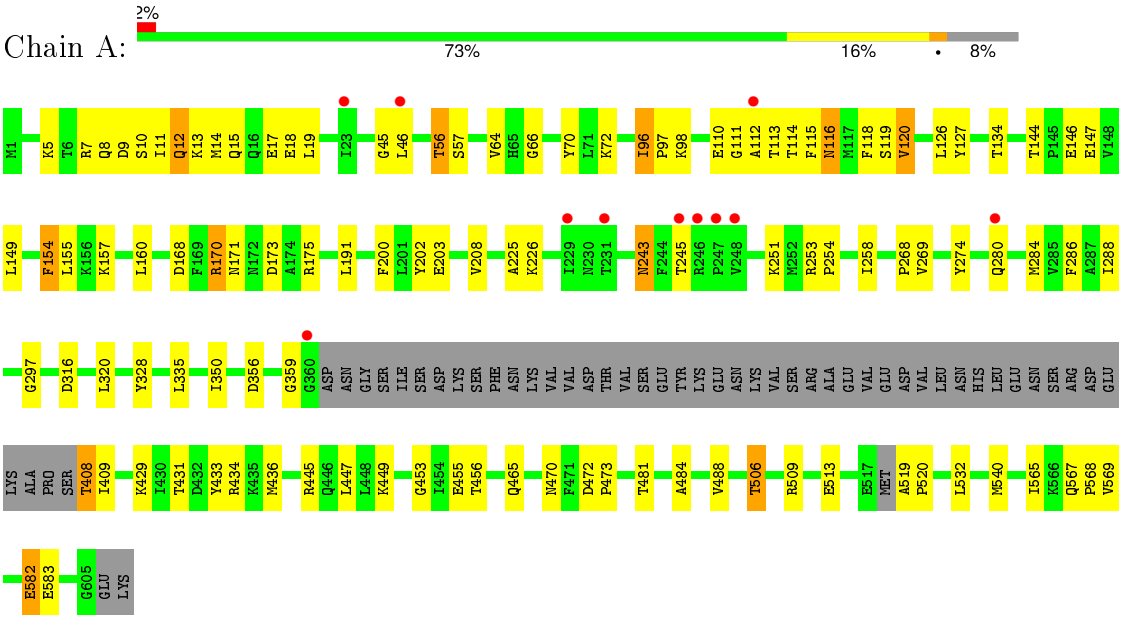
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	183	Total O 183 183	0	0
3	B	49	Total O 49 49	0	0

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 (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.

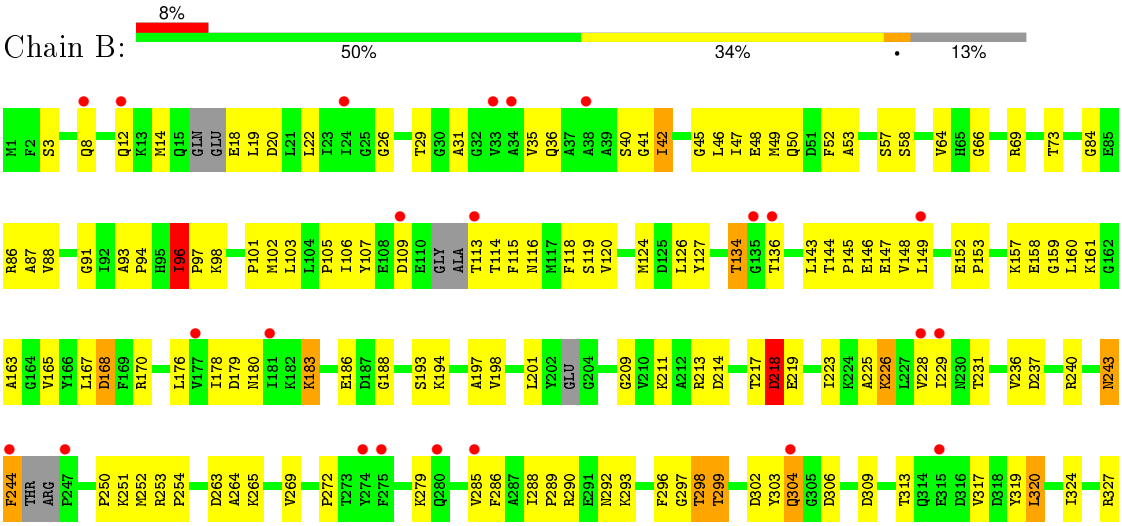
- Molecule 1: Alpha-Glycerophosphate Oxidase

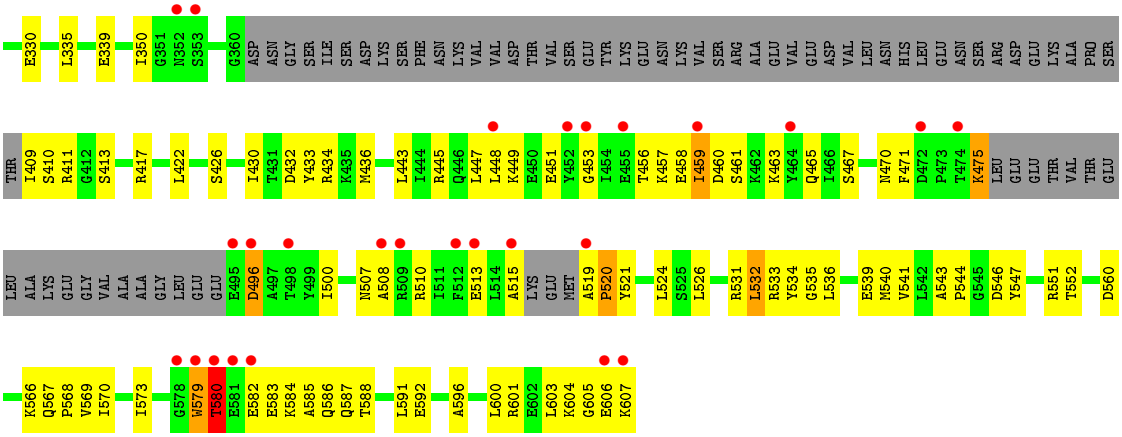
Chain A:



- Molecule 1: Alpha-Glycerophosphate Oxidase

Chain B:




E330 L335 E339 I350 G351 N352 S353 G360
ASP ASN GLY SER ILE SER ASP LYS SER PHE ASN LYS VAL VAL ASP THR VAL SER GLU TYR LYS GLU ASN LYS VAL SER ARG ALA GLU VAL GLU ASP VAL LEU ASN HIS LEU GLU ASN SER ARG ASP GLU LYS ALA PRO SER
THR I409 S410 R411 G412 S413 R417 L422 S426 I430 T431 D432 Y433 R434 K435 M436 L443 I444 R445 Q446 L447 L448 K449 E450 E451 Y452 G453 I454 E455 T456 K457 E458 I459 D460 S461 K462 K463 Y464 Q465 I466 S467 N470 F471 D472 P473 T474 K475 LEU GLU GLU THR VAL THR GLU
LEU ALA LYS GLU GLY VAL ALA ALA GLY LEU GLU GLU E495 D496 A497 T498 Y499 I500 N507 A508 R509 R510 I511 F512 E513 L514 A515 LYS GLU MET A519 P520 Y521 L524 S525 L526 R531 L532 R533 Y534 G535 L536 E539 M540 V541 L542 A543 P544 G545 D546 Y547 R551 T552 D560
K566 Q567 P568 V569 I570 I573 G578 W579 T580 E581 E582 E583 K584 A585 Q586 Q587 T588 L591 E592 A596 L600 R601 E602 L603 K604 G605 E606 K607

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.36Å 106.78Å 58.89Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40 29.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (12.00-2.40) 94.4 (29.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.238 , 0.247 0.229 , 0.273	Depositor DCC
R_{free} test set	2876 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 72.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 57943 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8862	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	0/4434	0.79	0/5991
1	B	0.48	0/4231	0.66	0/5706
All	All	0.59	0/8665	0.73	0/11697

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	GLY	Peptide
1	A	328	TYR	Mainchain
1	B	297	GLY	Peptide
1	B	298	THR	Peptide

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	4361	0	4361	85	0
1	B	4163	0	4167	196	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0
3	A	183	0	0	3	0
3	B	49	0	0	2	0
All	All	8862	0	8590	282	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 16.

All (282) 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:B:144:THR:HG22	1:B:147:GLU:HG2	1.15	1.13
1:B:109:ASP:OD2	1:B:159:GLY:HA3	1.70	0.90
1:A:449:LYS:HE2	1:A:455:GLU:HG2	1.53	0.89
1:B:46:LEU:HD23	1:B:47:ILE:N	1.90	0.87
1:B:471:PHE:HE1	1:B:475:LYS:HG2	1.44	0.83
1:B:579:TRP:O	1:B:580:THR:HG23	1.78	0.83
1:B:22:LEU:HD12	1:B:45:GLY:O	1.78	0.82
1:B:144:THR:HG22	1:B:147:GLU:CG	2.05	0.81
1:B:3:SER:HB3	1:B:536:LEU:O	1.79	0.80
1:B:460:ASP:OD2	1:B:463:LYS:HB2	1.82	0.79
1:B:566:LYS:O	1:B:569:VAL:HG12	1.82	0.79
1:B:20:ASP:HA	1:B:226:LYS:HD3	1.66	0.77
1:B:228:VAL:O	1:B:422:LEU:HD12	1.84	0.77
1:B:116:ASN:HD22	1:B:118:PHE:H	1.32	0.77
1:A:116:ASN:HD22	1:A:118:PHE:H	1.35	0.74
1:A:203:GLU:HG3	1:A:203:GLU:O	1.86	0.73
1:A:98:LYS:HG3	1:A:170:ARG:NH1	2.03	0.72
1:B:144:THR:CG2	1:B:147:GLU:HG2	2.09	0.72
1:B:14:MET:HE1	1:B:223:ILE:HD12	1.72	0.71
1:B:410:SER:HB3	1:B:413:SER:OG	1.90	0.71
1:B:544:PRO:HG2	1:B:591:LEU:HD21	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HB	1:B:97:PRO:CD	2.21	0.69
1:B:47:ILE:HD11	1:B:197:ALA:HB2	1.73	0.69
1:B:73:THR:HG22	1:B:73:THR:O	1.93	0.69
1:B:243:ASN:HD22	1:B:243:ASN:C	1.95	0.68
1:A:251:LYS:O	1:A:350:ILE:HG13	1.94	0.68
1:B:115:PHE:HB3	1:B:120:VAL:HG13	1.76	0.68
1:B:31:ALA:O	1:B:35:VAL:HG23	1.93	0.68
1:B:443:LEU:O	1:B:443:LEU:HG	1.94	0.67
1:A:116:ASN:HD22	1:A:118:PHE:N	1.92	0.67
1:B:515:ALA:O	1:B:526:LEU:HD11	1.94	0.67
1:B:269:VAL:O	1:B:269:VAL:HG23	1.94	0.66
1:B:584:LYS:C	1:B:584:LYS:HD3	2.16	0.66
1:B:106:ILE:HD11	1:B:120:VAL:HG11	1.79	0.65
1:B:584:LYS:HD3	1:B:585:ALA:N	2.11	0.65
1:A:116:ASN:ND2	1:A:118:PHE:H	1.95	0.65
1:B:103:LEU:HD12	1:B:165:VAL:HG22	1.78	0.64
1:B:532:LEU:HD11	1:B:569:VAL:HG23	1.79	0.64
1:B:298:THR:OG1	1:B:299:THR:N	2.31	0.64
1:B:47:ILE:O	1:B:47:ILE:HG13	1.98	0.64
1:B:14:MET:CE	1:B:223:ILE:HD12	2.28	0.64
1:B:237:ASP:OD1	1:B:240:ARG:NH1	2.31	0.63
1:B:510:ARG:HH21	1:B:513:GLU:HB2	1.63	0.63
1:A:243:ASN:HD22	1:A:243:ASN:C	2.02	0.63
1:B:14:MET:HG2	1:B:19:LEU:HD11	1.81	0.63
1:B:335:LEU:O	1:B:335:LEU:HD23	1.99	0.63
1:B:532:LEU:HD21	1:B:573:ILE:HD11	1.81	0.62
1:A:116:ASN:ND2	1:A:119:SER:H	1.98	0.62
1:A:203:GLU:HG2	1:A:208:VAL:HG11	1.82	0.62
1:A:509:ARG:O	1:A:513:GLU:HG3	2.00	0.62
1:B:579:TRP:CG	1:B:583:GLU:HG2	2.34	0.61
1:B:569:VAL:O	1:B:573:ILE:HG12	2.00	0.61
1:B:471:PHE:CE1	1:B:475:LYS:HG2	2.32	0.61
1:A:445:ARG:HD3	1:A:456:THR:OG1	2.00	0.61
1:B:40:SER:OG	1:B:459:ILE:HG12	2.00	0.61
1:A:258:ILE:HD13	1:A:316:ASP:HB3	1.82	0.61
1:B:217:THR:O	1:B:219:GLU:N	2.31	0.61
1:A:116:ASN:HD21	1:A:118:PHE:HB3	1.66	0.61
1:A:98:LYS:HG3	1:A:170:ARG:HH12	1.65	0.60
1:B:19:LEU:O	1:B:225:ALA:HA	2.00	0.60
1:A:154:PHE:CZ	1:A:268:PRO:O	2.55	0.60
1:A:116:ASN:ND2	1:A:118:PHE:N	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HG23	1:A:115:PHE:CD1	2.37	0.59
1:B:52:PHE:CZ	1:B:193:SER:HB3	2.38	0.59
1:A:449:LYS:CE	1:A:455:GLU:HG2	2.29	0.59
1:B:18:GLU:OE2	1:B:226:LYS:HG3	2.02	0.59
1:B:263:ASP:OD2	1:B:265:LYS:HG2	2.02	0.59
1:B:98:LYS:HB2	1:B:170:ARG:HD3	1.83	0.59
1:B:567:GLN:HB3	1:B:568:PRO:HD3	1.85	0.59
1:A:519:ALA:N	1:A:520:PRO:HD3	2.18	0.58
1:B:417:ARG:CZ	1:B:447:LEU:HD21	2.33	0.58
1:A:286:PHE:HB3	1:A:288:ILE:HD11	1.84	0.58
1:A:46:LEU:HB3	1:A:191:LEU:HD23	1.83	0.58
1:B:179:ASP:O	1:B:467:SER:HB3	2.04	0.58
1:B:243:ASN:ND2	1:B:243:ASN:C	2.57	0.58
1:B:432:ASP:O	1:B:436:MET:HG3	2.04	0.58
1:A:540:MET:HG3	1:A:540:MET:O	2.03	0.57
1:A:56:THR:HG23	2:A:1001:FAD:O2A	2.04	0.57
1:B:288:ILE:HG23	1:B:289:PRO:HD2	1.86	0.57
1:B:531:ARG:NH2	1:B:552:THR:HG22	2.19	0.57
1:A:408:THR:HG23	1:A:409:ILE:H	1.68	0.57
1:B:540:MET:HG3	1:B:540:MET:O	2.05	0.57
1:A:9:ASP:O	1:A:13:LYS:HD3	2.05	0.57
1:B:116:ASN:ND2	1:B:119:SER:H	2.03	0.57
1:B:109:ASP:CG	1:B:159:GLY:HA3	2.26	0.56
1:A:66:GLY:HA3	1:A:127:TYR:OH	2.05	0.56
1:B:586:GLN:NE2	1:B:586:GLN:HA	2.21	0.56
1:B:496:ASP:O	1:B:500:ILE:CD1	2.54	0.56
1:A:154:PHE:CD1	1:A:154:PHE:N	2.73	0.56
1:A:115:PHE:CB	1:A:120:VAL:HG13	2.36	0.56
1:A:116:ASN:O	1:A:120:VAL:HG22	2.06	0.55
1:A:115:PHE:HB2	1:A:120:VAL:HG13	1.87	0.55
1:B:145:PRO:HG3	1:B:161:LYS:C	2.26	0.55
1:B:519:ALA:N	1:B:520:PRO:HD3	2.22	0.55
1:B:417:ARG:NH1	1:B:447:LEU:HD11	2.22	0.55
1:B:596:ALA:HB2	1:B:601:ARG:HH21	1.73	0.55
1:B:201:LEU:HD12	1:B:209:GLY:HA3	1.89	0.54
1:B:144:THR:HG23	1:B:146:GLU:H	1.72	0.54
1:A:114:THR:HG23	1:A:115:PHE:N	2.22	0.54
1:B:475:LYS:C	1:B:475:LYS:HD2	2.28	0.54
1:B:579:TRP:O	1:B:580:THR:CG2	2.55	0.54
1:B:586:GLN:HE21	1:B:586:GLN:HA	1.72	0.54
1:B:583:GLU:O	1:B:587:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HB	1:B:97:PRO:HD3	1.90	0.54
1:B:551:ARG:HG2	1:B:551:ARG:HH11	1.73	0.53
1:A:175:ARG:HB3	3:A:1076:HOH:O	2.09	0.53
1:B:217:THR:C	1:B:219:GLU:H	2.12	0.52
1:A:149:LEU:HD21	1:A:160:LEU:HD23	1.90	0.52
1:B:105:PRO:HA	1:B:163:ALA:HB2	1.91	0.52
1:B:113:THR:OG1	1:B:114:THR:N	2.42	0.52
1:B:252:MET:O	1:B:350:ILE:HD11	2.09	0.52
1:B:448:LEU:HD12	1:B:456:THR:HG21	1.92	0.51
1:B:97:PRO:HA	1:B:170:ARG:O	2.10	0.51
1:B:457:LYS:HG2	1:B:458:GLU:H	1.75	0.51
1:A:8:GLN:O	1:A:12:GLN:HG2	2.09	0.51
1:B:145:PRO:O	1:B:149:LEU:HD23	2.10	0.51
1:B:496:ASP:O	1:B:500:ILE:HG13	2.10	0.51
1:B:236:VAL:HG21	1:B:426:SER:HB3	1.93	0.51
1:A:433:TYR:HA	1:A:436:MET:HE3	1.92	0.51
1:B:244:PHE:HD1	1:B:244:PHE:H	1.58	0.51
1:B:8:GLN:O	1:B:12:GLN:HG2	2.10	0.51
1:A:96:ILE:HB	1:A:97:PRO:CD	2.41	0.51
1:B:36:GLN:CD	1:B:461:SER:HB3	2.30	0.50
1:B:335:LEU:HD22	1:B:604:LYS:HG2	1.91	0.50
1:A:582:GLU:HG2	1:A:583:GLU:N	2.25	0.50
1:B:600:LEU:HB3	1:B:603:LEU:HD12	1.94	0.50
1:B:449:LYS:HA	1:B:453:GLY:H	1.76	0.50
1:A:484:ALA:O	1:A:488:VAL:HG23	2.12	0.50
1:A:203:GLU:CG	1:A:203:GLU:O	2.57	0.50
1:A:465:GLN:OE1	1:A:470:ASN:HA	2.11	0.50
1:A:96:ILE:HB	1:A:97:PRO:HD2	1.94	0.50
1:B:143:LEU:HB3	1:B:148:VAL:HG23	1.94	0.50
1:B:102:MET:HG3	1:B:272:PRO:HB2	1.93	0.50
1:B:604:LYS:HB3	1:B:607:LYS:OXT	2.12	0.49
1:B:604:LYS:HD2	1:B:607:LYS:HA	1.94	0.49
1:A:18:GLU:OE1	1:A:226:LYS:HG3	2.11	0.49
1:B:604:LYS:HZ2	1:B:607:LYS:CE	2.26	0.49
1:A:144:THR:HG23	1:A:147:GLU:OE1	2.13	0.49
1:B:167:LEU:HD12	1:B:168:ASP:H	1.76	0.49
1:A:243:ASN:HD21	1:A:245:THR:HB	1.78	0.49
1:A:243:ASN:HD22	1:A:245:THR:H	1.59	0.49
1:A:154:PHE:HZ	1:A:268:PRO:O	1.95	0.49
1:B:253:ARG:NH1	1:B:253:ARG:HG2	2.27	0.49
1:B:120:VAL:O	1:B:124:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:HG3	1:B:50:GLN:O	2.13	0.48
1:B:98:LYS:HB2	1:B:170:ARG:CG	2.44	0.48
1:B:288:ILE:CG2	1:B:289:PRO:HD2	2.44	0.48
1:B:457:LYS:HG2	1:B:458:GLU:N	2.29	0.48
1:B:320:LEU:O	1:B:324:ILE:HD12	2.14	0.48
1:A:11:ILE:O	1:A:15:GLN:HG3	2.13	0.48
1:B:605:GLY:O	1:B:606:GLU:HB3	2.13	0.48
1:A:14:MET:HE3	1:A:45:GLY:HA3	1.94	0.48
1:B:98:LYS:HB2	1:B:170:ARG:CD	2.44	0.48
1:B:510:ARG:HH21	1:B:513:GLU:CB	2.26	0.48
1:A:70:TYR:CZ	1:A:359:GLY:HA2	2.49	0.48
1:B:532:LEU:CD1	1:B:569:VAL:HG23	2.43	0.47
1:B:46:LEU:HD23	1:B:46:LEU:C	2.34	0.47
1:A:116:ASN:C	1:A:116:ASN:HD22	2.17	0.47
1:A:7:ARG:HD3	3:A:1080:HOH:O	2.15	0.47
1:B:500:ILE:HG22	1:B:508:ALA:HB1	1.96	0.47
1:B:279:LYS:NZ	1:B:319:TYR:HA	2.29	0.47
1:A:19:LEU:O	1:A:225:ALA:HA	2.15	0.47
1:B:250:PRO:O	1:B:251:LYS:HD2	2.15	0.47
1:A:154:PHE:HD1	1:A:154:PHE:H	1.55	0.47
1:B:244:PHE:CD1	1:B:244:PHE:N	2.83	0.47
1:B:531:ARG:O	1:B:547:TYR:HE1	1.98	0.46
1:B:14:MET:HE1	1:B:223:ILE:CD1	2.43	0.46
1:B:22:LEU:HD13	1:B:223:ILE:HG21	1.97	0.46
1:B:465:GLN:OE1	1:B:470:ASN:O	2.34	0.46
1:A:57:SER:O	1:A:173:ASP:HB2	2.15	0.46
1:A:208:VAL:HG23	1:A:208:VAL:O	2.13	0.46
1:B:229:ILE:HG23	1:B:229:ILE:O	2.16	0.46
1:B:579:TRP:HB3	1:B:583:GLU:HG2	1.96	0.46
1:B:198:VAL:HG22	1:B:211:LYS:O	2.16	0.46
1:B:116:ASN:HD22	1:B:118:PHE:N	2.07	0.46
1:A:243:ASN:ND2	1:A:245:THR:H	2.13	0.46
1:B:178:ILE:HG23	1:B:179:ASP:N	2.31	0.46
1:A:429:LYS:HB2	2:A:1001:FAD:O2	2.16	0.46
1:B:26:GLY:HA3	1:B:48:GLU:HB2	1.98	0.46
1:B:73:THR:CG2	1:B:73:THR:O	2.62	0.46
1:B:69:ARG:HB2	3:B:1036:HOH:O	2.16	0.46
1:B:579:TRP:HB3	1:B:583:GLU:CG	2.46	0.46
1:B:543:ALA:HB1	1:B:544:PRO:HD2	1.97	0.46
1:B:107:TYR:CE2	1:B:327:ARG:NH1	2.84	0.46
1:A:64:VAL:HG23	1:A:171:ASN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LYS:HD2	1:B:607:LYS:HD2	1.98	0.45
1:B:285:VAL:CG1	1:B:286:PHE:N	2.80	0.45
1:A:567:GLN:HB3	1:A:568:PRO:HD3	1.98	0.45
1:B:29:THR:CG2	1:B:231:THR:HB	2.47	0.45
1:B:293:LYS:HE3	1:B:339:GLU:OE1	2.17	0.45
1:B:183:LYS:HZ3	1:B:183:LYS:HB2	1.82	0.45
1:B:66:GLY:HA3	1:B:127:TYR:OH	2.16	0.45
1:B:507:ASN:HB3	1:B:534:TYR:OH	2.17	0.45
1:A:253:ARG:N	1:A:254:PRO:HD3	2.30	0.45
1:A:146:GLU:CD	1:A:146:GLU:H	2.19	0.45
1:B:19:LEU:HB2	1:B:225:ALA:HB2	1.99	0.45
1:B:433:TYR:CG	1:B:434:ARG:N	2.85	0.45
1:B:35:VAL:HG21	1:B:180:ASN:OD1	2.17	0.44
1:B:313:THR:O	1:B:317:VAL:HG23	2.16	0.44
1:B:535:GLY:O	1:B:541:VAL:HG23	2.17	0.44
1:A:565:ILE:O	1:A:569:VAL:HG23	2.17	0.44
1:B:116:ASN:HD21	1:B:118:PHE:HB3	1.83	0.44
1:B:324:ILE:H	1:B:324:ILE:HD12	1.83	0.44
1:B:64:VAL:HG11	1:B:86:ARG:HG3	1.98	0.44
1:A:472:ASP:HA	1:A:473:PRO:HD2	1.89	0.44
1:B:269:VAL:CG2	1:B:269:VAL:O	2.65	0.44
1:B:569:VAL:HG13	1:B:570:ILE:N	2.33	0.44
1:A:5:LYS:HA	1:A:5:LYS:HD3	1.82	0.44
1:B:41:GLY:O	1:B:42:ILE:C	2.56	0.43
1:B:320:LEU:O	1:B:324:ILE:CD1	2.66	0.43
1:A:10:SER:O	1:A:14:MET:HG3	2.18	0.43
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.84	0.43
1:B:49:MET:HB2	2:B:1001:FAD:C2A	2.48	0.43
1:B:532:LEU:HD21	1:B:573:ILE:CD1	2.47	0.43
1:A:433:TYR:CG	1:A:434:ARG:N	2.87	0.43
1:A:157:LYS:HE3	3:A:1104:HOH:O	2.18	0.43
1:B:350:ILE:N	1:B:350:ILE:HD12	2.34	0.43
1:B:296:PHE:CD2	1:B:324:ILE:HD11	2.54	0.43
1:B:116:ASN:ND2	1:B:118:PHE:HB3	2.34	0.43
1:A:116:ASN:HD21	1:A:119:SER:H	1.67	0.43
1:A:470:ASN:OD1	1:A:506:THR:HG21	2.19	0.43
1:B:84:GLY:O	1:B:87:ALA:HB3	2.19	0.43
1:A:114:THR:CG2	1:A:115:PHE:N	2.82	0.42
1:B:324:ILE:HD12	1:B:324:ILE:N	2.34	0.42
1:B:496:ASP:O	1:B:500:ILE:HD12	2.18	0.42
1:A:203:GLU:HG2	1:A:208:VAL:CG1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:O	1:B:170:ARG:HG2	2.18	0.42
1:A:12:GLN:HE21	1:A:12:GLN:HB3	1.63	0.42
1:B:167:LEU:HD12	1:B:168:ASP:N	2.34	0.42
1:B:253:ARG:NH2	1:B:302:ASP:OD1	2.51	0.42
2:B:1001:FAD:H1'1	2:B:1001:FAD:H9	1.77	0.42
1:B:579:TRP:CZ3	1:B:587:GLN:HG3	2.55	0.42
1:B:449:LYS:C	1:B:451:GLU:H	2.22	0.42
1:B:53:ALA:O	1:B:58:SER:HB3	2.19	0.42
1:B:588:THR:O	1:B:592:GLU:HG2	2.19	0.42
1:B:535:GLY:HA2	1:B:539:GLU:HG3	2.02	0.42
1:B:306:ASP:OD2	1:B:309:ASP:N	2.42	0.42
1:B:430:ILE:HG22	2:B:1001:FAD:N1	2.35	0.42
1:B:521:TYR:HB2	1:B:524:LEU:HD12	2.01	0.42
1:B:579:TRP:CG	1:B:583:GLU:CG	3.03	0.42
1:B:546:ASP:O	1:B:551:ARG:HG2	2.19	0.42
1:A:70:TYR:OH	1:A:356:ASP:O	2.36	0.42
1:B:586:GLN:HE21	1:B:586:GLN:CA	2.28	0.42
1:B:29:THR:HG22	1:B:231:THR:HB	2.02	0.42
1:B:445:ARG:NE	1:B:457:LYS:O	2.53	0.42
1:B:214:ASP:HB3	1:B:217:THR:O	2.20	0.42
1:B:42:ILE:HD12	1:B:448:LEU:HD11	2.02	0.41
1:A:245:THR:O	1:A:245:THR:CG2	2.67	0.41
1:A:429:LYS:HE3	2:A:1001:FAD:O2	2.20	0.41
1:A:408:THR:HG23	1:A:409:ILE:N	2.35	0.41
1:A:72:LYS:HD2	1:A:72:LYS:HA	1.80	0.41
1:A:274:TYR:CE1	1:A:284:MET:HB3	2.55	0.41
1:B:579:TRP:CB	1:B:583:GLU:HG2	2.51	0.41
1:B:579:TRP:CD1	1:B:583:GLU:HG2	2.55	0.41
1:A:111:GLY:O	1:A:112:ALA:HB3	2.20	0.41
1:B:304:GLN:NE2	1:B:304:GLN:N	2.69	0.41
1:B:157:LYS:O	1:B:159:GLY:N	2.54	0.41
1:B:531:ARG:HH21	1:B:552:THR:HG22	1.84	0.41
1:A:116:ASN:ND2	1:A:116:ASN:C	2.74	0.41
1:B:201:LEU:HB2	1:B:209:GLY:CA	2.50	0.41
1:B:253:ARG:N	1:B:254:PRO:HD3	2.35	0.41
1:B:604:LYS:NZ	1:B:607:LYS:NZ	2.68	0.41
1:A:431:THR:HG23	2:A:1001:FAD:O2	2.21	0.41
1:B:519:ALA:O	1:B:520:PRO:O	2.38	0.41
1:B:194:LYS:HD3	1:B:194:LYS:HA	1.95	0.41
1:B:152:GLU:HA	1:B:153:PRO:HD2	1.84	0.41
1:B:532:LEU:HA	1:B:547:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:NH1	1:B:551:ARG:HG2	2.34	0.41
1:B:303:TYR:C	1:B:304:GLN:NE2	2.74	0.41
1:B:20:ASP:CB	1:B:42:ILE:HG23	2.50	0.41
1:B:134:THR:O	1:B:134:THR:HG23	2.21	0.41
1:B:604:LYS:CD	1:B:607:LYS:HA	2.51	0.40
1:A:200:PHE:HB2	1:A:202:TYR:OH	2.22	0.40
1:B:53:ALA:HA	3:B:1010:HOH:O	2.20	0.40
1:B:290:ARG:HA	1:B:290:ARG:HD3	1.96	0.40
1:B:213:ARG:NH2	1:B:218:ASP:HB3	2.35	0.40
1:B:93:ALA:N	1:B:94:PRO:CD	2.85	0.40
1:B:264:ALA:HB2	1:B:292:ASN:O	2.21	0.40
1:B:449:LYS:C	1:B:451:GLU:N	2.74	0.40
1:A:269:VAL:O	1:A:269:VAL:HG23	2.21	0.40
1:A:429:LYS:O	1:A:436:MET:HE1	2.21	0.40
1:B:88:VAL:O	1:B:91:GLY:N	2.54	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	551/607 (91%)	522 (95%)	27 (5%)	2 (0%)	39	56
1	B	514/607 (85%)	449 (87%)	52 (10%)	13 (2%)	7	7
All	All	1065/1214 (88%)	971 (91%)	79 (7%)	15 (1%)	14	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ILE
1	B	158	GLU
1	B	218	ASP

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Mol	Chain	Res	Type
1	B	520	PRO
1	B	579	TRP
1	B	42	ILE
1	B	134	THR
1	B	560	ASP
1	B	580	THR
1	B	57	SER
1	B	96	ILE
1	B	136	THR
1	B	186	GLU
1	B	188	GLY
1	A	453	GLY

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	465/512 (91%)	442 (95%)	23 (5%)	31	48
1	B	445/512 (87%)	421 (95%)	24 (5%)	27	43
All	All	910/1024 (89%)	863 (95%)	47 (5%)	29	45

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	17	GLU
1	A	56	THR
1	A	110	GLU
1	A	113	THR
1	A	116	ASN
1	A	120	VAL
1	A	126	LEU
1	A	134	THR
1	A	154	PHE
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	168	ASP
1	A	170	ARG
1	A	243	ASN
1	A	280	GLN
1	A	320	LEU
1	A	335	LEU
1	A	408	THR
1	A	447	LEU
1	A	481	THR
1	A	506	THR
1	A	532	LEU
1	A	582	GLU
1	B	96	ILE
1	B	101	PRO
1	B	126	LEU
1	B	160	LEU
1	B	168	ASP
1	B	176	LEU
1	B	183	LYS
1	B	218	ASP
1	B	226	LYS
1	B	243	ASN
1	B	244	PHE
1	B	299	THR
1	B	304	GLN
1	B	320	LEU
1	B	330	GLU
1	B	409	ILE
1	B	411	ARG
1	B	459	ILE
1	B	475	LYS
1	B	496	ASP
1	B	532	LEU
1	B	533	ARG
1	B	580	THR
1	B	582	GLU

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	4	ASN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	243	ASN
1	A	280	GLN
1	A	554	HIS
1	B	8	GLN
1	B	12	GLN
1	B	116	ASN
1	B	241	ASN
1	B	243	ASN
1	B	304	GLN
1	B	554	HIS
1	B	586	GLN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	1001	-	48,58,58	1.94	14 (29%)	54,89,89	2.89	18 (33%)
2	FAD	B	1001	-	48,58,58	1.35	5 (10%)	54,89,89	2.02	8 (14%)

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	1001	-	-	0/30/50/50	0/6/6/6
2	FAD	B	1001	-	-	0/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	P-O2P	-2.71	1.43	1.54
2	A	1001	FAD	C5A-N7A	-2.31	1.31	1.39
2	A	1001	FAD	C2A-N3A	2.04	1.35	1.32
2	B	1001	FAD	O4B-C1B	2.12	1.43	1.41
2	A	1001	FAD	C4X-N5	2.22	1.36	1.33
2	A	1001	FAD	C6-C7	2.32	1.44	1.37
2	A	1001	FAD	O2B-C2B	2.47	1.48	1.43
2	A	1001	FAD	C7M-C7	2.51	1.56	1.51
2	A	1001	FAD	C9-C9A	2.54	1.46	1.40
2	A	1001	FAD	C4X-C10	2.58	1.45	1.41
2	A	1001	FAD	C5X-N5	2.74	1.39	1.35
2	A	1001	FAD	C10-N1	2.86	1.40	1.35
2	B	1001	FAD	C10-N1	2.95	1.40	1.35
2	B	1001	FAD	C5X-N5	3.10	1.40	1.35
2	A	1001	FAD	C4-N3	3.55	1.39	1.33
2	B	1001	FAD	C4-N3	3.95	1.40	1.33
2	B	1001	FAD	C4X-N5	4.42	1.40	1.33
2	A	1001	FAD	C10-N10	5.25	1.45	1.39
2	A	1001	FAD	C9A-N10	6.25	1.47	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	FAD	N3A-C2A-N1A	-13.21	118.78	128.89
2	B	1001	FAD	N3A-C2A-N1A	-9.68	121.48	128.89
2	A	1001	FAD	C4X-C10-N10	-5.55	117.25	120.52
2	B	1001	FAD	C4B-O4B-C1B	-5.43	103.75	109.72
2	B	1001	FAD	P-O3P-PA	-3.59	122.64	132.73
2	A	1001	FAD	O2P-P-O3P	-3.07	91.14	105.09
2	A	1001	FAD	C4X-C4-N3	-2.77	119.80	123.59
2	A	1001	FAD	C1B-N9A-C4A	-2.62	122.98	126.94
2	B	1001	FAD	C4X-C4-N3	-2.59	120.05	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	FAD	C4-C4X-C10	-2.58	118.29	119.94
2	A	1001	FAD	O5B-C5B-C4B	-2.52	99.82	109.12
2	A	1001	FAD	O3'-C3'-C4'	-2.49	102.47	108.75
2	B	1001	FAD	C4A-C5A-N7A	-2.42	107.25	109.48
2	A	1001	FAD	C9A-C5X-N5	-2.40	118.80	122.36
2	A	1001	FAD	O4B-C1B-N9A	2.29	112.90	108.10
2	A	1001	FAD	O4B-C4B-C5B	2.31	117.57	109.32
2	A	1001	FAD	C4-C4X-N5	2.38	121.61	118.72
2	B	1001	FAD	C4X-N5-C5X	2.42	119.55	116.76
2	A	1001	FAD	O2P-P-O1P	2.60	126.61	112.53
2	A	1001	FAD	P-O3P-PA	3.08	141.39	132.73
2	A	1001	FAD	O3P-PA-O5B	3.14	111.27	102.94
2	B	1001	FAD	C5X-C9A-N10	3.62	120.37	117.62
2	B	1001	FAD	C4-N3-C2	5.20	119.74	115.25
2	A	1001	FAD	C4X-N5-C5X	5.42	123.00	116.76
2	A	1001	FAD	O3P-P-O5'	6.36	119.80	102.94
2	A	1001	FAD	C4-N3-C2	6.90	121.21	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	FAD	4	0
2	B	1001	FAD	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

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, 95^{th} 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	557/607 (91%)	-0.07	11 (1%)	68	68	17, 45, 72, 103	0
1	B	530/607 (87%)	0.53	49 (9%)	11	11	43, 78, 120, 157	1 (0%)
All	All	1087/1214 (89%)	0.22	60 (5%)	29	29	17, 59, 109, 157	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	PHE	7.3
1	B	113	THR	6.4
1	A	247	PRO	6.2
1	B	515	ALA	5.3
1	B	352	ASN	4.6
1	B	452	TYR	4.3
1	B	508	ALA	4.3
1	B	495	GLU	4.0
1	B	149	LEU	4.0
1	A	246	ARG	3.9
1	B	353	SER	3.8
1	B	280	GLN	3.7
1	B	34	ALA	3.6
1	B	459	ILE	3.5
1	B	496	ASP	3.4
1	B	229	ILE	3.4
1	B	33	VAL	3.4
1	B	606	GLU	3.3
1	B	509	ARG	3.3
1	A	248	VAL	3.3
1	A	245	THR	3.3
1	B	607	LYS	3.3
1	B	24	ILE	3.2
1	A	23	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	304	GLN	3.2
1	B	472	ASP	3.1
1	B	12	GLN	3.1
1	B	455	GLU	3.1
1	B	498	THR	3.1
1	B	38	ALA	3.0
1	B	135	GLY	3.0
1	B	474	THR	3.0
1	A	280	GLN	2.9
1	B	247	PRO	2.9
1	B	244	PHE	2.8
1	A	112	ALA	2.8
1	B	274	TYR	2.7
1	B	136	THR	2.6
1	B	581	GLU	2.4
1	B	8	GLN	2.4
1	B	181	ILE	2.4
1	B	453	GLY	2.4
1	A	46	LEU	2.4
1	B	177	VAL	2.4
1	B	285	VAL	2.3
1	A	360	GLY	2.3
1	B	275	PHE	2.3
1	B	315	GLU	2.3
1	B	228	VAL	2.3
1	B	109	ASP	2.3
1	B	464	TYR	2.2
1	A	229	ILE	2.2
1	B	578	GLY	2.2
1	B	519	ALA	2.1
1	B	513	GLU	2.1
1	A	231	THR	2.1
1	B	580	THR	2.1
1	B	582	GLU	2.0
1	B	579	TRP	2.0
1	B	448	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, 95^{th} 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
2	FAD	B	1001	53/53	0.95	0.12	-0.69	29,44,50,50	0
2	FAD	A	1001	53/53	0.97	0.12	-0.78	12,22,29,33	0

6.5 Other polymers (i)

There are no such residues in this entry.