



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:16 PM GMT

PDB ID : 1Y56
Title : Crystal structure of L-proline dehydrogenase from P.horikoshii
Authors : Tsuge, H.; Kawakami, R.; Sakuraba, H.; Ago, H.; Miyano, M.; Aki, K.;
Katunuma, N.; Ohshima, T.
Deposited on : 2004-12-02
Resolution : 2.86 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

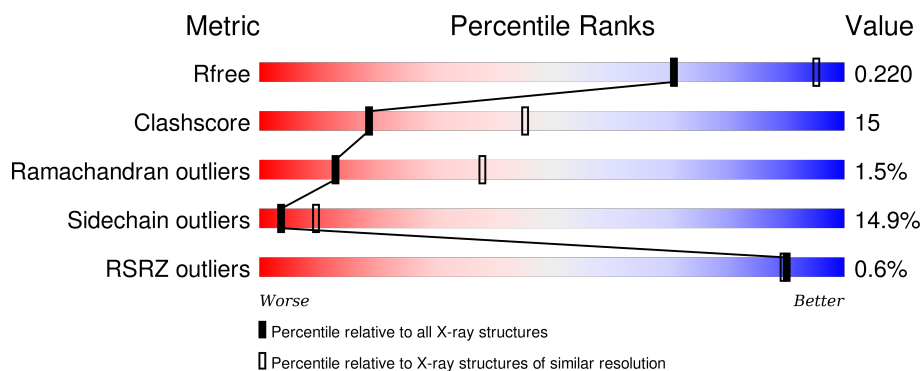
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	493	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>8%</div> <div>.</div> </div> </div>
2	B	382	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>6%</div> <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
7	FMN	A	802	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7147 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 hypothetical protein PH1363.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3844	2458	665	706	15			

- Molecule 2 is a protein called sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	0	0
			2961	1923	486	545	7			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

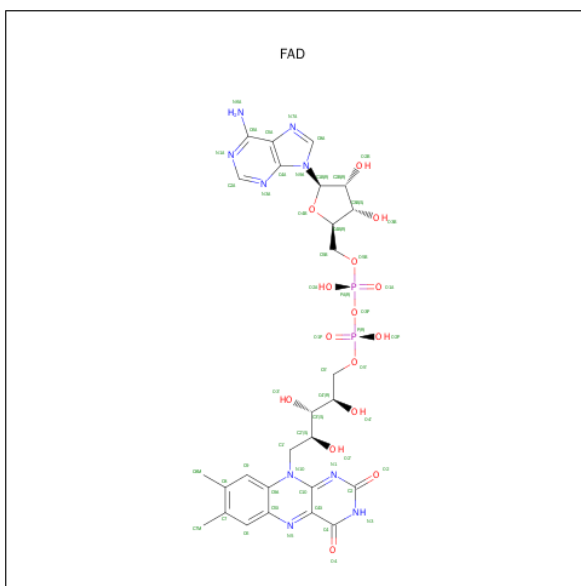
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



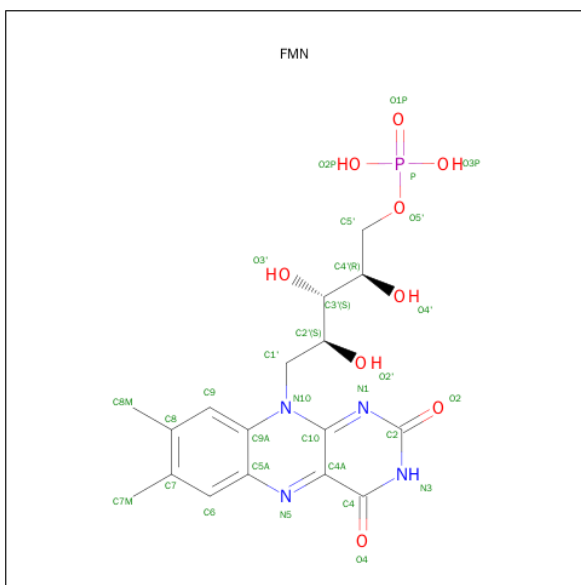
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



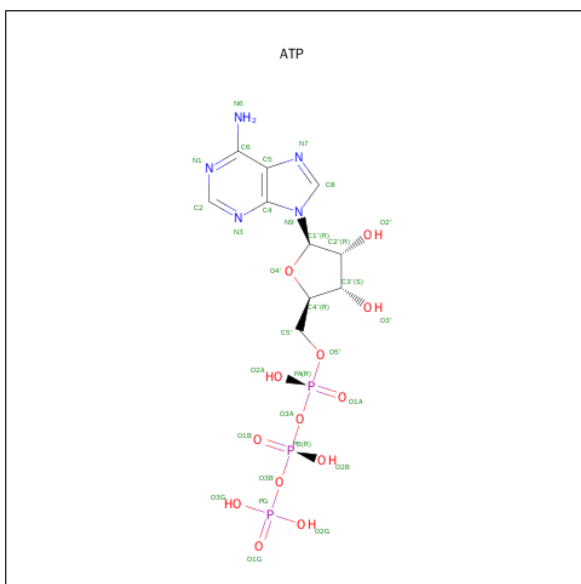
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0
			53	27	9	15	2	0

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



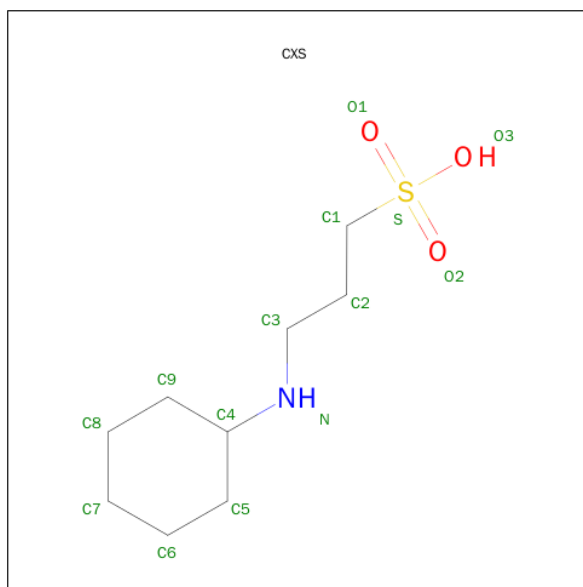
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 9 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

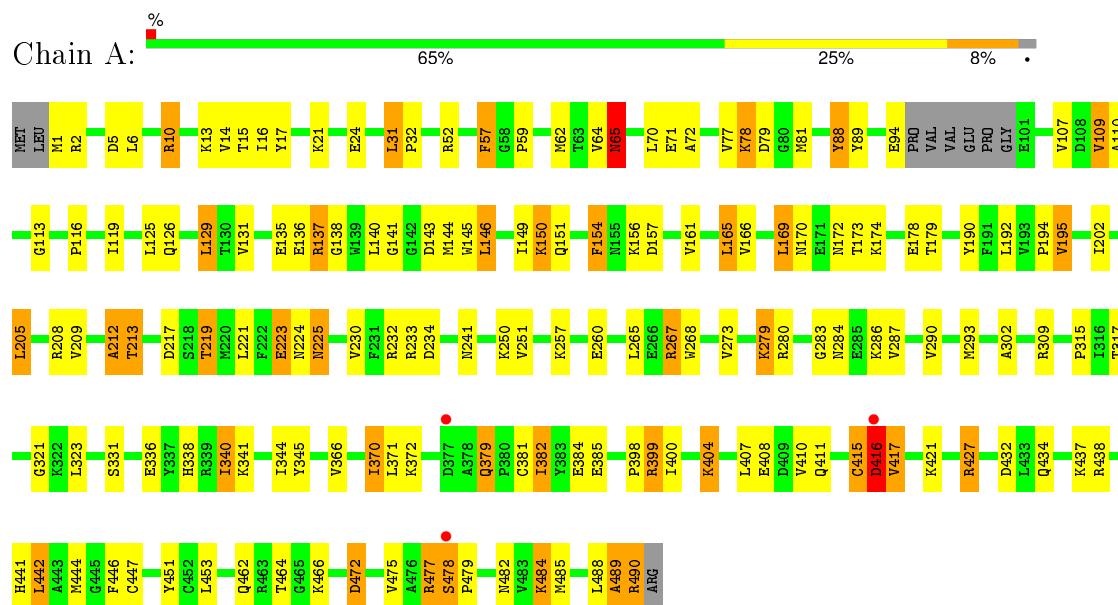
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	129	Total	O	0	0
			129	129		
10	B	77	Total	O	0	0
			77	77		

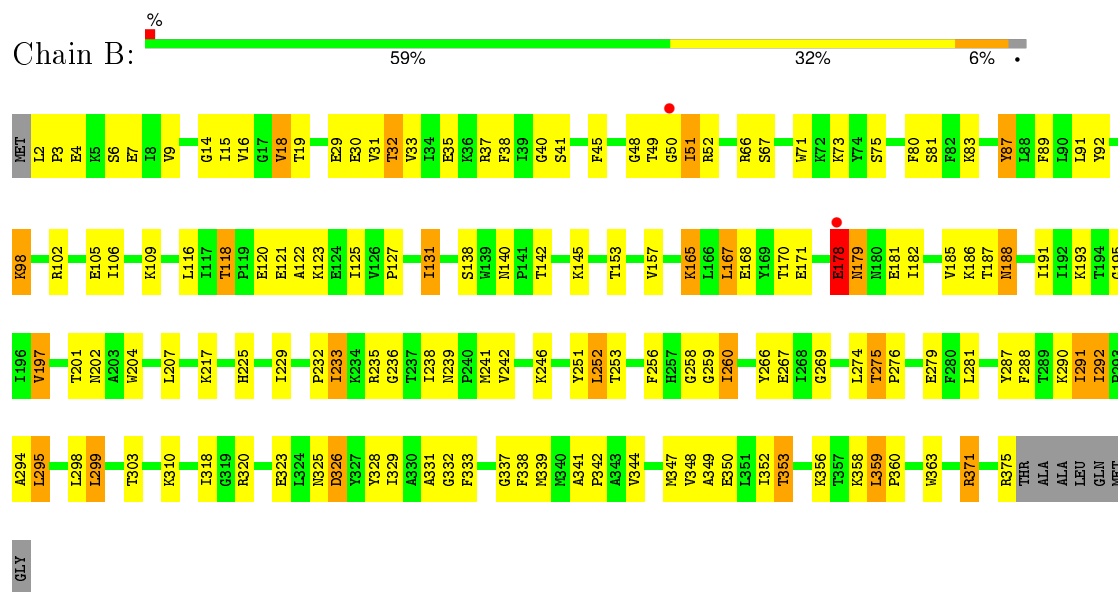
3 Residue-property plots

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: hypothetical protein PH1363



• Molecule 2: sarcosine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.22Å 172.22Å 175.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.86 149.15 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.85-2.86) 98.6 (149.15-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.226 0.203 , 0.220	Depositor DCC
R_{free} test set	1777 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 38541 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CXS, CL, FMN, FE, ATP, FAD, SO4

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	0.56	2/3914 (0.1%)	0.73	3/5275 (0.1%)
2	B	0.54	0/3031	0.72	3/4103 (0.1%)
All	All	0.55	2/6945 (0.0%)	0.73	6/9378 (0.1%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	CYS	CB-SG	6.50	1.93	1.82
1	A	444	MET	C-N	5.40	1.42	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	MET	N-CA-C	-9.27	85.97	111.00
1	A	446	PHE	CB-CA-C	-6.39	97.63	110.40
2	B	359	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	447	CYS	N-CA-C	6.12	127.51	111.00
2	B	252	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	51	ILE	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ALA	Peptide
1	A	484	LYS	Peptide
1	A	489	ALA	Peptide

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	3844	0	3918	118	0
2	B	2961	0	2993	101	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
6	B	53	0	31	5	0
7	A	31	0	17	0	0
8	A	31	0	12	3	0
9	A	14	0	19	0	0
10	A	129	0	0	17	1
10	B	77	0	0	7	1
All	All	7147	0	6990	215	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 15.

All (215) 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)
2:B:371:ARG:HH21	2:B:371:ARG:HG2	1.24	1.02
1:A:317:THR:HB	1:A:475:VAL:HG23	1.47	0.94
1:A:478:SER:HB3	1:A:479:PRO:HD3	1.53	0.91
2:B:118:THR:HG22	2:B:121:GLU:H	1.38	0.88
1:A:399:ARG:HH11	1:A:399:ARG:H	1.25	0.83
1:A:427:ARG:HG3	10:A:881:HOH:O	1.78	0.82
1:A:478:SER:HB3	2:B:303:THR:HB	1.64	0.79
2:B:217:LYS:HG2	10:B:880:HOH:O	1.84	0.78
1:A:94:GLU:HB3	10:A:878:HOH:O	1.85	0.76
1:A:170:ASN:HB3	1:A:172:ASN:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ARG:CG	2:B:371:ARG:HH21	1.99	0.75
2:B:6:SER:OG	2:B:32:THR:HG23	1.88	0.73
1:A:478:SER:CB	2:B:303:THR:HB	2.19	0.72
1:A:64:VAL:HB	1:A:70:LEU:HD12	1.71	0.72
2:B:349:ALA:O	2:B:353:THR:HB	1.90	0.72
2:B:202:ASN:HB2	2:B:332:GLY:H	1.53	0.71
1:A:217:ASP:HB2	1:A:232:ARG:HD3	1.72	0.71
1:A:2:ARG:HD3	1:A:5:ASP:OD1	1.91	0.71
1:A:224:ASN:N	10:A:929:HOH:O	2.24	0.71
2:B:3:PRO:HD2	2:B:167:LEU:HD21	1.73	0.70
2:B:29:GLU:OE2	2:B:29:GLU:HA	1.93	0.69
1:A:135:GLU:HG3	1:A:137:ARG:H	1.57	0.69
2:B:236:GLY:HA2	2:B:239:ASN:HD21	1.57	0.69
1:A:398:PRO:HA	10:A:875:HOH:O	1.92	0.68
1:A:219:THR:HG21	1:A:451:TYR:HB3	1.73	0.68
1:A:62:MET:HE2	1:A:72:ALA:HB2	1.74	0.68
2:B:195:GLY:O	2:B:326:ASP:HB2	1.93	0.68
1:A:232:ARG:HD2	1:A:234:ASP:OD1	1.93	0.67
2:B:89:PHE:HB2	2:B:138:SER:HB3	1.76	0.67
2:B:35:GLU:O	2:B:168:GLU:O	2.13	0.67
2:B:7:GLU:HB3	2:B:30:GLU:HG3	1.77	0.67
1:A:16:ILE:HG21	1:A:77:VAL:HG22	1.77	0.66
2:B:276:PRO:HB3	2:B:303:THR:HG22	1.77	0.66
1:A:213:THR:HG21	1:A:315:PRO:HG2	1.78	0.66
1:A:381:CYS:HA	1:A:384:GLU:HB2	1.78	0.66
2:B:50:GLY:HA2	6:B:800:FAD:HN3	1.60	0.65
1:A:179:THR:CG2	1:A:195:VAL:HG13	2.26	0.65
2:B:171:GLU:H	2:B:188:ASN:ND2	1.95	0.64
1:A:16:ILE:HG21	1:A:77:VAL:CG2	2.28	0.64
1:A:399:ARG:NH1	1:A:399:ARG:H	1.96	0.63
2:B:363:TRP:CZ2	2:B:375:ARG:HB3	2.34	0.62
2:B:288:PHE:HB3	2:B:295:LEU:HD23	1.80	0.62
1:A:179:THR:HG23	1:A:195:VAL:HG13	1.82	0.61
2:B:80:PHE:O	2:B:81:SER:HB3	1.99	0.61
1:A:59:PRO:HD2	1:A:88:TYR:OH	1.99	0.61
1:A:190:TYR:CE2	1:A:205:LEU:HD12	2.35	0.61
1:A:379:GLN:O	1:A:382:ILE:HD13	2.01	0.60
2:B:253:THR:O	2:B:260:ILE:HA	2.01	0.60
2:B:41:SER:O	10:B:816:HOH:O	2.16	0.60
1:A:241:ASN:HD21	1:A:267:ARG:HH12	1.47	0.60
1:A:135:GLU:OE2	1:A:137:ARG:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:HE2	10:A:858:HOH:O	2.01	0.60
2:B:371:ARG:HG2	2:B:371:ARG:NH2	2.03	0.59
1:A:233:ARG:HD2	10:A:912:HOH:O	2.03	0.58
2:B:292:ILE:O	2:B:292:ILE:HG13	2.03	0.58
1:A:109:VAL:O	1:A:208:ARG:O	2.21	0.58
1:A:478:SER:HB3	1:A:479:PRO:CD	2.30	0.58
1:A:400:ILE:H	1:A:462:GLN:HE22	1.50	0.58
1:A:109:VAL:HG21	1:A:125:LEU:HD13	1.83	0.58
1:A:233:ARG:NH2	1:A:309:ARG:HD3	2.19	0.58
1:A:78:LYS:O	1:A:81:MET:HB2	2.04	0.58
2:B:122:ALA:O	2:B:125:ILE:O	2.21	0.58
2:B:49:THR:O	2:B:145:LYS:HA	2.05	0.57
2:B:2:LEU:HD13	2:B:3:PRO:O	2.04	0.57
2:B:318:ILE:HA	2:B:329:ILE:O	2.05	0.57
2:B:71:TRP:O	2:B:75:SER:HB2	2.05	0.57
1:A:427:ARG:HD2	10:A:845:HOH:O	2.05	0.56
1:A:241:ASN:ND2	1:A:268:TRP:HE1	2.03	0.56
1:A:482:ASN:HB3	2:B:299:LEU:HG	1.87	0.56
1:A:225:ASN:HD21	1:A:411:GLN:H	1.52	0.56
1:A:225:ASN:N	1:A:225:ASN:HD22	2.03	0.56
1:A:209:VAL:HG22	1:A:344:ILE:HG23	1.88	0.56
1:A:421:LYS:HG3	10:A:931:HOH:O	2.04	0.56
2:B:16:VAL:O	2:B:19:THR:HG22	2.06	0.55
2:B:52:ARG:HG3	2:B:87:TYR:CD1	2.42	0.55
2:B:38:PHE:HA	2:B:168:GLU:HG2	1.88	0.55
2:B:320:ARG:HH11	2:B:325:ASN:HA	1.71	0.55
2:B:66:ARG:HG2	2:B:359:LEU:HD21	1.88	0.55
2:B:140:ASN:ND2	2:B:142:THR:H	2.05	0.54
1:A:257:LYS:HE3	1:A:260:GLU:OE2	2.07	0.54
1:A:478:SER:CB	1:A:479:PRO:HD3	2.33	0.54
1:A:65:ASN:N	10:A:923:HOH:O	2.41	0.54
1:A:317:THR:HB	1:A:475:VAL:CG2	2.29	0.53
2:B:236:GLY:HA2	2:B:239:ASN:ND2	2.24	0.53
2:B:48:GLY:H	6:B:800:FAD:C5X	2.22	0.53
1:A:464:THR:HG22	1:A:466:LYS:H	1.74	0.53
1:A:126:GLN:NE2	1:A:173:THR:OG1	2.41	0.52
1:A:338:HIS:HD2	10:A:815:HOH:O	1.93	0.52
2:B:14:GLY:O	2:B:18:VAL:HG13	2.09	0.52
1:A:141:GLY:HA3	1:A:145:TRP:HB2	1.90	0.52
2:B:188:ASN:HD22	2:B:188:ASN:H	1.58	0.52
1:A:219:THR:CG2	1:A:451:TYR:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:PHE:HB3	2:B:337:GLY:CA	2.40	0.51
1:A:57:PHE:HD1	1:A:57:PHE:O	1.94	0.50
1:A:129:LEU:HD22	1:A:371:LEU:HD12	1.92	0.50
1:A:109:VAL:HG21	1:A:125:LEU:CD1	2.41	0.49
1:A:283:GLY:HA3	1:A:286:LYS:O	2.12	0.49
2:B:287:TYR:O	2:B:291:ILE:HG23	2.11	0.49
2:B:350:GLU:HA	2:B:353:THR:HG22	1.94	0.49
1:A:125:LEU:HD21	1:A:370:ILE:HG13	1.95	0.49
1:A:225:ASN:ND2	1:A:225:ASN:N	2.61	0.48
2:B:201:THR:O	2:B:202:ASN:C	2.51	0.48
2:B:259:GLY:O	2:B:260:ILE:HB	2.13	0.48
2:B:320:ARG:NH1	2:B:325:ASN:HA	2.28	0.48
2:B:40:GLY:O	2:B:45:PHE:HB2	2.13	0.48
1:A:126:GLN:HB2	1:A:170:ASN:HD22	1.78	0.48
1:A:64:VAL:CG1	1:A:64:VAL:O	2.61	0.48
1:A:490:ARG:HG3	10:A:825:HOH:O	2.13	0.48
2:B:98:LYS:O	2:B:98:LYS:HE2	2.14	0.48
1:A:31:LEU:HB3	1:A:32:PRO:HD3	1.95	0.48
2:B:9:VAL:HG11	2:B:185:VAL:HG11	1.96	0.47
2:B:92:TYR:CG	2:B:246:LYS:HD3	2.50	0.47
2:B:348:VAL:O	2:B:352:ILE:HG12	2.14	0.47
1:A:309:ARG:NH1	8:A:801:ATP:O1G	2.48	0.47
1:A:62:MET:CE	1:A:72:ALA:HB2	2.42	0.47
8:A:801:ATP:O3G	8:A:801:ATP:O1A	2.33	0.47
1:A:336:GLU:HG2	10:A:883:HOH:O	2.14	0.47
1:A:399:ARG:HH11	1:A:399:ARG:N	2.05	0.47
1:A:217:ASP:CB	1:A:232:ARG:HD3	2.42	0.47
2:B:71:TRP:CE2	2:B:342:PRO:HG2	2.50	0.47
2:B:83:LYS:HG2	2:B:256:PHE:CE1	2.49	0.47
1:A:321:GLY:HA3	1:A:340:ILE:HG13	1.97	0.47
2:B:241:MET:HE2	2:B:251:TYR:HB2	1.97	0.47
2:B:182:ILE:HD13	2:B:197:VAL:HG13	1.97	0.47
2:B:202:ASN:HA	2:B:331:ALA:HB1	1.97	0.47
2:B:51:ILE:HA	2:B:339:MET:HB3	1.96	0.47
1:A:192:LEU:HG	1:A:194:PRO:HD3	1.97	0.46
2:B:170:THR:HA	2:B:188:ASN:HD21	1.80	0.46
1:A:10:ARG:HB3	1:A:10:ARG:HH11	1.80	0.46
2:B:204:TRP:CD2	6:B:800:FAD:H8A	2.50	0.46
2:B:333:PHE:CB	2:B:337:GLY:HA3	2.46	0.46
1:A:434:GLN:NE2	10:A:808:HOH:O	2.48	0.46
2:B:118:THR:CG2	2:B:120:GLU:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:THR:CB	1:A:475:VAL:HG23	2.32	0.46
1:A:478:SER:HB2	2:B:303:THR:HB	1.95	0.45
1:A:150:LYS:HD3	1:A:156:LYS:N	2.30	0.45
1:A:116:PRO:HG2	8:A:801:ATP:O3B	2.16	0.45
1:A:125:LEU:HD21	1:A:370:ILE:CG1	2.47	0.45
1:A:340:ILE:HA	1:A:340:ILE:HD12	1.67	0.45
2:B:71:TRP:O	2:B:75:SER:CB	2.64	0.45
2:B:52:ARG:HG3	2:B:87:TYR:CE1	2.52	0.45
1:A:464:THR:CG2	1:A:466:LYS:HB2	2.46	0.45
1:A:293:MET:CE	1:A:404:LYS:HG2	2.47	0.45
1:A:138:GLY:HA2	1:A:178:GLU:HG2	1.99	0.45
1:A:119:ILE:HG21	1:A:165:LEU:HB3	1.99	0.45
2:B:292:ILE:HG13	2:B:295:LEU:HD22	1.99	0.45
2:B:347:MET:HE3	2:B:359:LEU:HB3	1.99	0.45
2:B:359:LEU:HB3	2:B:360:PRO:HD2	1.98	0.44
2:B:225:HIS:HD2	10:B:810:HOH:O	2.00	0.44
2:B:178:GLU:HB3	2:B:179:ASN:H	1.67	0.44
2:B:238:ILE:HD12	2:B:260:ILE:HG12	1.98	0.44
1:A:286:LYS:HB3	10:A:933:HOH:O	2.16	0.44
2:B:73:LYS:NZ	10:B:837:HOH:O	2.50	0.44
2:B:276:PRO:CB	2:B:303:THR:HG22	2.46	0.44
2:B:188:ASN:N	2:B:188:ASN:HD22	2.14	0.44
2:B:15:ILE:O	2:B:19:THR:HB	2.18	0.44
1:A:472:ASP:N	1:A:472:ASP:OD1	2.48	0.44
1:A:17:TYR:HA	1:A:21:LYS:O	2.17	0.44
2:B:123:LYS:O	2:B:127:PRO:HA	2.17	0.44
1:A:223:GLU:OE1	1:A:280:ARG:NH2	2.43	0.44
1:A:24:GLU:HG2	10:A:816:HOH:O	2.16	0.44
1:A:109:VAL:HG22	1:A:131:VAL:HG12	1.99	0.44
1:A:489:ALA:HA	10:B:879:HOH:O	2.17	0.44
1:A:113:GLY:HA3	1:A:212:ALA:O	2.18	0.43
2:B:37:ARG:HG2	2:B:37:ARG:HH21	1.83	0.43
2:B:229:ILE:HD11	2:B:259:GLY:HA3	1.99	0.43
1:A:109:VAL:O	1:A:110:ALA:HB3	2.18	0.43
2:B:225:HIS:CD2	10:B:810:HOH:O	2.71	0.43
2:B:232:PRO:HA	2:B:258:GLY:O	2.19	0.43
1:A:432:ASP:OD1	1:A:434:GLN:HB2	2.18	0.43
1:A:404:LYS:O	1:A:404:LYS:HG3	2.18	0.43
2:B:233:ILE:HD13	2:B:233:ILE:HA	1.68	0.43
2:B:105:GLU:O	2:B:109:LYS:HG2	2.18	0.43
2:B:131:ILE:HA	2:B:131:ILE:HD12	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HD2	10:A:888:HOH:O	2.19	0.43
2:B:3:PRO:CD	2:B:167:LEU:HD21	2.46	0.43
1:A:14:VAL:HG22	1:A:79:ASP:HB2	2.00	0.43
2:B:202:ASN:CB	2:B:332:GLY:H	2.29	0.42
2:B:338:PHE:HB3	6:B:800:FAD:C2	2.49	0.42
1:A:416:ASP:N	1:A:416:ASP:OD2	2.51	0.42
1:A:166:VAL:HA	1:A:169:LEU:HD22	2.00	0.42
6:B:800:FAD:H1'1	6:B:800:FAD:H9	1.68	0.42
2:B:19:THR:HG21	2:B:341:ALA:HB1	2.01	0.42
1:A:279:LYS:HB2	1:A:293:MET:SD	2.59	0.42
2:B:292:ILE:CD1	2:B:294:ALA:HB3	2.49	0.42
1:A:136:GLU:HA	1:A:179:THR:N	2.35	0.42
1:A:477:ARG:HH22	2:B:275:THR:HG22	1.84	0.42
2:B:118:THR:HG21	2:B:120:GLU:HG2	2.02	0.42
1:A:345:TYR:CE1	1:A:370:ILE:HG22	2.54	0.42
1:A:208:ARG:HA	1:A:208:ARG:HD3	1.85	0.42
1:A:126:GLN:NE2	1:A:170:ASN:H	2.17	0.42
1:A:195:VAL:HG12	1:A:202:ILE:HB	2.02	0.42
2:B:32:THR:HA	2:B:165:LYS:O	2.20	0.41
1:A:251:VAL:HG22	1:A:302:ALA:HB3	2.01	0.41
1:A:205:LEU:N	1:A:205:LEU:HD22	2.35	0.41
1:A:437:LYS:HG2	1:A:442:LEU:O	2.20	0.41
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.86	0.41
1:A:144:MET:HE1	1:A:161:VAL:HG11	2.02	0.41
2:B:267:GLU:OE2	2:B:310:LYS:HD2	2.21	0.41
1:A:154:PHE:O	1:A:156:LYS:N	2.54	0.41
2:B:328:TYR:CZ	2:B:352:ILE:HD13	2.55	0.41
2:B:225:HIS:HE1	2:B:267:GLU:OE2	2.04	0.41
2:B:371:ARG:CG	2:B:371:ARG:NH2	2.67	0.41
1:A:366:VAL:O	1:A:370:ILE:HG23	2.20	0.41
1:A:119:ILE:HD11	1:A:140:LEU:O	2.21	0.41
2:B:153:THR:O	2:B:157:VAL:HG13	2.20	0.41
1:A:126:GLN:HE22	1:A:170:ASN:H	1.69	0.41
2:B:29:GLU:CA	2:B:29:GLU:OE2	2.67	0.40
1:A:89:TYR:CE1	2:B:232:PRO:HB2	2.56	0.40
2:B:353:THR:HG21	10:B:859:HOH:O	2.21	0.40
1:A:62:MET:HE2	1:A:72:ALA:CB	2.49	0.40
1:A:478:SER:HA	10:A:892:HOH:O	2.21	0.40
1:A:464:THR:HG21	1:A:466:LYS:HB2	2.03	0.40
1:A:143:ASP:O	1:A:146:LEU:HB2	2.21	0.40
2:B:171:GLU:O	2:B:187:THR:HB	2.22	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)
10:A:925:HOH:O	10:B:877:HOH:O[2_655]	2.18	0.02

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	480/493 (97%)	448 (93%)	25 (5%)	7 (2%)	13	38
2	B	372/382 (97%)	350 (94%)	16 (4%)	6 (2%)	12	36
All	All	852/875 (97%)	798 (94%)	41 (5%)	13 (2%)	13	38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	GLU
2	B	326	ASP
1	A	415	CYS
2	B	266	TYR
2	B	269	GLY
1	A	65	ASN
2	B	178	GLU
1	A	284	ASN
1	A	478	SER
2	B	275	THR
1	A	416	ASP
2	B	260	ILE
1	A	417	VAL

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	408/416 (98%)	345 (85%)	63 (15%)	3	9
2	B	311/316 (98%)	267 (86%)	44 (14%)	4	11
All	All	719/732 (98%)	612 (85%)	107 (15%)	4	10

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LEU
1	A	10	ARG
1	A	13	LYS
1	A	15	THR
1	A	31	LEU
1	A	57	PHE
1	A	65	ASN
1	A	71	GLU
1	A	78	LYS
1	A	88	TYR
1	A	107	VAL
1	A	109	VAL
1	A	129	LEU
1	A	137	ARG
1	A	146	LEU
1	A	149	ILE
1	A	150	LYS
1	A	151	GLN
1	A	154	PHE
1	A	157	ASP
1	A	165	LEU
1	A	169	LEU
1	A	174	LYS
1	A	195	VAL
1	A	205	LEU
1	A	213	THR

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Mol	Chain	Res	Type
1	A	219	THR
1	A	221	LEU
1	A	225	ASN
1	A	230	VAL
1	A	265	LEU
1	A	267	ARG
1	A	273	VAL
1	A	279	LYS
1	A	287	VAL
1	A	290	VAL
1	A	323	LEU
1	A	331	SER
1	A	340	ILE
1	A	341	LYS
1	A	370	ILE
1	A	372	LYS
1	A	379	GLN
1	A	382	ILE
1	A	385	GLU
1	A	399	ARG
1	A	404	LYS
1	A	407	LEU
1	A	408	GLU
1	A	410	VAL
1	A	415	CYS
1	A	416	ASP
1	A	417	VAL
1	A	427	ARG
1	A	438	ARG
1	A	441	HIS
1	A	442	LEU
1	A	472	ASP
1	A	477	ARG
1	A	484	LYS
1	A	488	LEU
1	A	490	ARG
2	B	4	GLU
2	B	18	VAL
2	B	31	VAL
2	B	32	THR
2	B	33	VAL
2	B	67	SER

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Mol	Chain	Res	Type
2	B	87	TYR
2	B	91	LEU
2	B	98	LYS
2	B	102	ARG
2	B	106	ILE
2	B	116	LEU
2	B	118	THR
2	B	131	ILE
2	B	165	LYS
2	B	167	LEU
2	B	178	GLU
2	B	179	ASN
2	B	181	GLU
2	B	186	LYS
2	B	188	ASN
2	B	191	ILE
2	B	193	LYS
2	B	197	VAL
2	B	207	LEU
2	B	233	ILE
2	B	235	ARG
2	B	242	VAL
2	B	252	LEU
2	B	274	LEU
2	B	279	GLU
2	B	281	LEU
2	B	290	LYS
2	B	291	ILE
2	B	292	ILE
2	B	295	LEU
2	B	298	LEU
2	B	299	LEU
2	B	323	GLU
2	B	344	VAL
2	B	353	THR
2	B	356	LYS
2	B	358	LYS
2	B	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	126	GLN
1	A	151	GLN
1	A	170	ASN
1	A	172	ASN
1	A	225	ASN
1	A	241	ASN
1	A	284	ASN
1	A	294	ASN
1	A	338	HIS
1	A	406	ASN
1	A	434	GLN
1	A	462	GLN
2	B	22	HIS
2	B	108	ASN
2	B	140	ASN
2	B	188	ASN
2	B	199	ASN
2	B	225	HIS
2	B	239	ASN
2	B	257	HIS
2	B	297	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
8	ATP	A	801	-	26,33,33	0.69	0	26,52,52	2.17	3 (11%)
7	FMN	A	802	-	32,33,33	1.96	4 (12%)	34,50,50	2.26	10 (29%)
9	CXS	A	803	-	14,14,14	3.78	2 (14%)	17,18,18	2.55	5 (29%)
5	SO4	A	806	-	4,4,4	0.18	0	6,6,6	0.34	0
6	FAD	B	800	-	52,58,58	1.15	3 (5%)	52,89,89	2.47	12 (23%)

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
8	ATP	A	801	-	-	0/18/38/38	0/3/3/3
7	FMN	A	802	-	1/1/4/4	0/18/18/18	0/3/3/3
9	CXS	A	803	-	-	0/8/16/16	0/1/1/1
5	SO4	A	806	-	-	0/0/0/0	0/0/0/0
6	FAD	B	800	-	-	0/30/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	803	CXS	C1-S	-12.62	1.58	1.77
7	A	802	FMN	O4'-C4'	-9.15	1.23	1.43
9	A	803	CXS	C2-C1	-5.83	1.34	1.52
7	A	802	FMN	C1'-N10	-2.39	1.45	1.48
6	B	800	FAD	C9A-N10	-2.37	1.35	1.38
7	A	802	FMN	C4A-N5	2.09	1.36	1.33
6	B	800	FAD	C10-N10	2.49	1.42	1.39
7	A	802	FMN	C9A-N10	2.66	1.42	1.38
6	B	800	FAD	C4X-C10	4.70	1.49	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	800	FAD	N3A-C2A-N1A	-10.15	120.90	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	ATP	N3-C2-N1	-9.15	121.69	128.87
7	A	802	FMN	N3-C2-N1	-3.99	120.96	127.69
6	B	800	FAD	C4X-C10-N10	-3.95	117.65	120.52
6	B	800	FAD	C1B-N9A-C4A	-3.60	122.79	126.81
6	B	800	FAD	C4-C4X-C10	-3.54	117.67	119.94
6	B	800	FAD	C4X-C4-N3	-3.42	119.05	123.52
6	B	800	FAD	N3-C2-N1	-3.08	122.50	127.69
7	A	802	FMN	C4A-C4-N3	-2.79	119.88	123.52
8	A	801	ATP	C1'-N9-C4	-2.66	123.83	126.81
7	A	802	FMN	C4-C4A-C10	-2.20	118.53	119.94
6	B	800	FAD	C4B-O4B-C1B	-2.01	107.52	109.64
7	A	802	FMN	C4-C4A-N5	2.09	121.24	118.70
9	A	803	CXS	O2-S-C1	2.39	108.56	106.87
8	A	801	ATP	O4'-C1'-N9	2.42	112.67	108.11
7	A	802	FMN	C1'-N10-C9A	2.43	121.65	118.83
6	B	800	FAD	O4B-C1B-N9A	2.45	112.73	108.11
7	A	802	FMN	O2'-C2'-C3'	2.65	115.78	108.96
9	A	803	CXS	O1-S-C1	3.14	109.09	106.87
6	B	800	FAD	C4X-N5-C5X	3.27	120.57	116.72
6	B	800	FAD	C4-C4X-N5	3.31	122.73	118.70
9	A	803	CXS	O3-S-C1	3.31	111.88	104.99
9	A	803	CXS	C3-C2-C1	3.49	117.98	112.01
7	A	802	FMN	O4'-C4'-C3'	3.93	119.08	108.96
7	A	802	FMN	C4A-N5-C5A	4.68	122.24	116.72
7	A	802	FMN	O4'-C4'-C5'	5.10	121.22	110.09
6	B	800	FAD	C5X-C9A-N10	5.29	121.54	117.58
7	A	802	FMN	C4-N3-C2	6.17	120.31	115.16
9	A	803	CXS	C2-C1-S	7.66	125.64	113.15
6	B	800	FAD	C4-N3-C2	8.32	122.10	115.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	802	FMN	C4'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	ATP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	800	FAD	5	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	484/493 (98%)	0.18	3 (0%)	90 89	21, 34, 50, 56	0
2	B	374/382 (97%)	0.16	2 (0%)	91 90	24, 34, 46, 54	0
All	All	858/875 (98%)	0.17	5 (0%)	90 89	21, 34, 49, 56	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	50	GLY	3.9
1	A	478	SER	2.9
1	A	416	ASP	2.8
1	A	377	ASP	2.6
2	B	178	GLU	2.2

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(\AA^2)	Q<0.9
7	FMN	A	802	31/31	0.94	0.25	1.26	58,61,63,63	0
9	CXS	A	803	14/14	0.94	0.23	0.91	43,47,56,56	0
3	FE	A	805	1/1	0.94	0.24	0.88	33,33,33,33	1
5	SO4	A	806	5/5	0.85	0.18	-0.35	69,69,70,70	0
6	FAD	B	800	53/53	0.98	0.19	-0.63	21,24,25,26	0
8	ATP	A	801	31/31	0.99	0.16	-1.17	17,24,26,27	0
4	CL	B	804	1/1	0.97	0.15	-3.17	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.