Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:31 PM GMT

PDB ID	:	1KNP
Title	:	E. coli L-aspartate oxidase: mutant R386L in complex with succinate
Authors	:	Bossi, R.T.; Mattevi, A.
Deposited on	:	2001-12-19
Resolution	:	2.60 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:

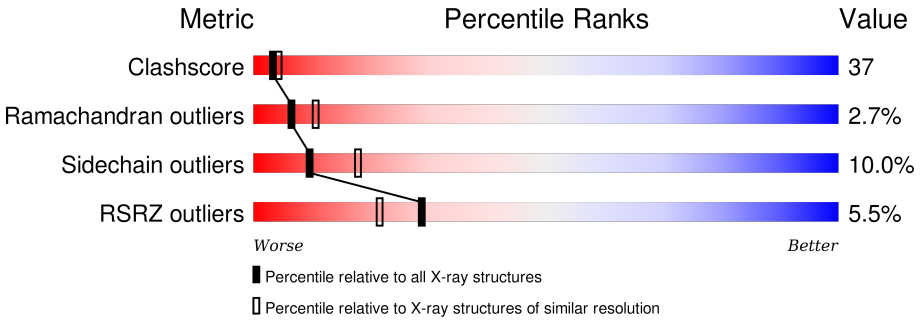
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	540	5% 50% 38% 8%

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	SIN	A	801	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4232 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-aspartate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4150	2607	749	773	21			

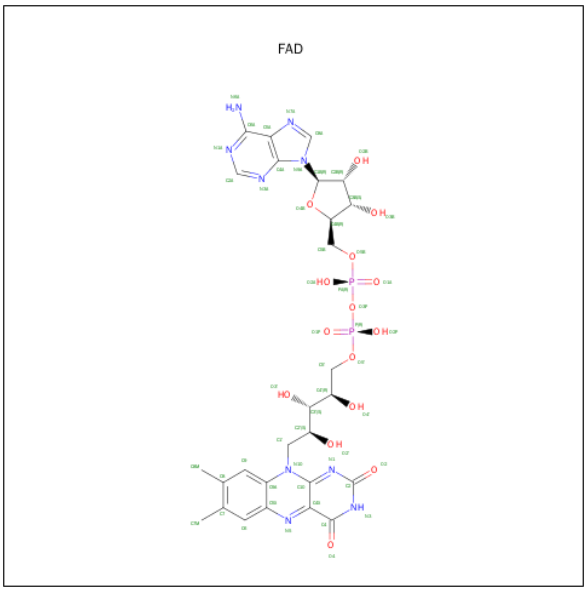
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	ARG	ENGINEERED	UNP P10902

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

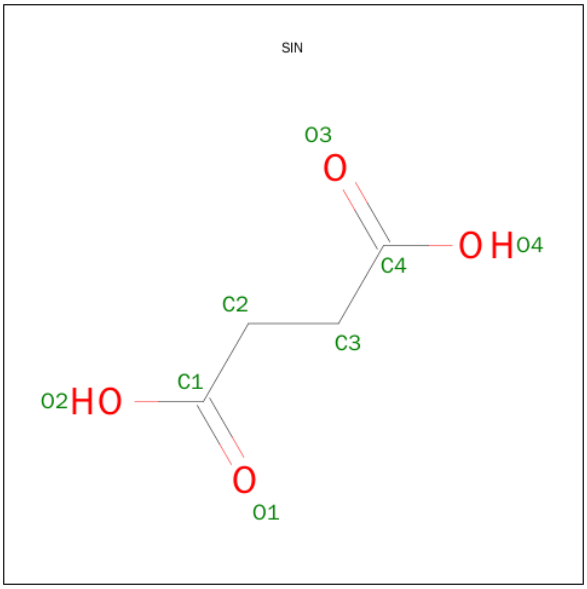
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

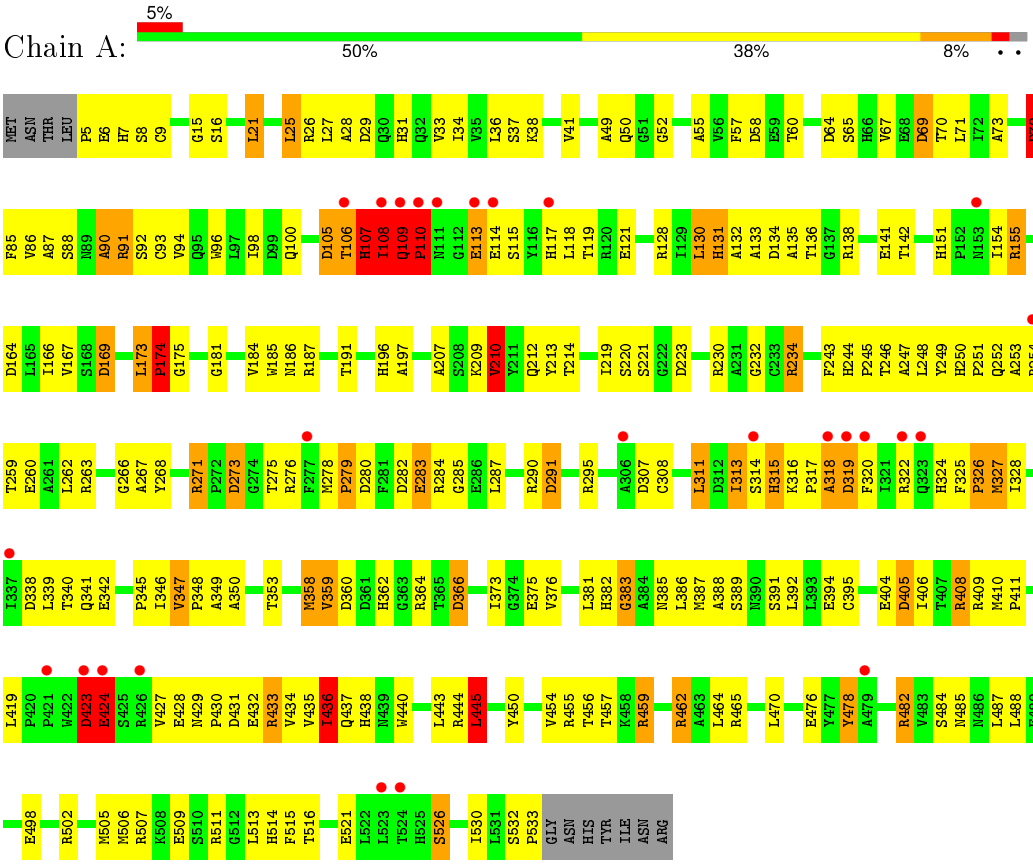
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		

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: L-aspartate oxidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	72.54Å 72.54Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 39.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.9 (40.00-2.60) 92.9 (39.48-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.230 , 0.281 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 91.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24658 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4232	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: NA, SIN, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.13	3/4244 (0.1%)	1.32	34/5767 (0.6%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	GLU	CD-OE2	6.93	1.33	1.25
1	A	210	VAL	CB-CG1	-6.71	1.38	1.52
1	A	454	VAL	CB-CG1	5.86	1.65	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	ASP	CB-CG-OD2	10.21	127.49	118.30
1	A	431	ASP	CB-CG-OD2	9.68	127.01	118.30
1	A	436	ILE	CG1-CB-CG2	-9.00	91.61	111.40
1	A	280	ASP	CB-CG-OD2	8.52	125.96	118.30
1	A	79	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	169	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	358	MET	CG-SD-CE	-7.70	87.88	100.20
1	A	273	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	210	VAL	CB-CA-C	-7.11	97.89	111.40
1	A	64	ASP	CB-CG-OD2	7.01	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	408	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	445	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	A	462	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	25	LEU	CA-CB-CG	-6.12	101.21	115.30
1	A	110	PRO	N-CA-C	-6.09	96.26	112.10
1	A	234	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	506	MET	CG-SD-CE	-5.89	90.78	100.20
1	A	109	GLN	N-CA-C	5.87	126.86	111.00
1	A	408	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	69	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	366	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	360	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	465	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	109	GLN	CB-CA-C	-5.33	99.74	110.40
1	A	291	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	405	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	175	GLY	N-CA-C	-5.29	99.88	113.10
1	A	279	PRO	N-CD-CG	-5.24	95.34	103.20
1	A	459	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	71	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	271	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	80	ARG	N-CA-C	5.06	124.67	111.00
1	A	311	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ILE	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	4150	0	4061	304	2
2	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	9	0
4	A	8	0	4	5	0
5	A	20	0	0	9	0
All	All	4232	0	4096	308	2

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 37.

All (308) 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:155:ARG:HH21	1:A:155:ARG:CB	1.11	1.57
1:A:327:MET:CE	1:A:327:MET:SD	2.01	1.48
1:A:155:ARG:NH2	1:A:155:ARG:HB3	1.13	1.40
2:A:541:NA:NA	5:A:812:HOH:O	0.90	1.35
1:A:502:ARG:HD2	5:A:811:HOH:O	1.38	1.23
1:A:91:ARG:HA	1:A:94:VAL:HB	1.19	1.18
1:A:109:GLN:CG	1:A:109:GLN:O	1.89	1.17
1:A:160:THR:CG2	1:A:184:VAL:HG11	1.77	1.15
1:A:155:ARG:CG	1:A:155:ARG:HH21	1.60	1.14
1:A:290:ARG:HH22	4:A:801:SIN:H32	1.13	1.13
1:A:313:ILE:N	1:A:313:ILE:HD12	1.58	1.11
1:A:250:HIS:CD2	1:A:252:GLN:H	1.67	1.11
1:A:91:ARG:N	5:A:818:HOH:O	1.88	1.06
1:A:416:ILE:HD12	1:A:416:ILE:H	1.17	1.06
1:A:478:TYR:O	1:A:491:ARG:NH2	1.93	1.02
1:A:487:LEU:HD21	1:A:491:ARG:HH21	1.21	1.01
1:A:424:GLU:HG2	1:A:424:GLU:O	1.55	1.00
1:A:313:ILE:H	1:A:313:ILE:CD1	1.73	1.00
1:A:327:MET:HG3	1:A:328:ILE:N	1.76	0.99
1:A:109:GLN:HG2	1:A:109:GLN:O	1.17	0.98
1:A:91:ARG:HG2	5:A:818:HOH:O	1.63	0.97
1:A:110:PRO:HD2	1:A:113:GLU:O	1.65	0.97
1:A:313:ILE:H	1:A:313:ILE:HD12	0.82	0.96
1:A:268:TYR:CE1	1:A:276:ARG:NH1	2.33	0.96
1:A:57:PHE:CD2	1:A:91:ARG:NH2	2.34	0.95
1:A:58:ASP:OD1	1:A:60:THR:HB	1.67	0.95
1:A:290:ARG:NH2	4:A:801:SIN:H32	1.83	0.94
1:A:250:HIS:HD2	1:A:252:GLN:N	1.64	0.93
1:A:327:MET:CE	1:A:327:MET:HB2	1.99	0.93
1:A:234:ARG:HB2	1:A:358:MET:HE3	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:O	1:A:93:CYS:N	2.04	0.90
1:A:33:VAL:CG1	1:A:154:ILE:HG12	2.02	0.89
1:A:134:ASP:OD2	1:A:328:ILE:HD12	1.72	0.89
1:A:90:ALA:O	1:A:94:VAL:N	2.05	0.89
1:A:91:ARG:CG	5:A:818:HOH:O	2.20	0.88
1:A:160:THR:CG2	1:A:184:VAL:CG1	2.50	0.88
1:A:268:TYR:CD1	1:A:276:ARG:NH1	2.41	0.87
1:A:96:TRP:O	1:A:100:GLN:HG2	1.75	0.87
1:A:424:GLU:O	1:A:424:GLU:CG	2.22	0.86
1:A:160:THR:HG22	1:A:184:VAL:HG11	1.58	0.86
1:A:416:ILE:H	1:A:416:ILE:CD1	1.77	0.86
1:A:160:THR:HG23	1:A:184:VAL:HG11	1.55	0.85
1:A:250:HIS:HD2	1:A:252:GLN:H	0.86	0.84
1:A:416:ILE:HD12	1:A:416:ILE:N	1.93	0.84
1:A:268:TYR:CE2	1:A:315:HIS:CD2	2.66	0.83
1:A:91:ARG:HA	1:A:94:VAL:CB	2.08	0.81
1:A:109:GLN:C	1:A:110:PRO:O	2.10	0.81
1:A:433:ARG:O	1:A:436:ILE:HG22	1.80	0.81
1:A:327:MET:HE2	1:A:327:MET:HB2	1.63	0.80
1:A:160:THR:HG23	1:A:184:VAL:CG1	2.11	0.80
1:A:173:LEU:HD23	1:A:174:PRO:CD	2.12	0.79
1:A:234:ARG:CB	1:A:358:MET:HE3	2.11	0.79
1:A:258:LEU:HD12	1:A:346:ILE:CG2	2.13	0.79
1:A:436:ILE:HG12	1:A:490:LEU:HD22	1.64	0.77
1:A:155:ARG:NH2	1:A:155:ARG:CB	1.91	0.77
1:A:314:SER:O	1:A:316:LYS:N	2.18	0.76
1:A:487:LEU:HD21	1:A:491:ARG:NH2	1.99	0.76
1:A:160:THR:HG22	1:A:184:VAL:CG1	2.15	0.76
1:A:57:PHE:CZ	1:A:91:ARG:HB3	2.21	0.75
1:A:266:GLY:O	1:A:315:HIS:HE1	1.70	0.75
1:A:260:GLU:HG3	1:A:263:ARG:NH2	2.02	0.75
1:A:290:ARG:HH22	4:A:801:SIN:C3	1.98	0.75
1:A:196:HIS:ND1	1:A:419:LEU:HD12	2.02	0.75
1:A:155:ARG:CG	1:A:155:ARG:NH2	2.29	0.75
1:A:159:ARG:HH21	1:A:187:ARG:HH11	1.34	0.74
1:A:331:LYS:O	1:A:331:LYS:HG3	1.85	0.74
1:A:173:LEU:HD23	1:A:174:PRO:HD3	1.69	0.74
1:A:424:GLU:N	1:A:424:GLU:CD	2.40	0.74
1:A:258:LEU:HD12	1:A:346:ILE:HG22	1.68	0.73
1:A:52:GLY:HA2	1:A:136:THR:HG21	1.70	0.73
1:A:314:SER:C	1:A:316:LYS:H	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:N	1:A:115:SER:O	2.16	0.72
1:A:291:ASP:HB3	1:A:513:LEU:HD23	1.70	0.71
1:A:106:THR:HG22	1:A:107:HIS:O	1.90	0.71
1:A:249:TYR:HB2	1:A:347:VAL:HG22	1.71	0.71
1:A:455:ARG:HH11	1:A:514:HIS:HD2	1.36	0.71
1:A:268:TYR:CD2	1:A:315:HIS:CD2	2.79	0.70
1:A:33:VAL:HG11	1:A:154:ILE:HG12	1.73	0.70
1:A:173:LEU:CD2	1:A:174:PRO:HD2	2.22	0.70
1:A:271:ARG:HD2	1:A:275:THR:OG1	1.91	0.70
3:A:800:FAD:C10	4:A:801:SIN:O4	2.41	0.69
1:A:90:ALA:C	1:A:94:VAL:H	1.96	0.69
1:A:266:GLY:O	1:A:315:HIS:CE1	2.46	0.69
1:A:262:LEU:HD13	1:A:311:LEU:CD2	2.23	0.69
1:A:487:LEU:CD2	1:A:491:ARG:HH21	2.02	0.68
1:A:254:ARG:O	1:A:255:ASN:OD1	2.12	0.68
1:A:69:ASP:HB3	1:A:387:MET:HE1	1.75	0.68
1:A:108:ILE:HG13	1:A:109:GLN:CB	2.23	0.68
1:A:38:LYS:HE2	1:A:223:ASP:OD2	1.94	0.68
1:A:28:ALA:HB1	1:A:151:HIS:CE1	2.29	0.68
1:A:327:MET:CB	1:A:327:MET:CE	2.72	0.67
1:A:478:TYR:O	1:A:491:ARG:CZ	2.42	0.67
1:A:404:GLU:HB3	1:A:408:ARG:HH12	1.60	0.67
1:A:359:VAL:HA	1:A:364:ARG:O	1.95	0.67
1:A:262:LEU:HD13	1:A:311:LEU:HD23	1.76	0.66
1:A:167:VAL:HG12	1:A:169:ASP:OD1	1.96	0.66
1:A:134:ASP:HB3	1:A:325:PHE:HD2	1.61	0.65
1:A:173:LEU:HD23	1:A:174:PRO:HD2	1.77	0.65
1:A:314:SER:C	1:A:316:LYS:N	2.50	0.65
1:A:131:HIS:CE1	5:A:808:HOH:O	2.50	0.64
1:A:423:ASP:O	1:A:424:GLU:C	2.36	0.64
1:A:405:ASP:O	1:A:409:ARG:HG3	1.98	0.64
1:A:433:ARG:CG	1:A:433:ARG:HH11	2.09	0.64
1:A:268:TYR:CD2	1:A:315:HIS:NE2	2.67	0.62
1:A:212:GLN:OE1	1:A:213:TYR:CZ	2.53	0.62
1:A:55:ALA:HB2	1:A:94:VAL:HG21	1.81	0.61
1:A:450:TYR:CD1	1:A:459:ARG:HB3	2.35	0.61
1:A:327:MET:CE	1:A:327:MET:CG	2.77	0.61
1:A:511:ARG:NH2	1:A:526:SER:HB2	2.14	0.61
1:A:81:HIS:HA	5:A:817:HOH:O	1.99	0.61
1:A:138:ARG:O	1:A:142:THR:HB	1.99	0.61
1:A:278:MET:N	1:A:279:PRO:HD3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:OE1	1:A:260:GLU:HB3	2.00	0.61
1:A:90:ALA:C	1:A:94:VAL:HG23	2.22	0.60
1:A:117:HIS:O	1:A:118:LEU:HD23	2.01	0.60
1:A:57:PHE:HD2	1:A:91:ARG:NH2	1.94	0.60
1:A:353:THR:N	1:A:375:GLU:OE2	2.30	0.60
1:A:432:GLU:HA	1:A:435:VAL:HG23	1.83	0.59
1:A:86:VAL:HG12	1:A:87:ALA:N	2.17	0.59
1:A:55:ALA:O	1:A:128:ARG:HB2	2.02	0.58
1:A:155:ARG:NH2	1:A:155:ARG:HG2	2.15	0.58
1:A:433:ARG:CG	1:A:433:ARG:NH1	2.66	0.58
1:A:325:PHE:N	1:A:326:PRO:HD3	2.18	0.58
1:A:110:PRO:CD	1:A:113:GLU:O	2.46	0.58
1:A:278:MET:HB3	1:A:285:GLY:HA2	1.85	0.58
1:A:106:THR:HG21	1:A:114:GLU:OE2	2.04	0.57
1:A:79:ASP:OD1	1:A:79:ASP:C	2.43	0.57
1:A:346:ILE:HD12	1:A:346:ILE:O	2.04	0.57
1:A:478:TYR:O	1:A:491:ARG:NH1	2.37	0.57
1:A:57:PHE:CE2	1:A:91:ARG:NH2	2.68	0.57
1:A:108:ILE:HG13	1:A:109:GLN:HB3	1.85	0.57
1:A:212:GLN:OE1	1:A:213:TYR:CE2	2.57	0.57
1:A:482:ARG:HG2	1:A:482:ARG:O	2.04	0.57
1:A:433:ARG:HG2	1:A:433:ARG:NH1	2.20	0.57
1:A:313:ILE:N	1:A:313:ILE:CD1	2.36	0.56
1:A:404:GLU:HB3	1:A:408:ARG:NH1	2.19	0.56
1:A:440:TRP:O	1:A:444:ARG:HG3	2.06	0.55
1:A:27:LEU:O	1:A:31:HIS:HD2	1.88	0.55
1:A:90:ALA:O	1:A:93:CYS:CA	2.54	0.55
1:A:250:HIS:C	1:A:250:HIS:CD2	2.80	0.55
1:A:7:HIS:O	1:A:196:HIS:HD2	1.89	0.55
1:A:427:VAL:HG12	1:A:428:GLU:N	2.22	0.54
1:A:219:ILE:O	1:A:221:SER:N	2.39	0.54
1:A:313:ILE:HD11	1:A:339:LEU:CD1	2.38	0.54
1:A:455:ARG:NH1	1:A:514:HIS:HD2	2.05	0.54
1:A:313:ILE:HD11	1:A:339:LEU:HD12	1.90	0.54
1:A:388:ALA:O	1:A:389:SER:HB2	2.08	0.54
1:A:36:LEU:HD22	1:A:160:THR:HG21	1.89	0.53
1:A:317:PRO:O	1:A:318:ALA:C	2.45	0.53
1:A:291:ASP:HB2	1:A:295:ARG:HH22	1.72	0.53
1:A:49:ALA:HB1	3:A:800:FAD:C4X	2.39	0.53
1:A:234:ARG:HG2	1:A:532:SER:HB3	1.91	0.52
1:A:258:LEU:CD1	1:A:346:ILE:HG22	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HG12	1:A:490:LEU:CD2	2.36	0.52
1:A:278:MET:N	1:A:279:PRO:CD	2.73	0.52
1:A:41:VAL:HG22	1:A:41:VAL:O	2.09	0.52
1:A:118:LEU:HD22	1:A:130:LEU:HD22	1.91	0.52
1:A:109:GLN:O	1:A:110:PRO:O	2.27	0.52
1:A:268:TYR:CE2	1:A:315:HIS:NE2	2.77	0.52
1:A:57:PHE:CE1	1:A:91:ARG:HB3	2.45	0.52
1:A:325:PHE:N	1:A:326:PRO:CD	2.73	0.51
1:A:173:LEU:HD22	1:A:174:PRO:HD2	1.92	0.51
1:A:260:GLU:HG3	1:A:263:ARG:CZ	2.40	0.51
1:A:187:ARG:HE	1:A:485:ASN:ND2	2.08	0.51
1:A:450:TYR:HD1	1:A:459:ARG:HB3	1.76	0.51
1:A:434:VAL:O	1:A:437:GLN:HB2	2.11	0.51
1:A:34:ILE:HG12	1:A:155:ARG:HB2	1.93	0.51
1:A:118:LEU:CD2	1:A:130:LEU:HD22	2.41	0.51
1:A:373:ILE:O	1:A:373:ILE:HG13	2.11	0.50
1:A:282:ASP:OD1	1:A:284:ARG:HB2	2.11	0.50
1:A:173:LEU:CD2	1:A:174:PRO:CD	2.83	0.50
1:A:258:LEU:HD12	1:A:346:ILE:HG21	1.93	0.50
1:A:69:ASP:HB3	1:A:387:MET:CE	2.40	0.50
1:A:340:THR:HG22	1:A:341:GLN:OE1	2.12	0.50
1:A:232:GLY:C	1:A:533:PRO:HG3	2.31	0.50
1:A:507:ARG:HG2	1:A:509:GLU:HG2	1.93	0.50
1:A:410:MET:N	1:A:411:PRO:CD	2.74	0.50
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.12	0.50
1:A:307:ASP:O	1:A:308:CYS:HB3	2.12	0.49
1:A:109:GLN:O	1:A:110:PRO:C	2.47	0.49
1:A:317:PRO:O	1:A:319:ASP:N	2.45	0.49
1:A:187:ARG:HE	1:A:485:ASN:HD21	1.60	0.49
1:A:262:LEU:HD13	1:A:311:LEU:HD21	1.94	0.49
1:A:263:ARG:HA	1:A:267:ALA:HB3	1.95	0.49
1:A:28:ALA:O	1:A:29:ASP:C	2.51	0.49
1:A:158:GLU:O	1:A:159:ARG:C	2.51	0.49
1:A:9:CYS:SG	1:A:197:ALA:HB2	2.53	0.49
1:A:273:ASP:OD2	1:A:273:ASP:C	2.51	0.48
1:A:250:HIS:CD2	1:A:252:GLN:N	2.51	0.48
1:A:392:LEU:HG	3:A:800:FAD:C2	2.43	0.48
1:A:15:GLY:HA2	3:A:800:FAD:H1B	1.94	0.48
1:A:291:ASP:CB	1:A:513:LEU:HD23	2.40	0.48
1:A:69:ASP:C	1:A:387:MET:HE3	2.33	0.48
1:A:106:THR:CG2	1:A:107:HIS:O	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:HB3	1:A:325:PHE:CD2	2.46	0.48
1:A:262:LEU:CD1	1:A:311:LEU:CD2	2.91	0.48
1:A:250:HIS:CD2	1:A:251:PRO:HD2	2.49	0.48
1:A:346:ILE:HD12	1:A:346:ILE:C	2.34	0.48
1:A:81:HIS:O	1:A:85:PHE:HB2	2.14	0.48
1:A:250:HIS:CD2	1:A:251:PRO:N	2.82	0.48
1:A:58:ASP:OD1	1:A:60:THR:CB	2.51	0.47
1:A:92:SER:O	1:A:96:TRP:N	2.41	0.47
1:A:381:LEU:HD23	1:A:382:HIS:CE1	2.50	0.47
1:A:358:MET:CE	1:A:530:ILE:HG23	2.44	0.47
1:A:234:ARG:HB3	1:A:358:MET:HE3	1.96	0.47
1:A:245:PRO:HG2	1:A:263:ARG:NH2	2.29	0.47
1:A:28:ALA:HB1	1:A:151:HIS:NE2	2.30	0.47
1:A:133:ALA:HB1	1:A:326:PRO:HG2	1.97	0.47
1:A:291:ASP:HB3	1:A:513:LEU:CD2	2.41	0.47
1:A:169:ASP:OD1	1:A:169:ASP:N	2.46	0.47
1:A:406:ILE:O	1:A:409:ARG:N	2.45	0.47
1:A:427:VAL:CG1	1:A:428:GLU:N	2.78	0.47
1:A:290:ARG:O	1:A:291:ASP:C	2.51	0.47
1:A:436:ILE:HG23	1:A:436:ILE:HD13	1.26	0.46
1:A:259:THR:HG23	1:A:262:LEU:H	1.79	0.46
1:A:423:ASP:C	1:A:424:GLU:CD	2.74	0.46
1:A:382:HIS:O	1:A:383:GLY:C	2.52	0.46
1:A:207:ALA:O	1:A:210:VAL:HG22	2.16	0.46
1:A:248:LEU:HD12	1:A:345:PRO:O	2.15	0.46
1:A:55:ALA:CB	1:A:94:VAL:HG21	2.46	0.46
3:A:800:FAD:C9A	3:A:800:FAD:O2'	2.53	0.46
1:A:291:ASP:OD1	1:A:291:ASP:N	2.48	0.46
1:A:25:LEU:O	1:A:26:ARG:C	2.49	0.46
1:A:257:LEU:HD22	3:A:800:FAD:HM73	1.96	0.46
1:A:362:HIS:CG	1:A:405:ASP:HB2	2.50	0.46
1:A:131:HIS:ND1	1:A:133:ALA:O	2.45	0.46
1:A:33:VAL:HG12	1:A:154:ILE:HG12	1.90	0.46
1:A:244:HIS:O	1:A:348:PRO:HA	2.16	0.46
1:A:209:LYS:HE3	1:A:444:ARG:CZ	2.46	0.45
1:A:187:ARG:NE	1:A:485:ASN:ND2	2.64	0.45
1:A:340:THR:HG22	1:A:341:GLN:CD	2.37	0.45
1:A:435:VAL:O	1:A:436:ILE:C	2.52	0.45
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.75	0.45
1:A:57:PHE:CZ	1:A:91:ARG:CB	2.95	0.45
1:A:185:TRP:CZ3	1:A:187:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:HG3	1:A:328:ILE:H	1.76	0.45
1:A:445:LEU:HD12	1:A:445:LEU:O	2.16	0.45
1:A:49:ALA:HA	3:A:800:FAD:C5X	2.47	0.45
1:A:60:THR:CG2	1:A:60:THR:O	2.62	0.45
1:A:214:THR:O	1:A:255:ASN:HB3	2.17	0.45
1:A:254:ARG:C	1:A:255:ASN:OD1	2.55	0.45
1:A:130:LEU:CD2	1:A:130:LEU:N	2.79	0.45
1:A:338:ASP:N	1:A:342:GLU:OE2	2.42	0.45
1:A:243:PHE:HA	1:A:349:ALA:O	2.17	0.45
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.70	0.45
1:A:134:ASP:CB	1:A:325:PHE:HD2	2.28	0.45
1:A:60:THR:HG22	1:A:60:THR:O	2.14	0.44
1:A:249:TYR:CD2	1:A:249:TYR:O	2.71	0.44
1:A:246:THR:O	1:A:246:THR:OG1	2.28	0.44
1:A:333:LEU:HA	1:A:333:LEU:HD12	1.79	0.44
1:A:424:GLU:N	1:A:424:GLU:OE1	2.50	0.44
1:A:320:PHE:CE1	1:A:324:HIS:HD2	2.36	0.44
1:A:131:HIS:HE1	5:A:808:HOH:O	1.95	0.44
1:A:38:LYS:CE	1:A:223:ASP:OD2	2.64	0.44
1:A:166:ILE:HG13	1:A:181:GLY:C	2.38	0.44
1:A:135:ALA:O	1:A:136:THR:C	2.54	0.44
1:A:434:VAL:O	1:A:437:GLN:N	2.50	0.44
1:A:250:HIS:O	1:A:253:ALA:N	2.36	0.44
1:A:41:VAL:N	1:A:158:GLU:HG2	2.32	0.44
1:A:230:ARG:HD3	5:A:813:HOH:O	2.17	0.43
1:A:234:ARG:HG3	1:A:366:ASP:OD2	2.18	0.43
1:A:456:THR:O	1:A:457:THR:C	2.53	0.43
1:A:33:VAL:HG13	1:A:154:ILE:HG23	2.00	0.43
1:A:244:HIS:CE1	1:A:257:LEU:HD11	2.54	0.43
1:A:455:ARG:HB2	1:A:515:PHE:O	2.18	0.43
1:A:105:ASP:OD1	1:A:132:ALA:HA	2.19	0.43
1:A:187:ARG:NE	1:A:485:ASN:HD21	2.17	0.43
1:A:338:ASP:C	1:A:340:THR:N	2.69	0.43
1:A:108:ILE:HG13	1:A:109:GLN:HB2	2.00	0.43
1:A:186:ASN:OD1	1:A:186:ASN:C	2.57	0.43
1:A:435:VAL:O	1:A:438:HIS:N	2.51	0.43
1:A:464:LEU:HD22	1:A:505:MET:HE1	2.00	0.43
1:A:507:ARG:CG	1:A:509:GLU:HG2	2.49	0.42
1:A:234:ARG:CB	1:A:358:MET:CE	2.93	0.42
1:A:84:GLU:O	1:A:88:SER:N	2.43	0.42
1:A:50:GLN:O	1:A:136:THR:OG1	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	3:A:800:FAD:C6	2.49	0.42
1:A:33:VAL:HG22	1:A:34:ILE:N	2.34	0.42
1:A:262:LEU:CD1	1:A:311:LEU:HD21	2.49	0.42
1:A:376:VAL:HG22	1:A:376:VAL:O	2.19	0.42
1:A:487:LEU:HD11	1:A:491:ARG:NH2	2.35	0.42
1:A:5:PRO:HB2	1:A:6:GLU:H	1.42	0.42
1:A:98:ILE:C	1:A:100:GLN:N	2.73	0.42
1:A:214:THR:OG1	1:A:350:ALA:O	2.28	0.42
1:A:433:ARG:HH11	1:A:433:ARG:HG3	1.83	0.41
1:A:70:THR:N	1:A:387:MET:HE3	2.35	0.41
1:A:247:ALA:O	1:A:347:VAL:N	2.38	0.41
1:A:38:LYS:HG2	1:A:38:LYS:O	2.20	0.41
1:A:73:ALA:O	1:A:385:ASN:HB3	2.20	0.41
1:A:50:GLN:NE2	1:A:257:LEU:O	2.47	0.41
1:A:106:THR:HG23	1:A:107:HIS:N	2.36	0.41
1:A:443:LEU:CD2	1:A:493:LEU:HB3	2.50	0.41
1:A:394:GLU:O	1:A:395:CYS:C	2.57	0.41
1:A:187:ARG:HH21	1:A:485:ASN:HD21	1.67	0.41
1:A:16:SER:HB2	1:A:21:LEU:HD11	2.02	0.41
1:A:498:GLU:HG2	1:A:502:ARG:HD3	2.03	0.41
1:A:185:TRP:HZ3	1:A:187:ARG:HD3	1.86	0.41
1:A:313:ILE:HD13	1:A:339:LEU:O	2.21	0.41
1:A:484:SER:O	1:A:488:LEU:HG	2.21	0.41
1:A:259:THR:OG1	4:A:801:SIN:O1	2.26	0.40
1:A:258:LEU:CD1	1:A:346:ILE:CG2	2.93	0.40
1:A:429:ASN:O	1:A:430:PRO:C	2.59	0.40
1:A:196:HIS:ND1	1:A:419:LEU:CD1	2.79	0.40
1:A:67:VAL:O	1:A:70:THR:N	2.55	0.40
1:A:291:ASP:HB2	1:A:295:ARG:NH2	2.36	0.40
3:A:800:FAD:H1'1	3:A:800:FAD:H9	1.89	0.40
1:A:358:MET:HE1	1:A:530:ILE:HG23	2.02	0.40
1:A:98:ILE:C	1:A:100:GLN:H	2.24	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:OE2	1:A:362:HIS:CE1[6_465]	2.03	0.17
1:A:432:GLU:OE2	1:A:462:ARG:NH2[7_556]	2.12	0.08

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	527/540 (98%)	468 (89%)	45 (8%)	14 (3%)	6 10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ALA
1	A	108	ILE
1	A	315	HIS
1	A	318	ALA
1	A	424	GLU
1	A	110	PRO
1	A	220	SER
1	A	326	PRO
1	A	423	ASP
1	A	107	HIS
1	A	174	PRO
1	A	383	GLY
1	A	109	GLN
1	A	416	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	441/452 (98%)	397 (90%)	44 (10%)	9 18

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	21	LEU
1	A	37	SER
1	A	65	SER
1	A	79	ASP
1	A	80	ARG
1	A	91	ARG
1	A	106	THR
1	A	107	HIS
1	A	113	GLU
1	A	119	THR
1	A	130	LEU
1	A	131	HIS
1	A	155	ARG
1	A	173	LEU
1	A	174	PRO
1	A	191	THR
1	A	210	VAL
1	A	255	ASN
1	A	257	LEU
1	A	283	GLU
1	A	287	LEU
1	A	313	ILE
1	A	319	ASP
1	A	322	ARG
1	A	327	MET
1	A	333	LEU
1	A	347	VAL
1	A	359	VAL
1	A	386	LEU
1	A	391	SER
1	A	415	ASP
1	A	416	ILE
1	A	423	ASP
1	A	424	GLU
1	A	433	ARG
1	A	436	ILE
1	A	445	LEU
1	A	476	GLU
1	A	478	TYR
1	A	482	ARG
1	A	516	THR
1	A	521	GLU

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Mol	Chain	Res	Type
1	A	526	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	32	GLN
1	A	196	HIS
1	A	250	HIS
1	A	315	HIS
1	A	324	HIS
1	A	414	HIS
1	A	485	ASN
1	A	514	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\|>2$
3	FAD	A	800	-	48,58,58	1.41	8 (16%)	54,89,89	2.48	14 (25%)
4	SIN	A	801	-	1,7,7	0.17	0	2,8,8	1.73	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	800	-	-	0/30/50/50	0/6/6/6
4	SIN	A	801	-	-	0/1/5/5	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	FAD	C10-N10	-3.23	1.35	1.39
3	A	800	FAD	C6-C5X	-3.22	1.36	1.41
3	A	800	FAD	O4B-C4B	-2.64	1.38	1.45
3	A	800	FAD	C5A-N7A	-2.02	1.32	1.39
3	A	800	FAD	C2A-N3A	2.12	1.35	1.32
3	A	800	FAD	C4-N3	2.57	1.37	1.33
3	A	800	FAD	C2A-N1A	2.64	1.38	1.33
3	A	800	FAD	C4X-N5	3.54	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	FAD	N3A-C2A-N1A	-11.15	120.36	128.89
3	A	800	FAD	O2'-C2'-C1'	-6.87	93.07	109.94
3	A	800	FAD	C2B-C1B-N9A	-5.71	105.56	114.29
4	A	801	SIN	C2-C3-C4	-2.45	108.26	112.75
3	A	800	FAD	C4X-C4-N3	-2.41	120.30	123.59
3	A	800	FAD	P-O3P-PA	-2.13	126.75	132.73
3	A	800	FAD	C4-C4X-C10	-2.06	118.62	119.94
3	A	800	FAD	N6A-C6A-N1A	2.06	123.63	119.20
3	A	800	FAD	O2A-PA-O3P	2.21	115.13	105.09
3	A	800	FAD	C2A-N1A-C6A	2.48	123.20	118.77
3	A	800	FAD	C1'-C2'-C3'	2.70	117.54	109.82
3	A	800	FAD	C4X-C10-N10	3.27	122.44	120.52
3	A	800	FAD	C1'-N10-C9A	3.61	122.91	118.86
3	A	800	FAD	C5X-C9A-N10	4.06	120.70	117.62
3	A	800	FAD	C4-N3-C2	4.13	118.82	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	FAD	9	0
4	A	801	SIN	5	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, 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	529/540 (97%)	0.31	29 (5%) 29 21	38, 66, 93, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	5.0
1	A	322	ARG	4.5
1	A	417	SER	4.4
1	A	110	PRO	4.3
1	A	111	ASN	3.8
1	A	106	THR	3.5
1	A	416	ILE	3.3
1	A	254	ARG	3.3
1	A	109	GLN	3.1
1	A	337	ILE	3.1
1	A	423	ASP	3.1
1	A	314	SER	3.0
1	A	426	ARG	2.9
1	A	424	GLU	2.9
1	A	323	GLN	2.8
1	A	333	LEU	2.8
1	A	318	ALA	2.6
1	A	113	GLU	2.6
1	A	114	GLU	2.5
1	A	319	ASP	2.5
1	A	320	PHE	2.3
1	A	277	PHE	2.2
1	A	523	LEU	2.2
1	A	108	ILE	2.2
1	A	117	HIS	2.1
1	A	421	PRO	2.1
1	A	306	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	153	ASN	2.0
1	A	524	THR	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
4	SIN	A	801	8/8	0.92	0.28	2.32	81,82,86,89	0
3	FAD	A	800	53/53	0.95	0.18	-0.20	53,61,67,70	0
2	NA	A	541	1/1	0.96	0.13	-3.12	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.