Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:31 AM GMT

PDB ID	:	2HKO
Title	:	Crystal structure of LSD1
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Deposited on	:	2006-07-05
Resolution	:	2.80 Å(reported)

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

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

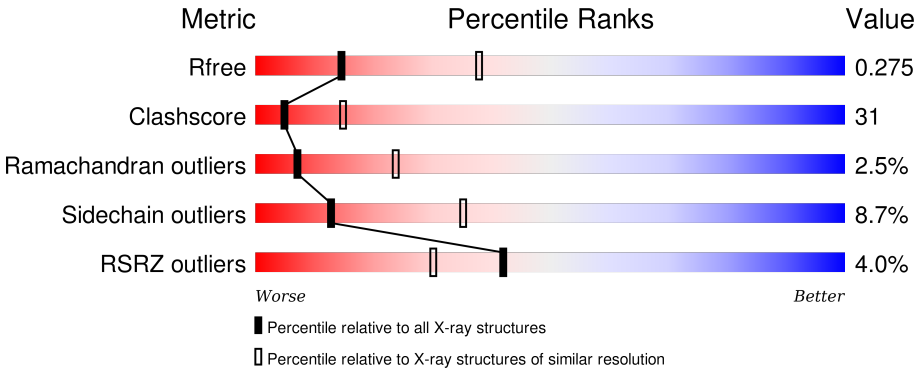
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	664	4%, 51%, 40%, 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5226 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.

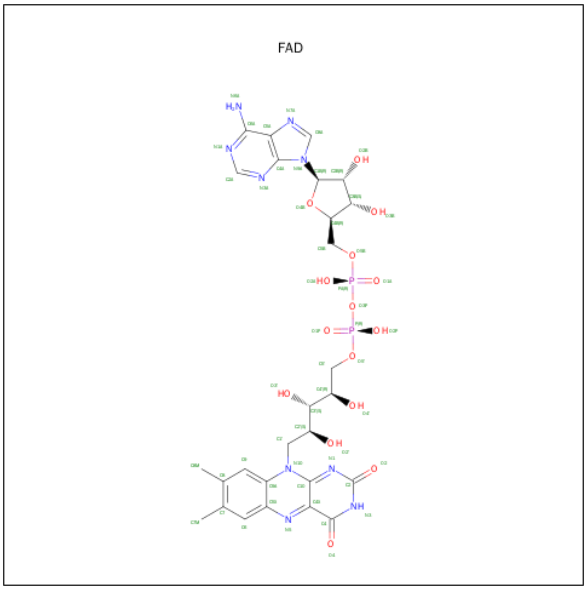
- Molecule 1 is a protein called Lysine-specific histone demethylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	0	0
			5072	3231	881	941	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	594	GLN	ARG	ENGINEERED	UNP O60341

- 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		

- Molecule 3 is water.

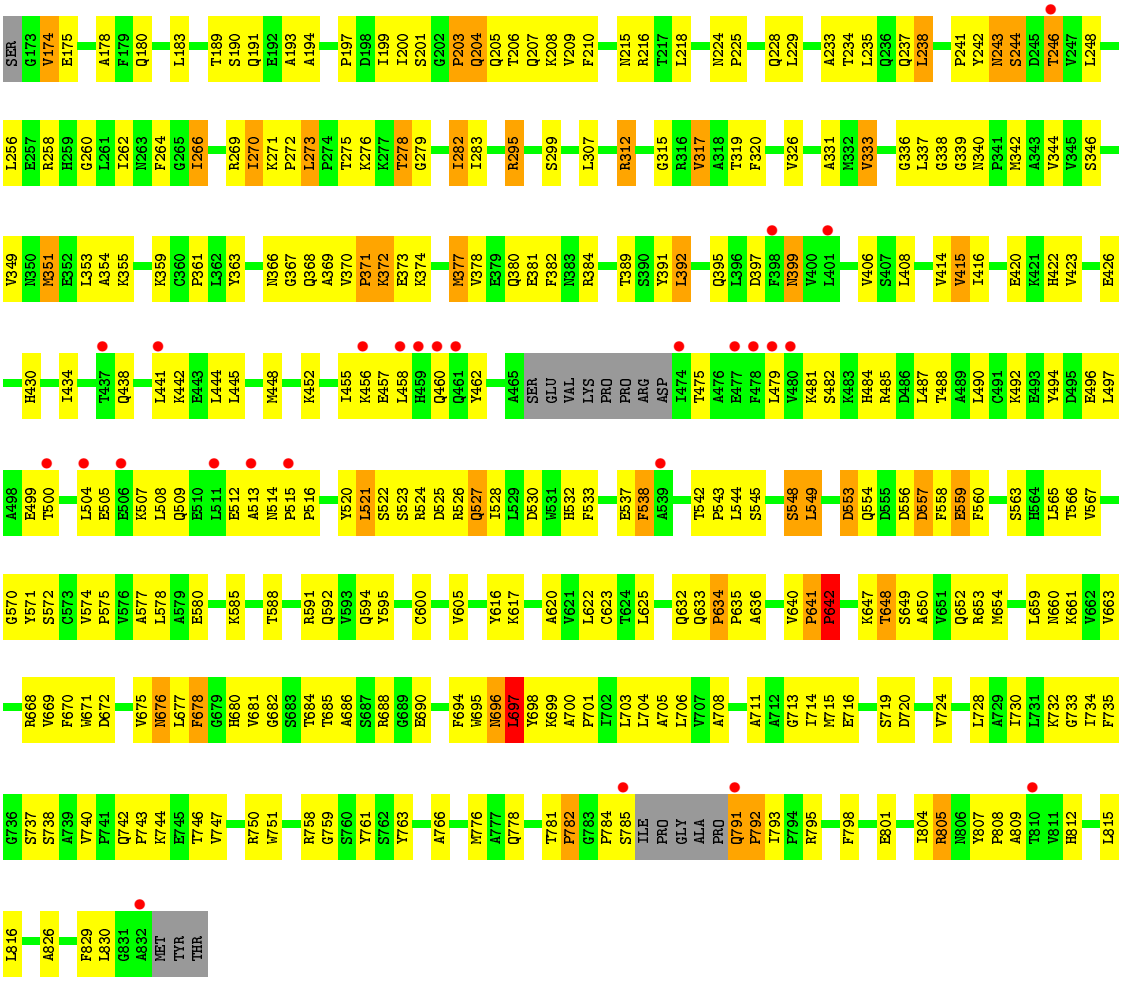
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		

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: Lysine-specific histone demethylase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	187.11Å 187.11Å 106.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 42.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 96.1 (42.83-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.283 0.225 , 0.275	Depositor DCC
R_{free} test set	2622 reflections (9.90%)	DCC
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 26475 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.49	5/5178 (0.1%)	0.71	9/7019 (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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	640	VAL	CB-CG1	-8.26	1.35	1.52
1	A	640	VAL	CB-CG2	-7.61	1.36	1.52
1	A	640	VAL	CA-CB	-6.73	1.40	1.54
1	A	642	PRO	CB-CG	-6.31	1.18	1.50
1	A	785	SER	CA-CB	5.34	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	785	SER	N-CA-C	-13.66	74.12	111.00
1	A	785	SER	N-CA-CB	9.79	125.18	110.50
1	A	782	PRO	N-CA-C	6.33	128.55	112.10
1	A	642	PRO	N-CD-CG	-6.03	94.16	103.20
1	A	641	PRO	N-CD-CG	-5.86	94.42	103.20
1	A	634	PRO	N-CA-C	-5.72	97.22	112.10
1	A	784	PRO	C-N-CA	5.70	135.95	121.70
1	A	784	PRO	CA-C-N	-5.40	105.31	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	ALA	N-CA-C	5.37	125.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	642	PRO	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	5072	0	5099	320	0
2	A	53	0	31	2	0
3	A	101	0	0	8	0
All	All	5226	0	5130	320	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 31.

All (320) 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:672:ASP:HB2	1:A:675:VAL:HG13	1.28	1.15
1:A:732:LYS:HG2	1:A:740:VAL:HG21	1.34	1.08
1:A:566:THR:HG21	1:A:697:LEU:HD11	1.34	1.07
1:A:742:GLN:HG3	1:A:743:PRO:HD2	1.27	1.07
1:A:174:VAL:HG13	1:A:215:ASN:HB3	1.47	0.96
1:A:420:GLU:OE2	1:A:521:LEU:HD21	1.67	0.94
1:A:566:THR:CB	1:A:697:LEU:HD21	1.97	0.94
1:A:204:GLN:HG2	1:A:208:LYS:HE3	1.52	0.89
1:A:672:ASP:O	1:A:675:VAL:HG22	1.76	0.85
1:A:408:LEU:HD23	1:A:544:LEU:HD22	1.59	0.84
1:A:537:GLU:CD	1:A:688:ARG:HH21	1.81	0.84
1:A:649:SER:HB3	1:A:653:ARG:HH12	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:THR:OG1	1:A:697:LEU:HD21	1.78	0.84
1:A:672:ASP:HB2	1:A:675:VAL:CG1	2.06	0.82
1:A:742:GLN:HG3	1:A:743:PRO:CD	2.09	0.81
1:A:685:THR:O	1:A:688:ARG:HG3	1.79	0.81
1:A:633:GLN:O	1:A:635:PRO:HD3	1.80	0.80
1:A:781:THR:HG22	1:A:792:PRO:HB2	1.64	0.79
1:A:434:ILE:HG22	1:A:438:GLN:NE2	1.97	0.79
1:A:566:THR:HG21	1:A:697:LEU:CD1	2.13	0.79
1:A:585:LYS:HD3	3:A:2793:HOH:O	1.81	0.79
1:A:452:LYS:HE3	1:A:494:TYR:OH	1.84	0.78
1:A:371:PRO:HD2	1:A:374:LYS:HG3	1.67	0.77
1:A:367:GLY:O	1:A:733:GLY:O	2.04	0.76
1:A:354:ALA:O	1:A:566:THR:HG22	1.86	0.75
1:A:553:ASP:HB3	1:A:556:ASP:OD2	1.86	0.74
1:A:781:THR:CG2	1:A:792:PRO:HB2	2.18	0.74
1:A:258:ARG:HH22	1:A:830:LEU:HD12	1.53	0.74
1:A:420:GLU:CD	1:A:521:LEU:HD21	2.09	0.73
1:A:370:VAL:HG13	1:A:374:LYS:HB2	1.68	0.73
1:A:538:PHE:HB2	1:A:708:ALA:HB2	1.71	0.73
1:A:660:ASN:HD21	1:A:751:TRP:H	1.37	0.72
1:A:595:TYR:HD2	1:A:782:PRO:HB3	1.54	0.72
1:A:633:GLN:OE1	1:A:633:GLN:HA	1.90	0.71
1:A:434:ILE:HG22	1:A:438:GLN:HE21	1.54	0.71
1:A:690:GLU:HG3	1:A:715:MET:SD	2.31	0.71
1:A:711:ALA:O	1:A:715:MET:HG3	1.90	0.71
1:A:233:ALA:O	1:A:237:GLN:HG3	1.91	0.70
1:A:276:LYS:HD2	1:A:276:LYS:N	2.06	0.70
1:A:633:GLN:O	1:A:635:PRO:CD	2.39	0.70
1:A:275:THR:C	1:A:276:LYS:HD2	2.12	0.70
1:A:557:ASP:N	1:A:557:ASP:OD1	2.25	0.70
1:A:275:THR:HB	1:A:276:LYS:NZ	2.07	0.69
1:A:677:LEU:O	1:A:678:PHE:HB3	1.91	0.69
1:A:359:LYS:HE2	1:A:361:PRO:HD3	1.73	0.69
1:A:566:THR:CG2	1:A:697:LEU:HD11	2.20	0.69
1:A:632:GLN:HG2	3:A:2840:HOH:O	1.93	0.68
1:A:592:GLN:NE2	1:A:594:GLN:NE2	2.41	0.68
1:A:481:LYS:O	1:A:485:ARG:HB2	1.93	0.68
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.75	0.68
1:A:278:THR:HG22	1:A:279:GLY:N	2.09	0.68
1:A:732:LYS:HD3	1:A:737:SER:HA	1.77	0.67
1:A:380:GLN:O	1:A:384:ARG:HG2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:O	1:A:445:LEU:HG	1.95	0.67
1:A:698:TYR:O	1:A:700:ALA:N	2.26	0.66
1:A:193:ALA:HB1	1:A:200:ILE:HD12	1.77	0.66
1:A:805:ARG:O	1:A:808:PRO:HD3	1.96	0.66
1:A:696:ASN:O	1:A:698:TYR:N	2.29	0.65
1:A:452:LYS:HE3	1:A:494:TYR:CZ	2.32	0.65
1:A:237:GLN:C	1:A:238:LEU:HD23	2.17	0.65
1:A:456:LYS:O	1:A:460:GLN:HG3	1.97	0.64
1:A:423:VAL:HG21	1:A:520:TYR:HB2	1.79	0.64
1:A:537:GLU:CD	1:A:688:ARG:NH2	2.51	0.63
1:A:438:GLN:O	1:A:442:LYS:HG3	1.98	0.63
1:A:793:ILE:HD11	1:A:795:ARG:NH2	2.14	0.62
1:A:266:ILE:HD13	1:A:577:ALA:HB1	1.81	0.62
1:A:178:ALA:HB2	1:A:215:ASN:OD1	1.99	0.62
1:A:653:ARG:HH11	1:A:653:ARG:HG3	1.64	0.62
1:A:720:ASP:OD1	1:A:750:ARG:NH2	2.32	0.62
1:A:295:ARG:HG3	3:A:2855:HOH:O	2.00	0.61
1:A:444:LEU:HD21	1:A:500:THR:HB	1.82	0.61
1:A:633:GLN:O	1:A:635:PRO:N	2.33	0.61
1:A:282:ILE:HD11	1:A:616:TYR:HB3	1.82	0.61
1:A:591:ARG:HD2	1:A:605:VAL:CG2	2.30	0.61
1:A:684:THR:HG22	1:A:686:ALA:H	1.66	0.61
1:A:595:TYR:CD2	1:A:782:PRO:HB3	2.35	0.61
1:A:695:TRP:HB2	1:A:704:LEU:HB2	1.83	0.61
1:A:671:TRP:NE1	1:A:696:ASN:OD1	2.30	0.60
1:A:342:MET:CE	1:A:815:LEU:HD13	2.32	0.60
1:A:632:GLN:OE1	1:A:636:ALA:HB2	2.00	0.60
1:A:355:LYS:N	1:A:565:LEU:HD23	2.17	0.60
1:A:530:ASP:O	1:A:533:PHE:HB2	2.02	0.60
1:A:434:ILE:O	1:A:438:GLN:HG3	2.03	0.59
1:A:275:THR:HB	1:A:276:LYS:HZ2	1.67	0.59
1:A:273:LEU:HD11	1:A:299:SER:HA	1.85	0.59
1:A:566:THR:CG2	1:A:697:LEU:HD21	2.32	0.59
1:A:392:LEU:N	1:A:392:LEU:HD23	2.17	0.59
1:A:632:GLN:HE22	1:A:758:ARG:HH21	1.51	0.59
1:A:342:MET:HE1	1:A:815:LEU:HD13	1.85	0.59
1:A:270:ILE:CD1	1:A:271:LYS:HG2	2.32	0.58
1:A:205:GLN:O	1:A:209:VAL:HG23	2.04	0.58
1:A:527:GLN:HG2	1:A:682:GLY:O	2.04	0.58
1:A:537:GLU:OE2	1:A:688:ARG:NH2	2.35	0.58
1:A:271:LYS:O	1:A:271:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:C	1:A:244:SER:H	2.05	0.58
1:A:680:HIS:HD2	1:A:730:ILE:HG23	1.69	0.58
1:A:209:VAL:HG13	1:A:242:TYR:CE1	2.39	0.57
1:A:270:ILE:HD13	1:A:271:LYS:HG2	1.85	0.57
1:A:319:THR:OG1	1:A:572:SER:HB3	2.05	0.57
1:A:381:GLU:OE1	1:A:520:TYR:OH	2.22	0.57
1:A:218:LEU:HD23	1:A:262:ILE:HG22	1.87	0.57
1:A:235:LEU:HD11	1:A:246:THR:HG22	1.86	0.57
1:A:548:SER:HA	1:A:766:ALA:HA	1.85	0.57
1:A:705:ALA:C	1:A:706:LEU:HD23	2.25	0.57
1:A:269:ARG:HH21	1:A:299:SER:HB3	1.70	0.57
1:A:633:GLN:HB3	1:A:634:PRO:HD3	1.86	0.57
1:A:391:TYR:O	1:A:395:GLN:HB2	2.05	0.56
1:A:537:GLU:OE2	1:A:543:PRO:HA	2.06	0.56
1:A:270:ILE:HD13	1:A:271:LYS:N	2.20	0.56
1:A:592:GLN:NE2	1:A:594:GLN:HE21	2.03	0.56
1:A:374:LYS:O	1:A:378:VAL:HG23	2.05	0.56
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.39	0.56
1:A:556:ASP:O	1:A:559:GLU:HG2	2.05	0.56
1:A:455:ILE:HD11	1:A:490:LEU:HB3	1.88	0.56
1:A:663:VAL:HG22	1:A:704:LEU:CD2	2.36	0.56
1:A:317:VAL:O	1:A:317:VAL:HG22	2.06	0.56
1:A:650:ALA:O	1:A:654:MET:HG3	2.05	0.55
1:A:194:ALA:O	1:A:197:PRO:HD3	2.07	0.55
1:A:566:THR:HG21	1:A:697:LEU:HD21	1.89	0.55
1:A:197:PRO:O	1:A:200:ILE:HG22	2.06	0.55
1:A:591:ARG:HD2	1:A:605:VAL:HG23	1.88	0.55
1:A:175:GLU:HA	1:A:175:GLU:OE1	2.07	0.55
1:A:355:LYS:HA	1:A:565:LEU:HD23	1.87	0.55
1:A:632:GLN:NE2	1:A:758:ARG:HE	2.04	0.54
1:A:475:THR:HG22	1:A:475:THR:O	2.07	0.54
1:A:422:HIS:O	1:A:426:GLU:HG3	2.08	0.54
1:A:258:ARG:HH12	1:A:830:LEU:CD1	2.21	0.54
1:A:174:VAL:HG13	1:A:215:ASN:CB	2.31	0.54
1:A:355:LYS:CA	1:A:565:LEU:HD23	2.38	0.53
1:A:189:THR:HG22	1:A:190:SER:N	2.23	0.53
1:A:782:PRO:HG3	1:A:795:ARG:HG3	1.90	0.53
1:A:672:ASP:CB	1:A:675:VAL:HG13	2.20	0.53
1:A:751:TRP:O	1:A:759:GLY:N	2.42	0.53
1:A:444:LEU:O	1:A:448:MET:HG3	2.09	0.53
1:A:623:CYS:SG	1:A:625:LEU:HD12	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:NH2	1:A:315:GLY:O	2.42	0.53
1:A:538:PHE:HB2	1:A:708:ALA:CB	2.39	0.52
1:A:475:THR:O	1:A:479:LEU:HB2	2.08	0.52
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.43	0.52
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.44	0.52
1:A:600:CYS:SG	1:A:795:ARG:HB3	2.49	0.52
1:A:336:GLY:C	1:A:337:LEU:HD23	2.30	0.52
1:A:270:ILE:HD13	1:A:271:LYS:H	1.75	0.52
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.73	0.52
1:A:361:PRO:HG2	1:A:678:PHE:HB2	1.91	0.51
1:A:678:PHE:O	1:A:678:PHE:CD1	2.64	0.51
1:A:238:LEU:HB2	1:A:243:ASN:HB3	1.92	0.51
1:A:654:MET:SD	1:A:776:MET:HG3	2.50	0.51
1:A:740:VAL:O	1:A:740:VAL:HG23	2.10	0.51
1:A:695:TRP:O	1:A:703:LEU:HD12	2.11	0.51
1:A:500:THR:HG22	1:A:504:LEU:HG	1.91	0.51
1:A:826:ALA:O	1:A:830:LEU:HG	2.11	0.51
1:A:342:MET:O	1:A:346:SER:HB2	2.11	0.51
1:A:556:ASP:C	1:A:558:PHE:H	2.13	0.51
1:A:487:LEU:HD23	1:A:487:LEU:O	2.10	0.51
1:A:378:VAL:HG11	1:A:528:ILE:HG22	1.93	0.51
1:A:353:LEU:HA	1:A:566:THR:O	2.11	0.50
1:A:420:GLU:OE2	1:A:521:LEU:HD11	2.11	0.50
1:A:807:TYR:N	1:A:808:PRO:CD	2.74	0.50
1:A:574:VAL:O	1:A:578:LEU:HG	2.12	0.50
1:A:382:PHE:CD1	1:A:532:HIS:HB3	2.47	0.50
1:A:496:GLU:O	1:A:499:GLU:HB3	2.12	0.50
1:A:180:GLN:NE2	1:A:339:GLY:H	2.09	0.50
1:A:653:ARG:NH1	1:A:653:ARG:HG3	2.27	0.50
1:A:620:ALA:HB2	1:A:829:PHE:CZ	2.47	0.50
1:A:482:SER:O	1:A:485:ARG:HB3	2.12	0.49
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.92	0.49
1:A:351:MET:HG2	1:A:353:LEU:HD21	1.93	0.49
1:A:684:THR:HG22	1:A:685:THR:N	2.27	0.49
1:A:488:THR:O	1:A:492:LYS:HG3	2.11	0.49
1:A:371:PRO:O	1:A:372:LYS:HB2	2.11	0.49
1:A:592:GLN:HE21	1:A:594:GLN:NE2	2.07	0.49
1:A:514:ASN:N	1:A:515:PRO:CD	2.75	0.49
1:A:370:VAL:CG1	1:A:374:LYS:HB2	2.41	0.49
1:A:641:PRO:O	1:A:642:PRO:O	2.29	0.49
1:A:648:THR:O	1:A:652:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:OE2	1:A:521:LEU:CD2	2.51	0.49
1:A:591:ARG:HD2	1:A:605:VAL:HG21	1.95	0.49
1:A:566:THR:HB	1:A:697:LEU:HD21	1.88	0.48
1:A:567:VAL:HG12	1:A:570:GLY:H	1.78	0.48
1:A:509:GLN:HA	1:A:512:GLU:OE1	2.13	0.48
1:A:522:SER:H	1:A:525:ASP:HB2	1.78	0.48
1:A:389:THR:HG22	1:A:549:LEU:HD12	1.95	0.48
1:A:751:TRP:HB3	1:A:759:GLY:O	2.14	0.48
1:A:270:ILE:H	1:A:270:ILE:HD13	1.78	0.48
1:A:650:ALA:HB3	1:A:776:MET:HE3	1.96	0.48
1:A:675:VAL:O	1:A:675:VAL:HG23	2.14	0.48
1:A:488:THR:O	1:A:488:THR:HG22	2.14	0.48
1:A:238:LEU:HD23	1:A:238:LEU:N	2.28	0.48
1:A:242:TYR:C	1:A:244:SER:N	2.67	0.47
1:A:189:THR:HG22	1:A:191:GLN:H	1.78	0.47
1:A:566:THR:CB	1:A:697:LEU:CD2	2.83	0.47
1:A:207:GLN:O	1:A:210:PHE:HB3	2.15	0.47
1:A:366:ASN:C	1:A:366:ASN:OD1	2.51	0.47
1:A:370:VAL:HG13	1:A:374:LYS:CB	2.41	0.47
1:A:333:VAL:HB	1:A:565:LEU:O	2.14	0.47
1:A:367:GLY:CA	1:A:733:GLY:O	2.63	0.47
1:A:538:PHE:CE1	1:A:706:LEU:CD1	2.97	0.47
1:A:675:VAL:O	1:A:675:VAL:CG2	2.63	0.47
1:A:728:LEU:O	1:A:732:LYS:HG3	2.14	0.47
1:A:363:TYR:O	1:A:681:VAL:HG23	2.14	0.47
1:A:791:GLN:HA	1:A:792:PRO:HD2	1.62	0.47
1:A:781:THR:HG23	1:A:793:ILE:C	2.35	0.47
1:A:258:ARG:HH12	1:A:830:LEU:HD11	1.79	0.47
1:A:197:PRO:C	1:A:200:ILE:HG22	2.34	0.47
1:A:415:VAL:HG12	1:A:416:ILE:N	2.28	0.47
1:A:734:ILE:HG22	1:A:735:PHE:CE1	2.50	0.47
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.49	0.47
1:A:389:THR:CG2	1:A:549:LEU:HD12	2.45	0.47
1:A:457:GLU:HA	1:A:460:GLN:OE1	2.15	0.47
1:A:641:PRO:C	1:A:642:PRO:O	2.45	0.47
1:A:694:PHE:HA	1:A:704:LEU:O	2.14	0.47
1:A:513:ALA:C	1:A:515:PRO:CD	2.84	0.47
1:A:225:PRO:HB2	1:A:344:VAL:HG13	1.97	0.47
1:A:430:HIS:NE2	1:A:434:ILE:HD11	2.30	0.46
1:A:266:ILE:HG23	1:A:295:ARG:NH2	2.30	0.46
1:A:548:SER:CA	1:A:766:ALA:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:LYS:CG	1:A:740:VAL:HG21	2.24	0.46
1:A:801:GLU:HG2	1:A:809:ALA:H	1.80	0.46
1:A:522:SER:HB2	1:A:525:ASP:H	1.80	0.46
1:A:275:THR:HB	1:A:276:LYS:HZ3	1.79	0.46
1:A:228:GLN:HE21	1:A:269:ARG:HA	1.81	0.46
1:A:363:TYR:N	1:A:363:TYR:CD1	2.84	0.46
1:A:793:ILE:HD11	1:A:795:ARG:CZ	2.45	0.46
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.51	0.46
1:A:337:LEU:HA	1:A:340:ASN:HB3	1.98	0.46
1:A:676:ASN:C	1:A:677:LEU:HD23	2.36	0.46
1:A:706:LEU:N	1:A:706:LEU:HD23	2.29	0.46
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.97	0.46
1:A:204:GLN:O	1:A:207:GLN:N	2.50	0.45
1:A:209:VAL:HG13	1:A:242:TYR:HE1	1.80	0.45
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.51	0.45
1:A:696:ASN:O	1:A:697:LEU:C	2.54	0.45
1:A:256:LEU:HB3	1:A:262:ILE:HG23	1.99	0.45
1:A:189:THR:CG2	1:A:190:SER:N	2.79	0.45
1:A:512:GLU:C	1:A:515:PRO:HD3	2.36	0.45
1:A:734:ILE:HG22	1:A:735:PHE:CD1	2.51	0.45
1:A:455:ILE:CD1	1:A:490:LEU:HB3	2.46	0.45
1:A:533:PHE:O	1:A:537:GLU:HG3	2.16	0.45
1:A:688:ARG:NH1	3:A:2825:HOH:O	2.48	0.45
1:A:732:LYS:NZ	1:A:740:VAL:HG23	2.31	0.45
1:A:698:TYR:C	1:A:700:ALA:N	2.70	0.45
1:A:457:GLU:HG3	1:A:460:GLN:OE1	2.17	0.45
1:A:720:ASP:O	1:A:724:VAL:HG23	2.17	0.45
1:A:282:ILE:CD1	1:A:616:TYR:HB3	2.46	0.45
1:A:349:VAL:HG21	1:A:574:VAL:HA	1.99	0.45
1:A:670:PHE:O	1:A:670:PHE:HD1	1.99	0.45
1:A:696:ASN:C	1:A:698:TYR:N	2.67	0.45
1:A:676:ASN:HD22	1:A:676:ASN:HA	1.48	0.44
1:A:200:ILE:HG23	1:A:201:SER:N	2.32	0.44
1:A:515:PRO:HA	1:A:516:PRO:HD3	1.81	0.44
1:A:225:PRO:CB	1:A:344:VAL:HG13	2.46	0.44
1:A:566:THR:HB	1:A:697:LEU:CD2	2.47	0.44
1:A:448:MET:HE2	1:A:497:LEU:HB2	2.00	0.44
1:A:320:PHE:O	1:A:326:VAL:HA	2.18	0.44
1:A:206:THR:O	1:A:209:VAL:HB	2.18	0.44
1:A:218:LEU:HD23	1:A:262:ILE:CG2	2.48	0.44
1:A:812:HIS:O	1:A:816:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ASN:ND2	1:A:697:LEU:HA	2.32	0.44
1:A:526:ARG:NH2	3:A:2825:HOH:O	2.51	0.44
1:A:781:THR:HG21	1:A:792:PRO:HB2	1.96	0.44
1:A:632:GLN:NE2	1:A:758:ARG:HH21	2.12	0.44
1:A:462:TYR:HH	1:A:484:HIS:CE1	2.35	0.44
1:A:567:VAL:HG12	1:A:570:GLY:N	2.32	0.43
1:A:269:ARG:NH2	3:A:2855:HOH:O	2.51	0.43
1:A:661:LYS:HG2	1:A:706:LEU:HD22	1.99	0.43
1:A:574:VAL:N	1:A:575:PRO:HD2	2.33	0.43
1:A:307:LEU:HD22	1:A:588:THR:HG21	2.01	0.43
1:A:556:ASP:OD1	1:A:559:GLU:OE2	2.36	0.43
1:A:377:MET:O	1:A:380:GLN:HB3	2.18	0.43
1:A:320:PHE:CE1	1:A:747:VAL:HG21	2.54	0.43
1:A:229:LEU:HA	3:A:2764:HOH:O	2.19	0.43
1:A:678:PHE:CD1	1:A:678:PHE:C	2.91	0.43
1:A:530:ASP:HA	1:A:533:PHE:CD2	2.54	0.43
1:A:542:THR:OG1	1:A:543:PRO:HD2	2.19	0.43
1:A:241:PRO:HG2	1:A:242:TYR:CD2	2.54	0.43
1:A:242:TYR:O	1:A:244:SER:N	2.52	0.43
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.85	0.43
1:A:675:VAL:HA	3:A:2852:HOH:O	2.19	0.42
1:A:210:PHE:CD1	1:A:210:PHE:C	2.92	0.42
1:A:441:LEU:HD11	1:A:505:GLU:HG2	2.00	0.42
1:A:738:SER:C	1:A:740:VAL:H	2.23	0.42
1:A:389:THR:HG21	1:A:408:LEU:HD12	2.00	0.42
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.49	0.42
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.02	0.42
1:A:434:ILE:C	1:A:438:GLN:HE21	2.22	0.42
1:A:199:ILE:HD11	1:A:248:LEU:CD1	2.49	0.42
1:A:632:GLN:NE2	1:A:758:ARG:NE	2.67	0.42
1:A:504:LEU:O	1:A:507:LYS:N	2.53	0.41
1:A:647:LYS:HE2	1:A:798:PHE:CE1	2.55	0.41
1:A:670:PHE:O	1:A:670:PHE:CD1	2.73	0.41
1:A:414:VAL:HG12	1:A:415:VAL:N	2.34	0.41
1:A:260:GLY:O	1:A:264:PHE:CD1	2.74	0.41
1:A:677:LEU:N	1:A:677:LEU:HD23	2.36	0.41
1:A:677:LEU:O	1:A:678:PHE:CB	2.63	0.41
1:A:204:GLN:O	1:A:205:GLN:C	2.58	0.41
1:A:406:VAL:CG1	1:A:549:LEU:HD22	2.50	0.41
1:A:235:LEU:HA	1:A:235:LEU:HD23	1.86	0.41
1:A:363:TYR:CE2	1:A:734:ILE:CG2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ILE:O	1:A:804:ILE:HG23	2.20	0.41
1:A:270:ILE:HD11	1:A:271:LYS:HG2	2.01	0.41
1:A:804:ILE:HD13	1:A:807:TYR:HB2	2.02	0.41
1:A:458:LEU:CB	1:A:487:LEU:HG	2.49	0.41
1:A:670:PHE:CD1	1:A:671:TRP:HE3	2.39	0.41
1:A:542:THR:HG21	1:A:763:TYR:CD2	2.56	0.41
1:A:482:SER:HA	1:A:485:ARG:HB3	2.03	0.41
1:A:508:LEU:HG	1:A:512:GLU:OE2	2.21	0.41
1:A:378:VAL:O	1:A:381:GLU:N	2.54	0.41
1:A:373:GLU:O	1:A:374:LYS:C	2.60	0.41
1:A:366:ASN:OD1	1:A:367:GLY:N	2.53	0.41
1:A:801:GLU:CG	1:A:809:ALA:HA	2.51	0.41
1:A:522:SER:C	1:A:524:ARG:N	2.71	0.41
1:A:399:ASN:C	1:A:406:VAL:HG23	2.41	0.40
1:A:258:ARG:NH2	1:A:830:LEU:HD12	2.28	0.40
1:A:337:LEU:HD23	1:A:337:LEU:N	2.36	0.40
1:A:270:ILE:H	1:A:270:ILE:CD1	2.35	0.40
1:A:234:THR:HG22	1:A:234:THR:O	2.20	0.40
1:A:713:GLY:O	1:A:716:GLU:HB2	2.21	0.40
1:A:331:ALA:HA	2:A:2762:FAD:C4X	2.50	0.40
1:A:801:GLU:HB2	2:A:2762:FAD:H5'2	2.02	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	641/664 (96%)	563 (88%)	62 (10%)	16 (2%)	7 24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	278	THR
1	A	678	PHE
1	A	697	LEU
1	A	372	LYS
1	A	699	LYS
1	A	243	ASN
1	A	371	PRO
1	A	548	SER
1	A	792	PRO
1	A	642	PRO
1	A	174	VAL
1	A	272	PRO
1	A	415	VAL
1	A	714	ILE
1	A	338	GLY

5.3.2 Protein sidechains (i)

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	549/564 (97%)	501 (91%)	48 (9%)	13 35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	203	PRO
1	A	204	GLN
1	A	216	ARG
1	A	224	ASN
1	A	238	LEU
1	A	244	SER
1	A	246	THR
1	A	266	ILE
1	A	270	ILE
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	282	ILE
1	A	295	ARG
1	A	312	ARG
1	A	317	VAL
1	A	333	VAL
1	A	351	MET
1	A	368	GLN
1	A	377	MET
1	A	392	LEU
1	A	397	ASP
1	A	399	ASN
1	A	521	LEU
1	A	523	SER
1	A	527	GLN
1	A	538	PHE
1	A	545	SER
1	A	549	LEU
1	A	553	ASP
1	A	554	GLN
1	A	557	ASP
1	A	559	GLU
1	A	563	SER
1	A	571	TYR
1	A	580	GLU
1	A	617	LYS
1	A	648	THR
1	A	659	LEU
1	A	668	ARG
1	A	676	ASN
1	A	696	ASN
1	A	697	LEU
1	A	719	SER
1	A	744	LYS
1	A	746	THR
1	A	778	GLN
1	A	791	GLN
1	A	805	ARG

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	224	ASN

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Mol	Chain	Res	Type
1	A	228	GLN
1	A	383	ASN
1	A	399	ASN
1	A	402	ASN
1	A	438	GLN
1	A	501	GLN
1	A	592	GLN
1	A	594	GLN
1	A	612	GLN
1	A	632	GLN
1	A	660	ASN
1	A	676	ASN
1	A	680	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	2762	-	48,58,58	1.77	8 (16%)	54,89,89	2.07	6 (11%)

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	2762	-	-	0/30/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2762	FAD	C5A-C4A	-2.32	1.35	1.40
2	A	2762	FAD	C4X-C10	2.01	1.44	1.41
2	A	2762	FAD	C9-C8	2.20	1.43	1.37
2	A	2762	FAD	C5X-N5	3.28	1.40	1.35
2	A	2762	FAD	C4A-N3A	3.80	1.41	1.35
2	A	2762	FAD	C4-N3	4.17	1.40	1.33
2	A	2762	FAD	C9A-N10	5.21	1.46	1.38
2	A	2762	FAD	C4X-N5	6.05	1.42	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2762	FAD	C4X-C4-N3	-6.02	115.35	123.59
2	A	2762	FAD	O5B-C5B-C4B	-2.44	100.14	109.12
2	A	2762	FAD	C4B-O4B-C1B	-2.10	107.41	109.72
2	A	2762	FAD	C2B-C1B-N9A	2.35	117.88	114.29
2	A	2762	FAD	O3P-P-O5'	2.59	109.82	102.94
2	A	2762	FAD	C4-N3-C2	11.13	124.87	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2762	FAD	2	0

5.7 Other polymers (i)

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	647/664 (97%)	0.15	26 (4%) 42 30	41, 79, 135, 166	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	ALA	4.9
1	A	477	GLU	4.8
1	A	785	SER	4.4
1	A	480	VAL	4.0
1	A	832	ALA	4.0
1	A	504	LEU	3.9
1	A	511	LEU	3.8
1	A	459	HIS	3.2
1	A	460	GLN	3.1
1	A	461	GLN	3.0
1	A	515	PRO	2.8
1	A	474	ILE	2.6
1	A	506	GLU	2.6
1	A	479	LEU	2.6
1	A	437	THR	2.5
1	A	478	PHE	2.5
1	A	791	GLN	2.4
1	A	810	THR	2.4
1	A	539	ALA	2.3
1	A	398	PHE	2.3
1	A	401	LEU	2.2
1	A	441	LEU	2.2
1	A	458	LEU	2.1
1	A	246	THR	2.1
1	A	456	LYS	2.0
1	A	500	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
2	FAD	A	2762	53/53	0.94	0.28	1.26	38,60,69,76	0

6.5 Other polymers (i)

There are no such residues in this entry.