Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:29 AM GMT

PDB ID	:	2XAJ
Title	:	CRYSTAL STRUCTURE OF LSD1-COREST IN COMPLEX WITH (-)-TRANS-2-PHENYLCYCLOPROPYL-1-AMINE
Authors	:	Binda, C.; Valente, S.; Romanenghi, M.; Pilotto, S.; Cirilli, R.; Karytinos, A.; Ciossani, G.; Botrugno, O.A.; Forneris, F.; Tardugno, M.; Edmondson, D.E.; Minucci, S.; Mattevi, A.; Mai, A.
Deposited on	:	2010-03-31
Resolution	:	3.30 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:

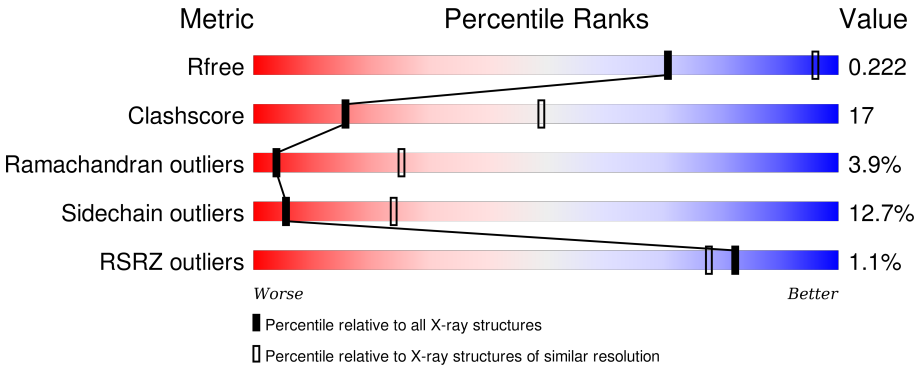
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	852	% 48% 27% • 22%
2	B	482	% 12% 12% • 72%

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	TCA	A	901	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6356 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.

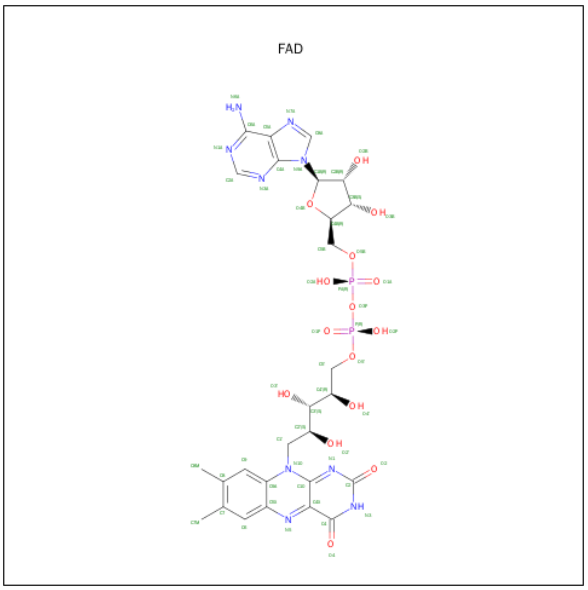
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

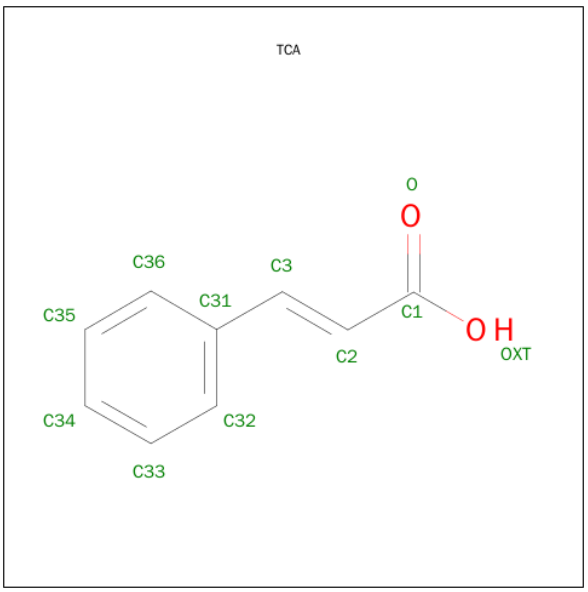
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is PHENYLETHYLENECARBOXYLIC ACID (three-letter code: TCA)

(formula: $C_9H_8O_2$).



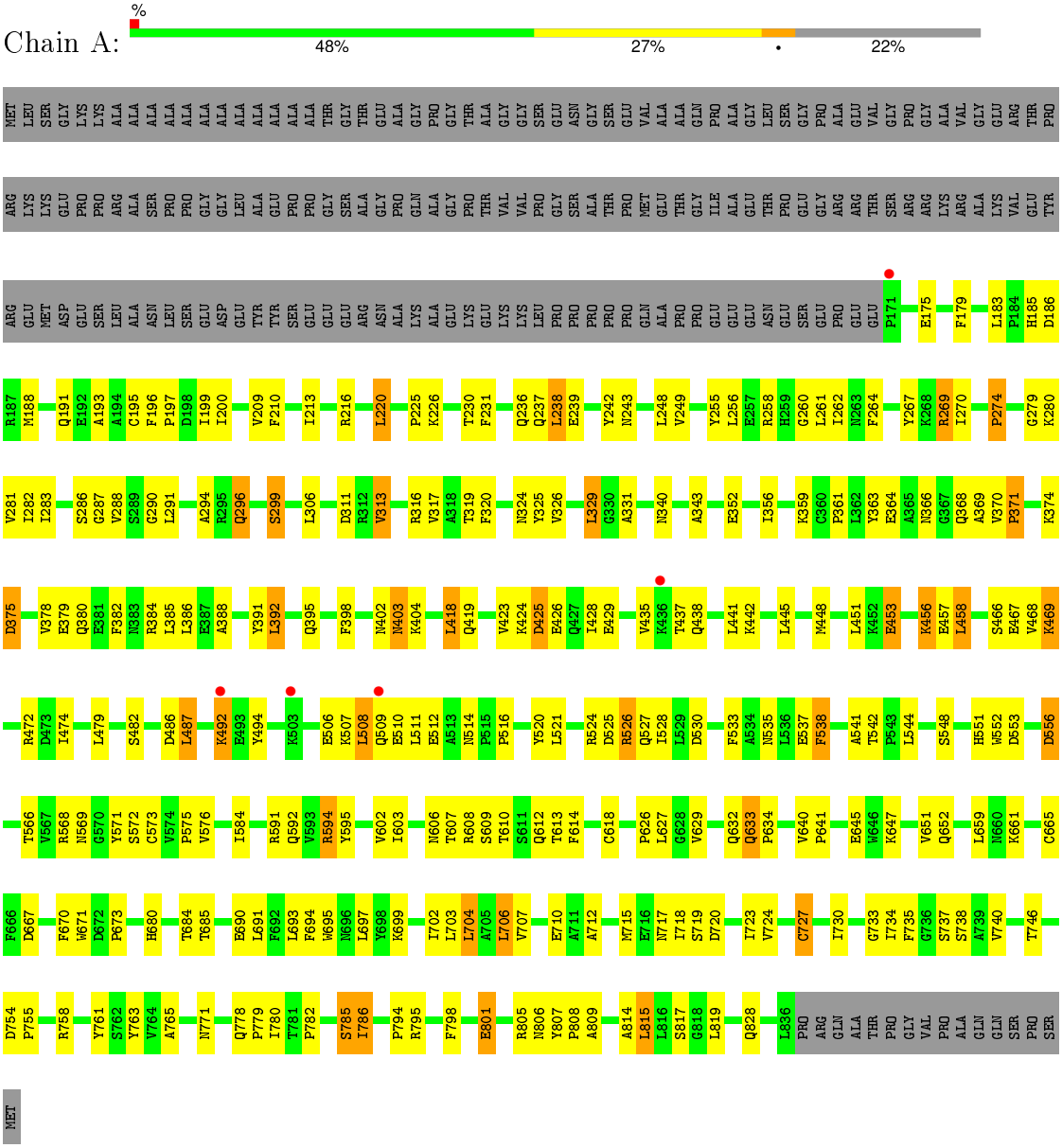
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 9 1	0	0

3 Residue-property plots (i)

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

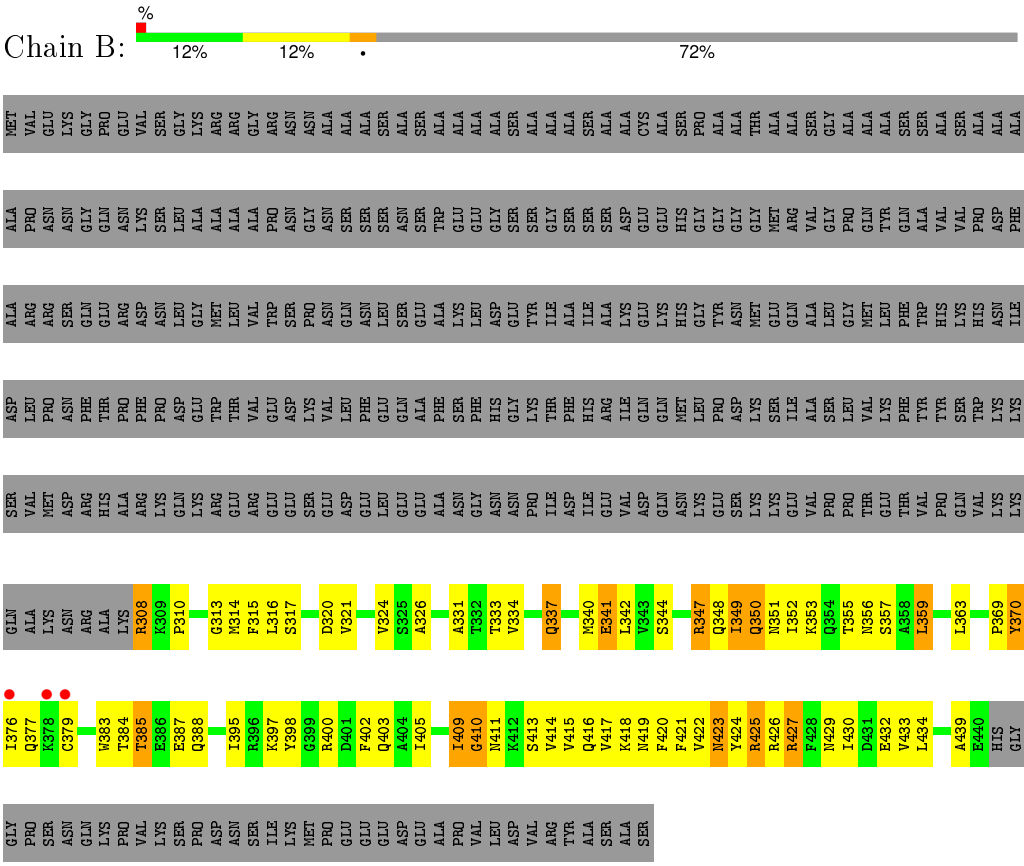
- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1

Chain A:



- Molecule 2: REST COREPRESSOR 1

Chain B:


%
12%
12%
72%
MET VAL GLU LYS GLY PRO GLU VAL SER GLY LYS ARG ARG GLY ARG ASN ASN ALA ALA ALA SER ALA SER ALA ALA ALA ALA SER ALA ALA ALA ALA ALA SER SER ALA ALA CYS ALA SER PRO ALA ALA THR ALA ALA SER GLY ALA ALA ALA SER SER ALA SER ALA ALA ALA ALA
ALA PRO ASN ASN GLY GLN ASN LYS SER LEU ALA ALA ALA ALA ALA PRO ASN GLY ASN SER SER SER ASN SER TRP GLU GLU GLY SER SER GLY SER SER SER ASP GLU GLU HIS GLY GLY GLY GLY MET ARG VAL GLY PRO GLN TYR GLN ALA VAL VAL PRO ASP PHE ASP PRO ALA LYS LEU
ALA ARG ARG SER GLN GLU ARG ASP ASN LEU GLY MET LEU VAL TRP SER PRO ASN GLN ASN LEU SER GLU ALA LYS LEU ASP GLU TYR ILE ALA ILE ALA LYS GLU LYS HIS GLY TYR ASN MET GLU GLN ALA LEU GLY MET LEU PHE TRP HIS LYS HIS ASN ILE GLU LYS SER LEU ALA
ASP LEU PRO ASN PHE THR PRO PHE PRO ASP GLU TRP THR VAL GLU ASP LYS VAL LEU PHE GLU GLN ALA PHE SER PHE HIS GLY LYS THR PHE HIS ARG ILE GLU GLN GLN MET LEU PRO ASP LYS SER ILE ALA SER LEU VAL LYS PHE TYR TYR SER TRP LYS LYS THR ARG THR LYS THR
SER VAL MET ASP ARG HIS ALA ARG LYS GLN LYS ARG GLU ARG GLU GLU SER GLU ASP GLU LEU GLU GLU ALA ASN GLY ASN ASN PRO ILE ASP ILE GLU VAL ASP GLN ASN LYS GLU SER LYS LYS GLU VAL PRO PRO THR GLU THR VAL PRO GLN VAL VAL LYS LYS GLU LYS HIS SER THR
GLN ALA LYS ASN ARG ALA LYS R308 K309 P310 G313 M314 F315 L316 S317 D320 V321 V324 S325 A326 A331 T332 T333 V334 Q337 M340 E341 L342 V343 S344 R347 Q348 I349 Q350 N351 I352 K353 Q354 T355 N356 S357 A358 L359 L363 P369 Y370 R371 L372 P373 E374 V375
I376 Q377 K378 C379 W383 T384 T385 E386 E387 Q388 I395 R396 K397 Y398 G399 R400 D401 F402 Q403 A404 I405 I409 G410 N411 K412 S413 V414 V415 Q416 V417 K418 N419 F420 F421 V422 N423 Y424 R425 R426 R427 F428 N429 I430 D431 E432 V433 L434 A439 E440 HIS GLY LYS GLU GLU THR ASN
GLY PRO SER ASN GLN LYS PRO VAL LYS SER PRO ASP ASN SER ILE LYS MET PRO GLU GLU GLU ASP GLU ALA PRO VAL LEU ASP VAL ARG TYR ALA SER ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.08Å 179.78Å 235.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.45 – 3.30 68.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.45-3.30) 99.8 (68.63-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.199 , 0.227 0.199 , 0.222	Depositor DCC
R_{free} test set	747 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 38323 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6356	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, TCA

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	0.72	0/5331	0.82	3/7232 (0.0%)
2	B	0.63	0/1091	0.74	1/1471 (0.1%)
All	All	0.70	0/6422	0.81	4/8703 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	258	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	258	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	359	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5217	0	5252	167	0
2	B	1076	0	1091	68	0
3	A	53	0	31	4	0
4	A	10	0	7	3	0
All	All	6356	0	6381	218	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 17.

All (218) 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:755:PRO:HA	1:A:758:ARG:NH1	1.61	1.14
1:A:286:SER:O	1:A:291:LEU:HD11	1.56	1.03
1:A:794:PRO:HD2	1:A:828:GLN:HE22	1.25	0.98
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.68	0.92
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.30	0.91
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.58	0.86
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.41	0.85
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.91	0.84
1:A:384:ARG:HH22	2:B:313:GLY:HA3	1.44	0.83
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.46	0.81
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.62	0.80
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.45	0.79
1:A:671:TRP:O	1:A:673:PRO:HD3	1.83	0.78
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.66	0.77
1:A:755:PRO:CA	1:A:758:ARG:HH12	1.98	0.77
1:A:548:SER:O	1:A:552:TRP:HB3	1.85	0.76
1:A:384:ARG:NH2	2:B:313:GLY:HA3	1.99	0.76
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.20	0.75
2:B:317:SER:O	2:B:321:VAL:HG23	1.88	0.73
1:A:286:SER:O	1:A:291:LEU:CD1	2.35	0.73
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.20	0.72
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.25	0.72
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.25	0.71
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.22	0.70
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.73	0.69
1:A:720:ASP:O	1:A:724:VAL:HG23	1.91	0.69
2:B:308:ARG:NH1	2:B:308:ARG:HA	2.09	0.67
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.78	0.65
1:A:195:CYS:C	1:A:197:PRO:HD3	2.17	0.65
1:A:209:VAL:O	1:A:213:ILE:HG13	1.97	0.65
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.78	0.65
1:A:807:TYR:N	1:A:808:PRO:HD3	2.12	0.64
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.32	0.64
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.80	0.63
1:A:469:LYS:HA	1:A:469:LYS:HE3	1.81	0.62
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.82	0.62
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HB3	2:B:356:ASN:HD21	1.65	0.62
2:B:337:GLN:O	2:B:341:GLU:HB2	1.98	0.61
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.46	0.61
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.63	0.61
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.82	0.60
1:A:594:ARG:HA	1:A:640:VAL:O	2.01	0.59
1:A:755:PRO:CA	1:A:758:ARG:NH1	2.50	0.59
1:A:419:GLN:HE22	2:B:315:PHE:H	1.52	0.58
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.67	0.58
1:A:287:GLY:HA3	3:A:900:FAD:O5B	2.03	0.58
2:B:397:LYS:O	2:B:397:LYS:HG2	2.03	0.58
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.67	0.58
1:A:441:LEU:O	1:A:445:LEU:HG	2.04	0.58
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.86	0.57
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.40	0.57
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.40	0.56
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.86	0.56
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.86	0.56
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.74	0.55
2:B:350:GLN:CA	2:B:350:GLN:HE21	2.19	0.55
1:A:506:GLU:O	1:A:508:LEU:N	2.38	0.55
2:B:370:TYR:N	2:B:370:TYR:HD2	2.04	0.55
1:A:801:GLU:CG	1:A:809:ALA:HA	2.37	0.55
2:B:370:TYR:CD2	2:B:370:TYR:N	2.73	0.55
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.41	0.55
1:A:761:TYR:CE2	4:A:901:TCA:H3	2.42	0.55
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.72	0.55
1:A:695:TRP:HE1	1:A:706:LEU:CD2	2.20	0.55
1:A:458:LEU:HD12	1:A:487:LEU:HD12	1.89	0.54
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.54
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.38	0.54
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.89	0.54
1:A:468:VAL:O	1:A:472:ARG:NH1	2.42	0.53
1:A:216:ARG:O	1:A:220:LEU:HD12	2.08	0.53
2:B:333:THR:HG22	2:B:334:VAL:N	2.23	0.53
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.73	0.53
2:B:377:GLN:NE2	2:B:410:GLY:HA3	2.24	0.53
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.09	0.52
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.92	0.52
1:A:196:PHE:N	1:A:197:PRO:HD3	2.25	0.52
1:A:525:ASP:O	1:A:528:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD23	2:B:356:ASN:ND2	2.24	0.52
1:A:445:LEU:HB2	2:B:359:LEU:HD12	1.91	0.52
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.92	0.51
2:B:418:LYS:O	2:B:421:PHE:HB2	2.09	0.51
2:B:383:TRP:HB3	2:B:388:GLN:HE21	1.75	0.51
1:A:319:THR:HB	1:A:572:SER:HB3	1.93	0.51
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.40	0.51
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.45	0.51
2:B:417:VAL:O	2:B:420:PHE:HB3	2.10	0.51
1:A:782:PRO:HG3	1:A:795:ARG:HG3	1.91	0.51
3:A:900:FAD:C4X	4:A:901:TCA:C3	2.88	0.51
1:A:255:TYR:CD2	1:A:256:LEU:HD23	2.45	0.51
2:B:369:PRO:C	2:B:370:TYR:HD2	2.14	0.50
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.47	0.50
1:A:269:ARG:HH12	1:A:299:SER:HB2	1.77	0.50
1:A:374:LYS:O	1:A:375:ASP:C	2.50	0.50
1:A:551:HIS:O	1:A:553:ASP:N	2.45	0.50
1:A:193:ALA:HB2	1:A:200:ILE:HD13	1.94	0.50
2:B:421:PHE:O	2:B:425:ARG:HB2	2.11	0.49
1:A:260:GLY:O	1:A:264:PHE:CD2	2.65	0.49
1:A:379:GLU:O	1:A:382:PHE:HB3	2.13	0.49
1:A:456:LYS:CG	2:B:370:TYR:HE1	2.25	0.49
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.93	0.49
2:B:347:ARG:HG3	2:B:348:GLN:N	2.28	0.49
1:A:693:LEU:HD12	1:A:694:PHE:N	2.27	0.48
1:A:724:VAL:O	1:A:727:CYS:HB2	2.13	0.48
1:A:458:LEU:CD1	1:A:487:LEU:HD12	2.43	0.48
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.94	0.48
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.95	0.48
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.95	0.48
2:B:415:VAL:HG22	2:B:419:ASN:HD21	1.77	0.48
1:A:740:VAL:O	1:A:740:VAL:HG12	2.13	0.48
1:A:331:ALA:HA	3:A:900:FAD:N5	2.29	0.48
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.49	0.48
1:A:541:ALA:O	1:A:542:THR:HB	2.14	0.48
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.95	0.48
1:A:606:ASN:HD22	1:A:609:SER:H	1.61	0.48
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.49	0.48
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.54	0.47
1:A:238:LEU:HD22	1:A:239:GLU:H	1.79	0.47
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:O	2:B:324:VAL:HG23	2.14	0.47
2:B:350:GLN:CA	2:B:350:GLN:NE2	2.77	0.47
2:B:405:ILE:O	2:B:409:ILE:HG13	2.15	0.47
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.97	0.47
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.65	0.47
1:A:364:GLU:OE2	1:A:370:VAL:HG22	2.15	0.47
1:A:626:PRO:HB2	1:A:629:VAL:HG23	1.97	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.46
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.45	0.46
1:A:525:ASP:O	1:A:527:GLN:N	2.48	0.46
1:A:647:LYS:O	1:A:651:VAL:HG23	2.16	0.46
1:A:418:LEU:HD13	2:B:324:VAL:HG21	1.98	0.46
1:A:807:TYR:N	1:A:808:PRO:CD	2.79	0.46
1:A:806:ASN:C	1:A:807:TYR:CD2	2.89	0.46
1:A:786:ILE:HD12	1:A:786:ILE:H	1.80	0.46
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.62	0.46
1:A:627:LEU:CD1	1:A:651:VAL:HG13	2.46	0.46
2:B:400:ARG:O	2:B:402:PHE:N	2.47	0.45
1:A:311:ASP:N	1:A:311:ASP:OD1	2.49	0.45
1:A:670:PHE:CD1	1:A:670:PHE:C	2.90	0.45
1:A:575:PRO:O	1:A:576:VAL:C	2.55	0.45
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.17	0.45
1:A:755:PRO:HA	1:A:758:ARG:CZ	2.39	0.45
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.81	0.45
2:B:385:THR:HA	2:B:388:GLN:HG3	1.97	0.45
1:A:320:PHE:O	1:A:326:VAL:HA	2.16	0.45
1:A:530:ASP:OD2	1:A:685:THR:HA	2.17	0.45
1:A:319:THR:CB	1:A:572:SER:HB3	2.47	0.44
2:B:416:GLN:O	2:B:419:ASN:HB2	2.17	0.44
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.98	0.44
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.47	0.44
1:A:492:LYS:HA	1:A:492:LYS:HE3	1.99	0.44
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.52	0.44
1:A:280:LYS:O	1:A:618:CYS:HB2	2.18	0.44
2:B:369:PRO:HB2	2:B:370:TYR:CE2	2.53	0.44
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.18	0.44
1:A:633:GLN:HA	1:A:634:PRO:HA	1.52	0.44
1:A:366:ASN:OD1	1:A:368:GLN:HG3	2.18	0.44
2:B:429:ASN:O	2:B:432:GLU:N	2.51	0.43
1:A:402:ASN:O	1:A:403:ASN:HB2	2.18	0.43
1:A:424:LYS:O	1:A:426:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.82	0.43
2:B:415:VAL:O	2:B:419:ASN:ND2	2.50	0.43
1:A:255:TYR:HD2	1:A:256:LEU:HD23	1.84	0.42
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.79	0.42
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.54	0.42
1:A:352:GLU:OE1	1:A:569:ASN:HB3	2.19	0.42
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.54	0.42
1:A:329:LEU:HA	1:A:661:LYS:HD2	2.02	0.42
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.85	0.42
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.83	0.42
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.84	0.42
2:B:413:SER:OG	2:B:415:VAL:HG12	2.20	0.42
1:A:340:ASN:O	1:A:343:ALA:HB3	2.19	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.77	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.77	0.42
1:A:374:LYS:O	1:A:378:VAL:HG23	2.18	0.42
2:B:420:PHE:HA	2:B:423:ASN:HD22	1.85	0.42
1:A:553:ASP:O	1:A:556:ASP:HB2	2.19	0.42
1:A:424:LYS:O	1:A:425:ASP:C	2.58	0.42
1:A:754:ASP:HA	1:A:755:PRO:HD2	1.63	0.42
2:B:415:VAL:HG22	2:B:419:ASN:ND2	2.35	0.42
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.84	0.42
2:B:340:MET:O	2:B:342:LEU:N	2.52	0.42
1:A:595:TYR:CE2	1:A:641:PRO:HD2	2.55	0.42
2:B:409:ILE:O	2:B:411:ASN:N	2.50	0.41
2:B:369:PRO:C	2:B:370:TYR:CD2	2.92	0.41
1:A:325:TYR:HA	1:A:702:ILE:HD11	2.03	0.41
1:A:691:LEU:CD2	1:A:727:CYS:SG	3.08	0.41
1:A:710:GLU:OE1	1:A:710:GLU:HA	2.20	0.41
1:A:366:ASN:OD1	1:A:368:GLN:N	2.53	0.41
1:A:296:GLN:HG2	1:A:819:LEU:HD22	2.01	0.41
1:A:317:VAL:HG12	1:A:317:VAL:O	2.20	0.41
3:A:900:FAD:C4	4:A:901:TCA:H36	2.51	0.41
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.02	0.41
1:A:814:ALA:O	1:A:817:SER:N	2.53	0.41
2:B:384:THR:O	2:B:387:GLU:N	2.54	0.41
2:B:419:ASN:HD22	2:B:419:ASN:N	2.19	0.41
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.86	0.41
1:A:419:GLN:HB3	1:A:520:TYR:CD1	2.54	0.41
1:A:239:GLU:OE1	1:A:239:GLU:HA	2.20	0.41
1:A:724:VAL:HG11	1:A:746:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:C	1:A:508:LEU:N	2.75	0.41
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.56	0.41
2:B:349:ILE:O	2:B:353:LYS:HB2	2.20	0.41
2:B:432:GLU:O	2:B:433:VAL:C	2.59	0.41
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.56	0.40
1:A:538:PHE:O	1:A:538:PHE:CG	2.72	0.40
2:B:350:GLN:NE2	2:B:350:GLN:HA	2.37	0.40
1:A:715:MET:CE	1:A:723:ILE:HG12	2.52	0.40
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.98	0.40
1:A:778:GLN:HA	1:A:779:PRO:HD2	1.87	0.40
1:A:613:THR:CG2	1:A:614:PHE:N	2.84	0.40
1:A:442:LYS:HE3	2:B:355:THR:HG21	2.03	0.40
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.03	0.40
1:A:287:GLY:O	1:A:290:GLY:N	2.55	0.40
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.74	0.40
2:B:310:PRO:HB3	2:B:316:LEU:HD12	2.04	0.40
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.36	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	664/852 (78%)	566 (85%)	75 (11%)	23 (4%)	4 29
2	B	131/482 (27%)	102 (78%)	21 (16%)	8 (6%)	2 14
All	All	795/1334 (60%)	668 (84%)	96 (12%)	31 (4%)	4 25

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP

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Mol	Chain	Res	Type
1	A	737	SER
1	A	801	GLU
2	B	326	ALA
2	B	341	GLU
1	A	279	GLY
1	A	288	VAL
1	A	507	LYS
1	A	526	ARG
1	A	573	CYS
1	A	738	SER
2	B	331	ALA
2	B	373	PRO
2	B	410	GLY
2	B	426	ARG
1	A	274	PRO
1	A	316	ARG
1	A	508	LEU
1	A	785	SER
1	A	236	GLN
1	A	313	VAL
1	A	375	ASP
1	A	403	ASN
1	A	516	PRO
1	A	225	PRO
1	A	369	ALA
2	B	425	ARG
2	B	439	ALA
1	A	371	PRO
1	A	428	ILE
1	A	733	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	566/699 (81%)	498 (88%)	68 (12%)	6 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	117/395 (30%)	98 (84%)	19 (16%)	3 14
All	All	683/1094 (62%)	596 (87%)	87 (13%)	5 24

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	PHE
1	A	183	LEU
1	A	191	GLN
1	A	220	LEU
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	267	TYR
1	A	269	ARG
1	A	274	PRO
1	A	281	VAL
1	A	296	GLN
1	A	299	SER
1	A	313	VAL
1	A	324	ASN
1	A	329	LEU
1	A	359	LYS
1	A	380	GLN
1	A	392	LEU
1	A	404	LYS
1	A	418	LEU
1	A	423	VAL
1	A	429	GLU
1	A	437	THR
1	A	438	GLN
1	A	453	GLU
1	A	456	LYS
1	A	457	GLU
1	A	458	LEU
1	A	466	SER
1	A	467	GLU
1	A	469	LYS
1	A	479	LEU
1	A	482	SER
1	A	487	LEU
1	A	492	LYS

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	512	GLU
1	A	514	ASN
1	A	524	ARG
1	A	526	ARG
1	A	535	ASN
1	A	538	PHE
1	A	556	ASP
1	A	568	ARG
1	A	571	TYR
1	A	591	ARG
1	A	594	ARG
1	A	607	THR
1	A	610	THR
1	A	612	GLN
1	A	632	GLN
1	A	633	GLN
1	A	645	GLU
1	A	652	GLN
1	A	659	LEU
1	A	667	ASP
1	A	684	THR
1	A	699	LYS
1	A	704	LEU
1	A	706	LEU
1	A	717	ASN
1	A	719	SER
1	A	727	CYS
1	A	780	ILE
1	A	785	SER
1	A	786	ILE
1	A	815	LEU
2	B	308	ARG
2	B	337	GLN
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	350	GLN
2	B	351	ASN
2	B	352	ILE
2	B	357	SER
2	B	370	TYR

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Mol	Chain	Res	Type
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	385	THR
2	B	409	ILE
2	B	414	VAL
2	B	422	VAL
2	B	423	ASN
2	B	427	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	410	GLN
1	A	419	GLN
1	A	422	HIS
1	A	438	GLN
1	A	484	HIS
1	A	535	ASN
1	A	564	HIS
1	A	828	GLN
2	B	337	GLN
2	B	348	GLN
2	B	350	GLN
2	B	388	GLN
2	B	419	ASN
2	B	423	ASN

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 (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	A	900	4	48,58,58	2.55	11 (22%)	54,89,89	3.47	12 (22%)
4	TCA	A	901	3	10,10,11	3.42	2 (20%)	10,11,13	3.79	2 (20%)

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	900	4	-	0/30/50/50	0/6/6/6
4	TCA	A	901	3	-	0/4/4/5	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C5'-C4'	2.09	1.54	1.51
3	A	900	FAD	C1'-N10	2.24	1.50	1.48
3	A	900	FAD	C4-C4X	2.50	1.46	1.41
4	A	901	TCA	C2-C1	3.07	1.53	1.44
3	A	900	FAD	C4X-C10	3.40	1.47	1.41
3	A	900	FAD	C10-N10	3.62	1.43	1.39
3	A	900	FAD	C5X-N5	4.09	1.41	1.35
3	A	900	FAD	C9A-N10	4.59	1.45	1.38
3	A	900	FAD	O4-C4	5.01	1.36	1.24
3	A	900	FAD	C2A-N1A	7.77	1.48	1.33
3	A	900	FAD	C2A-N3A	8.08	1.46	1.32
3	A	900	FAD	C4X-N5	8.32	1.46	1.33
4	A	901	TCA	C2-C3	9.94	1.52	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	N3A-C2A-N1A	-19.37	114.07	128.89
4	A	901	TCA	C31-C3-C2	-11.08	109.78	127.26
3	A	900	FAD	C4X-C10-N10	-6.19	116.87	120.52
3	A	900	FAD	C4-C4X-C10	-5.22	116.60	119.94
4	A	901	TCA	O-C1-C2	-3.83	115.73	125.51
3	A	900	FAD	C4X-C4-N3	-3.70	118.54	123.59
3	A	900	FAD	C4-C4X-N5	-3.50	114.47	118.72
3	A	900	FAD	C1B-N9A-C4A	-3.48	121.69	126.94
3	A	900	FAD	P-O3P-PA	-3.15	123.88	132.73
3	A	900	FAD	C4X-N5-C5X	-2.62	113.75	116.76
3	A	900	FAD	C6-C5X-N5	-2.61	115.60	118.96
3	A	900	FAD	C2A-N1A-C6A	2.18	122.66	118.77
3	A	900	FAD	C5X-C9A-N10	5.24	121.60	117.62
3	A	900	FAD	C4-N3-C2	8.43	122.54	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	4	0
4	A	901	TCA	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	666/852 (78%)	0.18	5 (0%)	87	84	34, 65, 93, 107	0
2	B	133/482 (27%)	0.49	4 (3%)	54	47	66, 94, 110, 118	0
All	All	799/1334 (59%)	0.23	9 (1%)	82	78	34, 70, 101, 118	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	2.7
2	B	376	ILE	2.5
1	A	509	GLN	2.4
2	B	374	GLU	2.4
2	B	378	LYS	2.3
1	A	436	LYS	2.3
1	A	503	LYS	2.2
2	B	379	CYS	2.1
1	A	492	LYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	TCA	A	901	10/11	0.96	0.38	2.46	59,69,71,71	0
3	FAD	A	900	53/53	0.99	0.23	-0.38	37,43,59,61	0

6.5 Other polymers

There are no such residues in this entry.