

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1XDI
Title	:	Crystal structure of LpdA (Rv3303c) from Mycobacterium tuberculosis
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Deposited on	:	2004-09-06
Resolution	:	2.81 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.81 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	499	57%	28%	7%	8%		
1	В	499	47%	38%	6% •	8%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6925 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	450	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	409	3356	2101	607	635	13	0	0	0	
1	Р	450	Total	С	Ν	0	S	0	0	0
I D	409	3356	2101	607	635	13	0	0	0	

• Molecule 1 is a protein called Rv3303c-lpdA.

Chain	Residue	Modelled	Actual	Comment	Reference
А	494	HIS	-	expression tag	UNP 053355
А	495	HIS	-	expression tag	UNP O53355
А	496	HIS	-	expression tag	UNP 053355
А	497	HIS	-	expression tag	UNP O53355
А	498	HIS	-	expression tag	UNP 053355
А	499	HIS	-	expression tag	UNP O53355
В	494	HIS	-	expression tag	UNP O53355
В	495	HIS	-	expression tag	UNP 053355
В	496	HIS	-	expression tag	UNP O53355
В	497	HIS	-	expression tag	UNP 053355
В	498	HIS	-	expression tag	UNP O53355
В	499	HIS	-	expression tag	UNP O53355

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\rm C_{27}H_{33}N_9O_{15}P_2).$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
0	Δ	1	Total	С	Ν	Ο	Р	0	0		
	1	53	27	9	15	2	0	0			
0	o D	D	Р	1	Total	С	Ν	Ο	Р	0	0
2 B		53	27	9	15	2	0	U			

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
3	В	50	Total O 50 50	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Rv3303c-lpdA



S424 S425 1425 1425 1425 1425 1425 1425 1425 1425 1425 1435 1425 1443 1443 1443 1445 1443 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1445 1455 1455 1455 1455 1455 1455 1455 1455 1455 1455 1456 1455 1455 1455 1456 1455 1455 1455 1456 1456 1457 1456 1456 1456 1457 1456 1456 1456 1457</t

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	244.20Å 244.20Å 104.80Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	50.00 - 2.81	Depositor
Resolution (A)	35.25 - 2.81	EDS
% Data completeness	98.9 (50.00-2.81)	Depositor
(in resolution range)	99.7 (35.25-2.81)	EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$6.31 (at 2.81 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
B B.	0.194 , 0.276	Depositor
II, II free	0.191 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	23.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 38.4	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.45, \langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6925	wwPDB-VP
Average B, all atoms $(Å^2)$	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.86	3/3404~(0.1%)	1.06	4/4637~(0.1%)	
1	В	0.87	0/3404	1.06	8/4637~(0.2%)	
All	All	0.86	3/6808~(0.0%)	1.06	12/9274~(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	А	0	1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	306	ARG	CB-CG	-5.17	1.38	1.52
1	А	434	VAL	CB-CG1	-5.05	1.42	1.52
1	А	201	TYR	CD2-CE2	5.04	1.47	1.39

All (3) bond length outliers are listed below:

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	306	ARG	CG-CD-NE	-6.36	98.45	111.80
1	В	183	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	В	262	ASP	CB-CA-C	-5.72	98.96	110.40
1	В	414	ILE	CG1-CB-CG2	-5.59	99.11	111.40
1	В	128	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	А	306	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	А	365	VAL	CB-CA-C	-5.32	101.29	111.40
1	В	166	GLY	N-CA-C	-5.27	99.93	113.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	306	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	А	302	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	В	387	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	В	113	ILE	CB-CA-C	-5.02	101.56	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	220	TYR	Sidechain

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	А	3356	0	3454	187	0
1	В	3356	0	3454	217	0
2	А	53	0	31	5	0
2	В	53	0	31	2	0
3	А	57	0	0	4	0
3	В	50	0	0	4	0
All	All	6925	0	6970	385	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 28.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:B:275:ILE:HG22	1:B:276:GLY:H	1.03	1.14
1:A:275:ILE:HG22	1:A:276:GLY:H	1.00	1.13
1:B:308:LEU:H	1:B:308:LEU:HD12	1.16	1.11
1:A:70:LEU:HD13	1:B:60:LEU:HD11	1.28	1.06
1:A:308:LEU:HD12	1:A:308:LEU:H	1.14	1.06
1:A:58:THR:HG22	1:A:359:ARG:HH12	1.20	1.03



	A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:275:ILE:HG22	1:A:276:GLY:N	1.72	1.01
1:B:433:ALA:HA	1:B:438:ILE:HD12	1.41	0.99
1:A:429:PRO:HG3	1:B:429:PRO:HG3	1.46	0.98
1:B:308:LEU:HD12	1:B:308:LEU:N	1.79	0.98
1:B:392:ALA:HA	1:B:397:MET:HE3	1.47	0.97
1:A:308:LEU:H	1:A:308:LEU:CD1	1.78	0.95
1:B:275:ILE:HG22	1:B:276:GLY:N	1.80	0.95
1:A:229:LEU:HD12	1:A:362:ILE:HD11	1.50	0.94
1:A:275:ILE:CG2	1:A:276:GLY:H	1.85	0.90
1:A:289:VAL:HG11	1:A:312:ILE:HD12	1.55	0.89
1:B:308:LEU:H	1:B:308:LEU:CD1	1.87	0.88
1:B:392:ALA:HA	1:B:397:MET:CE	2.03	0.87
1:A:308:LEU:HD12	1:A:308:LEU:N	1.89	0.87
1:A:439:THR:HG22	1:A:442:GLU:HB2	1.58	0.84
1:A:20:VAL:HG21	1:A:333:ARG:HG3	1.58	0.84
1:B:58:THR:HG23	1:B:203:GLU:HB2	1.60	0.83
1:B:303:ARG:HB3	1:B:346:PRO:HB3	1.61	0.83
1:A:439:THR:CG2	1:A:442:GLU:H	1.90	0.83
1:B:397:MET:HE1	1:B:453:LEU:HD21	1.60	0.83
1:B:66:ARG:HG2	1:B:69:HIS:HE1	1.43	0.83
1:B:123:THR:HG23	1:B:124:PRO:HD2	1.60	0.81
1:A:302:ASP:HB3	1:A:304:VAL:H	1.46	0.81
1:A:463:ARG:NH2	1:B:104:GLN:HE22	1.79	0.81
1:A:380:ARG:NH1	1:A:464:LEU:O	2.15	0.80
1:B:249:VAL:HG21	1:B:273:MET:HE1	1.63	0.79
1:A:274:THR:HG22	1:A:274:THR:O	1.81	0.79
1:B:58:THR:CG2	1:B:203:GLU:HB2	2.12	0.79
1:B:165:ASP:HB2	1:B:167:GLU:H	1.48	0.79
1:B:292:GLN:OE1	1:B:292:GLN:HA	1.83	0.78
1:B:321:LEU:HD12	1:B:331:GLN:NE2	1.98	0.78
1:B:130:ARG:HD2	1:B:144:GLU:OE2	1.84	0.78
1:A:347:ILE:HD12	1:A:347:ILE:H	1.50	0.76
1:B:88:ALA:O	1:B:92:THR:HB	1.85	0.75
1:B:410:THR:OG1	1:B:412:VAL:HG23	1.88	0.74
1:A:82:SER:OG	1:A:85:GLN:HG2	1.88	0.73
1:A:229:LEU:HD12	1:A:362:ILE:CD1	2.19	0.73
1:B:66:ARG:HG2	1:B:69:HIS:CE1	2.24	0.73
1:A:157:ARG:CD	1:A:275:ILE:HG21	2.18	0.73
1:B:252:THR:HG22	1:B:255:GLY:C	2.07	0.73
1:B:2:VAL:HG23	1:B:2:VAL:O	1.87	0.73
1:B:454:SER:HA	1:B:457:ILE:HD12	1.69	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:274:THR:O	1:A:274:THR:CG2	2.37	0.72
1:A:439:THR:HG22	1:A:442:GLU:H	1.55	0.72
1:B:249:VAL:HG21	1:B:273:MET:CE	2.18	0.72
1:B:241:PHE:CZ	1:B:266:VAL:HG22	2.25	0.72
1:A:302:ASP:HB2	1:A:306:ARG:H	1.55	0.72
1:A:321:LEU:HD22	1:A:349:LEU:HD11	1.71	0.71
1:B:380:ARG:NH1	1:B:466:ALA:HB3	2.05	0.71
1:A:393:LYS:HG2	1:B:93:LEU:HG	1.73	0.71
1:B:20:VAL:HG21	1:B:333:ARG:HG3	1.71	0.71
1:B:194:GLY:HA3	1:B:274:THR:HG21	1.71	0.71
1:A:66:ARG:HH12	1:A:396:GLU:HB2	1.54	0.71
1:B:52:LYS:HE3	1:B:357:PHE:CD2	2.25	0.70
1:A:58:THR:CG2	1:A:359:ARG:HH12	2.01	0.70
1:A:395:SER:HB2	1:A:397:MET:HE2	1.72	0.70
1:B:252:THR:CG2	1:B:255:GLY:H	2.05	0.70
1:A:17:ALA:O	1:A:336:MET:HG3	1.91	0.70
1:A:439:THR:HG23	1:A:442:GLU:H	1.57	0.69
1:B:302:ASP:OD2	1:B:306:ARG:HG2	1.92	0.69
1:B:25:HIS:HA	3:B:1005:HOH:O	1.92	0.68
1:A:194:GLY:HA3	1:A:274:THR:HG21	1.74	0.68
1:B:213:SER:O	1:B:243:ASN:HA	1.94	0.68
1:B:428:LEU:HB3	1:B:429:PRO:HD3	1.73	0.68
1:B:203:GLU:OE1	1:B:203:GLU:HA	1.93	0.67
1:B:275:ILE:CG2	1:B:276:GLY:H	1.91	0.67
1:A:463:ARG:NH2	1:B:104:GLN:NE2	2.42	0.67
1:B:213:SER:HB2	1:B:214:GLN:OE1	1.93	0.67
1:B:82:SER:OG	1:B:85:GLN:HG3	1.95	0.67
1:B:89:ARG:CG	1:B:89:ARG:HH11	2.08	0.66
1:B:433:ALA:HA	1:B:438:ILE:CD1	2.23	0.66
1:A:88:ALA:O	1:A:92:THR:HB	1.95	0.66
1:A:404:ILE:HD12	1:A:460:ALA:HB3	1.77	0.66
1:B:2:VAL:HA	1:B:28:THR:O	1.96	0.66
1:B:313:TYR:OH	1:B:338:HIS:HD2	1.79	0.66
1:B:433:ALA:CA	1:B:438:ILE:HD12	2.22	0.66
1:A:83:LEU:HG	1:A:181:LEU:HD23	1.77	0.65
1:A:439:THR:HG22	1:A:442:GLU:CB	2.26	0.65
1:A:447:LEU:HD21	1:B:330:MET:HG2	1.76	0.65
1:A:449:VAL:HG21	1:B:355:THR:CG2	2.27	0.65
1:B:380:ARG:HH12	1:B:466:ALA:HB3	1.60	0.64
1:A:182:PRO:HB3	1:A:270:HIS:CD2	2.32	0.64
1:B:66:ARG:CG	1:B:69:HIS:HE1	2.10	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:52:LYS:HE2	1:A:357:PHE:CD2	2.33	0.64
1:A:61:ARG:HD3	1:A:203:GLU:O	1.98	0.64
1:A:355:THR:HG21	1:A:424:SER:HA	1.78	0.64
1:A:295:ARG:NH1	1:A:295:ARG:HG3	2.13	0.63
1:B:7:ILE:HG23	1:B:149:LEU:HD23	1.80	0.63
1:A:249:VAL:HG21	1:A:273:MET:CE	2.29	0.63
1:A:295:ARG:HG3	1:A:295:ARG:HH11	1.62	0.62
1:A:43:ALA:HB2	2:A:999:FAD:O4'	1.99	0.62
1:A:397:MET:HE1	1:A:453:LEU:HD11	1.80	0.62
1:A:404:ILE:HG22	1:A:464:LEU:CD1	2.30	0.61
1:B:262:ASP:OD1	1:B:264:ARG:NH1	2.32	0.61
1:B:20:VAL:HG21	1:B:333:ARG:CG	2.31	0.61
1:B:274:THR:O	1:B:274:THR:CG2	2.47	0.61
1:B:61:ARG:HD3	1:B:203:GLU:O	2.00	0.61
1:A:157:ARG:HD3	1:A:275:ILE:HG21	1.81	0.61
1:B:66:ARG:HG2	1:B:66:ARG:O	2.00	0.61
1:A:169:ILE:HD12	1:A:249:VAL:HG12	1.83	0.61
1:A:334:ILE:CD1	1:A:347:ILE:HG13	2.30	0.60
1:A:209:THR:HG21	1:A:266:VAL:HG11	1.83	0.60
1:B:83:LEU:HG	1:B:181:LEU:HD23	1.84	0.60
1:A:25:HIS:N	1:A:26:PRO:HD3	2.17	0.60
1:A:19:LEU:HD13	1:A:105:LEU:HD23	1.83	0.60
1:A:193:THR:HG23	3:A:1013:HOH:O	2.02	0.60
1:A:247:ALA:H	1:A:260:MET:HA	1.65	0.60
1:B:25:HIS:NE2	1:B:342:GLU:OE2	2.34	0.59
1:B:34:ILE:HD13	1:B:133:ALA:HB2	1.85	0.59
1:B:439:THR:CG2	1:B:442:GLU:H	2.16	0.59
1:A:200:ALA:HA	1:A:359:ARG:HH22	1.68	0.59
1:A:404:ILE:HG22	1:A:464:LEU:HD12	1.84	0.59
1:B:301:VAL:CG2	1:B:314:ALA:HB3	2.33	0.59
1:A:130:ARG:HG3	1:A:144:GLU:OE2	2.03	0.59
1:B:89:ARG:HH11	1:B:89:ARG:HG2	1.67	0.58
1:A:55:ILE:HG12	1:A:200:ALA:HB2	1.84	0.58
1:A:83:LEU:HD13	1:A:87:HIS:CE1	2.39	0.58
1:B:275:ILE:CG2	1:B:276:GLY:N	2.54	0.58
1:A:169:ILE:HD12	1:A:249:VAL:CG1	2.34	0.58
1:A:157:ARG:HD2	1:A:275:ILE:HG21	1.84	0.58
1:B:91:LYS:NZ	1:B:177:ASP:OD1	2.32	0.57
1:B:242:LYS:O	1:B:264:ARG:NH2	2.36	0.57
1:B:365:VAL:O	1:B:415:GLY:HA2	2.03	0.57
1:A:428:LEU:HB3	1:A:429:PRO:HD3	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:8:LEU:HD22	1:B:117:GLY:HA3	1.84	0.57
1:B:123:THR:O	1:B:126:LEU:HG	2.03	0.57
1:B:321:LEU:HD22	1:B:349:LEU:HD21	1.86	0.57
1:B:186:ILE:HG21	1:B:258:VAL:HG21	1.86	0.57
1:B:59:GLY:O	1:B:62:THR:HB	2.03	0.57
1:A:15:TYR:CE2	1:A:101:ILE:HD13	2.40	0.56
1:A:215:ASP:HB3	1:A:216:HIS:ND1	2.20	0.56
1:A:299:LEU:HD13	1:A:314:ALA:HB2	1.88	0.56
1:B:123:THR:HG23	1:B:124:PRO:CD	2.34	0.56
1:A:2:VAL:N	3:A:1037:HOH:O	2.39	0.56
1:A:72:PHE:HE2	1:B:81:ILE:HD11	1.71	0.56
1:A:250:THR:HG22	1:A:251:ARG:N	2.21	0.56
1:A:330:MET:HG3	1:A:334:ILE:CD1	2.35	0.56
1:B:192:VAL:HG13	1:B:356:VAL:HG13	1.88	0.55
1:B:185:LEU:HB3	1:B:208:VAL:HG22	1.88	0.55
1:A:249:VAL:HG21	1:A:273:MET:HE1	1.89	0.55
1:B:262:ASP:CG	1:B:264:ARG:HH11	2.10	0.55
1:B:25:HIS:CD2	1:B:340:LEU:HD13	2.42	0.55
1:B:278:VAL:HG13	1:B:279:PRO:HD2	1.89	0.55
1:A:43:ALA:O	1:A:48:CYS:HB3	2.07	0.55
1:A:66:ARG:HG3	1:A:66:ARG:O	2.05	0.54
1:A:157:ARG:HD2	1:A:275:ILE:CG2	2.38	0.54
1:A:169:ILE:CD1	1:A:249:VAL:HG12	2.37	0.54
1:A:302:ASP:HB2	1:A:306:ARG:N	2.22	0.54
1:A:87:HIS:CE1	1:A:176:TYR:HA	2.43	0.54
1:A:245:ARG:O	1:A:260:MET:HB2	2.08	0.54
1:B:52:LYS:HE2	2:B:999:FAD:O4	2.07	0.54
1:B:286:LEU:CD1	1:B:293:LEU:HD21	2.37	0.54
1:A:330:MET:HG3	1:A:334:ILE:HD11	1.90	0.54
1:A:426:LEU:O	1:A:429:PRO:HD2	2.08	0.54
1:B:260:MET:HG2	1:B:264:ARG:HB3	1.89	0.54
1:B:321:LEU:CD2	1:B:349:LEU:HD21	2.37	0.54
1:B:164:PRO:HA	1:B:169:ILE:HG22	1.90	0.54
1:B:285:GLY:O	1:B:288:ARG:N	2.41	0.54
1:B:304:VAL:HG12	1:B:304:VAL:O	2.09	0.54
1:A:162:ALA:HB1	1:A:249:VAL:HB	1.89	0.53
1:B:301:VAL:HG13	1:B:305:SER:HA	1.89	0.53
1:B:441:ASN:HA	1:B:465:MET:HE3	1.90	0.53
1:A:194:GLY:CA	1:A:274:THR:HG21	2.38	0.53
1:A:391:ARG:HD2	3:B:1022:HOH:O	2.07	0.53
1:B:210:VAL:HG21	1:B:217:VAL:HG13	1.91	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:289:VAL:O	1:B:289:VAL:CG1	2.56	0.53
1:B:232:SER:O	1:B:236:ARG:HG3	2.08	0.53
1:B:274:THR:O	1:B:274:THR:HG23	2.08	0.53
1:A:295:ARG:HH11	1:A:295:ARG:CG	2.21	0.53
1:A:289:VAL:HG11	1:A:312:ILE:CD1	2.34	0.53
1:B:20:VAL:CG2	1:B:333:ARG:HG3	2.39	0.53
1:B:404:ILE:HD12	1:B:460:ALA:HB3	1.91	0.52
1:B:381:THR:HG22	1:B:405:PHE:CD1	2.44	0.52
1:B:439:THR:HG23	1:B:442:GLU:H	1.75	0.52
1:A:347:ILE:HD13	3:A:1049:HOH:O	2.09	0.52
1:B:83:LEU:HG	1:B:181:LEU:CD2	2.40	0.52
1:B:167:GLU:OE1	1:B:251:ARG:NH2	2.42	0.52
1:B:304:VAL:HG11	1:B:338:HIS:ND1	2.23	0.52
1:A:47:ASP:HB3	2:A:999:FAD:C8	2.39	0.52
1:A:315:ALA:HB1	1:A:331:GLN:HB3	1.92	0.52
1:B:458:THR:CG2	1:B:462:ARG:HH22	2.22	0.52
1:B:459:GLU:HG2	1:B:462:ARG:NH1	2.24	0.52
1:A:66:ARG:NH1	1:A:396:GLU:HB2	2.23	0.52
1:B:181:LEU:HD21	1:B:204:LEU:HD13	1.91	0.52
1:A:150:VAL:HG11	1:A:299:LEU:HD12	1.91	0.52
1:B:25:HIS:HB3	1:B:29:THR:HG23	1.92	0.52
1:B:216:HIS:C	1:B:218:LEU:N	2.62	0.51
1:B:286:LEU:HD12	1:B:293:LEU:HD21	1.92	0.51
1:B:370:SER:O	1:B:373:ASP:N	2.43	0.51
1:A:59:GLY:O	1:A:62:THR:HB	2.10	0.51
1:A:63:GLU:O	1:A:64:LEU:C	2.48	0.51
1:A:289:VAL:O	1:A:289:VAL:HG13	2.10	0.51
1:A:330:MET:HB2	1:B:447:LEU:HD21	1.93	0.51
1:B:248:SER:OG	1:B:259:THR:HG23	2.10	0.51
1:A:97:GLN:HG2	1:B:390:ALA:HB2	1.93	0.51
1:B:218:LEU:HD23	1:B:219:PRO:CD	2.41	0.51
1:B:233:PHE:CD1	1:B:238:VAL:HG21	2.46	0.51
1:B:382:ILE:HG13	1:B:383:MET:N	2.26	0.51
1:A:184:HIS:NE2	1:A:239:ARG:NH1	2.58	0.50
1:A:221:GLU:HB3	3:A:1055:HOH:O	2.12	0.50
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.76	0.50
1:B:252:THR:HG23	1:B:253:GLY:N	2.25	0.50
1:B:301:VAL:HG21	1:B:314:ALA:HB3	1.93	0.50
1:B:218:LEU:HD23	1:B:219:PRO:HD2	1.93	0.50
1:B:384:LEU:HG	3:B:1011:HOH:O	2.11	0.50
1:A:61:ARG:NH2	1:A:65:ARG:NH1	2.60	0.50



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:428:LEU:HD22	1:B:454:SER:HB2	1.92	0.50
1:B:189:GLY:HA3	1:B:274:THR:HG22	1.93	0.50
1:B:150:VAL:HG11	1:B:299:LEU:HD12	1.94	0.50
1:A:15:TYR:C	1:A:15:TYR:CD1	2.85	0.50
1:B:350:ARG:HB2	3:B:1028:HOH:O	2.11	0.50
1:A:67:ALA:HB3	1:A:68:PRO:HD3	1.93	0.49
1:A:83:LEU:HG	1:A:181:LEU:CD2	2.41	0.49
1:B:285:GLY:O	1:B:287:GLU:N	2.44	0.49
1:A:416:GLY:HA3	1:A:430:ILE:HG21	1.94	0.49
1:A:429:PRO:HG3	1:B:429:PRO:CG	2.29	0.49
1:B:218:LEU:C	1:B:218:LEU:CD2	2.80	0.49
1:A:182:PRO:HB3	1:A:270:HIS:HD2	1.77	0.49
1:B:150:VAL:HG11	1:B:299:LEU:CD1	2.43	0.49
1:B:355:THR:HG21	1:B:424:SER:HA	1.94	0.49
1:B:382:ILE:HG22	1:B:464:LEU:HD21	1.95	0.49
1:B:439:THR:HG23	1:B:441:ASN:HB2	1.94	0.49
1:B:252:THR:HG23	1:B:255:GLY:H	1.76	0.49
1:A:393:LYS:NZ	1:B:100:ASP:OD2	2.44	0.48
1:B:25:HIS:HD2	1:B:340:LEU:HD13	1.76	0.48
1:A:442:GLU:HG2	1:B:436:ASN:OD1	2.12	0.48
1:A:137:ASP:HB2	1:A:139:SER:OG	2.13	0.48
1:A:334:ILE:HD13	1:A:347:ILE:HG13	1.95	0.48
1:A:420:ALA:HB1	1:A:421:PRO:CD	2.44	0.48
1:B:87:HIS:O	1:B:91:LYS:HG3	2.13	0.48
1:B:301:VAL:HG23	1:B:314:ALA:HB3	1.96	0.48
1:A:439:THR:HG23	1:A:441:ASN:HB2	1.95	0.48
1:B:81:ILE:CG2	1:B:81:ILE:O	2.61	0.48
1:A:218:LEU:HD12	1:A:229:LEU:HD13	1.94	0.48
1:B:222:ASP:OD2	1:B:403:LYS:NZ	2.40	0.48
1:B:227:LEU:O	1:B:231:GLU:HG3	2.14	0.48
1:B:292:GLN:OE1	1:B:292:GLN:CA	2.60	0.48
1:A:52:LYS:HG2	1:B:451:PRO:HG2	1.96	0.47
1:A:67:ALA:HB1	1:A:72:PHE:HB2	1.96	0.47
1:B:395:SER:HB2	1:B:397:MET:CE	2.44	0.47
1:A:439:THR:HG22	1:A:442:GLU:N	2.27	0.47
1:B:395:SER:HB2	1:B:397:MET:HE3	1.97	0.47
1:A:249:VAL:HG21	1:A:273:MET:HE3	1.96	0.47
1:A:301:VAL:HG13	1:A:302:ASP:N	2.28	0.47
1:A:168:ARG:HD2	1:A:251:ARG:HE	1.80	0.47
1:B:58:THR:HG23	1:B:203:GLU:CB	2.37	0.47
1:A:168:ARG:HH11	1:A:251:ARG:HG2	1.80	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:235:GLU:C	1:A:237:GLY:H	2.18	0.47
1:A:371:VAL:HG13	1:A:376:SER:HB2	1.96	0.47
1:A:406:CYS:SG	1:A:464:LEU:HD13	2.54	0.47
1:B:2:VAL:O	1:B:2:VAL:CG2	2.58	0.47
1:A:365:VAL:HG23	1:A:427:ILE:HD11	1.97	0.47
1:A:315:ALA:HB1	1:A:331:GLN:CB	2.45	0.47
1:B:428:LEU:HD12	1:B:428:LEU:O	2.15	0.47
1.A.47.ASP.HB3	$2 \cdot A \cdot 999 \cdot FAD \cdot HM82$	1.97	0.47
1:A:83:LEU:CD1	1:A:87:HIS:CE1	2.98	0.47
1:A:362:ILE:HG23	1:A:419:VAL:HG22	1.97	0.46
1.A.162.ALA.CB	1·A·249·VAL·HB	2 45	0.46
1·A·302·ASP·HB3	1:A:304:VAL:N	2.24	0.46
1.A.361.GLU·HB2	1·A·420·ALA·O	2.14	0.46
1.B.439.THB.CG2	1.B.441.ASN.HB2	2.45	0.46
1:A:435:GLN:NE2	1·B·445·GLN·HB3	2.30	0.46
1.B.210.VAL:HG11	1·B·217·VAL·HG13	1.98	0.46
1.B.252.THB.HG22	1.B.255.GLY.H	1.30	0.46
1.A.72.PHE.CE2	1.B.200.011.11	2.51	0.46
1.A.302.ASP.OD2	1:A:306:ABG:HG2	2.51	0.46
1:A:292:GLN:OE1	1:A:292:GLN:HA	2.16	0.10
$1 \cdot A \cdot 404 \cdot ILE \cdot HD12$	1:A:460:ALA:CB	2.10	0.10
1:A:58:THB:HG22	1.A.359.ARG.NH1	2.06	0.45
1:A:168:ABG:HD2	1:A:251:ABG:NE	2.00	0.19
1.B.62.THB.HG22	1·B·63·GLU·N	2.31	0.45
1.B.382.ILE.CG2	$1 \cdot B \cdot 464 \cdot L E U \cdot H D 21$	2.30	0.45
1:A:97:GLN:O	$1 \cdot A \cdot 101 \cdot ILE \cdot HG13$	2.17	0.45
1.B.327.VAL:O	1·B·331·GLN·HG3	2.15	0.45
1·B·401·PHE·CD1	1·B·401·PHE·C	2.10	0.45
1.A.429.PRO.CG	1·B·429·PRO·HG3	2.32	0.45
1.B.182.PRO.HB3	1.B.270.HIS.CD2	2.52	0.45
1:A:451:PRO:0	1:A:451:PRO:HG2	2.02	0.44
1·B·209·THB·HG21	1.B.266.VAL.HG11	1 98	0.44
1:A:404:ILE:HG22	1:A:464:LEU:HD11	1.98	0.44
1.A.315.ALA.CB	1·A·331·GLN·HB3	2.47	0.44
1.B.148.VAL.HB	1.B.312.ILE.HG12	1 99	0.44
1:B:405:PHE:O	1:B:414:ILE:HG12	2.17	0.44
1.B.25.HIS.N	1·B·26·PRO·HD3	2.32	0.44
1:A:19·LEU·HD12	1:A:19:LEU·HA	1.73	0.44
1:A:70·LEU·HD13	1:B:60:LEU·CD1	2.21	0.44
1.B.80.LVS.HA	1.B.80.LVS.HD3	1 66	0.44
1:A:35:ASP:OD2	1:A:38:GLY:N	2.48	0.44



	A L C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:59:GLY:O	1:B:62:THR:N	2.42	0.44	
1:B:170:LEU:HD11	1:B:178:LEU:HD21	1.99	0.44	
1:B:194:GLY:CA	1:B:274:THR:HG21	2.43	0.44	
1:A:12:PRO:O	1:A:13:ALA:C	2.56	0.43	
1:A:391:ARG:O	1:A:394:MET:HB2	2.18	0.43	
1:A:435:GLN:O	1:A:435:GLN:HG3	2.16	0.43	
1:A:439:THR:CG2	1:A:441:ASN:HB2	2.48	0.43	
1:B:64:LEU:C	1:B:66:ARG:N	2.71	0.43	
1:B:164:PRO:HA	1:B:169:ILE:CG2	2.48	0.43	
1:A:49:VAL:HB	1:A:50:PRO:HD3	2.01	0.43	
1:B:439:THR:HG22	1:B:442:GLU:CD	2.39	0.43	
1:A:365:VAL:O	1:A:415:GLY:HA2	2.18	0.43	
1:B:370:SER:O	1:B:371:VAL:C	2.56	0.43	
1:B:441:ASN:O	1:B:445:GLN:HG3	2.19	0.43	
1:A:324:LEU:HD11	1:A:354:ALA:HB2	1.99	0.43	
1:B:97:GLN:OE1	1:B:97:GLN:HA	2.19	0.43	
1:B:229:LEU:HD11	1:B:358:THR:HG21	1.99	0.43	
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.72	0.43	
1:B:8:LEU:CD2	1:B:117:GLY:HA3	2.48	0.43	
1:B:192:VAL:O	1:B:196:GLU:HG3	2.19	0.43	
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.92	0.43	
1:B:52:LYS:N	1:B:52:LYS:CD	2.81	0.43	
1:B:158:ILE:HD13	1:B:164:PRO:HD2	2.01	0.43	
1:A:350:ARG:HA	1:A:350:ARG:HD3	1.74	0.43	
1:A:404:ILE:CG2	1:A:464:LEU:HD12	2.46	0.43	
1:B:81:ILE:O	1:B:81:ILE:HG23	2.18	0.42	
1:B:289:VAL:HG11	1:B:312:ILE:HD12	2.01	0.42	
1:A:130:ARG:NH1	1:A:144:GLU:OE2	2.52	0.42	
1:A:275:ILE:CG2	1:A:276:GLY:N	2.48	0.42	
1:B:249:VAL:HG21	1:B:273:MET:HE3	1.99	0.42	
1:A:256:VAL:HG11	1:A:271:ALA:HB2	2.00	0.42	
1:B:380:ARG:NH1	1:B:466:ALA:CB	2.78	0.42	
1:B:89:ARG:CG	1:B:89:ARG:NH1	2.75	0.42	
1:B:149:LEU:HA	1:B:313:TYR:O	2.19	0.42	
1:A:330:MET:CB	1:B:447:LEU:HD21	2.49	0.42	
1:A:347:ILE:H	1:A:347:ILE:CD1	2.27	0.42	
1:A:417:VAL:HG12	1:A:418:VAL:N	2.34	0.42	
1:B:157:ARG:HD2	1:B:275:ILE:HG21	2.02	0.42	
1:B:414:ILE:HG21	1:B:414:ILE:HD13	1.75	0.42	
1:A:25:HIS:N	1:A:26:PRO:CD	2.82	0.42	
1:A:324:LEU:HD11	1:A:354:ALA:CB	2.49	0.42	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:216:HIS:C	1:B:218:LEU:H	2.22	0.42	
1:A:64:LEU:O	1:A:66:ARG:N	2.53	0.42	
1:A:349:LEU:HD22	1:A:349:LEU:H	1.84	0.42	
1:A:365:VAL:CG2	1:A:427:ILE:HD11	2.50	0.42	
1:B:39:ILE:CG2	1:B:101:ILE:HG22	2.50	0.42	
1:B:198:VAL:HG21	1:B:210:VAL:HG22	2.01	0.42	
1:B:382:ILE:CG1	1:B:383:MET:N	2.82	0.42	
2:A:999:FAD:H1'1	2:A:999:FAD:H9	1.78	0.42	
1:A:64:LEU:C	1:A:66:ARG:H	2.24	0.42	
1:B:106:LEU:HD12	1:B:112:VAL:HG23	2.01	0.42	
2:B:999:FAD:H9	2:B:999:FAD:H1'1	1.92	0.42	
1:A:200:ALA:HA	1:A:359:ARG:NH2	2.34	0.41	
1:A:303:ARG:O	1:A:347:ILE:HD12	2.20	0.41	
1:B:159:LEU:HB3	1:B:162:ALA:HB3	2.02	0.41	
1:B:206:VAL:HA	1:B:207:PRO:HD3	1.96	0.41	
1:B:64:LEU:C	1:B:66:ARG:H	2.21	0.41	
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.84	0.41	
1:B:279:PRO:HB2	1:B:281:THR:HG23	2.02	0.41	
1:B:439:THR:HG22	1:B:442:GLU:H	1.84	0.41	
1:A:308:LEU:CD1	1:A:308:LEU:N	2.55	0.41	
1:A:459:GLU:O	1:A:460:ALA:C	2.59	0.41	
1:B:327:VAL:HG13	1:B:347:ILE:CD1	2.51	0.41	
1:A:224:ASP:OD2	1:A:403:LYS:NZ	2.47	0.41	
1:A:229:LEU:CD1	1:A:362:ILE:HD11	2.37	0.41	
1:B:285:GLY:O	1:B:286:LEU:C	2.58	0.41	
1:A:70:LEU:CD1	1:B:60:LEU:HD11	2.21	0.41	
1:A:260:MET:O	1:A:262:ASP:N	2.54	0.41	
1:A:316:GLY:HA3	2:A:999:FAD:O2P	2.21	0.41	
1:A:355:THR:HA	1:A:362:ILE:O	2.21	0.41	
1:B:52:LYS:N	1:B:52:LYS:HD3	2.36	0.41	
1:B:157:ARG:HB2	1:B:278:VAL:HG23	2.03	0.41	
1:B:218:LEU:C	1:B:218:LEU:HD22	2.40	0.41	
1:B:252:THR:HG22	1:B:255:GLY:N	2.36	0.41	
1:B:302:ASP:OD2	1:B:306:ARG:NH1	2.47	0.41	
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.91	0.40	
1:B:285:GLY:C	1:B:287:GLU:N	2.74	0.40	
1:B:367:VAL:HA	1:B:368:PRO:HD3	1.97	0.40	
1:A:310:THR:C	1:A:312:ILE:H	2.25	0.40	
1:B:214:GLN:CD	1:B:214:GLN:N	2.75	0.40	
1:B:260:MET:CG	1:B:264:ARG:HB3	2.51	0.40	
1:B:301:VAL:CG1	1:B:305:SER:HA	2.51	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:LEU:O	1:B:429:PRO:HD2	2.22	0.40
1:A:175:LEU:HD21	1:A:272:LEU:HG	2.03	0.40
1:A:355:THR:HG21	1:A:424:SER:CA	2.48	0.40
1:A:440:VAL:HB	1:A:461:ALA:HB1	2.03	0.40
1:B:241:PHE:CZ	1:B:266:VAL:CG2	3.00	0.40
1:B:322:LEU:HA	1:B:323:PRO:HD3	1.83	0.40
1:A:380:ARG:HB3	1:A:464:LEU:HD22	2.03	0.40
1:B:92:THR:HG22	1:B:93:LEU:N	2.36	0.40
1:B:289:VAL:O	1:B:289:VAL:HG13	2.22	0.40
1:B:340:LEU:HD23	1:B:340:LEU:HA	1.93	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	Perce	ntiles
1	А	455/499 (91%)	418 (92%)	30 (7%)	7(2%)	10	31
1	В	455/499 (91%)	413 (91%)	34 (8%)	8 (2%)	8	26
All	All	910/998~(91%)	831 (91%)	64 (7%)	15~(2%)	9	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	63	GLU
1	А	64	LEU
1	А	253	GLY
1	А	261	THR
1	А	275	ILE
1	В	286	LEU
1	А	65	ARG
1	А	48	CYS



Continued from previous page...

Mol	Chain	Res	Type
1	В	137	ASP
1	В	235	GLU
1	В	370	SER
1	В	41	GLY
1	В	371	VAL
1	В	138	GLY
1	В	275	ILE

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	352/386~(91%)	306~(87%)	46 (13%)	4 12
1	В	352/386~(91%)	301~(86%)	51 (14%)	3 9
All	All	704/772~(91%)	607~(86%)	97 (14%)	3 10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	THR
1	А	15	TYR
1	А	24	SER
1	А	52	LYS
1	А	60	LEU
1	А	73	HIS
1	А	83	LEU
1	А	92	THR
1	А	106	LEU
1	А	108	MET
1	А	118	GLU
1	А	123	THR
1	А	137	ASP
1	А	139	SER
1	A	157	ARG
1	А	183	ASP



Mol Chain Res Type					
1	А	186	ILE		
1	А	193	THR		
1	A	213	SER		
1	А	215	ASP		
1	A	218	LEU		
1	А	227	LEU		
1	А	260	MET		
1	А	264	ARG		
1	А	266	VAL		
1	А	272	LEU		
1	А	274	THR		
1	А	287	GLU		
1	А	289	VAL		
1	А	295	ARG		
1	А	299	LEU		
1	А	301	VAL		
1	А	302	ASP		
1	А	308	LEU		
1	А	321	LEU		
1	А	347	ILE		
1	А	355	THR		
1	А	358	THR		
1	А	359	ARG		
1	А	365	VAL		
1	А	376	SER		
1	А	439	THR		
1	А	442	GLU		
1	А	451	PRO		
1	A	456	SER		
1	A	459	GLU		
1	B	3	THR		
1	В	4	ARG		
1	В	15	TYR		
1	B	28	THR		
1	В	35	ASP		
1	В	58	THR		
1	В	62	THR		
1	В	65	ARG		
1	В	80	LYS		
1	В	81	ILE		
1	B	83	LEU		
1	В	85	GLN		



Mol	Chain	Res	Type
1	В	89	ARG
1	В	92	THR
1	В	97	GLN
1	В	122	SER
1	В	123	THR
1	В	130	ARG
1	В	132	LYS
1	В	161	SER
1	В	163	GLN
1	В	190	SER
1	В	218	LEU
1	В	227	LEU
1	В	229	LEU
1	В	239	ARG
1	В	240	LEU
1	В	257	LEU
1	В	259	THR
1	В	262	ASP
1	В	264	ARG
1	В	272	LEU
1	В	274	THR
1	В	295	ARG
1	В	299	LEU
1	В	301	VAL
1	В	306	ARG
1	В	308	LEU
1	В	321	LEU
1	В	322	LEU
1	B	349	LEU
1	В	355	THR
1	В	370	SER
1	В	376	SER
1	В	387	ARG
1	В	398	ARG
1	В	409	SER
1	В	432	VAL
1	В	439	THR
1	В	456	SER
1	В	458	THR

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



Mol	Chain	Res	Type
1	А	85	GLN
1	А	270	HIS
1	А	280	ASN
1	В	69	HIS
1	В	104	GLN
1	В	270	HIS
1	В	297	ASN
1	В	338	HIS
1	В	441	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 monosaccharides 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).

Mal	Trune	Turna Chain Dag Lim		Tinle	Bond lengths			B	ond ang	gles
INIOI	туре	Chain	nes	LIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	FAD	В	999	-	$53,\!58,\!58$	2.45	14 (26%)	68,89,89	1.47	13 (19%)
2	FAD	А	999	-	$53,\!58,\!58$	2.20	14 (26%)	68,89,89	1.43	11 (16%)

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



- means no outners of that kind were identified.									
Mol Type Chain Res Link Chirals Torsions Rings									
2	FAD	В	999	-	-	6/30/50/50	0/6/6/6		
2	FAD	А	999	-	-	7/30/50/50	0/6/6/6		

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	999	FAD	C4A-N3A	8.50	1.47	1.35
2	В	999	FAD	C4X-N5	7.23	1.44	1.30
2	А	999	FAD	C4X-N5	6.21	1.42	1.30
2	А	999	FAD	C4A-N3A	5.91	1.43	1.35
2	В	999	FAD	C9A-N10	5.11	1.50	1.41
2	В	999	FAD	C2A-N3A	5.00	1.40	1.32
2	В	999	FAD	C9A-C5X	4.61	1.48	1.41
2	А	999	FAD	C5'-C4'	-4.51	1.45	1.51
2	В	999	FAD	C5'-C4'	-4.49	1.45	1.51
2	А	999	FAD	C2A-N3A	4.40	1.39	1.32
2	А	999	FAD	C5A-C4A	-4.32	1.29	1.40
2	В	999	FAD	C5A-C4A	-4.08	1.30	1.40
2	А	999	FAD	C9A-N10	3.94	1.48	1.41
2	А	999	FAD	C3B-C4B	3.77	1.62	1.53
2	А	999	FAD	C9A-C5X	3.64	1.47	1.41
2	В	999	FAD	C1'-C2'	-3.56	1.47	1.52
2	В	999	FAD	C6-C7	3.09	1.44	1.39
2	А	999	FAD	C4X-C4	-2.98	1.33	1.44
2	В	999	FAD	C10-N1	2.83	1.39	1.33
2	А	999	FAD	C2B-C3B	-2.69	1.46	1.53
2	А	999	FAD	C1'-N10	-2.50	1.41	1.48
2	А	999	FAD	P-O1P	-2.48	1.42	1.50
2	А	999	FAD	O4'-C4'	2.28	1.48	1.43
2	В	999	FAD	C5X-N5	2.27	1.43	1.39
2	В	999	FAD	C2B-C1B	-2.21	1.50	1.53
2	В	999	FAD	C2B-C3B	-2.16	1.47	1.53
2	А	999	FAD	C7M-C7	2.14	1.55	1.51
2	В	999	FAD	C4X-C4	-2.11	1.36	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	999	FAD	O4'-C4'-C5'	-3.67	101.67	109.92
2	А	999	FAD	C3B-C2B-C1B	3.27	105.90	100.98



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	999	FAD	N3A-C2A-N1A	-3.13	123.78	128.68
2	А	999	FAD	O4'-C4'-C5'	-3.08	102.98	109.92
2	А	999	FAD	C5'-C4'-C3'	3.07	118.14	112.20
2	А	999	FAD	N3A-C2A-N1A	-3.07	123.88	128.68
2	А	999	FAD	O4'-C4'-C3'	-3.00	101.81	109.10
2	В	999	FAD	O3'-C3'-C4'	-2.97	101.64	108.81
2	А	999	FAD	O5B-C5B-C4B	-2.89	99.05	108.99
2	В	999	FAD	C3B-C2B-C1B	2.73	105.09	100.98
2	В	999	FAD	C5'-C4'-C3'	2.72	117.45	112.20
2	А	999	FAD	C1'-N10-C9A	-2.69	116.03	120.51
2	В	999	FAD	C5A-C6A-N6A	2.53	124.20	120.35
2	В	999	FAD	C9-C9A-N10	2.51	125.23	121.84
2	В	999	FAD	C5X-C9A-N10	-2.43	115.44	117.95
2	В	999	FAD	O4'-C4'-C3'	-2.39	103.29	109.10
2	А	999	FAD	C5X-C9A-N10	-2.36	115.52	117.95
2	А	999	FAD	C4-C4X-C10	2.26	120.59	116.79
2	В	999	FAD	C1'-C2'-C3'	2.25	116.06	109.79
2	А	999	FAD	C4X-C10-N10	2.22	119.73	116.48
2	А	999	FAD	O2B-C2B-C3B	2.21	118.98	111.82
2	В	999	FAD	O2'-C2'-C1'	-2.14	104.62	109.80
2	В	999	FAD	C4X-C10-N10	2.14	119.60	116.48
2	В	999	FAD	O2B-C2B-C3B	2.11	118.65	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	999	FAD	С5В-О5В-РА-О1А
2	А	999	FAD	C5B-O5B-PA-O3P
2	В	999	FAD	C5B-O5B-PA-O3P
2	А	999	FAD	P-O3P-PA-O1A
2	А	999	FAD	PA-O3P-P-O5'
2	В	999	FAD	PA-O3P-P-O5'
2	А	999	FAD	C5B-O5B-PA-O2A
2	В	999	FAD	C5B-O5B-PA-O1A
2	В	999	FAD	C5B-O5B-PA-O2A
2	В	999	FAD	P-O3P-PA-O2A
2	A	999	FAD	O4B-C4B-C5B-O5B
2	В	999	FAD	O4B-C4B-C5B-O5B
2	A	999	FAD	P-O3P-PA-O2A

There are no ring outliers.



Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
2	В	999	FAD	2	0
2	А	999	FAD	5	0

2 monomers are involved in 7 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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, 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	А	459/499 (91%)	-0.74	1 (0%) 95 94	1, 12, 34, 61	0
1	В	459/499 (91%)	-0.68	0 100 100	1, 12, 37, 51	0
All	All	918/998~(91%)	-0.71	1 (0%) 95 95	1, 12, 36, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	80	LYS	2.8

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 monosaccharides 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. 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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
2	FAD	А	999	53/53	0.97	0.13	$1,\!6,\!10,\!12$	0
2	FAD	В	999	53/53	0.98	0.12	1,8,12,12	0

The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

