



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:24 am BST

PDB ID : 1XDI
Title : Crystal structure of LpdA (Rv3303c) from Mycobacterium tuberculosis
Authors : Argyrou, A.; Vetting, M.W.; Blanchard, J.S.
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

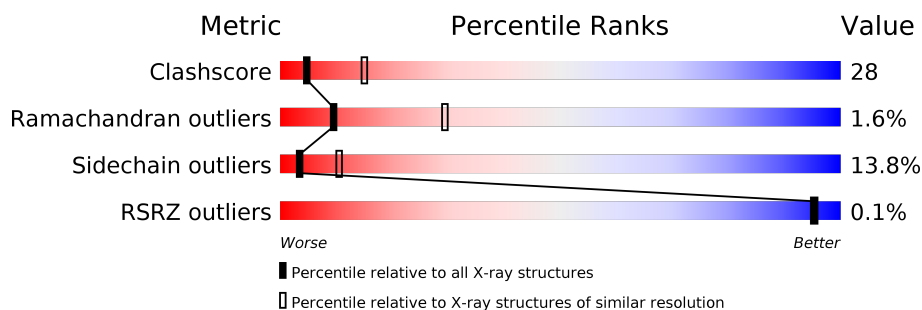
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	 57% 28% 7% 8%
1	B	499	 47% 38% 6% 8%

2 Entry composition

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.

- Molecule 1 is a protein called Rv3303c-lpdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3356	2101	607	635	13			
1	B	459	Total	C	N	O	S	0	0	0
			3356	2101	607	635	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	EXPRESSION TAG	UNP O53355
A	495	HIS	-	EXPRESSION TAG	UNP O53355
A	496	HIS	-	EXPRESSION TAG	UNP O53355
A	497	HIS	-	EXPRESSION TAG	UNP O53355
A	498	HIS	-	EXPRESSION TAG	UNP O53355
A	499	HIS	-	EXPRESSION TAG	UNP O53355
B	494	HIS	-	EXPRESSION TAG	UNP O53355
B	495	HIS	-	EXPRESSION TAG	UNP O53355
B	496	HIS	-	EXPRESSION TAG	UNP O53355
B	497	HIS	-	EXPRESSION TAG	UNP O53355
B	498	HIS	-	EXPRESSION TAG	UNP O53355
B	499	HIS	-	EXPRESSION TAG	UNP O53355

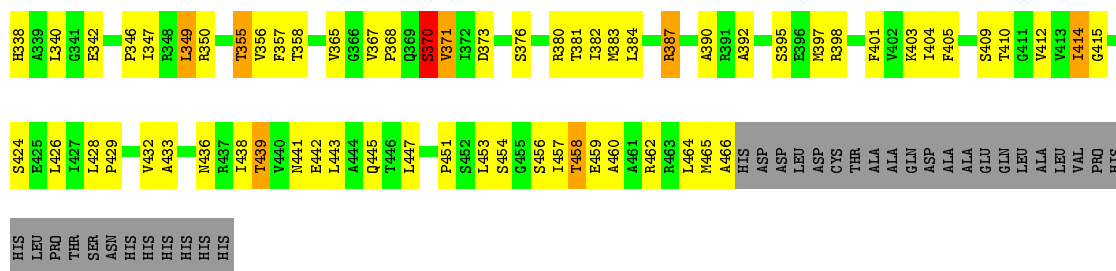
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	50	Total	O	0	0
			50	50		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	244.20 Å 244.20 Å 104.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.81 35.25 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.81) 99.7 (35.25-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.276 0.191 , (Not available)	Depositor 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.*

¹Intensities estimated from amplitudes.

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.

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	3/3404 (0.1%)	1.06	4/4637 (0.1%)
1	B	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	A	0	1

All (3) bond length outliers are listed below:

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

All (12) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	302	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	B	387	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	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	A	220	TYR	Sidechain

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	3356	0	3454	187	0
1	B	3356	0	3454	217	0
2	A	53	0	31	5	0
2	B	53	0	31	2	0
3	A	57	0	0	4	0
3	B	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 distance (Å)	Clash overlap (Å)
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:308:LEU:HD12	1:A:308:LEU:H	1.14	1.06
1:A:70:LEU:HD13	1:B:60:LEU:HD11	1.28	1.06
1:A:58:THR:HG22	1:A:359:ARG:HH12	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:CD1	1:A:308:LEU:H	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:CD1	1:B:308:LEU:H	1.87	0.88
1:B:392:ALA:HA	1:B:397:MET:CE	2.03	0.87
1:A:308:LEU:N	1:A:308:LEU:HD12	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:165:ASP:HB2	1:B:167:GLU:H	1.48	0.79
1:B:58:THR:CG2	1:B:203:GLU:HB2	2.12	0.79
1:B:292:GLN:HA	1:B:292:GLN:OE1	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:O	1:B:2:VAL:HG23	1.87	0.73
1:B:454:SER:HA	1:B:457:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:CG2	1:A:274:THR:O	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:HA	1:B:203:GLU:OE1	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:404:ILE:HD12	1:A:460:ALA:HB3	1.77	0.66
1:A:88:ALA:O	1:A:92:THR:HB	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:LYS:HE2	1:A:357:PHE:CD2	2.33	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:HH11	1:A:295:ARG:HG3	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:274:THR:CG2	1:B:274:THR:O	2.47	0.61
1:B:20:VAL:HG21	1:B:333:ARG:CG	2.31	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:HG2	1:B:89:ARG:HH11	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:242:LYS:O	1:B:264:ARG:NH2	2.36	0.57
1:B:91:LYS:NZ	1:B:177:ASP:OD1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:O	1:B:126:LEU:HG	2.03	0.57
1:B:8:LEU:HD22	1:B:117:GLY:HA3	1.84	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: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:A:72:PHE:HE2	1:B:81:ILE:HD11	1.71	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:O	1:A:66:ARG:HG3	2.05	0.54
1:A:169:ILE:CD1	1:A:249:VAL:HG12	2.37	0.54
1:A:157:ARG:HD2	1:A:275:ILE:CG2	2.38	0.54
1:A:302:ASP:HB2	1:A:306:ARG:N	2.22	0.54
1:A:245:ARG:O	1:A:260:MET:HB2	2.08	0.54
1:A:87:HIS:CE1	1:A:176:TYR:HA	2.43	0.54
1:B:286:LEU:CD1	1:B:293:LEU:HD21	2.37	0.54
1:B:52:LYS:HE2	2:B:999:FAD:O4	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:CG	1:A:295:ARG:HH11	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: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:B:83:LEU:HG	1:B:181:LEU:CD2	2.40	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: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:A:63:GLU:O	1:A:64:LEU:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:83:LEU:HG	1:A:181:LEU:CD2	2.41	0.49
1:A:67:ALA:HB3	1:A:68:PRO:HD3	1.93	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:439:THR:HG23	1:B:441:ASN:HB2	1.94	0.49
1:B:382:ILE:HG22	1:B:464:LEU:HD21	1.95	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:301:VAL:HG23	1:B:314:ALA:HB3	1.96	0.48
1:B:87:HIS:O	1:B:91:LYS:HG3	2.13	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:CA	1:B:292:GLN:OE1	2.60	0.48
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:52:LYS:HG2	1:B:451:PRO:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:C	1:A:237:GLY:H	2.18	0.47
1:A:406:CYS:SG	1:A:464:LEU:HD13	2.54	0.47
1:A:371:VAL:HG13	1:A:376:SER:HB2	1.96	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:83:LEU:CD1	1:A:87:HIS:CE1	2.98	0.47
1:A:47:ASP:HB3	2:A:999:FAD:HM82	1.97	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:THR:CG2	1:B:441:ASN:HB2	2.45	0.46
1:B:210:VAL:HG11	1:B:217:VAL:HG13	1.98	0.46
1:B:252:THR:HG22	1:B:255:GLY:H	1.78	0.46
1:A:435:GLN:NE2	1:B:445:GLN:HB3	2.30	0.46
1:A:302:ASP:OD2	1:A:306:ARG:HG2	2.15	0.46
1:A:72:PHE:CE2	1:B:81:ILE:HD11	2.51	0.46
1:A:292:GLN:HA	1:A:292:GLN:OE1	2.16	0.46
1:A:404:ILE:HD12	1:A:460:ALA:CB	2.44	0.46
1:A:58:THR:HG22	1:A:359:ARG:NH1	2.06	0.45
1:A:168:ARG:HD2	1:A:251:ARG:NE	2.31	0.45
1:B:382:ILE:CG2	1:B:464:LEU:HD21	2.47	0.45
1:B:62:THR:HG22	1:B:63:GLU:N	2.30	0.45
1:A:97:GLN:O	1:A:101:ILE: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	2.90	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:HG2	1:A:451:PRO:O	2.17	0.44
1:B:209:THR: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:HA	1:A:19:LEU:HD12	1.73	0.44
1:A:70:LEU:HD13	1:B:60:LEU:CD1	2.21	0.44
1:B:80:LYS:HD3	1:B:80:LYS:HA	1.66	0.44
1:A:35:ASP:OD2	1:A:38:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:59:GLY:O	1:B:62:THR:N	2.42	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: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:97:GLN:OE1	1:B:97:GLN:HA	2.19	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:HA	1:B:229:LEU:HD23	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:289:VAL:HG11	1:B:312:ILE:HD12	2.01	0.42
1:B:81:ILE:HG23	1:B:81:ILE:O	2.18	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:149:LEU:HA	1:B:313:TYR:O	2.19	0.42
1:B:89:ARG:NH1	1:B:89:ARG:CG	2.75	0.42
1:A:330:MET:CB	1:B:447:LEU:HD21	2.49	0.42
1:A:347:ILE:CD1	1:A:347:ILE:H	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:HD13	1:B:414:ILE:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:HIS:C	1:B:218:LEU:H	2.22	0.42
1:A:349:LEU:H	1:A:349:LEU:HD22	1.84	0.42
1:A:365:VAL:CG2	1:A:427:ILE:HD11	2.50	0.42
1:A:64:LEU:O	1:A:66:ARG:N	2.53	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
1:B:39:ILE:CG2	1:B:101:ILE:HG22	2.50	0.42
2:A:999:FAD:H9	2:A:999:FAD:H1'1	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:HA	1:A:299:LEU:HD23	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:316:GLY:HA3	2:A:999:FAD:O2P	2.21	0.41
1:B:157:ARG:HB2	1:B:278:VAL:HG23	2.03	0.41
1:B:218:LEU:HD22	1:B:218:LEU:C	2.40	0.41
1:A:260:MET:O	1:A:262:ASP:N	2.54	0.41
1:A:355:THR:HA	1:A:362:ILE:O	2.21	0.41
1:B:252:THR:HG22	1:B:255:GLY:N	2.36	0.41
1:B:52:LYS:N	1:B:52:LYS:HD3	2.36	0.41
1:B:302:ASP:OD2	1:B:306:ARG:NH1	2.47	0.41
1:A:322:LEU:HA	1:A:322:LEU:HD23	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:N	1:B:214:GLN:CD	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

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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:289:VAL:O	1:B:289:VAL:HG13	2.22	0.40
1:B:340:LEU:HA	1:B:340:LEU:HD23	1.93	0.40
1:B:92:THR:HG22	1:B:93:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/499 (91%)	418 (92%)	30 (7%)	7 (2%)	10	31
1	B	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	A	63	GLU
1	A	64	LEU
1	A	253	GLY
1	A	261	THR
1	A	275	ILE
1	B	286	LEU
1	A	65	ARG
1	A	48	CYS

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/386 (91%)	306 (87%)	46 (13%)	4	12
1	B	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	A	3	THR
1	A	15	TYR
1	A	24	SER
1	A	52	LYS
1	A	60	LEU
1	A	73	HIS
1	A	83	LEU
1	A	92	THR
1	A	106	LEU
1	A	108	MET
1	A	118	GLU
1	A	123	THR
1	A	137	ASP
1	A	139	SER
1	A	157	ARG
1	A	183	ASP

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

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

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

Mol	Chain	Res	Type
1	A	85	GLN
1	A	270	HIS
1	A	280	ASN
1	B	69	HIS
1	B	104	GLN
1	B	270	HIS
1	B	297	ASN
1	B	338	HIS
1	B	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 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	$\# Z > 2$
2	FAD	B	999	-	51,58,58	2.92	16 (31%)	60,89,89	2.35	15 (25%)
2	FAD	A	999	-	51,58,58	2.68	17 (33%)	60,89,89	2.45	14 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	999	-	-	6/30/50/50	0/6/6/6
2	FAD	A	999	-	-	7/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	FAD	C9A-N10	8.60	1.50	1.38
2	B	999	FAD	C4A-N3A	8.50	1.47	1.35
2	B	999	FAD	C4X-N5	8.04	1.44	1.33
2	A	999	FAD	C9A-N10	7.08	1.48	1.38
2	A	999	FAD	C4X-N5	6.65	1.42	1.33
2	A	999	FAD	C1'-N10	-6.25	1.41	1.48
2	A	999	FAD	C4A-N3A	5.91	1.43	1.35
2	B	999	FAD	C5X-N5	5.14	1.43	1.35
2	B	999	FAD	C2A-N3A	5.00	1.40	1.32
2	A	999	FAD	C4-C4X	-4.53	1.33	1.41
2	A	999	FAD	C5'-C4'	-4.51	1.45	1.51
2	B	999	FAD	C4-N3	4.51	1.40	1.33
2	B	999	FAD	C5'-C4'	-4.49	1.45	1.51
2	B	999	FAD	C10-N1	4.47	1.39	1.33
2	A	999	FAD	C2A-N3A	4.40	1.39	1.32
2	B	999	FAD	C4X-C10	4.37	1.43	1.38
2	A	999	FAD	C5A-C4A	-4.32	1.29	1.40
2	A	999	FAD	C5X-N5	4.21	1.42	1.35
2	A	999	FAD	C4X-C10	4.15	1.43	1.38
2	B	999	FAD	C5A-C4A	-4.08	1.30	1.40
2	A	999	FAD	C3B-C4B	3.77	1.62	1.53
2	B	999	FAD	C1'-N10	-3.62	1.44	1.48
2	B	999	FAD	C9A-C5X	3.17	1.48	1.42
2	A	999	FAD	C2B-C3B	-2.69	1.46	1.53
2	B	999	FAD	C4-C4X	-2.68	1.36	1.41
2	B	999	FAD	C6-C7	2.51	1.44	1.37
2	A	999	FAD	P-O1P	-2.48	1.42	1.50
2	A	999	FAD	C4-N3	2.36	1.37	1.33
2	A	999	FAD	C9A-C5X	2.35	1.47	1.42
2	A	999	FAD	O4'-C4'	2.28	1.48	1.43
2	B	999	FAD	C2B-C1B	-2.21	1.50	1.53
2	B	999	FAD	C2B-C3B	-2.16	1.47	1.53
2	A	999	FAD	C7M-C7	2.14	1.55	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C4-N3-C2	12.83	125.98	115.14
2	B	999	FAD	C4-N3-C2	12.25	125.48	115.14
2	A	999	FAD	C4X-C4-N3	-6.17	114.99	123.43
2	B	999	FAD	C4X-C4-N3	-5.88	115.39	123.43
2	A	999	FAD	C1'-N10-C10	4.13	122.11	118.41
2	B	999	FAD	O4'-C4'-C5'	-3.67	101.67	109.92
2	A	999	FAD	C3B-C2B-C1B	3.27	105.90	100.98
2	A	999	FAD	C10-C4X-N5	3.24	123.50	121.26
2	B	999	FAD	C10-C4X-N5	3.20	123.47	121.26
2	B	999	FAD	C5X-C9A-N10	-3.13	115.44	117.72
2	B	999	FAD	N3A-C2A-N1A	-3.13	123.78	128.68
2	A	999	FAD	O4'-C4'-C5'	-3.08	102.98	109.92
2	A	999	FAD	C5'-C4'-C3'	3.07	118.14	112.20
2	A	999	FAD	N3A-C2A-N1A	-3.07	123.88	128.68
2	A	999	FAD	C5X-C9A-N10	-3.03	115.52	117.72
2	A	999	FAD	O4'-C4'-C3'	-3.00	101.81	109.10
2	B	999	FAD	O3'-C3'-C4'	-2.97	101.64	108.81
2	A	999	FAD	O5B-C5B-C4B	-2.89	99.05	108.99
2	A	999	FAD	C1'-N10-C9A	-2.88	116.03	118.29
2	B	999	FAD	C3B-C2B-C1B	2.73	105.09	100.98
2	B	999	FAD	C5'-C4'-C3'	2.72	117.45	112.20
2	B	999	FAD	C5A-C6A-N6A	2.53	124.20	120.35
2	B	999	FAD	O4'-C4'-C3'	-2.39	103.29	109.10
2	A	999	FAD	C4-C4X-N5	-2.36	115.90	118.60
2	B	999	FAD	C1'-N10-C10	2.27	120.44	118.41
2	B	999	FAD	C1'-C2'-C3'	2.25	116.06	109.79
2	A	999	FAD	O2B-C2B-C3B	2.21	118.98	111.82
2	B	999	FAD	O2B-C2B-C3B	2.11	118.65	111.82
2	B	999	FAD	O2'-C2'-C1'	-2.06	104.62	109.59

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	999	FAD	C5B-O5B-PA-O3P
2	A	999	FAD	C5B-O5B-PA-O1A
2	A	999	FAD	C5B-O5B-PA-O3P
2	A	999	FAD	P-O3P-PA-O1A
2	B	999	FAD	PA-O3P-P-O5'
2	A	999	FAD	PA-O3P-P-O5'
2	B	999	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	999	FAD	C5B-O5B-PA-O2A
2	A	999	FAD	C5B-O5B-PA-O2A
2	B	999	FAD	P-O3P-PA-O2A
2	B	999	FAD	O4B-C4B-C5B-O5B
2	A	999	FAD	O4B-C4B-C5B-O5B
2	A	999	FAD	P-O3P-PA-O2A

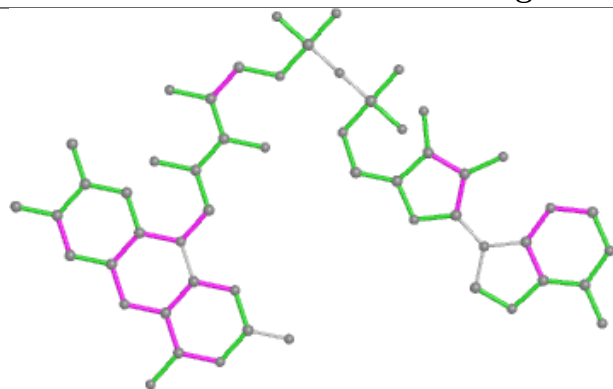
There are no ring outliers.

2 monomers are involved in 7 short contacts:

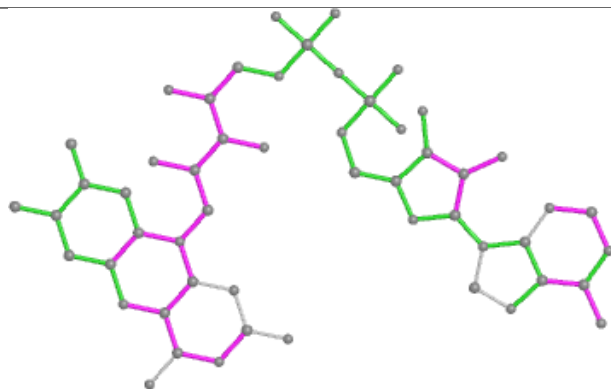
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	FAD	2	0
2	A	999	FAD	5	0

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 than 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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

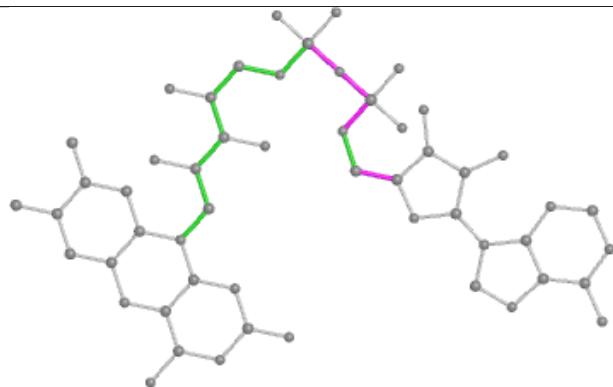
Ligand FAD B 999



Bond lengths



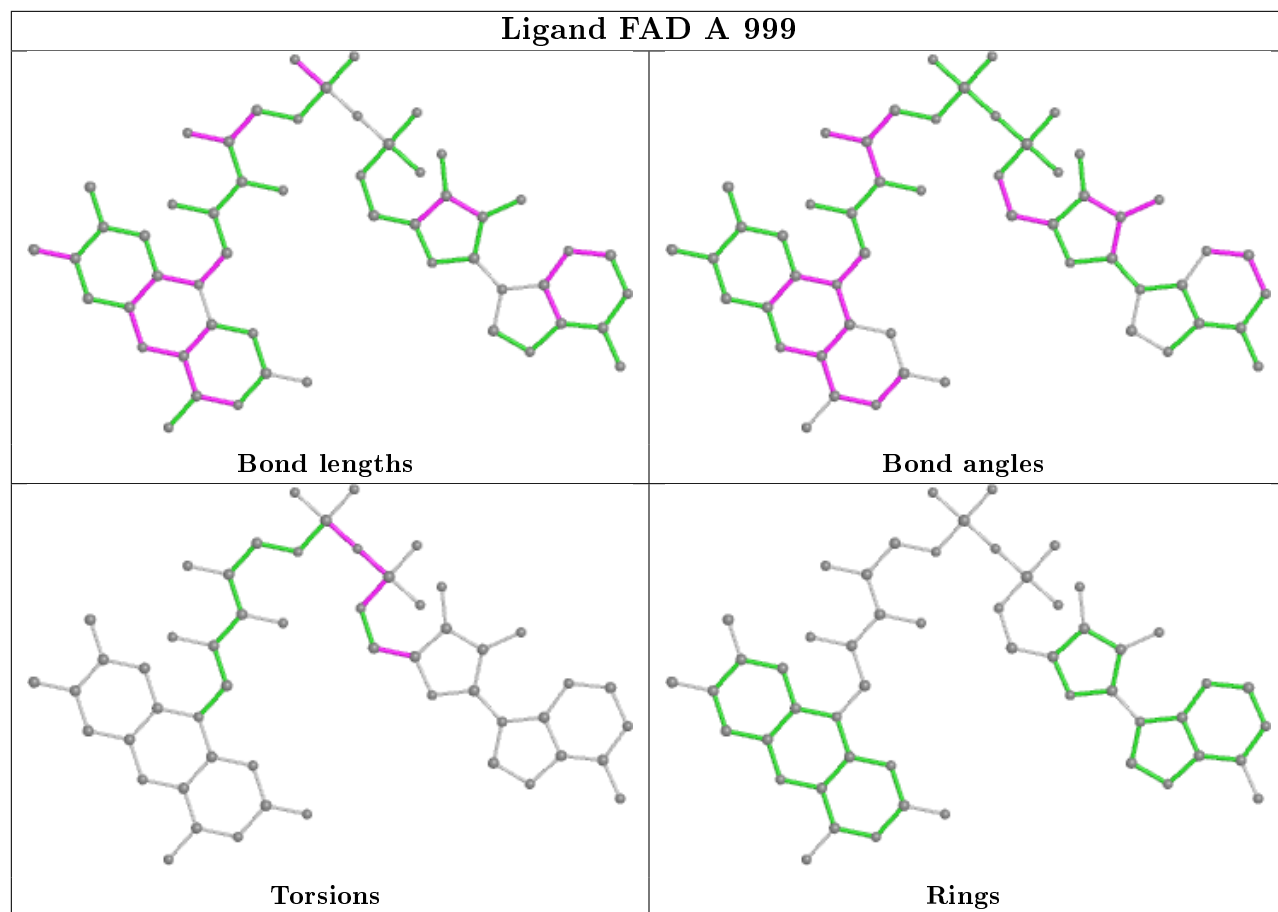
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/499 (91%)	-0.74	1 (0%) 95 94	1, 12, 34, 61	0
1	B	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	A	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 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

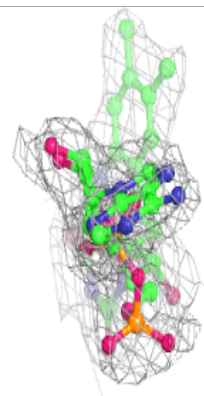
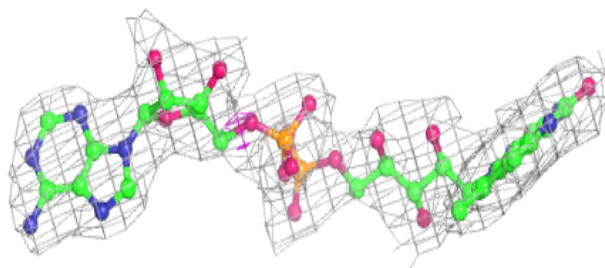
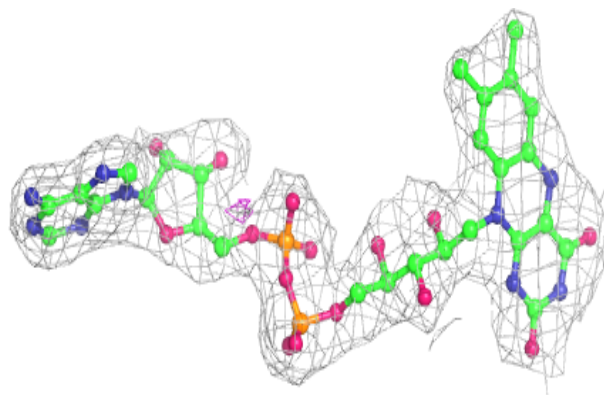
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	999	53/53	0.97	0.13	1,6,10,12	0
2	FAD	B	999	53/53	0.98	0.12	1,8,12,12	0

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.

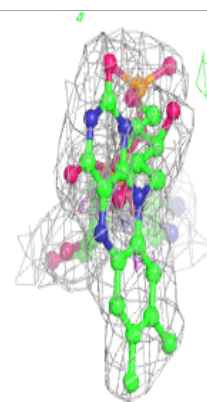
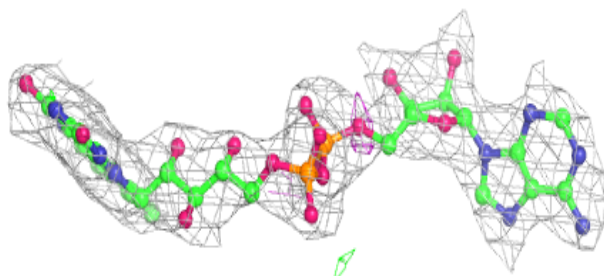
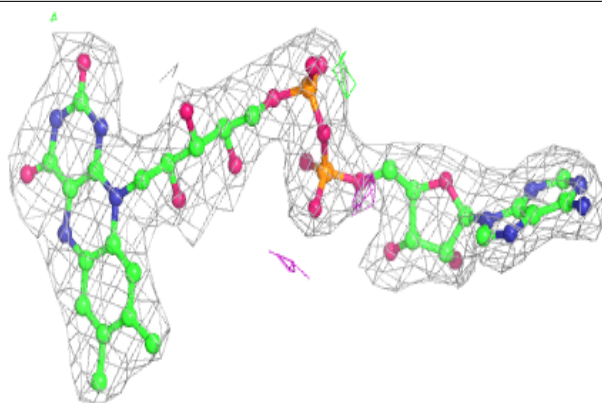
Electron density around FAD A 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD B 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.