



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 AM GMT

PDB ID : 2XAH
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.; Karytinis, 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 : 3.10 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 ⓘ symbol.

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

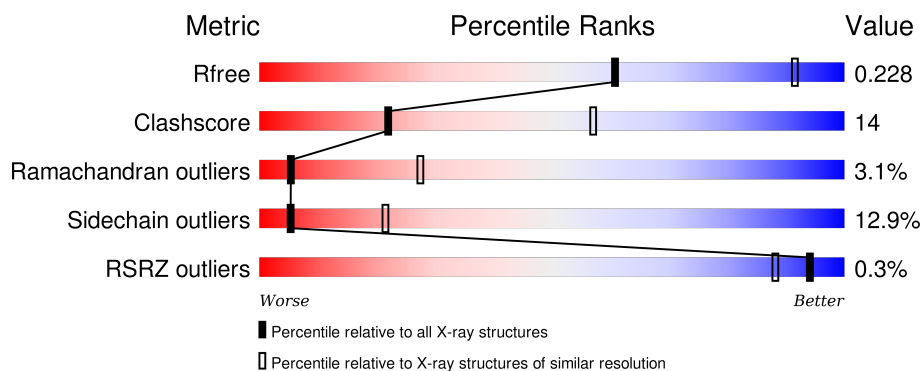
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 $\leq 5\%$. 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	852	 50% 24% • 22%
2	B	482	 18% 8% • 72%

2 Entry composition [i](#)

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.

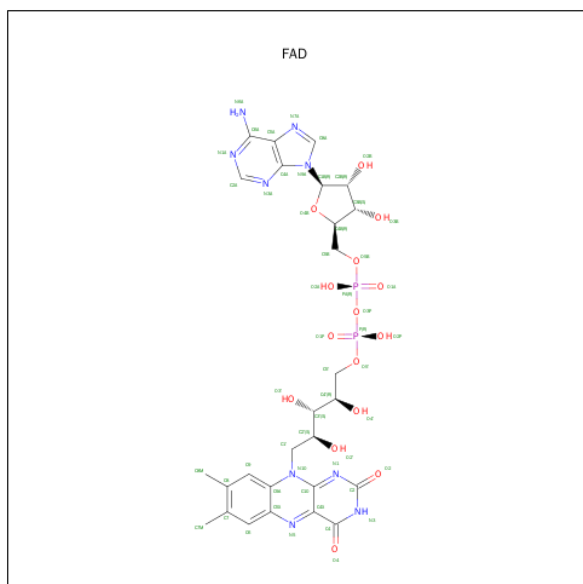
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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.

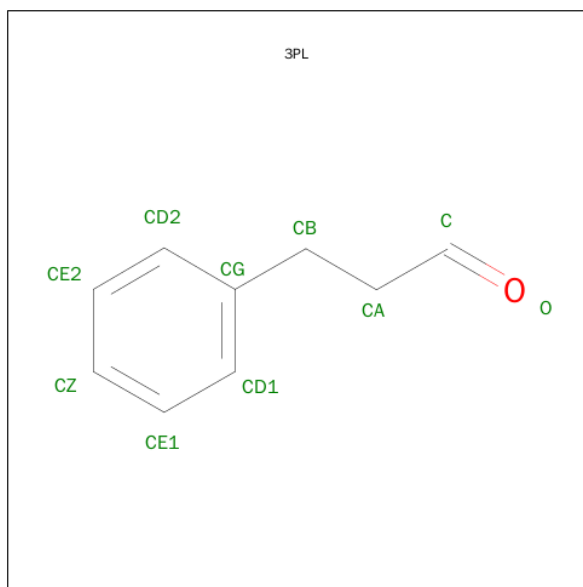
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- 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 3-PHENYLPROPANAL (three-letter code: 3PL) (formula: $C_9H_{10}O$).



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

• Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.96Å 181.50Å 234.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.75 – 3.10 71.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.75-3.10) 99.9 (71.84-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.208 , 0.228 0.206 , 0.228	Depositor DCC
R_{free} test set	900 reflections (1.96%)	DCC
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 46777 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6356	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.375 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: 3PL, 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	0.68	0/5331	0.77	0/7232
2	B	0.58	0/1091	0.69	1/1471 (0.1%)
All	All	0.67	0/6422	0.76	1/8703 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	359	LEU	CA-CB-CG	5.95	128.98	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	PRO	Peptide
1	A	792	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	160	0
2	B	1076	0	1091	31	0
3	A	53	0	31	3	0
4	A	10	0	9	2	0
All	All	6356	0	6383	177	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 14.

All (177) 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:794:PRO:HD2	1:A:828:GLN:HE22	1.11	1.10
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.15	1.07
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.69	1.07
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.39	1.04
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.20	0.99
1:A:758:ARG:HH11	1:A:758:ARG:HG2	1.25	0.97
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.80	0.95
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.07	0.90
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.11	0.86
1:A:494:TYR:CD2	1:A:494:TYR:O	2.31	0.84
1:A:671:TRP:O	1:A:673:PRO:HD3	1.80	0.81
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.62	0.81
1:A:437:THR:HG22	1:A:508:LEU:HD12	1.62	0.80
1:A:209:VAL:O	1:A:213:ILE:HG13	1.81	0.79
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.83	0.78
1:A:392:LEU:HD23	1:A:398:PHE:HB3	1.64	0.78
2:B:317:SER:O	2:B:321:VAL:HG23	1.83	0.76
1:A:758:ARG:HG2	1:A:758:ARG:NH1	1.95	0.74
1:A:384:ARG:NH2	2:B:312:LYS:O	2.20	0.74
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.70	0.71
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.73	0.69
1:A:260:GLY:O	1:A:264:PHE:CD2	2.47	0.68
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.75	0.67
1:A:755:PRO:CA	1:A:758:ARG:HH12	2.01	0.66
1:A:794:PRO:CD	1:A:828:GLN:HE22	2.00	0.65
1:A:761:TYR:CE2	4:A:901:3PL:HA2	2.31	0.64
1:A:437:THR:CG2	1:A:508:LEU:HD12	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:O	1:A:467:GLU:HG2	1.98	0.64
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.80	0.64
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.80	0.63
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.34	0.63
1:A:241:PRO:O	1:A:244:SER:HB3	1.99	0.63
1:A:392:LEU:CD2	1:A:398:PHE:HB3	2.29	0.63
1:A:760:SER:HB2	3:A:900:FAD:HM83	1.81	0.63
1:A:666:PHE:O	1:A:701:PRO:HG2	2.00	0.62
1:A:438:GLN:O	1:A:438:GLN:HG3	1.99	0.62
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.68	0.61
1:A:374:LYS:O	1:A:378:VAL:HG23	2.00	0.61
1:A:506:GLU:C	1:A:508:LEU:H	2.04	0.61
1:A:260:GLY:O	1:A:264:PHE:HD2	1.83	0.61
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.00	0.60
1:A:548:SER:O	1:A:552:TRP:HB3	2.01	0.60
1:A:437:THR:HG22	1:A:508:LEU:CD1	2.32	0.60
2:B:417:VAL:O	2:B:421:PHE:HD1	1.85	0.59
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.32	0.59
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.84	0.59
1:A:693:LEU:HD12	1:A:694:PHE:N	2.18	0.58
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.86	0.57
1:A:807:TYR:N	1:A:808:PRO:HD3	2.19	0.57
1:A:828:GLN:HG2	1:A:829:PHE:CE2	2.39	0.56
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.63	0.56
1:A:715:MET:HE3	1:A:723:ILE:HG12	1.87	0.56
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.35	0.56
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.88	0.55
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.42	0.55
1:A:736:GLY:O	1:A:738:SER:N	2.40	0.55
1:A:429:GLU:HA	1:A:432:LYS:HB2	1.89	0.54
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.43	0.54
1:A:715:MET:CE	1:A:723:ILE:HG12	2.38	0.54
1:A:377:MET:HE2	1:A:378:VAL:HG22	1.90	0.54
1:A:553:ASP:O	1:A:556:ASP:HB2	2.07	0.54
1:A:801:GLU:HG2	1:A:809:ALA:H	1.73	0.54
1:A:470:PRO:HB2	1:A:471:PRO:HA	1.89	0.54
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.73	0.54
1:A:295:ARG:O	1:A:299:SER:HB3	2.09	0.53
1:A:351:MET:HB3	1:A:567:VAL:HG13	1.90	0.53
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.39	0.53
1:A:419:GLN:HE22	2:B:315:PHE:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ASP:O	1:A:724:VAL:HG23	2.10	0.52
1:A:603:ILE:HG12	1:A:615:ILE:HD13	1.92	0.51
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.92	0.51
1:A:563:SER:O	1:A:565:LEU:HD12	2.11	0.51
1:A:530:ASP:OD2	1:A:685:THR:HA	2.11	0.51
1:A:750:ARG:NH1	1:A:750:ARG:HG3	2.25	0.50
1:A:392:LEU:CD2	1:A:398:PHE:CD2	2.94	0.50
1:A:801:GLU:HG2	1:A:809:ALA:N	2.25	0.50
1:A:494:TYR:HD2	1:A:494:TYR:O	1.89	0.50
1:A:594:ARG:HA	1:A:640:VAL:O	2.11	0.50
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.77	0.49
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.12	0.49
1:A:468:VAL:O	1:A:472:ARG:NH1	2.44	0.49
1:A:601:GLU:HA	1:A:616:TYR:O	2.12	0.49
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.94	0.49
1:A:455:ILE:HD11	1:A:490:LEU:O	2.13	0.49
1:A:385:LEU:O	1:A:388:ALA:HB3	2.12	0.49
1:A:716:GLU:CG	1:A:750:ARG:HG2	2.39	0.49
1:A:449:VAL:HG12	1:A:450:ASN:N	2.27	0.48
1:A:196:PHE:N	1:A:197:PRO:CD	2.76	0.48
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.43	0.48
1:A:693:LEU:HD12	1:A:694:PHE:H	1.79	0.48
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.49	0.48
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.29	0.48
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.96	0.48
2:B:337:GLN:HE21	2:B:337:GLN:CA	2.27	0.48
1:A:763:TYR:CE1	1:A:765:ALA:HB2	2.50	0.47
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.53	0.47
2:B:388:GLN:O	2:B:391:ALA:HB3	2.14	0.47
3:A:900:FAD:H1'1	3:A:900:FAD:H9	1.72	0.47
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.96	0.47
1:A:232:GLU:O	1:A:234:THR:N	2.48	0.47
1:A:770:GLY:O	1:A:773:TYR:HB2	2.14	0.47
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.50	0.47
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.97	0.47
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.96	0.46
1:A:758:ARG:NH1	1:A:758:ARG:CG	2.70	0.46
1:A:437:THR:C	1:A:439:GLU:H	2.19	0.46
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.97	0.46
1:A:776:MET:HB3	1:A:803:THR:HG22	1.97	0.46
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.81	0.46
1:A:422:HIS:HA	1:A:425:ASP:HB2	1.98	0.46
1:A:496:GLU:O	1:A:499:GLU:HB3	2.15	0.46
2:B:312:LYS:HE3	2:B:312:LYS:HA	1.98	0.45
1:A:640:VAL:HA	1:A:641:PRO:HA	1.80	0.45
1:A:364:GLU:HA	1:A:681:VAL:HB	1.98	0.45
1:A:392:LEU:HD23	1:A:398:PHE:CB	2.42	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.76	0.45
1:A:690:GLU:CG	1:A:691:LEU:HD12	2.44	0.45
2:B:324:VAL:HG12	2:B:324:VAL:O	2.17	0.45
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.27	0.45
1:A:567:VAL:HG11	1:A:571:TYR:HA	1.99	0.45
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.88	0.45
1:A:670:PHE:CZ	1:A:740:VAL:HG22	2.53	0.44
1:A:670:PHE:HD1	1:A:670:PHE:O	2.00	0.44
1:A:657:GLY:HA2	1:A:752:ARG:HH22	1.83	0.44
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.85	0.44
1:A:814:ALA:O	1:A:817:SER:N	2.50	0.44
1:A:670:PHE:CD1	1:A:670:PHE:C	2.91	0.44
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.47	0.44
1:A:374:LYS:O	1:A:375:ASP:C	2.55	0.44
1:A:506:GLU:C	1:A:508:LEU:N	2.68	0.43
1:A:297:LEU:HB2	1:A:304:VAL:HG21	2.01	0.43
1:A:449:VAL:HA	2:B:363:LEU:HD21	2.00	0.43
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.18	0.43
1:A:319:THR:HB	1:A:572:SER:HB3	2.01	0.43
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.50	0.43
1:A:331:ALA:HA	3:A:900:FAD:C4X	2.48	0.43
1:A:594:ARG:HB3	1:A:640:VAL:HB	2.00	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.49	0.43
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.49	0.43
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.52	0.43
1:A:800:GLY:O	1:A:803:THR:N	2.45	0.43
1:A:340:ASN:O	1:A:341:PRO:C	2.55	0.43
1:A:484:HIS:CD2	2:B:372:LEU:CD1	3.02	0.42
1:A:613:THR:HG22	1:A:614:PHE:N	2.32	0.42
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.52	0.42
1:A:548:SER:HB2	1:A:766:ALA:HA	2.00	0.42
1:A:828:GLN:HG3	1:A:828:GLN:O	2.18	0.42
2:B:329:THR:C	2:B:331:ALA:N	2.73	0.42
1:A:333:VAL:HG21	4:A:901:3PL:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HB3	1:A:565:LEU:HD23	2.01	0.42
1:A:295:ARG:NH2	1:A:580:GLU:O	2.53	0.42
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.01	0.42
1:A:613:THR:CG2	1:A:614:PHE:N	2.82	0.42
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.84	0.41
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.41
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.56	0.41
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.54	0.41
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.73	0.41
1:A:392:LEU:HD22	1:A:398:PHE:HD2	1.86	0.41
1:A:506:GLU:O	1:A:508:LEU:N	2.54	0.41
1:A:209:VAL:HG12	1:A:213:ILE:HD11	2.02	0.41
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.86	0.41
1:A:380:GLN:O	1:A:384:ARG:HD3	2.20	0.41
1:A:786:ILE:HD12	1:A:786:ILE:H	1.85	0.41
1:A:370:VAL:HA	1:A:371:PRO:HD3	1.85	0.41
1:A:808:PRO:O	1:A:810:THR:HG23	2.22	0.40
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.02	0.40
2:B:434:LEU:HA	2:B:434:LEU:HD23	2.00	0.40
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.95	0.40
2:B:418:LYS:O	2:B:421:PHE:HB2	2.22	0.40
1:A:633:GLN:HA	1:A:634:PRO:HA	1.51	0.40
1:A:747:VAL:HG12	1:A:748:VAL:N	2.36	0.40
1:A:797:PHE:CG	1:A:825:ILE:HD11	2.56	0.40
1:A:392:LEU:HD21	1:A:398:PHE:CD2	2.55	0.40
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.57	0.40
1:A:722:VAL:O	1:A:726:ARG:HG3	2.21	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%)	582 (88%)	63 (10%)	19 (3%)	6	29
2	B	131/482 (27%)	112 (86%)	13 (10%)	6 (5%)	3	17
All	All	795/1334 (60%)	694 (87%)	76 (10%)	25 (3%)	5	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	GLU
1	A	737	SER
1	A	233	ALA
1	A	425	ASP
1	A	438	GLN
1	A	468	VAL
1	A	507	LYS
1	A	801	GLU
2	B	326	ALA
1	A	232	GLU
1	A	244	SER
1	A	274	PRO
1	A	364	GLU
2	B	373	PRO
2	B	429	ASN
1	A	573	CYS
1	A	805	ARG
2	B	331	ALA
2	B	379	CYS
1	A	272	PRO
1	A	499	GLU
1	A	597	ALA
1	A	725	GLY
2	B	391	ALA
1	A	785	SER

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	566/699 (81%)	498 (88%)	68 (12%)	6	24
2	B	117/395 (30%)	97 (83%)	20 (17%)	2	11
All	All	683/1094 (62%)	595 (87%)	88 (13%)	5	21

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	191	GLN
1	A	195	CYS
1	A	200	ILE
1	A	205	GLN
1	A	236	GLN
1	A	237	GLN
1	A	247	VAL
1	A	263	ASN
1	A	268	LYS
1	A	271	LYS
1	A	278	THR
1	A	299	SER
1	A	313	VAL
1	A	351	MET
1	A	377	MET
1	A	380	GLN
1	A	402	ASN
1	A	423	VAL
1	A	426	GLU
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	438	GLN
1	A	458	LEU
1	A	467	GLU
1	A	469	LYS
1	A	472	ARG
1	A	473	ASP
1	A	479	LEU
1	A	482	SER
1	A	485	ARG
1	A	492	LYS
1	A	508	LEU
1	A	523	SER

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Mol	Chain	Res	Type
1	A	524	ARG
1	A	526	ARG
1	A	538	PHE
1	A	556	ASP
1	A	563	SER
1	A	568	ARG
1	A	571	TYR
1	A	580	GLU
1	A	591	ARG
1	A	594	ARG
1	A	612	GLN
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	648	THR
1	A	652	GLN
1	A	659	LEU
1	A	668	ARG
1	A	675	VAL
1	A	677	LEU
1	A	680	HIS
1	A	683	SER
1	A	684	THR
1	A	691	LEU
1	A	706	LEU
1	A	719	SER
1	A	727	CYS
1	A	758	ARG
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
1	A	821	GLU
1	A	828	GLN
2	B	312	LYS
2	B	332	THR
2	B	334	VAL
2	B	337	GLN
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	361	GLU

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Mol	Chain	Res	Type
2	B	362	LYS
2	B	368	GLU
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	386	GLU
2	B	414	VAL
2	B	422	VAL
2	B	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	259	HIS
1	A	419	GLN
1	A	484	HIS
1	A	778	GLN
1	A	828	GLN
2	B	337	GLN
2	B	419	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	$\# Z > 2$
3	FAD	A	900	4	48,58,58	1.57	6 (12%)	54,89,89	2.42	17 (31%)
4	3PL	A	901	3	10,10,10	1.02	0	10,11,11	1.80	3 (30%)

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	3PL	A	901	3	-	0/3/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C5'-C4'	2.89	1.56	1.51
3	A	900	FAD	C10-N10	3.24	1.42	1.39
3	A	900	FAD	C5X-N5	3.39	1.40	1.35
3	A	900	FAD	C4X-C10	4.28	1.49	1.41
3	A	900	FAD	C9A-N10	4.35	1.44	1.38
3	A	900	FAD	C4X-N5	4.87	1.41	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-9.86	121.35	128.89
3	A	900	FAD	C4X-C10-N10	-4.18	118.06	120.52
3	A	900	FAD	C1'-N10-C9A	-4.06	114.30	118.86
3	A	900	FAD	P-O3P-PA	-3.95	121.65	132.73
4	A	901	3PL	CB-CA-C	-3.11	103.55	111.70
3	A	900	FAD	C4X-N5-C5X	-3.00	113.31	116.76
3	A	900	FAD	C4X-C4-N3	-2.77	119.79	123.59
3	A	900	FAD	O5'-P-O1P	-2.63	99.41	109.62
4	A	901	3PL	CE1-CD1-CG	-2.43	116.79	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	3PL	CA-CB-CG	-2.33	106.81	113.04
3	A	900	FAD	C1B-N9A-C4A	-2.20	123.62	126.94
3	A	900	FAD	C4-C4X-C10	-2.02	118.65	119.94
3	A	900	FAD	C6-C5X-N5	-2.01	116.38	118.96
3	A	900	FAD	C6-C5X-C9A	2.10	121.74	118.98
3	A	900	FAD	O3P-P-O5'	2.15	108.65	102.94
3	A	900	FAD	O4'-C4'-C3'	2.20	114.56	109.02
3	A	900	FAD	O4'-C4'-C5'	2.27	115.15	110.19
3	A	900	FAD	O2A-PA-O1A	2.28	124.86	112.53
3	A	900	FAD	C5X-C9A-N10	4.35	120.93	117.62
3	A	900	FAD	C4-N3-C2	7.72	121.92	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	3	0
4	A	901	3PL	2	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 [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	666/852 (78%)	-0.21	2 (0%) 94 88	26, 56, 85, 101	0
2	B	133/482 (27%)	-0.02	0 100 100	58, 87, 99, 109	0
All	All	799/1334 (59%)	-0.18	2 (0%) 94 88	26, 61, 94, 109	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	GLN	2.3
1	A	171	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	3PL	A	901	10/10	0.94	0.26	0.92	54,57,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FAD	A	900	53/53	0.98	0.18	-0.99	23,31,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.