



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 AM GMT

PDB ID : 2XAG
Title : CRYSTAL STRUCTURE OF LSD1-COREST IN COMPLEX WITH PARA-BROMO-(-)-TRANS-2-PHENYLCYCLOPROPYL-1-AMINE
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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

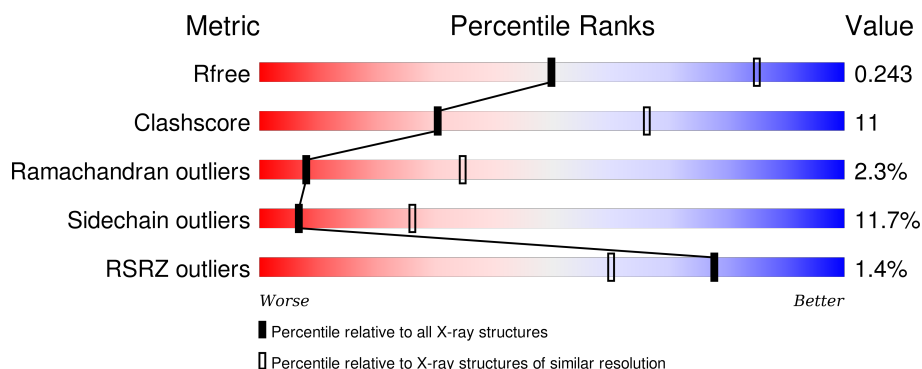
1 Overall quality at a glance

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	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>20%</div> <div>•</div> <div>22%</div> </div> </div>
2	B	482	<div> <div>%</div> <div> <div></div> <div>17%</div> <div>10%</div> <div>•</div> <div>72%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TCF	A	901	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6357 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.

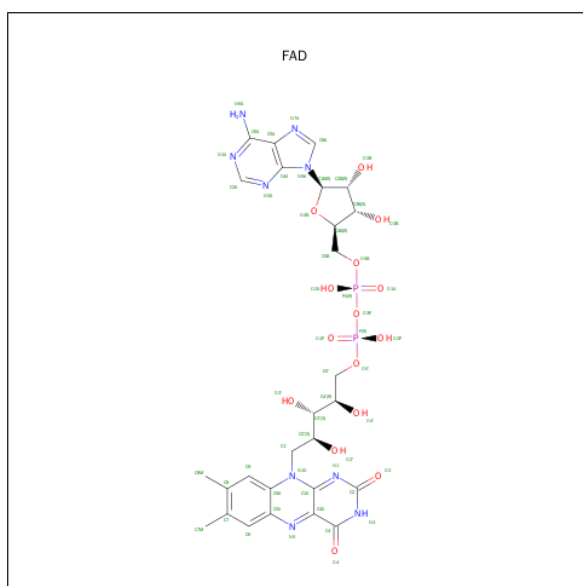
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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			

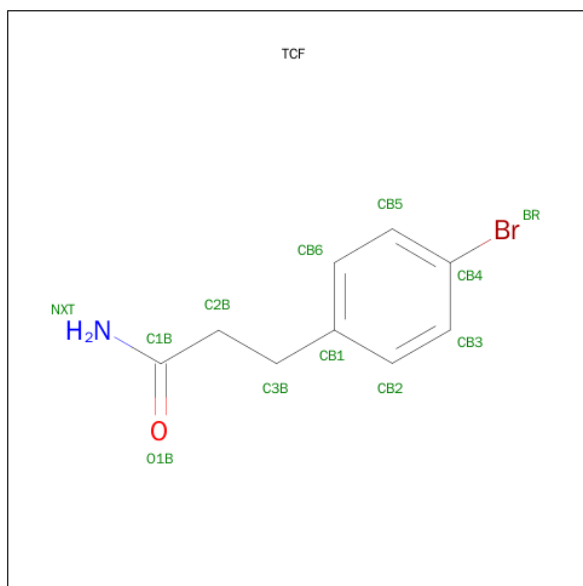
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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-(4-BROMOPHENYL)PROPANAMIDE (three-letter code: TCF) (formula:

C₉H₁₀BrNO).

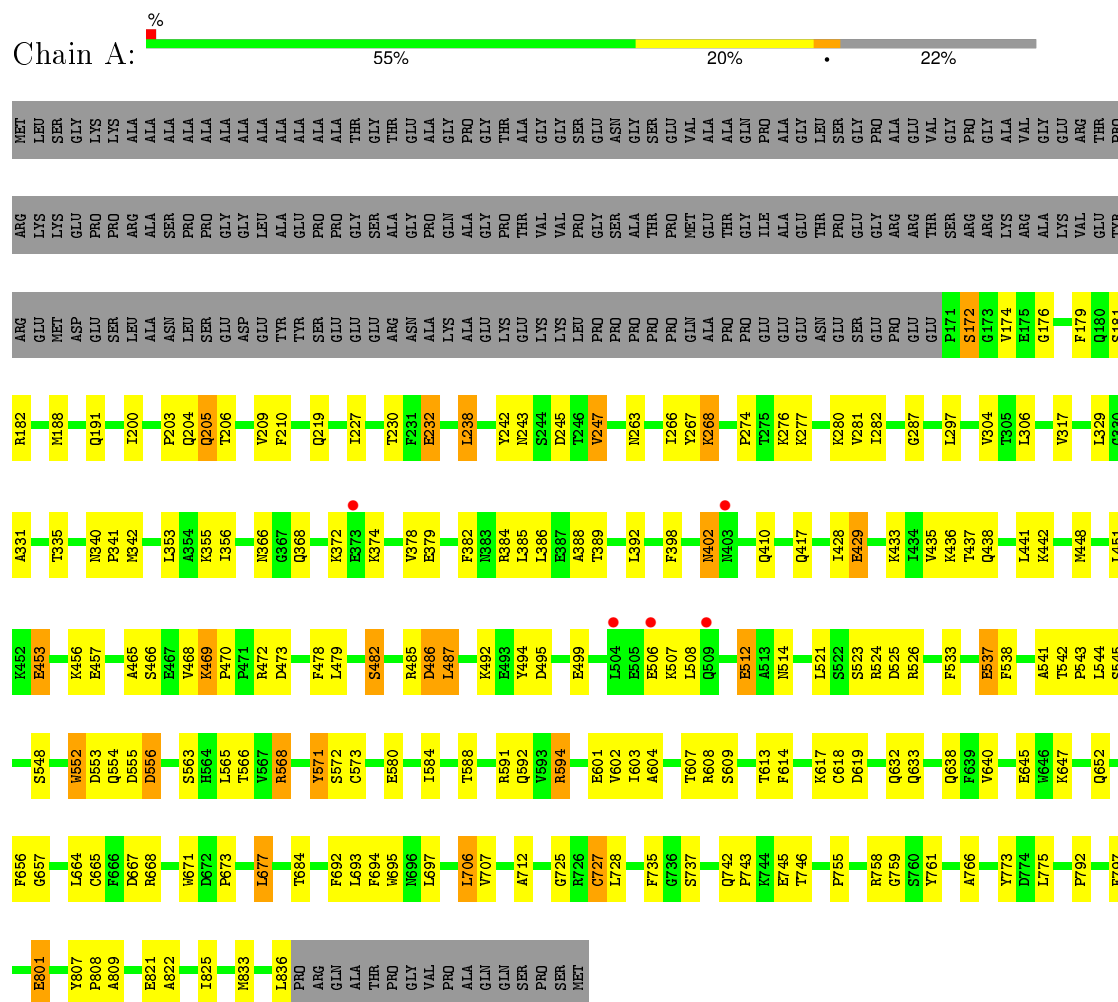


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
4	A	1	11	1	9	1	0	0

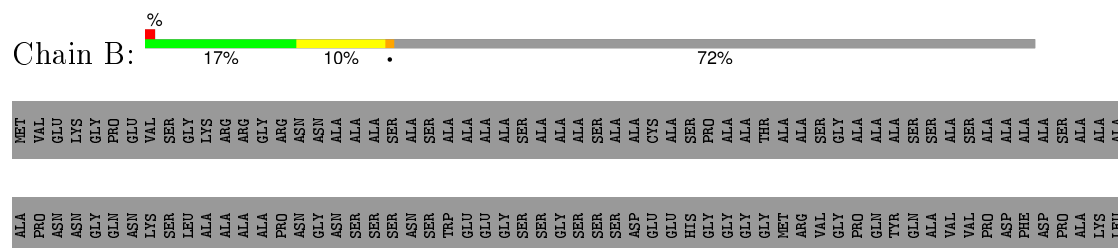
3 Residue-property plots

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

• Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1



• Molecule 2: REST COREPRESSOR 1



GLU	GLN	SER	ASP	ASP	ALA
ALA	ALA	VAL	GLN	GLU	LEU
PRO	T384	VAL	ASN	PRO	ARG
LEU	T385	ASN	ARG	PHE	GLN
ASP	Q388	ALA	HIS	THR	GLU
VAL	Q382	LYS	ALA	PHE	ARG
TYR	Q393	GLN	LYS	PRO	ASN
ALA	A394	P310	LYS	ASP	LEU
SER	Y398	P311	GLU	GLU	GLY
ALA	N411	K312	TRP	TRP	MET
SER	V414	G313	VAL	VAL	LEU
	V415	F315	GLU	GLU	TRP
	Q416	S317	GLU	ASP	SER
	V417	S317	LYS	LYS	PRO
	K418	Q318	GLU	VAL	ASN
	N419	E319	ASP	LEU	GLN
	F420	D320	GLU	PHE	ASN
	F421	V321	LEU	GLU	LEU
	V422	GLU	GLN	GLN	SER
	N423	ALA	ALA	ALA	GLU
	Y424	ASN	SER	PHE	LYS
	R426	GLY	PHE	ASP	LEU
	I430	ASN	ASN	GLY	GLU
	E440	ASN	ASN	LYS	TYR
HIS	GLY	ILE	THR	THR	ILE
LYS	LYS	ILE	PHE	PHE	ALA
GLU	Q348	GLU	GLU	HIS	ALA
GLU	I349	VAL	ILE	ILE	LYS
THR	Q350	ASP	GLN	GLN	GLY
ASN	N351	GLN	ASN	MET	LYS
GLY	T355	LYS	LYS	LEU	HIS
PRO	N356	GLU	PRO	LEU	GLY
SER		SER	ASP	VAL	MET
ASN	E361	LYS	LYS	SER	GLU
GLN	K362	GLU	ILE	ILE	GLN
LYS	L363	VAL	ALA	ALA	ALA
PRO	D364	PRO	SER	SER	LEU
VAL	G365	PRO	LEU	VAL	GLY
LYS		THR	VAL	VAL	MET
SER	Y370	GLU	LYS	LYS	LEU
PRO	R371	THR	PHE	PHE	PHE
ASN	L372	VAL	TYR	TYR	TRP
ASN	P373	PRO	TYR	TYR	HIS
SER	E374	GLN	GLN	TRP	LYS
ILE	V375	VAL	VAL	TRP	HIS
LYS	T376	LYS	LYS	LYS	ASN
MET	Q377	LYS	LYS	ILE	ILE
PRO	K378	GLU	THR	THR	GLU
GLU	C379	LYS	ARG	ARG	LYS
GLU	N380	HIS	THR	THR	SER
GLU	A381	SER	LYS	LYS	LEU
ASP	P382	THR	THR	THR	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.47Å 178.03Å 236.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.96 – 3.10 71.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (71.96-3.10) 95.0 (71.96-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.209 , 0.245 0.209 , 0.243	Depositor DCC
R_{free} test set	808 reflections (1.93%)	DCC
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 42606 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TCF, 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	0.66	0/5331	0.75	0/7232
2	B	0.60	0/1091	0.65	0/1471
All	All	0.65	0/6422	0.73	0/8703

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide

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	A	5217	0	5252	120	0
2	B	1076	0	1091	26	0
3	A	53	0	31	5	0
4	A	11	0	8	7	0
All	All	6357	0	6382	140	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 11.

All (140) 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:566:THR:HG21	1:A:697:LEU:HD22	1.32	1.07
3:A:900:FAD:C4X	4:A:901:TCF:H3B1	1.85	1.06
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.99	0.78
1:A:693:LEU:HD12	1:A:694:PHE:N	2.00	0.77
3:A:900:FAD:C10	4:A:901:TCF:H3B1	2.15	0.76
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.68	0.74
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.70	0.73
3:A:900:FAD:C4X	4:A:901:TCF:C3B	2.64	0.72
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.15	0.72
2:B:421:PHE:O	2:B:425:ARG:HB2	1.88	0.72
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.73	0.70
1:A:677:LEU:N	1:A:677:LEU:HD23	2.08	0.68
1:A:227:ILE:HG22	1:A:268:LYS:HB3	1.79	0.65
1:A:374:LYS:HE3	1:A:525:ASP:OD1	1.97	0.64
1:A:437:THR:CG2	1:A:508:LEU:HD21	2.27	0.64
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.28	0.63
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.36	0.61
1:A:548:SER:HB2	1:A:766:ALA:HA	1.82	0.61
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.31	0.61
1:A:693:LEU:HD12	1:A:694:PHE:H	1.66	0.60
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.32	0.60
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.82	0.60
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.85	0.58
1:A:553:ASP:O	1:A:556:ASP:HB2	2.02	0.58
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.05	0.57
1:A:588:THR:HG22	1:A:604:ALA:HB1	1.86	0.57
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.86	0.57
1:A:263:ASN:C	1:A:267:TYR:HE1	2.07	0.57
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.87	0.56
1:A:379:GLU:O	1:A:382:PHE:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PHE:O	1:A:482:SER:HB3	2.04	0.56
1:A:188:MET:SD	1:A:200:ILE:HG13	2.46	0.56
1:A:671:TRP:O	1:A:673:PRO:HD3	2.06	0.55
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.36	0.54
1:A:548:SER:O	1:A:552:TRP:HB3	2.07	0.54
1:A:263:ASN:C	1:A:267:TYR:CE1	2.81	0.54
2:B:317:SER:O	2:B:321:VAL:HG23	2.07	0.54
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.43	0.54
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.90	0.53
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.53
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.43	0.53
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.09	0.53
1:A:588:THR:HG22	1:A:604:ALA:CB	2.39	0.52
1:A:172:SER:HA	1:A:176:GLY:HA3	1.91	0.52
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.91	0.52
1:A:374:LYS:O	1:A:378:VAL:HG23	2.10	0.52
2:B:384:THR:O	2:B:388:GLN:HG3	2.10	0.51
2:B:347:ARG:HG3	2:B:348:GLN:N	2.26	0.51
1:A:677:LEU:CD2	1:A:677:LEU:N	2.73	0.51
2:B:361:GLU:O	2:B:364:ASP:HB2	2.12	0.51
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.11	0.51
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.76	0.50
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.11	0.50
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.47	0.49
1:A:677:LEU:H	1:A:677:LEU:HD23	1.76	0.49
1:A:563:SER:O	1:A:565:LEU:HD12	2.12	0.49
1:A:335:THR:HG21	4:A:901:TCF:HB3	1.95	0.49
1:A:797:PHE:CG	1:A:825:ILE:HD11	2.48	0.49
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.95	0.49
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.43	0.49
1:A:280:LYS:O	1:A:618:CYS:HB2	2.13	0.49
1:A:664:LEU:HD23	1:A:746:THR:HG22	1.95	0.48
2:B:380:ASN:O	2:B:416:GLN:NE2	2.46	0.48
1:A:707:VAL:HG12	1:A:712:ALA:CA	2.41	0.48
1:A:485:ARG:O	1:A:487:LEU:N	2.46	0.48
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.79	0.48
1:A:541:ALA:O	1:A:657:GLY:HA3	2.14	0.48
1:A:542:THR:OG1	1:A:543:PRO:HD2	2.13	0.47
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.47
2:B:350:GLN:HE21	2:B:350:GLN:HB3	1.51	0.47
1:A:807:TYR:N	1:A:808:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:CZ	1:A:640:VAL:HG11	2.45	0.46
1:A:473:ASP:OD1	1:A:473:ASP:C	2.54	0.46
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.98	0.46
1:A:521:LEU:HB3	1:A:525:ASP:HB2	1.98	0.46
2:B:417:VAL:O	2:B:420:PHE:HB3	2.16	0.46
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.51	0.45
1:A:366:ASN:OD1	1:A:368:GLN:N	2.48	0.45
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.64	0.45
1:A:667:ASP:N	1:A:667:ASP:OD1	2.44	0.45
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.81	0.44
2:B:362:LYS:C	2:B:364:ASP:H	2.20	0.44
1:A:203:PRO:C	1:A:205:GLN:N	2.70	0.44
1:A:775:LEU:HA	1:A:775:LEU:HD23	1.75	0.44
1:A:801:GLU:HG3	3:A:900:FAD:O3'	2.18	0.44
1:A:677:LEU:HB2	1:A:693:LEU:HD11	1.99	0.44
1:A:384:ARG:NH2	2:B:312:LYS:O	2.48	0.44
1:A:374:LYS:CE	1:A:525:ASP:OD1	2.65	0.44
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.99	0.44
1:A:601:GLU:OE1	1:A:617:LYS:HE3	2.18	0.44
1:A:266:ILE:O	1:A:266:ILE:HG22	2.17	0.44
1:A:773:TYR:HE1	1:A:808:PRO:HB3	1.82	0.43
1:A:533:PHE:O	1:A:537:GLU:CG	2.66	0.43
2:B:418:LYS:O	2:B:421:PHE:HB2	2.18	0.43
1:A:543:PRO:C	1:A:545:SER:H	2.22	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.48	0.43
1:A:728:LEU:HD21	1:A:743:PRO:HG3	1.99	0.43
1:A:568:ARG:HG2	1:A:568:ARG:HH11	1.84	0.43
1:A:340:ASN:OD1	1:A:342:MET:HG2	2.18	0.43
1:A:230:THR:OG1	1:A:232:GLU:HB2	2.18	0.43
2:B:414:VAL:O	2:B:418:LYS:HG3	2.19	0.43
2:B:394:ALA:O	2:B:398:TYR:N	2.51	0.43
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.91	0.43
1:A:465:ALA:HB1	1:A:479:LEU:HD23	2.01	0.42
1:A:410:GLN:HE21	1:A:410:GLN:HB3	1.72	0.42
1:A:203:PRO:C	1:A:205:GLN:H	2.22	0.42
1:A:485:ARG:O	1:A:486:ASP:C	2.57	0.42
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.02	0.42
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.34	0.42
1:A:537:GLU:OE2	1:A:544:LEU:N	2.50	0.42
1:A:297:LEU:HD21	1:A:822:ALA:HA	2.00	0.42
1:A:761:TYR:CZ	4:A:901:TCF:H3B2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:OE2	1:A:543:PRO:HA	2.19	0.42
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.90	0.42
1:A:386:LEU:O	1:A:389:THR:OG1	2.29	0.42
1:A:647:LYS:HE2	1:A:647:LYS:HB2	1.87	0.42
1:A:640:VAL:O	1:A:640:VAL:HG12	2.19	0.42
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.55	0.42
1:A:572:SER:O	1:A:573:CYS:C	2.58	0.41
2:B:310:PRO:O	2:B:311:PRO:C	2.59	0.41
1:A:172:SER:HA	1:A:176:GLY:CA	2.50	0.41
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.02	0.41
1:A:554:GLN:C	1:A:556:ASP:H	2.24	0.41
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.36	0.41
1:A:761:TYR:CE2	4:A:901:TCF:H3B2	2.56	0.41
1:A:179:PHE:C	1:A:181:SER:H	2.23	0.41
1:A:508:LEU:O	1:A:512:GLU:HB2	2.21	0.41
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.54	0.41
1:A:331:ALA:HA	3:A:900:FAD:N5	2.36	0.41
1:A:276:LYS:HE3	1:A:276:LYS:HB2	1.86	0.41
1:A:335:THR:CG2	4:A:901:TCF:HB3	2.50	0.40
1:A:533:PHE:O	1:A:537:GLU:HG2	2.21	0.40
1:A:280:LYS:N	1:A:619:ASP:OD2	2.51	0.40
1:A:613:THR:HG22	1:A:614:PHE:N	2.36	0.40
1:A:707:VAL:O	1:A:712:ALA:HB2	2.20	0.40
1:A:665:CYS:HB2	1:A:745:GLU:HB2	2.03	0.40
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.57	0.40
1:A:245:ASP:OD1	1:A:247:VAL:HG23	2.21	0.40
1:A:725:GLY:C	1:A:727:CYS:N	2.75	0.40
2:B:349:ILE:HG22	2:B:350:GLN:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/852 (78%)	573 (86%)	77 (12%)	14 (2%)	9	37
2	B	131/482 (27%)	104 (79%)	23 (18%)	4 (3%)	5	27
All	All	795/1334 (60%)	677 (85%)	100 (13%)	18 (2%)	8	35

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
1	A	486	ASP
1	A	428	ILE
1	A	287	GLY
1	A	402	ASN
1	A	555	ASP
1	A	608	ARG
2	B	314	MET
2	B	373	PRO
2	B	425	ARG
1	A	204	GLN
1	A	274	PRO
1	A	429	GLU
1	A	232	GLU
1	A	552	TRP
1	A	801	GLU
2	B	312	LYS
1	A	507	LYS

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%)	506 (89%)	60 (11%)	8	31
2	B	117/395 (30%)	97 (83%)	20 (17%)	2	11
All	All	683/1094 (62%)	603 (88%)	80 (12%)	7	26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	191	GLN
1	A	205	GLN
1	A	206	THR
1	A	238	LEU
1	A	247	VAL
1	A	268	LYS
1	A	277	LYS
1	A	281	VAL
1	A	304	VAL
1	A	329	LEU
1	A	355	LYS
1	A	372	LYS
1	A	402	ASN
1	A	417	GLN
1	A	429	GLU
1	A	433	LYS
1	A	436	LYS
1	A	438	GLN
1	A	453	GLU
1	A	457	GLU
1	A	466	SER
1	A	469	LYS
1	A	472	ARG
1	A	482	SER
1	A	487	LEU
1	A	492	LYS
1	A	499	GLU
1	A	506	GLU
1	A	512	GLU
1	A	514	ASN
1	A	523	SER
1	A	524	ARG
1	A	526	ARG
1	A	537	GLU
1	A	538	PHE
1	A	556	ASP
1	A	568	ARG
1	A	571	TYR
1	A	580	GLU
1	A	591	ARG
1	A	594	ARG
1	A	607	THR

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Mol	Chain	Res	Type
1	A	609	SER
1	A	632	GLN
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	652	GLN
1	A	668	ARG
1	A	677	LEU
1	A	684	THR
1	A	692	PHE
1	A	706	LEU
1	A	727	CYS
1	A	737	SER
1	A	742	GLN
1	A	821	GLU
1	A	833	MET
1	A	836	LEU
2	B	308	ARG
2	B	316	LEU
2	B	319	GLU
2	B	320	ASP
2	B	333	THR
2	B	337	GLN
2	B	345	VAL
2	B	347	ARG
2	B	350	GLN
2	B	351	ASN
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	392	VAL
2	B	415	VAL
2	B	423	ASN
2	B	425	ARG
2	B	426	ARG

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	395	GLN

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	427	GLN
1	A	438	GLN
1	A	540	ASN
2	B	348	GLN
2	B	350	GLN
2	B	419	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FAD	A	900	4	48,58,58	2.63	10 (20%)	54,89,89	3.38	11 (20%)
4	TCF	A	901	3	11,11,12	0.72	0	12,13,15	1.13	1 (8%)

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	TCF	A	901	3	-	0/3/4/5	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C5'-C4'	2.64	1.55	1.51
3	A	900	FAD	C10-N10	2.76	1.42	1.39
3	A	900	FAD	C4-C4X	3.35	1.48	1.41
3	A	900	FAD	C4X-C10	3.86	1.48	1.41
3	A	900	FAD	C5X-N5	4.69	1.42	1.35
3	A	900	FAD	O4-C4	4.96	1.36	1.24
3	A	900	FAD	C9A-N10	5.06	1.45	1.38
3	A	900	FAD	C2A-N1A	7.54	1.48	1.33
3	A	900	FAD	C2A-N3A	7.64	1.45	1.32
3	A	900	FAD	C4X-N5	9.10	1.47	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-19.69	113.82	128.89
3	A	900	FAD	C4X-C10-N10	-5.23	117.44	120.52
3	A	900	FAD	C4-C4X-C10	-4.54	117.04	119.94
3	A	900	FAD	C4X-C4-N3	-4.36	117.63	123.59
3	A	900	FAD	P-O3P-PA	-3.70	122.35	132.73
3	A	900	FAD	C1'-N10-C9A	-2.99	115.50	118.86
4	A	901	TCF	C3B-CB1-CB6	-2.09	115.95	121.25
3	A	900	FAD	C4X-N5-C5X	-2.00	114.46	116.76
3	A	900	FAD	C2A-N1A-C6A	2.08	122.47	118.77
3	A	900	FAD	O2A-PA-O1A	2.12	124.03	112.53
3	A	900	FAD	C5X-C9A-N10	4.73	121.21	117.62
3	A	900	FAD	C4-N3-C2	7.99	122.16	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	TCF	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.16	5 (0%) 87 75	34, 63, 92, 104	0
2	B	133/482 (27%)	0.54	6 (4%) 37 17	66, 93, 107, 113	0
All	All	799/1334 (59%)	0.22	11 (1%) 78 60	34, 67, 99, 113	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	308	ARG	3.0
1	A	373	GLU	3.0
2	B	376	ILE	2.8
1	A	506	GLU	2.7
2	B	365	GLY	2.7
1	A	509	GLN	2.4
1	A	504	LEU	2.2
2	B	378	LYS	2.2
2	B	379	CYS	2.2
1	A	403	ASN	2.1
2	B	375	VAL	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
3	FAD	A	900	53/53	0.98	0.22	-0.69	32,40,62,63	0
4	TCF	A	901	11/12	0.95	0.23	-0.70	64,75,82,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.