



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:49 PM UTC

PDB ID : 2XAF / pdb_00002xaf
Title : Crystal structure of LSD1-CoREST in complex with para-bromo-(+)-cis-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 : 3.25 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

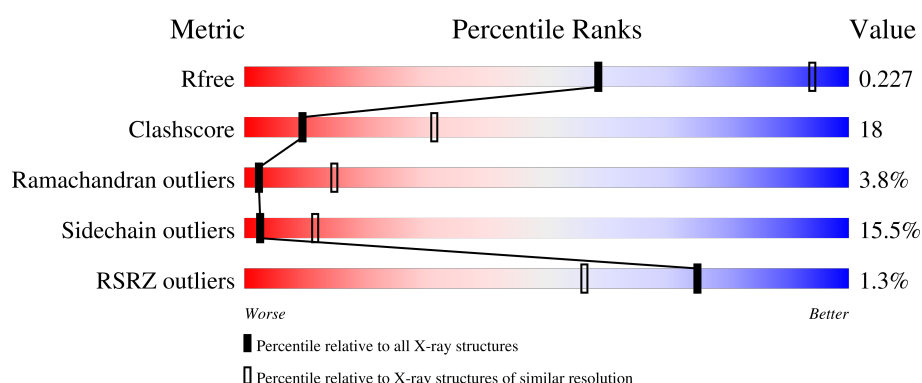
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 $\leq 5\%$. 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	
2	B	482	

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.

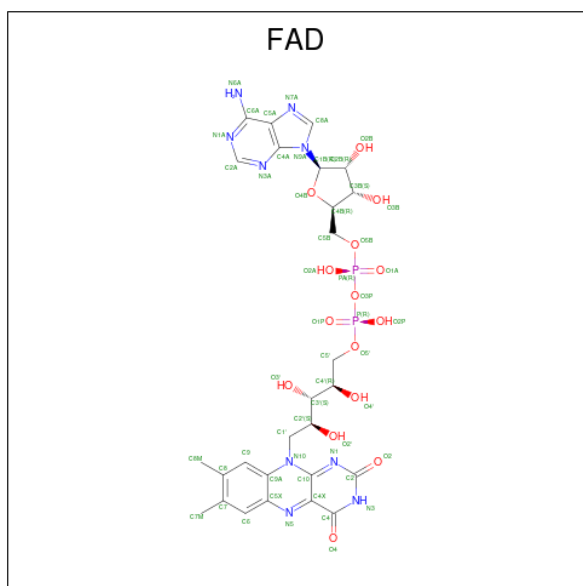
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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.

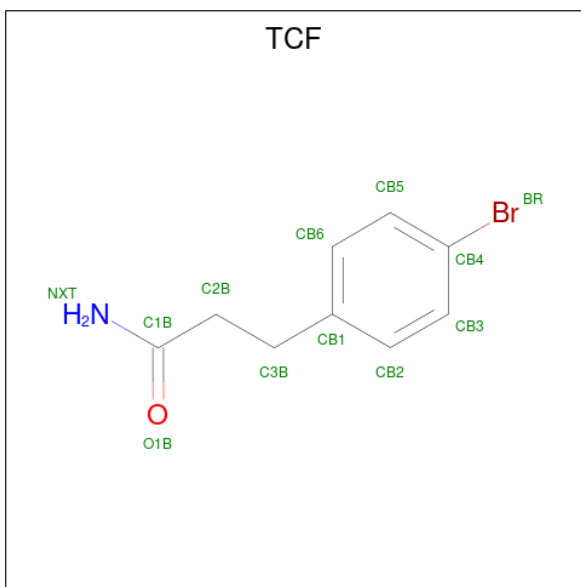
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 (CCD ID: TCF) (formula: $C_9H_{10}BrNO$).

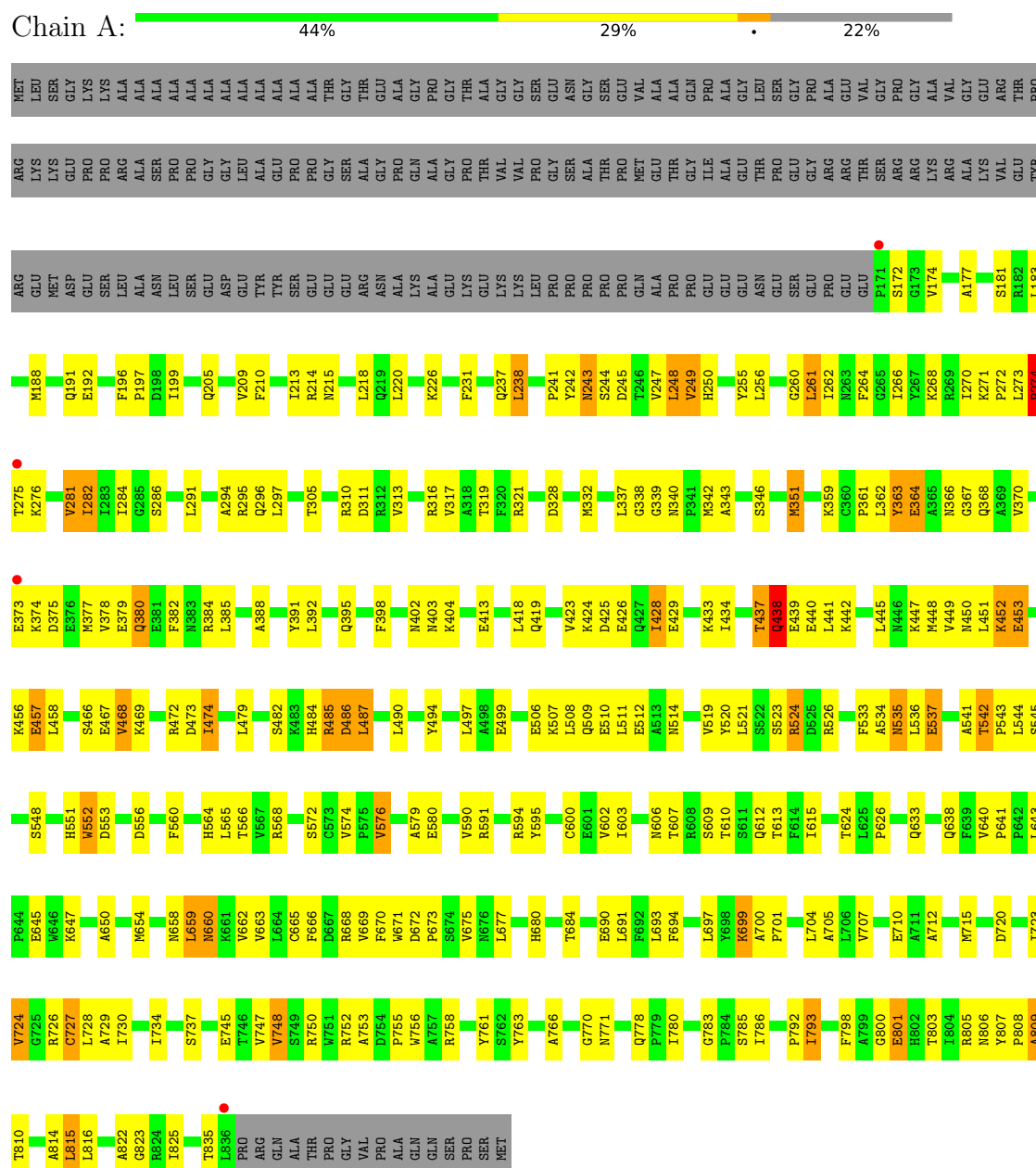


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
4	A	1	11	1	9	1	0	0

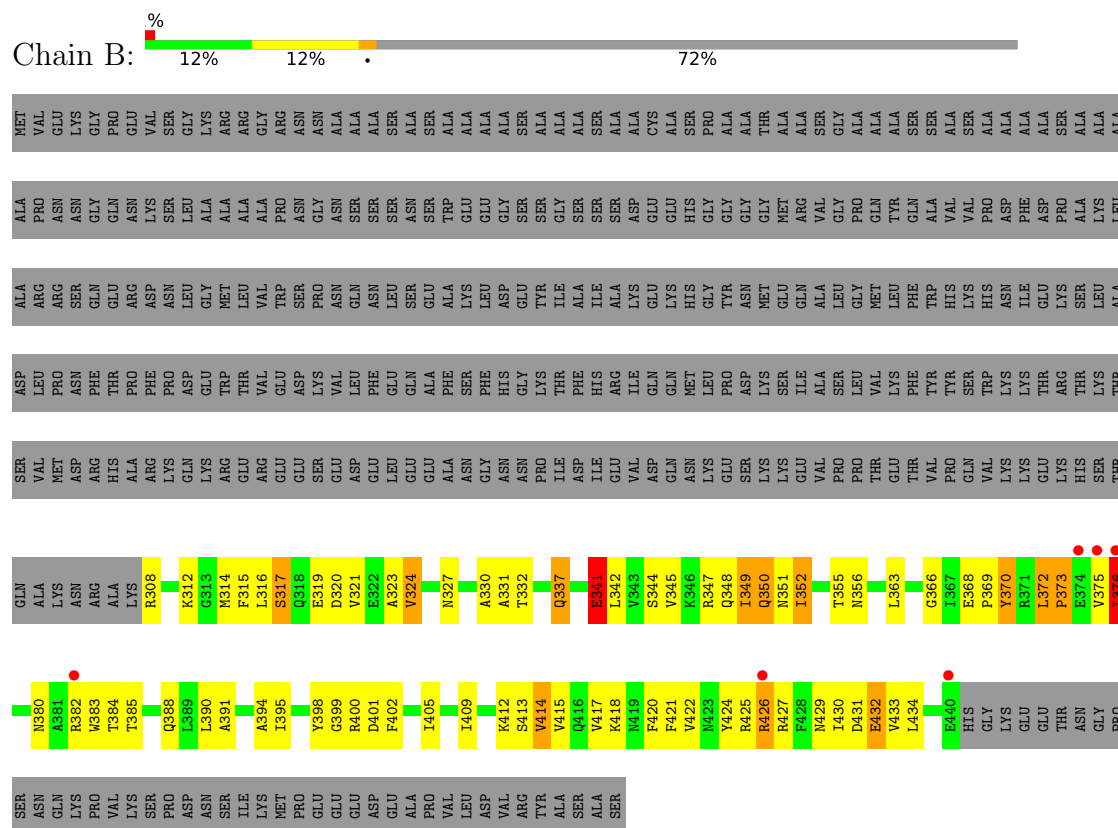
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1



- Molecule 2: REST COREPRESSOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.56Å 179.48Å 235.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.51 – 3.25 30.51 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.51-3.25) 94.5 (30.51-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.202 , 0.229 0.202 , 0.227	Depositor DCC
R_{free} test set	735 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, TCF

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	0.91	2/5331 (0.0%)	1.13	19/7232 (0.3%)
2	B	0.75	1/1091 (0.1%)	1.03	3/1471 (0.2%)
All	All	0.89	3/6422 (0.0%)	1.11	22/8703 (0.3%)

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	576	VAL	CA-CB	-5.24	1.48	1.54
2	B	376	ILE	CA-CB	5.14	1.58	1.53
1	A	363	TYR	CA-C	-5.04	1.47	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	N-CA-C	7.65	118.71	108.38
1	A	370	VAL	CA-C-N	7.63	127.69	119.90
1	A	370	VAL	C-N-CA	7.63	127.69	119.90
1	A	783	GLY	CA-C-N	-7.14	112.88	120.66
1	A	783	GLY	C-N-CA	-7.14	112.88	120.66
2	B	372	LEU	CA-C-N	6.65	128.16	119.84
2	B	372	LEU	C-N-CA	6.65	128.16	119.84
1	A	261	LEU	N-CA-C	-6.38	104.54	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	GLU	N-CA-C	-6.25	104.00	111.69
1	A	770	GLY	N-CA-C	-6.23	105.02	113.37
1	A	668	ARG	N-CA-C	5.99	119.26	108.48
1	A	281	VAL	CB-CA-C	-5.95	101.64	110.33
1	A	266	ILE	N-CA-C	5.81	114.72	106.53
1	A	613	THR	N-CA-C	5.58	119.16	110.17
2	B	345	VAL	N-CA-C	-5.57	106.24	111.48
1	A	474	ILE	N-CA-C	5.57	116.34	110.72
1	A	542	THR	CA-C-N	5.37	126.21	119.98
1	A	542	THR	C-N-CA	5.37	126.21	119.98
1	A	748	VAL	N-CA-C	5.20	115.53	107.78
1	A	660	ASN	N-CA-C	5.09	117.87	109.72
1	A	672	ASP	CA-C-N	5.03	126.13	119.84
1	A	672	ASP	C-N-CA	5.03	126.13	119.84

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

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	184	0
2	B	1076	0	1091	59	0
3	A	53	0	31	4	0
4	A	11	0	8	3	0
All	All	6357	0	6382	227	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 18.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.62	1.13
3:A:900:FAD:C4X	4:A:901:TCF:H3B1	1.78	1.11
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.16	1.11
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.56	1.01
1:A:671:TRP:O	1:A:673:PRO:HD3	1.62	0.99
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.27	0.98
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.03	0.93
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.47	0.92
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.53	0.89
1:A:209:VAL:O	1:A:213:ILE:HG13	1.76	0.85
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.47	0.83
1:A:658:ASN:ND2	1:A:752:ARG:HB2	1.94	0.82
1:A:801:GLU:CG	1:A:809:ALA:HA	2.10	0.81
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.16	0.81
1:A:755:PRO:CA	1:A:758:ARG:HH12	1.93	0.80
1:A:451:LEU:C	1:A:453:GLU:H	1.90	0.78
3:A:900:FAD:C4X	4:A:901:TCF:C3B	2.61	0.77
1:A:484:HIS:HD2	2:B:372:LEU:HD13	1.51	0.76
1:A:506:GLU:C	1:A:508:LEU:H	1.94	0.74
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.70	0.74
1:A:720:ASP:O	1:A:724:VAL:HG23	1.89	0.73
2:B:337:GLN:O	2:B:341:GLU:HB2	1.87	0.73
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.36	0.73
1:A:452:LYS:HE3	2:B:366:GLY:O	1.91	0.70
1:A:451:LEU:C	1:A:453:GLU:N	2.48	0.69
1:A:693:LEU:HD12	1:A:694:PHE:H	1.57	0.68
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.24	0.68
3:A:900:FAD:C10	4:A:901:TCF:H3B1	2.23	0.68
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.76	0.67
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.28	0.67
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.26	0.66
2:B:429:ASN:HB3	2:B:432:GLU:OE2	1.95	0.66
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.77	0.65
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.77	0.65
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.79	0.65
1:A:379:GLU:O	1:A:382:PHE:HB3	1.97	0.65
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.78	0.64
1:A:693:LEU:HD12	1:A:694:PHE:N	2.12	0.64
1:A:808:PRO:O	1:A:810:THR:HG23	1.97	0.64
1:A:343:ALA:O	1:A:346:SER:OG	2.15	0.64
1:A:506:GLU:O	1:A:508:LEU:N	2.27	0.64
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ARG:O	1:A:730:ILE:HG13	1.99	0.63
1:A:418:LEU:HD11	2:B:324:VAL:HG21	1.79	0.63
2:B:418:LYS:O	2:B:421:PHE:HB2	1.98	0.63
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.67	0.63
1:A:520:TYR:CD2	1:A:521:LEU:HG	2.33	0.63
2:B:426:ARG:HB3	2:B:427:ARG:HG3	1.79	0.62
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.35	0.62
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.65	0.61
1:A:665:CYS:HB2	1:A:745:GLU:O	2.00	0.61
1:A:270:ILE:O	1:A:272:PRO:HD3	2.00	0.60
1:A:659:LEU:HD12	1:A:660:ASN:N	2.16	0.60
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.83	0.60
1:A:807:TYR:N	1:A:808:PRO:HD3	2.17	0.60
1:A:533:PHE:O	1:A:537:GLU:HG2	2.01	0.60
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.84	0.59
1:A:385:LEU:O	1:A:388:ALA:HB3	2.01	0.59
1:A:377:MET:HE2	1:A:378:VAL:HG22	1.85	0.59
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.03	0.58
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.38	0.58
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.38	0.58
1:A:551:HIS:O	1:A:553:ASP:N	2.37	0.58
1:A:366:ASN:OD1	1:A:368:GLN:N	2.38	0.56
1:A:694:PHE:HA	1:A:704:LEU:O	2.05	0.56
1:A:473:ASP:C	1:A:473:ASP:OD1	2.47	0.56
1:A:715:MET:HE3	1:A:723:ILE:HG12	1.86	0.56
1:A:541:ALA:O	1:A:542:THR:HB	2.05	0.56
1:A:346:SER:HA	1:A:351:MET:SD	2.45	0.56
1:A:402:ASN:O	1:A:403:ASN:HB2	2.06	0.56
2:B:388:GLN:O	2:B:391:ALA:HB3	2.05	0.56
1:A:362:LEU:C	1:A:363:TYR:CD1	2.85	0.55
1:A:363:TYR:CD2	1:A:734:ILE:HG13	2.42	0.55
1:A:295:ARG:NH2	1:A:580:GLU:O	2.40	0.55
1:A:710:GLU:HA	1:A:710:GLU:OE1	2.06	0.55
1:A:374:LYS:O	1:A:375:ASP:C	2.50	0.54
2:B:399:GLY:O	2:B:434:LEU:HD21	2.08	0.54
1:A:548:SER:HB2	1:A:766:ALA:HA	1.89	0.54
1:A:548:SER:O	1:A:552:TRP:HB3	2.08	0.54
2:B:350:GLN:H	2:B:350:GLN:HE21	1.54	0.54
2:B:337:GLN:HE21	2:B:337:GLN:HA	1.71	0.54
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.43	0.54
2:B:370:TYR:CD2	2:B:370:TYR:N	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ARG:O	2:B:402:PHE:N	2.41	0.54
1:A:506:GLU:C	1:A:508:LEU:N	2.60	0.53
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.74	0.53
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.73	0.53
2:B:413:SER:C	2:B:415:VAL:H	2.16	0.52
2:B:421:PHE:O	2:B:425:ARG:HB2	2.09	0.52
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.91	0.52
1:A:340:ASN:HA	1:A:560:PHE:CZ	2.45	0.52
1:A:177:ALA:HB1	1:A:218:LEU:HB3	1.92	0.52
2:B:413:SER:O	2:B:415:VAL:N	2.42	0.51
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.92	0.51
2:B:369:PRO:HB2	2:B:370:TYR:CE2	2.45	0.51
1:A:724:VAL:O	1:A:728:LEU:HG	2.10	0.51
1:A:761:TYR:HB2	1:A:809:ALA:HB1	1.92	0.51
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.46	0.51
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.74	0.51
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.40	0.51
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.94	0.50
1:A:800:GLY:O	1:A:803:THR:N	2.37	0.50
1:A:761:TYR:HB2	1:A:809:ALA:CB	2.42	0.49
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.95	0.49
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.13	0.48
1:A:384:ARG:NH2	2:B:312:LYS:O	2.46	0.48
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.31	0.48
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.78	0.48
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.95	0.48
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.28	0.48
1:A:377:MET:O	1:A:377:MET:HG2	2.12	0.48
1:A:419:GLN:NE2	2:B:315:PHE:O	2.44	0.48
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.54	0.48
1:A:241:PRO:O	1:A:244:SER:HB3	2.14	0.48
1:A:337:LEU:O	1:A:339:GLY:N	2.46	0.47
2:B:417:VAL:O	2:B:420:PHE:HB3	2.14	0.47
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.96	0.47
2:B:317:SER:O	2:B:321:VAL:HG23	2.14	0.47
2:B:349:ILE:O	2:B:350:GLN:C	2.57	0.47
1:A:260:GLY:O	1:A:264:PHE:CD2	2.67	0.47
1:A:384:ARG:NH1	2:B:312:LYS:O	2.45	0.47
1:A:374:LYS:O	1:A:378:VAL:HG23	2.15	0.47
1:A:448:MET:CB	2:B:363:LEU:HD11	2.43	0.47
1:A:666:PHE:O	1:A:701:PRO:HG2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:O	1:A:249:VAL:C	2.57	0.47
1:A:650:ALA:O	1:A:654:MET:HG3	2.15	0.47
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.97	0.47
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.50	0.47
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.50	0.47
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.76	0.46
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.15	0.46
1:A:468:VAL:O	1:A:472:ARG:NH1	2.45	0.46
1:A:485:ARG:O	1:A:487:LEU:N	2.49	0.46
2:B:368:GLU:HB2	2:B:369:PRO:HD3	1.98	0.46
2:B:370:TYR:N	2:B:370:TYR:HD2	2.14	0.46
1:A:457:GLU:O	1:A:457:GLU:HG2	2.15	0.46
2:B:352:ILE:O	2:B:352:ILE:CG2	2.63	0.46
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.51	0.46
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.98	0.46
2:B:424:TYR:O	2:B:425:ARG:C	2.59	0.46
1:A:566:THR:HG21	1:A:697:LEU:HD21	1.98	0.45
1:A:594:ARG:HA	1:A:640:VAL:O	2.16	0.45
1:A:520:TYR:CE2	1:A:521:LEU:HG	2.51	0.45
1:A:437:THR:HG22	1:A:438:GLN:N	2.30	0.45
1:A:450:ASN:HA	1:A:453:GLU:HB2	1.96	0.45
1:A:286:SER:HB2	1:A:291:LEU:HD21	1.99	0.45
1:A:310:ARG:NH2	1:A:756:TRP:HB2	2.31	0.45
1:A:380:GLN:HE21	1:A:380:GLN:HB3	1.52	0.45
1:A:424:LYS:O	1:A:426:GLU:N	2.49	0.45
1:A:814:ALA:O	1:A:815:LEU:C	2.59	0.45
2:B:376:ILE:H	2:B:376:ILE:HG13	1.52	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.81	0.45
1:A:340:ASN:OD1	1:A:342:MET:N	2.45	0.45
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.99	0.45
1:A:209:VAL:HG13	1:A:242:TYR:CD1	2.49	0.44
1:A:317:VAL:HG12	1:A:317:VAL:O	2.17	0.44
1:A:451:LEU:O	1:A:453:GLU:N	2.50	0.44
1:A:366:ASN:OD1	1:A:367:GLY:N	2.51	0.44
1:A:568:ARG:NH2	1:A:699:LYS:HA	2.32	0.44
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.52	0.44
2:B:394:ALA:O	2:B:398:TYR:HB2	2.17	0.44
1:A:806:ASN:C	1:A:807:TYR:CD2	2.95	0.44
1:A:535:ASN:HD22	1:A:535:ASN:HA	1.51	0.44
1:A:572:SER:O	1:A:576:VAL:HG23	2.18	0.44
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.52	0.43
1:A:807:TYR:N	1:A:808:PRO:CD	2.81	0.43
1:A:447:LYS:HD3	1:A:497:LEU:HD21	2.00	0.43
1:A:606:ASN:ND2	1:A:609:SER:H	2.15	0.43
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.54	0.43
2:B:420:PHE:CD2	2:B:420:PHE:C	2.95	0.43
1:A:245:ASP:O	1:A:249:VAL:HG23	2.19	0.43
1:A:291:LEU:H	1:A:291:LEU:HG	1.69	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.72	0.43
2:B:383:TRP:O	2:B:384:THR:C	2.62	0.43
2:B:425:ARG:NH1	2:B:431:ASP:OD1	2.51	0.43
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.53	0.43
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.76	0.43
1:A:181:SER:OG	1:A:218:LEU:HD22	2.19	0.43
1:A:319:THR:HA	1:A:328:ASP:HA	2.01	0.43
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.53	0.43
1:A:659:LEU:HD12	1:A:659:LEU:C	2.43	0.43
1:A:603:ILE:HG12	1:A:615:ILE:HD13	2.00	0.43
1:A:801:GLU:HG2	1:A:809:ALA:HA	1.96	0.43
1:A:196:PHE:N	1:A:197:PRO:CD	2.83	0.42
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.55	0.42
1:A:564:HIS:CD2	1:A:564:HIS:N	2.87	0.42
1:A:294:ALA:O	1:A:295:ARG:C	2.60	0.42
1:A:565:LEU:HD12	1:A:565:LEU:N	2.35	0.42
1:A:670:PHE:CD1	1:A:670:PHE:C	2.97	0.42
1:A:728:LEU:O	1:A:729:ALA:C	2.62	0.42
1:A:800:GLY:O	1:A:801:GLU:C	2.62	0.42
1:A:543:PRO:C	1:A:545:SER:H	2.27	0.42
1:A:284:ILE:HD13	1:A:590:VAL:HG11	2.02	0.42
1:A:364:GLU:OE1	1:A:524:ARG:NE	2.53	0.42
1:A:378:VAL:O	1:A:379:GLU:C	2.62	0.42
1:A:543:PRO:C	1:A:545:SER:N	2.76	0.42
1:A:640:VAL:HA	1:A:641:PRO:HA	1.87	0.42
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.69	0.42
1:A:456:LYS:HG2	2:B:370:TYR:OH	2.19	0.42
1:A:822:ALA:O	1:A:823:GLY:C	2.59	0.42
1:A:606:ASN:HD22	1:A:609:SER:H	1.68	0.42
1:A:319:THR:HG21	1:A:321:ARG:NH2	2.35	0.42
1:A:319:THR:OG1	1:A:572:SER:HB3	2.20	0.41
1:A:747:VAL:HG12	1:A:748:VAL:N	2.35	0.41
1:A:669:VAL:HG11	1:A:673:PRO:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ARG:HG2	1:A:758:ARG:HH11	1.86	0.41
1:A:374:LYS:O	1:A:377:MET:N	2.53	0.41
1:A:533:PHE:O	1:A:537:GLU:CG	2.69	0.41
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.90	0.41
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.35	0.41
2:B:413:SER:C	2:B:415:VAL:N	2.79	0.41
1:A:377:MET:CE	1:A:378:VAL:HG22	2.51	0.41
1:A:437:THR:C	1:A:439:GLU:N	2.79	0.41
1:A:467:GLU:O	1:A:468:VAL:C	2.63	0.41
1:A:311:ASP:OD1	1:A:311:ASP:N	2.53	0.41
1:A:750:ARG:O	1:A:753:ALA:HB3	2.21	0.41
1:A:485:ARG:C	1:A:487:LEU:N	2.78	0.40
2:B:320:ASP:O	2:B:323:ALA:HB3	2.21	0.40
1:A:763:TYR:CD1	1:A:763:TYR:C	2.99	0.40
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.56	0.40
1:A:494:TYR:CD2	1:A:494:TYR:O	2.74	0.40
1:A:568:ARG:NH1	1:A:699:LYS:HE3	2.36	0.40
3:A:900:FAD:HM81	3:A:900:FAD:HM73	1.80	0.40
1:A:448:MET:HG3	1:A:497:LEU:HD23	2.04	0.40
2:B:349:ILE:HG22	2:B:350:GLN:N	2.37	0.40
2:B:405:ILE:O	2:B:409:ILE:HG13	2.22	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	664/852 (78%)	575 (87%)	65 (10%)	24 (4%)	2	16
2	B	131/482 (27%)	99 (76%)	26 (20%)	6 (5%)	2	11
All	All	795/1334 (60%)	674 (85%)	91 (11%)	30 (4%)	2	15

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	PRO
1	A	507	LYS
2	B	341	GLU
2	B	373	PRO
1	A	275	THR
1	A	425	ASP
1	A	438	GLN
1	A	452	LYS
1	A	482	SER
1	A	486	ASP
1	A	499	GLU
1	A	552	TRP
1	A	579	ALA
1	A	785	SER
1	A	793	ILE
1	A	801	GLU
2	B	414	VAL
2	B	426	ARG
1	A	243	ASN
1	A	373	GLU
1	A	428	ILE
1	A	737	SER
1	A	809	ALA
2	B	331	ALA
1	A	338	GLY
1	A	364	GLU
2	B	401	ASP
1	A	316	ARG
1	A	332	MET
1	A	468	VAL

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/699 (81%)	486 (86%)	80 (14%)	3	15
2	B	117/395 (30%)	91 (78%)	26 (22%)	1	4
All	All	683/1094 (62%)	577 (84%)	106 (16%)	2	12

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	VAL
1	A	183	LEU
1	A	191	GLN
1	A	205	GLN
1	A	220	LEU
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	247	VAL
1	A	248	LEU
1	A	249	VAL
1	A	268	LYS
1	A	271	LYS
1	A	274	PRO
1	A	276	LYS
1	A	281	VAL
1	A	282	ILE
1	A	296	GLN
1	A	305	THR
1	A	313	VAL
1	A	351	MET
1	A	359	LYS
1	A	380	GLN
1	A	404	LYS
1	A	413	GLU
1	A	423	VAL
1	A	428	ILE
1	A	429	GLU
1	A	433	LYS
1	A	434	ILE
1	A	437	THR
1	A	438	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	445	LEU
1	A	449	VAL
1	A	453	GLU
1	A	457	GLU
1	A	458	LEU
1	A	466	SER
1	A	469	LYS
1	A	479	LEU
1	A	485	ARG
1	A	487	LEU
1	A	490	LEU
1	A	509	GLN
1	A	512	GLU
1	A	514	ASN
1	A	519	VAL
1	A	523	SER
1	A	524	ARG
1	A	526	ARG
1	A	535	ASN
1	A	537	GLU
1	A	556	ASP
1	A	574	VAL
1	A	591	ARG
1	A	600	CYS
1	A	607	THR
1	A	610	THR
1	A	612	GLN
1	A	624	THR
1	A	626	PRO
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	659	LEU
1	A	663	VAL
1	A	675	VAL
1	A	677	LEU
1	A	684	THR
1	A	699	LYS
1	A	724	VAL
1	A	727	CYS
1	A	778	GLN
1	A	780	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	786	ILE
1	A	793	ILE
1	A	815	LEU
1	A	816	LEU
1	A	825	ILE
1	A	835	THR
2	B	308	ARG
2	B	316	LEU
2	B	317	SER
2	B	319	GLU
2	B	324	VAL
2	B	332	THR
2	B	337	GLN
2	B	341	GLU
2	B	342	LEU
2	B	344	SER
2	B	347	ARG
2	B	348	GLN
2	B	349	ILE
2	B	350	GLN
2	B	351	ASN
2	B	352	ILE
2	B	370	TYR
2	B	375	VAL
2	B	376	ILE
2	B	380	ASN
2	B	382	ARG
2	B	385	THR
2	B	390	LEU
2	B	414	VAL
2	B	422	VAL
2	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	HIS
1	A	380	GLN
1	A	395	GLN
1	A	402	ASN
1	A	417	GLN
1	A	422	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	438	GLN
1	A	484	HIS
1	A	509	GLN
1	A	535	ASN
1	A	564	HIS
1	A	828	GLN
2	B	337	GLN
2	B	348	GLN
2	B	350	GLN
2	B	380	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 oligosaccharides 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	$\# Z > 2$
4	TCF	A	901	3	10,11,12	0.89	0	13,13,15	2.18	5 (38%)
3	FAD	A	900	4	58,58,58	2.35	13 (22%)	85,89,89	1.93	24 (28%)

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
4	TCF	A	901	3	-	1/4/4/5	0/1/1/1
3	FAD	A	900	4	-	3/34/50/50	0/5/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C2A-N1A	8.62	1.49	1.33
3	A	900	FAD	C4X-N5	7.38	1.46	1.30
3	A	900	FAD	C2A-N3A	7.24	1.46	1.33
3	A	900	FAD	O4-C4	6.18	1.35	1.23
3	A	900	FAD	O2-C2	5.95	1.36	1.24
3	A	900	FAD	C8A-N7A	2.53	1.36	1.31
3	A	900	FAD	P-O3P	2.39	1.62	1.59
3	A	900	FAD	C5A-N7A	-2.36	1.34	1.39
3	A	900	FAD	C4A-N9A	-2.31	1.32	1.37
3	A	900	FAD	C9A-N10	2.26	1.45	1.41
3	A	900	FAD	C10-N10	2.12	1.41	1.37
3	A	900	FAD	C5'-C4'	2.12	1.54	1.51
3	A	900	FAD	C4-N3	-2.06	1.35	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-9.37	114.40	128.58
4	A	901	TCF	BR-CB4-CB3	4.87	125.93	119.30
3	A	900	FAD	C9A-N10-C10	-4.31	114.17	120.75
3	A	900	FAD	C5X-C9A-N10	3.89	121.48	117.97
3	A	900	FAD	O4-C4-C4X	-3.77	116.59	126.53
3	A	900	FAD	C2A-N3A-C4A	3.51	120.41	111.83
3	A	900	FAD	C5A-C4A-N3A	-2.96	122.64	126.72
3	A	900	FAD	O3P-P-O1P	-2.92	101.91	110.70
3	A	900	FAD	N9A-C8A-N7A	-2.89	109.84	113.94
4	A	901	TCF	C3B-CB1-CB6	-2.87	113.84	121.18
4	A	901	TCF	BR-CB4-CB5	-2.84	115.43	119.30
3	A	900	FAD	C4X-C10-N1	-2.67	118.05	124.59
3	A	900	FAD	O5'-C5'-C4'	2.42	115.83	109.36
3	A	900	FAD	C5X-N5-C4X	-2.42	114.17	118.09
4	A	901	TCF	C3B-CB1-CB2	2.40	127.32	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	O2A-PA-O1A	2.32	123.25	112.44
3	A	900	FAD	C2A-N1A-C6A	2.28	122.48	118.73
3	A	900	FAD	C4A-N9A-C8A	2.27	108.13	105.74
3	A	900	FAD	C4X-C4-N3	2.26	119.02	113.25
3	A	900	FAD	O4B-C1B-N9A	2.21	112.32	108.09
3	A	900	FAD	C9-C9A-C5X	-2.19	116.17	120.03
3	A	900	FAD	C4-N3-C2	-2.18	121.77	125.64
3	A	900	FAD	N10-C10-N1	2.14	124.80	118.51
3	A	900	FAD	C6A-C5A-C4A	2.12	120.08	117.18
3	A	900	FAD	C10-N1-C2	2.08	121.36	116.85
3	A	900	FAD	C4A-N9A-C1B	-2.08	121.77	126.63
3	A	900	FAD	C4A-C5A-N7A	-2.07	108.22	110.58
3	A	900	FAD	O3'-C3'-C4'	-2.03	104.32	108.93
4	A	901	TCF	CB2-CB3-CB4	2.02	121.60	119.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	FAD	PA-O3P-P-O5'
4	A	901	TCF	C1B-C2B-C3B-CB1
3	A	900	FAD	C2'-C1'-N10-C10
3	A	900	FAD	P-O3P-PA-O2A

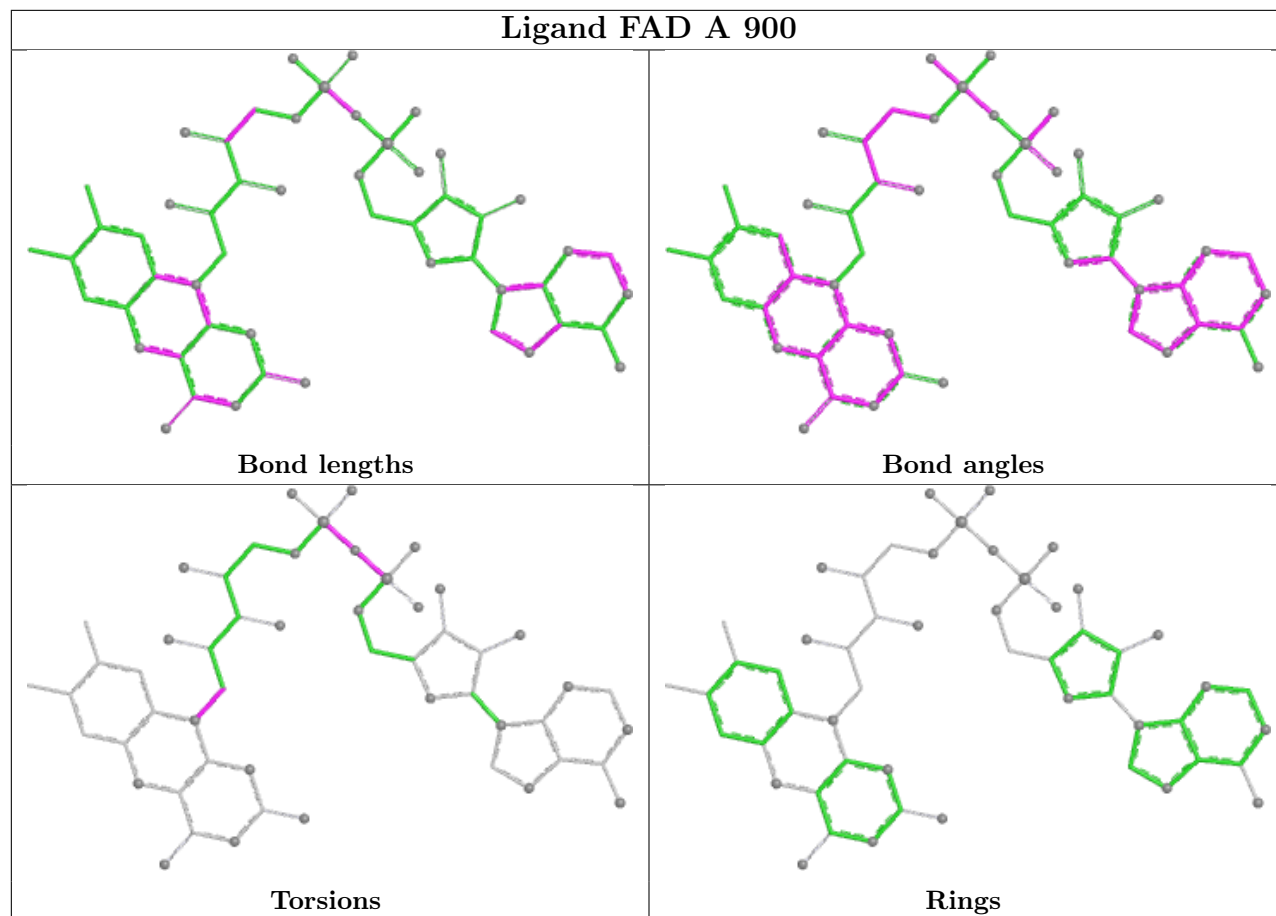
There are no ring outliers.

2 monomers are involved in 4 short contacts:

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



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%)	-0.29	4 (0%) 85 73	28, 62, 91, 105	0
2	B	133/482 (27%)	0.37	6 (4%) 38 25	64, 93, 108, 115	0
All	All	799/1334 (59%)	-0.18	10 (1%) 75 56	28, 67, 98, 115	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	3.7
2	B	374	GLU	3.5
2	B	375	VAL	3.4
1	A	171	PRO	3.0
1	A	373	GLU	2.8
2	B	440	GLU	2.8
2	B	376	ILE	2.3
2	B	426	ARG	2.3
2	B	382	ARG	2.1
1	A	275	THR	2.1

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](#)

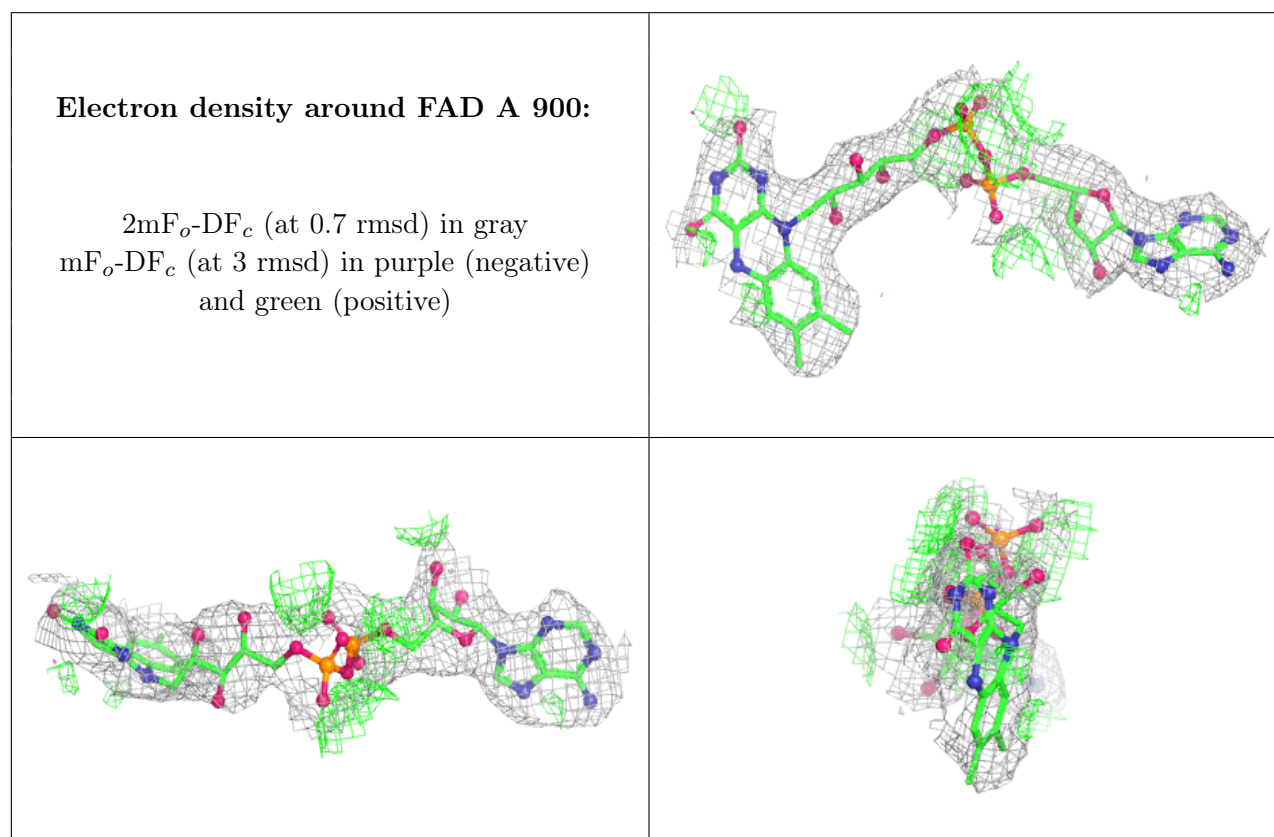
There are no oligosaccharides in this entry.

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
4	TCF	A	901	11/12	0.97	0.11	57,64,72,80	0
3	FAD	A	900	53/53	0.98	0.07	28,41,58,59	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.