



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 PM UTC

PDB ID : 8Q1J / pdb_00008q1j
Title : LSD1 Y391K-CoREST bound to Acetylated K14 of Histone H3
Authors : Barone, M.; Mattevi, A.
Deposited on : 2023-07-31
Resolution : 2.87 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 ⓘ](#)) 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

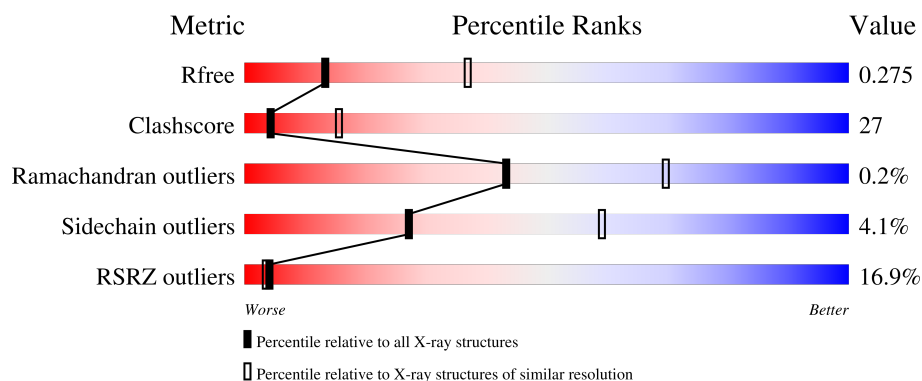
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	730	14% 49% 39% 9%
2	B	178	17% 32% 39% 28%
3	C	21	19% 24% 43% 5% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6419 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 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5214	3321	907	966	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	LYS	TYR	conflict	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			1042	654	186	199	3			

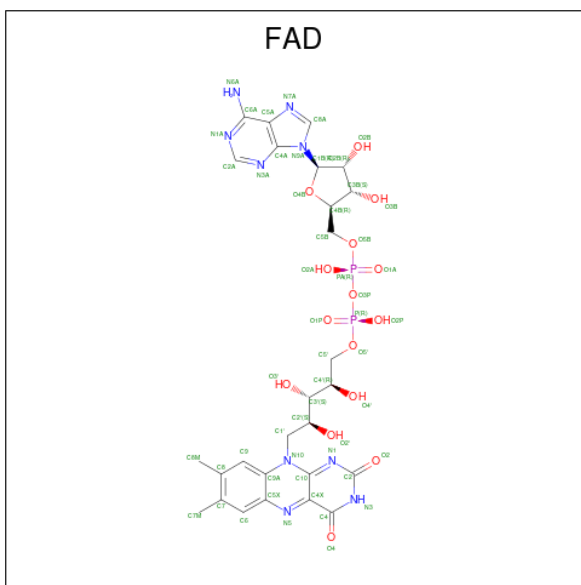
- Molecule 3 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	S	0	0	0
			110	64	24	21	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	LYS	conflict	UNP Q6NXT2

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).

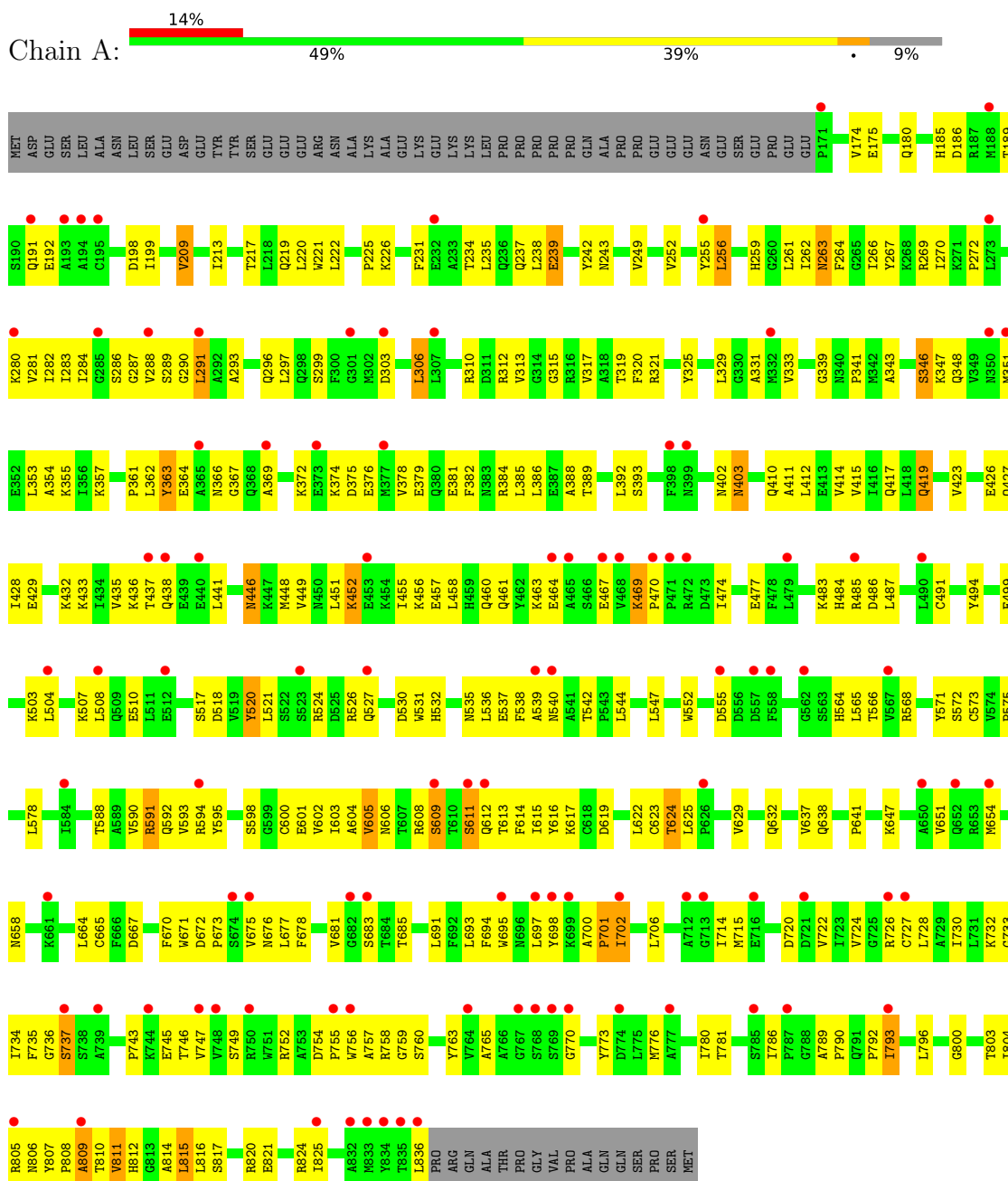


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

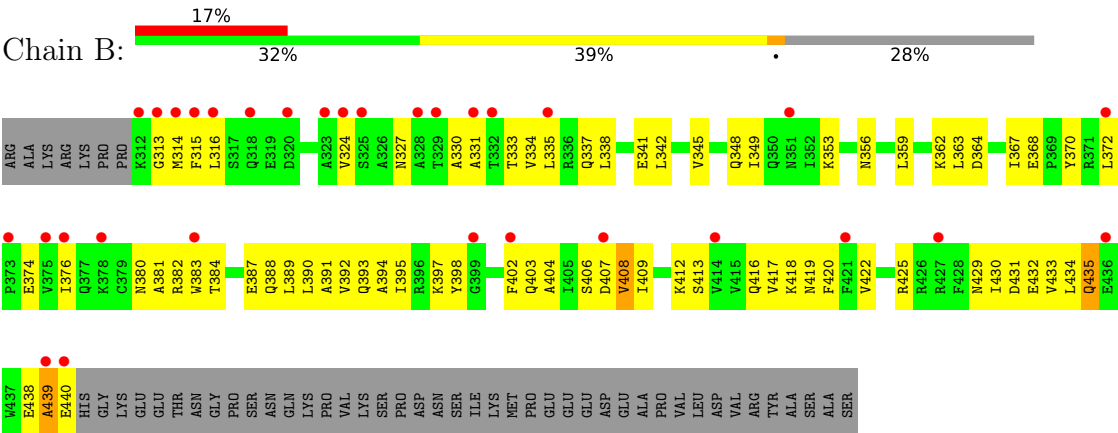
3 Residue-property plots

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.

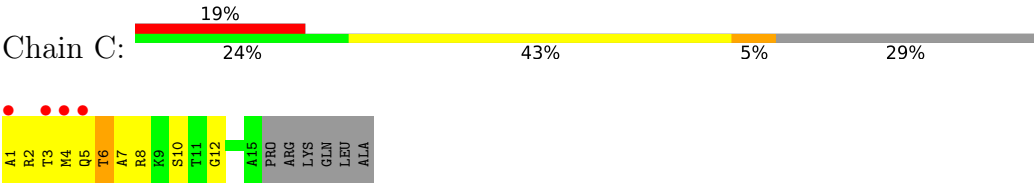
- Molecule 1: Lysine-specific histone demethylase 1A



● Molecule 2: REST corepressor 1



● Molecule 3: Histone H3.3C



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.60Å 180.15Å 232.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.87 48.87 – 2.87	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.87-2.87) 96.8 (48.87-2.87)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.240 , 0.272 0.249 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6419	wwPDB-VP
Average B, all atoms (Å ²)	107.0	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: ALY, 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	0.46	0/5327	0.90	23/7225 (0.3%)
2	B	0.37	0/1055	1.02	4/1422 (0.3%)
3	C	0.91	0/96	1.45	1/124 (0.8%)
All	All	0.46	0/6478	0.93	28/8771 (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
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	ALA	N-CA-C	-25.59	70.09	109.25
1	A	609	SER	N-CA-C	-17.83	84.09	110.48
1	A	609	SER	CB-CA-C	13.59	134.46	109.46
1	A	611	SER	N-CA-C	12.87	129.76	112.90
1	A	825	ILE	CB-CA-C	-11.97	96.36	112.04
1	A	702	ILE	N-CA-C	-11.54	93.12	108.35
1	A	209	VAL	CB-CA-C	-10.89	94.62	112.26
1	A	737	SER	CB-CA-C	10.17	127.63	110.74
1	A	209	VAL	N-CA-C	9.34	122.76	111.09
2	B	439	ALA	CA-C-N	8.93	137.78	121.70
2	B	439	ALA	C-N-CA	8.93	137.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	LYS	CB-CA-C	8.85	125.72	110.68
1	A	809	ALA	CB-CA-C	-8.62	93.28	110.42
1	A	611	SER	CB-CA-C	-7.71	94.18	109.67
1	A	369	ALA	CB-CA-C	-6.76	97.10	109.54
1	A	702	ILE	N-CA-CB	6.57	122.13	111.36
1	A	520	TYR	N-CA-C	6.47	119.29	111.40
1	A	702	ILE	CB-CA-C	6.33	123.02	111.30
1	A	520	TYR	CB-CA-C	-6.01	100.69	110.79
1	A	701	PRO	N-CA-C	-5.75	101.64	110.95
1	A	375	ASP	CB-CA-C	-5.61	99.26	110.42
3	C	6	THR	N-CA-C	-5.55	107.15	114.31
1	A	263	ASN	N-CA-C	5.35	122.20	110.80
1	A	313	VAL	CA-C-N	-5.33	113.63	120.34
1	A	313	VAL	C-N-CA	-5.33	113.63	120.34
2	B	439	ALA	CB-CA-C	5.29	118.97	110.29
1	A	825	ILE	N-CA-C	5.18	116.53	110.62
1	A	591	ARG	CB-CA-C	5.16	120.70	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide
2	B	439	ALA	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	5214	0	5256	300	1
2	B	1042	0	1051	78	0
3	C	110	0	119	13	0
4	A	53	0	31	9	0
All	All	6419	0	6457	346	1

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 27.

All (346) 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:664:LEU:HD11	1:A:727:CYS:SG	1.44	1.54
1:A:664:LEU:CD1	1:A:727:CYS:SG	2.17	1.30
1:A:485:ARG:HD3	2:B:407:ASP:CG	1.63	1.24
1:A:485:ARG:HD3	2:B:407:ASP:OD2	1.10	1.23
1:A:485:ARG:CD	2:B:407:ASP:OD2	1.86	1.23
1:A:209:VAL:O	1:A:213:ILE:HD12	1.39	1.21
1:A:520:TYR:O	1:A:521:LEU:HD23	1.58	1.03
1:A:594:ARG:HD2	1:A:601:GLU:CD	1.89	0.96
1:A:280:LYS:HD2	1:A:303:ASP:HB3	1.48	0.94
1:A:651:VAL:HG22	1:A:776:MET:HE1	1.47	0.94
1:A:263:ASN:O	1:A:267:TYR:CE2	2.24	0.90
1:A:564:HIS:ND1	3:C:6:THR:HG22	1.85	0.90
1:A:281:VAL:HG21	1:A:297:LEU:HD13	1.52	0.89
1:A:594:ARG:HD2	1:A:601:GLU:OE2	1.74	0.87
1:A:664:LEU:HD12	1:A:727:CYS:SG	2.17	0.85
1:A:263:ASN:C	1:A:267:TYR:HE2	1.87	0.83
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.14	0.83
1:A:594:ARG:HD2	1:A:601:GLU:CG	2.08	0.82
1:A:217:THR:HG22	1:A:234:THR:HG21	1.61	0.82
1:A:333:VAL:HG11	3:C:6:THR:HG21	1.62	0.81
1:A:357:LYS:H	1:A:676:ASN:HD22	1.29	0.80
1:A:263:ASN:C	1:A:267:TYR:CE2	2.59	0.80
1:A:381:GLU:OE1	1:A:384:ARG:NH1	2.15	0.79
1:A:539:ALA:HB2	3:C:5:GLN:HG2	1.64	0.79
1:A:388:ALA:HB2	2:B:314:MET:HG2	1.64	0.78
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.65	0.77
1:A:319:THR:HB	1:A:572:SER:HB3	1.66	0.77
1:A:594:ARG:HD2	1:A:601:GLU:HG3	1.67	0.76
1:A:310:ARG:HH12	1:A:756:TRP:HB2	1.50	0.76
1:A:606:ASN:O	1:A:609:SER:O	2.04	0.76
1:A:594:ARG:CD	1:A:601:GLU:OE2	2.34	0.76
1:A:355:LYS:H	1:A:355:LYS:HD2	1.50	0.75
1:A:331:ALA:HA	4:A:901:FAD:C4X	2.17	0.75
1:A:263:ASN:O	1:A:267:TYR:HE2	1.64	0.75
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.50	0.75
1:A:664:LEU:HD21	1:A:724:VAL:HG13	1.69	0.74
1:A:310:ARG:NH1	1:A:756:TRP:HB2	2.01	0.74
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.71	0.73
1:A:213:ILE:HG22	1:A:252:VAL:HG11	1.70	0.73
1:A:325:TYR:HE2	1:A:665:CYS:HB3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.73	0.71
1:A:226:LYS:HE3	1:A:347:LYS:O	1.90	0.70
1:A:367:GLY:HA2	1:A:734:ILE:HD12	1.73	0.70
1:A:341:PRO:HG3	1:A:816:LEU:HD13	1.73	0.69
1:A:527:GLN:NE2	1:A:683:SER:O	2.25	0.69
1:A:384:ARG:NH2	1:A:419:GLN:OE1	2.26	0.69
1:A:266:ILE:N	1:A:348:GLN:OE1	2.24	0.69
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.73	0.69
1:A:526:ARG:NH1	1:A:685:THR:HG22	2.08	0.68
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.08	0.68
2:B:422:VAL:HA	2:B:425:ARG:HG3	1.76	0.68
1:A:714:ILE:HG22	1:A:715:MET:HE2	1.74	0.67
1:A:315:GLY:HA2	4:A:901:FAD:H3B	1.75	0.67
1:A:800:GLY:O	1:A:803:THR:OG1	2.12	0.67
1:A:728:LEU:HD11	1:A:743:PRO:HD3	1.75	0.67
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.60	0.66
2:B:402:PHE:CD2	2:B:418:LYS:HG2	2.31	0.66
1:A:331:ALA:HA	4:A:901:FAD:N5	2.10	0.66
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.31	0.66
1:A:283:ILE:HG22	1:A:622:LEU:HB3	1.76	0.66
1:A:672:ASP:HB3	1:A:675:VAL:HG12	1.77	0.66
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.09	0.65
2:B:382:ARG:O	2:B:412:LYS:NZ	2.29	0.65
1:A:677:LEU:HD11	3:C:7:ALA:HB2	1.77	0.65
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.79	0.65
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.28	0.65
2:B:413:SER:O	2:B:417:VAL:HG23	1.96	0.65
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.79	0.64
1:A:485:ARG:HD3	2:B:407:ASP:OD1	1.95	0.64
1:A:226:LYS:CE	1:A:347:LYS:O	2.45	0.64
1:A:402:ASN:O	1:A:403:ASN:HB2	1.98	0.63
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.81	0.63
1:A:452:LYS:HZ2	2:B:363:LEU:C	2.06	0.63
2:B:387:GLU:HA	2:B:390:LEU:HB2	1.80	0.62
2:B:389:LEU:O	2:B:393:GLN:HG3	1.99	0.62
1:A:362:LEU:HD11	1:A:531:TRP:CE2	2.34	0.62
1:A:221:TRP:HE1	1:A:264:PHE:HE1	1.47	0.62
1:A:437:THR:HG21	1:A:507:LYS:HE3	1.82	0.62
2:B:394:ALA:O	2:B:398:TYR:N	2.28	0.62
1:A:571:TYR:O	1:A:572:SER:C	2.42	0.62
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:HE2	2:B:363:LEU:HD12	1.80	0.61
1:A:571:TYR:O	1:A:573:CYS:N	2.33	0.61
1:A:382:PHE:HA	1:A:385:LEU:HD12	1.83	0.61
1:A:664:LEU:HD11	1:A:727:CYS:HG	1.60	0.61
1:A:698:TYR:HB2	1:A:702:ILE:HD12	1.81	0.61
1:A:452:LYS:NZ	2:B:363:LEU:C	2.59	0.61
1:A:287:GLY:HA3	4:A:901:FAD:O5B	2.01	0.60
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.36	0.60
1:A:325:TYR:CD2	1:A:665:CYS:HB3	2.37	0.60
1:A:665:CYS:HB2	1:A:745:GLU:O	2.01	0.60
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.67	0.60
1:A:209:VAL:O	1:A:213:ILE:CD1	2.32	0.60
2:B:334:VAL:HA	2:B:337:GLN:NE2	2.17	0.60
1:A:594:ARG:HB3	1:A:601:GLU:HG3	1.84	0.60
2:B:384:THR:OG1	2:B:387:GLU:OE2	2.15	0.60
1:A:485:ARG:NE	2:B:407:ASP:OD2	2.34	0.59
2:B:407:ASP:OD1	2:B:408:VAL:N	2.36	0.59
2:B:429:ASN:HB3	2:B:432:GLU:HG3	1.83	0.59
1:A:374:LYS:O	1:A:378:VAL:HG23	2.01	0.59
1:A:283:ILE:HD11	1:A:306:LEU:HD21	1.85	0.58
1:A:263:ASN:O	1:A:267:TYR:CZ	2.56	0.58
1:A:357:LYS:H	1:A:676:ASN:ND2	2.00	0.58
1:A:449:VAL:HG23	2:B:363:LEU:HD21	1.85	0.58
1:A:724:VAL:HG11	1:A:746:THR:HG21	1.85	0.58
2:B:333:THR:HG22	2:B:337:GLN:HE22	1.68	0.58
2:B:380:ASN:OD1	2:B:381:ALA:N	2.36	0.58
1:A:452:LYS:NZ	2:B:363:LEU:HA	2.19	0.58
1:A:320:PHE:CE2	1:A:747:VAL:HG21	2.39	0.58
1:A:695:TRP:HH2	3:C:6:THR:HG1	1.52	0.57
1:A:536:LEU:HB3	1:A:544:LEU:HD21	1.87	0.57
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.20	0.57
1:A:417:GLN:HG2	2:B:331:ALA:HB1	1.87	0.57
1:A:647:LYS:O	1:A:651:VAL:HG23	2.05	0.57
1:A:219:GLN:O	1:A:222:LEU:N	2.38	0.56
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.41	0.56
2:B:404:ALA:O	2:B:407:ASP:OD1	2.23	0.56
1:A:752:ARG:HE	1:A:759:GLY:HA2	1.70	0.56
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.87	0.56
1:A:487:LEU:HD22	2:B:372:LEU:HD22	1.86	0.56
2:B:345:VAL:HA	2:B:348:GLN:OE1	2.06	0.56
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:VAL:HG23	4:A:901:FAD:H2'	1.87	0.56
1:A:381:GLU:OE2	1:A:520:TYR:OH	2.20	0.55
1:A:290:GLY:HA2	1:A:624:THR:HG21	1.88	0.55
1:A:385:LEU:HD23	1:A:415:VAL:CG1	2.35	0.55
1:A:757:ALA:O	1:A:758:ARG:HB2	2.05	0.55
1:A:485:ARG:HG2	2:B:398:TYR:HE2	1.72	0.55
1:A:537:GLU:HG2	1:A:542:THR:O	2.06	0.55
1:A:805:ARG:O	1:A:808:PRO:HD3	2.07	0.55
1:A:263:ASN:O	1:A:267:TYR:OH	2.23	0.55
1:A:464:GLU:HA	1:A:467:GLU:HG2	1.86	0.55
1:A:588:THR:HG22	1:A:604:ALA:HB1	1.88	0.55
1:A:601:GLU:HB3	1:A:617:LYS:HD3	1.88	0.55
1:A:720:ASP:O	1:A:724:VAL:HG23	2.05	0.55
1:A:808:PRO:O	1:A:810:THR:HG23	2.06	0.55
1:A:287:GLY:H	4:A:901:FAD:H4B	1.71	0.55
1:A:821:GLU:O	1:A:824:ARG:N	2.40	0.55
1:A:198:ASP:OD1	1:A:199:ILE:N	2.40	0.54
1:A:379:GLU:HG3	1:A:532:HIS:NE2	2.22	0.54
2:B:406:SER:HB2	2:B:417:VAL:HG21	1.89	0.54
1:A:441:LEU:HB3	2:B:356:ASN:ND2	2.22	0.54
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.23	0.54
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.43	0.54
1:A:591:ARG:O	1:A:637:VAL:HA	2.06	0.54
1:A:734:ILE:HG22	1:A:735:PHE:CD2	2.43	0.54
1:A:320:PHE:CD2	1:A:747:VAL:HG21	2.42	0.54
1:A:438:GLN:HE22	2:B:353:LYS:HA	1.73	0.53
1:A:601:GLU:HA	1:A:616:TYR:O	2.08	0.53
1:A:672:ASP:HB3	1:A:675:VAL:CG1	2.38	0.53
1:A:237:GLN:N	1:A:237:GLN:OE1	2.42	0.53
1:A:389:THR:O	1:A:393:SER:N	2.40	0.53
1:A:566:THR:OG1	1:A:697:LEU:HD22	2.09	0.53
1:A:571:TYR:C	1:A:573:CYS:N	2.66	0.52
1:A:572:SER:O	1:A:575:PRO:HD2	2.09	0.52
1:A:623:CYS:SG	1:A:625:LEU:HB2	2.49	0.52
1:A:310:ARG:NH2	1:A:754:ASP:OD1	2.42	0.52
1:A:410:GLN:O	1:A:414:VAL:HG23	2.09	0.52
1:A:474:ILE:HD12	1:A:477:GLU:HB3	1.91	0.52
1:A:456:LYS:HG2	2:B:370:TYR:CE2	2.45	0.52
1:A:329:LEU:HD21	1:A:747:VAL:HG12	1.91	0.52
1:A:664:LEU:CD1	1:A:727:CYS:HG	2.15	0.52
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:GLN:NE2	1:A:758:ARG:HH21	2.08	0.52
1:A:595:TYR:CE2	1:A:641:PRO:HD2	2.45	0.51
1:A:441:LEU:HB3	2:B:356:ASN:HD21	1.75	0.51
1:A:736:GLY:O	1:A:737:SER:C	2.52	0.51
1:A:456:LYS:HG2	2:B:370:TYR:HE2	1.76	0.51
1:A:457:GLU:O	1:A:461:GLN:HG3	2.11	0.50
1:A:217:THR:HA	1:A:220:LEU:HD12	1.92	0.50
1:A:592:GLN:HG3	1:A:638:GLN:HB3	1.93	0.50
1:A:217:THR:CG2	1:A:234:THR:HG21	2.39	0.50
1:A:362:LEU:C	1:A:363:TYR:HD1	2.20	0.50
1:A:518:ASP:OD1	1:A:518:ASP:N	2.43	0.50
3:C:2:ARG:NH1	3:C:10:SER:OG	2.44	0.50
3:C:3:THR:O	3:C:3:THR:HG22	2.12	0.50
1:A:474:ILE:HG23	2:B:393:GLN:NE2	2.22	0.50
1:A:423:VAL:HG11	1:A:520:TYR:HA	1.93	0.50
1:A:283:ILE:CG2	1:A:622:LEU:HB3	2.40	0.50
1:A:535:ASN:ND2	3:C:7:ALA:O	2.37	0.50
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.47	0.49
1:A:593:VAL:HG22	1:A:602:VAL:HG22	1.94	0.49
1:A:389:THR:HA	1:A:392:LEU:HB3	1.94	0.49
1:A:452:LYS:HZ3	2:B:363:LEU:HA	1.77	0.49
1:A:701:PRO:O	1:A:702:ILE:HG13	2.12	0.49
1:A:364:GLU:HA	1:A:681:VAL:HB	1.94	0.49
1:A:270:ILE:O	1:A:272:PRO:HD3	2.13	0.49
1:A:438:GLN:OE1	1:A:508:LEU:HD11	2.13	0.49
1:A:531:TRP:CH2	3:C:8:ARG:HG3	2.48	0.49
1:A:591:ARG:HG3	1:A:605:VAL:HG13	1.95	0.49
1:A:815:LEU:C	1:A:815:LEU:HD23	2.37	0.49
1:A:310:ARG:NH1	4:A:901:FAD:O2B	2.43	0.49
1:A:384:ARG:HD2	2:B:313:GLY:O	2.12	0.49
2:B:349:ILE:O	2:B:353:LYS:HB2	2.13	0.49
1:A:354:ALA:HB2	1:A:568:ARG:HG3	1.95	0.48
1:A:678:PHE:CD1	1:A:678:PHE:C	2.91	0.48
2:B:383:TRP:CH2	2:B:412:LYS:HG3	2.48	0.48
1:A:614:PHE:O	1:A:615:ILE:HD13	2.14	0.48
1:A:231:PHE:CE2	1:A:249:VAL:HG12	2.49	0.48
1:A:238:LEU:HD21	1:A:242:TYR:HB2	1.95	0.48
1:A:283:ILE:HD11	1:A:306:LEU:CD2	2.44	0.48
1:A:484:HIS:ND1	2:B:372:LEU:HD23	2.28	0.48
1:A:732:LYS:HG2	1:A:737:SER:HA	1.95	0.48
1:A:594:ARG:HD3	1:A:601:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:PHE:CD1	1:A:670:PHE:C	2.92	0.47
1:A:760:SER:O	4:A:901:FAD:HM81	2.14	0.47
1:A:189:THR:HG23	1:A:192:GLU:OE1	2.13	0.47
1:A:366:ASN:OD1	1:A:367:GLY:N	2.47	0.47
1:A:485:ARG:CD	2:B:407:ASP:CG	2.57	0.47
1:A:315:GLY:HA3	4:A:901:FAD:O2A	2.14	0.47
1:A:808:PRO:O	1:A:809:ALA:C	2.57	0.47
2:B:412:LYS:HB3	2:B:416:GLN:HG2	1.95	0.47
1:A:346:SER:HA	1:A:351:MET:HE2	1.96	0.47
2:B:435:GLN:HA	2:B:438:GLU:HG3	1.96	0.47
1:A:438:GLN:HE22	2:B:353:LYS:CA	2.27	0.47
1:A:452:LYS:NZ	2:B:364:ASP:O	2.39	0.47
1:A:526:ARG:HG2	1:A:526:ARG:HH11	1.80	0.47
1:A:537:GLU:HG3	1:A:544:LEU:HG	1.97	0.47
1:A:555:ASP:OD2	1:A:808:PRO:HD2	2.14	0.47
2:B:363:LEU:HD23	2:B:363:LEU:N	2.30	0.47
1:A:238:LEU:HD22	1:A:243:ASN:HB3	1.97	0.47
1:A:540:ASN:CG	1:A:547:LEU:HD11	2.39	0.47
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.46	0.46
1:A:319:THR:HG22	1:A:321:ARG:HG3	1.98	0.46
2:B:403:GLN:O	2:B:406:SER:N	2.45	0.46
2:B:341:GLU:HG3	2:B:341:GLU:O	2.15	0.46
1:A:317:VAL:HG22	1:A:331:ALA:HB3	1.98	0.46
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.97	0.46
1:A:458:LEU:HD11	1:A:486:ASP:HB3	1.98	0.46
1:A:671:TRP:O	1:A:673:PRO:HD3	2.15	0.46
2:B:425:ARG:HA	2:B:430:ILE:CD1	2.46	0.46
1:A:280:LYS:NZ	1:A:303:ASP:OD2	2.46	0.46
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.83	0.45
1:A:319:THR:CB	1:A:572:SER:HB3	2.39	0.45
1:A:428:ILE:O	1:A:432:LYS:HB2	2.15	0.45
1:A:485:ARG:CZ	2:B:407:ASP:OD2	2.64	0.45
1:A:781:THR:HG23	1:A:793:ILE:O	2.17	0.45
1:A:367:GLY:HA3	1:A:733:GLY:O	2.16	0.45
1:A:310:ARG:HE	1:A:312:ARG:HH21	1.62	0.45
1:A:325:TYR:CD1	1:A:325:TYR:N	2.85	0.45
1:A:538:PHE:O	1:A:539:ALA:C	2.58	0.45
1:A:451:LEU:O	1:A:452:LYS:C	2.60	0.45
1:A:180:GLN:HE22	1:A:343:ALA:HB3	1.82	0.45
2:B:387:GLU:HB2	2:B:409:ILE:HD13	1.98	0.45
1:A:460:GLN:O	1:A:464:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:MET:HE3	1:A:776:MET:SD	2.57	0.45
1:A:372:LYS:H	1:A:372:LYS:HD3	1.82	0.45
1:A:175:GLU:OE2	1:A:185:HIS:CG	2.70	0.45
1:A:329:LEU:HD23	1:A:749:SER:HB3	1.98	0.45
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.71	0.45
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.81	0.45
1:A:255:TYR:HD1	1:A:256:LEU:HD12	1.82	0.45
1:A:427:GLN:NE2	1:A:517:SER:O	2.39	0.45
1:A:603:ILE:HG23	1:A:615:ILE:CD1	2.46	0.45
1:A:701:PRO:C	1:A:702:ILE:HG13	2.42	0.44
1:A:217:THR:HG22	1:A:234:THR:CG2	2.40	0.44
1:A:288:VAL:HA	1:A:291:LEU:HD12	1.98	0.44
1:A:221:TRP:CZ3	1:A:225:PRO:HA	2.52	0.44
1:A:752:ARG:HE	1:A:759:GLY:CA	2.31	0.44
1:A:293:ALA:O	1:A:296:GLN:N	2.50	0.44
1:A:392:LEU:HD23	1:A:411:ALA:HB1	2.00	0.44
1:A:693:LEU:HD12	1:A:694:PHE:H	1.83	0.44
1:A:491:CYS:SG	2:B:367:ILE:HD12	2.58	0.44
1:A:238:LEU:HD23	1:A:239:GLU:N	2.33	0.44
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.53	0.44
2:B:333:THR:CG2	2:B:337:GLN:HE22	2.31	0.44
1:A:286:SER:O	1:A:291:LEU:HD11	2.18	0.43
2:B:431:ASP:OD1	2:B:431:ASP:N	2.51	0.43
2:B:374:GLU:OE1	2:B:376:ILE:HG23	2.18	0.43
1:A:325:TYR:N	1:A:325:TYR:HD1	2.17	0.43
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.57	0.43
1:A:526:ARG:HH12	1:A:685:THR:HG22	1.79	0.43
1:A:625:LEU:HD22	1:A:629:VAL:HG11	2.00	0.43
1:A:691:LEU:N	1:A:691:LEU:HD12	2.34	0.43
1:A:770:GLY:O	1:A:805:ARG:HG3	2.18	0.43
1:A:452:LYS:NZ	2:B:363:LEU:CA	2.81	0.43
1:A:539:ALA:HB1	3:C:1:ALA:O	2.19	0.43
1:A:606:ASN:HD21	1:A:608:ARG:HH21	1.65	0.43
1:A:722:VAL:O	1:A:726:ARG:HG3	2.18	0.43
2:B:324:VAL:HG13	2:B:331:ALA:HB2	2.00	0.43
1:A:346:SER:HB3	1:A:351:MET:HE3	2.00	0.43
2:B:362:LYS:C	2:B:363:LEU:HD23	2.44	0.43
1:A:520:TYR:CD1	1:A:520:TYR:C	2.94	0.43
1:A:730:ILE:O	1:A:734:ILE:HD13	2.19	0.43
1:A:433:LYS:HD3	1:A:436:LYS:HD3	2.00	0.43
2:B:434:LEU:O	2:B:438:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD13	1:A:565:LEU:HD22	2.00	0.42
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.19	0.42
2:B:388:GLN:O	2:B:392:VAL:HG23	2.19	0.42
1:A:289:SER:HB3	1:A:814:ALA:HB1	2.00	0.42
1:A:507:LYS:HA	1:A:510:GLU:HG3	2.01	0.42
1:A:804:ILE:CD1	1:A:816:LEU:HB3	2.48	0.42
1:A:423:VAL:HG21	1:A:520:TYR:HB2	2.01	0.42
1:A:700:ALA:HB3	1:A:702:ILE:HD11	2.01	0.42
1:A:235:LEU:HD13	1:A:249:VAL:HG11	2.00	0.42
1:A:264:PHE:HD1	1:A:264:PHE:H	1.67	0.42
1:A:362:LEU:HD13	1:A:362:LEU:HA	1.76	0.42
1:A:266:ILE:HD11	1:A:578:LEU:HD12	2.01	0.42
1:A:363:TYR:HD2	1:A:734:ILE:HG13	1.84	0.42
1:A:693:LEU:HD12	1:A:694:PHE:N	2.35	0.42
2:B:407:ASP:OD1	2:B:407:ASP:C	2.61	0.42
1:A:494:TYR:CD1	1:A:494:TYR:C	2.98	0.42
2:B:416:GLN:O	2:B:420:PHE:N	2.45	0.42
1:A:310:ARG:HE	1:A:312:ARG:NH2	2.18	0.42
2:B:315:PHE:O	2:B:316:LEU:HD23	2.20	0.42
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.50	0.41
1:A:354:ALA:HB2	1:A:568:ARG:HD2	2.02	0.41
1:A:374:LYS:HE2	1:A:524:ARG:HH11	1.84	0.41
1:A:817:SER:HB2	1:A:820:ARG:NH2	2.35	0.41
1:A:355:LYS:H	1:A:355:LYS:CD	2.23	0.41
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.20	0.41
1:A:664:LEU:HA	1:A:664:LEU:HD23	1.66	0.41
1:A:226:LYS:HE2	1:A:347:LYS:O	2.21	0.41
1:A:280:LYS:O	1:A:619:ASP:N	2.49	0.41
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.02	0.41
1:A:262:ILE:HG13	1:A:263:ASN:ND2	2.36	0.41
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.85	0.41
1:A:419:GLN:HE21	1:A:419:GLN:HA	1.86	0.41
2:B:425:ARG:HA	2:B:430:ILE:HD13	2.02	0.41
1:A:191:GLN:HE21	1:A:259:HIS:CD2	2.39	0.41
1:A:604:ALA:O	1:A:614:PHE:N	2.50	0.41
1:A:714:ILE:CG2	1:A:715:MET:HE2	2.49	0.41
1:A:269:ARG:HH12	1:A:299:SER:HB2	1.85	0.41
1:A:386:LEU:HB3	3:C:12:GLY:HA3	2.03	0.41
1:A:566:THR:HG21	1:A:697:LEU:HD13	2.03	0.41
3:C:4:MET:HE3	3:C:4:MET:HA	2.02	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:GLN:H	2:B:337:GLN:CD	2.28	0.41
1:A:463:LYS:HD2	1:A:463:LYS:HA	1.78	0.41
1:A:469:LYS:HD3	1:A:470:PRO:HD2	2.03	0.41
1:A:483:LYS:HA	1:A:483:LYS:HD2	1.91	0.41
1:A:530:ASP:OD2	1:A:685:THR:HA	2.21	0.41
1:A:806:ASN:C	1:A:807:TYR:CD1	2.99	0.41
1:A:261:LEU:HA	1:A:261:LEU:HD23	1.77	0.40
1:A:503:LYS:HG3	1:A:504:LEU:HD13	2.03	0.40
1:A:667:ASP:OD1	1:A:667:ASP:N	2.38	0.40
2:B:397:LYS:C	2:B:398:TYR:HD1	2.29	0.40
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.74	0.40
1:A:372:LYS:O	1:A:376:GLU:HG3	2.22	0.40
1:A:255:TYR:CD1	1:A:256:LEU:HD12	2.57	0.40
1:A:455:ILE:HD11	1:A:491:CYS:HA	2.03	0.40
1:A:600:CYS:O	1:A:617:LYS:HA	2.21	0.40
1:A:811:VAL:HG12	1:A:812:HIS:N	2.36	0.40
2:B:368:GLU:C	2:B:370:TYR:H	2.29	0.40
1:A:238:LEU:HD21	1:A:242:TYR:CB	2.52	0.40
1:A:695:TRP:HH2	3:C:6:THR:OG1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:NH1	1:A:611:SER:O[2_565]	1.98	0.22

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	664/730 (91%)	613 (92%)	49 (7%)	2 (0%)	36 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	127/178 (71%)	118 (93%)	9 (7%)	0	100	100
3	C	12/21 (57%)	10 (83%)	2 (17%)	0	100	100
All	All	803/929 (86%)	741 (92%)	60 (8%)	2 (0%)	43	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ASN
1	A	793	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	566/623 (91%)	544 (96%)	22 (4%)	28	60
2	B	113/156 (72%)	107 (95%)	6 (5%)	20	49
3	C	9/14 (64%)	9 (100%)	0	100	100
All	All	688/793 (87%)	660 (96%)	28 (4%)	27	59

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	256	LEU
1	A	291	LEU
1	A	306	LEU
1	A	346	SER
1	A	363	TYR
1	A	419	GLN
1	A	426	GLU
1	A	429	GLU
1	A	446	ASN
1	A	469	LYS
1	A	499	GLU

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Mol	Chain	Res	Type
1	A	598	SER
1	A	605	VAL
1	A	612	GLN
1	A	613	THR
1	A	624	THR
1	A	706	LEU
1	A	786	ILE
1	A	811	VAL
1	A	815	LEU
1	A	836	LEU
2	B	335	LEU
2	B	338	LEU
2	B	342	LEU
2	B	408	VAL
2	B	435	GLN
2	B	440	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	191	GLN
1	A	394	HIS
1	A	399	ASN
1	A	460	GLN
1	A	509	GLN
1	A	592	GLN
1	A	632	GLN
1	A	638	GLN
1	A	676	ASN
1	A	806	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ALY	C	14	3	10,11,12	0.39	0	7,12,14	0.31	0

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	ALY	C	14	3	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	14	ALY	CH3-CH-NZ-CE
3	C	14	ALY	CE-CD-CG-CB
3	C	14	ALY	OH-CH-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	FAD	A	901	-	58,58,58	0.42	0	85,89,89	0.72	3 (3%)

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	FAD	A	901	-	-	12/34/50/50	0/6/6/6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	FAD	O5'-P-O1P	-3.49	95.12	108.94
4	A	901	FAD	O2P-P-O5'	2.86	120.53	107.57
4	A	901	FAD	O2A-PA-O1A	2.83	125.61	112.44

There are no chirality outliers.

All (12) torsion outliers are listed below:

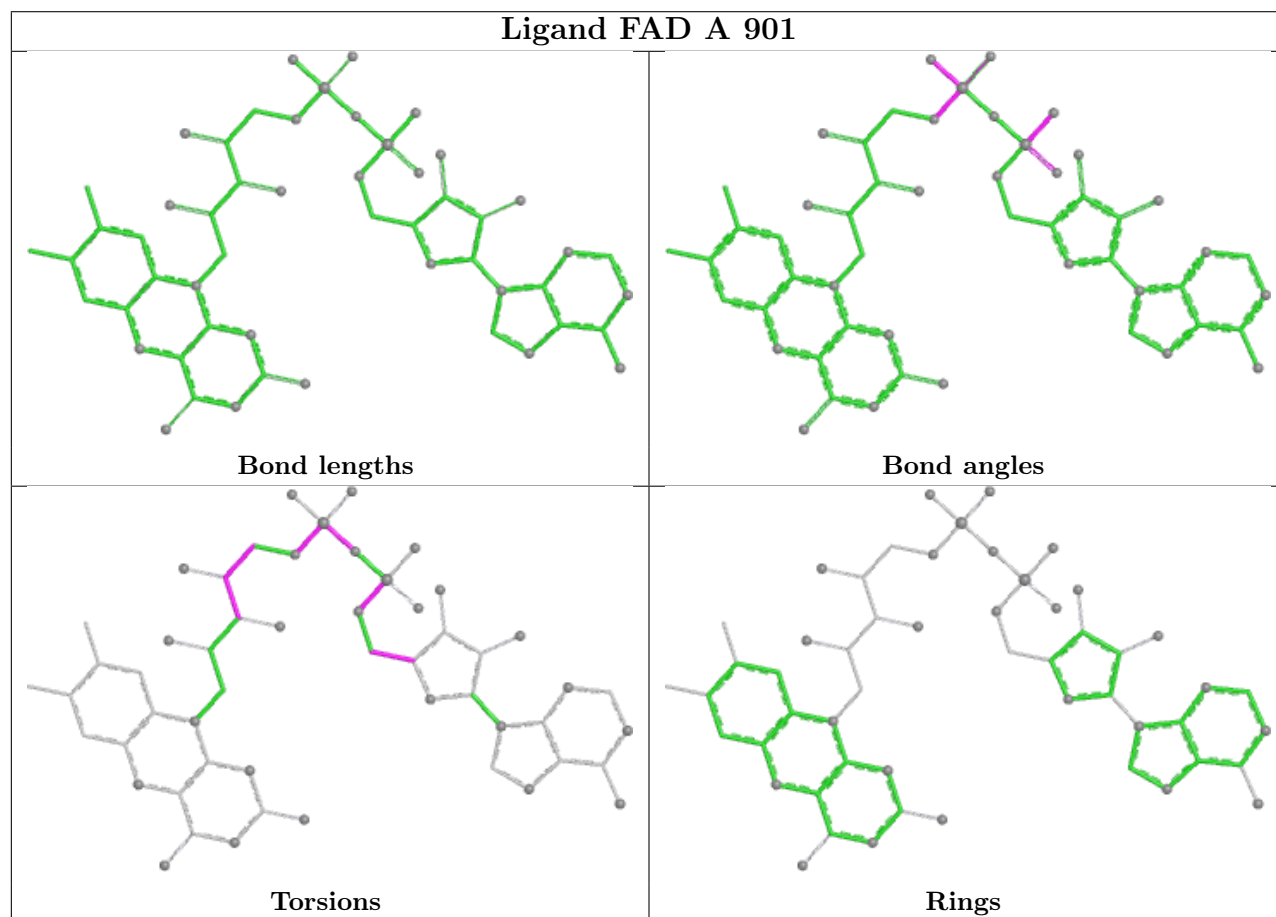
Mol	Chain	Res	Type	Atoms
4	A	901	FAD	C5B-O5B-PA-O1A
4	A	901	FAD	C5'-O5'-P-O2P
4	A	901	FAD	C2'-C3'-C4'-O4'
4	A	901	FAD	O3'-C3'-C4'-C5'
4	A	901	FAD	C2'-C3'-C4'-C5'
4	A	901	FAD	O4'-C4'-C5'-O5'
4	A	901	FAD	C3'-C4'-C5'-O5'
4	A	901	FAD	PA-O3P-P-O5'
4	A	901	FAD	O3'-C3'-C4'-O4'
4	A	901	FAD	C5B-O5B-PA-O3P
4	A	901	FAD	C5'-O5'-P-O3P
4	A	901	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	FAD	9	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

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	666/730 (91%)	1.19	102 (15%) 5 4	66, 100, 134, 155	0
2	B	129/178 (72%)	1.41	31 (24%) 2 2	101, 135, 159, 172	0
3	C	14/21 (66%)	1.75	4 (28%) 1 1	86, 94, 103, 106	0
All	All	809/929 (87%)	1.23	137 (16%) 4 3	66, 106, 144, 172	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	8.2
1	A	557	ASP	6.3
1	A	744	LYS	5.4
2	B	375	VAL	4.9
1	A	683	SER	4.5
2	B	376	ILE	4.5
1	A	674	SER	4.5
2	B	407	ASP	4.4
1	A	835	THR	4.3
1	A	770	GLY	4.3
1	A	833	MET	3.9
1	A	512	GLU	3.9
3	C	1	ALA	3.9
2	B	312	LYS	3.8
1	A	834	TYR	3.8
1	A	373	GLU	3.7
3	C	4	MET	3.7
2	B	324	VAL	3.7
1	A	285	GLY	3.5
1	A	682	GLY	3.4
2	B	331	ALA	3.4
2	B	315	PHE	3.4
1	A	698	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	3.4
1	A	787	PRO	3.4
1	A	727	CYS	3.3
1	A	555	ASP	3.2
1	A	194	ALA	3.2
1	A	540	ASN	3.1
1	A	558	PHE	3.1
1	A	307	LEU	3.1
1	A	809	ALA	3.1
1	A	398	PHE	3.1
1	A	793	ILE	3.0
1	A	654	MET	3.0
1	A	825	ILE	3.0
1	A	768	SER	3.0
2	B	332	THR	3.0
1	A	527	GLN	3.0
1	A	232	GLU	2.9
1	A	774	ASP	2.9
2	B	323	ALA	2.9
1	A	365	ALA	2.9
1	A	785	SER	2.9
1	A	764	VAL	2.9
2	B	329	THR	2.9
1	A	713	GLY	2.8
1	A	377	MET	2.8
2	B	314	MET	2.8
2	B	439	ALA	2.8
2	B	440	GLU	2.8
2	B	383	TRP	2.8
1	A	471	PRO	2.8
1	A	465	ALA	2.7
1	A	453	GLU	2.7
1	A	467	GLU	2.7
1	A	832	ALA	2.7
2	B	372	LEU	2.7
1	A	567	VAL	2.7
3	C	3	THR	2.7
1	A	191	GLN	2.6
1	A	612	GLN	2.6
1	A	750	ARG	2.6
2	B	325	SER	2.6
1	A	695	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	767	GLY	2.6
1	A	650	ALA	2.6
2	B	414	VAL	2.6
1	A	350	ASN	2.6
1	A	611	SER	2.5
1	A	508	LEU	2.5
1	A	756	TRP	2.5
2	B	320	ASP	2.5
1	A	769	SER	2.5
1	A	440	GLU	2.5
1	A	399	ASN	2.5
2	B	427	ARG	2.5
1	A	437	THR	2.4
1	A	755	PRO	2.4
1	A	739	ALA	2.4
2	B	328	ALA	2.4
1	A	470	PRO	2.4
1	A	594	ARG	2.4
1	A	661	LYS	2.4
1	A	255	TYR	2.3
1	A	504	LEU	2.3
2	B	313	GLY	2.3
1	A	369	ALA	2.3
1	A	747	VAL	2.3
1	A	539	ALA	2.3
1	A	712	ALA	2.3
1	A	726	ARG	2.3
2	B	373	PRO	2.3
1	A	188	MET	2.3
1	A	464	GLU	2.3
1	A	280	LYS	2.3
2	B	399	GLY	2.3
2	B	436	GLU	2.2
1	A	652	GLN	2.2
1	A	195	CYS	2.2
1	A	288	VAL	2.2
1	A	523	SER	2.2
1	A	351	MET	2.2
2	B	335	LEU	2.2
1	A	303	ASP	2.2
2	B	421	PHE	2.2
1	A	479	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	378	LYS	2.2
1	A	697	LEU	2.2
1	A	702	ILE	2.2
2	B	402	PHE	2.2
2	B	316	LEU	2.2
1	A	805	ARG	2.1
1	A	332	MET	2.1
1	A	193	ALA	2.1
1	A	737	SER	2.1
1	A	472	ARG	2.1
1	A	675	VAL	2.1
1	A	721	ASP	2.1
1	A	273	LEU	2.1
1	A	777	ALA	2.1
1	A	716	GLU	2.1
1	A	609	SER	2.1
1	A	301	GLY	2.1
1	A	584	ILE	2.1
1	A	438	GLN	2.0
1	A	699	LYS	2.0
2	B	318	GLN	2.0
1	A	468	VAL	2.0
1	A	291	LEU	2.0
2	B	351	ASN	2.0
1	A	485	ARG	2.0
1	A	562	GLY	2.0
3	C	5	GLN	2.0
1	A	626	PRO	2.0
1	A	490	LEU	2.0
1	A	748	VAL	2.0

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

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
3	ALY	C	14	12/13	0.80	0.29	91,105,121,126	0

6.3 Carbohydrates [i](#)

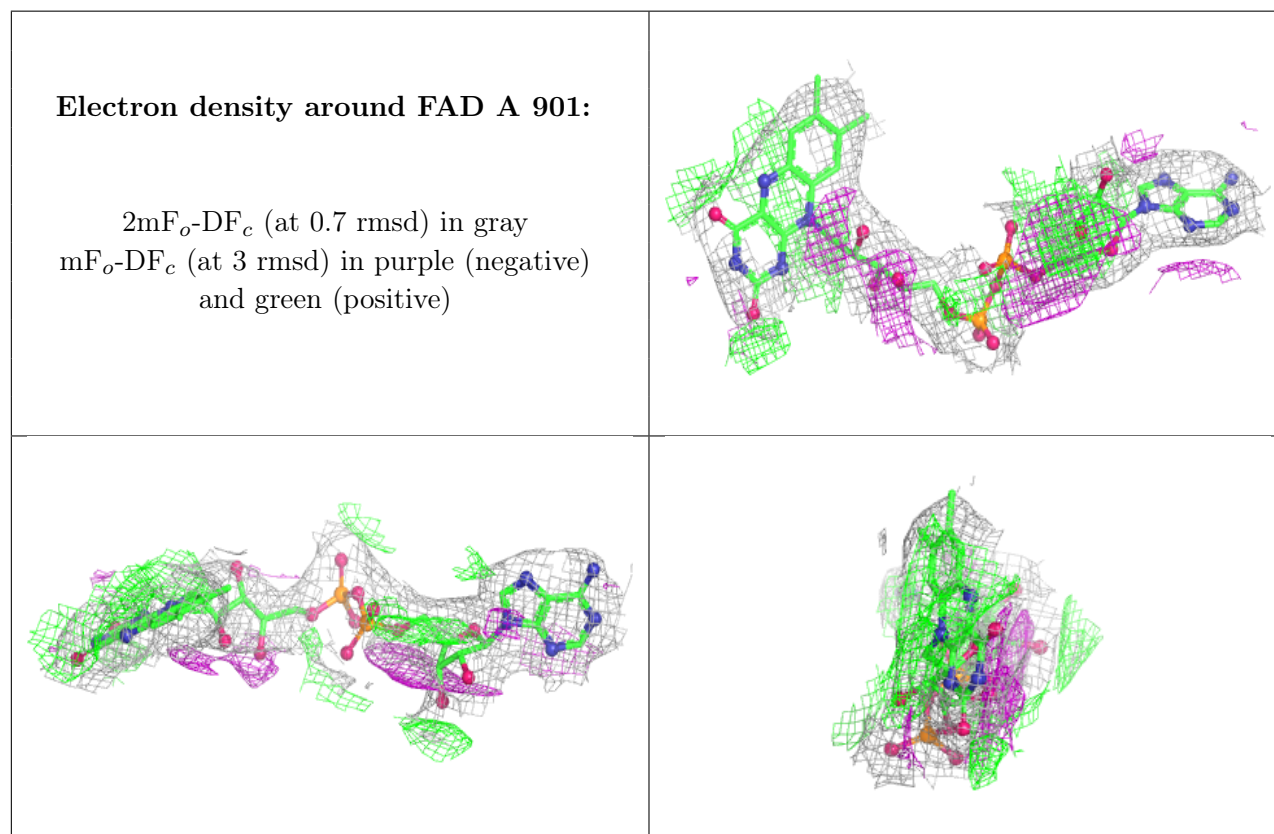
There are no oligosaccharides in this entry.

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	FAD	A	901	53/53	0.90	0.15	66,78,91,93	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.