



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:09 PM UTC

PDB ID : 4UXN / pdb_00004uxn
Title : LSD1(KDM1A)-CoREST in complex with Z-Pro derivative of MC2580
Authors : Rodriguez, V.; Valente, S.; Stazi, G.; Lucidi, A.; Mercurio, C.; Vianello, P.; Ciossani, G.; Mattevi, A.; Botrugno, O.A.; Dessanti, P.; Minucci, S.; Varasi, M.; Mai, A.
Deposited on : 2014-08-27
Resolution : 2.85 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

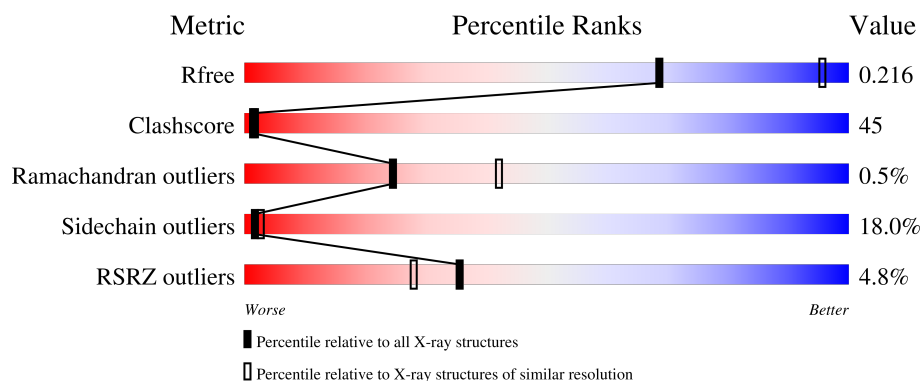
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	 3% 34% 34% 10% 22%
2	B	482	 2% 9% 13% 5% 72%

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	M8A	A	901	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6374 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.

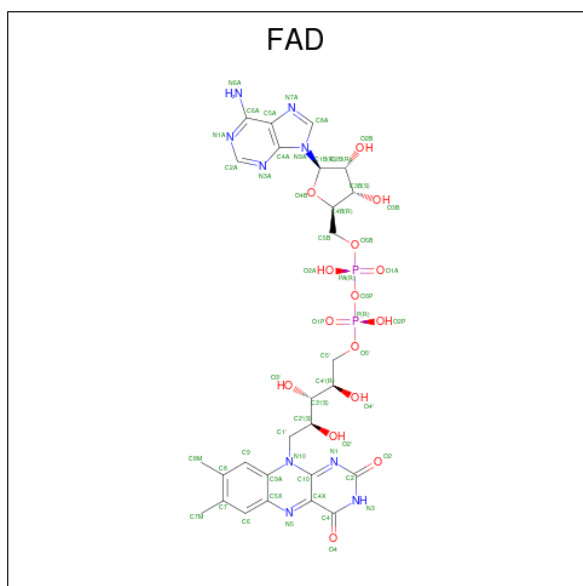
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

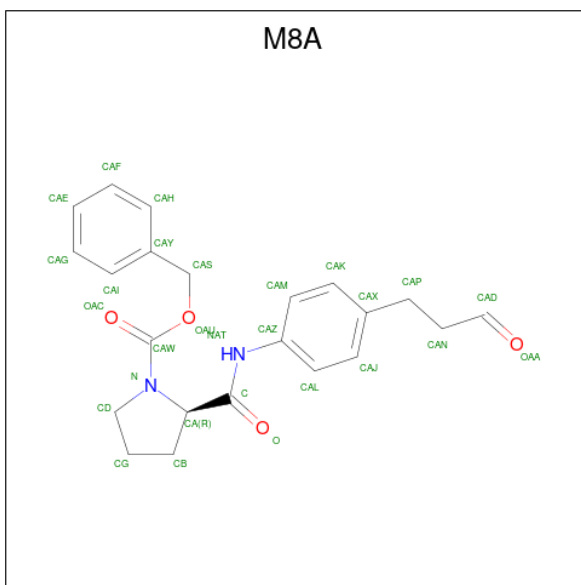
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- 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 benzyl (2R)-2-{[4-(3-oxopropyl)phenyl]carbamoyl}pyrrolidine-1-carboxylate (CCD ID: M8A) (formula: $C_{22}H_{24}N_2O_4$).

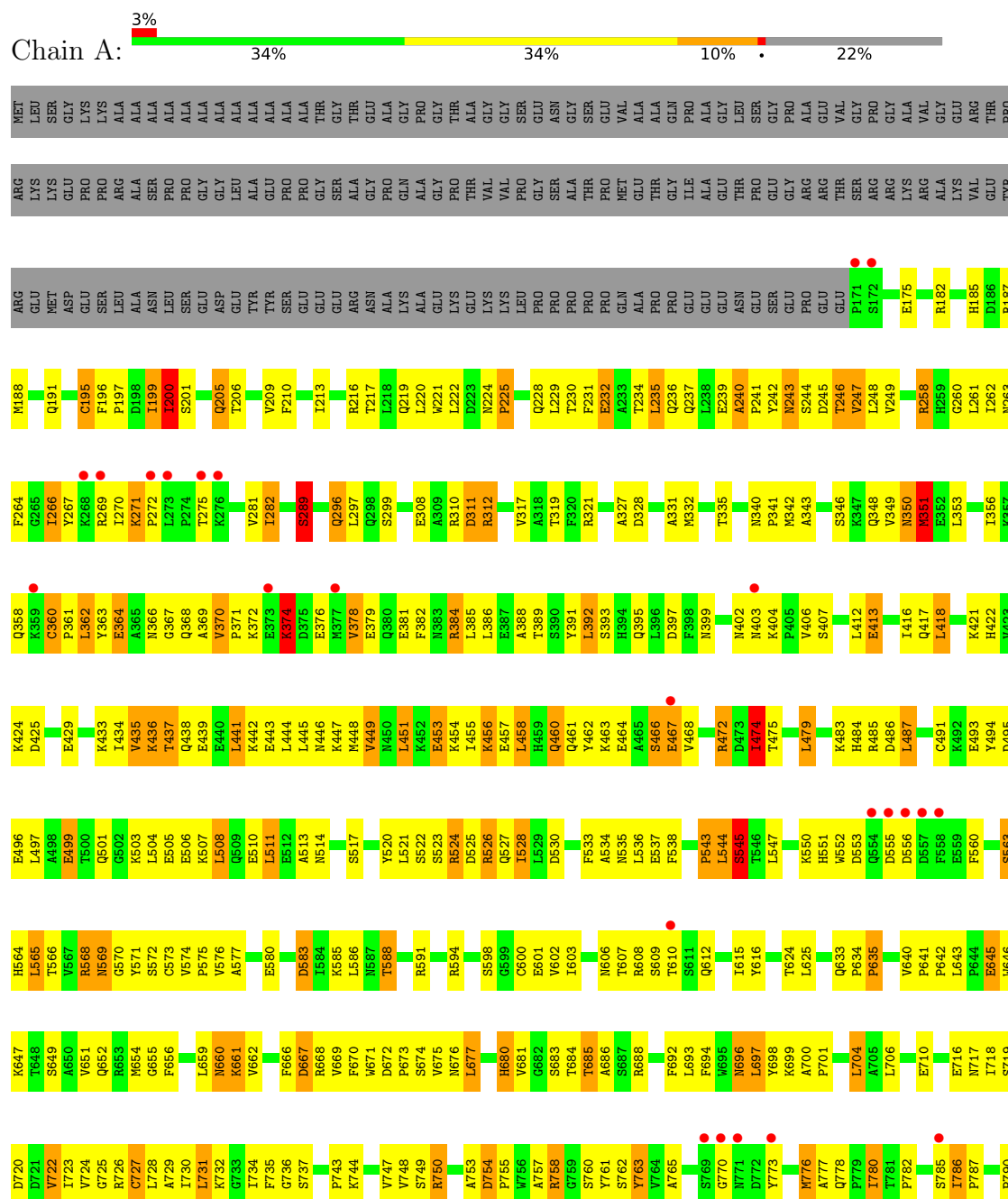


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	2	4		

3 Residue-property plots

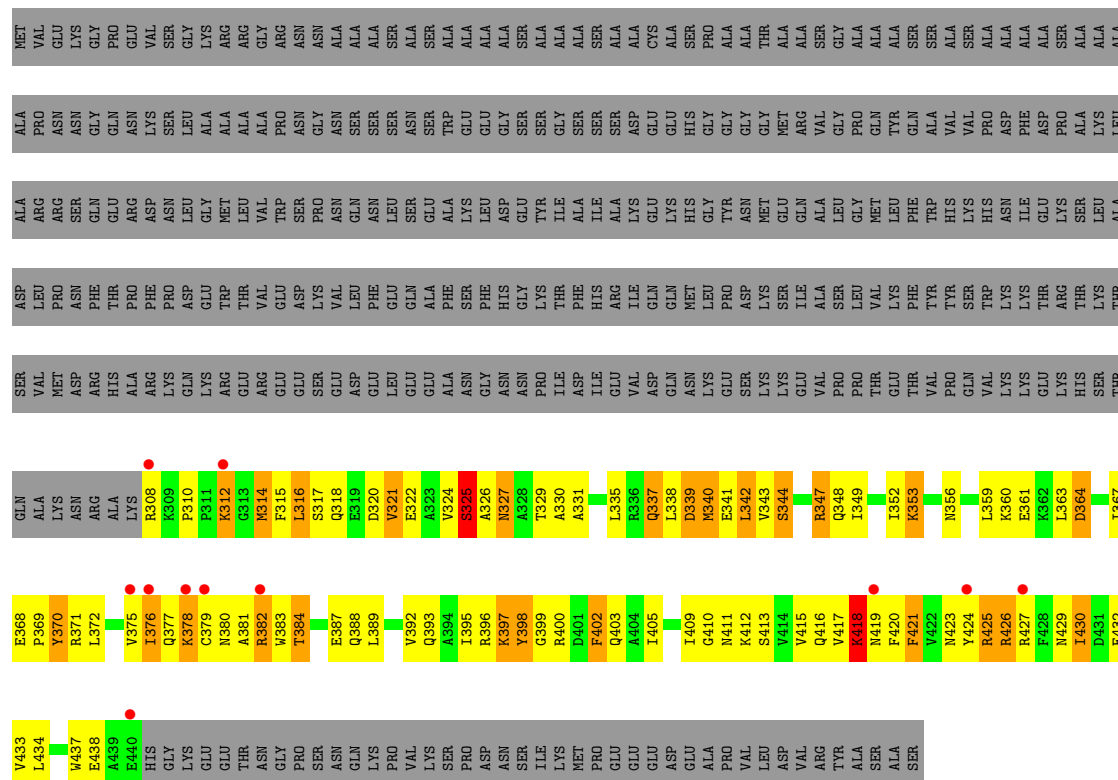
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.98Å 177.76Å 233.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.49 – 2.85 141.49 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (141.49-2.85) 98.9 (141.49-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.215 (Not available) , 0.216	Depositor DCC
R_{free} test set	1103 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, M8A

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	1.48	19/5331 (0.4%)	1.40	46/7232 (0.6%)
2	B	1.16	1/1091 (0.1%)	1.28	7/1471 (0.5%)
All	All	1.43	20/6422 (0.3%)	1.38	53/8703 (0.6%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	GLN	C-O	-7.88	1.14	1.24
1	A	635	PRO	C-O	-6.43	1.15	1.23
1	A	777	ALA	C-O	6.29	1.32	1.24
1	A	790	PRO	N-CA	-6.08	1.39	1.47
1	A	656	PHE	C-O	-6.01	1.17	1.24
1	A	661	LYS	CE-NZ	5.80	1.66	1.49
1	A	565	LEU	CA-C	-5.79	1.45	1.52
1	A	825	ILE	C-O	-5.78	1.17	1.24
1	A	299	SER	C-O	-5.59	1.17	1.24
1	A	794	PRO	N-CA	-5.57	1.41	1.46
1	A	297	LEU	CA-C	-5.46	1.46	1.52
1	A	200	ILE	C-O	-5.35	1.17	1.24
1	A	586	LEU	CA-C	-5.30	1.45	1.53
1	A	348	GLN	C-O	-5.27	1.17	1.24
1	A	545	SER	CA-C	-5.20	1.45	1.52
1	A	576	VAL	CA-CB	-5.13	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	THR	N-CA	-5.06	1.40	1.46
1	A	392	LEU	CA-C	-5.05	1.46	1.52
2	B	397	LYS	CA-C	-5.03	1.46	1.52
1	A	507	LYS	CA-C	5.02	1.59	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	LEU	CA-C-N	9.02	129.07	119.78
1	A	625	LEU	C-N-CA	9.02	129.07	119.78
1	A	474	ILE	N-CA-C	7.78	118.55	110.62
1	A	661	LYS	CD-CE-NZ	7.30	135.26	111.90
1	A	240	ALA	N-CA-C	-7.29	99.71	110.20
1	A	281	VAL	CB-CA-C	-7.20	99.90	110.62
2	B	353	LYS	N-CA-C	-6.91	103.67	111.07
1	A	435	VAL	CB-CA-C	-6.63	103.36	112.04
1	A	360	CYS	CA-C-N	6.58	128.06	119.84
1	A	360	CYS	C-N-CA	6.58	128.06	119.84
1	A	247	VAL	CB-CA-C	-6.37	103.54	112.14
1	A	195	CYS	N-CA-C	6.32	119.15	111.82
1	A	815	LEU	CA-CB-CG	6.25	138.19	116.30
1	A	722	VAL	CB-CA-C	-6.16	104.00	111.88
2	B	418	LYS	N-CA-C	-6.11	104.70	111.36
1	A	791	GLN	N-CA-C	6.05	117.01	109.57
1	A	791	GLN	CA-C-N	-6.01	114.42	120.31
1	A	791	GLN	C-N-CA	-6.01	114.42	120.31
1	A	793	ILE	CA-C-N	-6.00	114.13	120.66
1	A	793	ILE	C-N-CA	-6.00	114.13	120.66
1	A	289	SER	N-CA-C	-5.94	104.50	110.97
1	A	266	ILE	N-CA-C	5.91	115.25	106.85
2	B	398	TYR	N-CA-C	5.80	120.37	112.88
1	A	809	ALA	N-CA-C	5.76	119.61	112.24
1	A	652	GLN	CB-CA-C	-5.75	101.25	110.79
1	A	737	SER	N-CA-C	5.72	118.29	111.71
1	A	551	HIS	N-CA-C	5.70	120.94	113.30
1	A	351	MET	N-CA-C	-5.70	99.89	109.07
1	A	370	VAL	N-CA-C	-5.68	101.26	107.73
1	A	378	VAL	CB-CA-C	-5.67	104.72	111.97
1	A	669	VAL	CB-CA-C	-5.62	103.80	111.33
1	A	201	SER	N-CA-C	-5.57	106.44	113.18
2	B	339	ASP	N-CA-C	-5.56	105.12	111.07
2	B	325	SER	N-CA-C	5.54	117.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ARG	N-CA-C	-5.51	105.27	111.28
1	A	583	ASP	CA-C-N	-5.37	116.11	123.14
1	A	583	ASP	C-N-CA	-5.37	116.11	123.14
1	A	370	VAL	CA-C-N	5.35	126.53	119.84
1	A	370	VAL	C-N-CA	5.35	126.53	119.84
2	B	326	ALA	N-CA-C	5.27	118.50	111.75
1	A	312	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	763	TYR	CA-C-N	-5.20	115.98	122.48
1	A	763	TYR	C-N-CA	-5.20	115.98	122.48
1	A	528	ILE	N-CA-C	-5.19	105.47	110.72
1	A	199	ILE	N-CA-C	5.19	115.40	110.42
1	A	660	ASN	N-CA-C	5.18	117.69	109.50
2	B	392	VAL	CB-CA-C	-5.14	105.31	112.04
1	A	434	ILE	N-CA-C	5.13	115.56	110.23
1	A	374	LYS	N-CA-C	-5.13	105.58	111.07
1	A	754	ASP	CA-C-N	5.11	124.90	119.28
1	A	754	ASP	C-N-CA	5.11	124.90	119.28
1	A	232	GLU	N-CA-C	-5.08	105.44	110.97
1	A	747	VAL	CB-CA-C	-5.04	102.74	110.50

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	5250	431	0
2	B	1076	0	1089	157	0
3	A	53	0	31	20	0
4	A	28	0	23	17	0
All	All	6374	0	6393	569	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 45.

All (569) 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:363:TYR:CD2	1:A:734:ILE:HG23	1.55	1.40
1:A:240:ALA:N	1:A:243:ASN:OD1	1.60	1.33
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.42	1.32
3:A:900:FAD:C10	4:A:901:M8A:HAP1	1.59	1.30
1:A:216:ARG:O	1:A:220:LEU:HD12	1.35	1.25
1:A:437:THR:HG22	1:A:508:LEU:CD2	1.70	1.21
1:A:216:ARG:O	1:A:220:LEU:CD1	1.86	1.20
1:A:437:THR:CG2	1:A:508:LEU:HD21	1.70	1.20
1:A:332:MET:HE1	1:A:704:LEU:HD22	1.25	1.19
2:B:317:SER:O	2:B:321:VAL:HG23	1.37	1.18
1:A:437:THR:CG2	1:A:508:LEU:CD2	2.21	1.17
1:A:363:TYR:CD2	1:A:734:ILE:CG2	2.29	1.16
1:A:491:CYS:O	1:A:495:ASP:OD1	1.61	1.16
1:A:755:PRO:CA	1:A:758:ARG:HH12	1.58	1.16
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.32	1.12
1:A:332:MET:HE1	1:A:704:LEU:CD2	1.80	1.11
1:A:343:ALA:O	1:A:346:SER:OG	1.68	1.10
1:A:720:ASP:O	1:A:724:VAL:HG23	1.51	1.10
2:B:416:GLN:O	2:B:419:ASN:HB3	1.48	1.10
1:A:437:THR:HG21	1:A:508:LEU:HD23	1.33	1.09
1:A:366:ASN:OD1	1:A:368:GLN:N	1.84	1.09
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.32	1.09
1:A:239:GLU:C	1:A:243:ASN:OD1	1.97	1.08
1:A:731:LEU:HA	1:A:734:ILE:HD13	1.32	1.07
3:A:900:FAD:C4X	4:A:901:M8A:HAP1	1.82	1.07
1:A:384:ARG:NH2	2:B:312:LYS:O	1.87	1.07
2:B:340:MET:O	2:B:343:VAL:HG12	1.54	1.06
1:A:240:ALA:CA	1:A:243:ASN:OD1	2.03	1.05
1:A:716:GLU:HG2	1:A:750:ARG:HB3	1.38	1.05
1:A:526:ARG:NH2	1:A:530:ASP:OD1	1.89	1.04
1:A:564:HIS:C	1:A:565:LEU:HD12	1.82	1.04
2:B:416:GLN:C	2:B:419:ASN:HB3	1.81	1.04
3:A:900:FAD:C10	4:A:901:M8A:CAP	2.37	1.01
1:A:537:GLU:HG2	1:A:544:LEU:CD2	1.89	1.01
1:A:786:ILE:HG22	1:A:787:PRO:HD2	1.43	0.99
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.26	0.99
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.60	0.99
1:A:232:GLU:N	1:A:232:GLU:OE1	1.94	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:PRO:HA	1:A:758:ARG:HH12	0.82	0.99
2:B:411:ASN:O	2:B:412:LYS:NZ	1.96	0.99
1:A:289:SER:OG	3:A:900:FAD:O2P	1.80	0.98
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.45	0.97
1:A:693:LEU:HD12	1:A:694:PHE:H	1.26	0.97
2:B:413:SER:N	2:B:416:GLN:OE1	1.97	0.97
1:A:308:GLU:OE2	3:A:900:FAD:O2B	1.83	0.97
2:B:416:GLN:O	2:B:420:PHE:N	1.98	0.96
1:A:758:ARG:HG2	1:A:758:ARG:HH11	1.31	0.96
3:A:900:FAD:C4	4:A:901:M8A:HAP1	1.96	0.95
1:A:220:LEU:HD12	1:A:220:LEU:H	1.30	0.95
2:B:416:GLN:CA	2:B:419:ASN:HB3	1.98	0.94
2:B:416:GLN:HA	2:B:419:ASN:CB	1.98	0.94
1:A:363:TYR:CE2	1:A:734:ILE:CG2	2.51	0.94
1:A:241:PRO:O	1:A:244:SER:HB3	1.68	0.93
1:A:386:LEU:O	1:A:389:THR:OG1	1.85	0.93
1:A:693:LEU:HD12	1:A:694:PHE:N	1.83	0.93
1:A:362:LEU:C	1:A:363:TYR:HD1	1.77	0.93
1:A:719:SER:OG	1:A:722:VAL:HG23	1.69	0.92
2:B:321:VAL:O	2:B:325:SER:OG	1.86	0.92
1:A:363:TYR:HD2	1:A:734:ILE:HG23	0.85	0.92
1:A:731:LEU:HD12	1:A:731:LEU:H	1.35	0.92
1:A:660:ASN:OD1	1:A:749:SER:OG	1.86	0.91
1:A:437:THR:HG22	1:A:508:LEU:HD21	0.91	0.91
1:A:734:ILE:HD12	1:A:734:ILE:H	1.32	0.91
1:A:537:GLU:CG	1:A:544:LEU:HD21	2.00	0.91
2:B:377:GLN:CB	2:B:410:GLY:O	2.19	0.91
1:A:331:ALA:HA	3:A:900:FAD:C4X	2.00	0.91
1:A:263:ASN:C	1:A:267:TYR:CE2	2.50	0.89
1:A:530:ASP:OD2	1:A:685:THR:OG1	1.89	0.89
1:A:441:LEU:HD23	2:B:356:ASN:ND2	1.89	0.88
2:B:368:GLU:N	2:B:369:PRO:HD2	1.88	0.88
2:B:415:VAL:O	2:B:419:ASN:HB2	1.72	0.86
2:B:317:SER:O	2:B:321:VAL:CG2	2.24	0.85
2:B:318:GLN:O	2:B:322:GLU:HG3	1.75	0.85
1:A:496:GLU:O	1:A:499:GLU:HB3	1.77	0.85
2:B:411:ASN:OD1	2:B:412:LYS:NZ	2.09	0.85
1:A:645:GLU:OE1	1:A:649:SER:OG	1.93	0.84
1:A:263:ASN:O	1:A:267:TYR:OH	1.95	0.84
1:A:526:ARG:HH21	1:A:530:ASP:CG	1.84	0.83
2:B:416:GLN:HA	2:B:419:ASN:HB3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ARG:O	1:A:730:ILE:HG13	1.79	0.83
1:A:755:PRO:CA	1:A:758:ARG:NH1	2.29	0.82
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.11	0.81
1:A:716:GLU:CG	1:A:750:ARG:HB3	2.11	0.81
2:B:416:GLN:CA	2:B:419:ASN:CB	2.59	0.81
1:A:684:THR:HG22	1:A:686:ALA:H	1.47	0.80
1:A:533:PHE:CB	1:A:688:ARG:NH1	2.44	0.80
1:A:363:TYR:HD2	1:A:734:ILE:CG2	1.73	0.80
2:B:429:ASN:HB3	2:B:432:GLU:OE1	1.81	0.80
1:A:332:MET:CE	1:A:704:LEU:HD22	2.11	0.80
2:B:347:ARG:HG3	2:B:348:GLN:N	1.95	0.79
2:B:379:CYS:SG	2:B:413:SER:N	2.54	0.79
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.64	0.79
1:A:209:VAL:O	1:A:213:ILE:HG13	1.83	0.79
1:A:213:ILE:O	1:A:217:THR:OG1	2.00	0.79
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.65	0.78
1:A:216:ARG:O	1:A:220:LEU:HD11	1.83	0.78
1:A:728:LEU:HA	1:A:731:LEU:HD13	1.65	0.78
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.48	0.78
1:A:402:ASN:O	1:A:403:ASN:HB2	1.84	0.77
2:B:377:GLN:HB3	2:B:410:GLY:O	1.84	0.76
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.18	0.76
1:A:814:ALA:O	1:A:817:SER:OG	2.02	0.76
3:A:900:FAD:N3	4:A:901:M8A:HAJ	2.01	0.75
1:A:666:PHE:O	1:A:701:PRO:CG	2.34	0.75
2:B:317:SER:HB3	2:B:320:ASP:OD2	1.87	0.75
1:A:731:LEU:CA	1:A:734:ILE:HD13	2.15	0.75
1:A:240:ALA:HA	1:A:243:ASN:OD1	1.86	0.74
2:B:340:MET:CE	2:B:341:GLU:HA	2.17	0.74
1:A:437:THR:CG2	1:A:508:LEU:HD23	1.96	0.74
2:B:416:GLN:HA	2:B:419:ASN:HD22	1.51	0.74
1:A:216:ARG:HG3	1:A:220:LEU:HD11	1.69	0.74
1:A:384:ARG:CZ	2:B:312:LYS:O	2.35	0.74
1:A:340:ASN:OD1	1:A:342:MET:N	2.21	0.74
1:A:800:GLY:O	1:A:803:THR:OG1	2.06	0.74
1:A:680:HIS:HD2	1:A:730:ILE:HG23	1.52	0.74
1:A:392:LEU:N	1:A:392:LEU:HD12	2.03	0.73
1:A:677:LEU:N	1:A:677:LEU:HD23	2.04	0.73
2:B:340:MET:HE3	2:B:341:GLU:HA	1.69	0.73
1:A:346:SER:O	1:A:349:VAL:O	2.07	0.73
1:A:510:GLU:O	1:A:513:ALA:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HA	1:A:220:LEU:HD13	1.70	0.72
1:A:606:ASN:HD22	1:A:609:SER:H	1.37	0.72
1:A:458:LEU:HB3	1:A:487:LEU:HD12	1.72	0.72
1:A:220:LEU:HD12	1:A:220:LEU:N	2.04	0.72
1:A:666:PHE:O	1:A:701:PRO:HG2	1.90	0.72
1:A:188:MET:SD	1:A:200:ILE:HG13	2.30	0.72
2:B:378:LYS:N	2:B:378:LYS:HD2	2.05	0.72
1:A:754:ASP:OD1	1:A:755:PRO:CD	2.36	0.71
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.58	0.71
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.71	0.71
2:B:416:GLN:O	2:B:419:ASN:CB	2.36	0.71
1:A:364:GLU:OE1	1:A:370:VAL:HG22	1.89	0.71
1:A:437:THR:HG21	1:A:508:LEU:CD2	1.98	0.70
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.89	0.70
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.25	0.70
1:A:374:LYS:O	1:A:378:VAL:HG23	1.90	0.70
1:A:565:LEU:HD12	1:A:565:LEU:N	2.06	0.70
1:A:240:ALA:N	1:A:243:ASN:CG	2.50	0.69
1:A:270:ILE:O	1:A:272:PRO:HD3	1.91	0.69
1:A:734:ILE:HD12	1:A:734:ILE:N	2.06	0.69
1:A:786:ILE:CG2	1:A:787:PRO:HD2	2.20	0.69
2:B:415:VAL:O	2:B:419:ASN:N	2.22	0.69
1:A:258:ARG:HD2	1:A:827:ASP:OD1	1.93	0.68
2:B:426:ARG:HG2	2:B:426:ARG:HH11	1.59	0.68
2:B:342:LEU:HD23	2:B:343:VAL:N	2.07	0.68
2:B:382:ARG:HG3	2:B:382:ARG:HH11	1.58	0.68
1:A:332:MET:HE1	1:A:704:LEU:HD21	1.70	0.68
1:A:384:ARG:NH1	2:B:312:LYS:O	2.26	0.68
1:A:392:LEU:HD12	1:A:392:LEU:H	1.56	0.68
1:A:468:VAL:O	1:A:472:ARG:NH1	2.27	0.68
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.26	0.68
4:A:901:M8A:OAU	4:A:901:M8A:NAT	2.24	0.68
2:B:400:ARG:CB	2:B:402:PHE:HE1	2.07	0.67
2:B:426:ARG:HG2	2:B:426:ARG:NH1	2.09	0.67
1:A:220:LEU:CD1	1:A:220:LEU:H	2.06	0.67
1:A:435:VAL:HG23	1:A:436:LYS:N	2.09	0.67
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.10	0.67
1:A:445:LEU:HB2	2:B:359:LEU:HD12	1.77	0.67
1:A:533:PHE:HB3	1:A:688:ARG:NH1	2.08	0.67
1:A:240:ALA:HA	1:A:241:PRO:C	2.20	0.67
2:B:402:PHE:HD2	2:B:418:LYS:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HG13	1:A:263:ASN:HD22	1.60	0.66
1:A:448:MET:HE3	2:B:363:LEU:HD13	1.77	0.66
1:A:685:THR:O	1:A:688:ARG:HG2	1.96	0.66
1:A:464:GLU:O	1:A:467:GLU:HB2	1.96	0.66
2:B:396:ARG:HD2	2:B:396:ARG:O	1.96	0.65
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.78	0.65
4:A:901:M8A:CAW	4:A:901:M8A:HAT	2.08	0.65
2:B:416:GLN:HA	2:B:419:ASN:ND2	2.11	0.65
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.79	0.65
1:A:235:LEU:HD21	1:A:246:THR:CG2	2.25	0.65
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.80	0.64
1:A:522:SER:N	1:A:525:ASP:HB2	2.13	0.64
2:B:399:GLY:N	2:B:437:TRP:NE1	2.45	0.64
1:A:451:LEU:O	1:A:455:ILE:HG13	1.97	0.64
1:A:606:ASN:ND2	1:A:608:ARG:HB2	2.13	0.64
2:B:340:MET:HE2	2:B:341:GLU:N	2.12	0.64
1:A:216:ARG:C	1:A:220:LEU:CD1	2.71	0.64
1:A:413:GLU:O	1:A:417:GLN:HG3	1.96	0.64
1:A:533:PHE:HB2	1:A:688:ARG:NH1	2.12	0.64
1:A:633:GLN:OE1	1:A:634:PRO:HA	1.98	0.64
2:B:337:GLN:O	2:B:341:GLU:HB2	1.96	0.64
2:B:370:TYR:N	2:B:370:TYR:CD1	2.63	0.63
2:B:340:MET:HE2	2:B:341:GLU:CA	2.28	0.63
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.26	0.63
2:B:370:TYR:N	2:B:370:TYR:HD1	1.96	0.63
1:A:258:ARG:CD	1:A:827:ASP:OD1	2.47	0.63
1:A:524:ARG:O	1:A:528:ILE:HD12	1.99	0.63
2:B:377:GLN:HG3	2:B:410:GLY:O	1.97	0.63
1:A:448:MET:HE3	2:B:363:LEU:CD1	2.28	0.63
1:A:462:TYR:O	1:A:466:SER:OG	2.15	0.63
1:A:362:LEU:C	1:A:363:TYR:CD1	2.69	0.62
1:A:666:PHE:O	1:A:701:PRO:HG3	1.97	0.62
2:B:402:PHE:N	2:B:402:PHE:HD1	1.97	0.62
2:B:377:GLN:CG	2:B:410:GLY:O	2.47	0.62
1:A:362:LEU:HD23	1:A:362:LEU:N	2.13	0.62
1:A:372:LYS:O	1:A:376:GLU:HG3	1.99	0.62
1:A:510:GLU:HG2	1:A:511:LEU:HD23	1.81	0.62
1:A:263:ASN:O	1:A:267:TYR:CZ	2.51	0.62
2:B:327:ASN:ND2	2:B:329:THR:H	1.97	0.62
1:A:503:LYS:O	1:A:506:GLU:HG2	2.00	0.62
1:A:755:PRO:HA	1:A:758:ARG:CZ	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:HB	1:A:575:PRO:CD	2.30	0.62
2:B:415:VAL:O	2:B:419:ASN:CB	2.46	0.61
2:B:413:SER:OG	2:B:415:VAL:HG13	2.00	0.61
1:A:563:SER:O	1:A:565:LEU:CD1	2.48	0.61
1:A:667:ASP:OD1	1:A:667:ASP:N	2.24	0.61
2:B:376:ILE:HD12	2:B:376:ILE:H	1.65	0.61
2:B:399:GLY:CA	2:B:437:TRP:CE2	2.83	0.61
2:B:416:GLN:C	2:B:419:ASN:CB	2.65	0.61
1:A:553:ASP:O	1:A:556:ASP:HB2	2.00	0.61
1:A:661:LYS:NZ	4:A:901:M8A:OAA	2.31	0.61
1:A:731:LEU:HD12	1:A:731:LEU:N	2.13	0.61
2:B:340:MET:CE	2:B:341:GLU:CA	2.79	0.61
2:B:377:GLN:OE1	2:B:377:GLN:HA	2.00	0.61
1:A:522:SER:OG	1:A:525:ASP:N	2.31	0.61
1:A:555:ASP:OD2	4:A:901:M8A:HB2C	2.01	0.61
2:B:400:ARG:HB3	2:B:402:PHE:HE1	1.64	0.61
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.36	0.60
1:A:786:ILE:HG22	1:A:787:PRO:CD	2.24	0.60
2:B:402:PHE:N	2:B:402:PHE:CD1	2.68	0.60
1:A:361:PRO:C	1:A:362:LEU:HD23	2.27	0.60
1:A:535:ASN:HD22	1:A:692:PHE:HE2	1.48	0.60
2:B:415:VAL:C	2:B:419:ASN:HB2	2.25	0.60
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.83	0.60
1:A:263:ASN:C	1:A:267:TYR:HE2	2.07	0.60
1:A:675:VAL:O	1:A:696:ASN:ND2	2.34	0.60
1:A:247:VAL:HG23	1:A:248:LEU:N	2.17	0.60
1:A:731:LEU:HA	1:A:734:ILE:CD1	2.20	0.59
1:A:732:LYS:O	1:A:736:GLY:N	2.34	0.59
2:B:368:GLU:OE1	2:B:371:ARG:HG3	2.01	0.59
1:A:243:ASN:OD1	1:A:243:ASN:N	2.34	0.59
1:A:670:PHE:HD1	1:A:670:PHE:O	1.85	0.59
1:A:350:ASN:O	1:A:350:ASN:ND2	2.35	0.59
1:A:533:PHE:HB2	1:A:688:ARG:HH11	1.66	0.58
2:B:376:ILE:HD12	2:B:376:ILE:N	2.19	0.58
2:B:382:ARG:HG3	2:B:382:ARG:NH1	2.15	0.58
2:B:425:ARG:NH1	2:B:425:ARG:HG3	2.18	0.58
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.85	0.58
1:A:308:GLU:OE2	3:A:900:FAD:O3B	2.21	0.58
1:A:392:LEU:H	1:A:392:LEU:CD1	2.16	0.58
1:A:493:GLU:O	1:A:497:LEU:HD13	2.03	0.58
1:A:263:ASN:O	1:A:267:TYR:CE2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:HG3	2:B:352:ILE:CD1	2.34	0.58
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.36	0.58
2:B:368:GLU:N	2:B:369:PRO:CD	2.63	0.58
2:B:405:ILE:O	2:B:409:ILE:HG13	2.04	0.58
1:A:449:VAL:HG23	2:B:363:LEU:HG	1.85	0.58
1:A:526:ARG:NH2	1:A:530:ASP:CG	2.53	0.58
1:A:758:ARG:NH1	1:A:758:ARG:HG2	2.05	0.58
1:A:666:PHE:CE1	1:A:743:PRO:HB3	2.39	0.57
1:A:807:TYR:N	1:A:808:PRO:CD	2.67	0.57
2:B:396:ARG:O	2:B:437:TRP:HD1	1.87	0.57
2:B:402:PHE:CE2	2:B:418:LYS:HD2	2.39	0.57
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.38	0.57
1:A:641:PRO:HB2	1:A:642:PRO:CD	2.35	0.57
1:A:537:GLU:HG2	1:A:544:LEU:HD23	1.78	0.57
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.87	0.57
1:A:311:ASP:OD1	1:A:311:ASP:N	2.30	0.57
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.21	0.57
1:A:801:GLU:HG2	1:A:809:ALA:H	1.69	0.57
1:A:262:ILE:HG13	1:A:263:ASN:ND2	2.20	0.57
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.40	0.57
2:B:399:GLY:HA3	2:B:437:TRP:CE2	2.39	0.57
1:A:574:VAL:HB	1:A:575:PRO:HD2	1.87	0.56
1:A:750:ARG:O	1:A:753:ALA:HB3	2.05	0.56
1:A:680:HIS:CD2	1:A:730:ILE:HD13	2.40	0.56
1:A:731:LEU:H	1:A:731:LEU:CD1	2.14	0.56
1:A:319:THR:HG21	1:A:570:GLY:HA3	1.88	0.56
1:A:569:ASN:OD1	1:A:569:ASN:N	2.32	0.56
2:B:425:ARG:HG3	2:B:425:ARG:HH11	1.71	0.56
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.88	0.56
1:A:379:GLU:O	1:A:382:PHE:HB3	2.06	0.56
1:A:755:PRO:N	1:A:758:ARG:HH12	2.01	0.56
1:A:308:GLU:CD	3:A:900:FAD:O3B	2.50	0.55
2:B:327:ASN:OD1	2:B:330:ALA:HB2	2.07	0.55
1:A:670:PHE:CD1	1:A:670:PHE:C	2.84	0.55
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.89	0.55
3:A:900:FAD:C4	4:A:901:M8A:HAJ	2.37	0.55
2:B:400:ARG:CA	2:B:402:PHE:HE1	2.20	0.55
1:A:801:GLU:CG	1:A:809:ALA:HA	2.34	0.55
2:B:344:SER:O	2:B:347:ARG:HG2	2.07	0.55
2:B:367:ILE:C	2:B:369:PRO:HD2	2.32	0.55
2:B:402:PHE:CD2	2:B:418:LYS:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:900:FAD:C4	4:A:901:M8A:CAP	2.80	0.54
1:A:407:SER:CB	1:A:545:SER:O	2.56	0.54
1:A:335:THR:HG21	4:A:901:M8A:HAL	1.89	0.54
1:A:495:ASP:OD2	2:B:371:ARG:NH2	2.39	0.54
2:B:399:GLY:HA3	2:B:437:TRP:CZ2	2.42	0.54
2:B:399:GLY:H	2:B:437:TRP:CD1	2.26	0.54
1:A:684:THR:HG22	1:A:686:ALA:N	2.20	0.54
1:A:363:TYR:CD2	1:A:734:ILE:HG21	2.33	0.54
1:A:544:LEU:HD23	1:A:544:LEU:N	2.23	0.54
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.72	0.54
1:A:647:LYS:O	1:A:651:VAL:HG23	2.08	0.54
1:A:241:PRO:O	1:A:244:SER:CB	2.51	0.54
1:A:680:HIS:ND1	1:A:680:HIS:C	2.65	0.54
1:A:366:ASN:HD21	1:A:368:GLN:HB2	1.72	0.53
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.72	0.53
2:B:342:LEU:HD23	2:B:342:LEU:C	2.34	0.53
2:B:389:LEU:O	2:B:393:GLN:HG3	2.08	0.53
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.44	0.53
1:A:235:LEU:CD2	1:A:246:THR:HG22	2.35	0.53
1:A:381:GLU:OE2	1:A:520:TYR:OH	2.21	0.53
3:A:900:FAD:O4	4:A:901:M8A:CAD	2.56	0.53
2:B:419:ASN:O	2:B:423:ASN:HB2	2.08	0.53
1:A:245:ASP:OD1	1:A:247:VAL:HG22	2.08	0.53
1:A:501:GLN:O	1:A:505:GLU:HG3	2.08	0.53
2:B:417:VAL:O	2:B:420:PHE:HB3	2.08	0.53
1:A:196:PHE:N	1:A:197:PRO:CD	2.71	0.53
1:A:399:ASN:O	1:A:406:VAL:HG23	2.09	0.53
1:A:750:ARG:HH11	1:A:750:ARG:CG	2.22	0.52
2:B:315:PHE:CD1	2:B:315:PHE:N	2.77	0.52
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.09	0.52
1:A:363:TYR:HD1	1:A:363:TYR:N	2.05	0.52
1:A:445:LEU:CB	2:B:359:LEU:HD12	2.39	0.52
1:A:319:THR:HB	1:A:572:SER:HB3	1.91	0.52
1:A:447:LYS:HD3	1:A:497:LEU:HD21	1.90	0.52
1:A:448:MET:CE	2:B:363:LEU:HD13	2.40	0.52
1:A:435:VAL:CG2	1:A:436:LYS:N	2.73	0.52
2:B:430:ILE:HG22	2:B:434:LEU:CD1	2.38	0.52
1:A:363:TYR:CD1	1:A:363:TYR:N	2.75	0.52
1:A:439:GLU:HG3	2:B:352:ILE:HD13	1.92	0.52
1:A:510:GLU:O	1:A:513:ALA:CB	2.58	0.52
1:A:510:GLU:O	1:A:513:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:ASN:CB	2:B:432:GLU:OE1	2.56	0.52
1:A:422:HIS:CE1	2:B:315:PHE:CZ	2.98	0.52
1:A:677:LEU:N	1:A:677:LEU:CD2	2.73	0.52
1:A:734:ILE:H	1:A:734:ILE:CD1	2.12	0.52
1:A:563:SER:O	1:A:565:LEU:HD11	2.10	0.52
1:A:641:PRO:HB2	1:A:642:PRO:HD2	1.91	0.51
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.40	0.51
1:A:534:ALA:HB2	1:A:688:ARG:HB2	1.91	0.51
1:A:388:ALA:O	1:A:392:LEU:CD1	2.59	0.51
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.92	0.51
2:B:369:PRO:HG2	2:B:370:TYR:CD1	2.46	0.51
1:A:566:THR:CG2	1:A:697:LEU:HD22	2.30	0.51
1:A:388:ALA:O	1:A:391:TYR:HB3	2.11	0.51
1:A:391:TYR:CE1	1:A:395:GLN:HG3	2.45	0.51
1:A:491:CYS:C	1:A:495:ASP:OD1	2.48	0.51
2:B:324:VAL:HG13	2:B:331:ALA:HA	1.93	0.51
2:B:377:GLN:HB2	2:B:410:GLY:O	2.08	0.51
2:B:384:THR:HG1	2:B:387:GLU:CD	2.19	0.51
1:A:448:MET:CB	2:B:363:LEU:HD11	2.41	0.50
1:A:716:GLU:CD	1:A:750:ARG:HB3	2.36	0.50
1:A:230:THR:O	1:A:234:THR:OG1	2.26	0.50
1:A:308:GLU:HG3	1:A:310:ARG:H	1.76	0.50
1:A:633:GLN:OE1	1:A:635:PRO:HD3	2.11	0.50
2:B:416:GLN:CA	2:B:419:ASN:HB2	2.41	0.50
1:A:349:VAL:HG12	1:A:350:ASN:N	2.26	0.50
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.93	0.50
1:A:460:GLN:HE21	1:A:460:GLN:CA	2.25	0.50
2:B:402:PHE:HD1	2:B:402:PHE:H	1.59	0.50
2:B:384:THR:O	2:B:388:GLN:HG3	2.12	0.50
2:B:400:ARG:HB3	2:B:402:PHE:CE1	2.44	0.50
1:A:221:TRP:O	1:A:224:ASN:O	2.29	0.49
1:A:479:LEU:O	1:A:483:LYS:HB2	2.12	0.49
1:A:666:PHE:CD1	1:A:743:PRO:HA	2.46	0.49
1:A:804:ILE:O	1:A:808:PRO:HD3	2.11	0.49
1:A:385:LEU:O	1:A:388:ALA:HB3	2.10	0.49
1:A:750:ARG:HH11	1:A:750:ARG:HG3	1.77	0.49
3:A:900:FAD:C2	4:A:901:M8A:HAJ	2.43	0.49
1:A:574:VAL:CB	1:A:575:PRO:CD	2.90	0.49
1:A:231:PHE:HE1	1:A:249:VAL:CG1	2.26	0.49
1:A:728:LEU:O	1:A:729:ALA:C	2.55	0.49
1:A:264:PHE:CD1	1:A:264:PHE:C	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ARG:O	2:B:402:PHE:N	2.46	0.49
1:A:366:ASN:OD1	1:A:367:GLY:N	2.46	0.49
1:A:363:TYR:HE2	1:A:734:ILE:CG2	2.20	0.49
2:B:327:ASN:ND2	2:B:329:THR:OG1	2.45	0.49
1:A:321:ARG:NH2	1:A:569:ASN:O	2.46	0.49
1:A:399:ASN:C	1:A:406:VAL:HG23	2.37	0.49
1:A:670:PHE:O	1:A:670:PHE:CD1	2.65	0.49
1:A:724:VAL:O	1:A:727:CYS:HB2	2.13	0.49
1:A:817:SER:O	1:A:820:ARG:HB3	2.13	0.49
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.90	0.49
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.48	0.48
2:B:413:SER:OG	2:B:415:VAL:CG1	2.61	0.48
1:A:364:GLU:OE2	1:A:524:ARG:NE	2.46	0.48
1:A:460:GLN:CA	1:A:460:GLN:NE2	2.76	0.48
1:A:728:LEU:CA	1:A:731:LEU:HD13	2.40	0.48
1:A:806:ASN:C	1:A:807:TYR:CD1	2.92	0.48
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.48	0.48
1:A:660:ASN:OD1	1:A:749:SER:C	2.57	0.48
1:A:641:PRO:CB	1:A:642:PRO:CD	2.91	0.48
1:A:346:SER:HA	1:A:351:MET:SD	2.54	0.48
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.95	0.48
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.49	0.48
3:A:900:FAD:C10	4:A:901:M8A:HAP2	2.36	0.48
2:B:315:PHE:C	2:B:316:LEU:HG	2.38	0.47
1:A:222:LEU:O	1:A:225:PRO:HD3	2.14	0.47
1:A:448:MET:CE	2:B:363:LEU:CD1	2.91	0.47
1:A:761:TYR:CZ	4:A:901:M8A:HAK	2.49	0.47
1:A:296:GLN:HA	1:A:296:GLN:OE1	2.13	0.47
1:A:310:ARG:NH1	1:A:754:ASP:OD2	2.25	0.47
1:A:392:LEU:N	1:A:392:LEU:CD1	2.72	0.47
1:A:445:LEU:O	1:A:446:ASN:C	2.57	0.47
2:B:402:PHE:CD2	2:B:418:LYS:HG2	2.43	0.47
2:B:361:GLU:O	2:B:364:ASP:HB3	2.14	0.47
1:A:308:GLU:OE1	3:A:900:FAD:O3B	2.32	0.47
1:A:565:LEU:N	1:A:565:LEU:CD1	2.76	0.47
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.96	0.47
1:A:782:PRO:HG3	1:A:795:ARG:HG3	1.95	0.47
1:A:195:CYS:HB2	1:A:196:PHE:CD1	2.49	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.47
1:A:572:SER:O	1:A:573:CYS:C	2.54	0.47
1:A:758:ARG:NH1	1:A:758:ARG:CG	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:O	1:A:600:CYS:HB3	2.15	0.47
1:A:594:ARG:HA	1:A:640:VAL:O	2.15	0.47
1:A:520:TYR:CD2	1:A:521:LEU:HG	2.50	0.47
1:A:729:ALA:O	1:A:730:ILE:C	2.58	0.47
1:A:435:VAL:CG1	2:B:349:ILE:HG12	2.45	0.47
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.83	0.47
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.62	0.47
1:A:601:GLU:HA	1:A:616:TYR:O	2.15	0.46
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.46
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.50	0.46
1:A:524:ARG:HH11	1:A:524:ARG:CG	2.29	0.46
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.45	0.46
1:A:677:LEU:HD23	1:A:677:LEU:H	1.77	0.46
2:B:399:GLY:N	2:B:437:TRP:CD1	2.84	0.46
2:B:369:PRO:C	2:B:370:TYR:HD1	2.22	0.46
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.80	0.46
1:A:389:THR:HA	1:A:392:LEU:HD13	1.96	0.46
1:A:513:ALA:C	1:A:514:ASN:OD1	2.59	0.46
1:A:786:ILE:CG2	1:A:787:PRO:CD	2.91	0.46
1:A:366:ASN:OD1	1:A:368:GLN:CB	2.63	0.46
1:A:524:ARG:NH1	1:A:524:ARG:HG2	2.31	0.46
1:A:725:GLY:O	1:A:726:ARG:C	2.59	0.46
1:A:358:GLN:OE1	1:A:358:GLN:HA	2.16	0.46
1:A:701:PRO:HG2	1:A:701:PRO:O	2.16	0.46
1:A:393:SER:O	1:A:397:ASP:HA	2.15	0.46
1:A:460:GLN:HE21	1:A:460:GLN:C	2.24	0.46
1:A:834:TYR:CD1	1:A:835:THR:HG22	2.51	0.46
1:A:216:ARG:O	1:A:219:GLN:HB3	2.16	0.45
1:A:340:ASN:HA	1:A:341:PRO:HD2	1.80	0.45
1:A:513:ALA:CB	1:A:514:ASN:OD1	2.65	0.45
1:A:568:ARG:HG2	1:A:699:LYS:HZ3	1.81	0.45
2:B:379:CYS:SG	2:B:412:LYS:C	2.99	0.45
2:B:416:GLN:HA	2:B:419:ASN:CG	2.39	0.45
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.64	0.45
2:B:314:MET:HE2	2:B:314:MET:HA	1.97	0.45
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.17	0.45
1:A:564:HIS:CA	1:A:565:LEU:HD12	2.46	0.45
2:B:312:LYS:HD2	2:B:312:LYS:HA	1.69	0.45
2:B:400:ARG:CA	2:B:402:PHE:CE1	2.99	0.45
1:A:677:LEU:HB2	1:A:693:LEU:HD11	1.98	0.45
1:A:763:TYR:CD1	1:A:763:TYR:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.51	0.45
1:A:258:ARG:HD3	1:A:827:ASP:OD1	2.17	0.45
1:A:260:GLY:O	1:A:264:PHE:CD2	2.70	0.45
1:A:269:ARG:HG2	1:A:271:LYS:O	2.16	0.45
1:A:474:ILE:HG23	1:A:475:THR:N	2.32	0.45
1:A:524:ARG:HH11	1:A:524:ARG:HG2	1.81	0.45
1:A:719:SER:HG	1:A:722:VAL:HG23	1.74	0.45
1:A:217:THR:HG23	1:A:234:THR:HG21	1.99	0.44
1:A:754:ASP:HA	1:A:755:PRO:HD3	1.82	0.44
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.71	0.44
1:A:317:VAL:HG13	1:A:571:TYR:HB3	1.98	0.44
1:A:442:LYS:HB2	2:B:356:ASN:OD1	2.17	0.44
1:A:717:ASN:O	1:A:718:ILE:HG13	2.16	0.44
1:A:217:THR:HG23	1:A:234:THR:CG2	2.47	0.44
1:A:351:MET:HA	1:A:569:ASN:HD21	1.83	0.44
2:B:368:GLU:OE1	2:B:368:GLU:HA	2.16	0.44
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.71	0.44
1:A:205:GLN:O	1:A:209:VAL:HG23	2.18	0.44
1:A:228:GLN:HA	1:A:263:ASN:OD1	2.17	0.44
1:A:457:GLU:O	1:A:461:GLN:HG3	2.18	0.44
1:A:645:GLU:O	1:A:646:TRP:C	2.58	0.44
2:B:378:LYS:O	2:B:411:ASN:HB2	2.17	0.44
2:B:397:LYS:HD3	2:B:398:TYR:CZ	2.52	0.44
1:A:441:LEU:CD2	2:B:356:ASN:HD22	2.14	0.44
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.82	0.44
1:A:216:ARG:C	1:A:220:LEU:HD11	2.40	0.44
1:A:366:ASN:ND2	1:A:368:GLN:HB2	2.32	0.44
1:A:444:LEU:HD23	1:A:501:GLN:HB2	2.00	0.44
1:A:460:GLN:NE2	1:A:460:GLN:HA	2.32	0.44
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.99	0.44
1:A:750:ARG:CG	1:A:750:ARG:NH1	2.78	0.44
1:A:350:ASN:ND2	1:A:350:ASN:C	2.75	0.44
1:A:676:ASN:HB2	1:A:677:LEU:CD2	2.48	0.44
2:B:327:ASN:HD22	2:B:329:THR:H	1.64	0.44
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.53	0.43
1:A:372:LYS:O	1:A:376:GLU:CG	2.65	0.43
1:A:425:ASP:OD1	2:B:338:LEU:CD1	2.66	0.43
1:A:308:GLU:OE2	3:A:900:FAD:H1B	2.18	0.43
2:B:389:LEU:HD23	2:B:389:LEU:HA	1.87	0.43
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.48	0.43
1:A:776:MET:HE3	1:A:776:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASN:OD1	2:B:381:ALA:N	2.51	0.43
2:B:426:ARG:CD	2:B:426:ARG:H	2.31	0.43
1:A:445:LEU:O	1:A:449:VAL:N	2.46	0.43
1:A:448:MET:HG2	1:A:497:LEU:HD23	2.01	0.43
1:A:484:HIS:HD2	2:B:372:LEU:HD13	1.81	0.43
1:A:195:CYS:C	1:A:197:PRO:HD3	2.44	0.43
1:A:229:LEU:N	1:A:263:ASN:OD1	2.41	0.43
1:A:523:SER:O	1:A:527:GLN:HG3	2.18	0.43
1:A:308:GLU:OE2	3:A:900:FAD:C2B	2.65	0.43
1:A:456:LYS:CG	2:B:370:TYR:HE2	2.32	0.43
1:A:536:LEU:HD23	1:A:544:LEU:HD13	1.99	0.43
3:A:900:FAD:HM71	3:A:900:FAD:HM83	1.80	0.43
1:A:205:GLN:C	1:A:205:GLN:NE2	2.77	0.43
1:A:603:ILE:HG12	1:A:615:ILE:CD1	2.49	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.74	0.42
1:A:455:ILE:O	1:A:456:LYS:C	2.62	0.42
1:A:522:SER:O	1:A:525:ASP:HB2	2.20	0.42
1:A:760:SER:HA	3:A:900:FAD:HM81	2.01	0.42
1:A:188:MET:HE3	1:A:210:PHE:CD2	2.55	0.42
1:A:513:ALA:HB3	1:A:514:ASN:OD1	2.20	0.42
1:A:538:PHE:CD1	1:A:706:LEU:HD23	2.53	0.42
1:A:381:GLU:O	1:A:385:LEU:N	2.47	0.42
1:A:655:GLY:O	1:A:762:SER:HA	2.19	0.42
1:A:671:TRP:O	1:A:673:PRO:HD3	2.18	0.42
1:A:332:MET:CE	1:A:704:LEU:CD2	2.72	0.42
1:A:362:LEU:O	1:A:363:TYR:HD1	1.99	0.42
1:A:407:SER:HB3	1:A:545:SER:O	2.20	0.42
2:B:437:TRP:CE3	2:B:437:TRP:C	2.97	0.42
1:A:199:ILE:CD1	1:A:248:LEU:HD11	2.49	0.42
1:A:327:ALA:HA	1:A:698:TYR:CE2	2.55	0.42
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.78	0.42
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.49	0.42
1:A:319:THR:OG1	1:A:328:ASP:OD1	2.30	0.42
1:A:424:LYS:O	1:A:425:ASP:C	2.62	0.42
1:A:232:GLU:N	1:A:232:GLU:CD	2.73	0.42
1:A:205:GLN:O	1:A:205:GLN:NE2	2.53	0.42
1:A:718:ILE:HG22	1:A:723:ILE:CG1	2.48	0.42
1:A:672:ASP:OD1	1:A:674:SER:N	2.51	0.42
1:A:716:GLU:HG2	1:A:750:ARG:CB	2.29	0.42
1:A:514:ASN:OD1	1:A:514:ASN:N	2.51	0.41
1:A:537:GLU:HG3	1:A:544:LEU:HD21	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TRP:O	1:A:224:ASN:C	2.63	0.41
1:A:503:LYS:HE3	1:A:503:LYS:HB2	1.82	0.41
1:A:719:SER:O	1:A:723:ILE:HG13	2.20	0.41
1:A:808:PRO:O	1:A:810:THR:HG23	2.21	0.41
1:A:195:CYS:C	1:A:197:PRO:CD	2.93	0.41
1:A:360:CYS:HA	1:A:361:PRO:HD2	1.67	0.41
1:A:392:LEU:HD11	2:B:316:LEU:HD22	2.02	0.41
1:A:676:ASN:HB2	1:A:677:LEU:HD23	2.00	0.41
2:B:413:SER:O	2:B:416:GLN:HB2	2.19	0.41
1:A:366:ASN:OD1	1:A:366:ASN:C	2.63	0.41
1:A:594:ARG:HG2	1:A:640:VAL:HB	2.03	0.41
1:A:684:THR:HG22	1:A:685:THR:N	2.36	0.41
1:A:757:ALA:O	1:A:758:ARG:HB2	2.20	0.41
1:A:412:LEU:O	1:A:416:ILE:HG13	2.21	0.41
1:A:770:GLY:O	1:A:773:TYR:HB2	2.20	0.41
2:B:318:GLN:HG3	2:B:322:GLU:OE2	2.20	0.41
2:B:347:ARG:HG3	2:B:348:GLN:H	1.82	0.41
2:B:344:SER:O	2:B:347:ARG:CG	2.68	0.41
1:A:654:MET:HB3	1:A:654:MET:HE2	1.38	0.41
1:A:793:ILE:N	1:A:793:ILE:HD12	2.36	0.41
1:A:609:SER:O	1:A:609:SER:OG	2.39	0.41
1:A:247:VAL:CG2	1:A:248:LEU:N	2.83	0.41
1:A:308:GLU:HG3	1:A:310:ARG:N	2.36	0.41
1:A:494:TYR:CD1	1:A:494:TYR:C	2.98	0.41
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.02	0.41
1:A:804:ILE:HD13	1:A:804:ILE:HG21	1.90	0.41
1:A:832:ALA:HB1	1:A:834:TYR:CE2	2.56	0.41
1:A:282:ILE:HA	1:A:282:ILE:HD13	1.70	0.41
1:A:728:LEU:CA	1:A:731:LEU:CD1	2.98	0.41
1:A:467:GLU:OE1	1:A:467:GLU:CA	2.69	0.40
1:A:543:PRO:HG3	1:A:710:GLU:HG2	2.02	0.40
1:A:564:HIS:CE1	4:A:901:M8A:HAI	2.56	0.40
1:A:754:ASP:O	1:A:758:ARG:NH1	2.54	0.40
2:B:331:ALA:O	2:B:335:LEU:HG	2.21	0.40
1:A:364:GLU:HA	1:A:681:VAL:HB	2.03	0.40
1:A:388:ALA:O	1:A:392:LEU:HD12	2.20	0.40
1:A:537:GLU:CG	1:A:544:LEU:CD2	2.73	0.40
1:A:312:ARG:HH11	1:A:312:ARG:HD2	1.68	0.40
1:A:794:PRO:HD3	1:A:828:GLN:NE2	2.37	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%)	639 (96%)	21 (3%)	4 (1%)	21	38
2	B	131/482 (27%)	128 (98%)	3 (2%)	0	100	100
All	All	795/1334 (60%)	767 (96%)	24 (3%)	4 (0%)	24	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	ILE
1	A	831	GLY
1	A	369	ALA
1	A	225	PRO

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%)	472 (83%)	94 (17%)	2	4
2	B	117/395 (30%)	88 (75%)	29 (25%)	1	0
All	All	683/1094 (62%)	560 (82%)	123 (18%)	2	3

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	200	ILE
1	A	205	GLN
1	A	206	THR
1	A	235	LEU
1	A	236	GLN
1	A	237	GLN
1	A	243	ASN
1	A	246	THR
1	A	258	ARG
1	A	271	LYS
1	A	275	THR
1	A	282	ILE
1	A	289	SER
1	A	296	GLN
1	A	311	ASP
1	A	350	ASN
1	A	351	MET
1	A	362	LEU
1	A	364	GLU
1	A	374	LYS
1	A	404	LYS
1	A	413	GLU
1	A	418	LEU
1	A	429	GLU
1	A	433	LYS
1	A	436	LYS
1	A	437	THR
1	A	438	GLN
1	A	441	LEU
1	A	443	GLU
1	A	449	VAL
1	A	451	LEU
1	A	453	GLU
1	A	454	LYS
1	A	456	LYS
1	A	458	LEU
1	A	460	GLN
1	A	463	LYS
1	A	466	SER
1	A	467	GLU
1	A	472	ARG
1	A	474	ILE

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Mol	Chain	Res	Type
1	A	479	LEU
1	A	485	ARG
1	A	487	LEU
1	A	499	GLU
1	A	504	LEU
1	A	508	LEU
1	A	511	LEU
1	A	517	SER
1	A	524	ARG
1	A	526	ARG
1	A	543	PRO
1	A	544	LEU
1	A	545	SER
1	A	550	LYS
1	A	563	SER
1	A	568	ARG
1	A	569	ASN
1	A	580	GLU
1	A	588	THR
1	A	591	ARG
1	A	598	SER
1	A	607	THR
1	A	610	THR
1	A	612	GLN
1	A	624	THR
1	A	645	GLU
1	A	659	LEU
1	A	667	ASP
1	A	668	ARG
1	A	677	LEU
1	A	680	HIS
1	A	683	SER
1	A	685	THR
1	A	696	ASN
1	A	697	LEU
1	A	704	LEU
1	A	727	CYS
1	A	731	LEU
1	A	744	LYS
1	A	750	ARG
1	A	758	ARG
1	A	776	MET

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Mol	Chain	Res	Type
1	A	778	GLN
1	A	780	ILE
1	A	785	SER
1	A	786	ILE
1	A	801	GLU
1	A	815	LEU
1	A	833	MET
1	A	835	THR
2	B	308	ARG
2	B	312	LYS
2	B	314	MET
2	B	316	LEU
2	B	321	VAL
2	B	325	SER
2	B	327	ASN
2	B	337	GLN
2	B	339	ASP
2	B	340	MET
2	B	342	LEU
2	B	344	SER
2	B	347	ARG
2	B	353	LYS
2	B	360	LYS
2	B	364	ASP
2	B	370	TYR
2	B	375	VAL
2	B	376	ILE
2	B	378	LYS
2	B	382	ARG
2	B	384	THR
2	B	402	PHE
2	B	418	LYS
2	B	421	PHE
2	B	425	ARG
2	B	426	ARG
2	B	430	ILE
2	B	438	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN

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Mol	Chain	Res	Type
1	A	298	GLN
1	A	395	GLN
1	A	402	ASN
1	A	410	GLN
1	A	422	HIS
1	A	427	GLN
1	A	438	GLN
1	A	460	GLN
1	A	484	HIS
1	A	535	ASN
1	A	540	ASN
1	A	551	HIS
1	A	564	HIS
1	A	680	HIS
1	A	742	GLN
1	A	828	GLN
2	B	327	ASN
2	B	348	GLN
2	B	350	GLN
2	B	351	ASN
2	B	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	900	4	58,58,58	1.98	15 (25%)	85,89,89	2.22	23 (27%)
4	M8A	A	901	3	29,30,30	2.44	7 (24%)	39,39,39	2.73	13 (33%)

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	-	9/34/50/50	0/6/6/6
4	M8A	A	901	3	-	6/21/31/31	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C4X-N5	7.38	1.46	1.30
4	A	901	M8A	CA-C	-6.59	1.37	1.52
4	A	901	M8A	OAA-CAD	6.39	1.56	1.20
4	A	901	M8A	CAP-CAX	-5.69	1.35	1.51
3	A	900	FAD	PA-O3P	4.59	1.64	1.59
3	A	900	FAD	C5X-N5	-4.58	1.31	1.39
3	A	900	FAD	C5A-C4A	3.74	1.45	1.39
4	A	901	M8A	CAZ-NAT	-3.64	1.34	1.41
3	A	900	FAD	C9A-C5X	3.60	1.47	1.41
3	A	900	FAD	C5'-C4'	3.14	1.56	1.51
3	A	900	FAD	C4-N3	-3.10	1.33	1.38
3	A	900	FAD	C4A-N9A	-3.00	1.31	1.37
3	A	900	FAD	C8A-N9A	-2.86	1.32	1.37
4	A	901	M8A	CAG-CAI	2.74	1.43	1.38
3	A	900	FAD	C5A-N7A	-2.54	1.34	1.39
3	A	900	FAD	C2-N3	-2.50	1.33	1.39
3	A	900	FAD	C8A-N7A	2.49	1.36	1.31
3	A	900	FAD	C8-C7	2.38	1.46	1.40
4	A	901	M8A	CAS-CAY	-2.33	1.45	1.50
4	A	901	M8A	CD-N	-2.29	1.43	1.47
3	A	900	FAD	C6A-N1A	-2.08	1.30	1.35
3	A	900	FAD	C6-C5X	-2.02	1.36	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	M8A	OAU-CAW-N	10.22	122.85	111.02
3	A	900	FAD	C10-C4X-N5	-7.89	108.71	124.81
3	A	900	FAD	C4-C4X-C10	-6.69	105.47	116.93
4	A	901	M8A	OAU-CAW-OAC	-5.48	115.23	124.76
4	A	901	M8A	CA-N-CAW	5.05	134.60	122.67
3	A	900	FAD	C4A-N9A-C8A	4.90	110.88	105.74
4	A	901	M8A	CG-CD-N	4.79	111.47	103.24
4	A	901	M8A	CD-N-CA	-4.62	104.76	112.01
3	A	900	FAD	C9A-C5X-N5	-4.50	117.68	122.45
3	A	900	FAD	C5A-C4A-N3A	-4.50	120.52	126.72
3	A	900	FAD	N3A-C4A-N9A	4.38	134.62	127.17
4	A	901	M8A	CAZ-NAT-C	-4.15	117.89	127.37
3	A	900	FAD	O3P-P-O1P	-3.91	98.95	110.70
3	A	900	FAD	C9A-N10-C10	-3.87	114.85	120.75
4	A	901	M8A	OAC-CAW-N	-3.11	120.67	124.21
3	A	900	FAD	O2P-P-O3P	3.08	115.60	107.27
3	A	900	FAD	O4-C4-N3	-3.06	114.35	120.11
3	A	900	FAD	C5X-C9A-N10	3.04	120.72	117.97
3	A	900	FAD	C5'-C4'-C3'	-2.96	106.63	112.22
3	A	900	FAD	O2A-PA-O3P	2.89	115.07	107.27
3	A	900	FAD	C5X-N5-C4X	-2.77	113.60	118.09
4	A	901	M8A	CB-CA-N	2.76	107.06	103.02
3	A	900	FAD	C4-C4X-N5	-2.72	114.44	118.21
3	A	900	FAD	N9A-C8A-N7A	-2.67	110.14	113.94
3	A	900	FAD	O5'-P-O1P	2.66	119.46	108.94
4	A	901	M8A	CAS-OAU-CAW	2.65	122.18	115.51
4	A	901	M8A	OAU-CAS-CAY	-2.55	103.23	109.40
3	A	900	FAD	C4A-C5A-N7A	-2.39	107.85	110.58
3	A	900	FAD	C4X-C4-N3	2.35	119.23	113.25
3	A	900	FAD	C4'-C3'-C2'	2.26	117.33	113.57
3	A	900	FAD	C6-C5X-C9A	2.26	122.15	119.05
4	A	901	M8A	CAL-CAZ-CAM	-2.23	116.09	119.04
3	A	900	FAD	C2A-N3A-C4A	2.12	117.00	111.83
3	A	900	FAD	O5'-C5'-C4'	2.10	114.98	109.36
4	A	901	M8A	CAI-CAY-CAH	-2.06	115.17	118.23
4	A	901	M8A	CAJ-CAL-CAZ	2.00	122.61	120.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

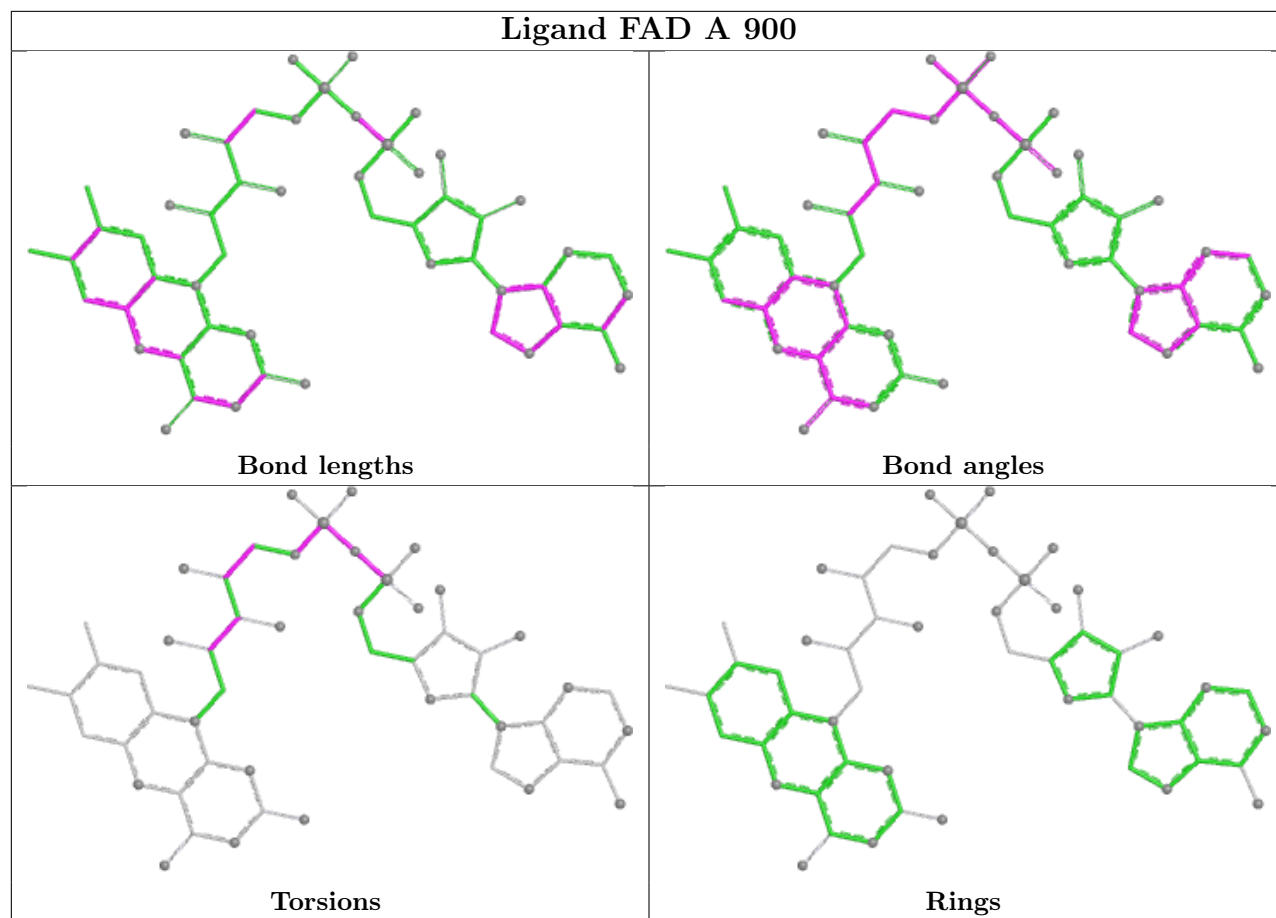
Mol	Chain	Res	Type	Atoms
3	A	900	FAD	O4'-C4'-C5'-O5'
3	A	900	FAD	C5'-O5'-P-O1P
4	A	901	M8A	N-CAW-OAU-CAS
4	A	901	M8A	OAC-CAW-OAU-CAS
3	A	900	FAD	PA-O3P-P-O5'
3	A	900	FAD	P-O3P-PA-O1A
3	A	900	FAD	P-O3P-PA-O2A
4	A	901	M8A	CAD-CAN-CAP-CAX
4	A	901	M8A	CAL-CAZ-NAT-C
3	A	900	FAD	C5'-O5'-P-O2P
3	A	900	FAD	C5'-O5'-P-O3P
4	A	901	M8A	CAM-CAZ-NAT-C
4	A	901	M8A	NAT-C-CA-CB
3	A	900	FAD	O2'-C2'-C3'-O3'
3	A	900	FAD	O2'-C2'-C3'-C4'

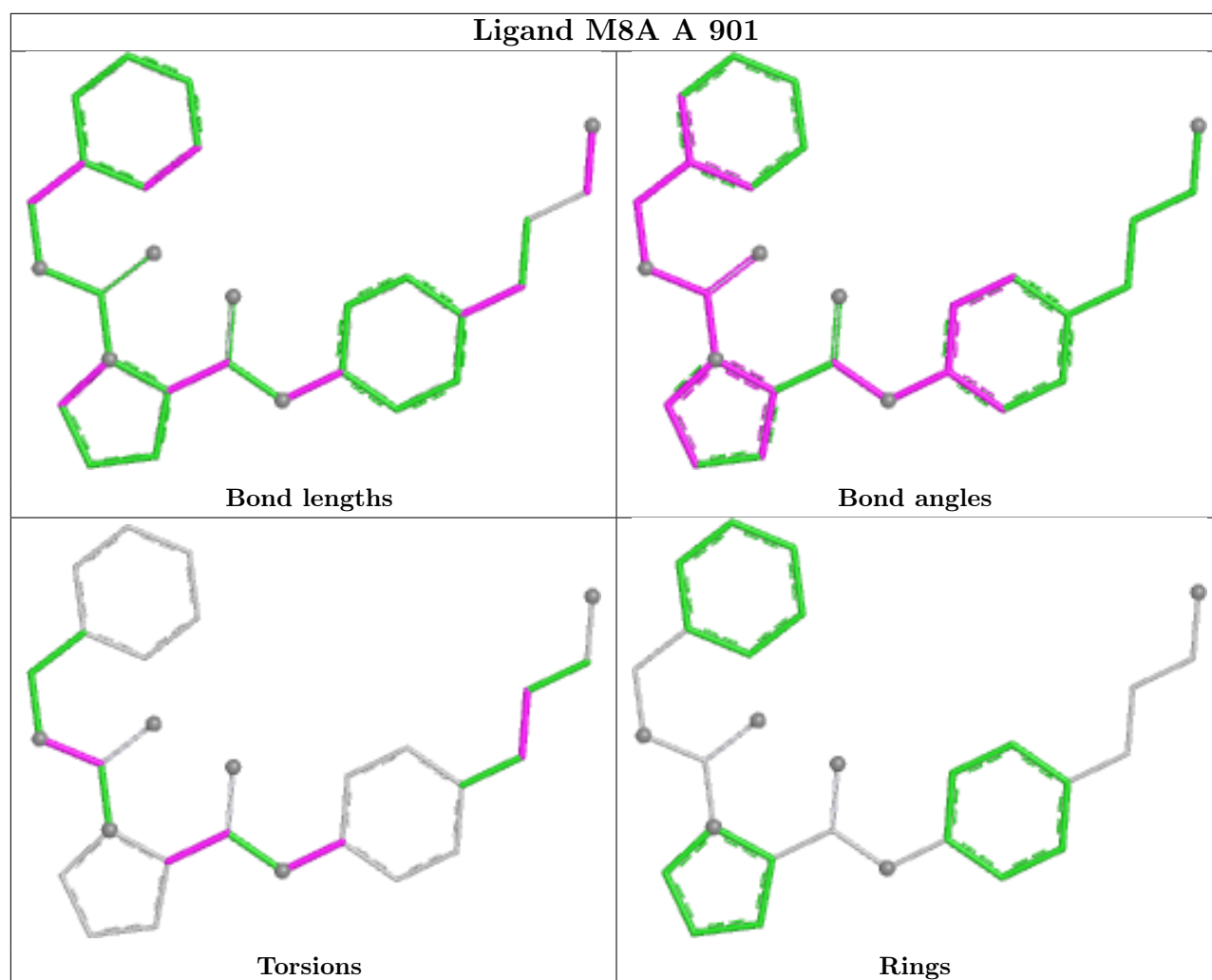
There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	20	0
4	A	901	M8A	17	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	666/852 (78%)	0.10	27 (4%)	41 32	39, 70, 112, 145	0
2	B	133/482 (27%)	0.53	11 (8%)	17 13	66, 103, 133, 156	0
All	All	799/1334 (59%)	0.17	38 (4%)	35 28	39, 76, 120, 156	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	7.7
1	A	557	ASP	7.2
1	A	833	MET	5.1
1	A	403	ASN	4.5
1	A	770	GLY	4.4
1	A	554	GLN	4.0
1	A	555	ASP	3.9
2	B	382	ARG	3.7
1	A	171	PRO	3.7
1	A	558	PHE	3.5
1	A	272	PRO	3.3
2	B	375	VAL	3.2
1	A	377	MET	3.1
2	B	308	ARG	3.0
2	B	378	LYS	3.0
2	B	440	GLU	2.8
2	B	376	ILE	2.8
1	A	275	THR	2.8
1	A	771	ASN	2.7
1	A	269	ARG	2.6
1	A	610	THR	2.5
1	A	172	SER	2.5
2	B	419	ASN	2.5
1	A	556	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	2.4
2	B	427	ARG	2.4
1	A	467	GLU	2.3
1	A	785	SER	2.3
2	B	424	TYR	2.3
1	A	276	LYS	2.3
1	A	373	GLU	2.2
1	A	769	SER	2.2
2	B	312	LYS	2.2
1	A	807	TYR	2.2
1	A	273	LEU	2.1
1	A	359	LYS	2.1
1	A	773	TYR	2.1
2	B	379	CYS	2.0

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](#)

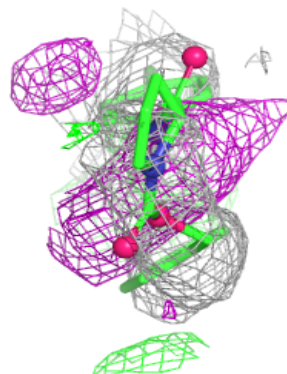
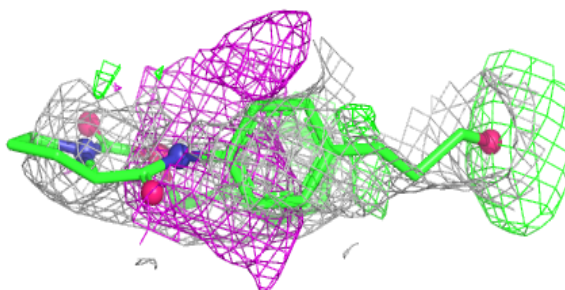
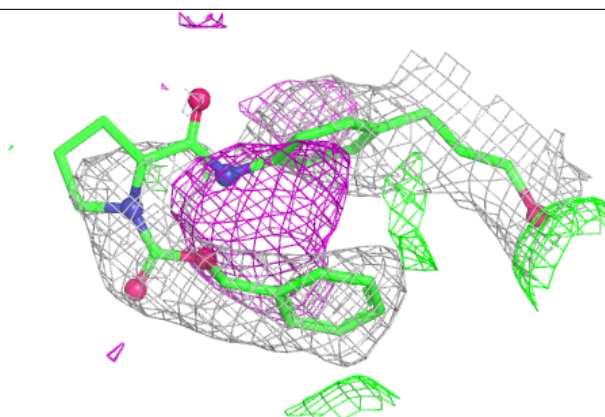
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	M8A	A	901	28/28	0.86	0.28	47,117,177,196	0
3	FAD	A	900	53/53	0.98	0.06	38,54,73,82	0

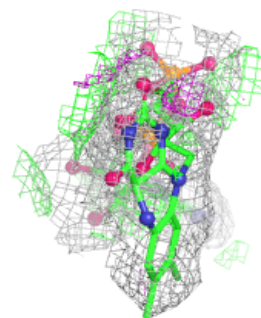
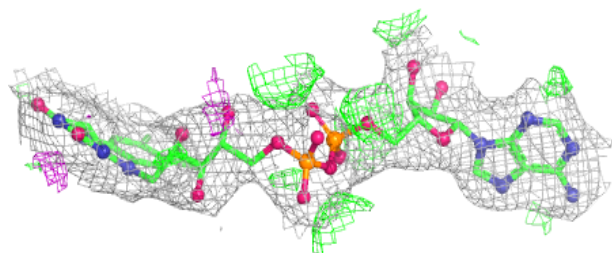
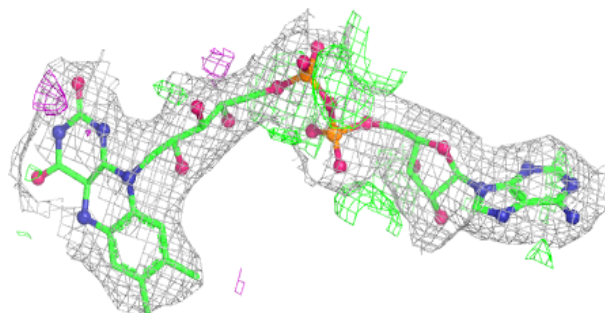
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around M8A A 901:

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

**Electron density around FAD A 900:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.