



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 4GU0 / pdb_00004gu0
Title : Crystal structure of LSD2 with H3
Authors : Chen, F.; Yang, H.; Dong, Z.; Fang, J.; Zhu, T.; Gong, W.; Xu, Y.
Deposited on : 2012-08-29
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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:

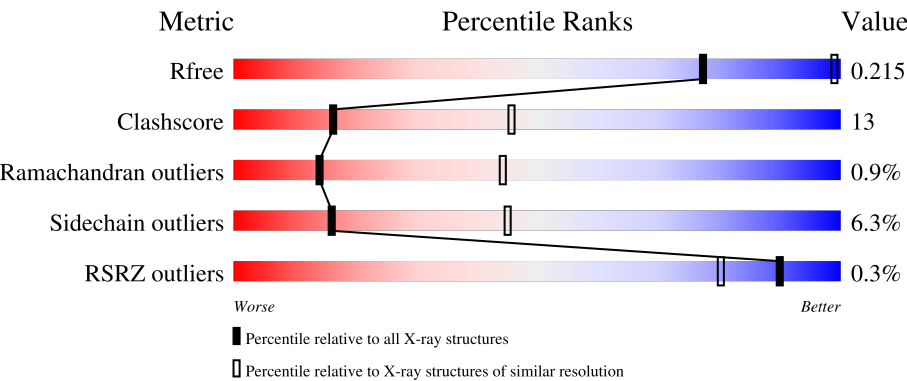
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	776	68%25%••
1	B	776	66%27%•••
1	C	776	70%22%•5%
1	D	776	66%26%•5%
2	E	26	50%42%8%

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Mol	Chain	Length	Quality of chain
2	F	26	8% 50% 42%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24156 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 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			5919	3780	1007	1091	41			
1	B	748	Total	C	N	O	S	0	0	0
			5919	3780	1007	1091	41			
1	C	736	Total	C	N	O	S	0	0	0
			5830	3724	992	1073	41			
1	D	735	Total	C	N	O	S	0	0	0
			5822	3718	991	1072	41			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	-	expression tag	UNP Q8NB78
A	48	LEU	-	expression tag	UNP Q8NB78
A	49	GLY	-	expression tag	UNP Q8NB78
A	50	SER	-	expression tag	UNP Q8NB78
B	47	PRO	-	expression tag	UNP Q8NB78
B	48	LEU	-	expression tag	UNP Q8NB78
B	49	GLY	-	expression tag	UNP Q8NB78
B	50	SER	-	expression tag	UNP Q8NB78
C	47	PRO	-	expression tag	UNP Q8NB78
C	48	LEU	-	expression tag	UNP Q8NB78
C	49	GLY	-	expression tag	UNP Q8NB78
C	50	SER	-	expression tag	UNP Q8NB78
D	47	PRO	-	expression tag	UNP Q8NB78
D	48	LEU	-	expression tag	UNP Q8NB78
D	49	GLY	-	expression tag	UNP Q8NB78
D	50	SER	-	expression tag	UNP Q8NB78

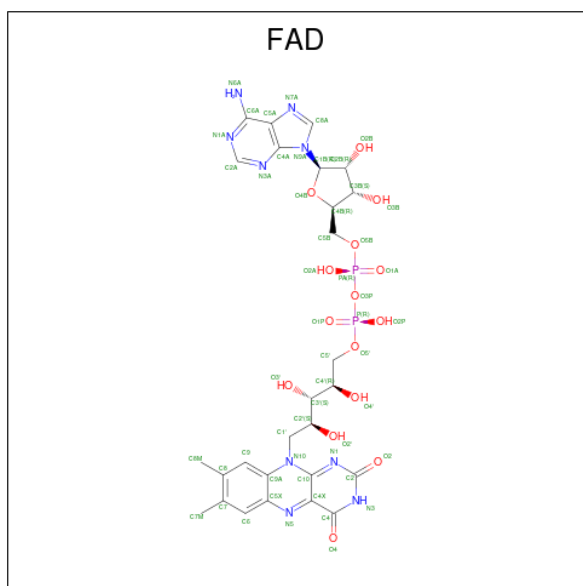
- Molecule 2 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	S	0	0	0
			193	115	44	33	1			
2	F	26	Total	C	N	O	S	0	0	0
			193	115	44	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	MET	LYS	engineered mutation	UNP P84243
F	4	MET	LYS	engineered mutation	UNP P84243

- 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		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Zn 3	0	0
4	B	3	Total 3	Zn 3	0	0
4	C	3	Total 3	Zn 3	0	0
4	D	3	Total 3	Zn 3	0	0

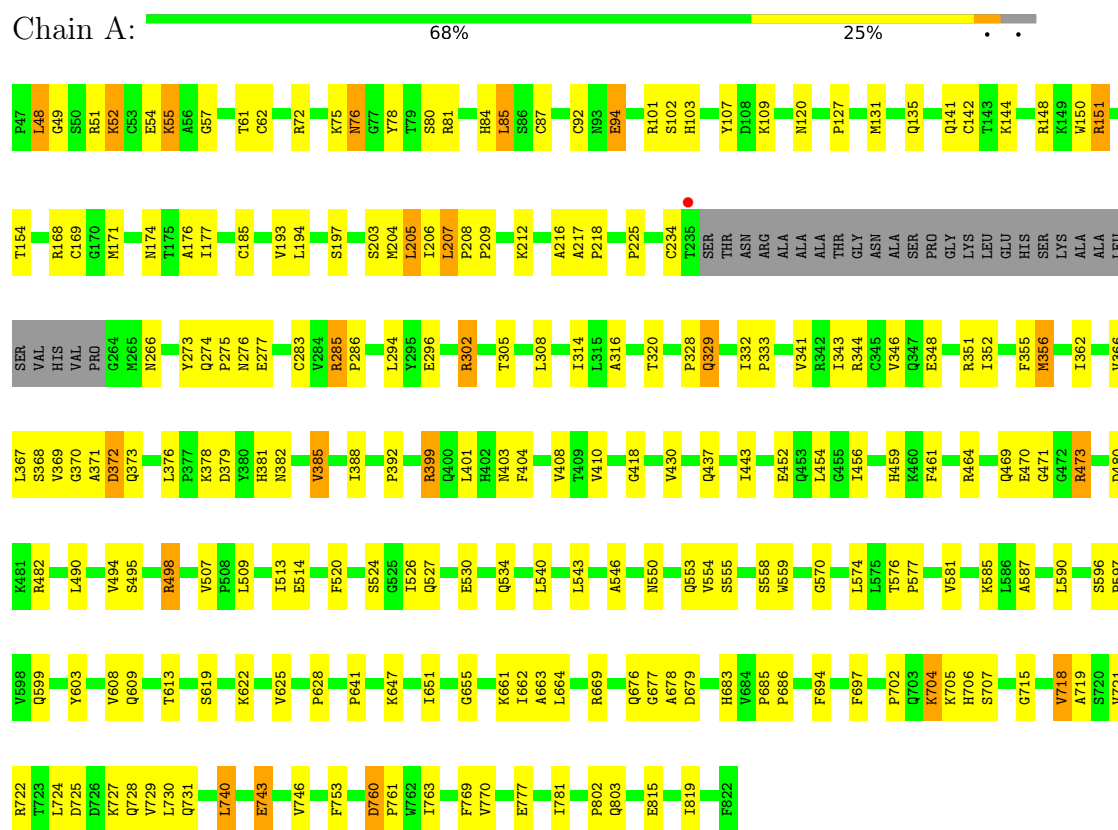
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	10	Total 10	O 10	0	0
5	C	16	Total 16	O 16	0	0
5	D	15	Total 15	O 15	0	0
5	E	1	Total 1	O 1	0	0
5	F	1	Total 1	O 1	0	0

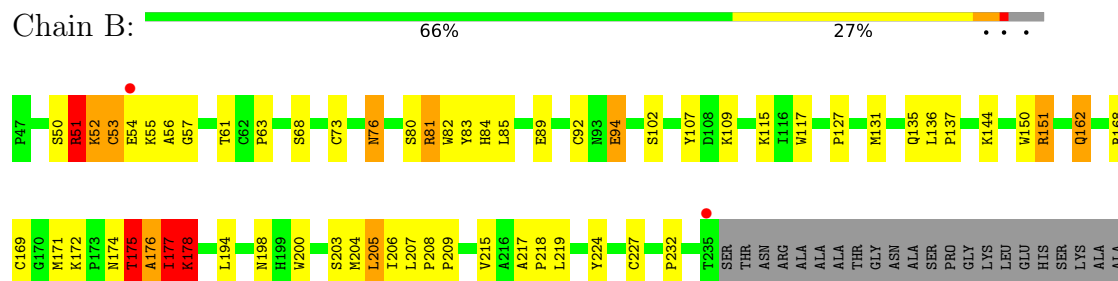
3 Residue-property plots

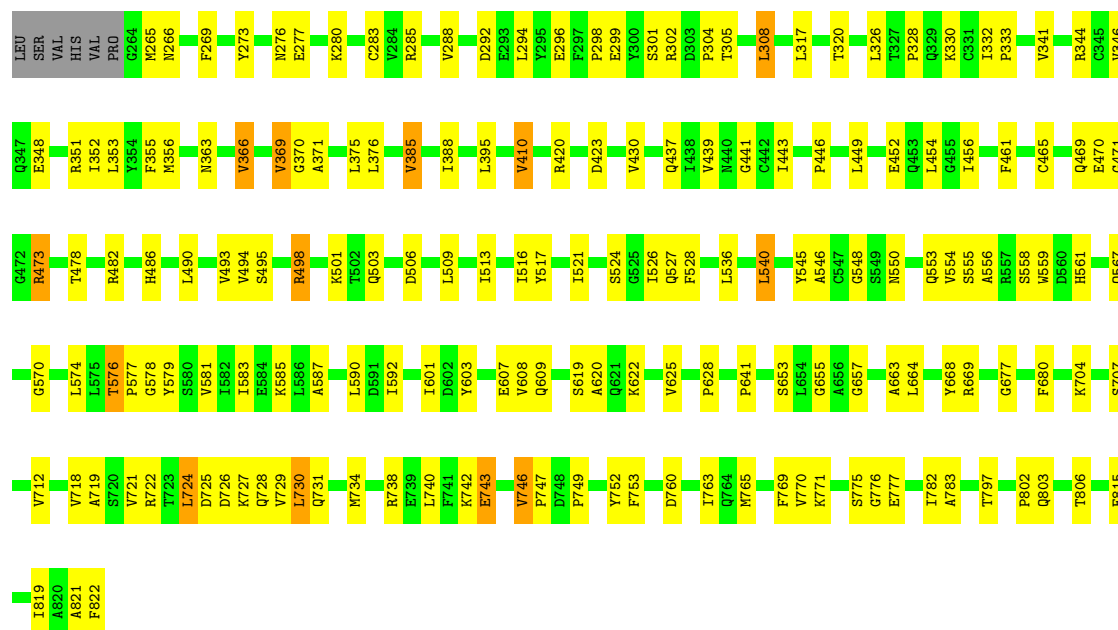
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1B



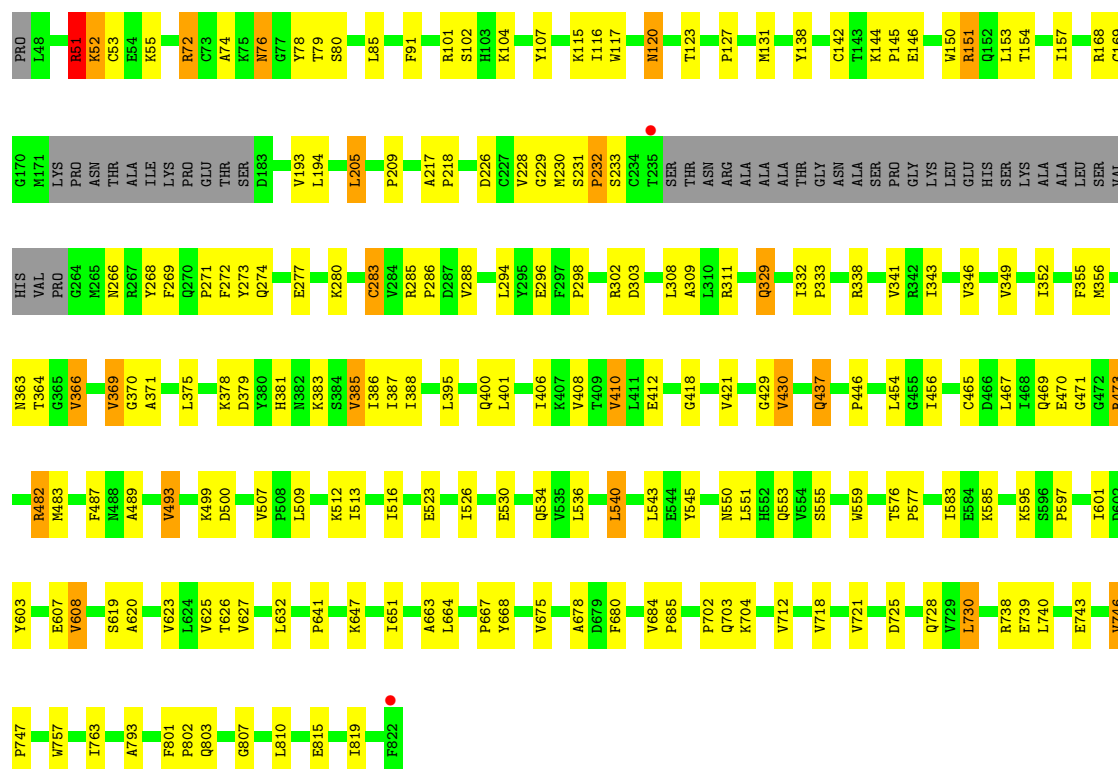
• Molecule 1: Lysine-specific histone demethylase 1B





- Molecule 1: Lysine-specific histone demethylase 1B

Chain C: 70% 22% 5%



- Molecule 1: Lysine-specific histone demethylase 1B

Chain D: 66% 26% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.84Å 108.93Å 120.83Å 94.47° 112.34° 117.95°	Depositor
Resolution (Å)	45.06 – 3.10 45.06 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.06-3.10) 98.7 (45.06-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.204 , 0.221 0.198 , 0.215	Depositor DCC
R_{free} test set	3633 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24156	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, ZN

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	0.30	0/6067	0.73	8/8221 (0.1%)
1	B	0.29	0/6067	0.70	2/8221 (0.0%)
1	C	0.30	0/5974	0.71	1/8092 (0.0%)
1	D	0.30	0/5966	0.72	5/8081 (0.1%)
2	E	0.57	0/193	1.03	0/254
2	F	0.62	0/193	0.96	0/254
All	All	0.31	0/24460	0.72	16/33123 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	CA-C-N	5.96	125.64	119.56
1	A	285	ARG	C-N-CA	5.96	125.64	119.56
1	C	51	ARG	N-CA-C	5.87	119.14	110.46
1	A	75	LYS	CB-CA-C	-5.69	110.00	116.54
1	D	303	ASP	CA-C-N	5.45	124.97	119.19
1	D	303	ASP	C-N-CA	5.45	124.97	119.19
1	D	270	GLN	CA-C-N	5.31	124.64	118.85
1	D	270	GLN	C-N-CA	5.31	124.64	118.85
1	D	277	GLU	N-CA-C	-5.21	103.81	110.53
1	B	760	ASP	CA-C-N	5.18	126.31	119.84
1	B	760	ASP	C-N-CA	5.18	126.31	119.84
1	A	207	LEU	CA-C-N	5.16	123.38	119.66
1	A	207	LEU	C-N-CA	5.16	123.38	119.66
1	A	176	ALA	N-CA-C	5.09	117.27	109.07
1	A	760	ASP	CA-C-N	5.03	125.30	119.47
1	A	760	ASP	C-N-CA	5.03	125.30	119.47

There are no chirality outliers.

There are no planarity outliers.

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	5919	0	5840	153	0
1	B	5919	0	5840	175	0
1	C	5830	0	5744	143	0
1	D	5822	0	5734	156	0
2	E	193	0	218	10	0
2	F	193	0	218	20	0
3	A	53	0	30	3	0
3	B	53	0	30	0	0
3	C	53	0	30	4	0
3	D	53	0	30	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	13	0	0	4	0
5	B	10	0	0	0	0
5	C	16	0	0	0	0
5	D	15	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24156	0	23714	621	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 13.

All (621) 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:C:72:ARG:HG2	1:C:72:ARG:HH11	1.15	1.11
1:B:302:ARG:HG2	1:D:526:ILE:HD11	1.10	1.10
1:B:203:SER:HA	1:B:302:ARG:HH22	1.19	1.04
3:A:901:FAD:O3B	5:A:1005:HOH:O	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:HA	2:E:19:GLN:HE21	1.27	0.99
1:B:276:ASN:HA	2:F:19:GLN:HE21	1.30	0.95
1:A:371:ALA:H	1:A:372:ASP:HB3	1.33	0.90
1:A:203:SER:HB3	1:A:302:ARG:HH12	1.38	0.88
1:A:371:ALA:N	1:A:372:ASP:HB3	1.86	0.88
1:C:51:ARG:HD3	1:C:79:THR:O	1.75	0.86
1:D:51:ARG:HG3	1:D:52:LYS:H	1.41	0.84
1:C:456:ILE:HG23	1:C:577:PRO:HG2	1.60	0.83
1:A:683:HIS:HD2	1:A:740:LEU:HD11	1.45	0.82
1:C:72:ARG:HH11	1:C:72:ARG:CG	1.93	0.79
1:B:276:ASN:CA	2:F:19:GLN:HE21	1.94	0.79
1:A:482:ARG:HG2	1:C:302:ARG:O	1.82	0.78
1:D:454:LEU:HD21	1:D:585:LYS:HG2	1.66	0.77
1:A:276:ASN:HA	2:E:19:GLN:NE2	2.01	0.76
1:B:550:ASN:HB3	1:B:553:GLN:HE22	1.51	0.76
1:C:209:PRO:HG3	1:C:341:VAL:HG21	1.69	0.73
1:C:352:ILE:HG22	1:C:356:MET:HE2	1.68	0.73
1:C:51:ARG:HD2	1:C:79:THR:H	1.53	0.73
1:C:72:ARG:HG2	1:C:72:ARG:NH1	1.95	0.73
1:A:266:ASN:HD22	1:A:452:GLU:HG2	1.52	0.72
1:A:144:LYS:HE2	1:A:168:ARG:HH11	1.53	0.72
1:D:51:ARG:HG3	1:D:52:LYS:N	2.05	0.72
1:D:626:THR:HG22	1:D:793:ALA:HB3	1.72	0.71
1:D:647:LYS:O	1:D:651:ILE:HG13	1.90	0.71
1:A:302:ARG:O	1:C:482:ARG:HG3	1.91	0.71
1:B:203:SER:HA	1:B:302:ARG:NH2	2.01	0.71
1:B:52:LYS:O	1:B:53:CYS:HB2	1.90	0.70
1:B:550:ASN:HB3	1:B:553:GLN:NE2	2.05	0.70
1:A:266:ASN:HD22	1:A:452:GLU:CG	2.06	0.69
1:B:276:ASN:HA	2:F:19:GLN:NE2	2.05	0.69
1:A:473:ARG:H	1:A:473:ARG:HD2	1.56	0.69
1:D:668:TYR:CE2	1:D:747:PRO:HG3	2.28	0.69
1:B:302:ARG:O	1:D:482:ARG:HB2	1.93	0.68
1:B:727:LYS:HE3	1:B:731:GLN:OE1	1.92	0.68
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.59	0.68
1:B:719:ALA:O	1:B:722:ARG:HG2	1.93	0.68
1:A:203:SER:HB3	1:A:302:ARG:NH1	2.09	0.67
1:A:454:LEU:HD21	1:A:585:LYS:HG2	1.77	0.67
1:A:576:THR:OG1	1:A:577:PRO:HD3	1.94	0.67
1:A:51:ARG:O	1:A:52:LYS:HB3	1.94	0.67
1:D:209:PRO:HG3	1:D:341:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ILE:HG23	1:D:577:PRO:HG2	1.76	0.67
1:D:603:TYR:HB3	1:D:608:VAL:HG12	1.75	0.67
1:B:473:ARG:H	1:B:473:ARG:HD2	1.60	0.67
1:C:576:THR:OG1	1:C:577:PRO:HD3	1.94	0.67
1:A:728:GLN:OE1	1:D:634:LYS:HD3	1.95	0.67
1:B:298:PRO:HB2	1:D:524:SER:HB3	1.77	0.66
1:D:555:SER:O	1:D:559:TRP:HB3	1.96	0.66
1:A:456:ILE:HG23	1:A:577:PRO:HG2	1.77	0.66
1:A:482:ARG:HE	1:C:303:ASP:HB2	1.60	0.66
1:A:683:HIS:CD2	1:A:740:LEU:HD11	2.30	0.66
1:C:74:ALA:HB2	1:C:79:THR:HB	1.78	0.66
1:A:76:ASN:HD22	1:A:76:ASN:H	1.42	0.65
1:B:171:MET:HG3	1:B:177:ILE:HD11	1.77	0.65
1:C:363:ASN:HB3	1:C:375:LEU:HD13	1.78	0.65
1:C:412:GLU:OE2	3:C:901:FAD:O3B	2.15	0.65
1:B:276:ASN:CB	2:F:19:GLN:HE21	2.09	0.65
1:A:150:TRP:HZ2	1:A:346:VAL:HG21	1.61	0.64
2:E:2:ARG:HD3	2:E:10:SER:O	1.97	0.64
1:A:87:CYS:SG	1:A:204:MET:HE3	2.37	0.64
1:A:550:ASN:HB3	1:A:553:GLN:HE22	1.61	0.64
1:B:302:ARG:HG2	1:D:526:ILE:CD1	2.06	0.64
1:C:76:ASN:H	1:C:76:ASN:HD22	1.44	0.64
1:C:543:LEU:HD11	1:C:559:TRP:CZ3	2.34	0.63
1:D:496:GLU:OE2	1:D:499:LYS:HE2	1.98	0.62
1:D:668:TYR:CZ	1:D:747:PRO:HG3	2.34	0.62
1:D:688:ALA:O	1:D:691:ARG:HG2	1.99	0.62
1:B:490:LEU:O	1:B:494:VAL:HG23	1.99	0.62
1:A:55:LYS:HZ1	1:A:204:MET:HG2	1.65	0.62
1:C:545:TYR:CE1	1:C:712:VAL:HG11	2.35	0.62
1:D:51:ARG:NH1	1:D:78:TYR:HE1	1.97	0.62
1:B:266:ASN:HD22	1:B:452:GLU:HG3	1.64	0.62
1:B:52:LYS:O	1:B:53:CYS:CB	2.47	0.61
1:D:483:MET:HE2	1:D:536:LEU:HB2	1.80	0.61
1:A:546:ALA:HB2	2:E:5:GLN:HG3	1.82	0.61
1:D:203:SER:HB2	1:D:302:ARG:HH21	1.66	0.61
1:C:401:LEU:HB2	1:C:408:VAL:HG21	1.83	0.61
1:D:509:LEU:HD23	1:D:551:LEU:HD22	1.83	0.60
1:B:495:SER:HA	1:B:498:ARG:HD2	1.83	0.60
1:D:576:THR:OG1	1:D:577:PRO:HD3	2.00	0.60
1:D:499:LYS:O	1:D:500:ASP:HB2	2.01	0.60
1:D:533:GLY:O	1:D:537:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:GLN:HB2	1:D:473:ARG:HG2	1.83	0.60
1:B:89:GLU:HG2	1:B:136:LEU:HD21	1.82	0.60
1:B:370:GLY:N	1:B:371:ALA:HA	2.16	0.60
1:A:461:PHE:CZ	1:A:574:LEU:HB2	2.37	0.60
1:D:587:ALA:HB1	1:D:592:ILE:CD1	2.32	0.59
1:B:721:VAL:HG23	1:B:724:LEU:HD12	1.84	0.59
1:C:273:TYR:CE1	1:C:283:CYS:HB3	2.37	0.59
1:C:483:MET:HE2	1:C:536:LEU:HB2	1.85	0.59
2:E:17:ARG:O	2:E:18:LYS:HG2	2.02	0.59
1:D:51:ARG:NH2	1:D:80:SER:O	2.36	0.59
1:B:56:ALA:O	1:B:204:MET:HE1	2.03	0.59
1:B:456:ILE:HG23	1:B:577:PRO:HG2	1.84	0.59
1:C:151:ARG:HD2	1:C:169:CYS:SG	2.43	0.59
1:A:490:LEU:O	1:A:494:VAL:HG23	2.01	0.59
1:A:92:CYS:SG	1:A:94:GLU:HG2	2.43	0.59
1:D:278:CYS:HB2	2:F:19:GLN:OE1	2.03	0.59
1:A:48:LEU:H	1:A:48:LEU:HD23	1.66	0.59
1:B:57:GLY:C	1:B:204:MET:HE2	2.27	0.59
1:C:456:ILE:CG2	1:C:577:PRO:HG2	2.33	0.58
1:D:521:ILE:HD11	1:D:528:PHE:CE2	2.39	0.58
2:F:22:THR:HG22	2:F:25:ALA:HB2	1.85	0.58
1:C:454:LEU:HD21	1:C:585:LYS:HG2	1.84	0.58
1:D:146:GLU:CD	1:D:146:GLU:H	2.12	0.58
1:D:715:GLY:O	1:D:718:VAL:HG22	2.03	0.58
1:A:628:PRO:HG2	1:A:763:ILE:HA	1.85	0.58
1:A:663:ALA:C	1:A:664:LEU:HD12	2.28	0.58
1:B:61:THR:O	1:B:63:PRO:HD3	2.03	0.58
1:B:175:THR:O	1:B:176:ALA:C	2.46	0.58
1:A:76:ASN:HD22	1:A:76:ASN:N	1.99	0.58
1:A:367:LEU:HA	5:A:1006:HOH:O	2.03	0.58
1:D:401:LEU:HB2	1:D:408:VAL:HG21	1.86	0.58
1:B:486:HIS:CE1	1:D:301:SER:HB2	2.39	0.57
1:D:265:MET:O	1:D:266:ASN:HB2	2.04	0.57
1:B:92:CYS:SG	1:B:94:GLU:HG2	2.45	0.57
1:D:123:THR:HG23	1:D:226:ASP:OD2	2.04	0.57
1:A:694:PHE:HB3	1:A:697:PHE:CZ	2.40	0.57
1:D:272:PHE:HB3	1:D:286:PRO:HG3	1.86	0.57
1:D:545:TYR:CD1	1:D:712:VAL:HG11	2.40	0.57
1:D:412:GLU:OE1	3:D:901:FAD:O3B	2.22	0.57
1:C:385:VAL:HG11	1:C:401:LEU:HD13	1.87	0.57
1:D:273:TYR:CE1	1:D:283:CYS:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LYS:O	1:C:406:ILE:HG23	2.05	0.56
1:D:228:VAL:HG23	1:D:230:MET:HG3	1.85	0.56
1:B:81:ARG:NH1	1:B:83:TYR:CE1	2.74	0.56
1:B:54:GLU:HG2	1:B:55:LYS:N	2.20	0.56
1:B:203:SER:CA	1:B:302:ARG:HH22	2.07	0.56
1:C:607:GLU:OE2	1:C:619:SER:HB2	2.05	0.56
1:B:730:LEU:HD21	1:B:749:PRO:HG3	1.86	0.56
1:C:209:PRO:HG3	1:C:341:VAL:CG2	2.34	0.56
1:D:738:ARG:HG2	1:D:746:VAL:HG13	1.88	0.56
1:A:84:HIS:HD2	1:A:206:ILE:HG12	1.70	0.56
1:C:395:LEU:HD12	1:C:583:ILE:HG23	1.88	0.55
1:C:489:ALA:O	1:C:493:VAL:HG12	2.05	0.55
1:A:705:LYS:HE3	1:A:706:HIS:CE1	2.42	0.55
1:B:266:ASN:HD22	1:B:452:GLU:CG	2.19	0.55
1:C:332:ILE:HB	1:C:333:PRO:HD3	1.88	0.55
1:B:150:TRP:HZ2	1:B:346:VAL:HG21	1.71	0.55
1:C:493:VAL:HG11	1:C:516:ILE:HG21	1.88	0.55
1:B:178:LYS:N	1:B:178:LYS:CD	2.69	0.55
1:A:127:PRO:O	1:A:131:MET:HG2	2.05	0.54
1:A:555:SER:O	1:A:559:TRP:HB3	2.07	0.54
1:A:603:TYR:CE2	1:A:641:PRO:HD2	2.41	0.54
1:B:555:SER:O	1:B:559:TRP:HB3	2.08	0.54
1:A:371:ALA:CA	1:A:372:ASP:HB3	2.36	0.54
1:D:493:VAL:HG13	1:D:516:ILE:HD13	1.88	0.54
1:D:622:LYS:HG3	1:D:819:ILE:HG23	1.88	0.54
1:C:473:ARG:H	1:C:473:ARG:HD2	1.73	0.54
1:D:603:TYR:CE2	1:D:641:PRO:HD2	2.42	0.54
1:A:296:GLU:HG2	1:A:355:PHE:CD1	2.43	0.54
1:C:555:SER:O	1:C:559:TRP:HB3	2.07	0.54
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.20	0.54
1:A:368:SER:HB2	5:A:1003:HOH:O	2.07	0.54
1:B:669:ARG:NH2	1:B:704:LYS:HG3	2.23	0.54
1:C:150:TRP:HZ2	1:C:346:VAL:HG21	1.73	0.54
1:C:370:GLY:H	1:C:371:ALA:HA	1.73	0.54
1:B:517:TYR:O	1:B:521:ILE:HG12	2.08	0.54
1:B:653:SER:O	1:B:771:LYS:HB2	2.08	0.54
1:D:51:ARG:CG	1:D:52:LYS:H	2.15	0.54
1:B:348:GLU:OE1	1:B:351:ARG:HD3	2.08	0.53
1:B:461:PHE:CZ	1:B:574:LEU:HB2	2.43	0.53
1:C:412:GLU:OE1	3:C:901:FAD:H1B	2.09	0.53
1:C:487:PHE:HE1	1:C:540:LEU:HD13	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ASN:HB3	1:B:375:LEU:HD13	1.89	0.53
1:B:727:LYS:O	1:B:731:GLN:HG3	2.08	0.53
1:C:229:GLY:HA3	1:C:309:ALA:HB2	1.89	0.53
1:C:668:TYR:CE2	1:C:747:PRO:HG3	2.43	0.53
1:A:208:PRO:CB	1:A:305:THR:HG21	2.39	0.53
1:B:454:LEU:HD21	1:B:585:LYS:HG2	1.91	0.53
1:B:558:SER:HB2	1:B:770:VAL:HG11	1.91	0.53
2:E:7:ALA:O	2:E:8:ARG:HB2	2.08	0.53
1:A:543:LEU:HD11	1:A:559:TRP:CZ3	2.44	0.53
1:C:757:TRP:HZ3	1:C:763:ILE:HD12	1.74	0.53
1:D:203:SER:HB2	1:D:302:ARG:NH2	2.23	0.53
1:A:371:ALA:HB3	1:A:372:ASP:HB2	1.91	0.53
1:C:51:ARG:CD	1:C:79:THR:H	2.21	0.53
1:A:102:SER:HA	1:A:107:TYR:CG	2.44	0.52
1:A:494:VAL:O	1:A:498:ARG:HG2	2.09	0.52
1:A:550:ASN:HB3	1:A:553:GLN:NE2	2.22	0.52
1:D:461:PHE:CZ	1:D:574:LEU:HB2	2.43	0.52
1:B:388:ILE:CD1	1:B:601:ILE:HD11	2.39	0.52
1:A:378:LYS:HA	1:A:381:HIS:CG	2.45	0.52
1:A:509:LEU:O	1:A:513:ILE:HG13	2.09	0.52
1:B:219:LEU:HD21	1:B:265:MET:HE1	1.90	0.52
1:C:668:TYR:CZ	1:C:747:PRO:HG3	2.45	0.52
1:A:144:LYS:HE2	1:A:168:ARG:NH1	2.24	0.52
1:B:410:VAL:HG13	1:B:592:ILE:HG12	1.91	0.52
1:B:209:PRO:HG3	1:B:341:VAL:HG21	1.90	0.52
1:B:603:TYR:CE2	1:B:641:PRO:HD2	2.45	0.52
1:B:61:THR:C	1:B:63:PRO:HD3	2.34	0.52
1:D:730:LEU:O	1:D:734:MET:HG2	2.08	0.52
1:A:725:ASP:OD2	1:A:728:GLN:HG3	2.09	0.52
1:B:208:PRO:HB3	1:B:305:THR:HB	1.92	0.52
1:B:217:ALA:HB3	1:B:218:PRO:HD3	1.91	0.52
1:B:276:ASN:OD1	2:F:19:GLN:NE2	2.43	0.52
1:C:370:GLY:N	1:C:371:ALA:HA	2.25	0.52
1:C:388:ILE:CD1	1:C:601:ILE:HD11	2.39	0.52
1:C:418:GLY:HA2	1:C:583:ILE:HG21	1.90	0.52
1:A:217:ALA:HB3	1:A:218:PRO:HD3	1.92	0.52
1:B:81:ARG:NH1	1:B:81:ARG:HG2	2.24	0.52
1:C:154:THR:OG1	1:C:157:ILE:HG13	2.10	0.52
1:D:423:ASP:HA	1:D:433:GLY:HA2	1.92	0.52
1:B:276:ASN:HA	2:F:19:GLN:HG2	1.91	0.51
1:C:647:LYS:O	1:C:651:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:CB	1:A:302:ARG:HH12	2.16	0.51
1:B:743:GLU:H	1:B:743:GLU:CD	2.16	0.51
1:D:370:GLY:N	1:D:371:ALA:HA	2.24	0.51
1:D:388:ILE:CD1	1:D:601:ILE:HD11	2.40	0.51
1:A:48:LEU:HD23	1:A:48:LEU:N	2.25	0.51
1:B:81:ARG:HG2	1:B:81:ARG:HH11	1.75	0.51
1:D:222:ALA:HB1	1:D:275:PRO:HG2	1.92	0.51
1:C:675:VAL:HG13	1:C:678:ALA:HB3	1.92	0.51
1:D:439:VAL:HG22	1:D:579:TYR:OH	2.11	0.51
1:A:150:TRP:CZ2	1:A:346:VAL:HG21	2.45	0.51
1:A:302:ARG:CZ	1:C:526:ILE:HG21	2.40	0.51
1:A:274:GLN:HB2	1:A:277:GLU:HG3	1.92	0.51
1:B:561:HIS:ND1	1:B:776:GLY:HA3	2.26	0.51
1:A:371:ALA:HB3	1:A:372:ASP:CB	2.41	0.51
1:B:51:ARG:O	1:B:52:LYS:HB3	2.11	0.51
1:B:55:LYS:HG3	1:B:204:MET:HE3	1.93	0.51
1:B:227:CYS:HB3	2:F:24:ALA:HB1	1.93	0.51
1:C:285:ARG:NH2	1:C:288:VAL:HG21	2.25	0.51
1:C:509:LEU:HD23	1:C:551:LEU:HD22	1.93	0.51
1:C:738:ARG:HG2	1:C:746:VAL:HG22	1.91	0.51
1:D:718:VAL:O	1:D:721:VAL:HG12	2.11	0.51
1:D:102:SER:HA	1:D:107:TYR:CD1	2.45	0.51
1:D:154:THR:OG1	1:D:157:ILE:HG13	2.09	0.51
1:B:269:PHE:CZ	1:B:449:LEU:HD12	2.46	0.51
1:C:120:ASN:N	1:C:120:ASN:HD22	2.09	0.51
1:D:66:PHE:CE2	1:D:131:MET:HE3	2.46	0.51
1:B:304:PRO:HG3	1:D:485:PHE:CE1	2.46	0.50
1:A:48:LEU:O	1:A:78:TYR:HB2	2.12	0.50
1:A:151:ARG:HD2	1:A:169:CYS:SG	2.51	0.50
1:C:493:VAL:HG22	1:C:516:ILE:HD13	1.93	0.50
1:D:370:GLY:H	1:D:371:ALA:HA	1.76	0.50
1:B:176:ALA:O	1:B:177:ILE:HB	2.09	0.50
1:B:536:LEU:O	1:B:540:LEU:HD22	2.11	0.50
1:B:821:ALA:O	1:B:822:PHE:HB2	2.12	0.50
1:C:150:TRP:CZ2	1:C:346:VAL:HG21	2.46	0.50
1:C:296:GLU:HG2	1:C:355:PHE:CD1	2.47	0.50
1:D:459:HIS:ND1	1:D:702:PRO:HB3	2.26	0.50
1:B:162:GLN:CD	1:B:162:GLN:H	2.17	0.50
1:C:79:THR:O	1:C:80:SER:C	2.54	0.50
1:A:275:PRO:O	1:A:276:ASN:HB2	2.11	0.50
1:A:480:ASP:CG	2:E:8:ARG:HH22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:GLY:HA3	1:A:769:PHE:CZ	2.47	0.50
1:C:388:ILE:HD12	1:C:601:ILE:HD11	1.93	0.50
1:C:545:TYR:HE1	1:C:712:VAL:HG11	1.75	0.50
1:C:217:ALA:HB3	1:C:218:PRO:HD3	1.94	0.50
1:A:376:LEU:HD12	1:A:404:PHE:HB3	1.93	0.50
1:A:388:ILE:N	1:A:388:ILE:HD12	2.26	0.50
1:D:663:ALA:O	1:D:752:TYR:HA	2.12	0.50
1:A:169:CYS:HB2	1:A:185:CYS:SG	2.50	0.50
1:A:352:ILE:O	1:A:356:MET:HG2	2.12	0.50
1:B:178:LYS:N	1:B:178:LYS:HD3	2.26	0.50
1:B:663:ALA:O	1:B:752:TYR:HA	2.12	0.50
1:C:576:THR:HG21	1:C:702:PRO:HG2	1.93	0.50
1:D:725:ASP:OD2	1:D:728:GLN:HG3	2.11	0.50
1:B:607:GLU:HB2	1:B:620:ALA:O	2.11	0.49
1:C:603:TYR:CE2	1:C:641:PRO:HD2	2.47	0.49
1:B:51:ARG:NH2	1:B:80:SER:O	2.42	0.49
1:C:802:PRO:O	1:C:803:GLN:HB2	2.12	0.49
1:D:738:ARG:HG2	1:D:746:VAL:CG1	2.42	0.49
1:B:509:LEU:O	1:B:513:ILE:HG13	2.12	0.49
1:C:53:CYS:SG	1:C:55:LYS:HB3	2.53	0.49
1:C:664:LEU:N	1:C:664:LEU:HD12	2.27	0.49
1:B:109:LYS:HE2	1:B:135:GLN:OE1	2.12	0.49
1:B:725:ASP:O	1:B:729:VAL:HG23	2.13	0.49
1:C:138:TYR:CE2	1:C:338:ARG:HG2	2.47	0.49
1:C:469:GLN:HB2	1:C:473:ARG:HG2	1.93	0.49
1:D:217:ALA:HB3	1:D:218:PRO:HD3	1.95	0.49
1:D:366:VAL:HG12	1:D:453:GLN:OE1	2.12	0.49
1:D:550:ASN:HB3	1:D:553:GLN:NE2	2.28	0.49
1:D:550:ASN:HB3	1:D:553:GLN:HE22	1.78	0.49
1:A:587:ALA:HA	1:A:590:LEU:HD12	1.95	0.49
1:B:84:HIS:HD2	1:B:206:ILE:HG12	1.78	0.49
1:D:127:PRO:O	1:D:131:MET:HG2	2.11	0.49
1:C:231:SER:C	1:C:233:SER:H	2.20	0.49
1:A:208:PRO:HB2	1:A:305:THR:HG21	1.95	0.49
1:C:421:VAL:HG11	1:C:583:ILE:HG13	1.95	0.49
1:C:465:CYS:HB2	1:C:680:PHE:CE1	2.48	0.49
1:D:595:LYS:C	1:D:597:PRO:HD3	2.37	0.49
1:B:102:SER:HA	1:B:107:TYR:CG	2.48	0.48
1:B:738:ARG:O	1:B:742:LYS:HD2	2.12	0.48
1:C:499:LYS:O	1:C:500:ASP:HB2	2.13	0.48
1:C:550:ASN:HB3	1:C:553:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:PHE:O	1:D:807:GLY:HA3	2.13	0.48
1:B:609:GLN:HE22	1:B:619:SER:HB3	1.78	0.48
1:C:272:PHE:HB3	1:C:286:PRO:HG3	1.94	0.48
1:D:328:PRO:O	1:D:332:ILE:HG13	2.13	0.48
1:D:376:LEU:HD12	1:D:404:PHE:HB3	1.96	0.48
1:A:329:GLN:CD	1:A:329:GLN:H	2.20	0.48
1:B:276:ASN:CB	2:F:19:GLN:NE2	2.74	0.48
1:B:285:ARG:NH2	1:B:288:VAL:HG21	2.28	0.48
1:D:49:GLY:O	1:D:78:TYR:HB2	2.13	0.48
1:A:469:GLN:HB2	1:A:473:ARG:HG2	1.96	0.48
1:B:446:PRO:HD2	1:B:806:THR:HG23	1.96	0.48
1:B:782:ILE:HG22	1:B:797:THR:HG22	1.96	0.48
2:E:23:LYS:C	2:E:25:ALA:H	2.22	0.48
1:B:55:LYS:CG	1:B:204:MET:HE3	2.43	0.48
1:B:68:SER:HA	1:B:73:CYS:SG	2.54	0.48
1:B:370:GLY:H	1:B:371:ALA:HA	1.78	0.48
1:B:663:ALA:C	1:B:664:LEU:HD12	2.39	0.48
1:C:386:ILE:HG13	1:C:620:ALA:HB3	1.94	0.48
1:C:595:LYS:C	1:C:597:PRO:HD3	2.38	0.48
1:D:587:ALA:HB1	1:D:592:ILE:HD11	1.95	0.48
1:A:205:LEU:HD22	1:A:207:LEU:O	2.14	0.48
1:A:456:ILE:HD11	1:A:581:VAL:HG11	1.95	0.47
1:C:626:THR:HG22	1:C:793:ALA:HB3	1.96	0.47
1:D:51:ARG:NH1	1:D:78:TYR:CE1	2.81	0.47
1:A:802:PRO:O	1:A:803:GLN:HB2	2.13	0.47
1:B:802:PRO:O	1:B:803:GLN:HB2	2.12	0.47
1:A:52:LYS:HA	1:A:61:THR:O	2.14	0.47
1:B:815:GLU:O	1:B:819:ILE:HG13	2.14	0.47
1:D:545:TYR:CE1	1:D:712:VAL:HG11	2.49	0.47
1:A:461:PHE:HA	1:A:679:ASP:OD2	2.14	0.47
1:A:662:ILE:HG21	1:A:694:PHE:HE2	1.78	0.47
1:B:348:GLU:OE1	1:B:348:GLU:HA	2.15	0.47
1:A:470:GLU:HA	1:A:471:GLY:HA2	1.58	0.47
1:C:51:ARG:NE	1:C:78:TYR:CE1	2.81	0.47
1:A:51:ARG:O	1:A:52:LYS:CB	2.62	0.47
1:A:120:ASN:O	1:A:225:PRO:HD2	2.15	0.47
1:A:727:LYS:HE3	1:A:731:GLN:OE1	2.15	0.47
1:B:76:ASN:C	1:B:76:ASN:HD22	2.22	0.47
1:C:153:LEU:HD13	1:C:157:ILE:HG21	1.97	0.47
1:C:274:GLN:O	1:C:277:GLU:HB2	2.15	0.47
1:D:383:LYS:HB2	1:D:621:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:LEU:N	1:D:664:LEU:HD12	2.30	0.47
1:A:456:ILE:CG2	1:A:577:PRO:HG2	2.42	0.47
1:D:85:LEU:O	1:D:205:LEU:HD23	2.15	0.47
1:A:715:GLY:O	1:A:718:VAL:HG13	2.14	0.47
1:A:212:LYS:HE2	5:A:1010:HOH:O	2.15	0.47
1:A:495:SER:HA	1:A:498:ARG:HG2	1.97	0.46
1:B:54:GLU:CG	1:B:55:LYS:N	2.77	0.46
1:B:276:ASN:CG	2:F:19:GLN:HE21	2.22	0.46
1:B:177:ILE:CG2	1:B:178:LYS:N	2.78	0.46
1:B:509:LEU:HA	1:B:556:ALA:HB2	1.97	0.46
1:A:459:HIS:CG	1:A:702:PRO:HB3	2.50	0.46
1:B:352:ILE:O	1:B:356:MET:HG3	2.16	0.46
1:C:85:LEU:O	1:C:205:LEU:HD23	2.16	0.46
1:B:668:TYR:CE2	1:B:747:PRO:HG3	2.51	0.46
1:C:545:TYR:CD1	1:C:712:VAL:HG11	2.51	0.46
2:E:22:THR:HG22	2:E:25:ALA:HB2	1.96	0.46
1:B:150:TRP:CZ2	1:B:346:VAL:HG21	2.50	0.46
1:A:216:ALA:HB2	1:A:316:ALA:HB2	1.98	0.46
1:A:370:GLY:HA2	1:A:371:ALA:C	2.40	0.46
1:B:215:VAL:HG21	1:B:317:LEU:HD21	1.97	0.46
1:A:193:VAL:HG13	1:A:343:ILE:HD13	1.96	0.46
1:B:725:ASP:OD2	1:B:728:GLN:HG3	2.14	0.46
1:C:603:TYR:CZ	1:C:641:PRO:HD2	2.50	0.46
1:C:608:VAL:HG21	1:C:623:VAL:HB	1.98	0.46
1:A:719:ALA:O	1:A:722:ARG:HG2	2.16	0.46
1:C:102:SER:HA	1:C:107:TYR:CD1	2.51	0.46
1:C:127:PRO:O	1:C:131:MET:HG2	2.15	0.46
1:C:378:LYS:HA	1:C:381:HIS:CD2	2.51	0.46
1:A:141:GLN:HB2	1:A:150:TRP:CE2	2.51	0.46
1:A:609:GLN:NE2	1:A:619:SER:HB3	2.31	0.46
1:B:526:ILE:HD11	1:D:302:ARG:HB3	1.97	0.46
1:C:576:THR:CG2	1:C:702:PRO:HG2	2.45	0.46
1:D:746:VAL:HA	1:D:747:PRO:HD3	1.86	0.46
1:A:530:GLU:O	1:A:534:GLN:HG3	2.16	0.46
1:C:364:THR:HA	1:C:400:GLN:HE22	1.80	0.46
1:C:730:LEU:HD22	1:C:730:LEU:O	2.16	0.45
1:A:662:ILE:HD12	1:A:729:VAL:HG12	1.97	0.45
1:A:721:VAL:HG23	1:A:724:LEU:HD12	1.97	0.45
1:A:743:GLU:CD	1:A:743:GLU:H	2.24	0.45
1:A:464:ARG:HH22	1:A:676:GLN:HB2	1.81	0.45
1:A:704:LYS:HD2	1:A:704:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:GLN:O	3:A:901:FAD:O3'	2.35	0.45
1:B:205:LEU:HD22	1:B:207:LEU:O	2.16	0.45
1:B:276:ASN:HA	2:F:19:GLN:CG	2.46	0.45
1:B:299:GLU:HA	1:D:526:ILE:HD12	1.97	0.45
1:D:76:ASN:H	1:D:76:ASN:ND2	2.13	0.45
1:D:473:ARG:H	1:D:473:ARG:HD2	1.81	0.45
1:B:655:GLY:HA3	1:B:769:PHE:CZ	2.51	0.45
1:C:123:THR:HG23	1:C:226:ASP:OD2	2.17	0.45
1:C:412:GLU:CD	3:C:901:FAD:O3B	2.59	0.45
1:D:101:ARG:HB2	1:D:104:LYS:HG2	1.98	0.45
1:B:54:GLU:HG2	1:B:55:LYS:H	1.80	0.45
1:B:395:LEU:HD12	1:B:583:ILE:HG23	1.99	0.45
1:C:101:ARG:HB2	1:C:104:LYS:HG2	1.97	0.45
1:D:691:ARG:HG3	1:D:691:ARG:O	2.16	0.45
1:A:76:ASN:H	1:A:76:ASN:ND2	2.14	0.45
1:C:507:VAL:HG21	1:C:512:LYS:HE2	1.99	0.45
1:C:815:GLU:O	1:C:819:ILE:HG13	2.17	0.45
1:A:669:ARG:CG	1:A:707:SER:HB3	2.46	0.45
1:B:587:ALA:HA	1:B:590:LEU:HD12	1.97	0.45
1:C:273:TYR:CD1	1:C:283:CYS:HB3	2.52	0.45
1:D:349:VAL:O	1:D:353:LEU:HB2	2.17	0.45
1:D:456:ILE:CG2	1:D:577:PRO:HG2	2.46	0.45
1:D:805:VAL:HG23	3:D:901:FAD:H2'	1.99	0.45
1:A:101:ARG:HB3	1:A:103:HIS:CE1	2.52	0.45
1:B:117:TRP:CZ3	1:B:232:PRO:HD2	2.52	0.45
1:B:410:VAL:CG1	1:B:592:ILE:HG12	2.47	0.45
1:D:274:GLN:HB3	1:D:275:PRO:HD2	1.98	0.45
1:D:544:GLU:HG2	1:D:551:LEU:HG	1.99	0.45
1:A:285:ARG:HA	1:A:286:PRO:HD3	1.78	0.45
1:B:461:PHE:CE2	1:B:574:LEU:HB2	2.52	0.45
1:D:300:TYR:OH	1:D:348:GLU:HG3	2.17	0.45
1:A:443:ILE:HG13	1:A:570:GLY:HA3	1.99	0.45
1:C:534:GLN:HB3	1:C:684:VAL:HG12	1.99	0.45
1:D:151:ARG:NH2	1:D:189:GLU:HA	2.32	0.45
1:A:369:VAL:CG1	1:A:403:ASN:HA	2.47	0.44
1:B:775:SER:OG	1:B:777:GLU:HG3	2.15	0.44
1:C:366:VAL:O	1:C:366:VAL:HG13	2.17	0.44
1:D:459:HIS:CE1	1:D:702:PRO:HB3	2.52	0.44
1:A:524:SER:OG	1:A:526:ILE:HG22	2.17	0.44
1:A:661:LYS:HE3	3:A:901:FAD:H6	2.00	0.44
1:C:346:VAL:O	1:C:349:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:VAL:HA	1:C:370:GLY:HA3	1.65	0.44
1:C:487:PHE:CE1	1:C:540:LEU:HD13	2.51	0.44
1:C:801:PHE:O	1:C:807:GLY:HA3	2.17	0.44
1:D:66:PHE:HE2	1:D:131:MET:HE3	1.81	0.44
1:D:265:MET:O	1:D:266:ASN:CB	2.65	0.44
1:D:385:VAL:HB	1:D:622:LYS:HB2	1.99	0.44
1:D:395:LEU:HD12	1:D:583:ILE:HG23	1.99	0.44
1:A:209:PRO:HG3	1:A:341:VAL:HG21	1.99	0.44
1:A:669:ARG:HG2	1:A:707:SER:HB3	1.99	0.44
1:A:677:GLY:O	1:A:678:ALA:C	2.58	0.44
1:B:198:ASN:HB3	1:B:200:TRP:NE1	2.31	0.44
1:B:576:THR:OG1	1:B:577:PRO:HD3	2.17	0.44
1:B:609:GLN:NE2	1:B:619:SER:HB3	2.32	0.44
1:C:607:GLU:OE2	1:C:608:VAL:O	2.36	0.44
1:D:540:LEU:HD12	1:D:540:LEU:HA	1.85	0.44
1:B:332:ILE:HB	1:B:333:PRO:HD3	1.98	0.44
1:B:664:LEU:HD12	1:B:664:LEU:N	2.32	0.44
1:D:418:GLY:HA2	1:D:583:ILE:HG21	2.00	0.44
1:A:609:GLN:HE22	1:A:619:SER:HB3	1.82	0.44
1:A:662:ILE:HG21	1:A:694:PHE:CE2	2.53	0.44
1:C:91:PHE:CE2	1:C:131:MET:HG3	2.53	0.44
1:D:51:ARG:HB3	1:D:82:TRP:HE1	1.83	0.44
1:D:76:ASN:H	1:D:76:ASN:HD22	1.66	0.44
1:D:791:PHE:CE1	1:D:819:ILE:HG12	2.52	0.44
1:A:777:GLU:O	1:A:781:ILE:HG13	2.18	0.44
1:C:228:VAL:CG2	1:C:230:MET:HE2	2.48	0.44
1:C:266:ASN:HB3	1:C:269:PHE:CD2	2.53	0.44
1:C:470:GLU:HA	1:C:471:GLY:HA2	1.58	0.44
1:D:387:ILE:O	1:D:410:VAL:HA	2.18	0.44
1:D:524:SER:O	1:D:526:ILE:HG22	2.18	0.44
1:C:228:VAL:HG21	1:C:230:MET:HE2	1.99	0.44
1:C:663:ALA:C	1:C:664:LEU:HD12	2.43	0.44
1:C:725:ASP:OD2	1:C:728:GLN:HG3	2.18	0.44
1:A:382:ASN:CG	1:A:382:ASN:O	2.61	0.43
1:A:369:VAL:HG11	1:A:403:ASN:HA	2.00	0.43
1:A:520:PHE:CE1	1:C:298:PRO:HB3	2.53	0.43
1:B:298:PRO:HB2	1:D:524:SER:CB	2.47	0.43
1:D:469:GLN:HB2	1:D:473:ARG:CG	2.48	0.43
2:F:16:PRO:C	2:F:17:ARG:O	2.55	0.43
1:A:72:ARG:CG	1:A:72:ARG:NH1	2.80	0.43
1:B:175:THR:O	1:B:177:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TRP:H	1:B:200:TRP:CD1	2.35	0.43
1:A:328:PRO:O	1:A:332:ILE:HG13	2.18	0.43
1:D:215:VAL:HG21	1:D:317:LEU:HD21	1.99	0.43
1:D:506:ASP:OD2	1:D:557:ARG:HG3	2.18	0.43
2:F:2:ARG:HD3	2:F:10:SER:O	2.19	0.43
1:A:144:LYS:HG2	1:A:168:ARG:HD3	2.00	0.43
1:B:663:ALA:HB3	1:B:753:PHE:CE2	2.53	0.43
1:C:193:VAL:HG13	1:C:343:ILE:HD13	2.01	0.43
1:C:437:GLN:O	1:C:437:GLN:HG2	2.19	0.43
1:D:169:CYS:HB2	1:D:185:CYS:SG	2.59	0.43
1:D:215:VAL:O	1:D:218:PRO:HD2	2.18	0.43
1:D:509:LEU:O	1:D:513:ILE:HG13	2.18	0.43
1:D:545:TYR:HD1	1:D:712:VAL:HG11	1.83	0.43
1:A:647:LYS:O	1:A:651:ILE:HG13	2.18	0.43
1:A:815:GLU:O	1:A:819:ILE:HG13	2.17	0.43
1:B:102:SER:HA	1:B:107:TYR:CD1	2.54	0.43
1:B:276:ASN:CA	2:F:19:GLN:NE2	2.71	0.43
1:B:493:VAL:HG11	1:B:516:ILE:HG21	2.00	0.43
1:C:429:GLY:O	1:C:430:VAL:HG23	2.18	0.43
1:D:821:ALA:O	1:D:822:PHE:C	2.61	0.43
1:B:470:GLU:HA	1:B:471:GLY:HA2	1.54	0.43
1:D:684:VAL:HA	1:D:685:PRO:HD3	1.90	0.43
1:A:685:PRO:HA	1:A:686:PRO:HD3	1.91	0.43
1:B:503:GLN:O	1:B:506:ASP:HB2	2.19	0.43
1:C:72:ARG:CG	1:C:72:ARG:NH1	2.62	0.43
1:D:76:ASN:HD22	1:D:76:ASN:N	2.17	0.43
1:D:274:GLN:HB2	1:D:277:GLU:HG3	1.99	0.43
1:A:49:GLY:O	1:A:78:TYR:HB2	2.19	0.43
1:B:456:ILE:HD11	1:B:581:VAL:HG11	2.00	0.43
1:B:734:MET:O	1:B:738:ARG:HG3	2.19	0.43
1:B:366:VAL:CG2	1:B:585:LYS:HB3	2.49	0.43
1:B:495:SER:HA	1:B:498:ARG:CD	2.49	0.43
1:C:142:CYS:SG	1:C:168:ARG:HA	2.59	0.43
1:A:558:SER:HB2	1:A:770:VAL:HG11	2.01	0.42
1:B:52:LYS:HB2	1:B:61:THR:HA	2.00	0.42
1:B:704:LYS:N	1:B:704:LYS:HD2	2.34	0.42
1:C:684:VAL:HA	1:C:685:PRO:HD3	1.86	0.42
1:D:356:MET:HB2	1:D:362:ILE:HG12	2.01	0.42
1:A:348:GLU:OE1	1:A:351:ARG:HD3	2.19	0.42
1:C:412:GLU:CD	3:C:901:FAD:HO3A	2.26	0.42
1:A:151:ARG:NH1	1:A:169:CYS:SG	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:ND2	1:A:452:GLU:HG2	2.26	0.42
1:B:81:ARG:HG3	1:B:82:TRP:N	2.32	0.42
1:B:127:PRO:O	1:B:131:MET:HG2	2.19	0.42
1:C:738:ARG:HG2	1:C:746:VAL:CG2	2.50	0.42
1:D:139:TRP:O	1:D:342:ARG:HD3	2.19	0.42
1:A:344:ARG:HA	1:A:344:ARG:HD3	1.93	0.42
1:D:725:ASP:O	1:D:729:VAL:HG23	2.20	0.42
1:A:208:PRO:HB3	1:A:305:THR:HG21	2.02	0.42
1:A:480:ASP:OD2	2:E:8:ARG:NH2	2.50	0.42
1:B:144:LYS:HG3	1:B:168:ARG:HD3	2.02	0.42
1:B:224:TYR:CD1	2:F:26:ARG:HG3	2.54	0.42
1:B:465:CYS:HB2	1:B:680:PHE:CE1	2.55	0.42
1:D:399:ARG:HD2	1:D:586:LEU:O	2.20	0.42
1:A:57:GLY:O	1:A:204:MET:HE1	2.20	0.42
1:C:746:VAL:HA	1:C:747:PRO:HD3	1.88	0.42
1:B:115:LYS:C	1:B:115:LYS:HD3	2.45	0.42
1:B:172:LYS:C	1:B:174:ASN:H	2.27	0.42
1:C:117:TRP:CH2	1:C:232:PRO:HD2	2.55	0.42
1:C:329:GLN:CD	1:C:329:GLN:H	2.27	0.42
1:A:168:ARG:O	1:A:171:MET:HB2	2.20	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.85	0.42
1:B:677:GLY:HA2	1:B:704:LYS:HZ2	1.84	0.42
1:B:721:VAL:HA	1:B:724:LEU:HG	2.01	0.42
1:B:136:LEU:HD23	1:B:137:PRO:HD2	2.01	0.42
1:B:385:VAL:HB	1:B:622:LYS:HB2	2.02	0.42
1:C:144:LYS:HA	1:C:145:PRO:HD3	1.83	0.42
1:C:280:LYS:O	1:C:283:CYS:HB2	2.20	0.42
1:C:446:PRO:CG	1:C:810:LEU:HD21	2.50	0.42
1:B:395:LEU:CD1	1:B:583:ILE:HG23	2.50	0.42
1:B:465:CYS:HB2	1:B:680:PHE:HE1	1.83	0.42
1:C:285:ARG:HA	1:C:286:PRO:HD3	1.87	0.42
1:A:85:LEU:O	1:A:205:LEU:HD23	2.20	0.41
1:B:63:PRO:HB2	1:B:82:TRP:CE2	2.55	0.41
1:B:524:SER:OG	1:B:526:ILE:HG22	2.19	0.41
1:C:369:VAL:HG23	1:C:370:GLY:O	2.20	0.41
1:C:627:VAL:HG23	1:C:632:LEU:HG	2.01	0.41
1:A:599:GLN:HB2	1:A:613:THR:HG22	2.02	0.41
1:A:753:PHE:CD1	1:A:753:PHE:C	2.98	0.41
1:B:486:HIS:CE1	1:D:301:SER:CB	3.03	0.41
1:B:738:ARG:HG2	1:B:746:VAL:HG22	2.00	0.41
1:C:470:GLU:HB3	1:C:739:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:TRP:CZ3	1:C:763:ILE:HD12	2.53	0.41
1:D:86:SER:OG	1:D:89:GLU:HB2	2.20	0.41
1:D:285:ARG:HA	1:D:286:PRO:HD3	1.84	0.41
1:D:470:GLU:HA	1:D:471:GLY:HA2	1.62	0.41
1:B:277:GLU:OE2	1:B:280:LYS:HE2	2.20	0.41
1:B:567:GLN:HG3	2:F:3:THR:HG21	2.02	0.41
1:B:669:ARG:CG	1:B:707:SER:HB3	2.50	0.41
1:D:150:TRP:CD2	1:D:343:ILE:HG12	2.56	0.41
1:A:273:TYR:HD1	1:A:285:ARG:HG2	1.86	0.41
1:B:296:GLU:HG2	1:B:355:PHE:CD1	2.56	0.41
1:C:115:LYS:HD3	1:C:116:ILE:N	2.35	0.41
1:C:509:LEU:O	1:C:513:ILE:HG13	2.20	0.41
1:D:497:TRP:O	1:D:501:LYS:NZ	2.52	0.41
1:D:802:PRO:O	1:D:803:GLN:HB2	2.20	0.41
1:C:52:LYS:NZ	1:C:52:LYS:HB2	2.36	0.41
1:C:266:ASN:OD1	1:C:268:TYR:HB2	2.20	0.41
1:C:269:PHE:O	1:C:271:PRO:HD3	2.21	0.41
1:D:310:LEU:HD22	1:D:349:VAL:HG23	2.01	0.41
1:D:343:ILE:O	1:D:347:GLN:HG3	2.21	0.41
1:B:375:LEU:O	1:B:376:LEU:HD23	2.20	0.41
1:C:385:VAL:HG13	1:C:408:VAL:HG22	2.03	0.41
1:C:387:ILE:O	1:C:410:VAL:HA	2.21	0.41
1:C:703:GLN:O	1:C:704:LYS:HB2	2.20	0.41
1:D:73:CYS:O	1:D:75:LYS:HG2	2.20	0.41
1:D:498:ARG:O	1:D:499:LYS:C	2.62	0.41
1:D:627:VAL:HG23	1:D:632:LEU:HG	2.02	0.41
1:D:659:ILE:HD13	1:D:767:TYR:OH	2.21	0.41
1:A:142:CYS:O	1:A:148:ARG:HD2	2.20	0.41
1:B:546:ALA:HB2	2:F:5:GLN:HG3	2.03	0.41
1:D:303:ASP:HB3	5:D:1001:HOH:O	2.21	0.41
1:D:369:VAL:HA	1:D:370:GLY:HA3	1.71	0.41
1:D:459:HIS:CG	1:D:702:PRO:HB3	2.55	0.41
1:A:109:LYS:HE2	1:A:135:GLN:OE1	2.21	0.41
1:A:401:LEU:HB2	1:A:408:VAL:HG21	2.03	0.41
1:A:760:ASP:HA	1:A:761:PRO:HD3	1.89	0.41
1:B:326:LEU:HA	1:B:330:LYS:HD2	2.02	0.41
1:B:344:ARG:HA	1:B:344:ARG:HD3	1.93	0.41
1:C:52:LYS:NZ	1:C:52:LYS:CB	2.84	0.41
1:C:76:ASN:HD22	1:C:76:ASN:N	2.06	0.41
1:D:479:ILE:HG12	1:D:482:ARG:HH12	1.86	0.41
1:B:423:ASP:OD1	1:B:578:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ILE:HG13	1:B:570:GLY:HA3	2.03	0.41
1:B:628:PRO:HG2	1:B:763:ILE:HA	2.02	0.41
1:B:738:ARG:HG2	1:B:746:VAL:CG2	2.50	0.41
1:B:783:ALA:HB2	1:B:797:THR:HB	2.03	0.41
1:C:667:PRO:HD2	1:C:747:PRO:HB2	2.01	0.41
1:D:166:THR:O	1:D:167:TYR:C	2.64	0.41
1:D:366:VAL:HG21	1:D:585:LYS:HB3	2.02	0.41
1:D:443:ILE:O	1:D:444:ASN:HB2	2.21	0.41
1:D:658:ILE:HG12	1:D:758:SER:HB2	2.02	0.41
1:D:663:ALA:C	1:D:664:LEU:HD12	2.46	0.41
1:D:667:PRO:HD2	1:D:747:PRO:HB2	2.01	0.41
1:A:207:LEU:HA	1:A:208:PRO:HD3	1.91	0.41
1:A:314:ILE:CG2	1:A:362:ILE:HD13	2.51	0.41
1:A:392:PRO:HD3	1:A:418:GLY:O	2.21	0.41
1:A:664:LEU:HD12	1:A:664:LEU:N	2.36	0.41
1:B:328:PRO:HD3	1:B:353:LEU:HD23	2.02	0.41
1:B:521:ILE:HD11	1:B:528:PHE:HE2	1.86	0.41
1:D:215:VAL:HG21	1:D:317:LEU:CD2	2.51	0.41
2:F:22:THR:CG2	2:F:25:ALA:HB2	2.49	0.41
1:B:420:ARG:HH12	1:B:765:MET:HE2	1.86	0.40
1:B:545:TYR:CD1	1:B:712:VAL:HG11	2.57	0.40
1:B:548:GLY:O	1:B:657:GLY:HA2	2.21	0.40
1:C:76:ASN:H	1:C:76:ASN:ND2	2.16	0.40
1:D:470:GLU:HB3	1:D:739:GLU:OE1	2.20	0.40
1:A:385:VAL:HB	1:A:622:LYS:HB2	2.03	0.40
1:A:399:ARG:O	1:A:399:ARG:HG3	2.20	0.40
1:A:596:SER:N	1:A:597:PRO:HD3	2.37	0.40
1:B:276:ASN:CG	2:F:19:GLN:NE2	2.80	0.40
1:B:439:VAL:HG22	1:B:579:TYR:OH	2.21	0.40
1:D:223:TYR:CE2	1:D:286:PRO:HG2	2.57	0.40
1:D:381:HIS:CD2	1:D:381:HIS:N	2.89	0.40
1:D:608:VAL:HG21	1:D:623:VAL:HB	2.03	0.40
1:D:815:GLU:O	1:D:819:ILE:HG13	2.21	0.40
1:A:332:ILE:HB	1:A:333:PRO:HD3	2.04	0.40
1:A:576:THR:CG2	1:A:702:PRO:HG2	2.52	0.40
1:B:151:ARG:NH1	1:B:169:CYS:SG	2.89	0.40
1:C:51:ARG:CD	1:C:79:THR:O	2.58	0.40
1:D:278:CYS:O	1:D:279:GLY:C	2.64	0.40
1:D:342:ARG:O	1:D:346:VAL:HG13	2.21	0.40
1:D:354:TYR:CE2	1:D:377:PRO:HG3	2.57	0.40
1:D:476:ASP:HA	1:D:477:PRO:HD2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:THR:O	1:B:482:ARG:HB2	2.22	0.40
1:D:124:GLU:HA	1:D:125:PRO:HD3	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/776 (96%)	682 (92%)	56 (8%)	6 (1%)	16	47
1	B	744/776 (96%)	695 (93%)	38 (5%)	11 (2%)	8	32
1	C	730/776 (94%)	677 (93%)	50 (7%)	3 (0%)	30	61
1	D	729/776 (94%)	678 (93%)	45 (6%)	6 (1%)	16	47
2	E	24/26 (92%)	20 (83%)	4 (17%)	0	100	100
2	F	24/26 (92%)	20 (83%)	3 (12%)	1 (4%)	2	13
All	All	2995/3156 (95%)	2772 (93%)	196 (6%)	27 (1%)	14	44

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	LYS
1	A	177	ILE
1	A	373	GLN
1	B	50	SER
1	B	51	ARG
1	B	53	CYS
1	B	176	ALA
1	B	177	ILE
1	D	266	ASN

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Mol	Chain	Res	Type
1	B	52	LYS
1	C	369	VAL
1	D	369	VAL
1	D	526	ILE
1	A	437	GLN
1	B	175	THR
1	B	437	GLN
1	C	437	GLN
1	D	275	PRO
1	D	437	GLN
1	A	372	ASP
1	D	743	GLU
1	C	232	PRO
2	F	17	ARG
1	B	178	LYS
1	B	369	VAL
1	B	441	GLY

5.3.2 Protein sidechains [i](#)

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	642/662 (97%)	599 (93%)	43 (7%)	15	43
1	B	642/662 (97%)	601 (94%)	41 (6%)	16	44
1	C	631/662 (95%)	597 (95%)	34 (5%)	20	50
1	D	630/662 (95%)	594 (94%)	36 (6%)	18	49
2	E	18/18 (100%)	14 (78%)	4 (22%)	1	4
2	F	18/18 (100%)	14 (78%)	4 (22%)	1	4
All	All	2581/2684 (96%)	2419 (94%)	162 (6%)	16	45

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	55	LYS
1	A	62	CYS
1	A	76	ASN
1	A	80	SER
1	A	81	ARG
1	A	85	LEU
1	A	94	GLU
1	A	151	ARG
1	A	154	THR
1	A	174	ASN
1	A	194	LEU
1	A	197	SER
1	A	205	LEU
1	A	234	CYS
1	A	283	CYS
1	A	294	LEU
1	A	302	ARG
1	A	308	LEU
1	A	320	THR
1	A	329	GLN
1	A	356	MET
1	A	366	VAL
1	A	379	ASP
1	A	385	VAL
1	A	399	ARG
1	A	410	VAL
1	A	430	VAL
1	A	473	ARG
1	A	498	ARG
1	A	507	VAL
1	A	514	GLU
1	A	527	GLN
1	A	540	LEU
1	A	554	VAL
1	A	608	VAL
1	A	625	VAL
1	A	704	LYS
1	A	718	VAL
1	A	730	LEU
1	A	740	LEU
1	A	743	GLU
1	A	746	VAL

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Mol	Chain	Res	Type
1	B	51	ARG
1	B	76	ASN
1	B	81	ARG
1	B	85	LEU
1	B	94	GLU
1	B	151	ARG
1	B	162	GLN
1	B	175	THR
1	B	177	ILE
1	B	178	LYS
1	B	194	LEU
1	B	205	LEU
1	B	273	TYR
1	B	283	CYS
1	B	292	ASP
1	B	294	LEU
1	B	301	SER
1	B	308	LEU
1	B	320	THR
1	B	366	VAL
1	B	369	VAL
1	B	385	VAL
1	B	410	VAL
1	B	430	VAL
1	B	469	GLN
1	B	473	ARG
1	B	498	ARG
1	B	501	LYS
1	B	527	GLN
1	B	540	LEU
1	B	554	VAL
1	B	576	THR
1	B	608	VAL
1	B	625	VAL
1	B	718	VAL
1	B	724	LEU
1	B	726	ASP
1	B	730	LEU
1	B	740	LEU
1	B	743	GLU
1	B	746	VAL
1	C	51	ARG

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Mol	Chain	Res	Type
1	C	52	LYS
1	C	72	ARG
1	C	76	ASN
1	C	120	ASN
1	C	146	GLU
1	C	151	ARG
1	C	194	LEU
1	C	205	LEU
1	C	283	CYS
1	C	294	LEU
1	C	308	LEU
1	C	311	ARG
1	C	329	GLN
1	C	366	VAL
1	C	379	ASP
1	C	385	VAL
1	C	410	VAL
1	C	430	VAL
1	C	467	LEU
1	C	473	ARG
1	C	482	ARG
1	C	493	VAL
1	C	523	GLU
1	C	530	GLU
1	C	540	LEU
1	C	608	VAL
1	C	625	VAL
1	C	718	VAL
1	C	721	VAL
1	C	730	LEU
1	C	740	LEU
1	C	743	GLU
1	C	746	VAL
1	D	76	ASN
1	D	87	CYS
1	D	151	ARG
1	D	183	ASP
1	D	184	HIS
1	D	194	LEU
1	D	205	LEU
1	D	283	CYS
1	D	294	LEU

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Mol	Chain	Res	Type
1	D	302	ARG
1	D	308	LEU
1	D	329	GLN
1	D	346	VAL
1	D	356	MET
1	D	379	ASP
1	D	385	VAL
1	D	410	VAL
1	D	467	LEU
1	D	473	ARG
1	D	493	VAL
1	D	498	ARG
1	D	502	THR
1	D	527	GLN
1	D	530	GLU
1	D	553	GLN
1	D	554	VAL
1	D	576	THR
1	D	625	VAL
1	D	638	GLN
1	D	704	LYS
1	D	721	VAL
1	D	724	LEU
1	D	730	LEU
1	D	740	LEU
1	D	743	GLU
1	D	746	VAL
2	E	11	THR
2	E	18	LYS
2	E	20	LEU
2	E	22	THR
2	F	17	ARG
2	F	18	LYS
2	F	20	LEU
2	F	22	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	134	GLN
1	A	158	GLN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	503	GLN
1	A	527	GLN
1	A	553	GLN
1	A	593	GLN
1	A	609	GLN
1	A	638	GLN
1	A	665	GLN
1	A	683	HIS
1	A	706	HIS
1	A	732	GLN
1	B	76	ASN
1	B	93	ASN
1	B	103	HIS
1	B	134	GLN
1	B	162	GLN
1	B	321	ASN
1	B	400	GLN
1	B	486	HIS
1	B	503	GLN
1	B	527	GLN
1	B	553	GLN
1	B	593	GLN
1	B	609	GLN
1	B	683	HIS
1	B	706	HIS
1	B	732	GLN
1	C	76	ASN
1	C	120	ASN
1	C	134	GLN
1	C	158	GLN
1	C	162	GLN
1	C	199	HIS
1	C	329	GLN
1	C	400	GLN
1	C	440	ASN
1	C	503	GLN
1	C	527	GLN
1	C	552	HIS
1	C	553	GLN
1	C	562	ASN
1	C	593	GLN

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Mol	Chain	Res	Type
1	C	599	GLN
1	C	731	GLN
1	C	732	GLN
1	D	76	ASN
1	D	93	ASN
1	D	134	GLN
1	D	135	GLN
1	D	162	GLN
1	D	199	HIS
1	D	440	ASN
1	D	503	GLN
1	D	553	GLN
1	D	593	GLN
1	D	609	GLN
1	D	638	GLN
1	D	706	HIS
1	D	728	GLN
1	D	732	GLN
2	E	19	GLN
2	F	19	GLN

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](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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	901	-	58,58,58	3.24	31 (53%)	85,89,89	1.83	20 (23%)
3	FAD	B	901	-	58,58,58	3.25	31 (53%)	85,89,89	1.83	20 (23%)
3	FAD	C	901	-	58,58,58	3.25	31 (53%)	85,89,89	1.83	20 (23%)
3	FAD	D	901	-	58,58,58	3.25	31 (53%)	85,89,89	1.83	20 (23%)

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	901	-	-	2/34/50/50	0/6/6/6
3	FAD	B	901	-	-	2/34/50/50	0/6/6/6
3	FAD	C	901	-	-	2/34/50/50	0/6/6/6
3	FAD	D	901	-	-	2/34/50/50	0/6/6/6

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	FAD	PA-O3P	-12.75	1.45	1.59
3	D	901	FAD	PA-O3P	-12.74	1.45	1.59
3	B	901	FAD	PA-O3P	-12.71	1.45	1.59
3	A	901	FAD	PA-O3P	-12.71	1.45	1.59
3	B	901	FAD	P-O3P	-11.24	1.47	1.59
3	A	901	FAD	P-O3P	-11.18	1.47	1.59
3	D	901	FAD	P-O3P	-11.18	1.47	1.59
3	C	901	FAD	P-O3P	-11.16	1.47	1.59
3	B	901	FAD	C5A-N7A	-5.36	1.29	1.39
3	D	901	FAD	C5A-N7A	-5.36	1.29	1.39
3	A	901	FAD	C5A-N7A	-5.34	1.29	1.39
3	C	901	FAD	C5A-N7A	-5.32	1.29	1.39
3	C	901	FAD	PA-O5B	-5.21	1.39	1.59
3	A	901	FAD	PA-O5B	-5.19	1.39	1.59
3	B	901	FAD	PA-O5B	-5.19	1.39	1.59
3	D	901	FAD	PA-O5B	-5.18	1.39	1.59
3	D	901	FAD	C8A-N9A	-4.12	1.30	1.37
3	A	901	FAD	C8A-N9A	-4.09	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	FAD	C8A-N9A	-4.08	1.30	1.37
3	B	901	FAD	C8A-N9A	-4.08	1.30	1.37
3	A	901	FAD	PA-O1A	-4.03	1.36	1.50
3	D	901	FAD	PA-O1A	-4.01	1.36	1.50
3	C	901	FAD	PA-O1A	-4.00	1.36	1.50
3	B	901	FAD	PA-O1A	-4.00	1.37	1.50
3	C	901	FAD	P-O2P	-3.89	1.37	1.55
3	A	901	FAD	P-O2P	-3.88	1.37	1.55
3	B	901	FAD	P-O2P	-3.86	1.37	1.55
3	D	901	FAD	P-O2P	-3.85	1.37	1.55
3	D	901	FAD	PA-O2A	-3.63	1.38	1.55
3	A	901	FAD	PA-O2A	-3.63	1.38	1.55
3	B	901	FAD	PA-O2A	-3.63	1.38	1.55
3	C	901	FAD	PA-O2A	-3.63	1.38	1.55
3	D	901	FAD	P-O1P	-3.60	1.38	1.50
3	B	901	FAD	P-O1P	-3.59	1.38	1.50
3	C	901	FAD	P-O1P	-3.58	1.38	1.50
3	A	901	FAD	P-O1P	-3.56	1.38	1.50
3	B	901	FAD	C5X-N5	-3.45	1.33	1.39
3	D	901	FAD	C5X-N5	-3.45	1.33	1.39
3	C	901	FAD	C5X-N5	-3.41	1.33	1.39
3	A	901	FAD	C5X-N5	-3.39	1.33	1.39
3	D	901	FAD	C4A-N9A	-3.30	1.30	1.37
3	C	901	FAD	C4A-N9A	-3.29	1.30	1.37
3	A	901	FAD	C4A-N9A	-3.26	1.30	1.37
3	B	901	FAD	C4A-N9A	-3.25	1.30	1.37
3	D	901	FAD	P-O5'	-3.20	1.46	1.59
3	B	901	FAD	P-O5'	-3.19	1.46	1.59
3	A	901	FAD	P-O5'	-3.19	1.46	1.59
3	C	901	FAD	P-O5'	-3.18	1.46	1.59
3	D	901	FAD	C5A-C4A	-2.92	1.33	1.39
3	C	901	FAD	C5A-C4A	-2.89	1.33	1.39
3	A	901	FAD	C5A-C4A	-2.86	1.34	1.39
3	B	901	FAD	C5A-C4A	-2.86	1.34	1.39
3	D	901	FAD	C2-N3	-2.84	1.32	1.39
3	A	901	FAD	C2-N3	-2.83	1.32	1.39
3	B	901	FAD	C2-N3	-2.83	1.32	1.39
3	C	901	FAD	C2-N3	-2.83	1.32	1.39
3	C	901	FAD	O3'-C3'	-2.68	1.36	1.43
3	A	901	FAD	C2A-N1A	-2.68	1.29	1.33
3	D	901	FAD	O3'-C3'	-2.67	1.36	1.43
3	B	901	FAD	C2A-N1A	-2.67	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	FAD	O3'-C3'	-2.66	1.36	1.43
3	A	901	FAD	O4B-C1B	-2.65	1.35	1.42
3	D	901	FAD	O4B-C1B	-2.65	1.35	1.42
3	B	901	FAD	O4B-C1B	-2.65	1.35	1.42
3	C	901	FAD	C2A-N1A	-2.65	1.29	1.33
3	A	901	FAD	O3'-C3'	-2.64	1.36	1.43
3	C	901	FAD	O4B-C1B	-2.64	1.35	1.42
3	A	901	FAD	C4X-C10	-2.61	1.36	1.44
3	C	901	FAD	C4X-C10	-2.60	1.36	1.44
3	B	901	FAD	C4X-C10	-2.59	1.36	1.44
3	D	901	FAD	C9A-C5X	-2.59	1.37	1.41
3	D	901	FAD	C4X-C10	-2.59	1.36	1.44
3	D	901	FAD	C2A-N1A	-2.59	1.29	1.33
3	B	901	FAD	O5B-C5B	-2.57	1.34	1.44
3	A	901	FAD	C9A-C5X	-2.57	1.37	1.41
3	C	901	FAD	O5B-C5B	-2.56	1.34	1.44
3	D	901	FAD	O5B-C5B	-2.56	1.34	1.44
3	A	901	FAD	O5B-C5B	-2.55	1.34	1.44
3	C	901	FAD	C9A-C5X	-2.55	1.37	1.41
3	C	901	FAD	C9-C8	-2.53	1.36	1.39
3	B	901	FAD	C9A-C5X	-2.53	1.37	1.41
3	D	901	FAD	C9-C8	-2.52	1.36	1.39
3	A	901	FAD	O2-C2	-2.50	1.19	1.24
3	B	901	FAD	C9-C8	-2.48	1.36	1.39
3	A	901	FAD	C9-C8	-2.48	1.36	1.39
3	C	901	FAD	O4'-C4'	-2.46	1.38	1.43
3	B	901	FAD	O4'-C4'	-2.46	1.38	1.43
3	A	901	FAD	O4'-C4'	-2.46	1.38	1.43
3	D	901	FAD	O4'-C4'	-2.45	1.38	1.43
3	D	901	FAD	O2-C2	-2.44	1.19	1.24
3	C	901	FAD	O2-C2	-2.43	1.19	1.24
3	A	901	FAD	C6-C5X	-2.43	1.36	1.40
3	B	901	FAD	C6-C5X	-2.42	1.36	1.40
3	B	901	FAD	C4-N3	-2.41	1.34	1.38
3	B	901	FAD	O2-C2	-2.41	1.19	1.24
3	C	901	FAD	C6-C5X	-2.41	1.36	1.40
3	A	901	FAD	C4-N3	-2.40	1.34	1.38
3	C	901	FAD	C4-N3	-2.36	1.34	1.38
3	D	901	FAD	C6-C5X	-2.35	1.36	1.40
3	D	901	FAD	C4-N3	-2.34	1.34	1.38
3	B	901	FAD	C9-C9A	-2.33	1.35	1.39
3	A	901	FAD	C9-C9A	-2.32	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	FAD	C6A-N6A	-2.32	1.28	1.34
3	D	901	FAD	C9-C9A	-2.31	1.35	1.39
3	B	901	FAD	C6A-N6A	-2.30	1.28	1.34
3	D	901	FAD	C6A-N6A	-2.30	1.28	1.34
3	C	901	FAD	C6A-N6A	-2.29	1.28	1.34
3	B	901	FAD	C4X-C4	-2.29	1.36	1.44
3	C	901	FAD	C4X-C4	-2.29	1.36	1.44
3	D	901	FAD	C4X-C4	-2.29	1.36	1.44
3	C	901	FAD	C9-C9A	-2.29	1.35	1.39
3	A	901	FAD	C4X-C4	-2.27	1.36	1.44
3	C	901	FAD	C6-C7	-2.25	1.36	1.39
3	A	901	FAD	C6-C7	-2.24	1.36	1.39
3	D	901	FAD	C6-C7	-2.24	1.36	1.39
3	B	901	FAD	C6-C7	-2.18	1.36	1.39
3	C	901	FAD	C9A-N10	-2.11	1.37	1.41
3	D	901	FAD	C9A-N10	-2.10	1.37	1.41
3	A	901	FAD	C2A-N3A	-2.08	1.30	1.33
3	B	901	FAD	C9A-N10	-2.08	1.37	1.41
3	D	901	FAD	C2A-N3A	-2.08	1.30	1.33
3	A	901	FAD	C9A-N10	-2.07	1.37	1.41
3	C	901	FAD	C2A-N3A	-2.06	1.30	1.33
3	B	901	FAD	C2A-N3A	-2.04	1.30	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	C5A-C4A-N3A	-6.20	118.17	126.72
3	D	901	FAD	C5A-C4A-N3A	-6.20	118.19	126.72
3	C	901	FAD	C5A-C4A-N3A	-6.19	118.20	126.72
3	B	901	FAD	C5A-C4A-N3A	-6.16	118.23	126.72
3	A	901	FAD	O2A-PA-O3P	-4.43	95.31	107.27
3	D	901	FAD	O2A-PA-O3P	-4.41	95.34	107.27
3	C	901	FAD	O2A-PA-O3P	-4.41	95.35	107.27
3	B	901	FAD	O2A-PA-O3P	-4.41	95.36	107.27
3	D	901	FAD	N3A-C2A-N1A	-3.89	122.69	128.58
3	B	901	FAD	N3A-C2A-N1A	-3.87	122.72	128.58
3	A	901	FAD	N3A-C2A-N1A	-3.86	122.74	128.58
3	C	901	FAD	N3A-C2A-N1A	-3.85	122.76	128.58
3	A	901	FAD	N3A-C4A-N9A	3.82	133.67	127.17
3	D	901	FAD	N3A-C4A-N9A	3.80	133.64	127.17
3	C	901	FAD	N3A-C4A-N9A	3.80	133.63	127.17
3	B	901	FAD	N3A-C4A-N9A	3.79	133.62	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	FAD	C2A-N3A-C4A	3.74	120.96	111.83
3	A	901	FAD	C2A-N3A-C4A	3.73	120.94	111.83
3	B	901	FAD	C2A-N3A-C4A	3.72	120.91	111.83
3	C	901	FAD	C2A-N3A-C4A	3.71	120.89	111.83
3	C	901	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
3	A	901	FAD	N9A-C8A-N7A	-3.65	108.75	113.94
3	D	901	FAD	N9A-C8A-N7A	-3.65	108.76	113.94
3	B	901	FAD	N9A-C8A-N7A	-3.64	108.77	113.94
3	A	901	FAD	C5A-N7A-C8A	3.61	109.12	103.45
3	C	901	FAD	C5A-N7A-C8A	3.60	109.11	103.45
3	B	901	FAD	C5A-N7A-C8A	3.59	109.09	103.45
3	D	901	FAD	C5A-N7A-C8A	3.55	109.02	103.45
3	B	901	FAD	C4X-C10-N10	3.48	121.47	116.48
3	C	901	FAD	C4X-C10-N10	3.44	121.41	116.48
3	D	901	FAD	C4X-C10-N10	3.43	121.40	116.48
3	A	901	FAD	C4X-C10-N10	3.42	121.38	116.48
3	A	901	FAD	C4A-C5A-N7A	-3.40	106.70	110.58
3	C	901	FAD	C4A-C5A-N7A	-3.39	106.70	110.58
3	B	901	FAD	C4A-C5A-N7A	-3.36	106.74	110.58
3	D	901	FAD	C4A-C5A-N7A	-3.34	106.77	110.58
3	D	901	FAD	C4-N3-C2	-3.04	120.23	125.64
3	B	901	FAD	C4-N3-C2	-3.04	120.25	125.64
3	C	901	FAD	C4-N3-C2	-3.03	120.27	125.64
3	A	901	FAD	C4-N3-C2	-3.00	120.31	125.64
3	A	901	FAD	C9A-N10-C10	-2.94	116.27	120.75
3	B	901	FAD	C9A-N10-C10	-2.94	116.28	120.75
3	D	901	FAD	C9A-N10-C10	-2.93	116.28	120.75
3	A	901	FAD	C5X-C9A-N10	2.92	120.61	117.97
3	C	901	FAD	C9A-N10-C10	-2.91	116.31	120.75
3	D	901	FAD	C5X-C9A-N10	2.91	120.60	117.97
3	B	901	FAD	C5X-C9A-N10	2.90	120.59	117.97
3	C	901	FAD	C5X-C9A-N10	2.89	120.58	117.97
3	A	901	FAD	C4'-C3'-C2'	2.74	118.13	113.57
3	D	901	FAD	C4'-C3'-C2'	2.73	118.11	113.57
3	C	901	FAD	C4'-C3'-C2'	2.71	118.09	113.57
3	B	901	FAD	C4'-C3'-C2'	2.70	118.07	113.57
3	A	901	FAD	C4X-C4-N3	2.67	120.06	113.25
3	B	901	FAD	C4X-C4-N3	2.67	120.06	113.25
3	D	901	FAD	C4X-C4-N3	2.67	120.06	113.25
3	C	901	FAD	C4X-C4-N3	2.67	120.04	113.25
3	D	901	FAD	O4'-C4'-C5'	-2.36	104.78	109.99
3	C	901	FAD	O4'-C4'-C5'	-2.35	104.80	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	O4'-C4'-C5'	-2.35	104.80	109.99
3	B	901	FAD	O4'-C4'-C5'	-2.35	104.81	109.99
3	B	901	FAD	C10-C4X-N5	-2.22	120.27	124.81
3	D	901	FAD	C10-C4X-N5	-2.20	120.31	124.81
3	C	901	FAD	C10-C4X-N5	-2.19	120.34	124.81
3	D	901	FAD	C5A-C4A-N9A	2.17	108.18	105.81
3	A	901	FAD	C10-C4X-N5	-2.17	120.38	124.81
3	C	901	FAD	C5A-C4A-N9A	2.17	108.17	105.81
3	A	901	FAD	C5A-C4A-N9A	2.15	108.16	105.81
3	B	901	FAD	C5A-C4A-N9A	2.14	108.15	105.81
3	B	901	FAD	C4-C4X-N5	2.14	121.17	118.21
3	D	901	FAD	C4-C4X-N5	2.14	121.16	118.21
3	A	901	FAD	C4-C4X-N5	2.12	121.14	118.21
3	A	901	FAD	C9A-C5X-N5	-2.12	120.20	122.45
3	B	901	FAD	C9A-C5X-N5	-2.11	120.22	122.45
3	C	901	FAD	C9A-C5X-N5	-2.10	120.22	122.45
3	C	901	FAD	C4-C4X-N5	2.10	121.11	118.21
3	D	901	FAD	C9A-C5X-N5	-2.09	120.24	122.45
3	B	901	FAD	O3P-P-O1P	2.04	116.83	110.70
3	D	901	FAD	O3P-P-O1P	2.02	116.79	110.70
3	C	901	FAD	O3P-P-O1P	2.01	116.76	110.70
3	A	901	FAD	O3P-P-O1P	2.01	116.75	110.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FAD	C5'-O5'-P-O3P
3	B	901	FAD	C5'-O5'-P-O3P
3	C	901	FAD	C5'-O5'-P-O3P
3	D	901	FAD	C5'-O5'-P-O3P
3	A	901	FAD	P-O3P-PA-O2A
3	B	901	FAD	P-O3P-PA-O2A
3	C	901	FAD	P-O3P-PA-O2A
3	D	901	FAD	P-O3P-PA-O2A

There are no ring outliers.

3 monomers are involved in 9 short contacts:

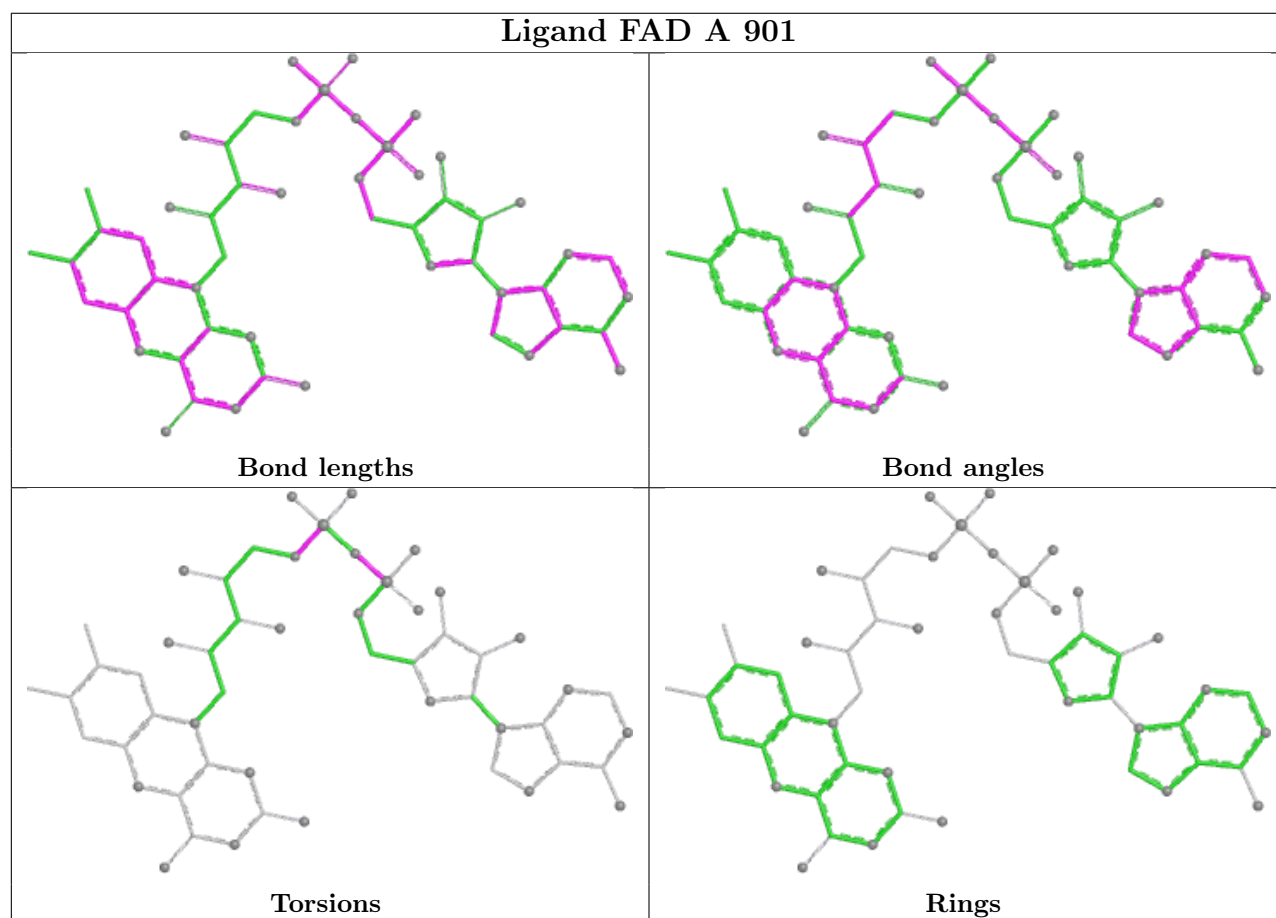
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	3	0

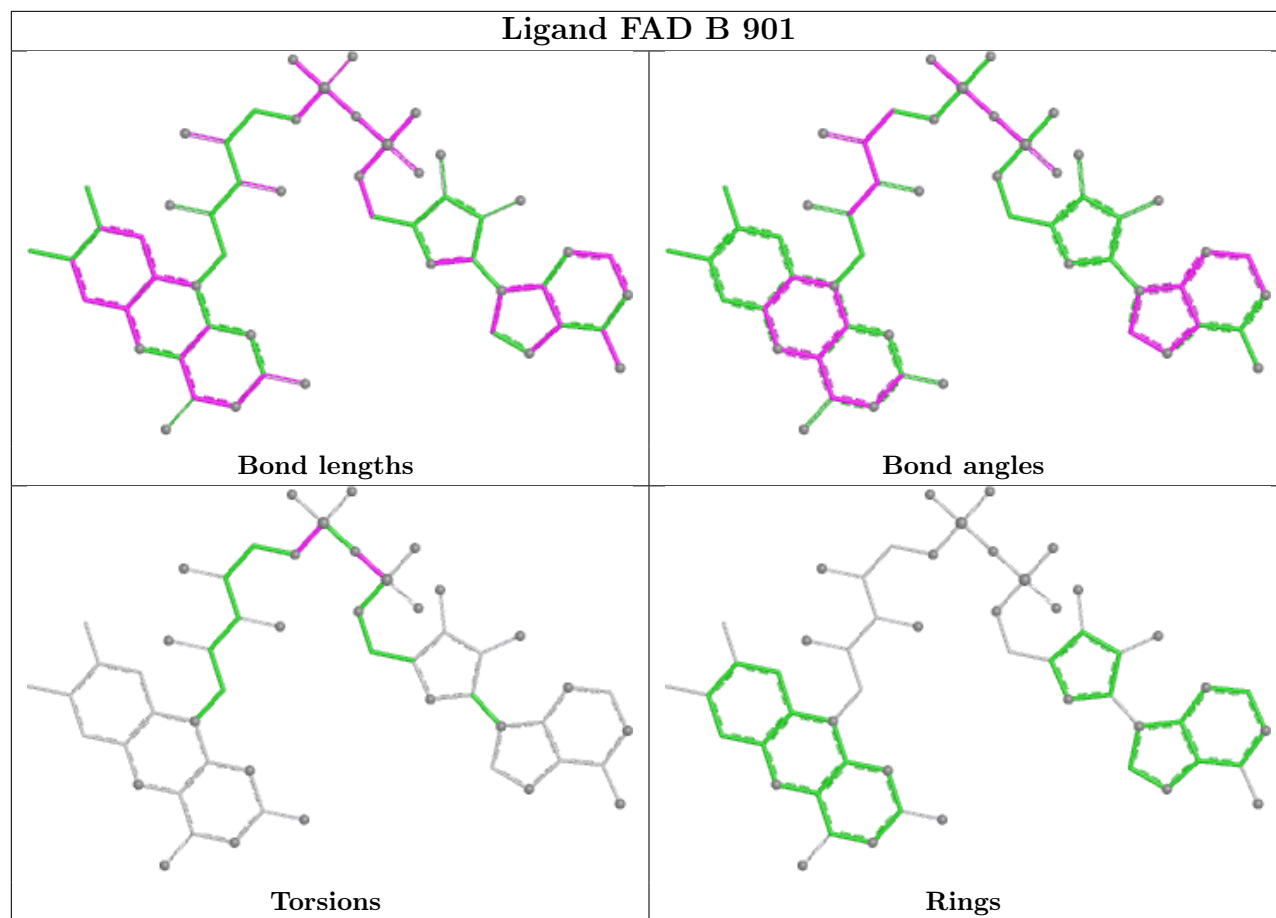
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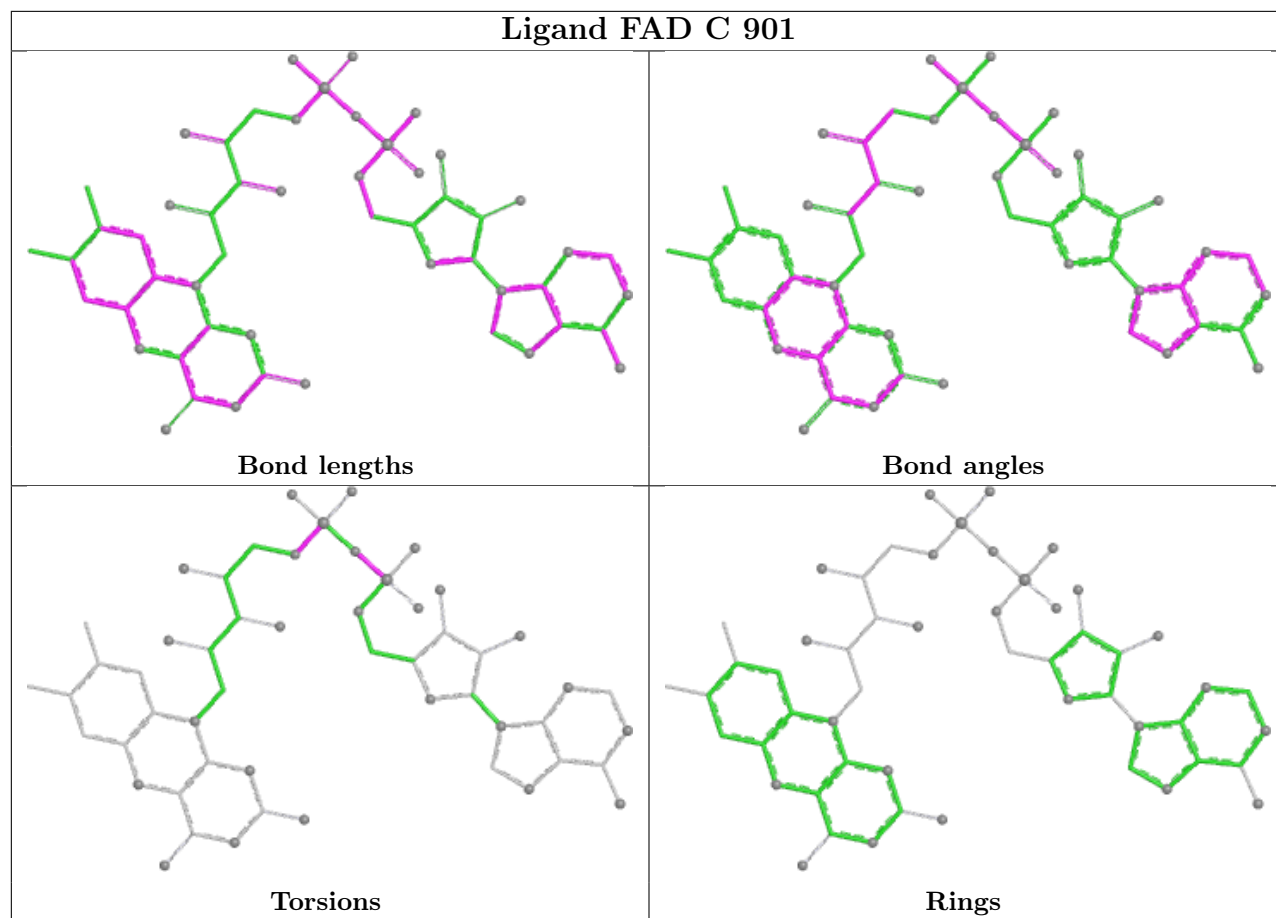
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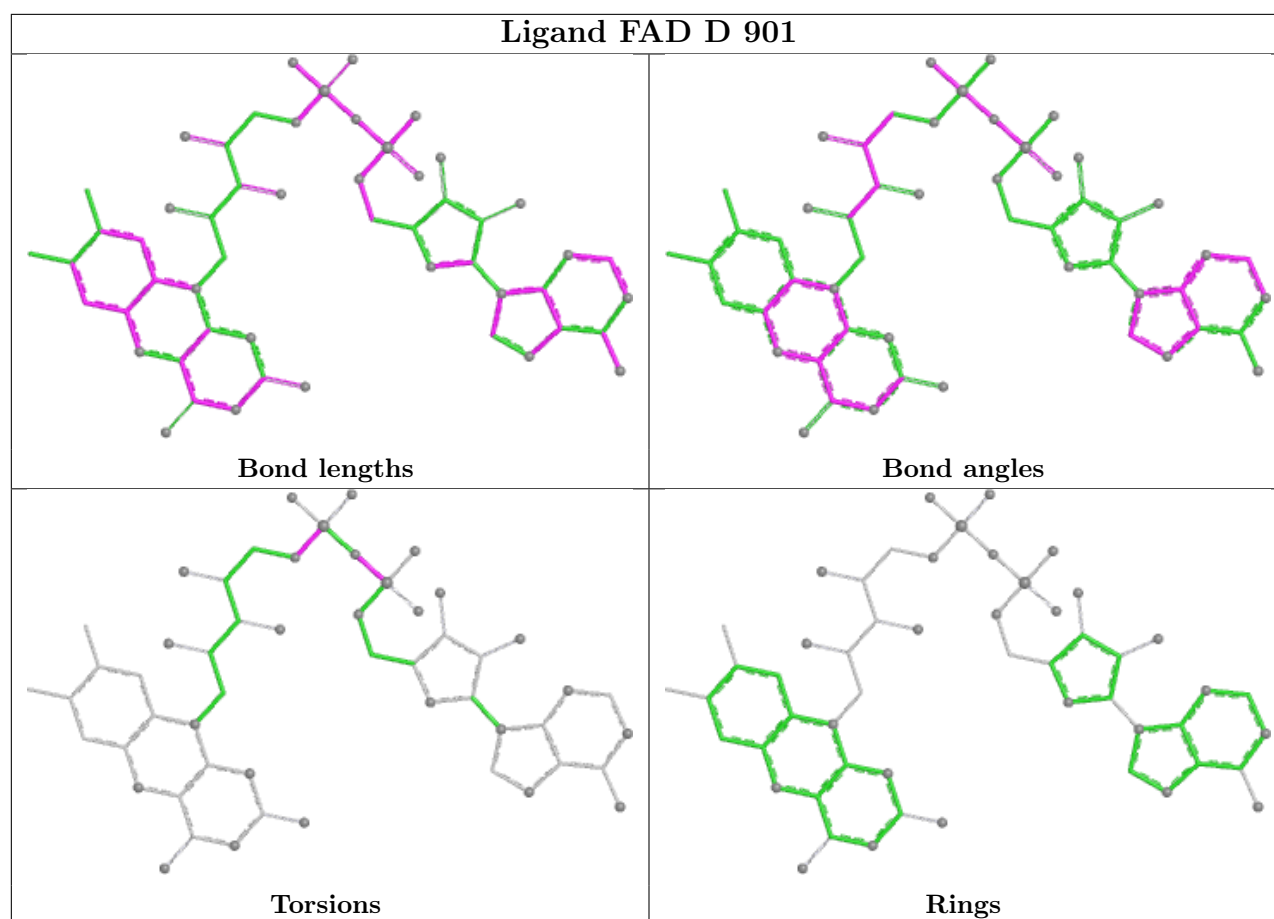
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	FAD	4	0
3	D	901	FAD	2	0

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	748/776 (96%)	-0.22	1 (0%) 92 86	51, 76, 115, 151	0
1	B	748/776 (96%)	-0.24	2 (0%) 90 80	52, 78, 114, 156	0
1	C	736/776 (94%)	-0.34	2 (0%) 90 80	42, 68, 104, 154	0
1	D	735/776 (94%)	-0.29	2 (0%) 90 80	45, 71, 107, 163	0
2	E	26/26 (100%)	0.61	0 100 100	83, 110, 143, 162	0
2	F	26/26 (100%)	0.49	2 (7%) 19 10	92, 110, 139, 149	0
All	All	3019/3156 (95%)	-0.26	9 (0%) 90 80	42, 73, 113, 163	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	THR	3.1
1	B	235	THR	3.1
1	D	235	THR	3.0
1	C	822	PHE	2.9
1	C	235	THR	2.6
2	F	20	LEU	2.4
2	F	1	ALA	2.3
1	D	49	GLY	2.2
1	B	54	GLU	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 ⓘ

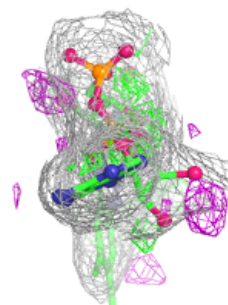
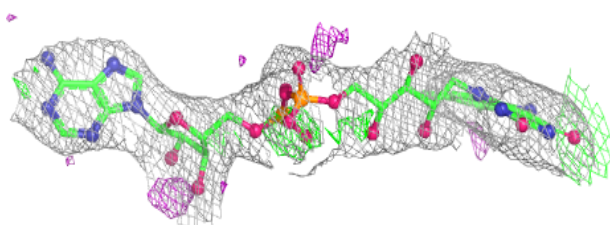
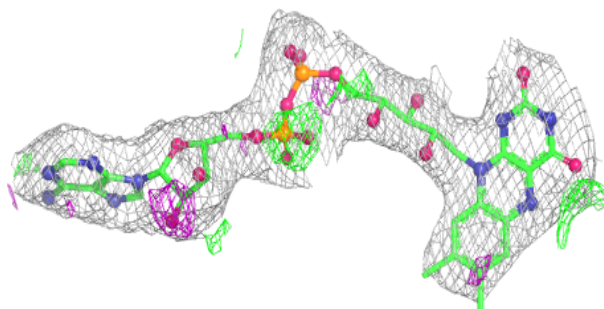
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FAD	A	901	53/53	0.91	0.10	56,67,82,172	0
3	FAD	B	901	53/53	0.94	0.09	52,65,73,124	0
3	FAD	C	901	53/53	0.95	0.08	43,52,61,75	0
3	FAD	D	901	53/53	0.95	0.08	45,55,65,95	0
4	ZN	C	903	1/1	0.96	0.22	147,147,147,147	0
4	ZN	D	904	1/1	0.98	0.04	95,95,95,95	0
4	ZN	A	904	1/1	0.99	0.06	65,65,65,65	0
4	ZN	B	902	1/1	0.99	0.03	57,57,57,57	0
4	ZN	B	903	1/1	0.99	0.02	53,53,53,53	0
4	ZN	B	904	1/1	0.99	0.04	67,67,67,67	0
4	ZN	C	902	1/1	0.99	0.09	71,71,71,71	0
4	ZN	A	902	1/1	0.99	0.09	77,77,77,77	0
4	ZN	D	902	1/1	0.99	0.05	69,69,69,69	0
4	ZN	D	903	1/1	0.99	0.04	63,63,63,63	0
4	ZN	A	903	1/1	0.99	0.02	53,53,53,53	0
4	ZN	C	904	1/1	1.00	0.04	96,96,96,96	0

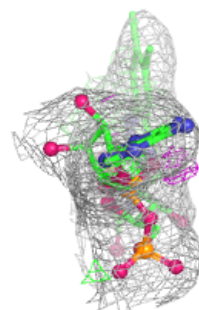
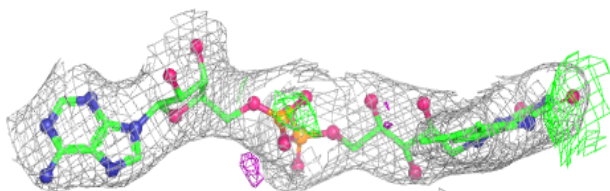
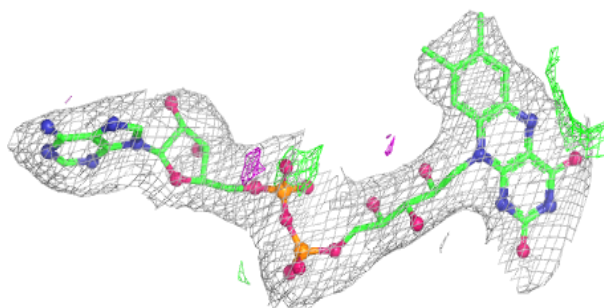
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

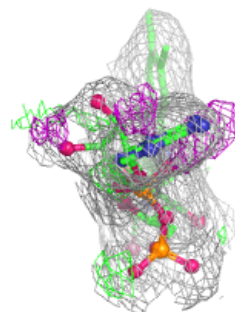
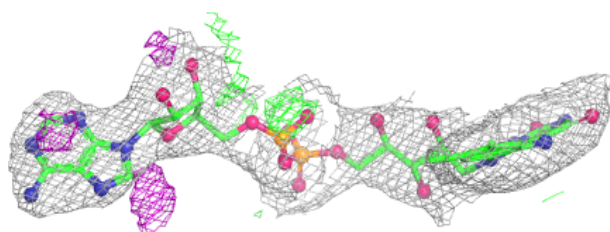
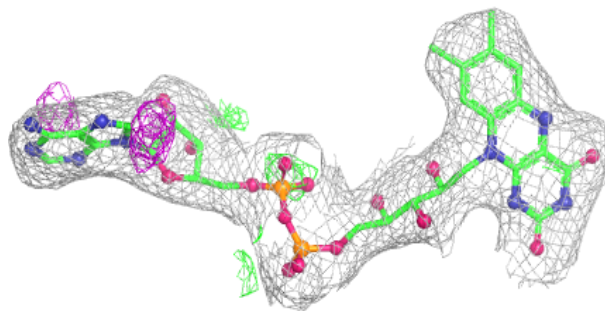
**Electron density around FAD B 901:**

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

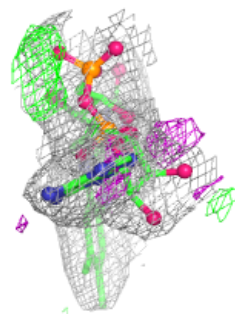
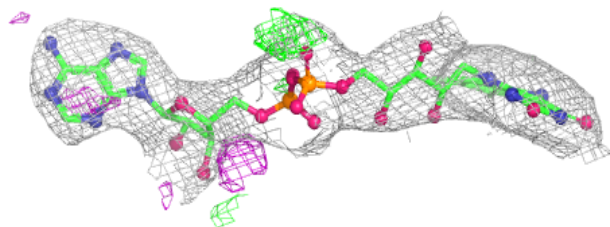
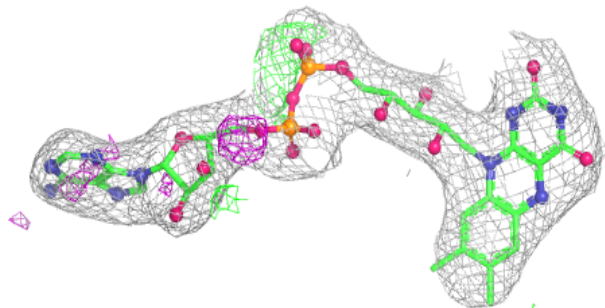


Electron density around FAD C 901:

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

**Electron density around FAD D 901:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.