



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:07 PM UTC

PDB ID : 2IPI / pdb_00002ipi
Title : Crystal Structure of Aclacinomycin Oxidoreductase
Authors : Sultana, A.; Kursula, I.; Schneider, G.; Alexeev, I.; Niemi, J.; Mantsala, P.
Deposited on : 2006-10-12
Resolution : 1.65 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

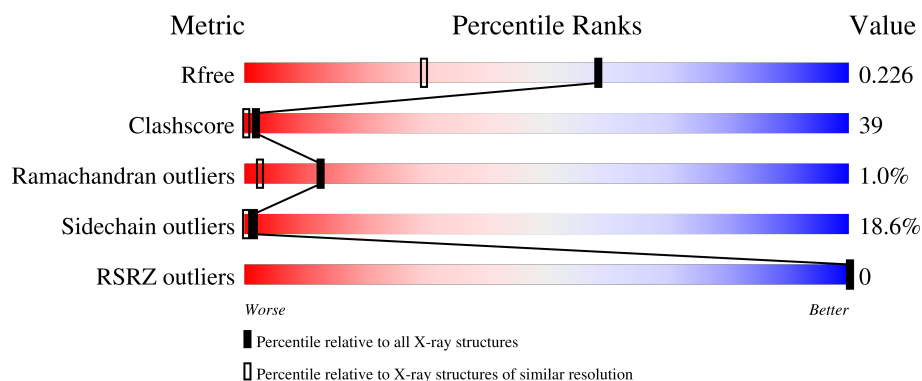
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	521	
1	B	521	
1	C	521	
1	D	521	

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
2	AKY	A	601[A]	X	-	-	-
3	FAD	B	801	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16589 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 Aclacinomycin oxidoreductase (AknOx).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	67	2	0
			3836	2423	693	712	8			
1	B	492	Total	C	N	O	S	67	0	0
			3823	2415	690	710	8			
1	C	492	Total	C	N	O	S	55	1	0
			3828	2418	690	712	8			
1	D	492	Total	C	N	O	S	70	0	0
			3823	2415	690	710	8			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q0PCD7
A	-17	ALA	-	cloning artifact	UNP Q0PCD7
A	-16	HIS	-	expression tag	UNP Q0PCD7
A	-15	HIS	-	expression tag	UNP Q0PCD7
A	-14	HIS	-	expression tag	UNP Q0PCD7
A	-13	HIS	-	expression tag	UNP Q0PCD7
A	-12	HIS	-	expression tag	UNP Q0PCD7
A	-11	HIS	-	expression tag	UNP Q0PCD7
A	-10	HIS	-	expression tag	UNP Q0PCD7
A	-9	ARG	-	cloning artifact	UNP Q0PCD7
A	-8	SER	-	cloning artifact	UNP Q0PCD7
A	-7	ALA	-	cloning artifact	UNP Q0PCD7
A	-6	ALA	-	cloning artifact	UNP Q0PCD7
A	-5	GLY	-	cloning artifact	UNP Q0PCD7
A	-4	THR	-	cloning artifact	UNP Q0PCD7
A	-3	ILE	-	cloning artifact	UNP Q0PCD7
A	-2	TRP	-	cloning artifact	UNP Q0PCD7
A	-1	GLU	-	cloning artifact	UNP Q0PCD7
A	0	PHE	-	cloning artifact	UNP Q0PCD7
B	-18	MET	-	initiating methionine	UNP Q0PCD7
B	-17	ALA	-	cloning artifact	UNP Q0PCD7

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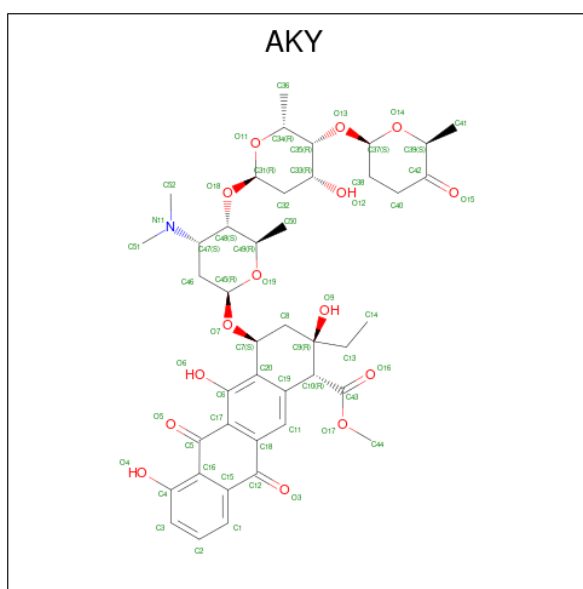
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q0PCD7
B	-15	HIS	-	expression tag	UNP Q0PCD7
B	-14	HIS	-	expression tag	UNP Q0PCD7
B	-13	HIS	-	expression tag	UNP Q0PCD7
B	-12	HIS	-	expression tag	UNP Q0PCD7
B	-11	HIS	-	expression tag	UNP Q0PCD7
B	-10	HIS	-	expression tag	UNP Q0PCD7
B	-9	ARG	-	cloning artifact	UNP Q0PCD7
B	-8	SER	-	cloning artifact	UNP Q0PCD7
B	-7	ALA	-	cloning artifact	UNP Q0PCD7
B	-6	ALA	-	cloning artifact	UNP Q0PCD7
B	-5	GLY	-	cloning artifact	UNP Q0PCD7
B	-4	THR	-	cloning artifact	UNP Q0PCD7
B	-3	ILE	-	cloning artifact	UNP Q0PCD7
B	-2	TRP	-	cloning artifact	UNP Q0PCD7
B	-1	GLU	-	cloning artifact	UNP Q0PCD7
B	0	PHE	-	cloning artifact	UNP Q0PCD7
C	-18	MET	-	initiating methionine	UNP Q0PCD7
C	-17	ALA	-	cloning artifact	UNP Q0PCD7
C	-16	HIS	-	expression tag	UNP Q0PCD7
C	-15	HIS	-	expression tag	UNP Q0PCD7
C	-14	HIS	-	expression tag	UNP Q0PCD7
C	-13	HIS	-	expression tag	UNP Q0PCD7
C	-12	HIS	-	expression tag	UNP Q0PCD7
C	-11	HIS	-	expression tag	UNP Q0PCD7
C	-10	HIS	-	expression tag	UNP Q0PCD7
C	-9	ARG	-	cloning artifact	UNP Q0PCD7
C	-8	SER	-	cloning artifact	UNP Q0PCD7
C	-7	ALA	-	cloning artifact	UNP Q0PCD7
C	-6	ALA	-	cloning artifact	UNP Q0PCD7
C	-5	GLY	-	cloning artifact	UNP Q0PCD7
C	-4	THR	-	cloning artifact	UNP Q0PCD7
C	-3	ILE	-	cloning artifact	UNP Q0PCD7
C	-2	TRP	-	cloning artifact	UNP Q0PCD7
C	-1	GLU	-	cloning artifact	UNP Q0PCD7
C	0	PHE	-	cloning artifact	UNP Q0PCD7
D	-18	MET	-	initiating methionine	UNP Q0PCD7
D	-17	ALA	-	cloning artifact	UNP Q0PCD7
D	-16	HIS	-	expression tag	UNP Q0PCD7
D	-15	HIS	-	expression tag	UNP Q0PCD7
D	-14	HIS	-	expression tag	UNP Q0PCD7
D	-13	HIS	-	expression tag	UNP Q0PCD7

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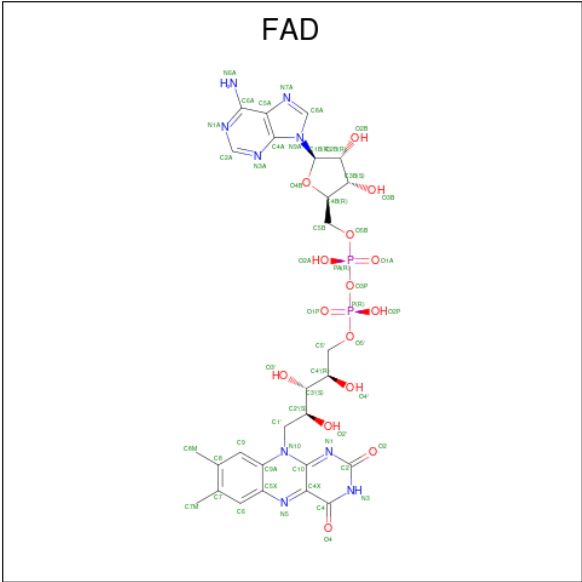
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q0PCD7
D	-11	HIS	-	expression tag	UNP Q0PCD7
D	-10	HIS	-	expression tag	UNP Q0PCD7
D	-9	ARG	-	cloning artifact	UNP Q0PCD7
D	-8	SER	-	cloning artifact	UNP Q0PCD7
D	-7	ALA	-	cloning artifact	UNP Q0PCD7
D	-6	ALA	-	cloning artifact	UNP Q0PCD7
D	-5	GLY	-	cloning artifact	UNP Q0PCD7
D	-4	THR	-	cloning artifact	UNP Q0PCD7
D	-3	ILE	-	cloning artifact	UNP Q0PCD7
D	-2	TRP	-	cloning artifact	UNP Q0PCD7
D	-1	GLU	-	cloning artifact	UNP Q0PCD7
D	0	PHE	-	cloning artifact	UNP Q0PCD7

- Molecule 2 is METHYL (2S,4R)-2-ETHYL-2,5,7-TRIHYDROXY-6,11-DIOXO-4-{[2,3,6-T RIDEOXY-4-O-{2,6-DIDEOXY-4-O-[(2S,6S)-6-METHYL-5-OXOTETRAHYDRO-2H -PY RAN-2-YL]-ALPHA-D-LYXO-HEXOPYRANOSYL}-3-(DIMETHYLAMINO)-D-RIBO-H EXOPYRANOSYL]OXY}-1,2,3,4,6,11-HEXAHYDROTETRACENE-1-C ARBOXYLATE (CCD ID: AKY) (formula: C₄₂H₅₃NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			58	42	1	15		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

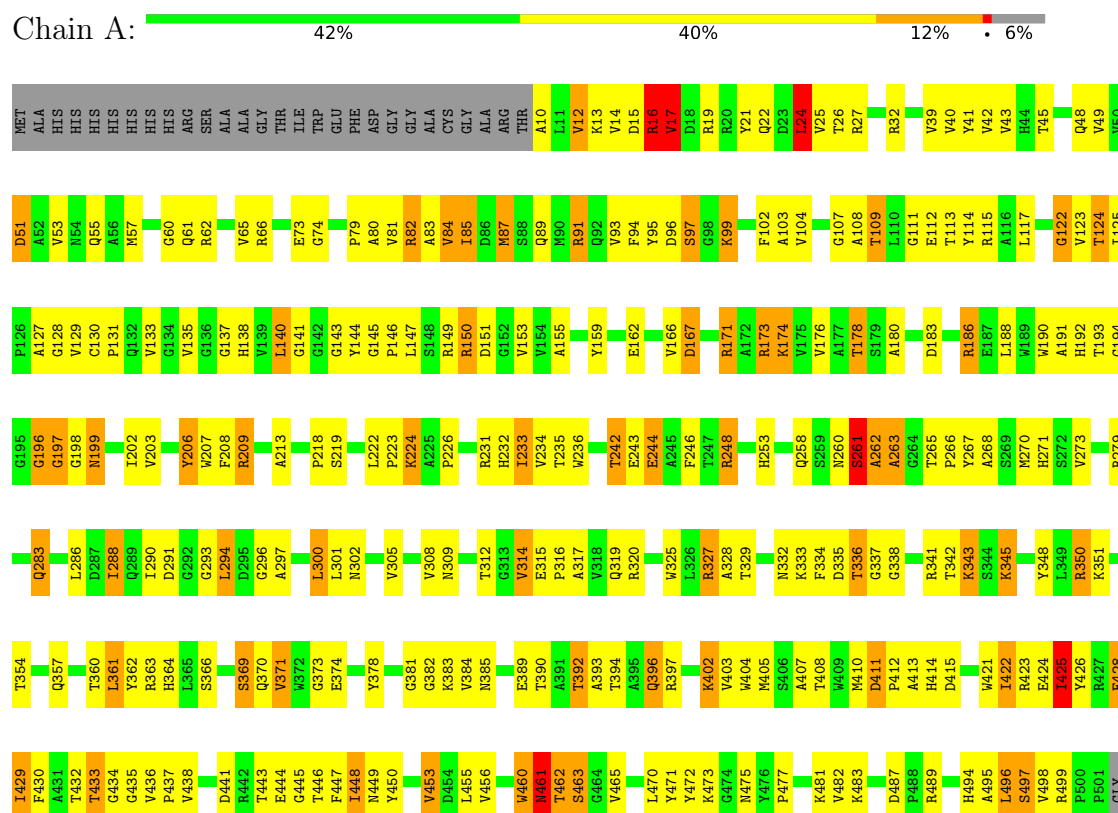
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	212	Total	O	0	0
			212	212		
4	C	317	Total	O	0	0
			317	317		
4	D	206	Total	O	0	0
			206	206		

3 Residue-property plots

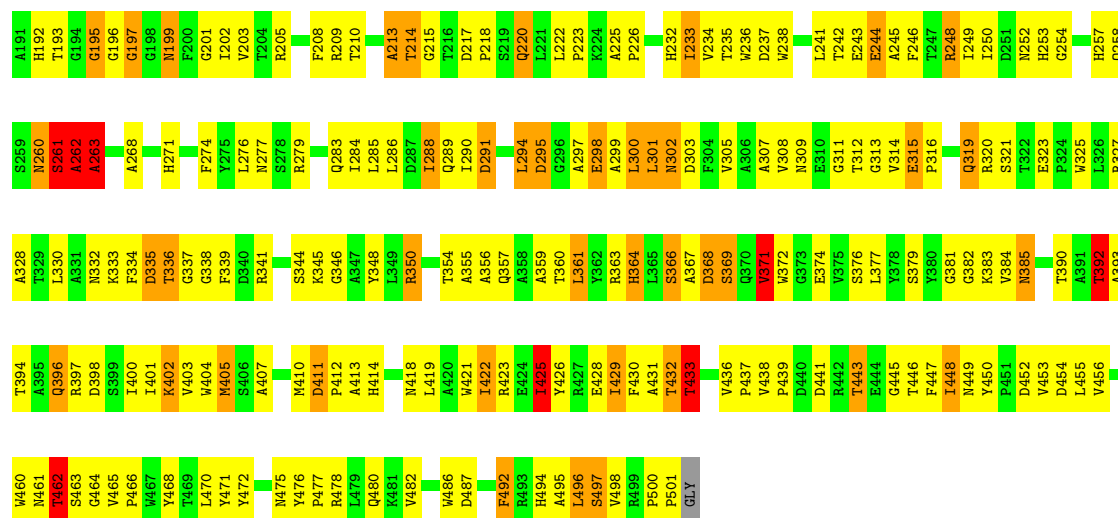
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



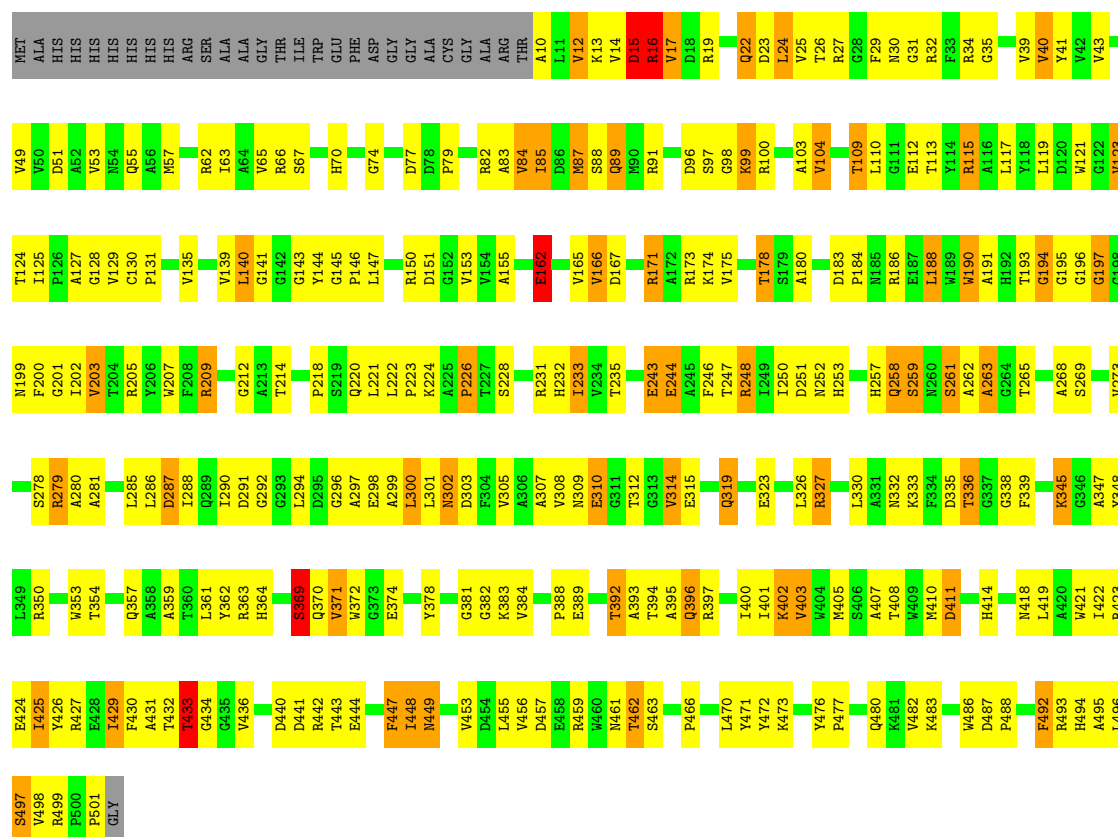
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)





• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain C: 41% 41% 11% • 6%



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain D: 39% 41% 13% • 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.50Å 266.20Å 68.70Å 90.00° 119.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-1.65) 98.5 (20.00-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.67Å)	Xtriage
Refinement program	REFMAC, SHELXL-97	Depositor
R, R_{free}	0.185 , 0.242 0.182 , 0.226	Depositor DCC
R_{free} test set	9546 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.128 for -h-l,k,h 0.128 for l,k,-h-l 0.130 for h,-k,-h-l 0.128 for -h-l,-k,l 0.430 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16589	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, AKY

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	0.51	1/3946 (0.0%)	1.48	48/5386 (0.9%)
1	B	0.53	1/3927 (0.0%)	1.54	47/5361 (0.9%)
1	C	0.56	2/3935 (0.1%)	1.61	51/5372 (0.9%)
1	D	0.51	0/3927	1.52	50/5361 (0.9%)
All	All	0.53	4/15735 (0.0%)	1.54	196/21480 (0.9%)

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	B	0	3
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLN	C-N	6.32	1.43	1.33
1	B	258	GLN	C-N	5.75	1.42	1.33
1	C	258	GLN	C-N	5.51	1.41	1.33
1	C	259	SER	C-N	-5.27	1.26	1.33

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	GLY	CA-C-N	18.66	140.69	119.98
1	C	196	GLY	C-N-CA	18.66	140.69	119.98
1	D	196	GLY	CA-C-N	13.20	147.28	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	GLY	C-N-CA	13.20	147.28	121.41
1	C	197	GLY	N-CA-C	11.88	126.98	112.73
1	B	263	ALA	CA-C-N	10.72	142.43	121.41
1	B	263	ALA	C-N-CA	10.72	142.43	121.41
1	B	166	VAL	CA-C-N	10.45	136.19	120.82
1	B	166	VAL	C-N-CA	10.45	136.19	120.82
1	C	194	GLY	CA-C-N	-10.33	106.29	122.51
1	C	194	GLY	C-N-CA	-10.33	106.29	122.51
1	C	194	GLY	O-C-N	-10.23	113.63	123.35
1	B	261	SER	CA-C-N	10.12	140.87	121.54
1	B	261	SER	C-N-CA	10.12	140.87	121.54
1	C	263	ALA	CA-C-N	9.51	140.06	121.41
1	C	263	ALA	C-N-CA	9.51	140.06	121.41
1	C	309	ASN	CA-CB-CG	9.29	121.89	112.60
1	C	197	GLY	O-C-N	-9.18	113.38	122.19
1	C	166	VAL	CA-C-N	8.84	133.81	120.82
1	C	166	VAL	C-N-CA	8.84	133.81	120.82
1	C	433	THR	CA-C-O	8.79	128.24	119.97
1	B	149	ARG	CD-NE-CZ	8.75	136.65	124.40
1	D	257	HIS	CA-C-O	8.69	129.96	119.97
1	D	493	ARG	CA-C-N	8.65	137.70	121.69
1	D	493	ARG	C-N-CA	8.65	137.70	121.69
1	D	17	VAL	CA-C-N	8.52	136.12	120.95
1	D	17	VAL	C-N-CA	8.52	136.12	120.95
1	B	253	HIS	CA-CB-CG	8.45	122.25	113.80
1	A	309	ASN	CA-CB-CG	8.41	121.01	112.60
1	B	102	PHE	CA-CB-CG	8.30	122.10	113.80
1	B	262	ALA	CA-C-N	8.28	134.47	121.72
1	B	262	ALA	C-N-CA	8.28	134.47	121.72
1	A	91	ARG	CD-NE-CZ	8.11	135.75	124.40
1	B	341	ARG	CD-NE-CZ	8.06	135.69	124.40
1	D	406	SER	CA-C-N	8.03	135.11	122.74
1	D	406	SER	C-N-CA	8.03	135.11	122.74
1	A	17	VAL	CA-C-N	8.00	134.38	120.87
1	A	17	VAL	C-N-CA	8.00	134.38	120.87
1	C	15	ASP	CA-C-O	-7.88	111.85	120.36
1	D	34	ARG	CD-NE-CZ	7.86	135.40	124.40
1	D	166	VAL	CA-C-N	7.76	132.24	120.82
1	D	166	VAL	C-N-CA	7.76	132.24	120.82
1	D	432	THR	CA-C-N	7.57	132.88	120.23
1	D	432	THR	C-N-CA	7.57	132.88	120.23
1	D	149	ARG	CD-NE-CZ	7.36	134.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ARG	CD-NE-CZ	7.36	134.70	124.40
1	A	369	SER	CA-C-N	-7.35	110.99	122.67
1	A	369	SER	C-N-CA	-7.35	110.99	122.67
1	D	82	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	B	495	ALA	CA-C-N	-7.20	111.75	122.83
1	B	495	ALA	C-N-CA	-7.20	111.75	122.83
1	D	446	THR	CA-C-N	7.18	133.10	123.05
1	D	446	THR	C-N-CA	7.18	133.10	123.05
1	A	196	GLY	CA-C-N	7.08	135.29	121.41
1	A	196	GLY	C-N-CA	7.08	135.29	121.41
1	D	194	GLY	O-C-N	-6.99	117.49	123.43
1	A	16	ARG	CD-NE-CZ	6.98	134.18	124.40
1	A	495	ALA	CA-C-N	-6.92	112.85	123.17
1	A	495	ALA	C-N-CA	-6.92	112.85	123.17
1	A	291	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	51	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	166	VAL	CA-C-N	6.74	130.93	120.75
1	A	166	VAL	C-N-CA	6.74	130.93	120.75
1	D	494	HIS	N-CA-C	6.73	119.45	108.55
1	C	16	ARG	N-CA-C	6.60	124.87	110.80
1	C	196	GLY	N-CA-C	6.59	121.22	112.65
1	C	433	THR	N-CA-C	-6.49	103.53	112.03
1	A	206	TYR	CA-C-O	-6.35	113.98	121.16
1	B	430	PHE	CA-CB-CG	-6.35	107.45	113.80
1	B	291	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	372	TRP	CA-C-N	6.25	128.43	122.36
1	C	372	TRP	C-N-CA	6.25	128.43	122.36
1	D	45	THR	CA-C-N	6.22	128.90	120.38
1	D	45	THR	C-N-CA	6.22	128.90	120.38
1	D	253	HIS	CA-CB-CG	6.20	120.00	113.80
1	D	257	HIS	O-C-N	-6.15	114.70	122.27
1	D	149	ARG	NE-CZ-NH2	6.15	124.73	119.20
1	B	134	GLY	CA-C-O	6.09	129.19	121.94
1	B	181	ALA	CA-C-N	6.03	132.49	122.54
1	B	181	ALA	C-N-CA	6.03	132.49	122.54
1	B	186	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	B	16	ARG	N-CA-C	5.99	120.89	112.93
1	B	91	ARG	CD-NE-CZ	5.99	132.78	124.40
1	C	15	ASP	N-CA-C	5.98	118.64	108.90
1	A	186	ARG	NE-CZ-NH1	-5.97	115.53	121.50
1	D	428	GLU	CA-C-N	-5.97	111.24	121.09
1	D	428	GLU	C-N-CA	-5.97	111.24	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	HIS	CA-CB-CG	5.96	119.76	113.80
1	A	122	GLY	CA-C-O	5.92	127.13	119.44
1	D	183	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	495	ALA	CA-C-N	-5.87	113.20	122.95
1	C	495	ALA	C-N-CA	-5.87	113.20	122.95
1	C	197	GLY	CA-C-N	-5.84	109.97	121.41
1	C	197	GLY	C-N-CA	-5.84	109.97	121.41
1	A	461	ASN	CA-CB-CG	5.83	118.44	112.60
1	C	447	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	439	PRO	CA-C-N	5.79	131.72	122.10
1	B	439	PRO	C-N-CA	5.79	131.72	122.10
1	A	308	VAL	CA-C-N	-5.79	113.36	122.79
1	A	308	VAL	C-N-CA	-5.79	113.36	122.79
1	D	213	ALA	N-CA-C	5.79	120.47	113.41
1	C	162	GLU	CA-CB-CG	5.76	125.62	114.10
1	C	74	GLY	CA-C-N	5.76	128.32	120.54
1	C	74	GLY	C-N-CA	5.76	128.32	120.54
1	C	258	GLN	O-C-N	-5.76	114.71	122.43
1	B	371	VAL	CA-C-N	5.76	132.53	121.54
1	B	371	VAL	C-N-CA	5.76	132.53	121.54
1	C	492	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	261	SER	CA-C-N	5.74	132.50	121.54
1	A	261	SER	C-N-CA	5.74	132.50	121.54
1	C	226	PRO	CA-C-N	5.74	128.24	120.44
1	C	226	PRO	C-N-CA	5.74	128.24	120.44
1	D	425	ILE	CB-CA-C	-5.70	104.44	112.14
1	C	110	LEU	CA-C-N	5.69	126.30	119.98
1	C	110	LEU	C-N-CA	5.69	126.30	119.98
1	C	287	ASP	CA-C-N	-5.65	115.26	123.06
1	C	287	ASP	C-N-CA	-5.65	115.26	123.06
1	D	327	ARG	CD-NE-CZ	5.63	132.29	124.40
1	B	213	ALA	O-C-N	5.62	129.34	122.14
1	A	102	PHE	CA-C-N	5.62	129.32	121.24
1	A	102	PHE	C-N-CA	5.62	129.32	121.24
1	A	135	VAL	CA-C-N	5.61	126.33	119.99
1	A	135	VAL	C-N-CA	5.61	126.33	119.99
1	D	215	GLY	N-CA-C	5.58	119.70	112.68
1	C	186	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	A	197	GLY	N-CA-C	5.54	126.30	113.18
1	B	27	ARG	CA-C-N	-5.54	114.41	120.44
1	B	27	ARG	C-N-CA	-5.54	114.41	120.44
1	D	320	ARG	CD-NE-CZ	5.53	132.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ALA	N-CA-C	-5.52	107.19	114.31
1	A	293	GLY	CA-C-N	-5.51	114.44	122.65
1	A	293	GLY	C-N-CA	-5.51	114.44	122.65
1	C	353	TRP	CA-CB-CG	5.51	124.06	113.60
1	C	209	ARG	CD-NE-CZ	5.50	132.10	124.40
1	A	461	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	B	487	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	197	GLY	O-C-N	-5.45	115.62	122.70
1	A	328	ALA	CA-C-N	5.44	128.12	120.28
1	A	328	ALA	C-N-CA	5.44	128.12	120.28
1	C	308	VAL	CA-C-N	-5.44	111.15	121.54
1	C	308	VAL	C-N-CA	-5.44	111.15	121.54
1	B	295	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	313	GLY	N-CA-C	-5.39	106.23	115.61
1	A	392	THR	CA-C-O	-5.39	115.42	121.40
1	A	60	GLY	CA-C-O	5.38	126.31	119.80
1	D	264	GLY	CA-C-N	5.36	134.88	121.80
1	D	264	GLY	C-N-CA	5.36	134.88	121.80
1	A	425	ILE	CB-CA-C	-5.36	104.91	112.14
1	B	213	ALA	CA-C-N	5.36	131.77	121.54
1	B	213	ALA	C-N-CA	5.36	131.77	121.54
1	C	40	VAL	CA-C-O	-5.34	114.82	120.48
1	A	24	LEU	CA-C-O	5.33	126.15	120.24
1	A	82	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	C	449	ASN	CA-C-N	5.30	130.17	123.34
1	C	449	ASN	C-N-CA	5.30	130.17	123.34
1	D	258	GLN	O-C-N	-5.29	115.34	122.43
1	C	139	VAL	N-CA-C	5.28	116.00	110.62
1	A	82	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	B	64	ALA	CA-C-N	5.28	129.73	123.19
1	B	64	ALA	C-N-CA	5.28	129.73	123.19
1	B	139	VAL	N-CA-C	5.28	116.05	110.72
1	D	397	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	D	495	ALA	CA-C-N	-5.27	115.31	123.17
1	D	495	ALA	C-N-CA	-5.27	115.31	123.17
1	D	37	PRO	O-C-N	-5.27	116.57	123.00
1	A	246	PHE	CA-CB-CG	5.27	119.07	113.80
1	C	310	GLU	CA-CB-CG	5.26	124.63	114.10
1	D	438	VAL	N-CA-C	5.25	113.90	109.02
1	B	425	ILE	CB-CA-C	-5.24	105.07	112.14
1	B	433	THR	CA-C-O	5.21	124.45	119.08
1	B	260	ASN	CA-CB-CG	-5.20	107.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	GLU	CA-C-N	-5.20	112.51	121.09
1	A	428	GLU	C-N-CA	-5.20	112.51	121.09
1	A	16	ARG	N-CA-C	5.19	119.24	112.13
1	D	205	ARG	CD-NE-CZ	5.17	131.65	124.40
1	A	74	GLY	CA-C-N	5.17	127.46	120.38
1	A	74	GLY	C-N-CA	5.17	127.46	120.38
1	B	366	SER	CA-C-N	5.16	128.18	120.90
1	B	366	SER	C-N-CA	5.16	128.18	120.90
1	D	194	GLY	CA-C-O	5.15	126.50	122.33
1	A	208	PHE	CA-CB-CG	-5.14	108.66	113.80
1	D	84	VAL	O-C-N	5.12	128.79	123.26
1	B	464	GLY	CA-C-N	-5.12	118.90	122.59
1	B	464	GLY	C-N-CA	-5.12	118.90	122.59
1	D	370	GLN	CA-C-O	5.10	126.63	119.80
1	D	353	TRP	CA-CB-CG	5.08	123.24	113.60
1	C	139	VAL	CB-CA-C	-5.07	105.29	112.14
1	C	369	SER	CA-C-N	-5.05	114.60	122.73
1	C	369	SER	C-N-CA	-5.05	114.60	122.73
1	B	65	VAL	CB-CA-C	-5.05	103.31	110.83
1	D	29	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	492	PHE	CA-CB-CG	-5.04	108.76	113.80
1	D	192	HIS	CA-CB-CG	-5.04	108.76	113.80
1	B	500	PRO	O-C-N	5.03	123.51	121.15
1	C	327	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	392	THR	CA-C-O	-5.02	115.67	121.49

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	SER	Peptide
1	B	262	ALA	Peptide
1	B	263	ALA	Peptide
1	D	261	SER	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	3836	0	3697	284	2
1	B	3823	0	3679	306	0
1	C	3828	0	3688	317	0
1	D	3823	0	3684	282	0
2	A	58	0	48	13	0
3	A	53	0	29	3	0
3	B	53	0	28	6	0
3	C	53	0	30	9	0
3	D	53	0	30	13	0
4	A	274	0	0	53	0
4	B	212	0	0	50	1
4	C	317	0	0	61	1
4	D	206	0	0	41	0
All	All	16589	0	14913	1166	2

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 39.

All (1166) 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:130:CYS:SG	3:C:801:FAD:H6	1.28	1.65
1:D:130:CYS:SG	3:D:801:FAD:H6	1.13	1.61
1:D:70:HIS:ND1	3:D:801:FAD:HM82	0.99	1.29
1:C:130:CYS:SG	3:C:801:FAD:C6	2.25	1.25
1:C:392:THR:HG21	1:C:397:ARG:HH21	1.23	1.02
1:D:70:HIS:CG	3:D:801:FAD:HM82	1.95	1.02
1:D:392:THR:HG21	1:D:397:ARG:HH21	1.22	1.02
1:A:392:THR:HG21	1:A:397:ARG:HH21	1.25	1.01
1:A:392:THR:HG23	1:A:394:THR:H	1.23	1.00
1:B:263:ALA:HB3	1:B:382:GLY:HA2	1.41	0.98
1:D:193:THR:HG23	1:D:393:ALA:H	1.30	0.95
1:B:392:THR:HG21	1:B:397:ARG:HH21	1.31	0.95
1:C:193:THR:HG23	1:C:393:ALA:H	1.27	0.94
1:C:392:THR:HG23	1:C:394:THR:H	1.30	0.94
1:C:434:GLY:HA3	1:C:463:SER:HB2	1.48	0.94
1:B:193:THR:HG23	1:B:393:ALA:H	1.34	0.93
1:C:291:ASP:HB3	1:C:294:LEU:HD23	1.48	0.92
1:D:231:ARG:HH12	1:D:289:GLN:HE21	1.16	0.91
1:C:178:THR:HG23	1:C:180:ALA:H	1.35	0.91
1:C:290:ILE:HG12	1:C:294:LEU:HD21	1.50	0.91
1:A:65:VAL:HG22	1:A:85:ILE:HD11	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HG23	1:A:393:ALA:H	1.34	0.90
1:B:392:THR:HG23	1:B:394:THR:H	1.36	0.90
1:C:436:VAL:HG13	1:C:461:ASN:HB3	1.54	0.89
1:B:65:VAL:HG22	1:B:85:ILE:HD11	1.55	0.89
1:A:354:THR:H	1:A:357:GLN:HE21	1.21	0.87
1:D:342:THR:HG22	1:D:408:THR:HG23	1.53	0.87
1:D:288:ILE:HD11	1:D:301:LEU:HG	1.56	0.86
1:C:354:THR:H	1:C:357:GLN:HE21	1.24	0.86
1:A:354:THR:HG23	1:A:357:GLN:H	1.38	0.85
1:C:251:ASP:HA	4:C:945:HOH:O	1.76	0.85
1:D:392:THR:HG23	1:D:394:THR:H	1.40	0.85
1:B:354:THR:H	1:B:357:GLN:HE21	1.24	0.85
1:B:24:LEU:HG	1:B:40:VAL:HG11	1.57	0.85
1:A:130:CYS:HB2	1:A:133:VAL:HG23	1.59	0.85
1:D:312:THR:HG22	1:D:314:VAL:HG13	1.58	0.85
1:D:130:CYS:HG	3:D:801:FAD:H6	1.37	0.84
1:B:195:GLY:HA3	1:B:472:TYR:HE1	1.40	0.84
1:B:300:LEU:HA	1:B:303:ASP:HB2	1.58	0.84
1:A:333:LYS:HB2	4:A:957:HOH:O	1.78	0.84
1:A:178:THR:HG23	1:A:180:ALA:H	1.40	0.84
1:B:109:THR:HG22	1:B:112:GLU:H	1.43	0.83
1:C:203:VAL:HG22	3:C:801:FAD:N6A	1.92	0.83
1:B:195:GLY:HA2	1:B:448:ILE:HG13	1.61	0.83
1:B:178:THR:HG23	1:B:180:ALA:H	1.42	0.82
1:B:354:THR:HG23	1:B:357:GLN:H	1.44	0.82
1:B:425:ILE:HB	4:B:957:HOH:O	1.80	0.82
1:D:257:HIS:O	1:D:261:SER:HB2	1.78	0.82
1:C:19:ARG:HH22	1:D:224:LYS:HB3	1.43	0.81
1:C:162:GLU:HG3	1:C:205:ARG:HB3	1.63	0.81
1:C:203:VAL:HG13	3:C:801:FAD:N1A	1.96	0.80
1:A:190:TRP:O	1:A:193:THR:HG22	1.83	0.79
1:A:233:ILE:HG23	1:A:319:GLN:HB2	1.64	0.79
1:C:129:VAL:HG22	1:C:146:PRO:HD3	1.62	0.79
1:B:51:ASP:O	1:B:55:GLN:HG3	1.83	0.79
1:D:396:GLN:H	1:D:396:GLN:HE21	1.31	0.78
1:B:425:ILE:O	1:B:429:ILE:HG23	1.83	0.78
1:A:290:ILE:HD13	1:A:300:LEU:HD13	1.64	0.78
1:A:84:VAL:HG23	4:A:960:HOH:O	1.83	0.78
1:A:392:THR:HG22	4:A:822:HOH:O	1.83	0.78
1:B:17:VAL:HA	4:B:884:HOH:O	1.82	0.78
1:B:226:PRO:HB3	1:B:291:ASP:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ILE:HG13	1:B:401:ILE:HG13	1.66	0.78
1:C:14:VAL:HG11	4:C:1046:HOH:O	1.83	0.78
1:A:244:GLU:HG2	4:A:1042:HOH:O	1.84	0.77
1:B:385:ASN:HB3	1:B:397:ARG:O	1.84	0.77
1:B:241:LEU:HD13	1:B:246:PHE:HD1	1.49	0.77
1:A:448:ILE:HG23	4:A:858:HOH:O	1.83	0.77
1:D:190:TRP:O	1:D:193:THR:HG22	1.83	0.77
1:D:365:LEU:HB2	4:D:945:HOH:O	1.83	0.77
1:B:448:ILE:HG23	4:B:878:HOH:O	1.85	0.77
1:B:93:VAL:HG11	4:B:937:HOH:O	1.84	0.76
1:D:296:GLY:O	1:D:300:LEU:HG	1.86	0.76
1:A:444:GLU:HG2	1:A:473:LYS:HZ3	1.51	0.76
1:D:381:GLY:O	1:D:384:VAL:HG12	1.86	0.76
1:B:190:TRP:O	1:B:193:THR:HG22	1.86	0.76
1:C:381:GLY:O	1:C:384:VAL:HG12	1.86	0.76
1:B:12:VAL:HG21	4:B:816:HOH:O	1.86	0.76
1:B:116:ALA:HB3	4:B:937:HOH:O	1.85	0.75
1:C:109:THR:O	1:C:113:THR:HG23	1.86	0.75
1:D:17:VAL:HG12	4:D:963:HOH:O	1.86	0.75
1:A:381:GLY:O	1:A:384:VAL:HG12	1.86	0.75
1:C:16:ARG:HB2	4:C:895:HOH:O	1.85	0.75
1:D:162:GLU:HG2	4:D:899:HOH:O	1.86	0.75
1:C:65:VAL:HG22	1:C:85:ILE:HD11	1.69	0.75
1:B:232:HIS:O	1:B:288:ILE:HG23	1.86	0.74
1:B:248:ARG:HB3	4:B:948:HOH:O	1.86	0.74
1:A:24:LEU:HD11	1:B:119:LEU:HD22	1.69	0.74
1:A:354:THR:HG22	1:A:357:GLN:HE21	1.53	0.74
1:A:312:THR:HG22	1:A:314:VAL:H	1.53	0.74
1:B:178:THR:HG22	1:B:183:ASP:OD2	1.87	0.74
1:A:477:PRO:HD2	4:A:1056:HOH:O	1.87	0.74
1:B:462:THR:HG22	1:B:465:VAL:O	1.88	0.74
1:C:263:ALA:HB3	1:C:268:ALA:HB2	1.70	0.74
1:C:212:GLY:HA3	4:C:881:HOH:O	1.88	0.73
1:B:141:GLY:O	1:B:448:ILE:HD11	1.88	0.73
1:D:242:THR:HG21	4:D:995:HOH:O	1.86	0.73
1:C:424:GLU:HB3	4:C:1003:HOH:O	1.86	0.73
1:B:350:ARG:HD3	1:B:441:ASP:O	1.89	0.73
1:C:224:LYS:HB2	4:C:812:HOH:O	1.88	0.73
1:A:103:ALA:HA	4:A:993:HOH:O	1.87	0.73
1:C:16:ARG:HD2	1:C:17:VAL:HG13	1.70	0.73
1:C:89:GLN:OE1	1:D:119:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:HB	4:C:1025:HOH:O	1.89	0.73
1:A:89:GLN:HE22	1:B:116:ALA:HA	1.54	0.73
1:C:190:TRP:O	1:C:193:THR:HG22	1.89	0.73
1:A:124:THR:HG23	4:A:820:HOH:O	1.87	0.73
1:B:65:VAL:HA	1:B:85:ILE:HG12	1.69	0.73
1:D:40:VAL:HG22	1:D:84:VAL:HG13	1.71	0.73
1:A:65:VAL:HG21	1:A:202:ILE:HG12	1.70	0.73
1:C:405:MET:HE1	1:C:429:ILE:HD12	1.71	0.73
1:B:25:VAL:HG23	4:B:930:HOH:O	1.88	0.72
1:D:25:VAL:HG23	4:D:853:HOH:O	1.90	0.72
1:D:371:VAL:HB	1:D:418:ASN:ND2	2.03	0.72
1:B:381:GLY:O	1:B:384:VAL:HG12	1.90	0.72
1:C:396:GLN:HA	1:C:444:GLU:OE2	1.89	0.72
1:C:51:ASP:O	1:C:55:GLN:HG3	1.88	0.72
1:D:354:THR:H	1:D:357:GLN:HE21	1.37	0.72
1:A:360:THR:HG23	1:A:428:GLU:OE2	1.90	0.72
1:A:404:TRP:CD2	2:A:601[A]:AKY:H413	2.24	0.72
1:C:89:GLN:HA	1:D:115:ARG:HH22	1.53	0.72
1:C:247:THR:HG21	1:C:248:ARG:HH11	1.55	0.72
1:B:345:LYS:HG3	1:B:405:MET:HB2	1.71	0.72
1:D:341:ARG:NH1	1:D:412:PRO:HB3	2.05	0.72
1:C:233:ILE:HG13	1:C:285:LEU:HD21	1.71	0.71
1:C:394:THR:HG22	4:C:1006:HOH:O	1.90	0.71
1:A:149:ARG:NH2	1:A:270:MET:HB3	2.06	0.71
1:A:297:ALA:HA	1:A:300:LEU:HD11	1.71	0.71
1:D:242:THR:HB	4:D:941:HOH:O	1.90	0.71
1:C:312:THR:HG22	1:C:314:VAL:H	1.54	0.71
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.55	0.71
1:D:143:GLY:O	1:D:153:VAL:HG13	1.91	0.71
1:C:444:GLU:OE2	1:C:473:LYS:HE2	1.91	0.71
1:D:178:THR:HG23	1:D:180:ALA:H	1.55	0.71
1:B:57:MET:HE3	4:B:902:HOH:O	1.89	0.71
1:C:167:ASP:HB2	1:C:171:ARG:H	1.55	0.71
1:A:297:ALA:O	1:A:300:LEU:HD12	1.90	0.70
1:B:297:ALA:O	1:B:300:LEU:HD12	1.91	0.70
1:C:140:LEU:HD23	1:C:203:VAL:HG11	1.71	0.70
1:A:494:HIS:O	1:A:497:SER:HB2	1.92	0.70
1:A:207:TRP:HA	4:A:993:HOH:O	1.90	0.70
1:C:392:THR:HG22	4:C:818:HOH:O	1.90	0.70
1:C:419:LEU:HB3	1:C:423:ARG:NH1	2.07	0.70
1:C:442:ARG:HG3	4:C:844:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:CB	1:B:382:GLY:HA2	2.18	0.70
1:A:193:THR:O	1:A:394:THR:HG23	1.91	0.69
1:C:31:GLY:HA2	1:C:34:ARG:NH2	2.07	0.69
1:A:432:THR:HG23	4:A:1027:HOH:O	1.92	0.69
1:D:244:GLU:O	1:D:248:ARG:HG2	1.92	0.69
1:C:203:VAL:HG22	3:C:801:FAD:H62A	1.58	0.69
1:B:137:GLY:HA3	3:B:801:FAD:H51A	1.75	0.69
1:D:384:VAL:HG13	1:D:385:ASN:OD1	1.92	0.69
1:D:427:ARG:HB2	4:D:942:HOH:O	1.93	0.69
1:A:93:VAL:HG13	1:A:104:VAL:HG12	1.76	0.68
1:A:460:TRP:HB3	1:A:461:ASN:OD1	1.93	0.68
1:C:14:VAL:HA	4:C:1033:HOH:O	1.91	0.68
1:C:178:THR:HG22	1:C:183:ASP:OD2	1.92	0.68
1:D:123:VAL:HG13	1:D:223:PRO:O	1.94	0.68
1:A:261:SER:HB2	4:A:826:HOH:O	1.92	0.68
1:A:354:THR:HG22	1:A:357:GLN:NE2	2.09	0.68
1:B:263:ALA:HB1	1:B:268:ALA:HB2	1.73	0.68
1:D:187:GLU:OE1	1:D:478:ARG:HD3	1.93	0.68
1:D:127:ALA:O	1:D:145:GLY:HA3	1.92	0.68
1:A:115:ARG:HH12	1:B:89:GLN:NE2	1.91	0.68
1:A:343:LYS:HE2	4:A:922:HOH:O	1.93	0.68
1:A:497:SER:HA	4:A:982:HOH:O	1.94	0.68
1:C:220:GLN:OE1	4:C:872:HOH:O	2.12	0.68
1:B:129:VAL:HG22	1:B:146:PRO:HD3	1.76	0.67
1:B:333:LYS:HA	4:B:978:HOH:O	1.93	0.67
1:D:114:TYR:OH	1:D:127:ALA:HB3	1.94	0.67
1:A:12:VAL:HG13	4:A:1040:HOH:O	1.93	0.67
1:A:366:SER:HA	4:A:916:HOH:O	1.94	0.67
1:B:354:THR:HG22	1:B:357:GLN:HE21	1.58	0.67
1:B:297:ALA:HA	1:B:300:LEU:HD11	1.75	0.67
1:D:108:ALA:O	1:D:135:VAL:HG23	1.95	0.67
1:A:66:ARG:HG3	4:A:985:HOH:O	1.93	0.67
1:C:119:LEU:HD22	1:D:24:LEU:HD11	1.77	0.67
1:C:212:GLY:HA2	4:C:969:HOH:O	1.95	0.67
1:C:231:ARG:HD3	1:C:287:ASP:OD2	1.94	0.67
1:C:232:HIS:HB2	1:C:288:ILE:HG12	1.77	0.67
1:D:352:PRO:HA	4:D:993:HOH:O	1.92	0.67
1:A:32:ARG:HG2	1:A:341:ARG:HH21	1.59	0.67
1:A:392:THR:HG23	1:A:394:THR:N	2.04	0.67
1:C:312:THR:HG22	1:C:314:VAL:HG13	1.76	0.67
1:C:493:ARG:HB3	4:C:1078:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ASP:HA	4:B:952:HOH:O	1.94	0.66
1:C:121:TRP:HB2	1:C:123:VAL:HG23	1.77	0.66
1:B:138:HIS:HB2	3:B:801:FAD:H4'	1.78	0.66
1:C:233:ILE:HD11	1:C:285:LEU:HD11	1.78	0.66
3:A:801:FAD:O2A	4:A:985:HOH:O	2.12	0.66
1:A:147:LEU:HD22	1:A:150:ARG:HD3	1.78	0.66
1:C:297:ALA:HA	1:C:300:LEU:HD11	1.77	0.66
1:D:231:ARG:HH12	1:D:289:GLN:NE2	1.92	0.66
1:B:65:VAL:HG21	1:B:202:ILE:HG12	1.78	0.65
1:A:444:GLU:HG2	1:A:473:LYS:NZ	2.12	0.65
1:B:426:TYR:O	1:B:429:ILE:HD13	1.97	0.65
1:C:244:GLU:HG2	1:C:248:ARG:HH22	1.60	0.65
1:C:184:PRO:HB2	4:C:980:HOH:O	1.96	0.65
1:A:133:VAL:HG13	3:A:801:FAD:H5'2	1.77	0.65
1:B:443:THR:HG21	4:B:961:HOH:O	1.97	0.65
1:A:32:ARG:HA	1:A:341:ARG:NH2	2.11	0.65
1:C:422:ILE:HD12	1:C:423:ARG:N	2.12	0.65
1:A:350[B]:ARG:HH11	1:A:441:ASP:HA	1.61	0.65
1:A:441:ASP:HB3	4:A:1006:HOH:O	1.97	0.65
1:B:150:ARG:O	1:B:383:LYS:HE2	1.96	0.65
1:B:431:ALA:HA	4:B:934:HOH:O	1.97	0.65
1:D:392:THR:HG21	1:D:397:ARG:NH2	2.04	0.65
1:A:436:VAL:HG13	1:A:462:THR:H	1.61	0.64
1:B:437:PRO:O	1:B:445:GLY:HA2	1.97	0.64
1:D:16:ARG:NE	1:D:17:VAL:H	1.95	0.64
1:A:279:ARG:HB2	4:A:916:HOH:O	1.96	0.64
1:A:288:ILE:HD11	1:A:301:LEU:HG	1.80	0.64
1:B:96:ASP:HA	4:B:855:HOH:O	1.95	0.64
1:C:43:VAL:HG21	1:C:87:MET:HE2	1.78	0.64
1:C:65:VAL:HG21	1:C:202:ILE:HG12	1.78	0.64
1:D:297:ALA:HA	1:D:300:LEU:HD11	1.78	0.64
1:D:68:GLY:HA3	3:D:801:FAD:O2P	1.97	0.64
1:B:124:THR:HG22	1:B:125:ILE:H	1.62	0.64
1:C:203:VAL:HB	4:C:1015:HOH:O	1.96	0.64
1:D:396:GLN:H	1:D:396:GLN:NE2	1.96	0.64
1:A:42:VAL:HG11	4:B:896:HOH:O	1.97	0.64
1:D:15:ASP:OD1	1:D:20:ARG:HB2	1.97	0.64
1:D:70:HIS:HB2	3:D:801:FAD:H5'1	1.79	0.64
1:B:121:TRP:O	1:B:123:VAL:HG23	1.97	0.64
1:D:32:ARG:HG2	1:D:341:ARG:HD3	1.78	0.64
1:B:354:THR:H	1:B:357:GLN:NE2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ARG:O	1:C:383:LYS:HE3	1.97	0.64
1:C:244:GLU:O	1:C:248:ARG:HG2	1.97	0.63
1:D:144:TYR:CE1	1:D:402:LYS:HE3	2.33	0.63
1:C:433:THR:HG22	1:C:436:VAL:O	1.98	0.63
1:B:400:ILE:HD11	4:B:953:HOH:O	1.97	0.63
1:C:220:GLN:HG2	4:C:905:HOH:O	1.98	0.63
1:C:350:ARG:NH1	1:C:444:GLU:HG2	2.13	0.63
1:B:188:LEU:HG	1:B:486:TRP:CD2	2.34	0.63
1:D:261:SER:HB3	1:D:400:ILE:HG22	1.79	0.63
1:A:178:THR:HG22	1:A:183:ASP:OD2	1.97	0.63
1:B:92:GLN:HB2	1:B:105:GLU:OE1	1.99	0.63
1:B:238:TRP:CD1	1:B:279:ARG:HA	2.34	0.63
1:B:288:ILE:HD11	1:B:301:LEU:HG	1.81	0.63
1:D:380:TYR:CE2	1:D:402:LYS:HE2	2.33	0.63
1:C:302:ASN:HA	1:C:305:VAL:HG22	1.80	0.62
1:A:186:ARG:HH12	1:A:190:TRP:HZ3	1.45	0.62
1:A:242:THR:HG22	4:A:1042:HOH:O	1.99	0.62
1:B:436:VAL:HG13	1:B:461:ASN:HB3	1.81	0.62
1:B:436:VAL:HG13	1:B:462:THR:H	1.63	0.62
1:C:130:CYS:CB	3:C:801:FAD:H6	2.28	0.62
1:D:216:THR:O	1:D:218:PRO:HD3	1.99	0.62
1:D:263:ALA:HB1	1:D:265:THR:OG1	1.99	0.62
1:D:436:VAL:HG22	4:D:950:HOH:O	1.99	0.62
1:B:233:ILE:HG23	1:B:319:GLN:HB2	1.79	0.62
1:D:150:ARG:NH2	1:D:226:PRO:HG3	2.14	0.62
1:C:359:ALA:O	1:C:363:ARG:HG3	1.99	0.62
1:B:245:ALA:HB1	1:B:312:THR:HG23	1.82	0.62
1:C:83:ALA:HB1	4:C:1011:HOH:O	1.99	0.62
1:C:155:ALA:HB1	1:C:193:THR:OG1	2.00	0.62
1:C:455:LEU:O	1:C:462:THR:HG21	2.00	0.62
1:D:25:VAL:HG21	1:D:35:GLY:O	2.00	0.62
1:D:31:GLY:HA3	1:D:340:ASP:OD1	1.99	0.62
1:D:150:ARG:O	1:D:383:LYS:HD2	2.00	0.62
1:A:373:GLY:HA3	1:A:421:TRP:CZ2	2.35	0.61
1:D:109:THR:HG22	1:D:112:GLU:HG3	1.82	0.61
1:D:124:THR:HG22	1:D:125:ILE:H	1.65	0.61
1:A:149:ARG:HD3	4:A:892:HOH:O	1.99	0.61
1:C:19:ARG:NH2	1:D:224:LYS:HB3	2.13	0.61
1:C:363:ARG:HB2	4:C:853:HOH:O	1.99	0.61
1:D:483:LYS:HD2	1:D:487:ASP:HB3	1.81	0.61
1:C:25:VAL:HG21	1:C:35:GLY:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:VAL:HG11	1:C:222:LEU:HB2	1.83	0.61
1:B:448:ILE:HD12	4:B:938:HOH:O	2.00	0.61
1:C:425:ILE:HD12	4:C:1025:HOH:O	2.00	0.61
1:D:150:ARG:HB2	4:D:836:HOH:O	2.01	0.61
1:A:167:ASP:HB2	1:A:171:ARG:H	1.66	0.61
1:B:18:ASP:OD2	1:B:20:ARG:HB2	2.00	0.61
1:D:16:ARG:HD2	1:D:17:VAL:HG13	1.83	0.61
1:A:109:THR:HG22	1:A:112:GLU:H	1.65	0.61
1:B:276:LEU:HD11	1:B:377:LEU:HD11	1.83	0.61
1:D:195:GLY:H	1:D:448:ILE:HD11	1.64	0.61
1:D:362:TYR:HA	4:D:945:HOH:O	2.00	0.60
1:A:124:THR:HG22	1:A:125:ILE:H	1.65	0.60
1:A:198:GLY:H	1:A:494:HIS:HE1	1.48	0.60
1:D:201:GLY:HA2	1:D:492:PHE:CE1	2.36	0.60
1:B:316:PRO:HG2	4:B:919:HOH:O	1.99	0.60
1:C:291:ASP:O	1:C:294:LEU:HG	2.00	0.60
1:B:422:ILE:HD12	1:B:423:ARG:N	2.16	0.60
1:C:388:PRO:HG3	4:C:832:HOH:O	2.00	0.60
1:D:84:VAL:HG11	4:D:975:HOH:O	2.01	0.60
1:A:336:THR:HA	2:A:601[A]:AKY:H503	1.84	0.60
1:D:188:LEU:HG	1:D:486:TRP:CD2	2.36	0.60
1:D:246:PHE:O	1:D:249:ILE:HB	2.02	0.60
1:C:345:LYS:HB2	1:C:426:TYR:CE2	2.35	0.60
1:B:478:ARG:HB2	4:B:834:HOH:O	2.02	0.60
1:B:480:GLN:HB3	1:B:501:PRO:HG3	1.84	0.60
1:C:199:ASN:ND2	1:C:498:VAL:HG22	2.16	0.60
1:D:84:VAL:HG21	4:D:975:HOH:O	2.02	0.60
1:D:195:GLY:HA2	1:D:472:TYR:HE1	1.66	0.60
1:D:231:ARG:HD3	1:D:287:ASP:OD2	2.02	0.60
1:D:421:TRP:CD1	1:D:422:ILE:HG23	2.37	0.60
1:C:99:LYS:HZ2	1:C:207:TRP:CD1	2.20	0.59
1:D:150:ARG:HH22	1:D:226:PRO:HG3	1.67	0.59
1:B:155:ALA:HB1	1:B:193:THR:OG1	2.02	0.59
1:D:99:LYS:HE3	1:D:207:TRP:CD1	2.37	0.59
1:B:348:TYR:CE1	1:B:402:LYS:HD3	2.37	0.59
1:D:103:ALA:HB2	1:D:207:TRP:CZ3	2.37	0.59
1:D:375:VAL:HG22	1:D:405:MET:HG2	1.84	0.59
1:A:290:ILE:HG21	1:A:301:LEU:HD11	1.83	0.59
1:A:384:VAL:O	1:A:397:ARG:HD2	2.02	0.59
1:C:150:ARG:HD2	1:C:151:ASP:OD1	2.02	0.59
1:C:233:ILE:HG23	1:C:319:GLN:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:THR:HG21	1:A:436:VAL:O	2.03	0.59
1:B:109:THR:CG2	1:B:112:GLU:H	2.16	0.59
1:C:396:GLN:H	1:C:396:GLN:HE21	1.47	0.59
1:B:354:THR:HG22	1:B:357:GLN:NE2	2.16	0.59
1:B:411:ASP:OD2	1:B:413:ALA:HB3	2.02	0.59
1:D:22:GLN:O	1:D:26:THR:HG23	2.03	0.59
1:D:133:VAL:HG13	3:D:801:FAD:H5'2	1.85	0.59
1:B:252:ASN:HB3	1:B:307:ALA:O	2.02	0.59
1:C:421:TRP:O	1:C:425:ILE:HG13	2.02	0.59
1:C:67:SER:HA	4:C:1000:HOH:O	2.02	0.59
1:C:297:ALA:O	1:C:300:LEU:HD12	2.03	0.59
1:A:45:THR:OG1	1:A:48:GLN:HG3	2.03	0.59
1:B:436:VAL:CG1	1:B:461:ASN:HB3	2.32	0.59
1:C:32:ARG:HD2	4:C:862:HOH:O	2.02	0.59
1:A:354:THR:H	1:A:357:GLN:NE2	1.97	0.58
1:D:85:ILE:HG12	1:D:85:ILE:O	2.03	0.58
1:A:411:ASP:OD2	1:A:413:ALA:HB3	2.04	0.58
1:A:446:THR:HG23	1:A:471:TYR:CE2	2.37	0.58
1:B:199:ASN:HB2	1:B:498:VAL:HG22	1.84	0.58
1:A:91:ARG:HB3	1:A:108:ALA:HA	1.85	0.58
1:A:123:VAL:HG13	1:A:223:PRO:O	2.03	0.58
1:A:297:ALA:O	1:A:301:LEU:HD13	2.04	0.58
1:B:226:PRO:HB3	1:B:291:ASP:CB	2.34	0.58
1:A:141:GLY:O	1:A:448:ILE:HD11	2.03	0.58
1:C:421:TRP:NE1	1:C:425:ILE:HD11	2.19	0.58
1:C:12:VAL:HB	4:C:1068:HOH:O	2.03	0.58
1:B:21:TYR:HB2	4:B:927:HOH:O	2.03	0.58
1:D:16:ARG:CZ	1:D:17:VAL:HG22	2.34	0.58
1:D:345:LYS:HD3	1:D:426:TYR:CG	2.38	0.58
1:D:478:ARG:O	1:D:482:VAL:HG23	2.04	0.58
1:D:455:LEU:O	1:D:462:THR:HG21	2.04	0.58
1:B:123:VAL:HG11	1:B:222:LEU:HB2	1.85	0.58
1:C:131:PRO:HG3	4:C:1057:HOH:O	2.04	0.58
1:C:312:THR:CG2	1:C:314:VAL:HG13	2.34	0.58
1:D:191:ALA:HB2	1:D:482:VAL:HG11	1.86	0.58
1:C:290:ILE:CG1	1:C:294:LEU:HD21	2.31	0.57
1:D:195:GLY:HA2	1:D:472:TYR:CE1	2.38	0.57
1:A:149:ARG:HH22	1:A:270:MET:HE2	1.68	0.57
1:B:244:GLU:O	1:B:248:ARG:HG2	2.04	0.57
1:D:40:VAL:HG22	1:D:84:VAL:CG1	2.34	0.57
1:B:354:THR:N	1:B:357:GLN:HE21	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG13	1:A:85:ILE:HG12	1.87	0.57
1:B:201:GLY:HA2	1:B:492:PHE:CD1	2.40	0.57
1:C:24:LEU:HB3	1:C:40:VAL:HG21	1.87	0.57
1:C:288:ILE:CD1	1:C:301:LEU:HG	2.34	0.57
1:C:14:VAL:HG13	1:C:39:VAL:HG21	1.86	0.57
1:A:109:THR:CG2	1:A:112:GLU:H	2.18	0.57
1:B:419:LEU:O	1:B:423:ARG:HG3	2.05	0.57
1:D:423:ARG:HD3	1:D:460:TRP:CZ2	2.40	0.57
1:C:294:LEU:HD11	1:C:300:LEU:HD11	1.87	0.56
1:A:149:ARG:NH2	1:A:270:MET:HE2	2.19	0.56
1:C:103:ALA:HB2	1:C:207:TRP:CZ3	2.40	0.56
1:A:350[B]:ARG:NH1	1:A:441:ASP:HA	2.21	0.56
1:A:433:THR:HG21	1:A:438:VAL:HG23	1.87	0.56
1:D:294:LEU:HD12	1:D:297:ALA:HB2	1.87	0.56
1:D:65:VAL:HG23	4:D:949:HOH:O	2.06	0.56
1:C:115:ARG:HB2	1:C:326:LEU:HD21	1.87	0.56
1:C:389:GLU:OE2	1:C:473:LYS:HE3	2.06	0.56
1:A:16:ARG:HG3	1:A:17:VAL:N	2.20	0.56
1:C:103:ALA:HB1	1:C:205:ARG:HD3	1.87	0.56
1:C:456:VAL:HG12	4:C:1056:HOH:O	2.05	0.56
1:A:248:ARG:HD3	4:A:967:HOH:O	2.06	0.56
1:C:244:GLU:HB2	4:C:804:HOH:O	2.06	0.56
1:D:178:THR:HG22	1:D:183:ASP:OD2	2.05	0.56
3:B:801:FAD:H2'	3:B:801:FAD:H9	1.88	0.56
1:D:130:CYS:CB	3:D:801:FAD:C6	2.84	0.56
1:A:140:LEU:HD21	1:A:197:GLY:HA2	1.88	0.56
1:A:389:GLU:OE2	1:A:473:LYS:HE2	2.05	0.56
1:B:233:ILE:HD11	1:B:285:LEU:HD11	1.88	0.56
1:C:109:THR:HG22	1:C:112:GLU:H	1.70	0.56
1:D:96:ASP:HB3	1:D:207:TRP:CZ3	2.40	0.56
1:D:494:HIS:O	1:D:497:SER:HB2	2.06	0.56
1:B:368:ASP:HA	4:B:862:HOH:O	2.05	0.56
1:C:299:ALA:HA	1:C:302:ASN:OD1	2.05	0.56
1:D:81:VAL:HB	4:D:948:HOH:O	2.05	0.56
1:B:254:GLY:HA2	4:B:953:HOH:O	2.05	0.55
1:B:436:VAL:CG1	1:B:462:THR:H	2.18	0.55
1:B:360:THR:CG2	1:B:429:ILE:HG22	2.37	0.55
1:C:201:GLY:HA2	1:C:492:PHE:CE1	2.41	0.55
1:B:161:VAL:HG23	1:B:203:VAL:HG13	1.89	0.55
1:C:147:LEU:HA	4:C:939:HOH:O	2.05	0.55
1:C:22:GLN:O	1:C:26:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:SER:HB2	1:D:323:GLU:O	2.06	0.55
1:D:238:TRP:HH2	4:D:945:HOH:O	1.88	0.55
1:A:122:GLY:O	1:A:224:LYS:HG3	2.05	0.55
1:B:18:ASP:HB2	4:B:815:HOH:O	2.05	0.55
1:B:301:LEU:O	1:B:305:VAL:HG13	2.06	0.55
1:B:432:THR:HG22	4:B:935:HOH:O	2.06	0.55
1:C:115:ARG:HE	1:D:91:ARG:NH2	2.04	0.55
1:C:201:GLY:HA2	1:C:492:PHE:CD1	2.42	0.55
1:C:364:HIS:CG	1:C:425:ILE:HG23	2.42	0.55
1:A:190:TRP:HZ2	1:A:390:THR:O	1.88	0.55
1:B:407:ALA:HB2	1:B:422:ILE:HG23	1.89	0.55
1:C:300:LEU:O	1:C:303:ASP:HB2	2.06	0.55
1:A:147:LEU:HD22	1:A:150:ARG:CD	2.36	0.55
2:A:601[A]:AKY:H141	4:A:1060:HOH:O	2.06	0.55
1:B:95:TYR:CE2	1:B:218:PRO:HG3	2.42	0.55
1:A:95:TYR:CE2	1:A:218:PRO:HG3	2.42	0.55
1:B:140:LEU:HD22	1:B:196:GLY:HA3	1.88	0.55
1:B:158:LEU:HD13	1:B:208:PHE:CE2	2.42	0.55
1:B:161:VAL:CG2	1:B:203:VAL:HG13	2.37	0.55
1:C:167:ASP:OD2	1:C:173:ARG:HD3	2.06	0.55
1:B:103:ALA:HB1	1:B:205:ARG:HD2	1.89	0.55
1:B:124:THR:HG23	4:B:936:HOH:O	2.07	0.55
1:A:243:GLU:HG3	1:A:362:TYR:CD2	2.42	0.55
1:B:323:GLU:HB2	1:B:328:ALA:HB2	1.89	0.55
1:D:267:TYR:CE1	1:D:300:LEU:HB2	2.42	0.54
1:B:27:ARG:HG2	1:B:27:ARG:HH21	1.71	0.54
1:B:140:LEU:H	1:B:140:LEU:HD12	1.72	0.54
1:B:392:THR:HG21	1:B:397:ARG:NH2	2.14	0.54
1:B:392:THR:CG2	1:B:394:THR:H	2.15	0.54
1:D:195:GLY:H	1:D:448:ILE:CD1	2.20	0.54
1:B:30:ASN:HD21	1:B:32:ARG:HG3	1.72	0.54
1:B:238:TRP:CD2	1:B:279:ARG:HG3	2.42	0.54
1:D:448:ILE:HG21	1:D:472:TYR:CE1	2.42	0.54
1:B:100:ARG:HD2	1:B:215:GLY:O	2.07	0.54
1:B:201:GLY:HA2	1:B:492:PHE:CE1	2.42	0.54
1:C:400:ILE:HG13	1:C:401:ILE:HG13	1.89	0.54
1:D:431:ALA:O	1:D:432:THR:HG22	2.07	0.54
1:B:291:ASP:O	1:B:294:LEU:HG	2.07	0.54
1:D:193:THR:O	1:D:394:THR:HG23	2.07	0.54
1:B:354:THR:CG2	1:B:357:GLN:H	2.17	0.54
1:C:195:GLY:HA2	1:C:472:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:VAL:HA	4:D:936:HOH:O	2.07	0.54
1:B:363:ARG:O	1:B:367:ALA:HB2	2.06	0.54
1:C:41:TYR:HA	4:C:1033:HOH:O	2.08	0.54
1:D:297:ALA:O	1:D:300:LEU:HD12	2.07	0.54
1:B:300:LEU:CA	1:B:303:ASP:HB2	2.35	0.54
1:C:65:VAL:HG22	1:C:85:ILE:CD1	2.38	0.54
1:A:17:VAL:HG23	1:A:17:VAL:O	2.06	0.54
1:A:404:TRP:CD2	2:A:601[A]:AKY:C41	2.91	0.54
1:B:146:PRO:HA	1:B:271:HIS:CG	2.42	0.54
1:A:40:VAL:HG13	1:A:84:VAL:HG22	1.90	0.54
1:A:423:ARG:HD3	1:A:460:TRP:CZ2	2.43	0.54
1:B:233:ILE:CG2	1:B:319:GLN:HB2	2.38	0.54
1:B:447:PHE:CE2	1:B:449:ASN:HB2	2.43	0.54
1:B:113:THR:HA	4:B:937:HOH:O	2.08	0.53
1:B:249:ILE:HG12	4:B:963:HOH:O	2.06	0.53
1:C:263:ALA:HB1	1:C:265:THR:OG1	2.08	0.53
1:A:144:TYR:CE2	1:A:402:LYS:HE3	2.43	0.53
1:B:15:ASP:HB3	1:B:18:ASP:OD2	2.09	0.53
1:B:92:GLN:HB2	1:B:105:GLU:CD	2.33	0.53
1:B:396:GLN:H	1:B:396:GLN:HE21	1.57	0.53
1:A:191:ALA:HB2	1:A:482:VAL:HG11	1.88	0.53
1:B:40:VAL:HG22	1:B:84:VAL:CG1	2.39	0.53
1:D:14:VAL:HG22	1:D:41:TYR:CD1	2.42	0.53
1:A:138:HIS:CE1	1:A:143:GLY:HA3	2.42	0.53
1:B:123:VAL:HG13	1:B:223:PRO:O	2.07	0.53
1:B:422:ILE:HD12	1:B:423:ARG:HG2	1.90	0.53
1:A:129:VAL:HG12	1:A:334:PHE:HZ	1.73	0.53
1:A:342:THR:HG22	1:A:408:THR:HG23	1.90	0.53
1:B:249:ILE:HA	4:B:963:HOH:O	2.07	0.53
1:C:143:GLY:O	1:C:153:VAL:HG13	2.08	0.53
1:B:112:GLU:O	1:B:115:ARG:HG2	2.07	0.53
1:B:245:ALA:HA	1:B:248:ARG:HG2	1.89	0.53
1:C:17:VAL:HG23	1:C:17:VAL:O	2.09	0.53
1:C:124:THR:HG22	1:C:125:ILE:H	1.74	0.53
1:D:123:VAL:HG11	1:D:222:LEU:HB2	1.91	0.53
1:D:419:LEU:HA	1:D:422:ILE:HD11	1.91	0.53
1:A:338:GLY:C	1:A:410:MET:HE2	2.33	0.53
1:B:249:ILE:HG23	4:B:963:HOH:O	2.07	0.53
1:D:302:ASN:HA	1:D:305:VAL:HG22	1.90	0.53
1:A:123:VAL:CG1	1:A:222:LEU:HB2	2.38	0.53
1:A:174:LYS:NZ	1:A:174:LYS:HB3	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:CG2	1:A:319:GLN:HB2	2.36	0.53
1:C:16:ARG:CD	1:C:17:VAL:HG13	2.37	0.53
1:C:364:HIS:O	1:C:421:TRP:HZ2	1.90	0.53
1:D:254:GLY:HA2	4:D:993:HOH:O	2.08	0.53
1:A:273:VAL:HG22	1:A:378:TYR:CD2	2.43	0.53
1:C:432:THR:HG23	4:C:1010:HOH:O	2.08	0.53
1:C:109:THR:HG22	1:C:112:GLU:HB2	1.91	0.53
1:C:115:ARG:HH12	1:C:119:LEU:HD12	1.73	0.53
1:C:422:ILE:HD12	1:C:423:ARG:HG3	1.89	0.53
1:A:407:ALA:HB2	1:A:421:TRP:HD1	1.74	0.52
3:B:801:FAD:H5'1	4:B:837:HOH:O	2.09	0.52
1:C:123:VAL:HG12	1:C:223:PRO:O	2.09	0.52
1:D:174:LYS:HD3	4:D:899:HOH:O	2.09	0.52
1:A:354:THR:CG2	1:A:357:GLN:H	2.17	0.52
1:A:494:HIS:HD2	1:A:496:LEU:H	1.56	0.52
1:B:197:GLY:O	3:B:801:FAD:H1B	2.09	0.52
1:D:433:THR:HG22	1:D:433:THR:O	2.10	0.52
1:B:226:PRO:HD2	1:B:325:TRP:CD1	2.44	0.52
1:C:140:LEU:HD23	1:C:203:VAL:CG1	2.38	0.52
1:C:482:VAL:HG13	1:C:486:TRP:CE3	2.44	0.52
1:D:17:VAL:HG23	1:D:17:VAL:O	2.09	0.52
1:A:91:ARG:HD3	1:A:112:GLU:OE1	2.09	0.52
1:A:162:GLU:HG3	1:A:176:VAL:HG22	1.92	0.52
1:C:115:ARG:NH1	1:C:119:LEU:HD12	2.25	0.52
1:C:65:VAL:CG2	1:C:202:ILE:HG12	2.39	0.52
1:C:421:TRP:CD1	1:C:425:ILE:HD11	2.44	0.52
1:D:91:ARG:HB3	1:D:108:ALA:HA	1.90	0.52
1:D:261:SER:OG	1:D:380:TYR:O	2.27	0.52
1:D:278:SER:HA	1:D:365:LEU:HD22	1.91	0.52
1:D:371:VAL:HG21	1:D:421:TRP:CG	2.44	0.52
1:A:394:THR:HB	4:A:812:HOH:O	2.08	0.52
1:C:421:TRP:CE2	1:C:425:ILE:HD11	2.45	0.52
1:C:447:PHE:CE2	1:C:449:ASN:HB2	2.44	0.52
1:A:40:VAL:HG22	1:A:84:VAL:HG13	1.92	0.52
1:A:123:VAL:HG11	1:A:222:LEU:HB2	1.91	0.52
1:C:25:VAL:O	1:C:25:VAL:HG22	2.10	0.52
1:C:89:GLN:HE21	1:D:115:ARG:HH22	1.58	0.52
1:C:43:VAL:CG2	1:C:87:MET:HE2	2.40	0.52
1:D:14:VAL:HG13	1:D:39:VAL:HG21	1.91	0.52
1:D:245:ALA:O	1:D:249:ILE:HG13	2.09	0.52
1:A:40:VAL:HG22	1:A:84:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:ND2	4:A:982:HOH:O	2.42	0.52
1:B:113:THR:HG21	1:B:135:VAL:HG21	1.92	0.51
1:B:354:THR:HG22	1:B:357:GLN:CG	2.40	0.51
1:B:396:GLN:H	1:B:396:GLN:NE2	2.07	0.51
1:C:30:ASN:ND2	1:C:32:ARG:HB2	2.26	0.51
1:D:45:THR:O	1:D:48:GLN:HB2	2.09	0.51
1:A:91:ARG:HH21	1:B:115:ARG:CZ	2.23	0.51
1:D:58:ALA:HB3	4:D:929:HOH:O	2.11	0.51
1:D:299:ALA:HA	1:D:302:ASN:OD1	2.10	0.51
1:A:327:ARG:HH12	1:B:34:ARG:HH22	1.57	0.51
1:C:247:THR:CG2	1:C:248:ARG:HH11	2.23	0.51
1:D:497:SER:HB3	4:D:909:HOH:O	2.10	0.51
1:B:150:ARG:NH1	1:B:226:PRO:HG3	2.25	0.51
1:B:262:ALA:H	1:B:263:ALA:CB	2.24	0.51
1:B:455:LEU:C	1:B:462:THR:HG1	2.18	0.51
1:A:115:ARG:HH12	1:B:89:GLN:HE21	1.57	0.51
1:A:422:ILE:HD12	1:A:423:ARG:N	2.25	0.51
1:C:22:GLN:HA	1:C:22:GLN:OE1	2.08	0.51
1:A:25:VAL:HG13	1:A:26:THR:HG23	1.92	0.51
1:A:434:GLY:O	1:A:461:ASN:HB3	2.10	0.51
1:B:153:VAL:HG12	1:B:155:ALA:H	1.74	0.51
1:B:279:ARG:HG2	1:B:279:ARG:O	2.09	0.51
1:C:462:THR:HG23	1:C:470:LEU:HD11	1.92	0.51
1:D:16:ARG:NH1	1:D:17:VAL:HG22	2.26	0.51
1:D:149:ARG:NH2	1:D:261:SER:OG	2.44	0.51
1:A:131:PRO:HD3	1:A:334:PHE:CE1	2.45	0.51
1:A:364:HIS:HE1	1:A:428:GLU:OE1	1.94	0.51
1:A:447:PHE:CE2	1:A:449:ASN:HB2	2.46	0.51
1:C:113:THR:HG21	1:C:135:VAL:HG21	1.92	0.51
1:D:56:ALA:HB3	1:D:63:ILE:HD11	1.93	0.51
1:D:233:ILE:HG22	1:D:319:GLN:O	2.09	0.51
1:A:89:GLN:HA	1:B:115:ARG:HH22	1.76	0.51
1:A:128:GLY:HA2	1:A:144:TYR:O	2.11	0.51
1:B:13:LYS:HB2	1:B:42:VAL:HB	1.93	0.51
1:B:16:ARG:HD3	4:B:844:HOH:O	2.11	0.51
1:B:431:ALA:O	1:B:432:THR:HG22	2.10	0.51
1:C:115:ARG:NH2	1:D:91:ARG:HH21	2.09	0.51
1:A:21:TYR:HB2	4:A:1061:HOH:O	2.10	0.51
1:A:196:GLY:O	1:A:199:ASN:OD1	2.29	0.51
1:A:288:ILE:HD11	1:A:301:LEU:CG	2.40	0.51
1:B:226:PRO:HD2	1:B:325:TRP:NE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD13	1:A:470:LEU:HD12	1.92	0.51
1:A:434:GLY:HA3	1:A:463:SER:HB2	1.92	0.50
1:A:456:VAL:HG12	1:A:456:VAL:O	2.11	0.50
1:B:237:ASP:HA	1:B:283:GLN:HB3	1.93	0.50
1:B:311:GLY:HA3	4:B:866:HOH:O	2.11	0.50
1:C:49:VAL:HG21	1:C:87:MET:HE1	1.94	0.50
1:D:299:ALA:O	1:D:302:ASN:OD1	2.29	0.50
1:D:494:HIS:HB2	1:D:497:SER:OG	2.12	0.50
1:A:91:ARG:HG2	1:A:107:GLY:C	2.36	0.50
1:A:408:THR:HG21	2:A:601[A]:AKY:H512	1.93	0.50
1:A:412:PRO:HA	1:A:415:ASP:OD1	2.12	0.50
1:B:433:THR:HB	4:B:935:HOH:O	2.12	0.50
1:C:338:GLY:O	1:C:410:MET:HB2	2.11	0.50
1:D:25:VAL:HG22	1:D:25:VAL:O	2.11	0.50
1:A:10:ALA:HB1	4:B:940:HOH:O	2.11	0.50
1:A:62:ARG:HD3	4:A:978:HOH:O	2.12	0.50
1:B:22:GLN:HA	1:B:25:VAL:HG12	1.92	0.50
1:D:350:ARG:HD2	1:D:444:GLU:HG3	1.94	0.50
1:A:149:ARG:HB3	1:A:268:ALA:O	2.12	0.50
1:B:123:VAL:HG12	1:B:124:THR:H	1.76	0.50
1:C:14:VAL:HG22	1:C:41:TYR:CD1	2.47	0.50
1:D:104:VAL:HG22	1:D:206:TYR:HB2	1.92	0.50
1:D:242:THR:HG22	1:D:243:GLU:H	1.77	0.50
1:A:209:ARG:HH11	1:A:209:ARG:HB3	1.77	0.50
1:A:296:GLY:O	1:A:300:LEU:HG	2.11	0.50
1:C:302:ASN:HB3	4:C:841:HOH:O	2.11	0.50
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.77	0.50
1:B:196:GLY:O	1:B:199:ASN:OD1	2.30	0.50
1:B:433:THR:HG21	4:B:961:HOH:O	2.11	0.50
1:B:462:THR:HG23	1:B:470:LEU:HD11	1.94	0.50
1:C:10:ALA:HB2	4:C:1031:HOH:O	2.12	0.50
1:C:41:TYR:HD2	4:C:1011:HOH:O	1.94	0.50
1:C:89:GLN:CD	1:D:115:ARG:HH12	2.20	0.50
1:D:368:ASP:O	1:D:368:ASP:OD1	2.30	0.50
1:A:199:ASN:HB3	1:A:498:VAL:HG22	1.93	0.49
1:A:363:ARG:NH1	4:A:1073:HOH:O	2.45	0.49
1:C:299:ALA:O	1:C:302:ASN:OD1	2.30	0.49
1:B:418:ASN:O	1:B:422:ILE:HG13	2.11	0.49
1:C:115:ARG:NE	1:D:91:ARG:HH21	2.09	0.49
1:C:258:GLN:HG2	4:C:971:HOH:O	2.12	0.49
1:C:301:LEU:O	1:C:305:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ILE:O	1:C:429:ILE:HG12	2.04	0.49
1:B:75:PHE:HZ	1:B:496:LEU:HD22	1.76	0.49
1:B:237:ASP:HA	1:B:283:GLN:CB	2.42	0.49
1:B:299:ALA:O	1:B:302:ASN:OD1	2.30	0.49
1:B:438:VAL:O	1:B:443:THR:OG1	2.30	0.49
1:C:124:THR:HG23	4:C:1009:HOH:O	2.11	0.49
1:A:85:ILE:HG13	1:A:202:ILE:HD13	1.95	0.49
1:A:150:ARG:HG3	1:A:151:ASP:CG	2.38	0.49
1:A:404:TRP:CG	2:A:601[A]:AKY:H413	2.47	0.49
1:C:121:TRP:CD1	1:C:218:PRO:HB2	2.47	0.49
1:C:244:GLU:HG2	1:C:248:ARG:NH2	2.26	0.49
1:D:427:ARG:HB3	1:D:461:ASN:CG	2.37	0.49
1:D:447:PHE:CE2	1:D:449:ASN:HB2	2.47	0.49
1:B:61:GLN:HB3	1:B:82:ARG:HB2	1.95	0.49
1:B:195:GLY:HA3	1:B:472:TYR:CE1	2.32	0.49
1:B:261:SER:N	1:B:262:ALA:HB2	2.27	0.49
1:C:180:ALA:HA	4:C:899:HOH:O	2.11	0.49
1:C:288:ILE:HD11	1:C:301:LEU:HG	1.95	0.49
1:C:384:VAL:O	1:C:397:ARG:HD2	2.12	0.49
1:A:232:HIS:O	1:A:288:ILE:HG23	2.12	0.49
1:A:394:THR:HG22	4:A:932:HOH:O	2.11	0.49
1:B:455:LEU:O	1:B:462:THR:OG1	2.30	0.49
1:B:472:TYR:O	1:B:475:ASN:HB2	2.13	0.49
1:C:89:GLN:NE2	1:D:115:ARG:HH22	2.11	0.49
1:C:109:THR:HG22	1:C:112:GLU:CB	2.42	0.49
1:C:262:ALA:HA	1:C:382:GLY:H	1.76	0.49
1:D:341:ARG:HH11	1:D:412:PRO:HB3	1.75	0.49
1:A:40:VAL:HG13	1:A:84:VAL:HG13	1.92	0.49
1:A:96:ASP:CG	1:A:99:LYS:HD2	2.38	0.49
1:B:447:PHE:HB3	1:B:450:TYR:CD1	2.47	0.49
1:C:441:ASP:HB3	4:C:844:HOH:O	2.12	0.49
1:A:407:ALA:HB2	1:A:422:ILE:HG23	1.94	0.49
2:A:601[A]:AKY:H513	2:A:601[A]:AKY:O18	2.12	0.49
1:C:30:ASN:ND2	1:C:32:ARG:H	2.11	0.49
1:C:153:VAL:HG12	1:C:155:ALA:H	1.78	0.49
1:D:274:PHE:CE2	1:D:284:ILE:HD12	2.47	0.49
1:A:137:GLY:HA2	1:A:140:LEU:HD11	1.94	0.49
1:A:226:PRO:HD2	1:A:325:TRP:CD1	2.48	0.49
1:A:193:THR:CG2	1:A:393:ALA:H	2.18	0.49
1:C:203:VAL:HG13	3:C:801:FAD:C2A	2.43	0.49
1:C:220:GLN:NE2	4:C:1002:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:HD13	4:C:828:HOH:O	2.12	0.49
1:D:419:LEU:O	1:D:422:ILE:HD12	2.12	0.49
1:D:466:PRO:HG2	1:D:469:THR:OG1	2.12	0.49
1:A:396:GLN:H	1:A:396:GLN:NE2	2.11	0.48
1:C:476:TYR:HB3	1:C:477:PRO:HD3	1.95	0.48
1:A:16:ARG:HG3	1:A:17:VAL:H	1.77	0.48
1:B:25:VAL:HG22	1:B:25:VAL:O	2.13	0.48
1:B:262:ALA:H	1:B:263:ALA:HB2	1.78	0.48
1:C:89:GLN:NE2	1:D:115:ARG:HH12	2.11	0.48
1:C:263:ALA:CB	1:C:268:ALA:HB2	2.39	0.48
1:D:174:LYS:HG3	4:D:899:HOH:O	2.13	0.48
1:D:291:ASP:O	1:D:294:LEU:HG	2.14	0.48
1:B:20:ARG:NH2	4:B:815:HOH:O	2.43	0.48
1:B:65:VAL:CG2	1:B:202:ILE:HG12	2.43	0.48
1:B:279:ARG:HB2	1:B:366:SER:HA	1.94	0.48
1:D:364:HIS:CG	1:D:425:ILE:HG23	2.49	0.48
1:A:14:VAL:HG22	1:A:41:TYR:CD1	2.48	0.48
1:A:345:LYS:HD3	1:A:426:TYR:CG	2.48	0.48
1:B:494:HIS:H	1:B:497:SER:HB2	1.78	0.48
1:C:109:THR:CG2	1:C:112:GLU:H	2.26	0.48
1:C:115:ARG:HE	1:D:91:ARG:HH21	1.60	0.48
1:C:195:GLY:HA2	1:C:472:TYR:HE1	1.78	0.48
1:A:65:VAL:HG22	1:A:85:ILE:CD1	2.35	0.48
1:B:40:VAL:HA	1:B:84:VAL:HG13	1.95	0.48
1:B:120:ASP:HB3	4:B:940:HOH:O	2.13	0.48
1:B:455:LEU:O	1:B:462:THR:HG21	2.14	0.48
1:C:115:ARG:HH21	1:D:91:ARG:HH21	1.61	0.48
1:A:143:GLY:HA2	3:A:801:FAD:O2	2.13	0.48
1:A:392:THR:HG21	1:A:394:THR:OG1	2.13	0.48
1:B:130:CYS:HB3	4:B:802:HOH:O	2.14	0.48
1:B:232:HIS:CE1	1:B:301:LEU:HB3	2.49	0.48
1:C:262:ALA:HA	1:C:382:GLY:N	2.29	0.48
1:D:343:LYS:HE2	4:D:956:HOH:O	2.13	0.48
1:A:370:GLN:NE2	4:A:1020:HOH:O	2.46	0.48
1:B:456:VAL:HG12	1:B:456:VAL:O	2.13	0.48
1:D:124:THR:HG21	4:D:935:HOH:O	2.13	0.48
1:B:199:ASN:CB	1:B:498:VAL:HG22	2.43	0.48
1:B:245:ALA:HA	1:B:248:ARG:CG	2.44	0.48
1:B:263:ALA:HB1	1:B:268:ALA:CB	2.43	0.48
1:C:389:GLU:OE2	1:C:395:ALA:O	2.30	0.48
1:D:193:THR:CG2	1:D:393:ALA:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:GLN:NE2	4:D:1004:HOH:O	2.47	0.48
1:B:195:GLY:HA2	1:B:448:ILE:CG1	2.39	0.48
1:B:338:GLY:O	1:B:410:MET:HG3	2.14	0.48
1:B:423:ARG:NH2	4:B:882:HOH:O	2.47	0.48
1:C:128:GLY:HA2	1:C:144:TYR:O	2.13	0.48
1:D:419:LEU:O	1:D:423:ARG:HD2	2.13	0.48
1:D:297:ALA:HA	1:D:300:LEU:CD1	2.42	0.48
1:A:146:PRO:HA	1:A:271:HIS:CG	2.49	0.47
1:A:422:ILE:HD12	1:A:423:ARG:HG3	1.96	0.47
1:B:277:ASN:HA	1:B:374:GLU:HB3	1.94	0.47
1:C:214:THR:O	1:C:221:LEU:HD21	2.14	0.47
1:D:109:THR:HG22	1:D:112:GLU:CG	2.44	0.47
1:C:40:VAL:HA	1:C:84:VAL:HG13	1.96	0.47
1:C:141:GLY:C	1:C:194:GLY:HA2	2.39	0.47
1:D:14:VAL:HG22	1:D:41:TYR:CE1	2.50	0.47
1:D:85:ILE:HG13	1:D:87:MET:HE3	1.96	0.47
1:D:128:GLY:HA2	1:D:144:TYR:O	2.14	0.47
1:D:429:ILE:O	1:D:429:ILE:HG12	2.08	0.47
1:A:159:TYR:OH	4:A:879:HOH:O	2.18	0.47
1:A:209:ARG:HB3	1:A:209:ARG:NH1	2.29	0.47
1:A:407:ALA:HB2	1:A:421:TRP:CD1	2.50	0.47
1:A:435:GLY:HA3	1:A:461:ASN:HB3	1.96	0.47
1:B:140:LEU:HA	1:B:192:HIS:O	2.14	0.47
1:B:288:ILE:HD11	1:B:301:LEU:CG	2.43	0.47
1:B:334:PHE:HE1	4:B:876:HOH:O	1.96	0.47
1:A:21:TYR:O	1:A:25:VAL:HG12	2.14	0.47
1:A:127:ALA:O	1:A:145:GLY:HA3	2.14	0.47
1:A:345:LYS:HE3	1:A:345:LYS:HB3	1.64	0.47
1:B:109:THR:HG21	4:B:926:HOH:O	2.14	0.47
1:B:290:ILE:HG22	1:B:301:LEU:HD21	1.97	0.47
1:B:433:THR:HG22	1:B:436:VAL:O	2.14	0.47
1:C:89:GLN:HA	1:D:115:ARG:NH2	2.26	0.47
1:B:305:VAL:HG21	4:B:913:HOH:O	2.13	0.47
1:B:344:SER:HB2	1:B:404:TRP:NE1	2.29	0.47
1:B:407:ALA:HB2	1:B:421:TRP:HD1	1.78	0.47
1:A:261:SER:OG	1:A:262:ALA:N	2.48	0.47
1:C:82:ARG:HH11	1:C:82:ARG:HD3	1.48	0.47
1:C:339:PHE:HB3	1:C:408:THR:HG22	1.95	0.47
1:A:81:VAL:HG23	4:A:978:HOH:O	2.13	0.47
1:B:10:ALA:HB3	1:B:44:HIS:CE1	2.50	0.47
1:B:411:ASP:HA	1:B:412:PRO:HD2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:HIS:HD2	1:B:496:LEU:H	1.62	0.47
1:C:23:ASP:OD1	1:D:324:PRO:HB2	2.15	0.47
1:C:30:ASN:HD22	1:C:32:ARG:H	1.62	0.47
1:C:433:THR:HB	4:C:848:HOH:O	2.14	0.47
1:D:173:ARG:HB2	4:D:862:HOH:O	2.15	0.47
1:A:290:ILE:CG2	1:A:301:LEU:HD11	2.45	0.47
1:B:45:THR:OG1	1:B:48:GLN:HG3	2.15	0.47
1:C:279:ARG:O	1:C:279:ARG:HG2	2.14	0.47
1:D:337:GLY:O	1:D:339:PHE:HD2	1.98	0.47
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.23	0.47
1:A:384:VAL:HG13	1:A:385:ASN:OD1	2.14	0.47
1:B:392:THR:CG2	1:B:397:ARG:HH21	2.14	0.47
1:C:296:GLY:O	1:C:299:ALA:HB3	2.15	0.47
1:D:103:ALA:HB2	1:D:207:TRP:CH2	2.49	0.47
1:A:405:MET:HE1	1:A:429:ILE:HD12	1.97	0.47
1:D:124:THR:OG1	1:D:225:ALA:HB2	2.15	0.47
1:D:162:GLU:HB3	1:D:204:THR:CG2	2.46	0.47
1:D:309:ASN:ND2	1:D:316:PRO:HD3	2.29	0.47
1:C:104:VAL:HG23	1:C:135:VAL:HG11	1.97	0.46
1:D:99:LYS:HE3	1:D:207:TRP:NE1	2.29	0.46
1:D:203:VAL:HG11	1:D:206:TYR:CZ	2.50	0.46
1:A:141:GLY:CA	1:A:448:ILE:HD11	2.45	0.46
1:C:66:ARG:HH22	1:C:77:ASP:CG	2.24	0.46
1:C:246:PHE:O	1:C:250:ILE:HG12	2.15	0.46
1:C:494:HIS:O	1:C:497:SER:HB2	2.15	0.46
1:D:394:THR:OG1	1:D:397:ARG:NH2	2.49	0.46
1:A:140:LEU:HA	1:A:192:HIS:O	2.14	0.46
1:A:213:ALA:N	4:A:954:HOH:O	2.48	0.46
1:B:17:VAL:O	1:B:17:VAL:HG23	2.15	0.46
1:B:237:ASP:OD1	1:B:283:GLN:NE2	2.49	0.46
1:C:65:VAL:HG22	1:C:85:ILE:CG1	2.45	0.46
1:D:100:ARG:HH22	1:D:213:ALA:HB1	1.79	0.46
1:D:162:GLU:HG3	1:D:176:VAL:HG22	1.97	0.46
1:B:163:VAL:HG22	1:B:203:VAL:HG22	1.96	0.46
1:B:217:ASP:OD2	1:B:220:GLN:NE2	2.49	0.46
1:C:252:ASN:HB3	1:C:307:ALA:O	2.15	0.46
1:C:197:GLY:O	3:C:801:FAD:N3A	2.49	0.46
1:A:290:ILE:HG12	1:A:294:LEU:HD11	1.97	0.46
1:B:232:HIS:HB2	1:B:288:ILE:HG12	1.98	0.46
1:A:16:ARG:NH1	4:A:824:HOH:O	2.49	0.46
1:A:290:ILE:HD13	1:A:300:LEU:CD1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:HIS:O	1:C:261:SER:OG	2.30	0.46
1:C:434:GLY:CA	1:C:463:SER:HB2	2.34	0.46
1:D:27:ARG:HH11	1:D:66:ARG:HD2	1.81	0.46
1:D:130:CYS:HG	3:D:801:FAD:C5X	2.28	0.46
1:A:421:TRP:HZ3	4:A:974:HOH:O	1.98	0.46
1:A:453:VAL:HG23	1:A:496:LEU:HD13	1.96	0.46
1:B:213:ALA:O	1:B:214:THR:OG1	2.29	0.46
1:C:231:ARG:HA	1:C:288:ILE:O	2.16	0.46
1:C:486:TRP:C	1:C:488:PRO:HD3	2.41	0.46
1:B:115:ARG:HG3	1:B:116:ALA:N	2.31	0.46
1:C:370:GLN:O	1:C:370:GLN:HG3	2.15	0.46
1:D:196:GLY:O	1:D:199:ASN:ND2	2.49	0.46
1:D:312:THR:CG2	1:D:314:VAL:HG13	2.37	0.46
1:B:67:SER:HB3	1:B:106:PRO:O	2.16	0.46
3:B:801:FAD:N1	3:B:801:FAD:O3'	2.49	0.46
1:C:88:SER:N	4:C:1000:HOH:O	2.49	0.46
1:C:103:ALA:HB2	1:C:207:TRP:CE3	2.51	0.46
1:C:199:ASN:ND2	1:C:497:SER:OG	2.49	0.46
1:C:462:THR:CG2	1:C:470:LEU:HD11	2.45	0.46
1:D:462:THR:N	4:D:950:HOH:O	2.47	0.46
1:A:162:GLU:CG	1:A:176:VAL:HG22	2.46	0.45
1:A:373:GLY:HA3	1:A:421:TRP:CE2	2.51	0.45
1:A:434:GLY:O	1:A:462:THR:N	2.50	0.45
1:A:437:PRO:O	1:A:445:GLY:HA2	2.15	0.45
1:C:62:ARG:NH2	1:C:494:HIS:HA	2.32	0.45
1:D:28:GLY:O	1:D:34:ARG:NH2	2.50	0.45
1:A:112:GLU:HA	1:A:115:ARG:HG2	1.98	0.45
1:A:149:ARG:NH1	1:A:267:TYR:O	2.49	0.45
1:A:261:SER:HB2	4:A:892:HOH:O	2.16	0.45
1:B:234:VAL:HG11	4:B:913:HOH:O	2.15	0.45
1:B:291:ASP:N	4:B:895:HOH:O	2.48	0.45
1:B:419:LEU:HD22	1:B:423:ARG:HH21	1.82	0.45
1:C:34:ARG:NH2	4:C:997:HOH:O	2.49	0.45
1:C:347:ALA:N	1:C:403:VAL:HG22	2.30	0.45
1:C:400:ILE:HD11	4:C:1007:HOH:O	2.17	0.45
1:C:422:ILE:HD12	1:C:423:ARG:H	1.81	0.45
1:D:232:HIS:CD2	1:D:320:ARG:HG2	2.51	0.45
1:A:14:VAL:HG22	1:A:41:TYR:CE1	2.51	0.45
1:A:335:ASP:OD2	1:A:337:GLY:N	2.49	0.45
1:B:65:VAL:HG22	1:B:85:ILE:CD1	2.37	0.45
1:B:252:ASN:HB2	1:B:308:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:OE2	1:B:320:ARG:NH1	2.50	0.45
1:D:78:ASP:N	4:D:948:HOH:O	2.49	0.45
1:D:427:ARG:O	1:D:431:ALA:N	2.49	0.45
1:A:265:THR:HB	1:A:266:PRO:HD2	1.98	0.45
1:A:405:MET:HE1	1:A:429:ILE:CD1	2.46	0.45
1:A:450:TYR:CE2	2:A:601[A]:AKY:H412	2.51	0.45
1:B:150:ARG:NH2	1:B:151:ASP:OD2	2.50	0.45
1:C:115:ARG:NH2	1:D:88:SER:O	2.50	0.45
1:C:233:ILE:HG22	4:C:1001:HOH:O	2.17	0.45
1:C:243:GLU:OE1	1:C:362:TYR:HB3	2.17	0.45
1:C:354:THR:H	1:C:357:GLN:NE2	2.03	0.45
1:D:341:ARG:NE	4:D:959:HOH:O	2.49	0.45
1:A:140:LEU:HD12	1:A:140:LEU:H	1.81	0.45
1:A:279:ARG:N	4:A:916:HOH:O	2.49	0.45
1:B:335:ASP:OD2	1:B:337:GLY:N	2.50	0.45
1:C:109:THR:HG22	1:C:112:GLU:HG3	1.99	0.45
1:C:188:LEU:HG	1:C:486:TRP:CD2	2.52	0.45
1:A:17:VAL:HA	4:A:852:HOH:O	2.16	0.45
1:A:114:TYR:OH	1:A:127:ALA:HB3	2.17	0.45
1:B:109:THR:HG22	1:B:112:GLU:HG3	1.98	0.45
1:C:66:ARG:NH2	1:C:77:ASP:OD2	2.48	0.45
1:C:79:PRO:O	1:C:82:ARG:NH1	2.49	0.45
1:C:109:THR:HG22	1:C:112:GLU:CG	2.47	0.45
1:C:171:ARG:NH2	4:C:877:HOH:O	2.50	0.45
1:D:354:THR:OG1	1:D:355:ALA:N	2.49	0.45
1:A:89:GLN:OE1	1:B:115:ARG:NH1	2.50	0.45
1:A:414:HIS:HA	4:A:853:HOH:O	2.17	0.45
2:A:601[A]:AKY:H143	2:A:601[A]:AKY:H81	1.70	0.45
1:B:96:ASP:OD2	1:B:98:GLY:N	2.49	0.45
1:B:299:ALA:HA	1:B:302:ASN:OD1	2.17	0.45
1:B:336:THR:OG1	1:B:339:PHE:O	2.29	0.45
1:C:127:ALA:O	1:C:145:GLY:HA3	2.16	0.45
1:C:429:ILE:HD11	1:C:430:PHE:CZ	2.52	0.45
1:D:350:ARG:HD2	4:D:915:HOH:O	2.16	0.45
1:A:155:ALA:HB1	1:A:193:THR:OG1	2.16	0.45
1:A:203:VAL:HG11	1:A:206:TYR:CZ	2.52	0.45
1:A:261:SER:OG	1:A:382:GLY:N	2.50	0.45
1:B:140:LEU:HD22	1:B:196:GLY:C	2.41	0.45
1:B:246:PHE:O	1:B:250:ILE:HG12	2.17	0.45
1:C:130:CYS:CB	3:C:801:FAD:C6	2.90	0.45
1:C:150:ARG:NH1	1:C:151:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:SER:HA	1:D:152:GLY:O	2.16	0.45
1:D:254:GLY:HA3	1:D:352:PRO:HB3	1.99	0.45
1:D:352:PRO:O	1:D:442:ARG:NH2	2.50	0.45
1:D:369:SER:OG	1:D:370:GLN:N	2.50	0.45
1:D:432:THR:HG23	1:D:432:THR:O	2.16	0.45
1:A:62:ARG:NH2	4:A:1011:HOH:O	2.49	0.45
1:B:140:LEU:HD12	1:B:140:LEU:N	2.32	0.45
1:C:162:GLU:CG	1:C:205:ARG:HB3	2.42	0.45
1:C:396:GLN:H	1:C:396:GLN:NE2	2.14	0.45
1:C:456:VAL:HG12	1:C:456:VAL:O	2.17	0.45
1:D:191:ALA:CB	1:D:482:VAL:HG11	2.47	0.45
1:D:341:ARG:NH2	1:D:415:ASP:OD2	2.50	0.45
1:A:463:SER:N	4:A:895:HOH:O	2.49	0.45
1:B:64:ALA:O	1:B:84:VAL:HA	2.17	0.45
1:B:392:THR:HG23	1:B:393:ALA:N	2.30	0.45
1:C:173:ARG:NH2	4:C:990:HOH:O	2.50	0.45
1:C:448:ILE:HG22	1:C:471:TYR:HB3	1.98	0.45
1:A:234:VAL:HA	1:A:317:ALA:O	2.17	0.44
2:A:601[A]:AKY:O16	2:A:601[A]:AKY:H82	2.14	0.44
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.85	0.44
1:B:354:THR:OG1	1:B:355:ALA:N	2.50	0.44
1:B:367:ALA:O	1:B:369:SER:N	2.50	0.44
1:B:446:THR:HG23	1:B:471:TYR:CE2	2.52	0.44
1:C:63:ILE:HG23	1:C:85:ILE:HD13	1.99	0.44
1:C:88:SER:O	1:D:115:ARG:NH2	2.50	0.44
1:D:70:HIS:CE1	3:D:801:FAD:C8M	2.86	0.44
1:D:425:ILE:H	1:D:425:ILE:HG13	1.58	0.44
1:D:427:ARG:HB3	1:D:461:ASN:ND2	2.32	0.44
1:A:61:GLN:HB3	1:A:83:ALA:HB2	2.00	0.44
4:A:937:HOH:O	1:B:327:ARG:NE	2.50	0.44
1:B:356:ALA:O	1:B:359:ALA:HB3	2.17	0.44
1:B:426:TYR:N	4:B:957:HOH:O	2.50	0.44
1:C:14:VAL:HG22	1:C:41:TYR:CE1	2.52	0.44
1:D:278:SER:OG	1:D:373:GLY:O	2.35	0.44
1:A:112:GLU:O	1:A:115:ARG:HG2	2.16	0.44
1:A:263:ALA:N	4:A:896:HOH:O	2.51	0.44
1:C:97:SER:O	1:C:100:ARG:N	2.50	0.44
1:C:175:VAL:N	4:C:929:HOH:O	2.50	0.44
1:C:253:HIS:HE1	4:C:850:HOH:O	2.01	0.44
1:D:372:TRP:NE1	4:D:858:HOH:O	2.49	0.44
1:D:435:GLY:O	1:D:461:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NE	4:A:1041:HOH:O	2.49	0.44
1:A:429:ILE:HD11	1:A:430:PHE:CE2	2.53	0.44
1:A:448:ILE:HD13	4:A:857:HOH:O	2.17	0.44
1:B:248:ARG:HG2	1:B:248:ARG:H	1.69	0.44
1:B:308:VAL:HG12	4:B:963:HOH:O	2.18	0.44
1:C:97:SER:C	1:C:100:ARG:H	2.25	0.44
1:C:499:ARG:HH11	1:C:499:ARG:HD3	1.51	0.44
1:B:127:ALA:O	1:B:145:GLY:HA3	2.17	0.44
1:D:193:THR:HG23	1:D:393:ALA:N	2.14	0.44
1:D:270:MET:HB2	1:D:290:ILE:HD12	1.99	0.44
1:D:279:ARG:O	1:D:279:ARG:HG2	2.18	0.44
1:B:123:VAL:HG12	1:B:124:THR:N	2.33	0.44
1:B:233:ILE:HG12	1:B:319:GLN:OE1	2.17	0.44
1:D:138:HIS:NE2	1:D:143:GLY:HA3	2.32	0.44
1:D:232:HIS:NE2	1:D:298:GLU:OE2	2.50	0.44
1:D:288:ILE:HD12	1:D:304:PHE:CD1	2.53	0.44
1:D:453:VAL:HG12	4:D:875:HOH:O	2.17	0.44
1:D:480:GLN:HG2	1:D:499:ARG:O	2.18	0.44
1:B:454:ASP:OD2	1:B:454:ASP:N	2.49	0.44
1:C:27:ARG:HD2	4:C:1030:HOH:O	2.16	0.44
1:D:89:GLN:HE21	1:D:89:GLN:HA	1.82	0.44
1:D:244:GLU:HB2	4:D:941:HOH:O	2.17	0.44
1:D:436:VAL:HG13	1:D:461:ASN:HB3	1.98	0.44
3:D:801:FAD:O4'	3:D:801:FAD:O2'	2.31	0.44
1:A:85:ILE:HG12	1:A:85:ILE:O	2.18	0.44
1:C:115:ARG:NH2	1:D:89:GLN:HE21	2.15	0.44
1:C:425:ILE:HG13	1:C:425:ILE:H	1.53	0.44
1:D:82:ARG:HD3	1:D:82:ARG:HA	1.80	0.44
1:D:89:GLN:HB2	4:D:845:HOH:O	2.18	0.44
1:D:109:THR:HG22	1:D:112:GLU:H	1.81	0.44
1:A:79:PRO:O	1:A:82:ARG:NH1	2.49	0.44
1:A:424:GLU:OE2	4:A:990:HOH:O	2.21	0.44
1:B:185:ASN:N	1:B:185:ASN:OD1	2.50	0.44
1:B:238:TRP:CG	1:B:279:ARG:HG3	2.53	0.44
1:C:29:PHE:HB2	1:C:70:HIS:HA	2.00	0.44
1:C:115:ARG:CZ	1:D:91:ARG:HH21	2.31	0.44
1:C:129:VAL:HG22	1:C:146:PRO:CD	2.39	0.44
1:D:263:ALA:HB1	1:D:265:THR:HG23	1.98	0.44
1:D:374:GLU:HG3	4:D:835:HOH:O	2.17	0.44
1:A:89:GLN:OE1	1:B:115:ARG:NH2	2.50	0.43
1:A:209:ARG:HD3	1:A:213:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HG	1:B:40:VAL:CG1	2.38	0.43
1:B:205:ARG:NH1	4:B:887:HOH:O	2.48	0.43
1:B:257:HIS:NE2	1:B:379:SER:HB3	2.33	0.43
1:D:140:LEU:HD13	1:D:197:GLY:H	1.83	0.43
1:D:209:ARG:HG3	1:D:221:LEU:HD13	1.99	0.43
1:A:94:PHE:O	1:A:103:ALA:N	2.49	0.43
1:A:383:LYS:N	4:A:972:HOH:O	2.50	0.43
1:A:483:LYS:HD3	1:A:498:VAL:HG23	1.99	0.43
1:B:123:VAL:CG1	1:B:222:LEU:HB2	2.47	0.43
1:C:480:GLN:HB3	1:C:501:PRO:HG3	1.98	0.43
1:D:51:ASP:O	1:D:55:GLN:HG3	2.17	0.43
1:B:193:THR:HG23	1:B:393:ALA:N	2.17	0.43
1:B:350:ARG:NE	4:B:811:HOH:O	2.42	0.43
1:B:385:ASN:OD1	1:B:385:ASN:N	2.50	0.43
1:B:466:PRO:HG2	1:B:468:TYR:CE2	2.53	0.43
1:C:457:ASP:HB2	4:C:882:HOH:O	2.17	0.43
1:D:70:HIS:ND1	3:D:801:FAD:HM81	2.12	0.43
1:A:62:ARG:NH1	1:A:80:ALA:HB3	2.33	0.43
1:B:236:TRP:NE1	1:B:309:ASN:OD1	2.50	0.43
1:C:113:THR:HG21	1:C:135:VAL:CG2	2.48	0.43
1:C:233:ILE:HD11	1:C:285:LEU:CD1	2.47	0.43
1:D:13:LYS:HB2	1:D:42:VAL:HB	2.00	0.43
1:B:144:TYR:CE2	1:B:402:LYS:HE2	2.54	0.43
1:C:305:VAL:HG21	4:C:987:HOH:O	2.18	0.43
1:A:95:TYR:CE2	1:A:97:SER:HA	2.53	0.43
1:A:236:TRP:CE2	1:A:316:PRO:HB3	2.54	0.43
1:C:312:THR:HG22	1:C:314:VAL:N	2.27	0.43
1:A:319:GLN:NE2	4:A:941:HOH:O	2.49	0.43
1:A:404:TRP:CE2	2:A:601[A]:AKY:C41	3.01	0.43
1:B:34:ARG:NE	4:B:970:HOH:O	2.49	0.43
1:B:241:LEU:HD11	1:B:284:ILE:HD13	2.00	0.43
1:B:315:GLU:HA	1:B:316:PRO:HD2	1.92	0.43
1:B:360:THR:HG21	1:B:429:ILE:HG22	2.01	0.43
1:C:53:VAL:HG12	1:C:57:MET:HE2	2.01	0.43
1:D:129:VAL:HG22	1:D:146:PRO:HD3	2.00	0.43
1:D:341:ARG:HD2	1:D:415:ASP:OD1	2.18	0.43
1:A:262:ALA:HA	1:A:382:GLY:CA	2.49	0.43
1:A:371:VAL:HG21	1:A:421:TRP:CD1	2.54	0.43
1:A:425:ILE:O	1:A:429:ILE:HG23	2.19	0.43
1:C:348:TYR:CD2	1:C:396:GLN:HG2	2.53	0.43
1:C:350:ARG:HH11	1:C:350:ARG:HD2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ASP:O	1:C:411:ASP:OD2	2.37	0.43
1:D:249:ILE:O	1:D:252:ASN:HB2	2.18	0.43
1:A:73:GLU:OE1	1:A:343:LYS:NZ	2.50	0.43
1:A:396:GLN:H	1:A:396:GLN:HE21	1.66	0.43
1:C:98:GLY:HA2	4:C:954:HOH:O	2.19	0.43
1:C:203:VAL:CB	4:C:1015:HOH:O	2.60	0.43
1:C:247:THR:HG22	1:C:248:ARG:HE	1.84	0.43
1:C:335:ASP:OD1	1:D:332:ASN:ND2	2.49	0.43
1:C:392:THR:CG2	1:C:394:THR:H	2.15	0.43
1:D:66:ARG:NH1	4:D:975:HOH:O	2.50	0.43
1:D:249:ILE:N	4:D:901:HOH:O	2.52	0.43
1:A:124:THR:HG22	1:A:125:ILE:N	2.32	0.43
1:A:361:LEU:HD12	1:A:361:LEU:HA	1.86	0.43
1:C:193:THR:HG23	1:C:393:ALA:N	2.12	0.43
1:C:233:ILE:CD1	1:C:285:LEU:HD11	2.48	0.43
1:C:422:ILE:CD1	1:C:423:ARG:HG3	2.49	0.43
1:A:14:VAL:HG13	1:A:39:VAL:HG21	2.00	0.42
1:A:140:LEU:HD12	1:A:140:LEU:N	2.34	0.42
1:A:147:LEU:O	1:A:150:ARG:HG2	2.18	0.42
1:A:279:ARG:HA	4:A:854:HOH:O	2.19	0.42
1:B:30:ASN:ND2	1:B:32:ARG:HB2	2.34	0.42
1:B:87:MET:O	1:B:107:GLY:HA3	2.19	0.42
1:B:381:GLY:C	1:B:384:VAL:HG12	2.43	0.42
1:C:336:THR:CG2	4:C:968:HOH:O	2.67	0.42
1:D:229:THR:O	1:D:322:THR:HA	2.19	0.42
3:D:801:FAD:H9	3:D:801:FAD:H1'2	1.65	0.42
1:A:25:VAL:O	1:A:25:VAL:HG22	2.19	0.42
1:A:290:ILE:CD1	1:A:300:LEU:HD13	2.43	0.42
1:A:354:THR:HG22	1:A:357:GLN:CG	2.49	0.42
1:B:364:HIS:HE1	1:B:428:GLU:OE2	2.03	0.42
1:B:411:ASP:HB3	1:B:414:HIS:CE1	2.54	0.42
1:C:65:VAL:HA	1:C:85:ILE:HG12	2.01	0.42
1:C:228:SER:OG	1:C:292:GLY:HA3	2.19	0.42
1:C:232:HIS:CE1	1:C:301:LEU:HB3	2.53	0.42
1:D:350:ARG:HG3	1:D:444:GLU:HG3	2.00	0.42
1:A:194:GLY:HA3	1:A:394:THR:HG22	2.00	0.42
1:A:336:THR:HG23	1:A:338:GLY:H	1.83	0.42
1:A:424:GLU:HG2	4:A:1053:HOH:O	2.19	0.42
1:C:231:ARG:NH1	1:C:287:ASP:OD2	2.50	0.42
1:C:281:ALA:HB2	4:C:817:HOH:O	2.20	0.42
1:C:297:ALA:HA	1:C:300:LEU:CD1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:CD	1:D:17:VAL:H	2.31	0.42
1:D:27:ARG:NE	1:D:86:ASP:OD1	2.50	0.42
1:D:265:THR:O	1:D:268:ALA:HB3	2.19	0.42
1:D:446:THR:HG23	1:D:471:TYR:CE2	2.54	0.42
1:B:131:PRO:HD3	1:B:334:PHE:CE1	2.55	0.42
1:B:147:LEU:HA	4:B:924:HOH:O	2.19	0.42
1:B:174:LYS:HB2	1:B:174:LYS:HE3	1.87	0.42
1:B:312:THR:HG22	1:B:313:GLY:N	2.33	0.42
1:C:165:VAL:HA	4:C:1050:HOH:O	2.19	0.42
1:C:466:PRO:O	1:C:470:LEU:HG	2.19	0.42
1:D:343:LYS:HD3	4:D:956:HOH:O	2.19	0.42
1:A:129:VAL:HG12	1:A:334:PHE:CZ	2.52	0.42
1:B:346:GLY:HA2	1:B:403:VAL:O	2.19	0.42
1:D:144:TYR:CD1	1:D:402:LYS:HE3	2.54	0.42
1:D:409:TRP:NE1	1:D:415:ASP:OD1	2.50	0.42
1:A:130:CYS:HB2	1:A:133:VAL:CG2	2.39	0.42
1:B:350:ARG:NE	1:B:398:ASP:OD1	2.52	0.42
1:B:482:VAL:HG13	1:B:486:TRP:CE3	2.55	0.42
1:C:96:ASP:HB3	1:C:207:TRP:HZ3	1.84	0.42
1:C:347:ALA:HB3	1:C:403:VAL:HG22	2.01	0.42
1:D:249:ILE:HG12	4:D:901:HOH:O	2.20	0.42
1:B:300:LEU:H	1:B:300:LEU:HG	1.63	0.42
1:B:312:THR:HG22	1:B:313:GLY:H	1.85	0.42
1:C:166:VAL:HG23	4:C:1050:HOH:O	2.19	0.42
1:C:294:LEU:O	1:C:297:ALA:HB2	2.20	0.42
1:C:405:MET:HE1	1:C:429:ILE:CD1	2.44	0.42
1:B:65:VAL:HG13	1:B:87:MET:HE3	2.01	0.42
1:C:191:ALA:HB1	1:C:200:PHE:CE2	2.55	0.42
1:D:263:ALA:HB1	1:D:265:THR:CG2	2.50	0.42
1:A:65:VAL:CG2	1:A:202:ILE:HG12	2.46	0.42
1:A:453:VAL:HG23	1:A:496:LEU:CD1	2.50	0.42
1:B:360:THR:HG22	1:B:429:ILE:HG22	2.01	0.42
1:C:27:ARG:NH2	4:C:854:HOH:O	2.51	0.42
1:C:290:ILE:HD13	1:C:300:LEU:CD1	2.50	0.42
1:C:348:TYR:OH	1:C:402:LYS:NZ	2.47	0.42
1:C:447:PHE:HA	4:C:900:HOH:O	2.20	0.42
1:D:375:VAL:HG22	1:D:405:MET:CG	2.50	0.42
1:D:422:ILE:HD12	1:D:423:ARG:H	1.85	0.42
1:A:62:ARG:HH11	1:A:80:ALA:HB3	1.85	0.42
1:B:476:TYR:HB3	1:B:477:PRO:HD3	2.01	0.42
1:D:99:LYS:HE2	4:D:980:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ARG:HG3	1:D:231:ARG:HH11	1.85	0.42
1:D:462:THR:HG22	1:D:465:VAL:O	2.20	0.42
1:A:236:TRP:HD1	1:A:314:VAL:HG22	1.85	0.41
1:B:25:VAL:HG21	1:B:35:GLY:O	2.20	0.41
1:B:210:THR:O	1:B:213:ALA:HB2	2.20	0.41
1:B:354:THR:HG22	1:B:357:GLN:HG3	2.01	0.41
1:C:144:TYR:CE1	1:C:402:LYS:HE3	2.55	0.41
1:C:300:LEU:HA	1:C:303:ASP:HB2	2.02	0.41
1:A:27:ARG:NH2	1:A:66:ARG:HG2	2.35	0.41
1:A:51:ASP:OD1	1:A:55:GLN:NE2	2.50	0.41
1:A:53:VAL:O	1:A:57:MET:HG3	2.20	0.41
1:A:421:TRP:CE2	1:A:425:ILE:HD11	2.55	0.41
1:A:421:TRP:NE1	4:A:904:HOH:O	2.49	0.41
1:B:236:TRP:NE1	1:B:316:PRO:HD3	2.35	0.41
1:B:260:ASN:C	1:B:262:ALA:HB2	2.45	0.41
1:B:356:ALA:HA	1:B:359:ALA:HB3	2.02	0.41
1:D:153:VAL:HG12	1:D:155:ALA:H	1.85	0.41
1:D:193:THR:OG1	1:D:392:THR:OG1	2.29	0.41
1:A:109:THR:HG23	1:A:111:GLY:N	2.35	0.41
1:A:115:ARG:HH21	1:B:91:ARG:HD2	1.84	0.41
1:A:203:VAL:HG11	1:A:206:TYR:CE1	2.55	0.41
1:A:243:GLU:N	4:A:1042:HOH:O	2.53	0.41
1:B:390:THR:HG23	1:B:390:THR:O	2.19	0.41
1:C:262:ALA:HA	1:C:382:GLY:CA	2.50	0.41
1:C:347:ALA:HB3	1:C:403:VAL:CG2	2.50	0.41
1:C:392:THR:HG21	1:C:397:ARG:NH2	2.08	0.41
1:C:455:LEU:HD22	1:C:470:LEU:CD1	2.50	0.41
1:D:115:ARG:HG3	1:D:116:ALA:N	2.33	0.41
1:D:381:GLY:C	1:D:384:VAL:HG12	2.43	0.41
1:D:417:ALA:O	1:D:420:ALA:HB3	2.19	0.41
1:D:456:VAL:HG12	1:D:456:VAL:O	2.20	0.41
1:A:262:ALA:HA	1:A:382:GLY:O	2.20	0.41
1:C:273:VAL:HG13	1:C:378:TYR:CD2	2.55	0.41
1:C:483:LYS:HD3	1:C:498:VAL:O	2.19	0.41
1:C:487:ASP:N	1:C:488:PRO:HD3	2.35	0.41
1:D:226:PRO:HD2	1:D:325:TRP:CD1	2.56	0.41
1:D:274:PHE:CZ	1:D:284:ILE:HD12	2.56	0.41
1:B:146:PRO:HA	1:B:271:HIS:CD2	2.55	0.41
1:B:426:TYR:OH	1:B:437:PRO:HD3	2.20	0.41
1:D:130:CYS:HB2	1:D:133:VAL:HG23	2.01	0.41
1:D:232:HIS:HB2	1:D:288:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:VAL:HG22	1:D:378:TYR:HD2	1.85	0.41
1:D:414:HIS:HB3	4:D:970:HOH:O	2.20	0.41
1:A:115:ARG:NH2	1:B:91:ARG:NE	2.69	0.41
1:A:325:TRP:O	1:A:329:THR:OG1	2.30	0.41
1:C:16:ARG:HE	1:C:17:VAL:HG22	1.85	0.41
1:C:49:VAL:CG2	1:C:87:MET:HE1	2.50	0.41
1:C:290:ILE:HD13	1:C:300:LEU:HD13	2.03	0.41
1:C:448:ILE:HA	1:C:471:TYR:CE2	2.56	0.41
1:D:418:ASN:O	1:D:421:TRP:HB3	2.20	0.41
1:A:404:TRP:CE2	2:A:601[A]:AKY:H411	2.55	0.41
1:A:462:THR:HG22	1:A:465:VAL:O	2.21	0.41
2:A:601[A]:AKY:O5	2:A:601[A]:AKY:O6	2.38	0.41
1:B:95:TYR:CZ	1:B:218:PRO:HG3	2.55	0.41
1:B:350:ARG:HG2	1:B:398:ASP:O	2.20	0.41
1:C:323:GLU:OE1	1:C:327:ARG:NH1	2.54	0.41
1:A:171:ARG:NH1	1:A:173:ARG:NH2	2.69	0.41
1:B:165:VAL:HG22	1:B:175:VAL:HG13	2.02	0.41
1:C:124:THR:HG22	1:C:125:ILE:N	2.34	0.41
1:D:288:ILE:HD12	1:D:304:PHE:HD1	1.85	0.41
1:A:231:ARG:O	1:A:320:ARG:HA	2.21	0.41
1:A:248:ARG:HB3	4:A:967:HOH:O	2.19	0.41
1:A:483:LYS:NZ	1:A:487:ASP:OD2	2.50	0.41
1:B:140:LEU:HD22	1:B:196:GLY:CA	2.51	0.41
1:B:179:SER:HB3	1:B:189:TRP:CE2	2.55	0.41
1:B:384:VAL:O	1:B:397:ARG:HD2	2.20	0.41
1:C:15:ASP:O	1:C:39:VAL:HA	2.20	0.41
1:C:296:GLY:O	1:C:300:LEU:HG	2.21	0.41
1:C:448:ILE:CG2	1:C:471:TYR:HB3	2.51	0.41
1:D:96:ASP:HB3	1:D:207:TRP:HZ3	1.83	0.41
1:D:109:THR:HG23	1:D:131:PRO:O	2.21	0.41
1:D:117:LEU:HD12	1:D:117:LEU:HA	1.90	0.41
1:D:252:ASN:HB3	1:D:308:VAL:HA	2.03	0.41
1:D:312:THR:HG22	1:D:314:VAL:H	1.85	0.41
1:D:411:ASP:HA	1:D:412:PRO:HD2	1.82	0.41
1:D:438:VAL:HG13	1:D:439:PRO:HD2	2.03	0.41
1:A:49:VAL:O	1:A:53:VAL:HG23	2.21	0.41
1:A:93:VAL:HG13	1:A:103:ALA:O	2.20	0.41
1:A:283:GLN:N	1:A:283:GLN:HE21	2.19	0.41
1:C:226:PRO:O	1:D:19:ARG:NH2	2.53	0.41
1:A:104:VAL:O	1:A:104:VAL:HG23	2.22	0.40
1:A:130:CYS:HA	1:A:131:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:TYR:CD2	1:A:396:GLN:HG2	2.56	0.40
1:B:91:ARG:HD3	1:B:112:GLU:OE1	2.22	0.40
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.95	0.40
1:B:193:THR:HG23	1:B:193:THR:O	2.21	0.40
1:B:371:VAL:HG23	1:B:372:TRP:N	2.36	0.40
1:D:27:ARG:NH1	1:D:66:ARG:HD2	2.36	0.40
1:D:38:ASP:OD1	1:D:82:ARG:HD2	2.21	0.40
1:D:405:MET:HE1	1:D:429:ILE:CD1	2.51	0.40
1:A:297:ALA:HA	1:A:300:LEU:CD1	2.45	0.40
1:B:124:THR:OG1	1:B:225:ALA:HB2	2.22	0.40
1:B:143:GLY:O	1:B:153:VAL:HG13	2.21	0.40
1:B:361:LEU:HD12	1:B:361:LEU:HA	1.93	0.40
1:C:98:GLY:HA3	4:C:978:HOH:O	2.22	0.40
1:C:359:ALA:HB1	1:C:363:ARG:NH1	2.36	0.40
1:C:371:VAL:HB	1:C:418:ASN:OD1	2.21	0.40
1:C:407:ALA:HB2	1:C:422:ILE:HG23	2.04	0.40
1:C:457:ASP:OD2	1:C:459:ARG:N	2.54	0.40
1:D:63:ILE:HA	1:D:83:ALA:O	2.21	0.40
1:D:364:HIS:O	1:D:421:TRP:HH2	2.04	0.40
1:D:433:THR:HG22	1:D:438:VAL:HG23	2.03	0.40
1:A:345:LYS:HD3	1:A:426:TYR:HB2	2.04	0.40
1:B:274:PHE:O	1:B:376:SER:HA	2.22	0.40
1:B:354:THR:H	1:B:357:GLN:HB2	1.85	0.40
1:C:278:SER:O	1:C:281:ALA:HB3	2.22	0.40
1:C:431:ALA:O	1:C:432:THR:HG22	2.21	0.40
1:A:109:THR:O	1:A:113:THR:HG23	2.21	0.40
1:A:199:ASN:OD1	1:A:199:ASN:N	2.53	0.40
1:B:188:LEU:HD22	1:B:192:HIS:CE1	2.57	0.40
1:C:89:GLN:NE2	1:D:115:ARG:NH1	2.70	0.40
1:C:199:ASN:HD21	1:C:498:VAL:H	1.68	0.40
1:D:427:ARG:HA	1:D:435:GLY:HA2	2.02	0.40
1:D:470:LEU:HD23	1:D:470:LEU:HA	1.93	0.40
1:A:43:VAL:HG21	1:A:87:MET:HE2	2.03	0.40
1:A:350[A]:ARG:NH1	1:A:444:GLU:HG2	2.36	0.40
1:A:472:TYR:O	1:A:475:ASN:HB2	2.22	0.40
1:C:129:VAL:CG2	1:C:146:PRO:HD3	2.43	0.40
1:C:448:ILE:HG23	4:C:900:HOH:O	2.22	0.40
1:D:354:THR:HG23	1:D:357:GLN:H	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LYS:CD	4:C:1070:HOH:O[2_655]	1.75	0.45
1:A:499:ARG:NH2	4:B:820:HOH:O[1_554]	2.18	0.02

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	492/521 (94%)	459 (93%)	29 (6%)	4 (1%)	16	4
1	B	490/521 (94%)	456 (93%)	27 (6%)	7 (1%)	9	1
1	C	491/521 (94%)	449 (91%)	39 (8%)	3 (1%)	21	8
1	D	490/521 (94%)	448 (91%)	37 (8%)	5 (1%)	12	2
All	All	1963/2084 (94%)	1812 (92%)	132 (7%)	19 (1%)	12	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ALA
1	B	195	GLY
1	B	214	THR
1	B	368	ASP
1	B	460	TRP
1	D	196	GLY
1	D	197	GLY
1	D	398	ASP
1	B	197	GLY
1	B	432	THR
1	A	261	SER
1	A	460	TRP
1	C	369	SER
1	D	214	THR
1	D	460	TRP
1	A	263	ALA

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Mol	Chain	Res	Type
1	B	462	THR
1	C	279	ARG
1	C	333	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/408 (96%)	318 (81%)	73 (19%)	1	0
1	B	389/408 (95%)	317 (82%)	72 (18%)	1	0
1	C	390/408 (96%)	321 (82%)	69 (18%)	2	0
1	D	389/408 (95%)	312 (80%)	77 (20%)	1	0
All	All	1559/1632 (96%)	1268 (81%)	291 (19%)	1	0

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	LYS
1	A	15	ASP
1	A	16	ARG
1	A	17	VAL
1	A	19	ARG
1	A	22	GLN
1	A	24	LEU
1	A	84	VAL
1	A	85	ILE
1	A	87	MET
1	A	97	SER
1	A	99	LYS
1	A	109	THR
1	A	117	LEU
1	A	124	THR
1	A	140	LEU
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	153	VAL
1	A	167	ASP
1	A	171	ARG
1	A	173	ARG
1	A	174	LYS
1	A	178	THR
1	A	188	LEU
1	A	199	ASN
1	A	209	ARG
1	A	219	SER
1	A	224	LYS
1	A	233	ILE
1	A	235	THR
1	A	242	THR
1	A	244	GLU
1	A	248	ARG
1	A	260	ASN
1	A	283	GLN
1	A	286	LEU
1	A	288	ILE
1	A	294	LEU
1	A	300	LEU
1	A	302	ASN
1	A	305	VAL
1	A	314	VAL
1	A	315	GLU
1	A	327	ARG
1	A	332	ASN
1	A	336	THR
1	A	343	LYS
1	A	345	LYS
1	A	350[A]	ARG
1	A	350[B]	ARG
1	A	351	LYS
1	A	361	LEU
1	A	369	SER
1	A	371	VAL
1	A	374	GLU
1	A	396	GLN
1	A	402	LYS
1	A	403	VAL
1	A	411	ASP

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Mol	Chain	Res	Type
1	A	422	ILE
1	A	425	ILE
1	A	429	ILE
1	A	433	THR
1	A	443	THR
1	A	448	ILE
1	A	453	VAL
1	A	461	ASN
1	A	462	THR
1	A	463	SER
1	A	489	ARG
1	A	496	LEU
1	A	497	SER
1	B	12	VAL
1	B	13	LYS
1	B	16	ARG
1	B	18	ASP
1	B	23	ASP
1	B	24	LEU
1	B	84	VAL
1	B	85	ILE
1	B	87	MET
1	B	89	GLN
1	B	92	GLN
1	B	97	SER
1	B	99	LYS
1	B	104	VAL
1	B	109	THR
1	B	115	ARG
1	B	117	LEU
1	B	125	ILE
1	B	140	LEU
1	B	167	ASP
1	B	171	ARG
1	B	174	LYS
1	B	178	THR
1	B	188	LEU
1	B	199	ASN
1	B	209	ARG
1	B	220	GLN
1	B	233	ILE
1	B	235	THR

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Mol	Chain	Res	Type
1	B	242	THR
1	B	243	GLU
1	B	244	GLU
1	B	248	ARG
1	B	286	LEU
1	B	288	ILE
1	B	289	GLN
1	B	294	LEU
1	B	295	ASP
1	B	298	GLU
1	B	300	LEU
1	B	301	LEU
1	B	302	ASN
1	B	314	VAL
1	B	315	GLU
1	B	319	GLN
1	B	321	SER
1	B	330	LEU
1	B	332	ASN
1	B	335	ASP
1	B	336	THR
1	B	350	ARG
1	B	361	LEU
1	B	364	HIS
1	B	369	SER
1	B	371	VAL
1	B	385	ASN
1	B	392	THR
1	B	396	GLN
1	B	402	LYS
1	B	405	MET
1	B	411	ASP
1	B	422	ILE
1	B	425	ILE
1	B	429	ILE
1	B	433	THR
1	B	443	THR
1	B	448	ILE
1	B	453	VAL
1	B	462	THR
1	B	463	SER
1	B	496	LEU

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Mol	Chain	Res	Type
1	B	497	SER
1	C	12	VAL
1	C	13	LYS
1	C	15	ASP
1	C	16	ARG
1	C	17	VAL
1	C	22	GLN
1	C	24	LEU
1	C	84	VAL
1	C	85	ILE
1	C	87	MET
1	C	89	GLN
1	C	91	ARG
1	C	99	LYS
1	C	104	VAL
1	C	109	THR
1	C	115	ARG
1	C	117	LEU
1	C	123	VAL
1	C	140	LEU
1	C	162	GLU
1	C	171	ARG
1	C	174	LYS
1	C	178	THR
1	C	188	LEU
1	C	190	TRP
1	C	203	VAL
1	C	209	ARG
1	C	233	ILE
1	C	235	THR
1	C	243	GLU
1	C	244	GLU
1	C	248	ARG
1	C	259	SER
1	C	261	SER
1	C	269	SER
1	C	286	LEU
1	C	298	GLU
1	C	300	LEU
1	C	302	ASN
1	C	310	GLU
1	C	314	VAL

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Mol	Chain	Res	Type
1	C	315	GLU
1	C	319	GLN
1	C	330	LEU
1	C	332	ASN
1	C	336	THR
1	C	345	LYS
1	C	361	LEU
1	C	369	SER
1	C	371	VAL
1	C	374	GLU
1	C	392	THR
1	C	396	GLN
1	C	402	LYS
1	C	403	VAL
1	C	411	ASP
1	C	414	HIS
1	C	425	ILE
1	C	427	ARG
1	C	429	ILE
1	C	433	THR
1	C	440[A]	ASP
1	C	440[B]	ASP
1	C	443	THR
1	C	448	ILE
1	C	453	VAL
1	C	462	THR
1	C	496	LEU
1	C	497	SER
1	D	12	VAL
1	D	13	LYS
1	D	16	ARG
1	D	17	VAL
1	D	22	GLN
1	D	24	LEU
1	D	29	PHE
1	D	30	ASN
1	D	65	VAL
1	D	84	VAL
1	D	85	ILE
1	D	87	MET
1	D	91	ARG
1	D	97	SER

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Mol	Chain	Res	Type
1	D	104	VAL
1	D	109	THR
1	D	117	LEU
1	D	129	VAL
1	D	140	LEU
1	D	162	GLU
1	D	163	VAL
1	D	167	ASP
1	D	171	ARG
1	D	173	ARG
1	D	174	LYS
1	D	178	THR
1	D	188	LEU
1	D	190	TRP
1	D	209	ARG
1	D	220	GLN
1	D	221	LEU
1	D	235	THR
1	D	243	GLU
1	D	248	ARG
1	D	261	SER
1	D	286	LEU
1	D	288	ILE
1	D	294	LEU
1	D	298	GLU
1	D	300	LEU
1	D	302	ASN
1	D	310	GLU
1	D	312	THR
1	D	314	VAL
1	D	315	GLU
1	D	319	GLN
1	D	320	ARG
1	D	323	GLU
1	D	327	ARG
1	D	332	ASN
1	D	336	THR
1	D	345	LYS
1	D	350	ARG
1	D	354	THR
1	D	361	LEU
1	D	364	HIS

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Mol	Chain	Res	Type
1	D	371	VAL
1	D	374	GLU
1	D	377	LEU
1	D	383	LYS
1	D	396	GLN
1	D	402	LYS
1	D	403	VAL
1	D	411	ASP
1	D	422	ILE
1	D	425	ILE
1	D	427	ARG
1	D	429	ILE
1	D	432	THR
1	D	440	ASP
1	D	443	THR
1	D	448	ILE
1	D	453	VAL
1	D	462	THR
1	D	478	ARG
1	D	496	LEU
1	D	497	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	253	HIS
1	A	283	GLN
1	A	319	GLN
1	A	332	ASN
1	A	357	GLN
1	A	364	HIS
1	A	396	GLN
1	A	494	HIS
1	B	22	GLN
1	B	30	ASN
1	B	89	GLN
1	B	220	GLN
1	B	253	HIS
1	B	260	ASN
1	B	283	GLN
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	357	GLN
1	B	364	HIS
1	B	396	GLN
1	B	414	HIS
1	B	494	HIS
1	C	30	ASN
1	C	89	GLN
1	C	199	ASN
1	C	220	GLN
1	C	253	HIS
1	C	283	GLN
1	C	357	GLN
1	C	364	HIS
1	C	396	GLN
1	C	494	HIS
1	D	30	ASN
1	D	55	GLN
1	D	89	GLN
1	D	258	GLN
1	D	271	HIS
1	D	283	GLN
1	D	289	GLN
1	D	319	GLN
1	D	357	GLN
1	D	370	GLN
1	D	396	GLN
1	D	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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
2	AKY	A	601[A]	-	62,64,64	1.97	16 (25%)	87,98,98	1.96	22 (25%)
3	FAD	B	801	1	58,58,58	1.85	15 (25%)	85,89,89	1.99	28 (32%)
3	FAD	D	801	1	58,58,58	1.88	23 (39%)	85,89,89	1.96	22 (25%)
3	FAD	C	801	1	58,58,58	1.79	15 (25%)	85,89,89	2.04	28 (32%)
3	FAD	A	801	1	58,58,58	1.59	11 (18%)	85,89,89	1.83	22 (25%)

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
2	AKY	A	601[A]	-	7/7/18/18	6/25/105/105	0/7/7/7
3	FAD	B	801	1	1/1/9/9	10/34/50/50	0/6/6/6
3	FAD	D	801	1	-	11/34/50/50	0/6/6/6
3	FAD	C	801	1	-	12/34/50/50	0/6/6/6
3	FAD	A	801	1	-	9/34/50/50	0/6/6/6

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	AKY	C32-C33	-6.61	1.40	1.52
2	A	601[A]	AKY	C41-C39	-5.28	1.34	1.51
3	A	801	FAD	O2-C2	-4.35	1.15	1.24
2	A	601[A]	AKY	O12-C33	4.30	1.52	1.43
3	B	801	FAD	P-O1P	-4.13	1.36	1.50
2	A	601[A]	AKY	O11-C31	3.91	1.52	1.42
2	A	601[A]	AKY	C32-C31	-3.80	1.41	1.50
3	D	801	FAD	O2-C2	-3.80	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	AKY	O11-C34	3.73	1.53	1.44
3	B	801	FAD	P-O3P	-3.72	1.55	1.59
3	C	801	FAD	P-O1P	-3.64	1.38	1.50
3	B	801	FAD	O2-C2	-3.62	1.17	1.24
3	C	801	FAD	P-O3P	3.47	1.63	1.59
3	D	801	FAD	P-O1P	-3.41	1.39	1.50
2	A	601[A]	AKY	C36-C34	-3.39	1.43	1.51
3	C	801	FAD	C8A-N9A	-3.35	1.31	1.37
3	B	801	FAD	C5A-N7A	-3.33	1.33	1.39
3	D	801	FAD	C4X-N5	3.32	1.37	1.30
3	B	801	FAD	PA-O3P	-3.31	1.55	1.59
2	A	601[A]	AKY	C18-C12	-3.29	1.41	1.48
2	A	601[A]	AKY	O9-C9	-3.26	1.39	1.44
3	A	801	FAD	P-O2P	-3.25	1.40	1.55
3	D	801	FAD	C5'-C4'	3.23	1.56	1.51
3	C	801	FAD	C6-C7	-3.21	1.35	1.39
3	D	801	FAD	C5A-N7A	-3.19	1.33	1.39
3	C	801	FAD	C5A-N7A	-3.12	1.33	1.39
3	D	801	FAD	O2'-C2'	-3.12	1.36	1.43
2	A	601[A]	AKY	C15-C12	-3.12	1.42	1.48
3	B	801	FAD	O4'-C4'	-3.09	1.36	1.43
3	B	801	FAD	O4B-C4B	-3.05	1.38	1.45
3	B	801	FAD	PA-O2A	-3.04	1.41	1.55
3	D	801	FAD	C9-C8	-3.03	1.35	1.39
3	D	801	FAD	O4B-C4B	-2.97	1.38	1.45
3	A	801	FAD	C5A-N7A	-2.92	1.33	1.39
3	C	801	FAD	PA-O2A	-2.91	1.41	1.55
3	B	801	FAD	C4X-N5	2.89	1.37	1.30
3	D	801	FAD	PA-O1A	-2.88	1.40	1.50
3	D	801	FAD	P-O3P	-2.83	1.56	1.59
3	A	801	FAD	C4X-N5	2.82	1.36	1.30
3	A	801	FAD	O4'-C4'	-2.80	1.37	1.43
3	C	801	FAD	O2-C2	-2.78	1.18	1.24
3	B	801	FAD	PA-O1A	-2.76	1.41	1.50
3	B	801	FAD	C6A-N6A	-2.74	1.27	1.34
2	A	601[A]	AKY	C40-C42	2.73	1.55	1.50
3	B	801	FAD	O2'-C2'	-2.72	1.37	1.43
3	A	801	FAD	PA-O1A	-2.69	1.41	1.50
3	C	801	FAD	PA-O1A	-2.68	1.41	1.50
3	D	801	FAD	C2'-C3'	-2.64	1.48	1.53
2	A	601[A]	AKY	C16-C5	-2.59	1.41	1.47
2	A	601[A]	AKY	C17-C5	-2.47	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FAD	P-O1P	-2.46	1.42	1.50
3	A	801	FAD	C10-N1	2.42	1.38	1.33
3	C	801	FAD	C5X-N5	-2.42	1.35	1.39
3	D	801	FAD	C9A-C5X	-2.41	1.37	1.41
3	D	801	FAD	C1'-C2'	-2.39	1.49	1.52
2	A	601[A]	AKY	C38-C40	-2.36	1.47	1.53
3	D	801	FAD	C6-C5X	-2.36	1.36	1.40
3	C	801	FAD	C4X-N5	2.35	1.35	1.30
3	A	801	FAD	C6A-N6A	-2.35	1.28	1.34
3	D	801	FAD	C9A-N10	-2.34	1.37	1.41
3	C	801	FAD	O3'-C3'	-2.33	1.37	1.43
3	D	801	FAD	C6-C7	-2.28	1.36	1.39
3	C	801	FAD	P-O2P	-2.27	1.44	1.55
3	D	801	FAD	O4'-C4'	-2.24	1.38	1.43
3	C	801	FAD	O2'-C2'	-2.20	1.38	1.43
3	C	801	FAD	C10-N1	2.19	1.37	1.33
3	B	801	FAD	C6-C7	-2.19	1.36	1.39
3	A	801	FAD	C4A-N3A	-2.18	1.30	1.34
3	B	801	FAD	P-O2P	-2.18	1.45	1.55
3	D	801	FAD	C9-C9A	-2.17	1.36	1.39
3	D	801	FAD	PA-O2A	-2.14	1.45	1.55
3	C	801	FAD	C9A-C5X	-2.11	1.37	1.41
3	D	801	FAD	C5X-N5	-2.11	1.35	1.39
3	B	801	FAD	O5B-C5B	-2.08	1.36	1.44
3	D	801	FAD	O2B-C2B	-2.06	1.37	1.43
3	D	801	FAD	C4X-C10	-2.06	1.38	1.44
3	D	801	FAD	C6A-N6A	-2.06	1.29	1.34
2	A	601[A]	AKY	C8-C7	-2.05	1.48	1.52
2	A	601[A]	AKY	C8-C9	-2.01	1.51	1.53
3	A	801	FAD	O4B-C4B	-2.00	1.40	1.45

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	AKY	O19-C49-C50	6.35	120.83	106.74
3	B	801	FAD	C5A-C4A-N3A	-5.78	118.75	126.72
3	A	801	FAD	C4'-C3'-C2'	-5.73	104.03	113.57
3	B	801	FAD	N3A-C2A-N1A	-5.67	120.00	128.58
3	C	801	FAD	N3A-C2A-N1A	-5.50	120.26	128.58
3	D	801	FAD	N3A-C2A-N1A	-5.32	120.53	128.58
2	A	601[A]	AKY	C14-C13-C9	-5.16	104.45	115.05
2	A	601[A]	AKY	O17-C43-C10	5.14	120.63	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	FAD	C4A-C5A-N7A	-5.12	104.73	110.58
3	B	801	FAD	C5'-C4'-C3'	5.05	121.75	112.22
2	A	601[A]	AKY	C45-O19-C49	5.04	127.64	113.82
3	C	801	FAD	O4B-C1B-N9A	4.95	117.61	108.09
3	D	801	FAD	C5A-C4A-N3A	-4.94	119.91	126.72
3	D	801	FAD	N3A-C4A-N9A	4.88	135.46	127.17
2	A	601[A]	AKY	C50-C49-C48	4.79	120.53	113.39
3	C	801	FAD	C9A-C5X-N5	-4.65	117.52	122.45
3	A	801	FAD	C5A-C4A-N3A	-4.57	120.42	126.72
3	B	801	FAD	C4'-C3'-C2'	-4.52	106.05	113.57
3	D	801	FAD	O5'-C5'-C4'	4.49	121.35	109.36
3	D	801	FAD	O4-C4-C4X	-4.43	114.85	126.53
3	C	801	FAD	C5X-C9A-N10	4.40	121.94	117.97
3	D	801	FAD	C2A-N3A-C4A	4.34	122.44	111.83
3	C	801	FAD	C5A-C4A-N3A	-4.15	121.00	126.72
3	C	801	FAD	C5A-N7A-C8A	4.14	109.96	103.45
2	A	601[A]	AKY	O18-C31-C32	4.04	116.05	108.28
3	B	801	FAD	C2A-N3A-C4A	3.95	121.48	111.83
3	A	801	FAD	C5'-C4'-C3'	3.90	119.58	112.22
3	D	801	FAD	C10-N1-C2	3.88	125.25	116.85
3	D	801	FAD	C4X-C4-N3	3.87	123.10	113.25
3	C	801	FAD	O3'-C3'-C2'	3.80	117.56	108.93
3	A	801	FAD	C9A-C5X-N5	-3.72	118.50	122.45
3	A	801	FAD	O3'-C3'-C4'	3.71	117.36	108.93
3	B	801	FAD	O4B-C1B-N9A	3.66	115.12	108.09
2	A	601[A]	AKY	C44-O17-C43	-3.65	107.63	115.92
3	D	801	FAD	C4-N3-C2	-3.62	119.21	125.64
3	B	801	FAD	C4X-C10-N10	3.56	121.58	116.48
3	A	801	FAD	N3A-C2A-N1A	-3.55	123.21	128.58
3	A	801	FAD	N3A-C4A-N9A	3.47	133.07	127.17
2	A	601[A]	AKY	O5-C5-C17	-3.47	115.65	121.44
3	D	801	FAD	C4-C4X-N5	3.42	122.93	118.21
3	B	801	FAD	N3A-C4A-N9A	3.37	132.90	127.17
3	B	801	FAD	C4-C4X-N5	3.30	122.77	118.21
3	B	801	FAD	N9A-C8A-N7A	-3.30	109.25	113.94
3	C	801	FAD	C2A-N3A-C4A	3.26	119.79	111.83
3	A	801	FAD	C2A-N3A-C4A	3.24	119.75	111.83
3	B	801	FAD	C10-C4X-N5	-3.21	118.26	124.81
2	A	601[A]	AKY	O14-C37-C38	3.18	118.01	111.23
2	A	601[A]	AKY	O17-C43-O16	-3.09	117.84	123.85
2	A	601[A]	AKY	O14-C39-C42	3.03	114.77	111.48
3	C	801	FAD	N9A-C8A-N7A	-3.03	109.64	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	AKY	O12-C33-C35	3.02	117.05	109.99
3	C	801	FAD	C4-N3-C2	-2.95	120.40	125.64
3	D	801	FAD	C3B-C2B-C1B	-2.93	95.91	101.46
3	A	801	FAD	O2A-PA-O3P	2.93	115.20	107.27
2	A	601[A]	AKY	O11-C34-C35	2.92	114.60	109.19
2	A	601[A]	AKY	O9-C9-C13	2.90	114.62	107.86
2	A	601[A]	AKY	O15-C42-C40	-2.88	117.01	122.13
3	A	801	FAD	C5X-C9A-N10	2.87	120.56	117.97
2	A	601[A]	AKY	C48-C47-N11	2.84	120.76	111.75
3	D	801	FAD	C1'-N10-C9A	-2.79	115.20	120.63
3	D	801	FAD	O3P-PA-O1A	-2.79	102.31	110.70
3	A	801	FAD	O4B-C1B-N9A	2.79	113.44	108.09
3	C	801	FAD	O4-C4-C4X	-2.79	119.18	126.53
3	B	801	FAD	N6A-C6A-N1A	2.77	124.55	118.38
3	C	801	FAD	C1'-C2'-C3'	2.75	117.10	109.66
3	D	801	FAD	O4B-C1B-C2B	2.74	112.48	106.62
3	D	801	FAD	C1'-C2'-C3'	2.74	117.09	109.66
3	A	801	FAD	C10-C4X-N5	-2.74	119.22	124.81
3	B	801	FAD	O5B-C5B-C4B	2.70	118.17	108.99
3	C	801	FAD	O2A-PA-O3P	2.69	114.53	107.27
3	C	801	FAD	C2A-N1A-C6A	2.69	123.14	118.73
3	A	801	FAD	O4'-C4'-C3'	2.69	115.53	109.25
3	A	801	FAD	C4-C4X-N5	2.68	121.91	118.21
3	D	801	FAD	O3'-C3'-C4'	2.66	114.98	108.93
3	B	801	FAD	C5A-C6A-N6A	-2.66	116.70	123.29
3	C	801	FAD	O3'-C3'-C4'	2.58	114.79	108.93
3	A	801	FAD	O4'-C4'-C5'	-2.56	104.33	109.99
3	B	801	FAD	C4-N3-C2	-2.56	121.10	125.64
3	B	801	FAD	C5A-N7A-C8A	2.56	107.47	103.45
3	A	801	FAD	N9A-C8A-N7A	-2.53	110.35	113.94
3	B	801	FAD	O4-C4-C4X	-2.52	119.89	126.53
3	B	801	FAD	C9A-C9-C8	2.51	124.26	119.22
2	A	601[A]	AKY	C46-C47-N11	2.44	122.45	115.59
3	B	801	FAD	C2B-C1B-N9A	-2.42	107.30	113.30
3	D	801	FAD	C5X-C9A-N10	2.41	120.15	117.97
3	B	801	FAD	O3B-C3B-C4B	-2.41	104.16	111.08
3	D	801	FAD	C4X-C10-N1	-2.40	118.70	124.59
3	B	801	FAD	O3B-C3B-C2B	-2.40	104.12	111.82
3	A	801	FAD	C4X-C10-N10	2.39	119.91	116.48
2	A	601[A]	AKY	O13-C35-C34	2.37	112.81	106.77
3	C	801	FAD	C5A-C4A-N9A	2.37	108.39	105.81
3	A	801	FAD	C10-N1-C2	2.36	121.96	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	FAD	C10-N1-C2	2.35	121.93	116.85
3	A	801	FAD	C4X-C4-N3	2.34	119.22	113.25
3	B	801	FAD	C5A-C4A-N9A	2.32	108.34	105.81
3	A	801	FAD	C5X-N5-C4X	2.32	121.84	118.09
3	D	801	FAD	O4B-C1B-N9A	2.30	112.51	108.09
3	D	801	FAD	C10-C4X-N5	-2.29	120.13	124.81
3	C	801	FAD	C4X-C4-N3	2.28	119.05	113.25
3	A	801	FAD	C5A-N7A-C8A	2.27	107.02	103.45
3	D	801	FAD	O2A-PA-O3P	2.25	113.36	107.27
2	A	601[A]	AKY	C52-N11-C47	2.23	119.57	113.15
3	B	801	FAD	C4A-C5A-N7A	-2.23	108.04	110.58
2	A	601[A]	AKY	O12-C33-C32	2.22	115.39	109.86
3	B	801	FAD	C4X-C10-N1	-2.21	119.17	124.59
3	B	801	FAD	C9-C9A-N10	2.21	124.82	121.85
3	B	801	FAD	C6A-C5A-C4A	2.20	120.18	117.18
3	D	801	FAD	C5A-N7A-C8A	2.20	106.90	103.45
3	C	801	FAD	O3B-C3B-C4B	-2.20	104.77	111.08
3	C	801	FAD	C5X-N5-C4X	2.19	121.64	118.09
2	A	601[A]	AKY	O16-C43-C10	-2.19	121.53	125.22
3	C	801	FAD	C2'-C1'-N10	2.14	120.30	110.20
3	C	801	FAD	C6A-C5A-N7A	2.13	136.19	132.09
3	B	801	FAD	C4X-C4-N3	2.11	118.63	113.25
3	A	801	FAD	C9A-C9-C8	2.09	123.42	119.22
2	A	601[A]	AKY	C9-C8-C7	-2.08	110.40	114.58
3	C	801	FAD	C6-C5X-N5	2.07	121.88	118.44
3	C	801	FAD	O2P-P-O3P	2.06	112.84	107.27
3	C	801	FAD	O5'-C5'-C4'	2.05	114.83	109.36
3	C	801	FAD	C4-C4X-C10	2.04	120.43	116.93
3	C	801	FAD	N3A-C4A-N9A	2.01	130.59	127.17
3	C	801	FAD	C4X-C10-N10	2.00	119.35	116.48

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601[A]	AKY	C31
2	A	601[A]	AKY	C33
2	A	601[A]	AKY	C49
2	A	601[A]	AKY	C39
2	A	601[A]	AKY	C35
2	A	601[A]	AKY	C34
2	A	601[A]	AKY	C37
3	B	801	FAD	C2'

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	AKY	C10-C43-O17-C44
2	A	601[A]	AKY	C46-C47-N11-C51
2	A	601[A]	AKY	C48-C47-N11-C52
3	A	801	FAD	N10-C1'-C2'-O2'
3	A	801	FAD	N10-C1'-C2'-C3'
3	A	801	FAD	C2'-C3'-C4'-C5'
3	A	801	FAD	O3'-C3'-C4'-C5'
3	A	801	FAD	C5'-O5'-P-O2P
3	B	801	FAD	C5B-O5B-PA-O1A
3	B	801	FAD	C5B-O5B-PA-O3P
3	C	801	FAD	N10-C1'-C2'-O2'
3	D	801	FAD	C1'-C2'-C3'-O3'
3	D	801	FAD	C1'-C2'-C3'-C4'
3	D	801	FAD	O2'-C2'-C3'-O3'
3	D	801	FAD	C3'-C4'-C5'-O5'
3	D	801	FAD	O4'-C4'-C5'-O5'
3	D	801	FAD	C5'-O5'-P-O2P
2	A	601[A]	AKY	O16-C43-O17-C44
3	A	801	FAD	O3'-C3'-C4'-O4'
3	C	801	FAD	O3'-C3'-C4'-O4'
3	A	801	FAD	C2'-C3'-C4'-O4'
3	D	801	FAD	O2'-C2'-C3'-C4'
3	C	801	FAD	O3'-C3'-C4'-C5'
2	A	601[A]	AKY	C48-C47-N11-C51
3	B	801	FAD	O2'-C2'-C3'-C4'
3	C	801	FAD	O2'-C2'-C3'-C4'
3	B	801	FAD	O2'-C2'-C3'-O3'
3	B	801	FAD	C3'-C4'-C5'-O5'
3	C	801	FAD	C3'-C4'-C5'-O5'
3	C	801	FAD	P-O3P-PA-O1A
3	D	801	FAD	P-O3P-PA-O5B
3	C	801	FAD	C2'-C3'-C4'-C5'
2	A	601[A]	AKY	C46-C47-N11-C52
3	C	801	FAD	N10-C1'-C2'-C3'
3	A	801	FAD	C5'-O5'-P-O1P
3	C	801	FAD	C5B-O5B-PA-O1A
3	C	801	FAD	C5B-O5B-PA-O2A
3	C	801	FAD	C5B-O5B-PA-O3P
3	D	801	FAD	C5'-O5'-P-O1P
3	D	801	FAD	C5'-O5'-P-O3P
3	D	801	FAD	C2'-C3'-C4'-O4'
3	B	801	FAD	C3B-C4B-C5B-O5B

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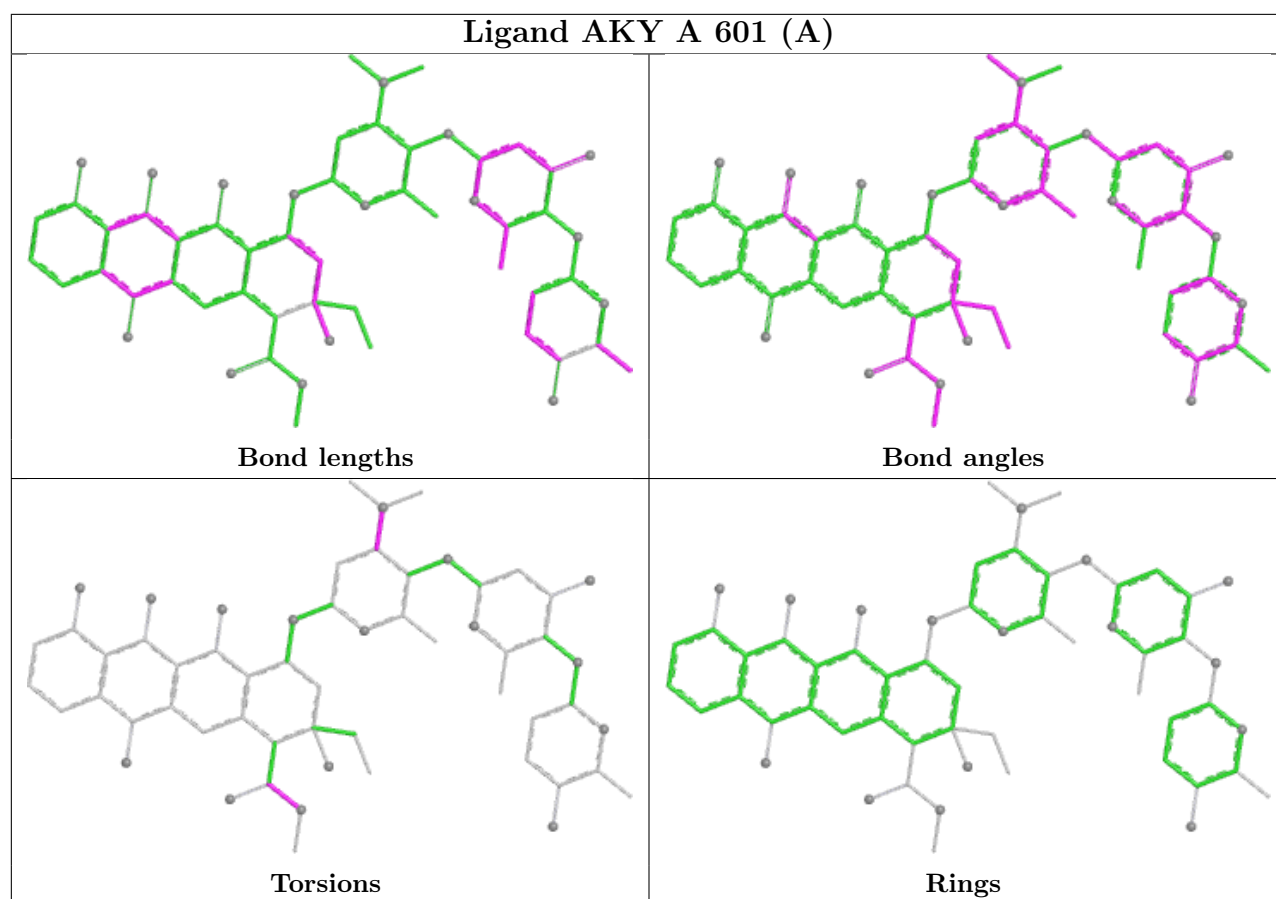
Mol	Chain	Res	Type	Atoms
3	B	801	FAD	C2'-C3'-C4'-C5'
3	C	801	FAD	P-O3P-PA-O2A
3	B	801	FAD	C1'-C2'-C3'-O3'
3	A	801	FAD	PA-O3P-P-O2P
3	B	801	FAD	O4B-C4B-C5B-O5B
3	B	801	FAD	O4'-C4'-C5'-O5'

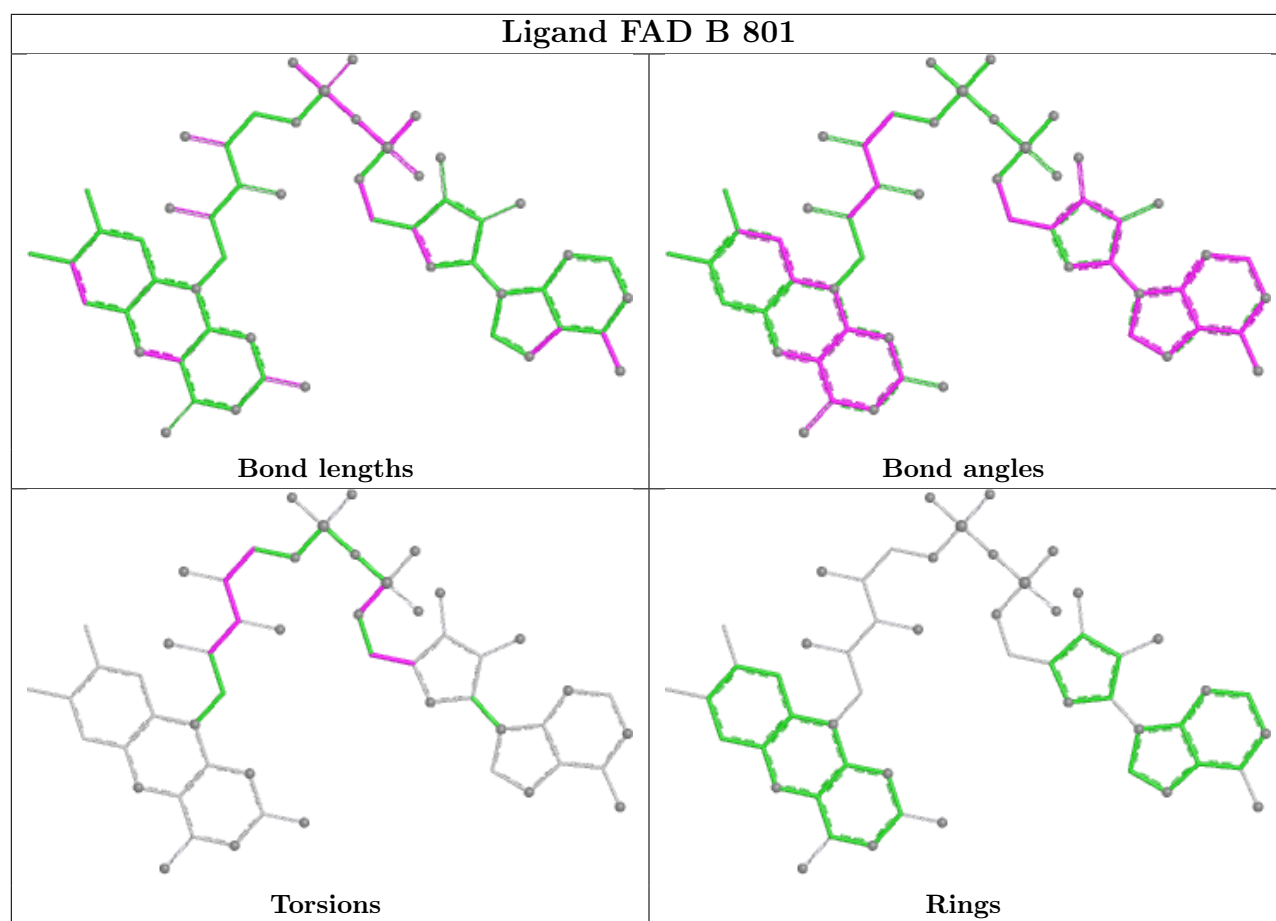
There are no ring outliers.

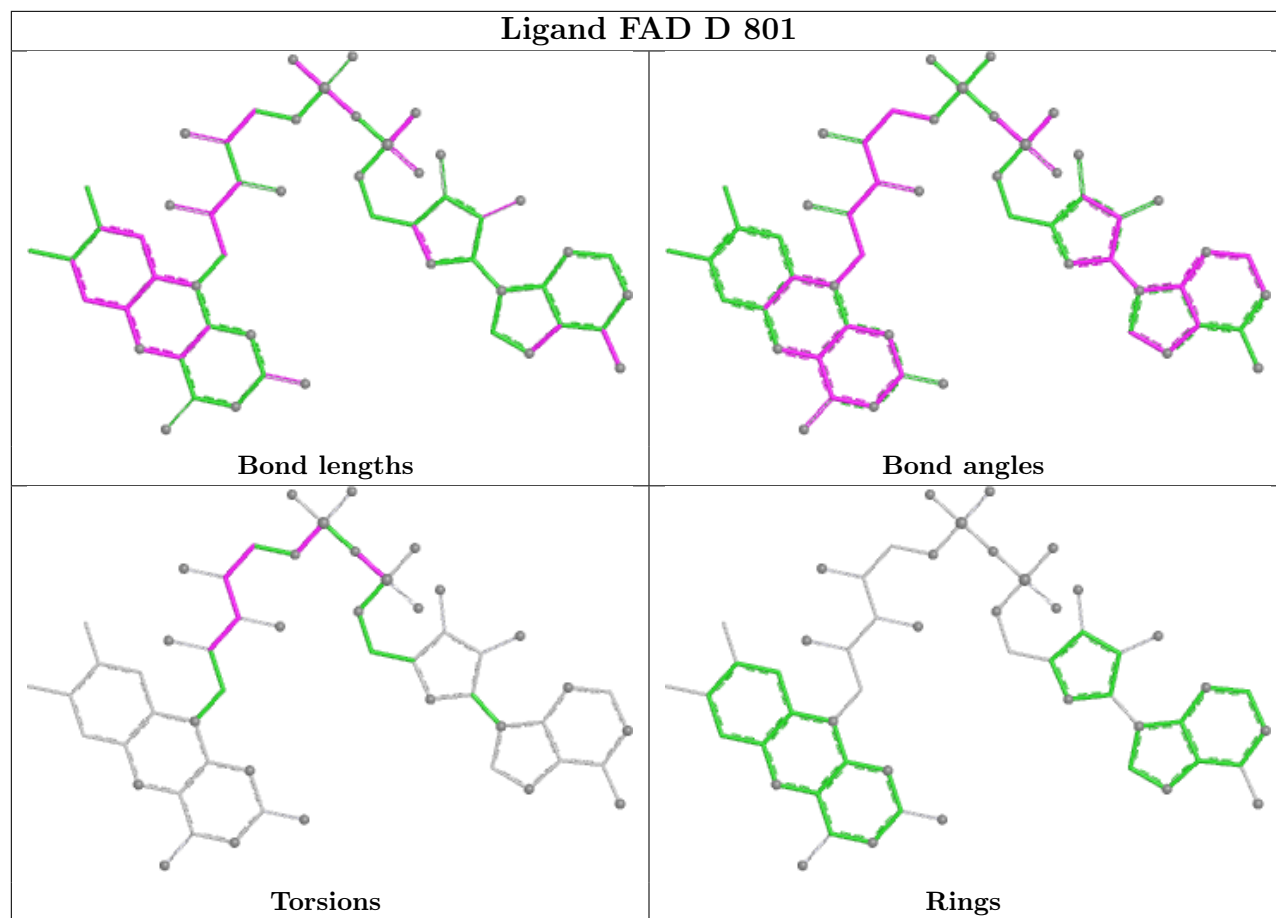
5 monomers are involved in 44 short contacts:

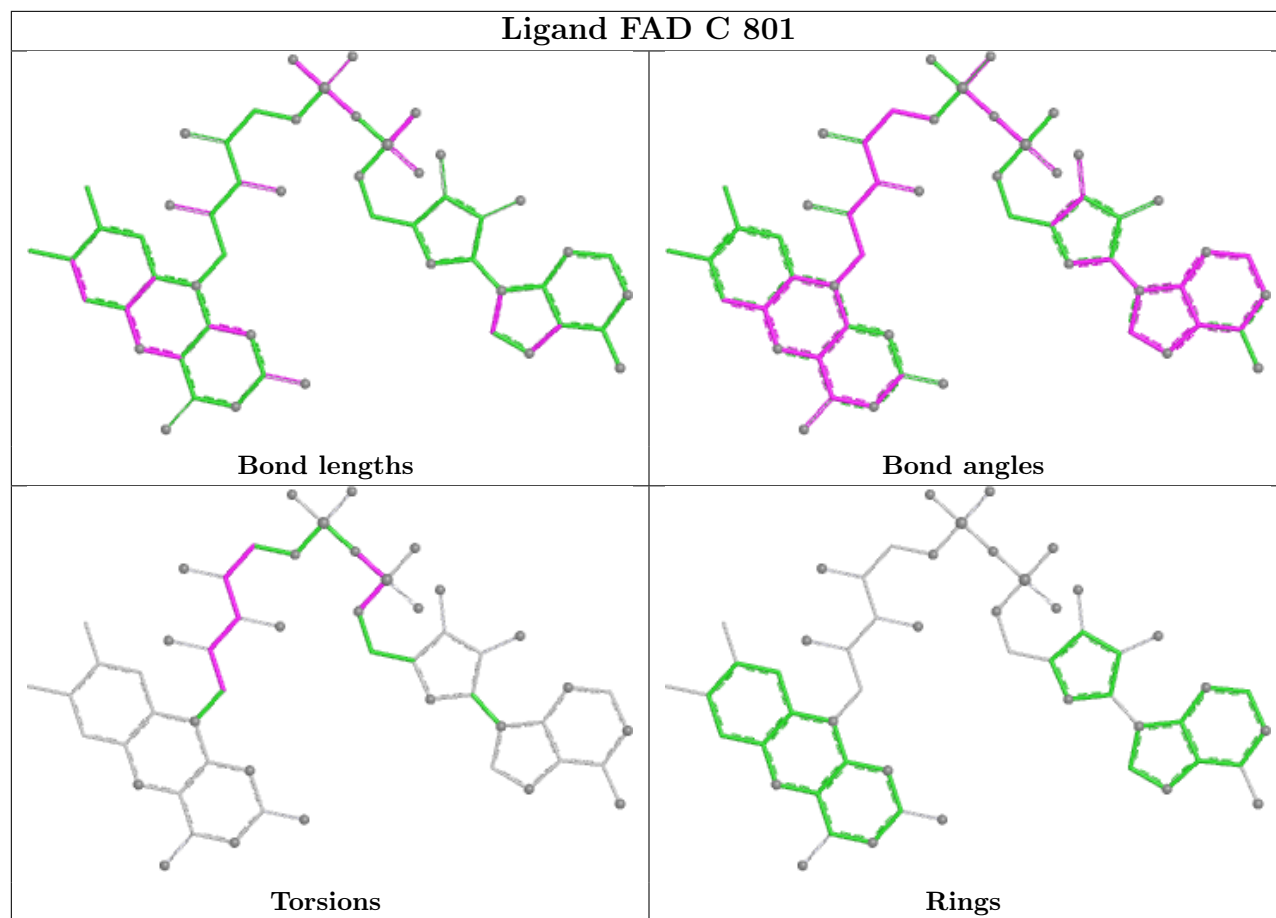
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601[A]	AKY	13	0
3	B	801	FAD	6	0
3	D	801	FAD	13	0
3	C	801	FAD	9	0
3	A	801	FAD	3	0

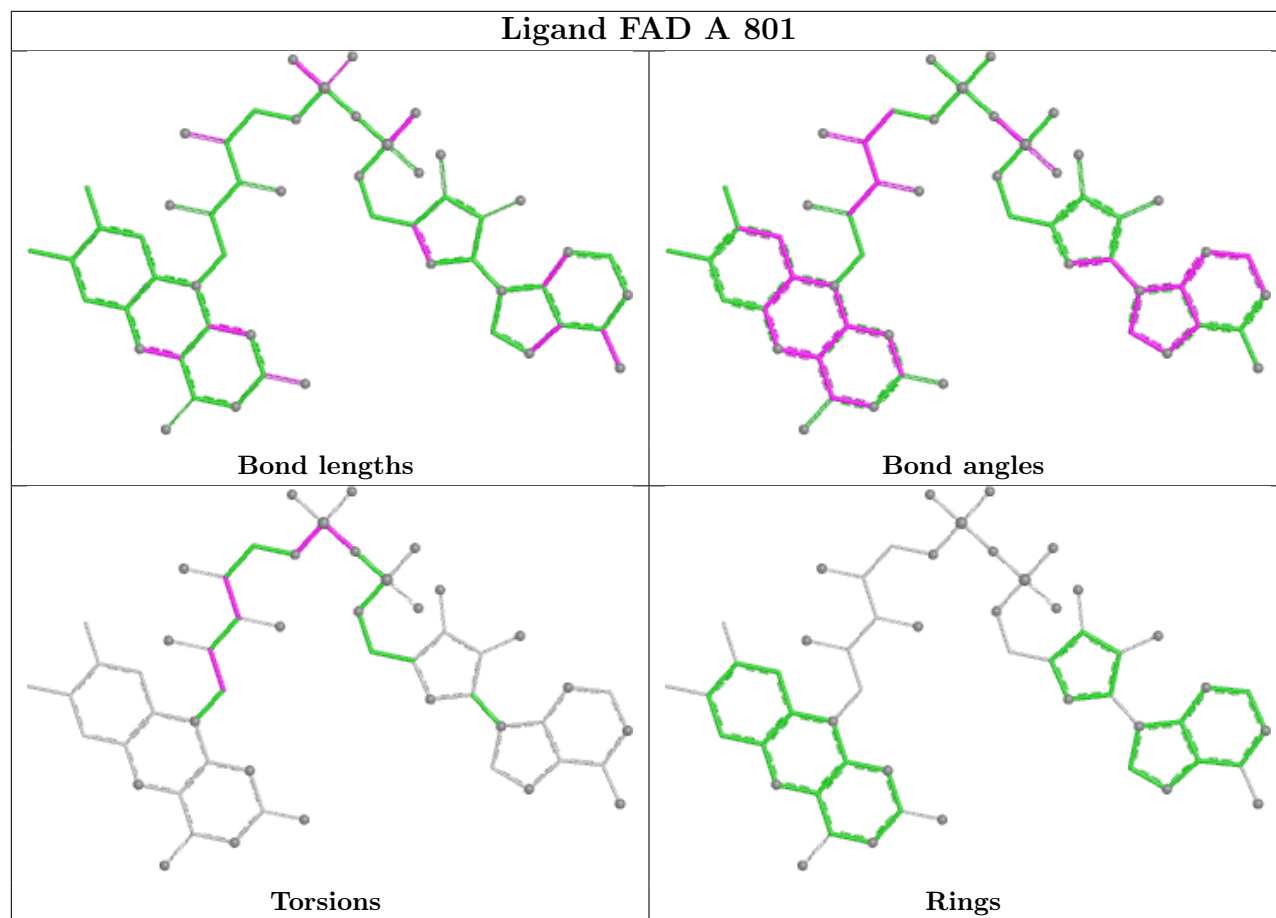
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	492/521 (94%)	-1.09	0 100 100	3, 16, 30, 39	16 (3%)
1	B	492/521 (94%)	-1.07	0 100 100	6, 17, 30, 39	14 (2%)
1	C	492/521 (94%)	-1.11	0 100 100	5, 16, 29, 40	13 (2%)
1	D	492/521 (94%)	-1.07	0 100 100	4, 16, 31, 43	15 (3%)
All	All	1968/2084 (94%)	-1.09	0 100 100	3, 16, 30, 43	58 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AKY	A	601[A]	58/58	0.98	0.05	10,20,34,38	58
3	FAD	A	801	53/53	0.99	0.03	7,14,19,24	0
3	FAD	B	801	53/53	0.99	0.03	4,14,23,36	0
3	FAD	C	801	53/53	0.99	0.03	3,11,25,37	0

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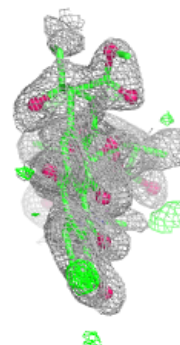
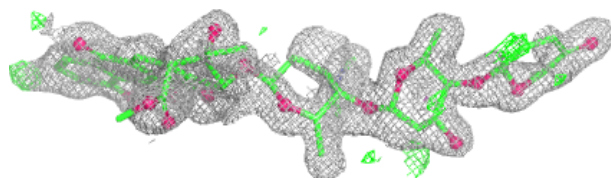
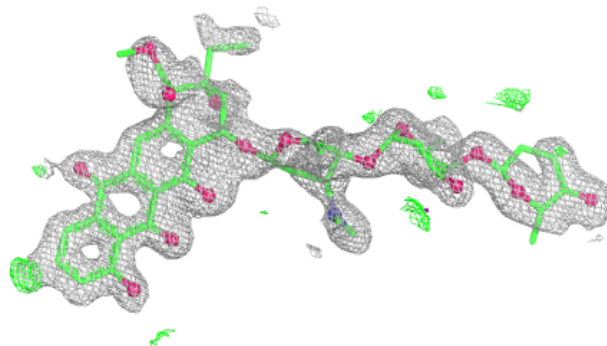
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	D	801	53/53	0.99	0.03	4,11,26,42	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.

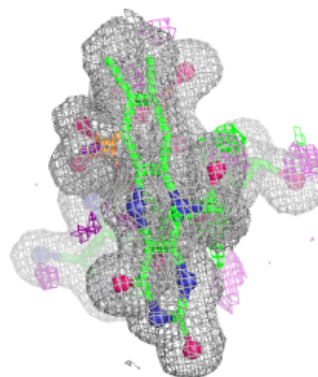
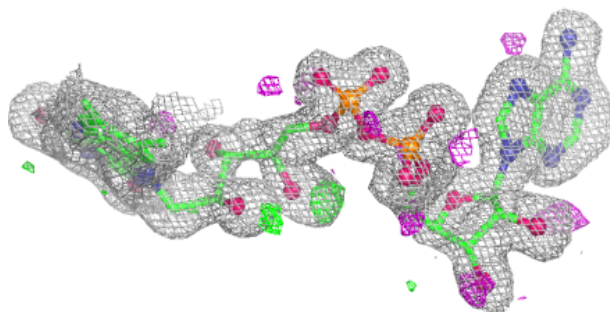
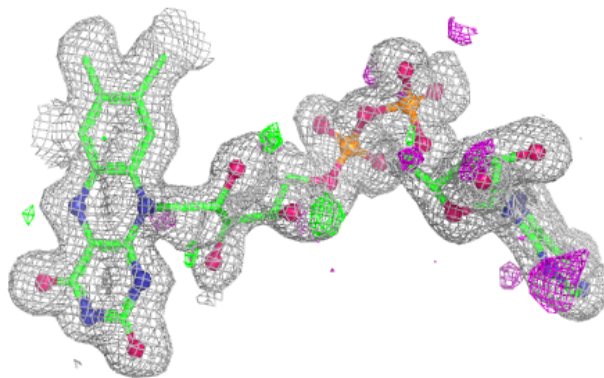
Electron density around AKY A 601 (A):

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

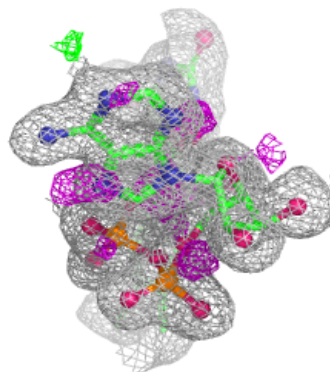
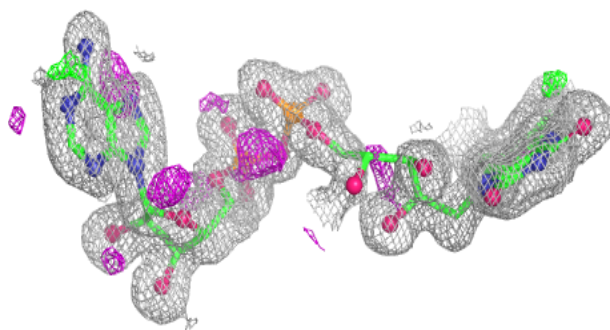
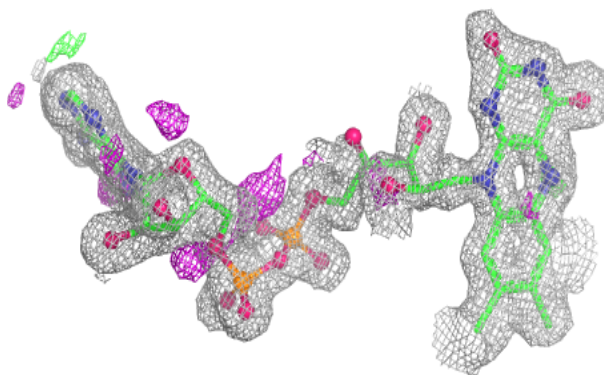


Electron density around FAD A 801:

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

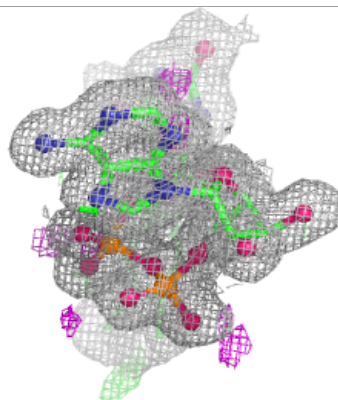
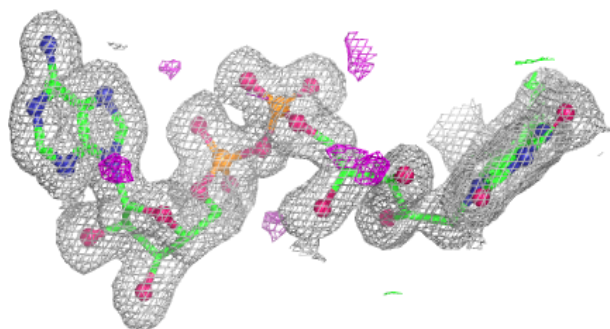
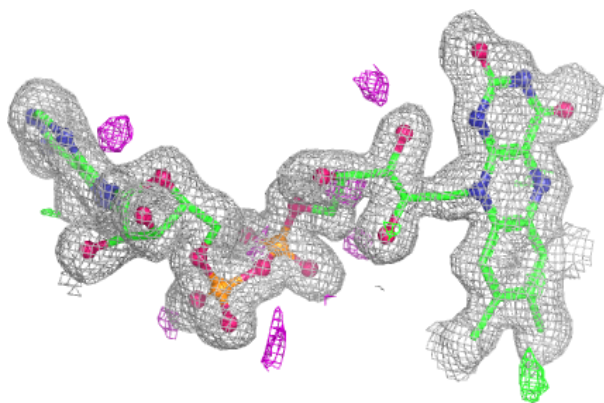
**Electron density around FAD B 801:**

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

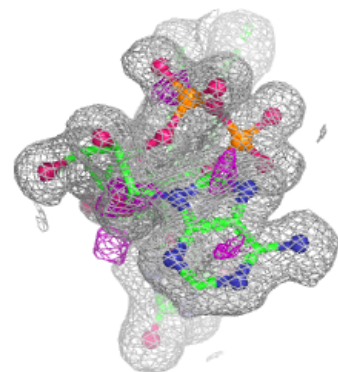
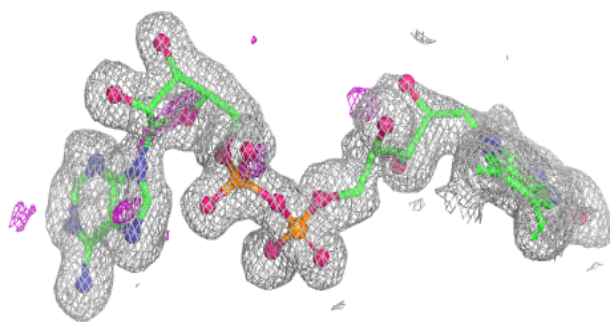
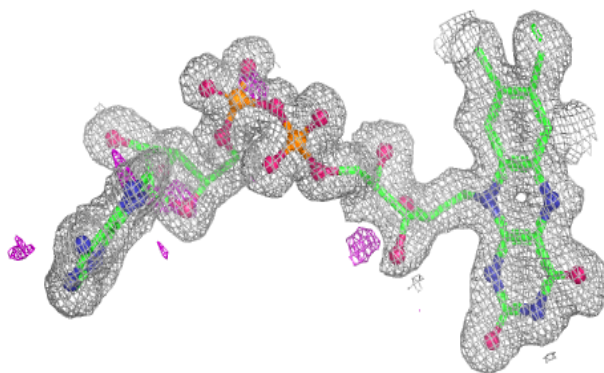


Electron density around FAD C 801:

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

**Electron density around FAD D 801:**

$2mF_o-DF_c$ (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.