Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:24 AM EDT

PDB ID	:	3W4K
Title	:	Crystal Structure of human DAAO in complex with coumpound 13
Authors	:	Hondo, T.; Warizaya, M.; Niimi, T.; Namatame, I.; Yamaguchi, T.; Nakanishi, K.; Hamajima, T.; Harada, K.; Sakashita, H.; Matsumoto, Y.; Orita, M.; Watanabe, T.; Takeuchi, M.
Deposited on	:	2013-01-09
Resolution	:	2.86 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:

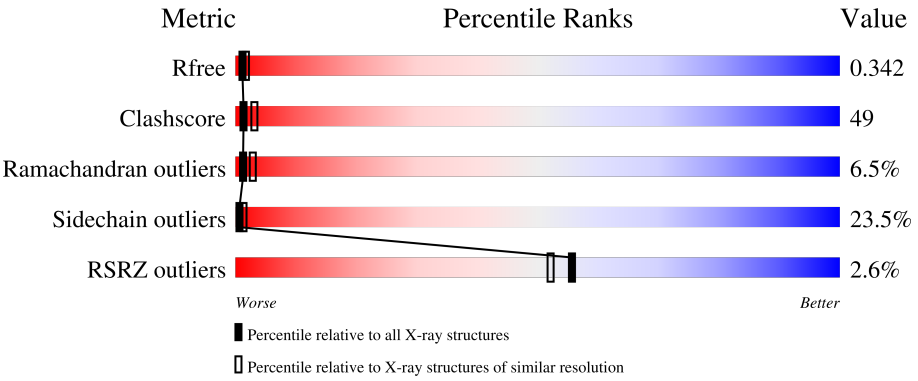
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	347	% 28% 48% 18% 5%
1	B	347	% 30% 50% 13% 5%
1	C	347	3% 26% 47% 21%
1	D	347	4% 29% 43% 22%

2 Entry composition (i)

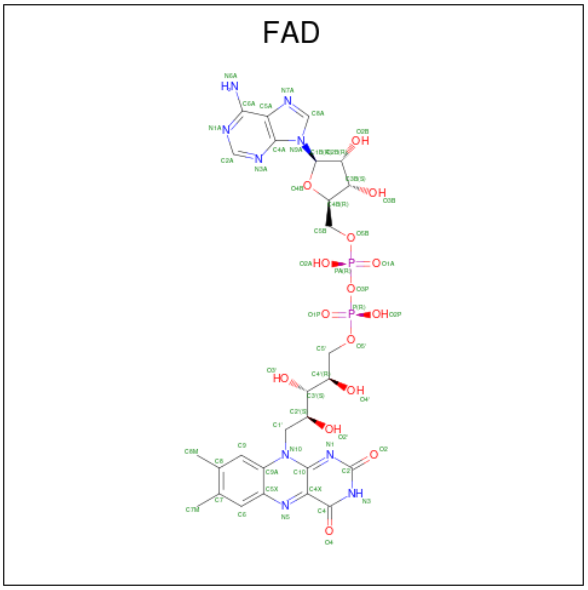
There are 3 unique types of molecules in this entry. The entry contains 11208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	B	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	C	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	D	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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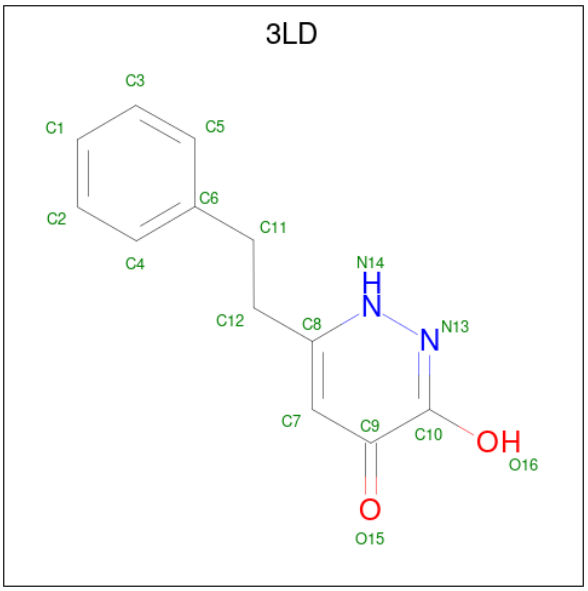
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-hydroxy-6-(2-phenylethyl)pyridazin-4(1H)-one (three-letter code: 3LD) (formula: $C_{12}H_{12}N_2O_2$).



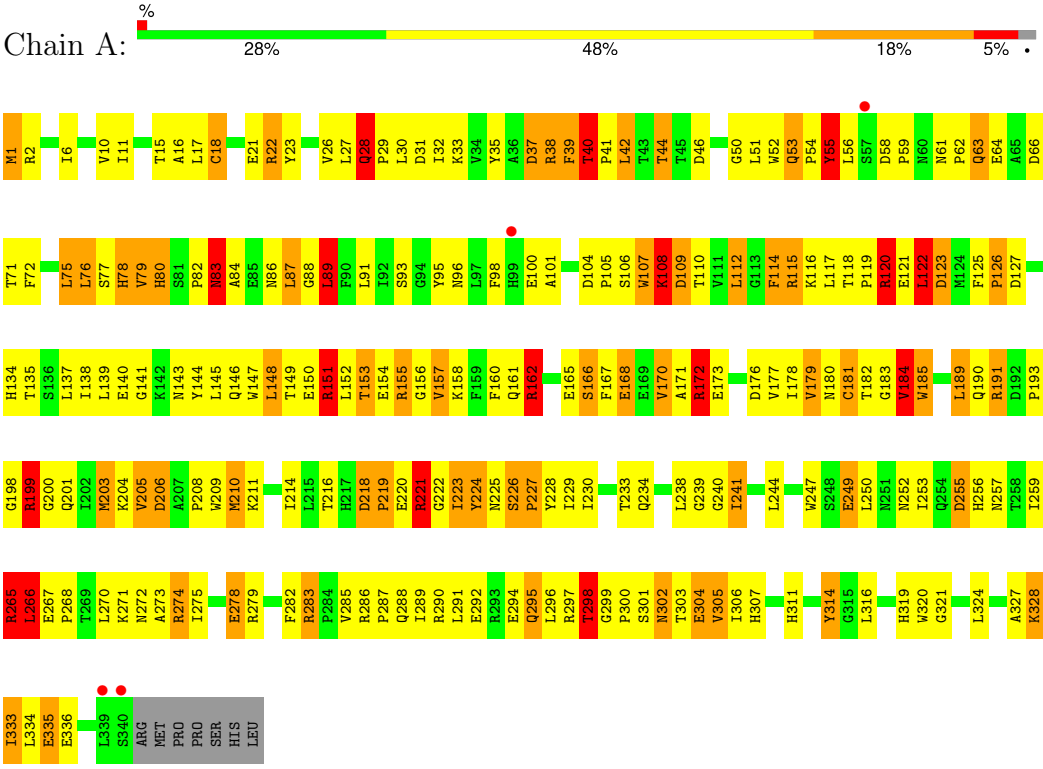
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	12	2	2		
3	B	1	Total	C	N	O	0	0
			16	12	2	2		
3	C	1	Total	C	N	O	0	0
			16	12	2	2		
3	D	1	Total	C	N	O	0	0
			16	12	2	2		

3 Residue-property plots (i)

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.

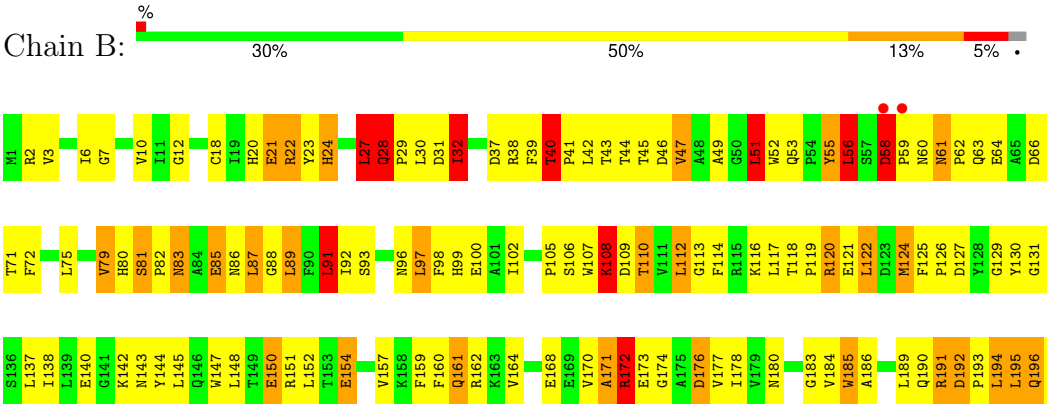
• Molecule 1: D-amino-acid oxidase

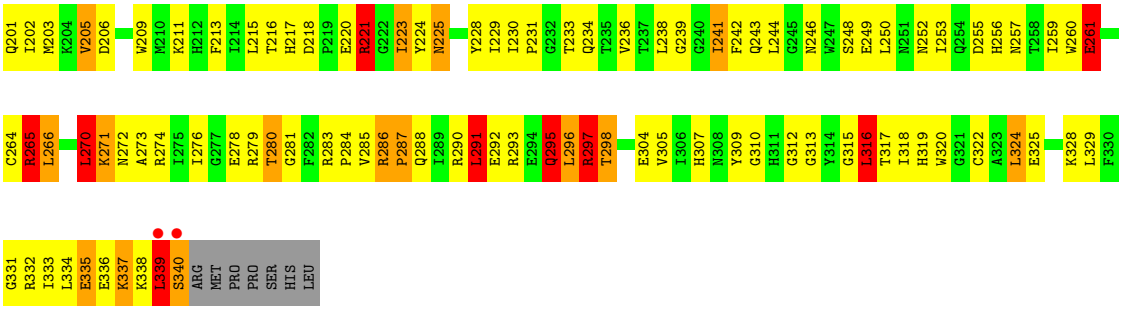
Chain A:



• Molecule 1: D-amino-acid oxidase

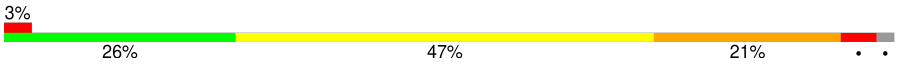
Chain B:

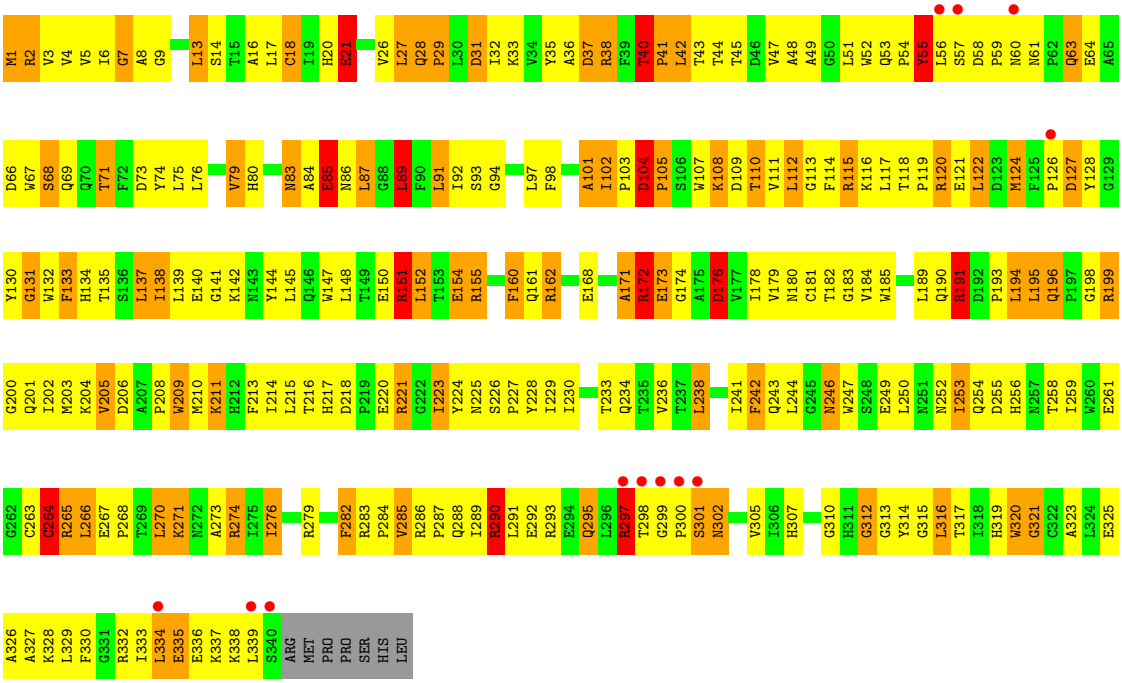




• Molecule 1: D-amino-acid oxidase

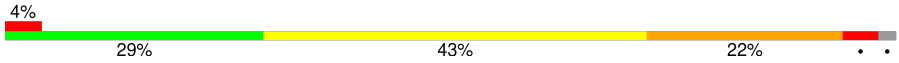
Chain C:

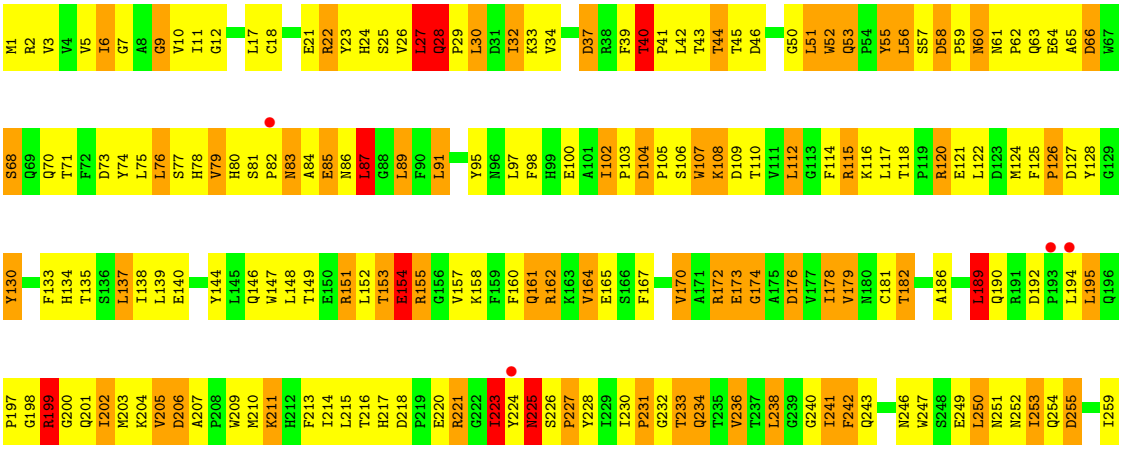


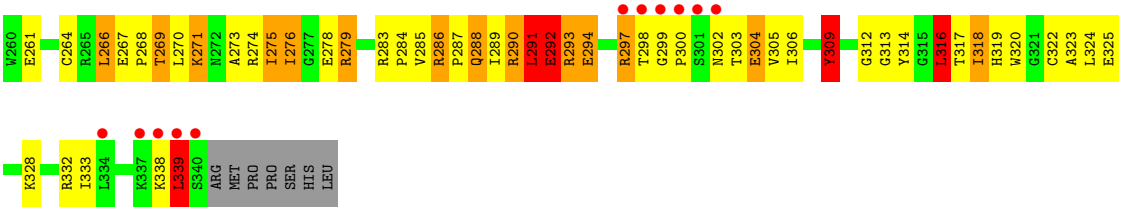


• Molecule 1: D-amino-acid oxidase

Chain D:






W260
E261
C264
R265
L266
E267
P268
T269
L270
K271
N272
A273
R274
I275
I276
G277
E278
R279
R283
P284
V285
R286
P287
Q288
I289
R290
L291
E292
R293
E294
R297
T298
G299
P300
S301
N302
T303
E304
V305
I306
Y309
G312
G313
Y314
G315
L316
T317
I318
H319
W320
G321
C322
A323
L324
E325
K328
R332
I333
L334
K337
K338
L339
S340
ARG
MET
PRO
PRO
SER
HIS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.66Å 182.46Å 50.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 2.86 38.95 – 2.86	Depositor EDS
% Data completeness (in resolution range)	92.9 (38.95-2.86) 92.9 (38.95-2.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.233 , 0.344 0.235 , 0.342	Depositor DCC
R_{free} test set	1566 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2218e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3LD, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.51	18/2810 (0.6%)	1.47	36/3824 (0.9%)
1	B	1.49	10/2810 (0.4%)	1.48	36/3824 (0.9%)
1	C	1.44	17/2810 (0.6%)	1.45	36/3824 (0.9%)
1	D	1.42	15/2810 (0.5%)	1.45	31/3824 (0.8%)
All	All	1.46	60/11240 (0.5%)	1.46	139/15296 (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	A	0	1
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	ILE	C-N	15.27	1.69	1.34
1	C	18	CYS	CB-SG	-12.32	1.61	1.82
1	A	18	CYS	CB-SG	-11.36	1.62	1.82
1	B	21	GLU	CG-CD	9.77	1.66	1.51
1	A	260	TRP	CB-CG	-8.28	1.35	1.50
1	A	21	GLU	CG-CD	7.62	1.63	1.51
1	D	181	CYS	CB-SG	-7.52	1.69	1.82
1	D	107	TRP	CB-CG	7.42	1.63	1.50
1	B	185	TRP	CE3-CZ3	7.32	1.50	1.38
1	B	261	GLU	CG-CD	7.12	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	PHE	CE2-CZ	7.04	1.50	1.37
1	A	35	TYR	CD1-CE1	-6.84	1.29	1.39
1	A	100	GLU	CG-CD	6.66	1.61	1.51
1	B	205	VAL	CB-CG2	-6.51	1.39	1.52
1	C	264	CYS	CB-SG	-6.46	1.71	1.82
1	B	297	ARG	CB-CG	6.43	1.70	1.52
1	A	28	GLN	CG-CD	6.36	1.65	1.51
1	C	21	GLU	CG-CD	6.35	1.61	1.51
1	A	185	TRP	CB-CG	-6.32	1.38	1.50
1	D	154	GLU	CG-CD	6.26	1.61	1.51
1	C	85	GLU	CG-CD	6.20	1.61	1.51
1	A	55	TYR	CE2-CZ	6.20	1.46	1.38
1	A	181	CYS	CB-SG	-6.07	1.72	1.82
1	D	21	GLU	CG-CD	5.89	1.60	1.51
1	D	52	TRP	CB-CG	5.87	1.60	1.50
1	B	72	PHE	CB-CG	-5.86	1.41	1.51
1	C	191	ARG	CG-CD	5.79	1.66	1.51
1	A	185	TRP	CE3-CZ3	5.74	1.48	1.38
1	A	314	TYR	CE1-CZ	-5.72	1.31	1.38
1	C	151	ARG	CB-CG	5.72	1.68	1.52
1	D	100	GLU	CG-CD	5.68	1.60	1.51
1	D	242	PHE	CE1-CZ	5.63	1.48	1.37
1	A	304	GLU	CB-CG	-5.63	1.41	1.52
1	D	309	TYR	CD1-CE1	5.63	1.47	1.39
1	C	55	TYR	CD2-CE2	5.56	1.47	1.39
1	D	278	GLU	CD-OE1	5.55	1.31	1.25
1	B	47	VAL	CA-CB	-5.54	1.43	1.54
1	C	79	VAL	CB-CG1	5.52	1.64	1.52
1	D	234	GLN	CG-CD	5.49	1.63	1.51
1	A	55	TYR	CD1-CE1	5.49	1.47	1.39
1	C	160	PHE	CB-CG	-5.49	1.42	1.51
1	C	220	GLU	CB-CG	5.47	1.62	1.52
1	A	18	CYS	N-CA	-5.39	1.35	1.46
1	D	236	VAL	CB-CG2	-5.38	1.41	1.52
1	B	260	TRP	CB-CG	-5.34	1.40	1.50
1	A	204	LYS	CD-CE	5.30	1.64	1.51
1	A	28	GLN	CB-CG	5.30	1.66	1.52
1	D	165	GLU	CG-CD	5.27	1.59	1.51
1	C	55	TYR	CE2-CZ	5.27	1.45	1.38
1	C	246	ASN	CB-CG	-5.22	1.39	1.51
1	D	278	GLU	CG-CD	5.16	1.59	1.51
1	D	55	TYR	CE2-CZ	5.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	TYR	CE1-CZ	5.12	1.45	1.38
1	A	278	GLU	CB-CG	-5.12	1.42	1.52
1	B	32	ILE	CA-CB	-5.12	1.43	1.54
1	C	4	VAL	CB-CG1	5.12	1.63	1.52
1	C	185	TRP	CB-CG	-5.11	1.41	1.50
1	A	335	GLU	CG-CD	-5.09	1.44	1.51
1	C	47	VAL	CB-CG1	-5.09	1.42	1.52
1	C	209	TRP	CB-CG	-5.01	1.41	1.50

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	199	ARG	NE-CZ-NH1	-13.38	113.61	120.30
1	D	199	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	A	122	LEU	CA-CB-CG	-10.86	90.33	115.30
1	B	265	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	D	291	LEU	CA-CB-CG	9.99	138.28	115.30
1	A	151	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	B	339	LEU	CA-CB-CG	9.41	136.93	115.30
1	C	199	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	C	339	LEU	CA-CB-CG	9.10	136.22	115.30
1	A	199	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	C	151	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	B	291	LEU	CA-CB-CG	8.78	135.48	115.30
1	C	18	CYS	CA-CB-SG	-8.39	98.91	114.00
1	A	189	LEU	CA-CB-CG	8.27	134.31	115.30
1	B	221	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	A	189	LEU	CB-CG-CD1	-8.13	97.18	111.00
1	A	151	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	B	206	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	18	CYS	CA-CB-SG	-7.95	99.68	114.00
1	D	89	LEU	CA-CB-CG	7.89	133.44	115.30
1	A	40	THR	N-CA-C	7.74	131.90	111.00
1	A	199	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	B	199	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	C	151	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	B	270	LEU	CB-CG-CD2	-7.56	98.14	111.00
1	C	42	LEU	CB-CG-CD2	-7.54	98.17	111.00
1	C	189	LEU	CA-CB-CG	7.54	132.64	115.30
1	D	137	LEU	CA-CB-CG	7.36	132.22	115.30
1	D	181	CYS	CA-CB-SG	-7.25	100.95	114.00
1	D	22	ARG	NE-CZ-NH2	7.25	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	120	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	B	324	LEU	CB-CG-CD2	7.13	123.12	111.00
1	B	192	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	B	265	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	B	91	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	C	189	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	B	221	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	C	279	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	223	ILE	CB-CA-C	-6.92	97.76	111.60
1	D	316	LEU	CA-CB-CG	6.91	131.20	115.30
1	B	316	LEU	CA-CB-CG	6.84	131.04	115.30
1	B	206	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	28	GLN	C-N-CD	6.58	142.22	128.40
1	C	89	LEU	CB-CG-CD2	6.54	122.12	111.00
1	C	40	THR	C-N-CD	6.54	142.13	128.40
1	D	211	LYS	CD-CE-NZ	6.51	126.68	111.70
1	B	40	THR	CB-CA-C	-6.45	94.18	111.60
1	D	40	THR	N-CA-C	6.43	128.37	111.00
1	A	206	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	89	LEU	CA-CB-CG	6.39	130.00	115.30
1	B	127	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	42	LEU	CB-CG-CD1	6.35	121.79	111.00
1	C	162	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	D	18	CYS	CA-CB-SG	-6.33	102.61	114.00
1	A	266	LEU	CA-CB-CG	6.28	129.75	115.30
1	D	51	LEU	CA-CB-CG	-6.24	100.95	115.30
1	A	329	LEU	CB-CG-CD1	6.23	121.58	111.00
1	D	255	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	28	GLN	C-N-CD	6.18	141.38	128.40
1	C	102	ILE	C-N-CD	6.17	141.35	128.40
1	C	40	THR	N-CA-C	6.16	127.64	111.00
1	C	37	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	283	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	B	276	ILE	N-CA-C	-6.11	94.50	111.00
1	A	265	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	C	102	ILE	N-CA-C	-6.04	94.69	111.00
1	C	270	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	126	PRO	N-CA-C	-5.99	96.54	112.10
1	D	303	THR	N-CA-C	-5.96	94.90	111.00
1	A	148	LEU	CA-CB-CG	5.94	128.96	115.30
1	B	120	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	C	334	LEU	CA-CB-CG	5.94	128.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	ASN	CB-CA-C	-5.89	98.61	110.40
1	B	297	ARG	CB-CA-C	5.89	122.18	110.40
1	C	238	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	89	LEU	CB-CG-CD2	5.87	120.97	111.00
1	A	109	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	263	CYS	CA-CB-SG	-5.83	103.51	114.00
1	A	328	LYS	CD-CE-NZ	5.79	125.01	111.70
1	C	199	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	B	91	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	B	21	GLU	CB-CA-C	5.76	121.93	110.40
1	C	131	GLY	N-CA-C	5.70	127.36	113.10
1	B	61	ASN	CB-CA-C	5.68	121.76	110.40
1	A	123	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	194	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	C	137	LEU	CA-CB-CG	-5.67	102.25	115.30
1	D	27	LEU	CB-CG-CD1	-5.67	101.37	111.00
1	C	276	ILE	CB-CA-C	-5.62	100.36	111.60
1	B	229	ILE	CG1-CB-CG2	-5.58	99.14	111.40
1	A	39	PHE	CB-CA-C	-5.55	99.30	110.40
1	B	296	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	C	37	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	D	339	LEU	CB-CG-CD2	5.54	120.41	111.00
1	B	51	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	C	9	GLY	N-CA-C	-5.51	99.31	113.10
1	D	232	GLY	N-CA-C	-5.51	99.32	113.10
1	D	314	TYR	N-CA-C	5.51	125.87	111.00
1	D	22	ARG	N-CA-C	5.50	125.84	111.00
1	D	266	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	B	91	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	199	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	B	270	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	44	THR	CA-CB-CG2	-5.44	104.79	112.40
1	C	42	LEU	CB-CA-C	-5.44	99.87	110.20
1	A	157	VAL	CB-CA-C	-5.43	101.07	111.40
1	A	265	ARG	CG-CD-NE	-5.43	100.39	111.80
1	B	280	THR	CB-CA-C	-5.43	96.94	111.60
1	A	162	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	206	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	189	LEU	CB-CG-CD2	5.41	120.20	111.00
1	D	66	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	221	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	293	ARG	NE-CZ-NH1	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	LEU	CB-CG-CD2	5.30	120.02	111.00
1	A	255	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	22	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	D	117	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	2	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	87	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	C	7	GLY	N-CA-C	-5.22	100.05	113.10
1	B	174	GLY	N-CA-C	5.21	126.11	113.10
1	C	176	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	40	THR	C-N-CD	5.20	139.32	128.40
1	D	9	GLY	N-CA-C	-5.19	100.12	113.10
1	B	21	GLU	CA-CB-CG	5.18	124.79	113.40
1	C	194	LEU	CB-CG-CD2	5.17	119.80	111.00
1	B	238	LEU	CB-CG-CD1	5.17	119.78	111.00
1	D	120	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	332	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	D	27	LEU	C-N-CA	-5.10	108.95	121.70
1	B	97	LEU	CA-CB-CG	-5.08	103.60	115.30
1	C	290	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	75	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	C	85	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	A	120	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	C	57	SER	N-CA-CB	-5.02	102.97	110.50
1	C	40	THR	C-N-CA	-5.01	100.95	122.00
1	B	195	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ASP	Peptide
1	B	58	ASP	Peptide
1	C	301	SER	Peptide
1	C	41	PRO	Peptide
1	C	60	ASN	Peptide
1	D	57	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2733	0	2680	263	0
1	B	2733	0	2680	265	0
1	C	2733	0	2680	308	0
1	D	2733	0	2680	261	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
2	C	53	0	31	17	0
2	D	53	0	31	5	0
3	A	16	0	11	2	0
3	B	16	0	11	5	0
3	C	16	0	11	4	0
3	D	16	0	11	5	0
All	All	11208	0	10888	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1080) 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:D:223:ILE:C	1:D:224:TYR:N	1.69	1.42
1:B:221:ARG:HH21	1:B:221:ARG:CB	1.43	1.31
1:C:264:CYS:SG	1:C:271:LYS:HD3	1.72	1.28
1:C:38:ARG:NH2	2:C:401:FAD:H2B	1.49	1.25
1:B:221:ARG:NH2	1:B:221:ARG:HB2	1.55	1.22
1:C:69:GLN:NE2	1:C:110:THR:HG23	1.60	1.17
1:D:221:ARG:HB2	1:D:221:ARG:HH21	1.08	1.12
1:B:335:GLU:HA	1:B:340:SER:HB3	1.31	1.11
1:C:38:ARG:NH2	2:C:401:FAD:C2B	2.14	1.09
1:C:17:LEU:O	1:C:21:GLU:HG2	1.51	1.09
1:D:264:CYS:SG	1:D:271:LYS:HD2	1.93	1.08
1:C:112:LEU:CD2	1:C:112:LEU:N	2.17	1.07
1:D:221:ARG:HH21	1:D:221:ARG:CB	1.67	1.06
1:A:140:GLU:OE1	1:A:233:THR:HB	1.53	1.06
1:D:264:CYS:SG	1:D:271:LYS:CD	2.44	1.06
1:A:274:ARG:HE	1:A:274:ARG:HA	1.23	1.03
1:D:40:THR:HG22	1:D:41:PRO:HD3	1.40	1.03
1:C:2:ARG:HG3	1:C:176:ASP:OD1	1.58	1.03
1:A:155:ARG:HG2	1:A:155:ARG:HH21	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HA	1:B:100:GLU:OE1	1.60	1.01
1:A:221:ARG:HB2	1:A:221:ARG:NH2	1.74	1.01
1:A:178:ILE:HB	1:A:305:VAL:HG22	1.39	1.01
1:D:83:ASN:O	1:D:86:ASN:HB2	1.62	0.99
1:A:168:GLU:O	1:A:172:ARG:HB2	1.62	0.99
1:B:224:TYR:O	1:B:242:PHE:HB2	1.61	0.99
1:A:61:ASN:OD1	1:A:63:GLN:HG3	1.63	0.98
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.46	0.98
1:B:284:PRO:HG2	1:B:312:GLY:H	1.27	0.98
1:B:241:ILE:HD12	1:B:255:ASP:HB3	1.45	0.98
1:C:2:ARG:HD3	1:C:174:GLY:O	1.64	0.98
1:A:221:ARG:HB2	1:A:221:ARG:CZ	1.92	0.97
1:C:38:ARG:HH22	2:C:401:FAD:H2B	1.18	0.97
1:C:332:ARG:O	1:C:336:GLU:HG3	1.62	0.97
1:B:55:TYR:HE1	1:B:224:TYR:OH	1.47	0.97
1:D:240:GLY:O	1:D:241:ILE:HD13	1.63	0.97
1:D:28:GLN:HB3	1:D:29:PRO:HD3	1.45	0.96
1:C:38:ARG:HH22	2:C:401:FAD:C2B	1.77	0.95
1:B:290:ARG:HD2	1:B:292:GLU:OE2	1.67	0.94
1:C:252:ASN:HD22	1:C:255:ASP:H	0.95	0.94
1:B:280:THR:HG22	1:B:281:GLY:N	1.79	0.94
1:C:111:VAL:C	1:C:112:LEU:HD22	1.89	0.93
1:C:112:LEU:N	1:C:112:LEU:HD23	1.83	0.93
1:B:180:ASN:HD22	1:B:307:HIS:CD2	1.87	0.93
1:B:264:CYS:SG	1:B:271:LYS:HG3	2.09	0.92
1:B:92:ILE:HD11	1:B:231:PRO:HG2	1.48	0.92
1:B:168:GLU:O	1:B:172:ARG:HB2	1.68	0.92
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.03	0.91
1:A:290:ARG:HD2	1:A:292:GLU:OE2	1.71	0.91
1:B:221:ARG:HH21	1:B:221:ARG:HB2	0.75	0.91
1:C:117:LEU:O	1:C:122:LEU:HD11	1.70	0.91
1:A:53:GLN:HE22	1:A:96:ASN:HD21	1.16	0.90
1:C:38:ARG:NH2	2:C:401:FAD:O2B	2.03	0.90
1:D:224:TYR:O	1:D:242:PHE:HB2	1.72	0.89
1:B:335:GLU:CA	1:B:340:SER:HB3	2.02	0.89
1:B:107:TRP:O	1:B:109:ASP:N	2.06	0.89
1:C:228:TYR:OH	3:C:402:3LD:O15	1.88	0.89
1:D:233:THR:CG2	1:D:234:GLN:HG2	2.03	0.89
1:C:69:GLN:NE2	1:C:110:THR:CG2	2.36	0.88
1:D:264:CYS:SG	1:D:271:LYS:HD3	2.12	0.88
1:A:178:ILE:HB	1:A:305:VAL:CG2	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:CYS:HG	1:C:271:LYS:HD3	1.35	0.88
1:D:40:THR:CG2	1:D:41:PRO:HD3	2.03	0.88
1:A:161:GLN:HG3	1:C:249:GLU:O	1.72	0.88
1:C:112:LEU:N	1:C:112:LEU:HD22	1.87	0.87
1:B:205:VAL:HG22	1:B:273:ALA:HB1	1.53	0.87
1:B:199:ARG:HH12	1:B:201:GLN:NE2	1.72	0.87
1:B:199:ARG:NH1	1:B:201:GLN:NE2	2.23	0.87
1:C:1:MET:N	1:C:29:PRO:O	2.07	0.87
1:B:55:TYR:HE1	1:B:224:TYR:CZ	1.92	0.86
1:B:199:ARG:HH12	1:B:201:GLN:HE22	1.22	0.86
1:C:150:GLU:O	1:C:154:GLU:HG2	1.75	0.86
1:C:221:ARG:HB2	1:C:221:ARG:NH2	1.91	0.86
1:A:335:GLU:HG3	1:A:336:GLU:H	1.36	0.86
1:C:229:ILE:HD12	1:C:266:LEU:HD13	1.57	0.86
1:B:221:ARG:CB	1:B:221:ARG:NH2	2.25	0.86
1:A:233:THR:HG23	1:A:234:GLN:N	1.90	0.85
1:C:52:TRP:NE1	1:C:317:THR:HG23	1.91	0.85
1:B:255:ASP:O	1:B:259:ILE:HG13	1.76	0.85
1:B:274:ARG:HH12	1:C:274:ARG:HD2	1.39	0.84
1:A:1:MET:HG2	1:A:27:LEU:HD13	1.59	0.84
1:D:221:ARG:CB	1:D:221:ARG:NH2	2.40	0.84
1:D:43:THR:O	1:D:46:ASP:HB2	1.78	0.84
1:C:242:PHE:HD1	1:C:243:GLN:N	1.75	0.84
1:C:243:GLN:HE22	1:C:246:ASN:HD22	1.26	0.83
1:B:150:GLU:O	1:B:154:GLU:HG2	1.78	0.83
1:B:203:MET:HE1	1:B:256:HIS:CE1	2.14	0.82
1:C:38:ARG:HH21	2:C:401:FAD:H2B	1.43	0.82
1:A:216:THR:O	1:A:226:SER:HB3	1.80	0.82
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.15	0.81
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.29	0.81
1:D:76:LEU:HG	1:D:76:LEU:O	1.81	0.80
1:D:201:GLN:HE22	1:D:252:ASN:H	1.28	0.80
1:C:79:VAL:HG22	1:C:80:HIS:CD2	2.17	0.80
1:C:252:ASN:ND2	1:C:255:ASP:H	1.78	0.80
1:C:79:VAL:HG22	1:C:80:HIS:HD2	1.47	0.80
1:B:49:ALA:HB1	1:B:230:ILE:HG21	1.64	0.79
1:D:201:GLN:NE2	1:D:252:ASN:H	1.79	0.79
1:B:2:ARG:N	1:B:176:ASP:OD1	2.12	0.79
1:B:298:THR:HG23	1:B:298:THR:O	1.82	0.79
1:C:79:VAL:HG21	1:C:91:LEU:HD11	1.63	0.79
1:D:81:SER:HB2	1:D:82:PRO:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLY:O	1:B:334:LEU:HB2	1.83	0.78
1:A:27:LEU:HD11	1:A:334:LEU:HD21	1.65	0.78
1:C:283:ARG:NE	3:C:402:3LD:O16	2.13	0.78
1:A:155:ARG:HG2	1:A:155:ARG:NH2	1.88	0.78
1:B:335:GLU:HG2	1:B:336:GLU:N	1.97	0.78
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.23	0.78
1:A:205:VAL:HG22	1:A:273:ALA:HB1	1.63	0.78
1:B:191:ARG:NH1	1:B:193:PRO:HG3	1.99	0.78
1:A:1:MET:HA	1:A:1:MET:CE	2.14	0.78
1:C:54:PRO:HG3	1:C:317:THR:HG21	1.66	0.78
1:A:69:GLN:NE2	1:A:110:THR:HG23	2.00	0.77
1:A:141:GLY:O	1:A:145:LEU:HB2	1.84	0.77
1:C:115:ARG:O	1:C:115:ARG:HG3	1.84	0.77
1:C:55:TYR:CE1	1:C:224:TYR:OH	2.36	0.77
1:A:69:GLN:HE22	1:A:110:THR:HG23	1.50	0.77
1:C:55:TYR:HE1	1:C:224:TYR:HH	1.30	0.77
1:C:117:LEU:HB3	1:C:122:LEU:HD21	1.67	0.77
1:A:233:THR:CG2	1:A:234:GLN:H	1.98	0.76
1:C:151:ARG:HH11	1:C:154:GLU:CD	1.88	0.76
1:D:52:TRP:CD1	1:D:317:THR:HG23	2.21	0.76
1:C:69:GLN:HE22	1:C:110:THR:HG23	1.46	0.76
1:A:108:LYS:HG3	1:A:109:ASP:N	1.99	0.76
1:B:81:SER:HB2	1:B:82:PRO:HD2	1.67	0.76
1:C:286:ARG:HG3	1:C:287:PRO:HD2	1.68	0.76
1:D:5:VAL:HA	1:D:179:VAL:HG23	1.68	0.76
1:B:293:ARG:NH2	1:B:304:GLU:OE2	2.19	0.76
1:C:69:GLN:CD	1:C:110:THR:HG23	2.06	0.76
1:C:252:ASN:ND2	1:C:254:GLN:H	1.84	0.76
1:A:223:ILE:O	1:A:223:ILE:HG23	1.85	0.75
1:B:336:GLU:C	1:B:338:LYS:H	1.89	0.75
1:B:28:GLN:HB3	1:B:29:PRO:HD3	1.68	0.75
1:B:291:LEU:HA	1:B:307:HIS:O	1.87	0.75
1:C:111:VAL:C	1:C:112:LEU:CD2	2.54	0.75
1:A:233:THR:CG2	1:A:234:GLN:N	2.49	0.75
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.69	0.75
1:B:203:MET:CE	1:B:256:HIS:CE1	2.69	0.75
1:A:53:GLN:HE22	1:A:96:ASN:ND2	1.84	0.74
1:D:240:GLY:C	1:D:241:ILE:HD13	2.07	0.74
1:D:50:GLY:HA2	1:D:316:LEU:HD23	1.69	0.74
1:B:55:TYR:HE1	1:B:224:TYR:HH	0.79	0.74
1:B:224:TYR:O	1:B:242:PHE:CB	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG2	1:D:27:LEU:HD11	1.70	0.74
1:B:39:PHE:O	1:B:41:PRO:CD	2.35	0.73
1:A:32:ILE:HB	1:A:157:VAL:HG22	1.71	0.73
1:A:291:LEU:HA	1:A:307:HIS:O	1.89	0.73
1:A:274:ARG:HA	1:A:274:ARG:NE	1.96	0.73
1:D:231:PRO:HA	1:D:236:VAL:HG22	1.71	0.73
1:A:168:GLU:O	1:A:172:ARG:CB	2.35	0.72
1:C:27:LEU:HD11	1:C:334:LEU:CD2	2.18	0.72
1:B:61:ASN:HB2	1:B:288:GLN:NE2	2.04	0.72
1:C:198:GLY:O	1:C:283:ARG:HG3	1.89	0.72
1:B:202:ILE:HD12	1:B:202:ILE:O	1.89	0.72
1:C:264:CYS:HB3	1:C:271:LYS:NZ	2.05	0.72
1:D:293:ARG:O	1:D:294:GLU:HB2	1.90	0.72
1:A:40:THR:CG2	1:A:41:PRO:HD3	2.20	0.72
1:D:199:ARG:O	1:D:283:ARG:NH2	2.22	0.72
1:B:55:TYR:CE1	1:B:224:TYR:CZ	2.77	0.71
1:C:252:ASN:HD22	1:C:255:ASP:N	1.80	0.71
1:B:55:TYR:CE1	1:B:224:TYR:CE1	2.79	0.71
1:C:55:TYR:HE1	1:C:224:TYR:OH	1.73	0.70
1:D:151:ARG:O	1:D:154:GLU:HG2	1.90	0.70
1:D:23:TYR:O	1:D:30:LEU:HD23	1.91	0.70
1:A:53:GLN:NE2	1:A:96:ASN:HD21	1.89	0.70
1:B:228:TYR:HD1	1:B:230:ILE:HD12	1.54	0.70
1:C:114:PHE:HZ	1:C:132:TRP:CD1	2.09	0.70
1:A:203:MET:HE3	1:A:259:ILE:HB	1.72	0.70
1:C:264:CYS:HB3	1:C:271:LYS:HZ3	1.57	0.70
1:D:167:PHE:CE1	1:D:189:LEU:HD12	2.27	0.70
1:A:179:VAL:HG13	1:A:306:ILE:HB	1.74	0.70
1:B:200:GLY:O	1:B:280:THR:HG23	1.92	0.70
1:C:5:VAL:HG22	1:C:179:VAL:HB	1.73	0.70
1:D:59:PRO:HG3	1:D:65:ALA:HB2	1.74	0.70
1:C:191:ARG:NH1	1:C:193:PRO:HG3	2.07	0.70
1:D:286:ARG:HH12	1:D:290:ARG:HD3	1.58	0.69
1:A:1:MET:HE1	1:A:176:ASP:HB3	1.73	0.69
1:A:59:PRO:HG2	1:A:62:PRO:HA	1.75	0.69
1:B:203:MET:CE	1:B:256:HIS:ND1	2.55	0.69
1:C:295:GLN:CD	1:C:295:GLN:H	1.94	0.69
1:B:295:GLN:H	1:B:295:GLN:HE21	1.40	0.69
1:B:180:ASN:ND2	1:B:307:HIS:HD2	1.86	0.69
1:D:3:VAL:HG12	1:D:32:ILE:HG23	1.75	0.69
1:D:233:THR:HG23	1:D:234:GLN:HE21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ARG:H	1:D:297:ARG:HD3	1.58	0.69
1:D:221:ARG:HB2	1:D:221:ARG:NH2	1.93	0.69
1:C:112:LEU:HB2	1:C:135:THR:HB	1.73	0.69
1:D:233:THR:HG22	1:D:234:GLN:HG2	1.74	0.69
1:B:280:THR:HG22	1:B:281:GLY:H	1.53	0.68
1:A:182:THR:O	2:A:401:FAD:H8A	1.93	0.68
1:B:43:THR:N	1:B:46:ASP:OD1	2.21	0.68
1:B:336:GLU:O	1:B:338:LYS:N	2.26	0.68
1:C:191:ARG:HH11	1:C:193:PRO:HG3	1.57	0.68
1:A:1:MET:HA	1:A:1:MET:HE2	1.75	0.68
1:C:286:ARG:HG3	1:C:287:PRO:CD	2.22	0.68
1:C:83:ASN:O	1:C:86:ASN:HB2	1.93	0.68
1:D:242:PHE:O	1:D:243:GLN:HG3	1.92	0.68
1:A:40:THR:O	1:A:40:THR:OG1	2.06	0.68
1:A:223:ILE:HG13	1:A:224:TYR:N	2.07	0.68
1:A:297:ARG:HG3	1:A:302:ASN:HD22	1.59	0.68
1:B:112:LEU:H	1:B:112:LEU:HD22	1.58	0.68
1:D:126:PRO:O	1:D:128:TYR:N	2.27	0.67
1:B:168:GLU:OE2	1:B:296:LEU:HD21	1.94	0.67
1:C:52:TRP:CE2	1:C:317:THR:HG23	2.29	0.67
1:D:83:ASN:O	1:D:86:ASN:CB	2.41	0.67
1:D:105:PRO:HD2	1:D:108:LYS:HB3	1.77	0.67
1:B:59:PRO:HG2	1:B:62:PRO:HA	1.76	0.67
1:B:150:GLU:O	1:B:154:GLU:CG	2.43	0.67
1:C:79:VAL:O	1:C:80:HIS:HD2	1.78	0.67
1:B:112:LEU:HD23	1:B:135:THR:O	1.94	0.67
1:C:332:ARG:HA	1:C:335:GLU:CG	2.25	0.67
1:A:38:ARG:HD2	2:A:401:FAD:O2B	1.94	0.66
1:A:335:GLU:HG3	1:A:336:GLU:N	2.07	0.66
1:B:231:PRO:HA	1:B:236:VAL:HG22	1.75	0.66
1:D:179:VAL:HG12	1:D:306:ILE:HB	1.76	0.66
1:C:241:ILE:HD12	1:C:255:ASP:HB3	1.77	0.66
1:A:200:GLY:CA	1:A:283:ARG:HH22	2.07	0.66
1:C:20:HIS:HD2	1:C:32:ILE:HD12	1.61	0.66
1:C:211:LYS:HD3	1:C:211:LYS:N	1.99	0.66
1:D:6:ILE:CD1	1:D:164:VAL:HG11	2.25	0.66
1:B:228:TYR:CD1	1:B:230:ILE:HD12	2.31	0.66
1:A:296:LEU:O	1:A:298:THR:HG22	1.95	0.66
1:C:87:LEU:HD23	1:C:147:TRP:CD2	2.31	0.66
1:C:117:LEU:CB	1:C:122:LEU:HD21	2.25	0.66
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LEU:HD13	1:C:287:PRO:HG2	1.77	0.65
1:C:242:PHE:CD1	1:C:243:GLN:N	2.63	0.65
1:B:22:ARG:HD2	1:B:23:TYR:CE2	2.31	0.65
1:B:325:GLU:OE1	1:B:325:GLU:HA	1.97	0.65
1:C:13:LEU:O	1:C:16:ALA:HB3	1.96	0.65
1:D:250:LEU:HD12	1:D:251:ASN:N	2.11	0.65
1:A:221:ARG:CZ	1:A:221:ARG:CB	2.73	0.65
1:B:22:ARG:HD2	1:B:23:TYR:CZ	2.31	0.65
1:B:184:VAL:HG21	1:B:197:PRO:HB3	1.79	0.65
1:B:203:MET:HE1	1:B:256:HIS:ND1	2.12	0.65
1:A:61:ASN:ND2	1:A:63:GLN:HE21	1.94	0.65
1:A:257:ASN:O	1:A:261:GLU:OE1	2.14	0.65
1:D:112:LEU:HB2	1:D:135:THR:HB	1.78	0.65
1:C:178:ILE:HB	1:C:305:VAL:HG22	1.79	0.65
2:C:401:FAD:O4	3:C:402:3LD:H9	1.96	0.65
1:B:196:GLN:O	1:B:285:VAL:HG23	1.97	0.65
1:B:274:ARG:NH1	1:C:274:ARG:HD2	2.11	0.65
1:C:223:ILE:HD12	1:C:224:TYR:H	1.61	0.65
1:D:40:THR:CG2	1:D:41:PRO:CD	2.76	0.64
1:C:150:GLU:HG3	1:C:151:ARG:NH1	2.12	0.64
1:D:201:GLN:HE22	1:D:252:ASN:N	1.94	0.64
1:B:3:VAL:HB	1:B:32:ILE:HG23	1.77	0.64
1:C:243:GLN:HE22	1:C:246:ASN:ND2	1.94	0.64
1:B:284:PRO:HG2	1:B:312:GLY:N	2.09	0.64
1:D:223:ILE:CA	1:D:224:TYR:N	2.60	0.64
1:A:298:THR:HG21	1:A:303:THR:HG23	1.78	0.64
1:C:71:THR:HG21	1:C:317:THR:O	1.97	0.64
1:B:280:THR:CG2	1:B:281:GLY:N	2.55	0.64
1:A:205:VAL:CG2	1:A:273:ALA:HB1	2.28	0.64
1:B:40:THR:O	1:B:40:THR:OG1	2.04	0.64
1:D:102:ILE:CG1	1:D:103:PRO:CD	2.76	0.64
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.46	0.63
1:B:242:PHE:CD1	1:B:242:PHE:C	2.71	0.63
1:B:216:THR:HG23	1:B:266:LEU:HD11	1.80	0.63
1:D:151:ARG:NE	1:D:154:GLU:OE2	2.30	0.63
1:C:264:CYS:CB	1:C:271:LYS:HZ3	2.11	0.63
1:D:202:ILE:HD11	1:D:279:ARG:HB2	1.79	0.63
1:B:112:LEU:HD22	1:B:112:LEU:N	2.14	0.63
1:C:291:LEU:HA	1:C:307:HIS:O	1.99	0.63
1:A:295:GLN:HE21	1:A:295:GLN:N	1.95	0.63
1:B:28:GLN:HB3	1:B:29:PRO:CD	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TYR:CD1	1:B:309:TYR:C	2.72	0.63
1:C:61:ASN:HD21	1:C:63:GLN:HB2	1.63	0.63
1:C:325:GLU:OE2	1:C:329:LEU:HD21	1.98	0.62
1:A:252:ASN:HD22	1:A:255:ASP:H	1.47	0.62
1:B:119:PRO:HA	1:B:122:LEU:HD12	1.80	0.62
1:B:159:PHE:N	1:B:159:PHE:HD2	1.95	0.62
1:B:298:THR:O	1:B:298:THR:CG2	2.47	0.62
1:C:264:CYS:SG	1:C:271:LYS:CD	2.67	0.62
1:A:193:PRO:HD2	1:A:194:LEU:H	1.62	0.62
1:B:38:ARG:NH1	1:B:249:GLU:OE2	2.32	0.62
1:B:221:ARG:HH21	1:B:221:ARG:HB3	1.57	0.62
1:C:221:ARG:HB2	1:C:221:ARG:HH21	1.64	0.62
1:D:140:GLU:OE1	1:D:233:THR:HB	1.99	0.62
1:A:199:ARG:HH12	1:A:201:GLN:NE2	1.96	0.62
1:C:284:PRO:O	1:C:312:GLY:N	2.31	0.62
1:B:24:HIS:H	1:B:24:HIS:CD2	2.17	0.62
1:D:58:ASP:OD2	1:D:59:PRO:HD2	1.99	0.62
1:D:252:ASN:HD21	1:D:254:GLN:HB2	1.65	0.62
1:C:40:THR:HG23	1:C:41:PRO:HD3	1.80	0.62
1:C:74:TYR:CD2	1:C:320:TRP:CD1	2.88	0.62
1:C:160:PHE:N	1:C:160:PHE:CD1	2.66	0.62
1:C:289:ILE:HG22	1:C:290:ARG:N	2.15	0.62
1:D:102:ILE:CG1	1:D:103:PRO:HD2	2.30	0.62
1:B:161:GLN:HG3	1:D:249:GLU:N	2.14	0.62
1:B:336:GLU:C	1:B:338:LYS:N	2.54	0.62
1:D:223:ILE:C	1:D:224:TYR:CA	2.67	0.61
1:A:42:LEU:HD22	1:C:42:LEU:CD2	2.27	0.61
1:A:286:ARG:HG2	1:A:288:GLN:O	1.99	0.61
1:C:80:HIS:CE1	1:D:267:GLU:OE2	2.53	0.61
1:B:161:GLN:HG3	1:D:249:GLU:H	1.65	0.61
1:C:27:LEU:HD11	1:C:334:LEU:HD22	1.83	0.61
1:B:85:GLU:O	1:B:85:GLU:HG2	2.00	0.61
1:C:332:ARG:HA	1:C:335:GLU:HG2	1.81	0.61
1:A:105:PRO:HB2	1:A:107:TRP:CE2	2.36	0.61
1:B:39:PHE:O	1:B:41:PRO:HD2	2.00	0.61
1:B:186:ALA:HB3	1:B:195:LEU:HD22	1.82	0.61
1:D:59:PRO:HG2	1:D:62:PRO:HA	1.80	0.61
1:C:223:ILE:HD12	1:C:224:TYR:N	2.15	0.61
1:A:40:THR:HG23	1:A:41:PRO:CD	2.31	0.61
1:A:40:THR:HG22	1:A:41:PRO:HD3	1.81	0.61
1:B:41:PRO:HD2	1:B:42:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PHE:N	1:B:159:PHE:CD2	2.65	0.61
1:C:284:PRO:HG2	1:C:312:GLY:H	1.65	0.61
1:A:239:GLY:HA2	1:A:259:ILE:CD1	2.31	0.61
1:C:274:ARG:HA	1:C:274:ARG:NE	2.16	0.61
1:B:51:LEU:HD23	3:B:402:3LD:H7	1.82	0.60
1:D:182:THR:HG22	2:D:401:FAD:C8A	2.31	0.60
1:B:55:TYR:HE1	1:B:224:TYR:CE1	2.17	0.60
1:B:241:ILE:CD1	1:B:255:ASP:HB3	2.27	0.60
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.31	0.60
1:C:289:ILE:CG2	1:C:290:ARG:N	2.64	0.60
1:D:170:VAL:CG1	1:D:178:ILE:HD13	2.31	0.60
1:D:172:ARG:C	1:D:174:GLY:H	2.04	0.60
1:A:223:ILE:O	1:A:223:ILE:CG2	2.49	0.60
1:C:114:PHE:CZ	1:C:132:TRP:CD1	2.89	0.60
1:A:61:ASN:HB2	1:A:288:GLN:OE1	2.02	0.60
1:C:51:LEU:HD23	3:C:402:3LD:H7	1.83	0.60
1:C:252:ASN:ND2	1:C:254:GLN:N	2.48	0.60
1:D:207:ALA:O	1:D:209:TRP:N	2.34	0.60
1:C:117:LEU:HB3	1:C:122:LEU:CD2	2.30	0.60
1:B:24:HIS:H	1:B:24:HIS:HD2	1.50	0.60
1:B:205:VAL:HG22	1:B:273:ALA:CB	2.31	0.60
1:D:242:PHE:C	1:D:243:GLN:HG3	2.22	0.60
1:C:61:ASN:HD21	1:C:63:GLN:HE21	1.48	0.60
1:C:320:TRP:O	1:C:321:GLY:C	2.40	0.60
1:D:241:ILE:HG12	1:D:259:ILE:HD11	1.84	0.60
1:D:293:ARG:O	1:D:294:GLU:CB	2.48	0.60
1:C:61:ASN:ND2	1:C:63:GLN:HB2	2.17	0.60
1:C:133:PHE:C	1:C:133:PHE:CD2	2.74	0.60
1:A:51:LEU:HD12	1:A:52:TRP:H	1.66	0.59
1:D:139:LEU:HD11	1:D:144:TYR:CD1	2.37	0.59
1:D:267:GLU:O	1:D:270:LEU:HB2	2.02	0.59
1:B:32:ILE:HB	1:B:157:VAL:HG13	1.84	0.59
1:B:117:LEU:O	1:B:122:LEU:HD11	2.01	0.59
1:C:112:LEU:HD23	1:C:112:LEU:H	1.67	0.59
1:D:28:GLN:HB3	1:D:29:PRO:CD	2.24	0.59
1:D:71:THR:HG23	1:D:320:TRP:H	1.67	0.59
1:D:153:THR:C	1:D:155:ARG:H	2.06	0.59
1:D:223:ILE:HD12	1:D:224:TYR:H	1.68	0.59
1:C:104:ASP:OD1	1:C:104:ASP:N	2.33	0.59
1:D:102:ILE:HG12	1:D:103:PRO:N	2.18	0.59
1:A:214:ILE:HG21	1:A:266:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLY:O	1:B:283:ARG:HD2	2.03	0.59
1:C:87:LEU:HD23	1:C:147:TRP:CE2	2.37	0.59
1:C:289:ILE:HD11	1:C:314:TYR:HE2	1.66	0.59
1:A:146:GLN:O	1:A:149:THR:HB	2.03	0.59
1:D:161:GLN:O	1:D:162:ARG:HB3	2.03	0.59
1:C:114:PHE:CD1	1:C:114:PHE:C	2.76	0.59
1:C:208:PRO:HG2	1:D:234:GLN:NE2	2.16	0.59
1:D:253:ILE:HD13	1:D:253:ILE:O	2.01	0.59
1:D:172:ARG:O	1:D:174:GLY:N	2.36	0.59
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.46	0.58
1:A:332:ARG:O	1:A:333:ILE:C	2.40	0.58
1:C:91:LEU:HD23	1:C:137:LEU:HD21	1.85	0.58
1:A:105:PRO:HD3	1:A:132:TRP:CE2	2.38	0.58
1:B:129:GLY:O	1:B:130:TYR:HB2	2.03	0.58
1:A:105:PRO:HD2	1:A:114:PHE:CZ	2.38	0.58
1:B:53:GLN:HE22	1:B:96:ASN:HD21	1.50	0.58
1:D:102:ILE:HG12	1:D:103:PRO:CD	2.33	0.58
1:D:32:ILE:O	1:D:157:VAL:HG13	2.03	0.58
1:D:52:TRP:NE1	1:D:317:THR:HG23	2.19	0.58
1:A:222:GLY:O	1:A:225:ASN:HB3	2.04	0.58
1:A:278:GLU:O	1:A:279:ARG:HG2	2.02	0.58
1:B:92:ILE:CD1	1:B:231:PRO:HG2	2.29	0.58
1:B:114:PHE:HZ	1:B:132:TRP:CD1	2.21	0.58
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.84	0.58
1:C:242:PHE:HD1	1:C:242:PHE:C	2.07	0.58
1:C:49:ALA:HB1	1:C:230:ILE:HG21	1.86	0.58
1:A:40:THR:HG23	1:A:41:PRO:HD3	1.86	0.58
1:C:97:LEU:CD2	1:C:117:LEU:CD1	2.82	0.58
1:D:144:TYR:OH	1:D:319:HIS:CE1	2.57	0.57
1:C:102:ILE:HG23	1:C:103:PRO:O	2.04	0.57
1:C:225:ASN:HD22	1:C:242:PHE:H	1.52	0.57
1:A:61:ASN:HD21	1:A:63:GLN:NE2	2.00	0.57
1:A:167:PHE:CE1	1:A:189:LEU:HD12	2.40	0.57
1:C:40:THR:HG23	1:C:41:PRO:CD	2.35	0.57
1:C:242:PHE:CD1	1:C:242:PHE:C	2.78	0.57
1:D:52:TRP:CE2	1:D:317:THR:HG23	2.40	0.57
1:A:203:MET:CE	1:A:259:ILE:HB	2.34	0.57
1:D:224:TYR:O	1:D:242:PHE:CB	2.51	0.57
1:A:1:MET:CE	1:A:1:MET:CA	2.82	0.57
1:A:69:GLN:NE2	1:A:110:THR:CG2	2.67	0.57
1:D:304:GLU:O	1:D:305:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD11	1:A:334:LEU:CD2	2.35	0.57
1:C:266:LEU:CD2	1:C:266:LEU:O	2.53	0.57
1:A:6:ILE:O	1:A:181:CYS:HB2	2.05	0.56
1:D:74:TYR:O	1:D:77:SER:OG	2.23	0.56
1:D:207:ALA:HA	1:D:209:TRP:CZ3	2.40	0.56
1:A:1:MET:HG2	1:A:27:LEU:CD1	2.34	0.56
1:A:51:LEU:HD12	1:A:52:TRP:N	2.20	0.56
1:A:83:ASN:O	1:A:86:ASN:N	2.38	0.56
1:B:218:ASP:OD1	1:B:220:GLU:HB2	2.05	0.56
1:D:167:PHE:O	1:D:170:VAL:HG12	2.05	0.56
1:A:39:PHE:O	1:A:41:PRO:HD2	2.05	0.56
1:A:41:PRO:HD2	1:A:42:LEU:HG	1.88	0.56
1:C:114:PHE:CD1	1:C:115:ARG:N	2.74	0.56
1:D:102:ILE:HG13	1:D:103:PRO:HD2	1.87	0.56
1:D:313:GLY:O	3:D:402:3LD:N13	2.38	0.56
2:B:401:FAD:C5X	3:B:402:3LD:C10	2.83	0.56
1:D:318:ILE:O	1:D:319:HIS:C	2.43	0.56
1:A:1:MET:HA	1:A:1:MET:HE3	1.86	0.56
1:A:107:TRP:O	1:A:110:THR:N	2.35	0.56
1:C:199:ARG:O	1:C:283:ARG:NH2	2.38	0.56
1:A:233:THR:HG23	1:A:234:GLN:H	1.55	0.56
1:C:119:PRO:HA	1:C:122:LEU:HD12	1.88	0.56
1:C:214:ILE:C	1:C:215:LEU:HD23	2.26	0.56
1:C:224:TYR:OH	1:C:313:GLY:HA3	2.06	0.56
1:C:244:LEU:HD21	1:C:285:VAL:HG11	1.86	0.56
1:D:147:TRP:CZ3	1:D:148:LEU:HD23	2.41	0.56
1:A:67:TRP:HB3	1:A:321:GLY:HA3	1.88	0.56
1:A:39:PHE:O	1:A:41:PRO:CD	2.54	0.56
1:A:200:GLY:CA	1:A:283:ARG:NH2	2.69	0.56
1:A:216:THR:HG23	1:A:266:LEU:HD11	1.87	0.56
2:A:401:FAD:O4	3:A:402:3LD:H9	2.06	0.56
1:B:205:VAL:CG2	1:B:273:ALA:HB1	2.31	0.56
1:B:328:LYS:O	1:B:331:GLY:N	2.39	0.56
1:C:1:MET:CE	1:C:176:ASP:HB2	2.36	0.56
1:C:180:ASN:HD22	1:C:307:HIS:CD2	2.24	0.56
1:A:210:MET:C	1:A:211:LYS:HD3	2.27	0.55
1:A:216:THR:CG2	1:A:266:LEU:HD11	2.36	0.55
1:C:94:GLY:HA3	1:C:213:PHE:O	2.06	0.55
1:D:37:ASP:N	2:D:401:FAD:N3A	2.51	0.55
1:A:221:ARG:NH2	1:A:221:ARG:CB	2.60	0.55
1:B:203:MET:HE2	1:B:256:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PRO:CD	1:C:105:PRO:O	2.53	0.55
1:C:144:TYR:OH	1:C:319:HIS:CE1	2.60	0.55
1:B:63:GLN:O	1:B:64:GLU:C	2.43	0.55
1:D:121:GLU:O	1:D:124:MET:HG2	2.07	0.55
1:D:153:THR:C	1:D:155:ARG:N	2.60	0.55
1:D:293:ARG:HD3	1:D:333:ILE:HD11	1.88	0.55
1:A:1:MET:HE2	1:A:176:ASP:OD1	2.07	0.55
1:B:6:ILE:HD13	1:B:164:VAL:HG21	1.88	0.55
1:B:27:LEU:O	1:B:28:GLN:O	2.25	0.55
1:D:318:ILE:O	1:D:320:TRP:N	2.40	0.55
1:A:72:PHE:C	1:A:72:PHE:CD2	2.81	0.55
1:A:144:TYR:CE2	1:A:148:LEU:HD11	2.41	0.55
1:A:331:GLY:HA2	1:A:334:LEU:HD12	1.89	0.55
1:B:180:ASN:HB3	1:B:307:HIS:HA	1.89	0.55
1:C:3:VAL:N	1:C:31:ASP:O	2.29	0.55
1:C:45:THR:OG1	2:C:401:FAD:O1A	2.16	0.55
1:C:297:ARG:NH2	1:C:297:ARG:HB2	2.20	0.55
1:D:152:LEU:HG	1:D:157:VAL:HG21	1.89	0.55
1:A:162:ARG:HG3	1:A:162:ARG:O	2.04	0.55
1:B:199:ARG:HB2	1:B:246:ASN:HB3	1.89	0.55
1:C:79:VAL:HG22	1:C:79:VAL:O	2.06	0.55
1:D:221:ARG:NH2	1:D:221:ARG:HB3	2.21	0.55
1:A:268:PRO:HG2	1:B:80:HIS:HB3	1.89	0.54
1:A:272:ASN:O	1:A:273:ALA:C	2.44	0.54
1:D:255:ASP:O	1:D:259:ILE:HG12	2.07	0.54
1:A:140:GLU:OE1	1:A:233:THR:CB	2.41	0.54
1:C:246:ASN:OD1	1:C:246:ASN:C	2.44	0.54
1:D:209:TRP:HE1	1:D:269:THR:HG1	1.55	0.54
1:A:193:PRO:CD	1:A:194:LEU:H	2.18	0.54
1:A:198:GLY:HA3	1:A:283:ARG:HB2	1.90	0.54
1:C:43:THR:O	1:C:44:THR:C	2.43	0.54
1:C:116:LYS:HD2	1:C:130:TYR:OH	2.06	0.54
1:D:1:MET:CG	1:D:27:LEU:HD11	2.35	0.54
1:C:27:LEU:HD11	1:C:334:LEU:HD21	1.89	0.54
1:D:186:ALA:HB1	1:D:309:TYR:CE2	2.42	0.54
1:D:216:THR:OG1	1:D:226:SER:OG	2.26	0.54
1:C:97:LEU:HD23	1:C:117:LEU:HD12	1.89	0.54
1:C:140:GLU:OE1	1:C:233:THR:CG2	2.56	0.54
1:D:286:ARG:HG2	1:D:287:PRO:HD2	1.90	0.54
1:A:252:ASN:ND2	1:A:255:ASP:H	2.04	0.54
1:C:320:TRP:HA	1:C:320:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:TRP:CG	1:D:317:THR:HG23	2.43	0.54
1:B:205:VAL:CG2	1:B:273:ALA:CB	2.86	0.54
1:B:284:PRO:HG2	1:B:284:PRO:O	2.08	0.54
1:C:155:ARG:HG2	1:C:155:ARG:HH21	1.73	0.54
1:D:52:TRP:O	1:D:53:GLN:HB2	2.08	0.54
1:D:215:LEU:HD23	1:D:215:LEU:N	2.23	0.54
1:B:81:SER:HB2	1:B:82:PRO:CD	2.36	0.53
1:D:122:LEU:HD22	1:D:130:TYR:HA	1.89	0.53
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.43	0.53
1:D:233:THR:HG23	1:D:234:GLN:HG2	1.84	0.53
1:A:178:ILE:O	1:A:305:VAL:HA	2.07	0.53
1:A:67:TRP:O	1:A:71:THR:OG1	2.12	0.53
1:A:267:GLU:O	1:A:270:LEU:HB2	2.08	0.53
1:A:297:ARG:CG	1:A:302:ASN:HD22	2.21	0.53
1:B:79:VAL:HG13	1:B:80:HIS:CD2	2.43	0.53
1:B:83:ASN:O	1:B:86:ASN:HB2	2.07	0.53
1:B:114:PHE:CD1	1:B:114:PHE:C	2.82	0.53
1:A:177:VAL:HG12	1:A:178:ILE:N	2.24	0.53
1:B:22:ARG:HB3	1:B:23:TYR:CD2	2.44	0.53
1:C:114:PHE:CZ	1:C:132:TRP:CG	2.96	0.53
1:D:199:ARG:HH22	1:D:201:GLN:HE21	1.56	0.53
1:A:115:ARG:NH1	1:B:113:GLY:HA3	2.24	0.53
1:B:61:ASN:OD1	1:B:63:GLN:HG2	2.09	0.53
1:B:286:ARG:O	1:B:287:PRO:C	2.46	0.53
1:B:309:TYR:HD1	1:B:310:GLY:N	2.05	0.53
1:C:206:ASP:HB2	1:C:276:ILE:HD11	1.91	0.53
1:D:102:ILE:HG13	1:D:103:PRO:CD	2.39	0.53
1:A:239:GLY:HA2	1:A:259:ILE:HD13	1.90	0.53
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.26	0.53
1:B:58:ASP:N	1:B:58:ASP:OD1	2.42	0.53
1:C:113:GLY:HA3	1:D:115:ARG:NH1	2.22	0.53
1:D:2:ARG:N	1:D:176:ASP:OD1	2.41	0.53
1:D:210:MET:HE3	1:D:210:MET:HA	1.91	0.53
1:B:38:ARG:N	2:B:401:FAD:O2B	2.41	0.53
1:B:66:ASP:O	1:B:69:GLN:HB3	2.09	0.53
1:B:147:TRP:O	1:B:150:GLU:N	2.42	0.53
1:B:47:VAL:HG12	1:B:47:VAL:O	2.09	0.53
1:D:17:LEU:HB2	1:D:152:LEU:CD1	2.39	0.53
1:C:1:MET:HE1	1:C:176:ASP:HB2	1.90	0.53
1:C:48:ALA:HB1	2:C:401:FAD:C4X	2.39	0.53
1:C:199:ARG:HH12	1:C:201:GLN:NE2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:HG2	1:D:289:ILE:HD12	1.90	0.53
1:D:6:ILE:HD12	1:D:164:VAL:HG11	1.90	0.52
1:A:194:LEU:HD22	1:A:287:PRO:HG2	1.92	0.52
1:B:270:LEU:C	1:B:272:ASN:N	2.61	0.52
1:B:316:LEU:O	1:B:319:HIS:HD2	1.91	0.52
1:C:40:THR:O	1:C:40:THR:OG1	2.24	0.52
1:D:9:GLY:HA3	2:D:401:FAD:O1P	2.09	0.52
1:A:116:LYS:HD2	1:A:130:TYR:OH	2.09	0.52
1:B:56:LEU:HD23	1:B:56:LEU:N	2.25	0.52
1:B:170:VAL:HA	1:B:173:GLU:HG2	1.91	0.52
1:C:225:ASN:ND2	1:C:242:PHE:H	2.08	0.52
1:D:152:LEU:HA	1:D:155:ARG:HD2	1.91	0.52
1:A:55:TYR:HE1	1:A:224:TYR:OH	1.92	0.52
1:B:171:ALA:O	1:B:172:ARG:C	2.48	0.52
1:C:107:TRP:O	1:C:109:ASP:N	2.42	0.52
1:C:286:ARG:NH2	1:C:290:ARG:HB2	2.25	0.52
1:A:69:GLN:HE22	1:A:110:THR:CG2	2.21	0.52
1:B:63:GLN:O	1:B:66:ASP:N	2.43	0.52
1:B:328:LYS:O	1:B:329:LEU:C	2.47	0.52
1:A:83:ASN:O	1:A:84:ALA:C	2.48	0.52
1:B:286:ARG:HD3	1:B:288:GLN:O	2.10	0.52
1:B:319:HIS:CG	1:B:320:TRP:N	2.78	0.52
1:C:97:LEU:HD23	1:C:117:LEU:CD1	2.39	0.52
1:C:268:PRO:C	1:C:270:LEU:H	2.13	0.52
1:D:98:PHE:CD1	1:D:217:HIS:HB2	2.45	0.52
1:D:186:ALA:HB3	1:D:195:LEU:CD2	2.39	0.52
1:A:199:ARG:NH1	1:A:201:GLN:NE2	2.57	0.52
1:B:140:GLU:OE1	1:B:233:THR:HB	2.10	0.52
1:C:56:LEU:HD11	1:C:98:PHE:HE1	1.74	0.52
1:C:139:LEU:HD21	1:C:144:TYR:CG	2.44	0.52
1:C:290:ARG:HD2	1:C:292:GLU:OE2	2.10	0.52
1:A:150:GLU:HG3	1:A:151:ARG:NH2	2.25	0.52
1:B:86:ASN:O	1:B:143:ASN:ND2	2.40	0.52
1:B:100:GLU:OE1	1:B:100:GLU:CA	2.43	0.52
1:C:114:PHE:HA	1:C:134:HIS:HB3	1.90	0.52
1:C:208:PRO:HG2	1:D:234:GLN:HE22	1.73	0.52
1:D:91:LEU:HD13	1:D:135:THR:HG21	1.92	0.52
1:A:27:LEU:HB3	1:A:30:LEU:HB2	1.91	0.52
1:B:96:ASN:O	1:B:131:GLY:HA3	2.10	0.52
1:C:316:LEU:HB2	2:C:401:FAD:O2	2.10	0.52
1:A:66:ASP:O	1:A:70:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:HG2	1:A:247:TRP:CE2	2.44	0.51
1:B:313:GLY:O	3:B:402:3LD:N13	2.43	0.51
1:B:93:SER:HA	1:B:135:THR:HA	1.92	0.51
1:D:66:ASP:O	1:D:70:GLN:HG3	2.10	0.51
1:D:68:SER:HB3	1:D:317:THR:HG22	1.91	0.51
1:D:213:PHE:O	1:D:214:ILE:HG13	2.10	0.51
1:D:297:ARG:H	1:D:297:ARG:CD	2.18	0.51
1:A:1:MET:CE	1:A:176:ASP:CB	2.88	0.51
1:B:112:LEU:CD2	1:B:135:THR:O	2.59	0.51
1:C:150:GLU:HG3	1:C:151:ARG:HH12	1.73	0.51
1:D:102:ILE:HG12	1:D:103:PRO:HD2	1.92	0.51
1:D:87:LEU:HD12	1:D:147:TRP:CD1	2.46	0.51
1:D:87:LEU:HD13	1:D:87:LEU:H	1.76	0.51
1:D:153:THR:O	1:D:155:ARG:N	2.44	0.51
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.92	0.51
1:A:221:ARG:O	1:A:225:ASN:HB3	2.10	0.51
1:C:105:PRO:O	1:C:105:PRO:HD2	2.10	0.51
1:D:192:ASP:C	1:D:192:ASP:OD1	2.49	0.51
1:A:167:PHE:CE1	1:A:189:LEU:CD1	2.93	0.51
1:B:75:LEU:O	1:B:89:LEU:HD11	2.10	0.51
1:D:107:TRP:O	1:D:110:THR:N	2.36	0.51
1:D:199:ARG:HH22	1:D:201:GLN:NE2	2.09	0.51
1:B:81:SER:CB	1:B:82:PRO:HD2	2.37	0.51
1:C:252:ASN:HD21	1:C:254:GLN:H	1.59	0.51
1:C:325:GLU:O	1:C:327:ALA:N	2.44	0.51
1:C:201:GLN:HE22	1:C:252:ASN:H	1.59	0.51
1:D:44:THR:O	1:D:45:THR:C	2.47	0.51
1:B:52:TRP:NE1	1:B:317:THR:HG23	2.25	0.51
1:C:133:PHE:CD2	1:C:134:HIS:N	2.78	0.51
1:C:205:VAL:HG12	1:C:236:VAL:HB	1.92	0.51
1:C:243:GLN:NE2	1:C:246:ASN:HD22	2.03	0.51
1:A:114:PHE:HA	1:A:134:HIS:HB3	1.93	0.51
1:B:322:CYS:O	1:B:325:GLU:HB3	2.10	0.51
1:C:266:LEU:O	1:C:266:LEU:HD22	2.10	0.51
1:C:297:ARG:HB2	1:C:297:ARG:CZ	2.40	0.51
1:C:325:GLU:O	1:C:326:ALA:C	2.47	0.51
1:D:122:LEU:CD2	1:D:130:TYR:HA	2.41	0.51
1:A:319:HIS:CG	1:A:320:TRP:N	2.79	0.50
1:B:42:LEU:HD22	1:D:42:LEU:HD22	1.92	0.50
1:C:216:THR:HG1	1:C:226:SER:HG	1.56	0.50
1:D:290:ARG:NH2	1:D:292:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HG2	1:A:23:TYR:CE2	2.47	0.50
1:C:17:LEU:HB2	1:C:152:LEU:CD1	2.42	0.50
1:C:59:PRO:HB2	1:C:61:ASN:H	1.76	0.50
1:C:205:VAL:HG22	1:C:273:ALA:HB1	1.92	0.50
1:A:107:TRP:O	1:A:109:ASP:N	2.44	0.50
1:B:215:LEU:HD23	1:B:228:TYR:HB2	1.93	0.50
1:B:305:VAL:O	1:B:305:VAL:HG12	2.08	0.50
1:C:71:THR:CG2	1:C:317:THR:O	2.59	0.50
1:C:191:ARG:NH1	1:C:193:PRO:CG	2.75	0.50
1:C:209:TRP:CZ3	1:D:85:GLU:HG3	2.46	0.50
1:D:215:LEU:HD13	3:D:402:3LD:C6	2.41	0.50
1:A:59:PRO:HG2	1:A:61:ASN:O	2.11	0.50
1:A:289:ILE:HG12	1:A:311:HIS:HA	1.94	0.50
1:C:201:GLN:NE2	1:C:252:ASN:H	2.10	0.50
1:D:182:THR:HG22	2:D:401:FAD:N7A	2.26	0.50
1:B:40:THR:HG23	1:B:41:PRO:N	2.25	0.50
1:C:104:ASP:HB3	1:C:105:PRO:CD	2.41	0.50
1:B:40:THR:O	1:B:46:ASP:OD2	2.30	0.50
1:B:315:GLY:HA3	2:B:401:FAD:O3'	2.11	0.50
1:C:316:LEU:HB2	2:C:401:FAD:C2	2.41	0.50
1:D:264:CYS:HG	1:D:271:LYS:HD2	1.71	0.50
1:A:1:MET:HE1	1:A:176:ASP:CB	2.41	0.50
1:A:296:LEU:O	1:A:302:ASN:HB3	2.11	0.50
1:C:208:PRO:HB2	1:D:233:THR:O	2.11	0.50
1:B:22:ARG:O	1:B:22:ARG:HD3	2.12	0.49
1:B:252:ASN:HD22	1:B:255:ASP:CG	2.15	0.49
1:C:200:GLY:CA	1:C:283:ARG:HH22	2.25	0.49
1:C:208:PRO:O	1:C:211:LYS:HE2	2.12	0.49
1:A:330:PHE:O	1:A:333:ILE:HB	2.11	0.49
1:B:114:PHE:CZ	1:B:132:TRP:CD1	3.00	0.49
1:C:44:THR:O	1:C:45:THR:C	2.50	0.49
1:D:5:VAL:HB	1:D:34:VAL:HG22	1.94	0.49
1:C:139:LEU:HD21	1:C:144:TYR:CD2	2.47	0.49
1:A:54:PRO:O	1:A:55:TYR:O	2.29	0.49
1:A:297:ARG:HG3	1:A:302:ASN:ND2	2.24	0.49
1:B:52:TRP:HA	1:B:317:THR:OG1	2.12	0.49
1:D:44:THR:C	1:D:46:ASP:N	2.61	0.49
1:C:18:CYS:HB2	1:C:323:ALA:HB1	1.94	0.49
1:D:286:ARG:O	1:D:287:PRO:C	2.49	0.49
1:A:203:MET:HE3	1:A:259:ILE:CG2	2.42	0.49
1:C:210:MET:C	1:C:211:LYS:HD3	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PRO:HB2	1:C:310:GLY:HA2	1.94	0.49
1:A:203:MET:HB3	1:A:238:LEU:HB2	1.94	0.49
1:D:198:GLY:O	1:D:283:ARG:HD2	2.13	0.49
1:D:228:TYR:CE1	3:D:402:3LD:H3	2.47	0.49
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.45	0.49
1:C:274:ARG:HA	1:C:274:ARG:HE	1.77	0.49
1:D:33:LYS:HG2	1:D:160:PHE:CE1	2.48	0.49
1:B:87:LEU:HD11	1:B:147:TRP:CE2	2.47	0.49
1:B:147:TRP:CZ3	1:B:148:LEU:HD23	2.48	0.49
1:D:162:ARG:O	2:D:401:FAD:H2A	2.13	0.49
1:A:79:VAL:HG13	1:A:80:HIS:HB2	1.95	0.48
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.12	0.48
1:D:28:GLN:CB	1:D:29:PRO:HD3	2.31	0.48
1:C:121:GLU:HA	1:C:124:MET:HE2	1.95	0.48
1:C:150:GLU:HG3	1:C:151:ARG:CZ	2.43	0.48
1:A:200:GLY:HA2	1:A:283:ARG:HH22	1.76	0.48
1:B:255:ASP:C	1:B:259:ILE:HG13	2.34	0.48
1:C:117:LEU:HD22	1:C:121:GLU:CB	2.43	0.48
1:A:133:PHE:C	1:A:133:PHE:CD2	2.86	0.48
1:B:52:TRP:CD1	1:B:317:THR:HG23	2.48	0.48
1:B:67:TRP:CH2	1:B:291:LEU:HD23	2.48	0.48
1:B:209:TRP:O	1:B:211:LYS:HG2	2.12	0.48
1:A:112:LEU:HB2	1:A:135:THR:HB	1.95	0.48
1:B:304:GLU:HB3	1:B:333:ILE:HD13	1.95	0.48
1:D:87:LEU:H	1:D:87:LEU:CD1	2.27	0.48
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.37	0.48
1:B:257:ASN:O	1:B:261:GLU:OE1	2.31	0.48
1:D:44:THR:O	1:D:46:ASP:N	2.47	0.48
1:D:75:LEU:HB3	1:D:89:LEU:HD21	1.94	0.48
1:D:114:PHE:HA	1:D:134:HIS:HB3	1.96	0.48
1:A:196:GLN:O	1:A:285:VAL:HB	2.13	0.48
1:A:272:ASN:O	1:A:273:ALA:O	2.31	0.48
1:C:199:ARG:HG3	1:C:282:PHE:CE1	2.49	0.48
1:C:221:ARG:CZ	1:C:221:ARG:CB	2.92	0.48
1:C:253:ILE:HG22	1:C:254:GLN:NE2	2.28	0.48
1:D:112:LEU:CD2	1:D:112:LEU:N	2.76	0.48
1:B:56:LEU:HD11	1:B:217:HIS:ND1	2.28	0.48
1:B:56:LEU:HD11	1:B:217:HIS:CE1	2.49	0.48
1:B:151:ARG:HA	1:B:154:GLU:HG3	1.95	0.48
1:B:183:GLY:O	1:B:184:VAL:C	2.52	0.48
1:C:114:PHE:CE2	1:C:132:TRP:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ARG:HG2	2:C:401:FAD:C8M	2.43	0.48
1:D:79:VAL:HG13	1:D:80:HIS:N	2.29	0.48
1:D:167:PHE:CZ	1:D:189:LEU:HB3	2.49	0.48
1:D:186:ALA:HB3	1:D:195:LEU:HD22	1.94	0.48
1:A:17:LEU:O	1:A:18:CYS:C	2.51	0.48
1:C:54:PRO:HG3	1:C:317:THR:CG2	2.42	0.48
1:D:95:TYR:CZ	1:D:133:PHE:HE1	2.32	0.48
1:A:1:MET:O	1:A:1:MET:HG3	2.13	0.48
1:A:52:TRP:O	1:A:53:GLN:HB2	2.14	0.48
1:A:30:LEU:HG	1:A:30:LEU:O	2.13	0.47
1:B:192:ASP:OD1	1:B:192:ASP:C	2.51	0.47
1:D:30:LEU:C	1:D:30:LEU:HD12	2.35	0.47
1:D:170:VAL:HG11	1:D:178:ILE:HD13	1.94	0.47
1:A:101:ALA:HA	1:A:130:TYR:CE2	2.49	0.47
1:B:39:PHE:C	1:B:41:PRO:CD	2.82	0.47
1:B:290:ARG:HD2	1:B:292:GLU:CD	2.33	0.47
1:C:325:GLU:C	1:C:327:ALA:N	2.65	0.47
1:A:95:TYR:HD1	1:A:214:ILE:HG12	1.79	0.47
1:B:335:GLU:HG2	1:B:336:GLU:H	1.77	0.47
1:A:328:LYS:O	1:A:332:ARG:HG3	2.15	0.47
1:D:200:GLY:HA3	1:D:283:ARG:NH2	2.30	0.47
1:D:286:ARG:NH1	1:D:290:ARG:HD3	2.28	0.47
1:A:160:PHE:CD1	1:A:160:PHE:N	2.82	0.47
1:A:199:ARG:HH12	1:A:201:GLN:HE22	1.62	0.47
1:B:91:LEU:HD23	1:B:137:LEU:CD2	2.43	0.47
1:C:117:LEU:HB2	1:C:131:GLY:O	2.14	0.47
1:A:114:PHE:HA	1:A:134:HIS:CB	2.45	0.47
1:B:335:GLU:HA	1:B:340:SER:CB	2.23	0.47
1:A:63:GLN:O	1:A:64:GLU:C	2.52	0.47
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.46	0.47
1:A:333:ILE:HG22	1:A:334:LEU:N	2.30	0.47
1:B:71:THR:OG1	1:B:318:ILE:O	2.32	0.47
1:B:255:ASP:O	1:B:259:ILE:CG1	2.55	0.47
1:C:208:PRO:HD2	1:C:209:TRP:CZ3	2.50	0.47
1:D:97:LEU:HD11	1:D:125:PHE:CD2	2.49	0.47
1:D:205:VAL:HG13	1:D:273:ALA:HB1	1.95	0.47
1:D:286:ARG:CZ	1:D:290:ARG:HB2	2.45	0.47
1:A:205:VAL:HG23	1:A:275:ILE:HA	1.97	0.47
2:A:401:FAD:O5B	2:A:401:FAD:O1P	2.30	0.47
1:B:87:LEU:CD1	1:B:147:TRP:CE2	2.98	0.47
1:C:178:ILE:CB	1:C:305:VAL:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:CZ	1:C:313:GLY:HA3	2.50	0.47
1:A:42:LEU:CD2	1:C:42:LEU:HD22	2.31	0.47
1:A:197:PRO:HG2	1:A:247:TRP:NE1	2.30	0.47
1:A:278:GLU:C	1:A:279:ARG:HG2	2.35	0.47
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.50	0.47
1:C:266:LEU:O	1:C:266:LEU:HD23	2.15	0.47
1:D:103:PRO:O	1:D:104:ASP:O	2.32	0.47
1:D:107:TRP:O	1:D:109:ASP:N	2.47	0.47
1:A:223:ILE:C	1:A:225:ASN:N	2.66	0.47
1:C:140:GLU:OE1	1:C:233:THR:HG22	2.14	0.47
1:C:171:ALA:O	1:C:172:ARG:C	2.52	0.47
1:C:320:TRP:O	1:C:321:GLY:O	2.33	0.47
1:D:286:ARG:NH1	1:D:290:ARG:HB2	2.30	0.47
1:B:243:GLN:HE21	1:B:243:GLN:HB2	1.27	0.46
1:C:265:ARG:O	1:C:266:LEU:C	2.52	0.46
1:C:265:ARG:O	1:C:267:GLU:N	2.48	0.46
1:D:98:PHE:CE1	1:D:217:HIS:HB2	2.50	0.46
1:A:195:LEU:HB2	1:A:286:ARG:HD2	1.97	0.46
1:B:107:TRP:O	1:B:108:LYS:C	2.51	0.46
1:C:208:PRO:HD2	1:C:209:TRP:CE3	2.50	0.46
1:D:63:GLN:O	1:D:66:ASP:N	2.44	0.46
1:D:264:CYS:HB3	1:D:271:LYS:NZ	2.30	0.46
1:B:59:PRO:HG2	1:B:62:PRO:CA	2.44	0.46
1:B:295:GLN:O	1:B:297:ARG:HD3	2.15	0.46
1:C:180:ASN:HD22	1:C:307:HIS:HD2	1.62	0.46
1:C:327:ALA:O	1:C:330:PHE:HB3	2.15	0.46
1:D:199:ARG:NH1	1:D:255:ASP:OD2	2.48	0.46
1:C:120:ARG:HA	1:C:120:ARG:HE	1.81	0.46
1:C:316:LEU:HD13	1:C:316:LEU:HA	1.44	0.46
1:A:98:PHE:HD2	1:A:131:GLY:HA2	1.79	0.46
1:A:203:MET:HE3	1:A:259:ILE:CB	2.42	0.46
1:C:133:PHE:C	1:C:133:PHE:HD2	2.16	0.46
1:C:168:GLU:HA	1:C:171:ALA:HB3	1.97	0.46
1:C:69:GLN:HG3	1:C:73:ASP:OD2	2.15	0.46
1:C:75:LEU:O	1:C:76:LEU:C	2.54	0.46
1:C:113:GLY:O	1:C:114:PHE:C	2.53	0.46
1:D:10:VAL:HB	1:D:45:THR:HG21	1.98	0.46
1:A:118:THR:HB	1:A:119:PRO:HD2	1.98	0.46
1:A:144:TYR:CD2	1:A:148:LEU:HD11	2.51	0.46
1:A:230:ILE:O	1:A:230:ILE:HG22	2.16	0.46
1:B:241:ILE:HD12	1:B:255:ASP:CB	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PHE:CD1	1:B:243:GLN:N	2.84	0.46
1:C:37:ASP:HB3	1:C:38:ARG:CZ	2.46	0.46
1:C:56:LEU:CD1	1:C:98:PHE:HE1	2.29	0.46
1:C:266:LEU:CD2	1:C:266:LEU:C	2.84	0.46
1:C:289:ILE:HD11	1:C:314:TYR:CE2	2.49	0.46
1:D:40:THR:HG23	1:D:41:PRO:CD	2.46	0.46
1:D:201:GLN:HA	1:D:279:ARG:O	2.16	0.46
1:A:311:HIS:O	1:A:314:TYR:CE1	2.69	0.46
1:B:203:MET:HE1	1:B:256:HIS:CG	2.51	0.46
1:B:270:LEU:O	1:B:272:ASN:N	2.49	0.46
1:B:332:ARG:O	1:B:333:ILE:C	2.52	0.46
1:C:93:SER:OG	1:C:135:THR:HA	2.16	0.46
1:C:205:VAL:CG2	1:C:273:ALA:HB1	2.45	0.46
1:D:144:TYR:CE2	1:D:148:LEU:HD11	2.51	0.46
1:D:291:LEU:O	1:D:292:GLU:HB3	2.16	0.46
1:A:157:VAL:HG12	1:A:158:LYS:N	2.31	0.46
1:C:202:ILE:HD13	1:C:204:LYS:HE2	1.98	0.46
1:D:126:PRO:C	1:D:128:TYR:H	2.19	0.46
1:A:165:GLU:O	1:A:166:SER:HB3	2.16	0.46
1:B:69:GLN:OE1	1:B:110:THR:HG23	2.16	0.46
1:B:121:GLU:O	1:B:124:MET:HG3	2.16	0.46
1:B:284:PRO:O	1:B:312:GLY:N	2.49	0.46
1:C:92:ILE:HG21	1:C:138:ILE:HG13	1.98	0.46
1:D:186:ALA:CB	1:D:309:TYR:CD2	2.99	0.46
1:D:267:GLU:HA	1:D:268:PRO:HD3	1.82	0.46
1:A:208:PRO:HD2	1:A:209:TRP:CE3	2.51	0.45
1:A:218:ASP:HA	1:A:219:PRO:HD2	1.49	0.45
1:B:52:TRP:CE2	1:B:317:THR:HG23	2.51	0.45
1:B:213:PHE:HA	1:B:231:PRO:HD2	1.98	0.45
1:C:79:VAL:HG21	1:C:91:LEU:HD21	1.97	0.45
1:A:70:GLN:O	1:A:71:THR:C	2.55	0.45
1:A:76:LEU:O	1:A:76:LEU:HG	2.15	0.45
1:A:239:GLY:HA2	1:A:259:ILE:HD12	1.97	0.45
1:B:64:GLU:O	1:B:67:TRP:N	2.49	0.45
1:B:144:TYR:CE2	1:B:319:HIS:CE1	3.04	0.45
1:D:224:TYR:CE2	1:D:313:GLY:HA3	2.51	0.45
1:A:328:LYS:HD2	1:A:332:ARG:NH1	2.32	0.45
1:D:284:PRO:HD2	1:D:312:GLY:O	2.17	0.45
1:C:20:HIS:ND1	1:C:155:ARG:NH2	2.64	0.45
1:C:55:TYR:CE1	1:C:314:TYR:HD1	2.35	0.45
1:C:205:VAL:HG13	1:C:273:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:C	1:A:295:GLN:HE21	2.20	0.45
1:B:92:ILE:HG21	1:B:138:ILE:CD1	2.46	0.45
1:B:97:LEU:HB2	1:B:216:THR:HG22	1.98	0.45
1:C:79:VAL:HG21	1:C:91:LEU:CD1	2.38	0.45
1:C:119:PRO:O	1:C:120:ARG:C	2.55	0.45
1:A:1:MET:HE2	1:A:1:MET:CA	2.46	0.45
1:A:93:SER:HA	1:A:135:THR:HA	1.99	0.45
1:C:68:SER:HB3	1:C:317:THR:HG22	1.99	0.45
1:C:217:HIS:CD2	1:C:217:HIS:N	2.84	0.45
1:C:293:ARG:HD3	1:C:333:ILE:HD11	1.99	0.45
1:C:314:TYR:O	1:C:317:THR:N	2.50	0.45
1:B:96:ASN:O	1:B:131:GLY:CA	2.64	0.45
1:C:6:ILE:HA	1:C:35:TYR:O	2.17	0.45
1:C:71:THR:O	1:C:74:TYR:HB3	2.17	0.45
1:D:324:LEU:O	1:D:328:LYS:HE2	2.17	0.45
1:A:61:ASN:OD1	1:A:61:ASN:C	2.54	0.45
1:B:43:THR:O	1:B:46:ASP:HB2	2.16	0.45
1:B:293:ARG:NH2	1:B:333:ILE:HG12	2.32	0.45
1:C:205:VAL:HG12	1:C:205:VAL:O	2.16	0.45
1:D:199:ARG:HG3	1:D:246:ASN:HB3	1.97	0.45
1:A:249:GLU:N	1:A:282:PHE:HZ	2.15	0.45
1:B:118:THR:HB	1:B:119:PRO:CD	2.46	0.45
1:C:13:LEU:HB2	1:C:148:LEU:HD13	1.99	0.45
1:C:128:TYR:N	1:C:128:TYR:CD1	2.83	0.45
1:C:184:VAL:O	1:C:195:LEU:HD21	2.17	0.45
1:C:190:GLN:O	1:C:191:ARG:C	2.55	0.45
1:D:223:ILE:HD12	1:D:224:TYR:N	2.31	0.45
1:A:52:TRP:CE2	1:A:72:PHE:HB2	2.52	0.44
1:A:203:MET:O	1:A:238:LEU:N	2.49	0.44
1:C:13:LEU:O	1:C:16:ALA:N	2.50	0.44
1:C:20:HIS:HD2	1:C:32:ILE:CD1	2.29	0.44
1:C:69:GLN:HE22	1:C:110:THR:CG2	2.13	0.44
1:D:61:ASN:HD21	1:D:63:GLN:HB2	1.82	0.44
1:D:138:ILE:HD12	1:D:231:PRO:O	2.17	0.44
1:A:286:ARG:O	1:A:287:PRO:C	2.55	0.44
1:B:223:ILE:O	1:B:224:TYR:C	2.53	0.44
1:C:114:PHE:CE2	1:C:132:TRP:CG	3.05	0.44
1:C:205:VAL:HG13	1:C:206:ASP:N	2.32	0.44
1:C:215:LEU:HD23	1:C:215:LEU:N	2.31	0.44
1:A:15:THR:O	1:A:16:ALA:C	2.54	0.44
1:A:50:GLY:O	1:A:138:ILE:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:NE2	1:A:244:LEU:HD22	2.32	0.44
1:B:83:ASN:HA	1:B:86:ASN:HD22	1.83	0.44
1:B:87:LEU:HD12	1:B:147:TRP:CD2	2.52	0.44
1:C:13:LEU:HD12	1:C:145:LEU:CD1	2.47	0.44
1:C:52:TRP:CD1	1:C:317:THR:HG23	2.50	0.44
1:D:27:LEU:HD12	1:D:30:LEU:HD22	1.99	0.44
1:D:51:LEU:HA	1:D:51:LEU:HD12	1.55	0.44
1:A:193:PRO:CD	1:A:194:LEU:N	2.81	0.44
1:B:10:VAL:HB	1:B:45:THR:HG21	1.99	0.44
1:B:168:GLU:CD	1:B:168:GLU:H	2.21	0.44
1:C:64:GLU:O	1:C:67:TRP:HB2	2.18	0.44
1:C:79:VAL:C	1:C:80:HIS:HD2	2.20	0.44
1:D:78:HIS:O	1:D:79:VAL:C	2.56	0.44
1:A:46:ASP:OD2	1:A:145:LEU:HD23	2.18	0.44
1:A:151:ARG:O	1:A:155:ARG:HD2	2.18	0.44
2:C:401:FAD:H1'1	2:C:401:FAD:H9	1.72	0.44
1:D:252:ASN:ND2	1:D:254:GLN:HB2	2.32	0.44
1:A:190:GLN:O	1:A:191:ARG:C	2.55	0.44
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.74	0.44
1:A:168:GLU:O	1:A:172:ARG:N	2.50	0.44
1:A:171:ALA:HB1	1:A:303:THR:HG21	1.98	0.44
1:B:108:LYS:HD2	1:B:109:ASP:CG	2.38	0.44
1:C:8:ALA:O	1:C:13:LEU:HD11	2.18	0.44
1:C:107:TRP:C	1:C:109:ASP:H	2.21	0.44
1:D:75:LEU:O	1:D:78:HIS:N	2.43	0.44
1:D:210:MET:HE3	1:D:210:MET:CA	2.48	0.44
1:D:63:GLN:O	1:D:66:ASP:HB2	2.18	0.44
1:A:10:VAL:HG13	1:A:11:ILE:N	2.32	0.44
1:A:28:GLN:HB3	1:A:29:PRO:CD	2.48	0.44
1:A:229:ILE:CD1	1:A:266:LEU:HD13	2.48	0.44
1:A:233:THR:HG22	1:A:234:GLN:H	1.80	0.44
1:B:265:ARG:HE	1:B:265:ARG:HB2	1.28	0.44
1:D:170:VAL:CG1	1:D:178:ILE:CD1	2.95	0.44
1:D:216:THR:OG1	1:D:227:PRO:O	2.33	0.44
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.67	0.43
1:A:121:GLU:HG3	1:B:112:LEU:HB3	2.00	0.43
1:B:177:VAL:HG22	1:B:304:GLU:HB2	2.00	0.43
1:C:213:PHE:HA	1:C:229:ILE:O	2.18	0.43
1:C:226:SER:HA	1:C:227:PRO:HD2	1.80	0.43
1:D:148:LEU:O	1:D:149:THR:C	2.55	0.43
1:D:178:ILE:HB	1:D:305:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HD13	1:A:11:ILE:HA	1.77	0.43
1:A:104:ASP:OD1	1:A:116:LYS:CE	2.65	0.43
1:A:274:ARG:HD2	1:D:274:ARG:HH12	1.83	0.43
1:B:7:GLY:O	1:B:12:GLY:HA3	2.17	0.43
1:B:125:PHE:HA	1:B:126:PRO:HD3	1.65	0.43
1:C:79:VAL:O	1:C:80:HIS:CD2	2.64	0.43
1:D:304:GLU:O	1:D:305:VAL:CG2	2.66	0.43
1:A:52:TRP:O	1:A:53:GLN:CB	2.65	0.43
1:A:138:ILE:CG2	1:A:139:LEU:N	2.77	0.43
1:A:180:ASN:ND2	1:A:307:HIS:HD2	2.14	0.43
1:A:200:GLY:HA3	1:A:283:ARG:NH2	2.32	0.43
1:B:39:PHE:C	1:B:41:PRO:HD3	2.38	0.43
1:B:117:LEU:CD2	1:B:133:PHE:HB2	2.48	0.43
1:C:101:ALA:HA	1:C:130:TYR:CD2	2.53	0.43
1:D:10:VAL:HG13	1:D:11:ILE:HG12	1.99	0.43
1:A:84:ALA:O	1:A:88:GLY:N	2.52	0.43
1:A:144:TYR:OH	1:A:319:HIS:HE1	2.01	0.43
1:D:225:ASN:ND2	1:D:241:ILE:HA	2.34	0.43
1:A:71:THR:HA	1:A:320:TRP:HB3	2.00	0.43
1:A:333:ILE:O	1:A:334:LEU:C	2.54	0.43
1:B:297:ARG:CZ	1:B:297:ARG:HB2	2.48	0.43
1:B:309:TYR:C	1:B:309:TYR:HD1	2.22	0.43
1:C:205:VAL:CG1	1:C:273:ALA:HB1	2.49	0.43
1:C:233:THR:HG23	1:C:234:GLN:N	2.34	0.43
1:C:68:SER:O	1:C:69:GLN:C	2.56	0.43
1:A:153:THR:O	1:A:156:GLY:N	2.46	0.43
1:A:197:PRO:CG	1:A:247:TRP:CE2	3.01	0.43
1:B:198:GLY:H	1:B:285:VAL:CG2	2.32	0.43
1:B:249:GLU:N	1:D:161:GLN:HG3	2.34	0.43
1:A:67:TRP:HA	1:A:70:GLN:OE1	2.19	0.43
1:A:229:ILE:HD12	1:A:266:LEU:HD13	2.01	0.43
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.01	0.43
1:B:203:MET:HE3	1:B:278:GLU:OE1	2.19	0.43
1:C:41:PRO:HG2	1:C:42:LEU:HG	1.99	0.43
1:A:87:LEU:HD11	1:A:147:TRP:CE2	2.54	0.43
1:A:114:PHE:CD1	1:A:114:PHE:C	2.92	0.43
1:A:218:ASP:OD1	1:A:218:ASP:C	2.57	0.43
1:B:309:TYR:CD1	1:B:310:GLY:N	2.85	0.43
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.46	0.43
1:C:178:ILE:CG2	1:C:305:VAL:HG22	2.49	0.43
1:D:17:LEU:CA	1:D:152:LEU:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HG3	1:A:262:GLY:HA3	2.00	0.43
1:A:233:THR:HG23	1:A:234:GLN:HG2	2.01	0.43
1:C:155:ARG:HG2	1:C:155:ARG:NH2	2.34	0.43
1:B:28:GLN:O	1:B:30:LEU:N	2.51	0.42
1:B:80:HIS:O	1:B:81:SER:HB3	2.19	0.42
1:B:144:TYR:OH	1:B:319:HIS:HE1	2.01	0.42
1:D:214:ILE:C	1:D:215:LEU:HD23	2.39	0.42
1:D:293:ARG:HA	1:D:305:VAL:O	2.19	0.42
1:A:120:ARG:HE	1:A:120:ARG:HA	1.84	0.42
1:B:81:SER:CB	1:B:82:PRO:CD	2.97	0.42
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.88	0.42
1:C:139:LEU:HD21	1:C:144:TYR:CD1	2.54	0.42
1:C:225:ASN:OD1	1:C:225:ASN:O	2.36	0.42
1:A:170:VAL:HA	1:A:173:GLU:HG2	2.01	0.42
1:A:228:TYR:CZ	3:A:402:3LD:H3	2.54	0.42
1:C:117:LEU:HD22	1:C:121:GLU:HB3	2.00	0.42
1:D:253:ILE:CG2	1:D:254:GLN:N	2.82	0.42
1:A:67:TRP:HD1	1:A:70:GLN:OE1	2.03	0.42
1:A:214:ILE:HG21	1:A:266:LEU:CD2	2.50	0.42
1:B:228:TYR:OH	3:B:402:3LD:O15	2.23	0.42
1:D:228:TYR:CE2	1:D:240:GLY:N	2.87	0.42
1:A:178:ILE:N	1:A:304:GLU:O	2.49	0.42
1:B:47:VAL:O	1:B:47:VAL:CG1	2.68	0.42
1:B:147:TRP:HE1	1:B:151:ARG:HH21	1.66	0.42
1:B:284:PRO:O	1:B:312:GLY:HA2	2.19	0.42
1:B:325:GLU:OE1	1:B:325:GLU:CA	2.59	0.42
1:C:7:GLY:HA3	1:C:181:CYS:O	2.19	0.42
1:C:150:GLU:O	1:C:154:GLU:CG	2.57	0.42
1:A:104:ASP:OD1	1:A:116:LYS:HE3	2.19	0.42
1:B:335:GLU:CB	1:B:340:SER:HB3	2.47	0.42
1:C:200:GLY:HA3	1:C:283:ARG:NH2	2.34	0.42
1:D:108:LYS:C	1:D:108:LYS:HD2	2.40	0.42
1:A:157:VAL:CG1	1:A:158:LYS:N	2.82	0.42
1:A:327:ALA:O	1:A:330:PHE:HB3	2.20	0.42
1:C:105:PRO:O	1:C:105:PRO:CG	2.67	0.42
1:C:127:ASP:N	1:C:127:ASP:OD1	2.52	0.42
1:B:213:PHE:HA	1:B:231:PRO:CD	2.49	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.71	0.42
1:D:95:TYR:O	1:D:215:LEU:N	2.43	0.42
1:D:206:ASP:HB2	1:D:274:ARG:HB3	2.02	0.42
1:D:323:ALA:C	1:D:325:GLU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLY:O	1:A:185:TRP:N	2.52	0.42
1:A:201:GLN:H	1:A:241:ILE:HG22	1.84	0.42
1:B:98:PHE:CE1	1:B:217:HIS:HB2	2.55	0.42
1:B:278:GLU:O	1:B:279:ARG:HG2	2.20	0.42
1:C:33:LYS:HE2	1:C:35:TYR:HE1	1.85	0.42
1:D:124:MET:HG2	1:D:124:MET:H	1.69	0.42
1:D:291:LEU:HD21	1:D:322:CYS:HA	2.02	0.42
1:A:18:CYS:SG	1:A:324:LEU:HD23	2.60	0.42
1:A:203:MET:SD	1:A:275:ILE:HD13	2.60	0.42
1:A:218:ASP:OD2	1:A:220:GLU:HB2	2.20	0.42
1:D:203:MET:HE3	1:D:259:ILE:CG2	2.50	0.42
1:D:283:ARG:NH1	3:D:402:3LD:O15	2.48	0.42
1:A:40:THR:CG2	1:A:41:PRO:CD	2.90	0.41
1:B:202:ILE:HG22	1:B:239:GLY:HA3	2.02	0.41
1:C:1:MET:CB	1:C:27:LEU:HD22	2.50	0.41
1:C:118:THR:OG1	1:C:121:GLU:HG3	2.20	0.41
1:C:336:GLU:C	1:C:338:LYS:H	2.23	0.41
1:D:17:LEU:O	1:D:17:LEU:HG	2.19	0.41
1:D:41:PRO:HB2	1:D:42:LEU:HD23	2.01	0.41
1:A:151:ARG:HA	1:A:151:ARG:HE	1.85	0.41
1:B:184:VAL:HG12	1:B:185:TRP:CD2	2.55	0.41
1:C:1:MET:HB2	1:C:27:LEU:HD22	2.02	0.41
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.81	0.41
1:C:316:LEU:CB	2:C:401:FAD:O2	2.68	0.41
1:D:10:VAL:HG13	1:D:11:ILE:H	1.86	0.41
1:D:28:GLN:O	1:D:30:LEU:N	2.53	0.41
1:D:60:ASN:OD1	1:D:60:ASN:C	2.58	0.41
1:D:95:TYR:CZ	1:D:133:PHE:CE1	3.08	0.41
1:C:196:GLN:OE1	1:C:244:LEU:HD21	2.20	0.41
1:C:253:ILE:O	1:C:256:HIS:HB3	2.21	0.41
1:D:186:ALA:HB1	1:D:309:TYR:CD2	2.56	0.41
1:B:114:PHE:HA	1:B:134:HIS:HB3	2.02	0.41
1:B:164:VAL:O	1:B:189:LEU:HD21	2.20	0.41
1:C:13:LEU:HD12	1:C:145:LEU:HD12	2.00	0.41
1:D:323:ALA:C	1:D:325:GLU:H	2.22	0.41
1:A:37:ASP:OD2	1:A:38:ARG:CZ	2.69	0.41
1:B:85:GLU:C	1:B:88:GLY:H	2.24	0.41
1:B:105:PRO:HD2	1:B:108:LYS:HB3	2.01	0.41
1:B:270:LEU:C	1:B:272:ASN:H	2.22	0.41
1:C:246:ASN:OD1	1:C:247:TRP:N	2.53	0.41
1:C:268:PRO:C	1:C:270:LEU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:HD2	1:D:288:GLN:O	2.21	0.41
1:A:87:LEU:HB3	1:A:89:LEU:HB2	2.03	0.41
1:A:117:LEU:HB2	1:A:122:LEU:HD11	2.02	0.41
1:A:184:VAL:HG12	1:A:185:TRP:CD2	2.55	0.41
1:D:73:ASP:O	1:D:74:TYR:C	2.59	0.41
1:D:178:ILE:O	1:D:306:ILE:N	2.38	0.41
1:D:201:GLN:NE2	1:D:252:ASN:N	2.57	0.41
1:D:205:VAL:HA	1:D:274:ARG:O	2.21	0.41
1:D:224:TYR:HE1	3:D:402:3LD:C1	2.34	0.41
1:D:283:ARG:HD2	1:D:283:ARG:HH21	1.73	0.41
1:A:200:GLY:HA2	1:A:241:ILE:HG22	2.03	0.41
1:B:108:LYS:HD2	1:B:109:ASP:OD1	2.20	0.41
1:D:10:VAL:HG13	1:D:11:ILE:N	2.35	0.41
1:D:27:LEU:CD2	1:D:339:LEU:HD22	2.51	0.41
1:D:51:LEU:CD1	1:D:138:ILE:HG12	2.50	0.41
1:A:255:ASP:O	1:A:256:HIS:C	2.57	0.41
1:B:221:ARG:NH2	1:B:221:ARG:HB3	2.24	0.41
1:C:271:LYS:HB2	1:C:271:LYS:HE2	1.87	0.41
1:D:33:LYS:HG2	1:D:160:PHE:HE1	1.86	0.41
1:D:51:LEU:HD13	1:D:138:ILE:HG12	2.03	0.41
1:D:172:ARG:C	1:D:174:GLY:N	2.71	0.41
1:B:92:ILE:O	1:B:92:ILE:HG23	2.21	0.41
1:B:199:ARG:NH2	1:B:248:SER:O	2.54	0.41
1:B:242:PHE:HA	1:B:283:ARG:NH2	2.36	0.41
1:B:337:LYS:HB3	1:B:339:LEU:HD22	2.03	0.41
2:B:401:FAD:C4X	3:B:402:3LD:N14	2.84	0.41
1:C:13:LEU:O	1:C:14:SER:C	2.58	0.41
1:C:74:TYR:CD1	1:C:74:TYR:C	2.89	0.41
1:D:52:TRP:CD2	1:D:317:THR:HG23	2.55	0.41
1:D:114:PHE:CD1	1:D:115:ARG:N	2.88	0.41
1:D:275:ILE:C	1:D:276:ILE:HD13	2.41	0.41
1:D:276:ILE:O	1:D:276:ILE:HG22	2.20	0.41
1:B:117:LEU:HD21	1:B:133:PHE:HB2	2.01	0.41
1:B:122:LEU:HD22	1:B:130:TYR:HA	2.01	0.41
1:C:61:ASN:HD21	1:C:63:GLN:CB	2.33	0.41
1:C:87:LEU:HD23	1:C:147:TRP:CG	2.56	0.41
1:C:253:ILE:HD13	1:C:253:ILE:HA	1.85	0.41
1:D:126:PRO:C	1:D:128:TYR:N	2.74	0.41
1:D:255:ASP:O	1:D:259:ILE:CG1	2.68	0.41
1:D:285:VAL:CG1	1:D:286:ARG:N	2.84	0.41
1:A:39:PHE:CE2	1:C:250:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:O	1:A:80:HIS:N	2.54	0.40
1:A:114:PHE:HB2	1:A:134:HIS:CB	2.51	0.40
1:A:123:ASP:C	1:A:125:PHE:H	2.24	0.40
1:A:177:VAL:HG21	1:A:330:PHE:CE1	2.56	0.40
1:B:203:MET:HE2	1:B:256:HIS:ND1	2.32	0.40
1:C:89:LEU:HA	1:C:138:ILE:O	2.21	0.40
1:C:120:ARG:HB3	1:D:112:LEU:HD13	2.02	0.40
1:C:141:GLY:O	1:C:145:LEU:HB2	2.21	0.40
1:A:333:ILE:O	1:A:335:GLU:N	2.55	0.40
1:C:36:ALA:HA	2:C:401:FAD:C2A	2.52	0.40
1:C:283:ARG:HG2	2:C:401:FAD:HM81	2.04	0.40
1:D:84:ALA:C	1:D:86:ASN:N	2.72	0.40
1:D:238:LEU:HD11	1:D:270:LEU:HD21	2.03	0.40
1:D:250:LEU:HD12	1:D:251:ASN:H	1.84	0.40
1:A:143:ASN:C	1:A:145:LEU:N	2.72	0.40
1:B:20:HIS:O	1:B:21:GLU:C	2.60	0.40
1:B:144:TYR:O	1:B:148:LEU:HG	2.21	0.40
1:B:223:ILE:HG13	1:B:224:TYR:N	2.35	0.40
1:B:295:GLN:H	1:B:295:GLN:NE2	2.15	0.40
1:D:3:VAL:O	1:D:32:ILE:HG23	2.22	0.40
1:A:145:LEU:HD12	1:A:145:LEU:HA	1.92	0.40
1:B:39:PHE:O	1:B:41:PRO:N	2.54	0.40
1:B:112:LEU:H	1:B:112:LEU:CD2	2.31	0.40
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.21	0.40
1:D:58:ASP:OD2	1:D:59:PRO:CD	2.67	0.40
1:D:71:THR:HA	1:D:320:TRP:HB3	2.04	0.40
1:D:87:LEU:CD1	1:D:87:LEU:N	2.84	0.40
1:B:107:TRP:C	1:B:109:ASP:H	2.21	0.40
1:B:200:GLY:HA2	1:B:241:ILE:O	2.22	0.40
1:C:36:ALA:HA	2:C:401:FAD:H2A	2.02	0.40
1:C:79:VAL:CG2	1:C:80:HIS:CD2	2.96	0.40
1:C:104:ASP:HB3	1:C:105:PRO:HD2	2.03	0.40
1:C:209:TRP:CE3	1:D:85:GLU:HG3	2.57	0.40
1:D:7:GLY:O	1:D:12:GLY:HA3	2.22	0.40
1:D:39:PHE:O	1:D:41:PRO:HD2	2.22	0.40
1:D:268:PRO:C	1:D:270:LEU:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	279 (82%)	38 (11%)	21 (6%)	1	3
1	B	338/347 (97%)	257 (76%)	63 (19%)	18 (5%)	2	5
1	C	338/347 (97%)	269 (80%)	44 (13%)	25 (7%)	1	2
1	D	338/347 (97%)	259 (77%)	55 (16%)	24 (7%)	1	2
All	All	1352/1388 (97%)	1064 (79%)	200 (15%)	88 (6%)	1	3

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	TYR
1	A	299	GLY
1	B	28	GLN
1	B	40	THR
1	B	108	LYS
1	B	191	ARG
1	B	223	ILE
1	B	337	LYS
1	C	40	THR
1	C	55	TYR
1	C	83	ASN
1	C	101	ALA
1	C	171	ALA
1	C	299	GLY
1	C	300	PRO
1	D	28	GLN
1	D	40	THR
1	D	56	LEU
1	D	79	VAL
1	D	104	ASP
1	D	118	THR

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Mol	Chain	Res	Type
1	D	127	ASP
1	D	199	ARG
1	A	79	VAL
1	A	108	LYS
1	A	184	VAL
1	A	224	TYR
1	A	333	ILE
1	B	87	LEU
1	B	253	ILE
1	C	21	GLU
1	C	84	ALA
1	C	85	GLU
1	C	108	LYS
1	C	127	ASP
1	C	183	GLY
1	C	297	ARG
1	C	315	GLY
1	C	321	GLY
1	D	154	GLU
1	D	173	GLU
1	D	225	ASN
1	D	294	GLU
1	D	299	GLY
1	D	300	PRO
1	A	191	ARG
1	B	225	ASN
1	B	295	GLN
1	C	104	ASP
1	C	105	PRO
1	D	115	ARG
1	D	126	PRO
1	D	220	GLU
1	D	292	GLU
1	D	298	THR
1	A	126	PRO
1	A	172	ARG
1	A	249	GLU
1	A	298	THR
1	A	300	PRO
1	B	99	HIS
1	B	171	ALA
1	B	190	GLN

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Mol	Chain	Res	Type
1	C	126	PRO
1	C	312	GLY
1	D	83	ASN
1	A	28	GLN
1	A	166	SER
1	B	27	LEU
1	B	81	SER
1	B	124	MET
1	B	194	LEU
1	C	53	GLN
1	C	173	GLU
1	C	302	ASN
1	D	53	GLN
1	D	55	TYR
1	D	174	GLY
1	A	53	GLN
1	A	227	PRO
1	B	172	ARG
1	C	172	ARG
1	A	82	PRO
1	A	240	GLY
1	C	29	PRO
1	A	219	PRO
1	D	223	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/299 (98%)	229 (78%)	63 (22%)	1	2
1	B	292/299 (98%)	237 (81%)	55 (19%)	1	3
1	C	292/299 (98%)	221 (76%)	71 (24%)	0	1
1	D	292/299 (98%)	207 (71%)	85 (29%)	0	1
All	All	1168/1196 (98%)	894 (76%)	274 (24%)	1	1

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	ARG
1	A	26	VAL
1	A	28	GLN
1	A	31	ASP
1	A	33	LYS
1	A	37	ASP
1	A	38	ARG
1	A	44	THR
1	A	56	LEU
1	A	63	GLN
1	A	76	LEU
1	A	77	SER
1	A	78	HIS
1	A	80	HIS
1	A	83	ASN
1	A	87	LEU
1	A	89	LEU
1	A	91	LEU
1	A	106	SER
1	A	107	TRP
1	A	108	LYS
1	A	112	LEU
1	A	114	PHE
1	A	115	ARG
1	A	120	ARG
1	A	122	LEU
1	A	127	ASP
1	A	133	PHE
1	A	137	LEU
1	A	151	ARG
1	A	152	LEU
1	A	153	THR
1	A	154	GLU
1	A	155	ARG
1	A	162	ARG
1	A	168	GLU
1	A	170	VAL
1	A	172	ARG
1	A	179	VAL
1	A	184	VAL
1	A	196	GLN

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Mol	Chain	Res	Type
1	A	199	ARG
1	A	203	MET
1	A	205	VAL
1	A	206	ASP
1	A	210	MET
1	A	218	ASP
1	A	221	ARG
1	A	226	SER
1	A	241	ILE
1	A	250	LEU
1	A	253	ILE
1	A	265	ARG
1	A	266	LEU
1	A	271	LYS
1	A	274	ARG
1	A	295	GLN
1	A	298	THR
1	A	301	SER
1	A	302	ASN
1	A	305	VAL
1	A	316	LEU
1	B	22	ARG
1	B	24	HIS
1	B	27	LEU
1	B	28	GLN
1	B	31	ASP
1	B	32	ILE
1	B	37	ASP
1	B	44	THR
1	B	51	LEU
1	B	56	LEU
1	B	58	ASP
1	B	60	ASN
1	B	79	VAL
1	B	83	ASN
1	B	85	GLU
1	B	89	LEU
1	B	91	LEU
1	B	102	ILE
1	B	106	SER
1	B	108	LYS
1	B	110	THR

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Mol	Chain	Res	Type
1	B	112	LEU
1	B	116	LYS
1	B	120	ARG
1	B	122	LEU
1	B	142	LYS
1	B	145	LEU
1	B	150	GLU
1	B	152	LEU
1	B	154	GLU
1	B	160	PHE
1	B	161	GLN
1	B	162	ARG
1	B	172	ARG
1	B	176	ASP
1	B	196	GLN
1	B	221	ARG
1	B	225	ASN
1	B	241	ILE
1	B	250	LEU
1	B	261	GLU
1	B	265	ARG
1	B	266	LEU
1	B	270	LEU
1	B	271	LYS
1	B	286	ARG
1	B	287	PRO
1	B	291	LEU
1	B	295	GLN
1	B	297	ARG
1	B	298	THR
1	B	316	LEU
1	B	335	GLU
1	B	339	LEU
1	B	340	SER
1	C	1	MET
1	C	2	ARG
1	C	13	LEU
1	C	26	VAL
1	C	27	LEU
1	C	28	GLN
1	C	31	ASP
1	C	38	ARG

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Mol	Chain	Res	Type
1	C	58	ASP
1	C	63	GLN
1	C	66	ASP
1	C	68	SER
1	C	71	THR
1	C	85	GLU
1	C	87	LEU
1	C	89	LEU
1	C	91	LEU
1	C	104	ASP
1	C	108	LYS
1	C	110	THR
1	C	112	LEU
1	C	115	ARG
1	C	120	ARG
1	C	122	LEU
1	C	124	MET
1	C	133	PHE
1	C	138	ILE
1	C	142	LYS
1	C	151	ARG
1	C	152	LEU
1	C	154	GLU
1	C	155	ARG
1	C	161	GLN
1	C	162	ARG
1	C	172	ARG
1	C	173	GLU
1	C	176	ASP
1	C	182	THR
1	C	191	ARG
1	C	195	LEU
1	C	196	GLN
1	C	203	MET
1	C	205	VAL
1	C	211	LYS
1	C	218	ASP
1	C	221	ARG
1	C	223	ILE
1	C	238	LEU
1	C	242	PHE
1	C	253	ILE

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Mol	Chain	Res	Type
1	C	258	THR
1	C	259	ILE
1	C	261	GLU
1	C	264	CYS
1	C	265	ARG
1	C	266	LEU
1	C	271	LYS
1	C	274	ARG
1	C	285	VAL
1	C	288	GLN
1	C	290	ARG
1	C	295	GLN
1	C	297	ARG
1	C	298	THR
1	C	301	SER
1	C	302	ASN
1	C	316	LEU
1	C	320	TRP
1	C	328	LYS
1	C	335	GLU
1	C	337	LYS
1	D	6	ILE
1	D	22	ARG
1	D	24	HIS
1	D	25	SER
1	D	26	VAL
1	D	27	LEU
1	D	28	GLN
1	D	30	LEU
1	D	32	ILE
1	D	37	ASP
1	D	40	THR
1	D	44	THR
1	D	56	LEU
1	D	58	ASP
1	D	60	ASN
1	D	68	SER
1	D	76	LEU
1	D	85	GLU
1	D	87	LEU
1	D	91	LEU
1	D	102	ILE

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Mol	Chain	Res	Type
1	D	106	SER
1	D	108	LYS
1	D	112	LEU
1	D	116	LYS
1	D	120	ARG
1	D	130	TYR
1	D	137	LEU
1	D	146	GLN
1	D	151	ARG
1	D	153	THR
1	D	155	ARG
1	D	158	LYS
1	D	161	GLN
1	D	162	ARG
1	D	164	VAL
1	D	170	VAL
1	D	172	ARG
1	D	173	GLU
1	D	176	ASP
1	D	178	ILE
1	D	179	VAL
1	D	182	THR
1	D	189	LEU
1	D	190	GLN
1	D	194	LEU
1	D	195	LEU
1	D	199	ARG
1	D	202	ILE
1	D	204	LYS
1	D	205	VAL
1	D	206	ASP
1	D	211	LYS
1	D	218	ASP
1	D	221	ARG
1	D	223	ILE
1	D	225	ASN
1	D	227	PRO
1	D	230	ILE
1	D	231	PRO
1	D	233	THR
1	D	238	LEU
1	D	241	ILE

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Mol	Chain	Res	Type
1	D	250	LEU
1	D	253	ILE
1	D	261	GLU
1	D	266	LEU
1	D	269	THR
1	D	271	LYS
1	D	275	ILE
1	D	276	ILE
1	D	279	ARG
1	D	286	ARG
1	D	288	GLN
1	D	290	ARG
1	D	291	LEU
1	D	292	GLU
1	D	297	ARG
1	D	302	ASN
1	D	304	GLU
1	D	309	TYR
1	D	316	LEU
1	D	318	ILE
1	D	338	LYS
1	D	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	63	GLN
1	A	69	GLN
1	A	80	HIS
1	A	134	HIS
1	A	161	GLN
1	A	196	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	295	GLN
1	A	302	ASN
1	A	307	HIS
1	A	319	HIS
1	B	24	HIS
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	78	HIS
1	B	80	HIS
1	B	96	ASN
1	B	134	HIS
1	B	201	GLN
1	B	243	GLN
1	B	252	ASN
1	B	272	ASN
1	B	288	GLN
1	B	295	GLN
1	B	307	HIS
1	B	319	HIS
1	C	53	GLN
1	C	61	ASN
1	C	63	GLN
1	C	69	GLN
1	C	80	HIS
1	C	96	ASN
1	C	134	HIS
1	C	190	GLN
1	C	201	GLN
1	C	225	ASN
1	C	243	GLN
1	C	252	ASN
1	C	254	GLN
1	C	302	ASN
1	C	307	HIS
1	C	319	HIS
1	D	24	HIS
1	D	53	GLN
1	D	61	ASN
1	D	63	GLN
1	D	69	GLN
1	D	96	ASN
1	D	99	HIS
1	D	161	GLN
1	D	201	GLN
1	D	225	ASN
1	D	234	GLN
1	D	243	GLN
1	D	252	ASN
1	D	302	ASN

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Mol	Chain	Res	Type
1	D	307	HIS
1	D	319	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	3LD	C	402	-	15,17,17	0.74	0	19,22,22	2.75	7 (36%)
2	FAD	C	401	-	54,58,58	1.53	6 (11%)	71,89,89	2.05	29 (40%)
3	3LD	D	402	-	15,17,17	0.75	0	19,22,22	2.74	7 (36%)
3	3LD	B	402	-	15,17,17	0.65	0	19,22,22	1.77	5 (26%)
2	FAD	B	401	-	54,58,58	1.69	9 (16%)	71,89,89	1.82	20 (28%)
2	FAD	D	401	-	54,58,58	1.85	9 (16%)	71,89,89	1.98	22 (30%)
3	3LD	A	402	-	15,17,17	0.74	0	19,22,22	2.74	7 (36%)
2	FAD	A	401	-	54,58,58	1.60	11 (20%)	71,89,89	2.03	28 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3LD	C	402	-	-	3/5/5/5	0/2/2/2
2	FAD	C	401	-	-	9/30/50/50	0/6/6/6
3	3LD	D	402	-	-	3/5/5/5	0/2/2/2
3	3LD	B	402	-	-	2/5/5/5	0/2/2/2
2	FAD	B	401	-	-	7/30/50/50	0/6/6/6
2	FAD	D	401	-	-	9/30/50/50	0/6/6/6
3	3LD	A	402	-	-	3/5/5/5	0/2/2/2
2	FAD	A	401	-	-	12/30/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	O4B-C1B	5.18	1.47	1.40
2	A	401	FAD	O4B-C1B	4.86	1.47	1.40
2	C	401	FAD	C1'-C2'	4.82	1.59	1.52
2	D	401	FAD	P-O3P	4.67	1.64	1.59
2	C	401	FAD	C9A-N10	-4.57	1.33	1.41
2	B	401	FAD	C9A-N10	-4.49	1.33	1.41
2	D	401	FAD	C9A-N10	-4.39	1.33	1.41
2	D	401	FAD	C10-N1	4.21	1.41	1.33
2	B	401	FAD	P-O3P	3.95	1.63	1.59
2	A	401	FAD	C9A-N10	-3.79	1.34	1.41
2	D	401	FAD	C5X-N5	-3.74	1.32	1.39
2	C	401	FAD	C5X-N5	-3.74	1.32	1.39
2	C	401	FAD	C4-N3	-3.36	1.32	1.38
2	A	401	FAD	C7M-C7	-3.31	1.44	1.51
2	B	401	FAD	O4B-C1B	3.18	1.45	1.40
2	B	401	FAD	C6-C7	-3.16	1.35	1.39
2	A	401	FAD	C2'-C3'	3.11	1.58	1.53
2	B	401	FAD	C5X-N5	-3.07	1.33	1.39
2	A	401	FAD	C10-N10	-3.01	1.30	1.37
2	B	401	FAD	C5'-C4'	2.98	1.55	1.51
2	D	401	FAD	C4A-N3A	-2.95	1.31	1.35
2	D	401	FAD	C4X-C4	2.85	1.55	1.44
2	B	401	FAD	C7M-C7	-2.73	1.45	1.51
2	A	401	FAD	PA-O3P	-2.62	1.56	1.59
2	A	401	FAD	C6-C7	-2.50	1.36	1.39
2	A	401	FAD	C5X-N5	-2.45	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FAD	C9-C9A	-2.31	1.35	1.39
2	A	401	FAD	C4X-C10	-2.25	1.37	1.44
2	D	401	FAD	C1B-N9A	-2.23	1.44	1.49
2	A	401	FAD	C8-C7	-2.14	1.35	1.40
2	C	401	FAD	O4B-C1B	2.11	1.43	1.40
2	C	401	FAD	C10-N10	-2.06	1.32	1.37
2	D	401	FAD	C5'-C4'	2.04	1.54	1.51
2	B	401	FAD	C9A-C5X	-2.02	1.38	1.41
2	A	401	FAD	C10-N1	2.00	1.37	1.33

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	3LD	C7-C8-N14	7.97	126.12	119.54
3	A	402	3LD	C7-C8-N14	7.92	126.08	119.54
3	D	402	3LD	C7-C8-N14	7.84	126.02	119.54
2	B	401	FAD	O3'-C3'-C4'	-4.92	97.75	108.93
2	D	401	FAD	C4B-O4B-C1B	-4.85	105.48	109.92
2	D	401	FAD	C8M-C8-C7	-4.84	110.88	120.76
2	A	401	FAD	C5X-N5-C4X	-4.80	110.32	118.09
2	A	401	FAD	C1'-N10-C9A	4.75	129.87	120.63
2	B	401	FAD	C4B-O4B-C1B	-4.67	105.65	109.92
2	C	401	FAD	O3'-C3'-C2'	-4.62	98.42	108.93
2	A	401	FAD	C5A-C6A-N6A	4.59	127.30	120.31
3	B	402	3LD	C7-C8-N14	4.50	123.26	119.54
2	D	401	FAD	O3'-C3'-C4'	-4.46	98.81	108.93
3	D	402	3LD	C10-N13-N14	-4.23	110.61	117.33
3	A	402	3LD	C10-N13-N14	-4.21	110.64	117.33
3	C	402	3LD	C10-N13-N14	-4.19	110.67	117.33
2	C	401	FAD	C5X-C9A-N10	4.15	121.72	117.97
2	C	401	FAD	O3'-C3'-C4'	-4.15	99.50	108.93
2	C	401	FAD	O4B-C1B-N9A	4.15	114.25	108.75
2	A	401	FAD	O3B-C3B-C4B	-3.98	99.64	111.08
2	A	401	FAD	C4'-C3'-C2'	3.94	120.13	113.57
2	C	401	FAD	O4'-C4'-C5'	-3.90	101.38	109.99
3	C	402	3LD	C2-C4-C6	-3.89	115.14	120.61
3	D	402	3LD	C2-C4-C6	-3.89	115.14	120.61
3	A	402	3LD	C2-C4-C6	-3.84	115.22	120.61
2	D	401	FAD	C7M-C7-C6	3.75	126.19	119.57
2	C	401	FAD	C5X-N5-C4X	-3.73	112.05	118.09
2	D	401	FAD	O3P-PA-O1A	-3.69	99.60	110.70
2	D	401	FAD	C7M-C7-C8	-3.64	113.32	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FAD	O4'-C4'-C5'	3.62	117.97	109.99
3	D	402	3LD	C12-C8-N14	-3.58	110.53	115.55
3	A	402	3LD	C12-C8-N14	-3.55	110.58	115.55
3	C	402	3LD	C12-C8-N14	-3.51	110.63	115.55
2	D	401	FAD	O2P-P-O5'	-3.43	92.02	107.57
2	D	401	FAD	O2A-PA-O3P	3.36	116.35	107.27
2	A	401	FAD	C8M-C8-C7	-3.35	113.93	120.76
2	C	401	FAD	C7M-C7-C6	-3.33	113.70	119.57
2	C	401	FAD	C5A-C6A-N6A	3.32	125.38	120.31
2	C	401	FAD	C7M-C7-C8	3.30	127.49	120.76
2	B	401	FAD	C4'-C3'-C2'	-3.28	108.11	113.57
2	C	401	FAD	C4-C4X-N5	-3.26	113.71	118.21
2	B	401	FAD	C4X-C10-N10	3.20	121.06	116.48
3	B	402	3LD	C10-N13-N14	-3.18	112.27	117.33
2	C	401	FAD	C8M-C8-C9	-3.16	114.01	119.57
2	C	401	FAD	C4B-O4B-C1B	-3.15	107.04	109.92
2	D	401	FAD	C9-C8-C7	3.13	124.29	119.69
2	B	401	FAD	C9-C8-C7	3.13	124.29	119.69
2	A	401	FAD	O2'-C2'-C3'	-3.10	101.99	109.25
3	A	402	3LD	C1-C3-C5	-3.09	116.43	120.24
2	A	401	FAD	C4X-C10-N10	3.05	120.85	116.48
3	D	402	3LD	C1-C3-C5	-3.05	116.48	120.24
3	C	402	3LD	C1-C3-C5	-3.04	116.48	120.24
2	D	401	FAD	C9-C9A-N10	-3.04	117.76	121.85
2	B	401	FAD	O4B-C1B-N9A	-3.04	104.71	108.75
2	C	401	FAD	C1B-N9A-C4A	-3.03	121.31	126.64
2	D	401	FAD	C8M-C8-C9	2.99	124.83	119.57
2	C	401	FAD	C8M-C8-C7	2.96	126.80	120.76
2	C	401	FAD	C9A-N10-C10	-2.95	116.25	120.75
2	B	401	FAD	O2A-PA-O3P	2.90	115.11	107.27
2	D	401	FAD	C4X-C10-N10	2.83	120.53	116.48
2	B	401	FAD	C1'-N10-C9A	2.80	126.08	120.63
2	A	401	FAD	N3-C2-N1	-2.80	113.56	119.50
2	A	401	FAD	C2B-C3B-C4B	2.76	107.95	102.61
2	A	401	FAD	C1'-C2'-C3'	2.70	116.98	109.66
2	A	401	FAD	C10-N1-C2	2.68	122.66	116.85
2	D	401	FAD	N3A-C2A-N1A	2.68	132.32	128.67
2	B	401	FAD	O5B-C5B-C4B	2.68	118.12	108.99
2	A	401	FAD	O3P-P-O1P	-2.65	102.72	110.70
2	C	401	FAD	N6A-C6A-N1A	-2.63	112.72	118.33
2	B	401	FAD	C10-N1-C2	2.62	122.53	116.85
2	A	401	FAD	PA-O5B-C5B	-2.60	106.44	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	3LD	C5-C6-C4	2.60	122.10	118.23
2	A	401	FAD	N6A-C6A-N1A	-2.60	112.79	118.33
3	A	402	3LD	C5-C6-C4	2.59	122.08	118.23
3	D	402	3LD	C1-C2-C4	2.58	123.42	120.24
2	B	401	FAD	O2P-P-O5'	-2.58	95.87	107.57
3	D	402	3LD	C5-C6-C4	2.57	122.05	118.23
2	A	401	FAD	O4-C4-C4X	-2.57	119.76	126.53
2	A	401	FAD	O2-C2-N3	2.56	123.49	118.58
3	B	402	3LD	C1-C2-C4	-2.54	117.10	120.24
3	A	402	3LD	C1-C2-C4	2.53	123.36	120.24
2	A	401	FAD	C9A-N10-C10	-2.53	116.89	120.75
3	C	402	3LD	C1-C2-C4	2.53	123.36	120.24
2	D	401	FAD	C9A-C9-C8	-2.52	114.16	119.22
2	D	401	FAD	O5'-P-O1P	2.50	118.83	108.94
2	C	401	FAD	C4X-C10-N10	2.49	120.05	116.48
2	A	401	FAD	O2'-C2'-C1'	-2.44	100.19	110.20
2	A	401	FAD	O2A-PA-O3P	2.43	113.84	107.27
2	D	401	FAD	C6-C5X-N5	-2.41	114.45	118.44
2	A	401	FAD	C7M-C7-C6	2.41	123.81	119.57
2	D	401	FAD	O2P-P-O1P	2.37	123.47	112.44
3	B	402	3LD	C3-C5-C6	-2.36	117.29	120.61
2	A	401	FAD	C5X-C9A-N10	2.35	120.10	117.97
2	C	401	FAD	C9-C9A-N10	-2.33	118.72	121.85
2	A	401	FAD	C9A-C5X-N5	2.33	124.93	122.45
2	A	401	FAD	C5B-C4B-C3B	-2.30	106.94	115.21
2	C	401	FAD	C1'-C2'-C3'	2.28	115.85	109.66
2	B	401	FAD	C4A-C5A-N7A	2.27	111.73	109.34
2	C	401	FAD	O5B-C5B-C4B	2.26	116.68	108.99
2	D	401	FAD	C1'-C2'-C3'	2.24	115.73	109.66
2	D	401	FAD	C1B-N9A-C4A	-2.23	122.72	126.64
2	D	401	FAD	C5X-C6-C7	-2.20	116.74	120.83
2	D	401	FAD	O4B-C1B-N9A	-2.20	105.83	108.75
2	C	401	FAD	C10-N1-C2	2.20	121.61	116.85
2	C	401	FAD	O5'-P-O1P	2.18	117.58	108.94
2	C	401	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	C	401	FAD	C5'-C4'-C3'	2.17	116.31	112.22
2	A	401	FAD	O4-C4-N3	2.15	124.17	120.11
2	C	401	FAD	C4-C4X-C10	2.15	120.62	116.93
2	B	401	FAD	O3B-C3B-C4B	-2.13	104.97	111.08
2	C	401	FAD	O2P-P-O3P	-2.13	101.52	107.27
2	C	401	FAD	O2A-PA-O1A	2.12	122.33	112.44
2	B	401	FAD	O2P-P-O1P	2.11	122.27	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FAD	PA-O5B-C5B	-2.11	109.27	121.35
2	A	401	FAD	C8M-C8-C9	2.11	123.29	119.57
2	B	401	FAD	C4-N3-C2	2.11	129.39	125.64
2	A	401	FAD	C9-C8-C7	2.11	122.78	119.69
2	B	401	FAD	C1'-C2'-C3'	2.10	115.35	109.66
2	D	401	FAD	C4X-C10-N1	-2.08	119.48	124.59
2	B	401	FAD	PA-O5B-C5B	-2.08	109.42	121.35
2	B	401	FAD	O2-C2-N3	2.07	122.56	118.58
3	B	402	3LD	C7-C9-C10	2.07	120.53	116.31
2	B	401	FAD	N3A-C2A-N1A	2.05	131.46	128.67
2	A	401	FAD	C1B-N9A-C4A	-2.05	123.03	126.64
2	C	401	FAD	O2'-C2'-C1'	2.03	118.55	110.20

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5B-O5B-PA-O1A
2	A	401	FAD	C5B-O5B-PA-O2A
2	A	401	FAD	C5B-O5B-PA-O3P
2	A	401	FAD	P-O3P-PA-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	C3B-C4B-C5B-O5B
2	A	401	FAD	C5'-O5'-P-O2P
2	A	401	FAD	C5'-O5'-P-O3P
2	B	401	FAD	C5B-O5B-PA-O2A
2	B	401	FAD	C5B-O5B-PA-O3P
2	C	401	FAD	C5B-O5B-PA-O3P
2	C	401	FAD	P-O3P-PA-O5B
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	C5B-O5B-PA-O2A
2	D	401	FAD	C5B-O5B-PA-O3P
2	D	401	FAD	C5'-O5'-P-O3P
3	A	402	3LD	C11-C12-C8-N14
3	C	402	3LD	C11-C12-C8-N14
3	D	402	3LD	C11-C12-C8-N14
2	C	401	FAD	C3B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O3'-C3'-C4'-C5'
2	A	401	FAD	O2'-C2'-C3'-O3'
2	B	401	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	O3'-C3'-C4'-O4'
3	A	402	3LD	C11-C12-C8-C7
3	B	402	3LD	C11-C12-C8-C7
3	C	402	3LD	C11-C12-C8-C7
3	D	402	3LD	C11-C12-C8-C7
2	D	401	FAD	P-O3P-PA-O5B
2	C	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	C5B-O5B-PA-O1A
2	C	401	FAD	C5B-O5B-PA-O1A
2	C	401	FAD	C5'-O5'-P-O3P
3	A	402	3LD	C6-C11-C12-C8
3	C	402	3LD	C6-C11-C12-C8
3	D	402	3LD	C6-C11-C12-C8
2	C	401	FAD	O3'-C3'-C4'-O4'
2	B	401	FAD	C2'-C3'-C4'-O4'
3	B	402	3LD	C11-C12-C8-N14
2	D	401	FAD	C3'-C4'-C5'-O5'
2	D	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	O2'-C2'-C3'-C4'
2	A	401	FAD	PA-O3P-P-O2P

There are no ring outliers.

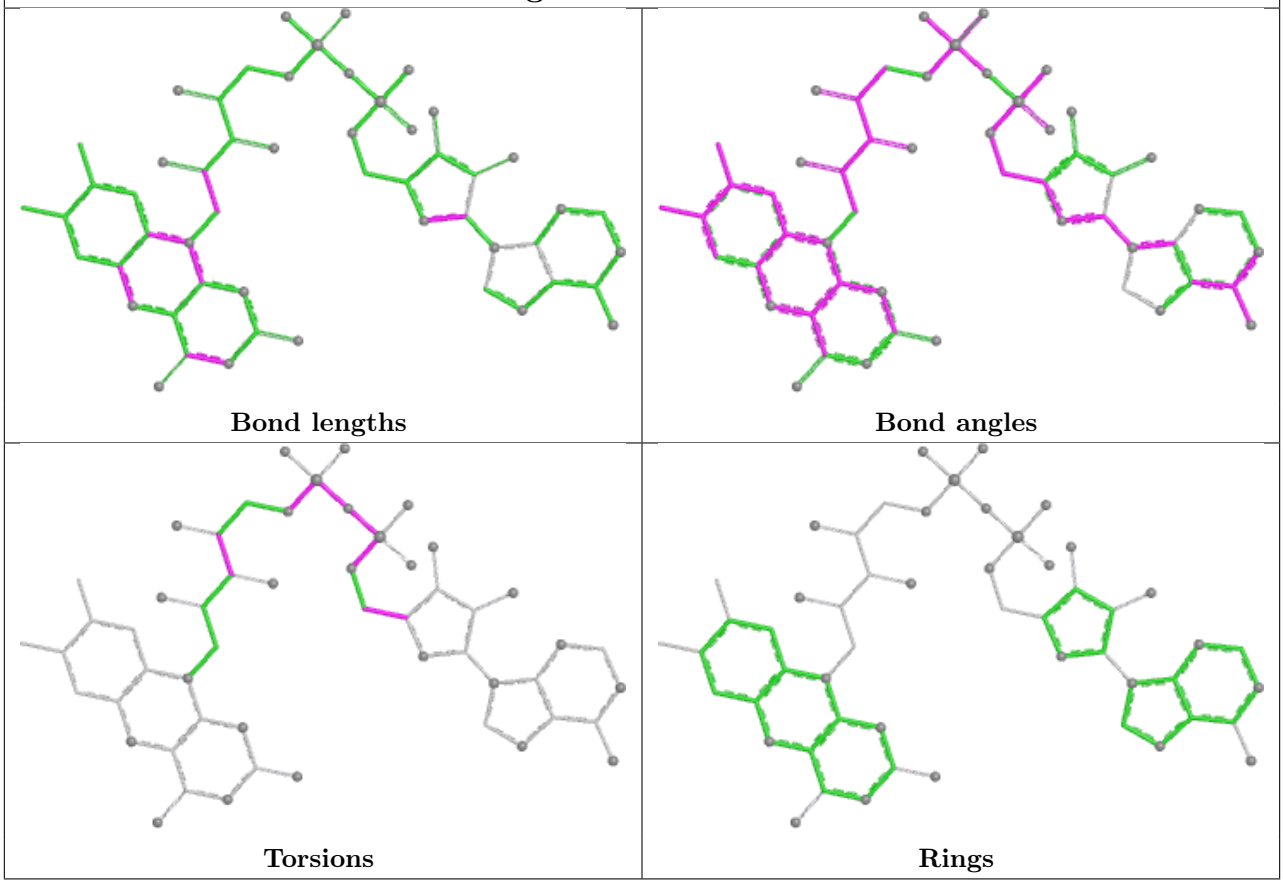
8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	3LD	4	0
2	C	401	FAD	17	0
3	D	402	3LD	5	0
3	B	402	3LD	5	0
2	B	401	FAD	4	0
2	D	401	FAD	5	0
3	A	402	3LD	2	0
2	A	401	FAD	4	0

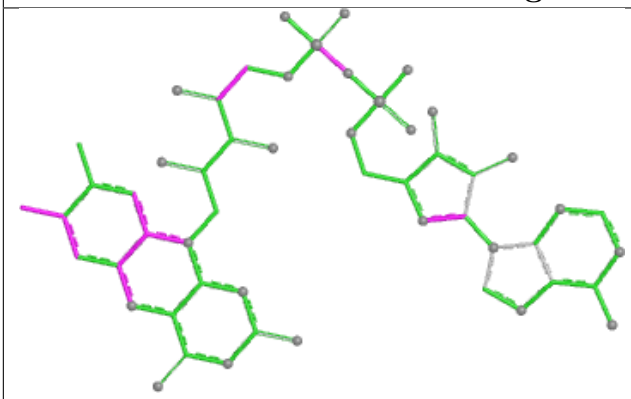
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

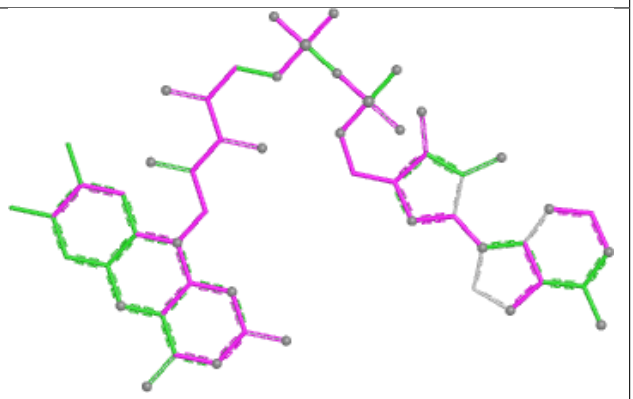
Ligand FAD C 401



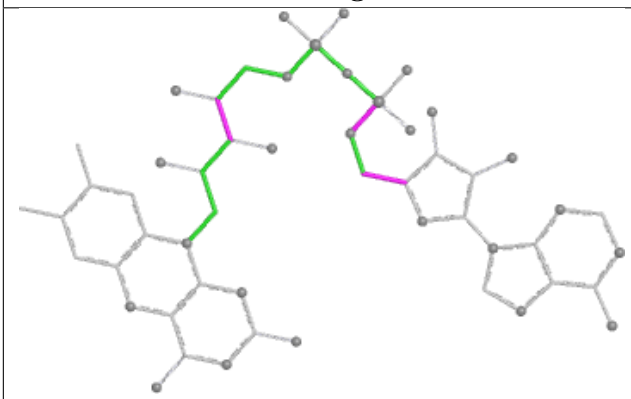
Ligand FAD B 401



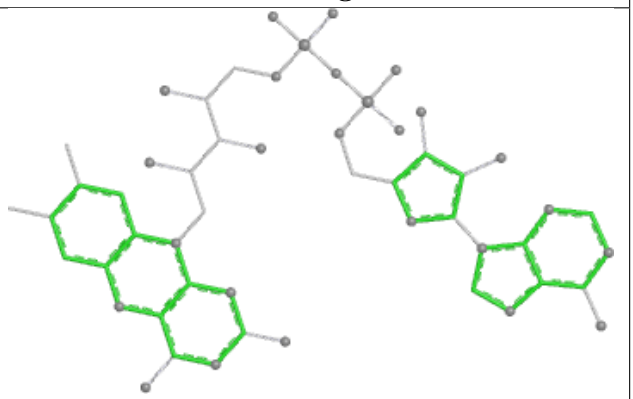
Bond lengths



Bond angles

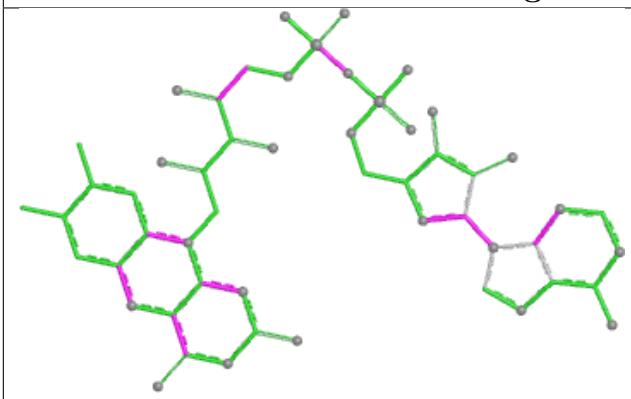


Torsions

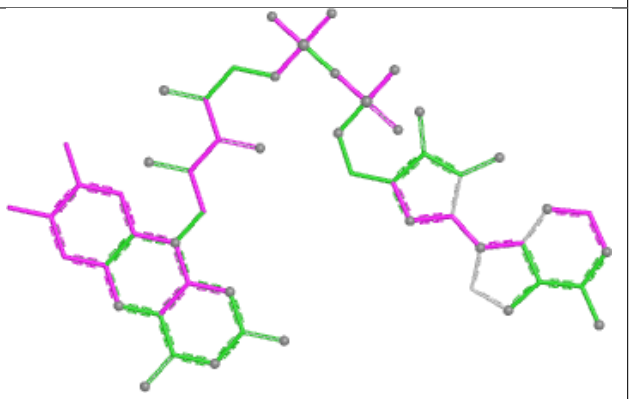


Rings

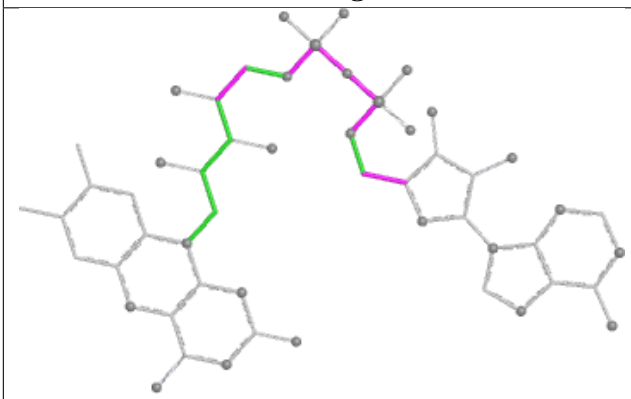
Ligand FAD D 401



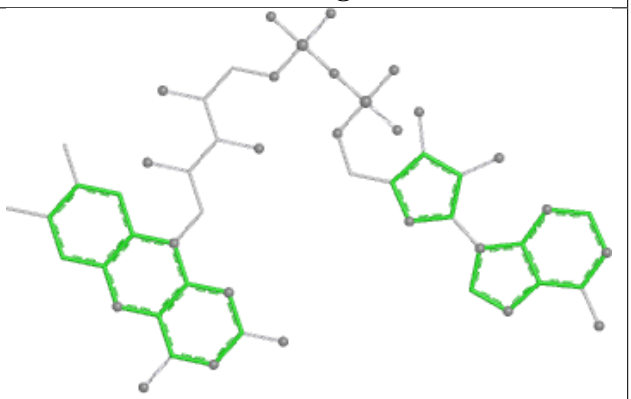
Bond lengths



Bond angles

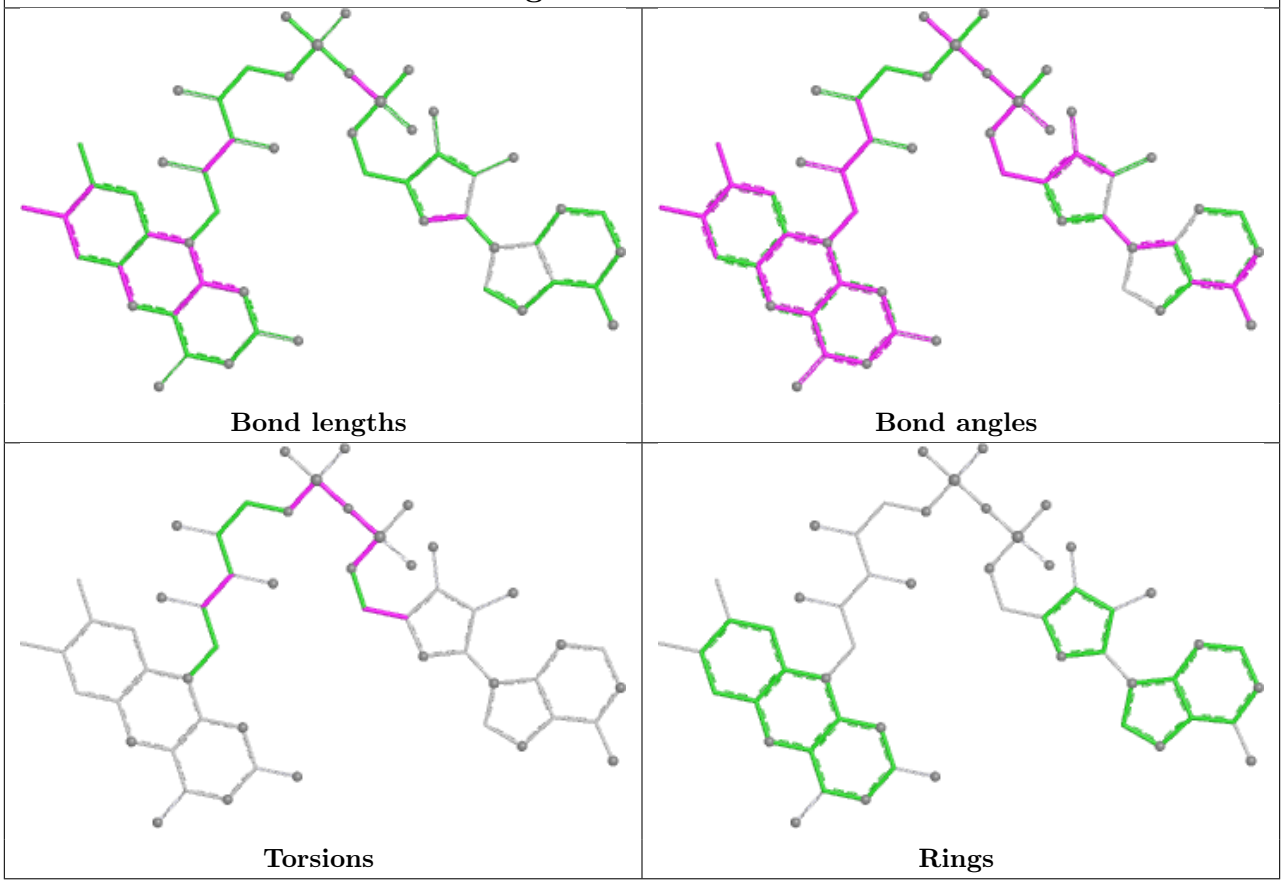


Torsions



Rings

Ligand FAD A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	223:ILE	C	224:TYR	N	1.69

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	340/347 (97%)	-0.22	4 (1%)	79	78	18, 41, 65, 75	0
1	B	340/347 (97%)	-0.16	4 (1%)	79	78	20, 40, 64, 77	0
1	C	340/347 (97%)	0.07	12 (3%)	44	38	27, 48, 74, 93	0
1	D	340/347 (97%)	0.04	15 (4%)	34	29	27, 49, 75, 90	0
All	All	1360/1388 (97%)	-0.07	35 (2%)	56	52	18, 44, 69, 93	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	340	SER	5.7
1	C	339	LEU	4.9
1	C	300	PRO	4.7
1	A	340	SER	4.3
1	D	300	PRO	4.2
1	D	339	LEU	4.1
1	D	299	GLY	3.8
1	D	340	SER	3.5
1	C	298	THR	3.4
1	D	301	SER	3.3
1	A	57	SER	3.1
1	B	339	LEU	3.1
1	D	224	TYR	3.0
1	C	299	GLY	2.9
1	B	59	PRO	2.8
1	C	334	LEU	2.7
1	D	298	THR	2.7
1	A	339	LEU	2.7
1	B	340	SER	2.6
1	D	194	LEU	2.6
1	D	82	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	297	ARG	2.6
1	D	338	LYS	2.5
1	D	302	ASN	2.5
1	B	58	ASP	2.4
1	C	60	ASN	2.3
1	C	297	ARG	2.3
1	D	193	PRO	2.2
1	D	337	LYS	2.2
1	C	301	SER	2.1
1	D	334	LEU	2.1
1	A	99	HIS	2.1
1	C	57	SER	2.1
1	C	126	PRO	2.1
1	C	56	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

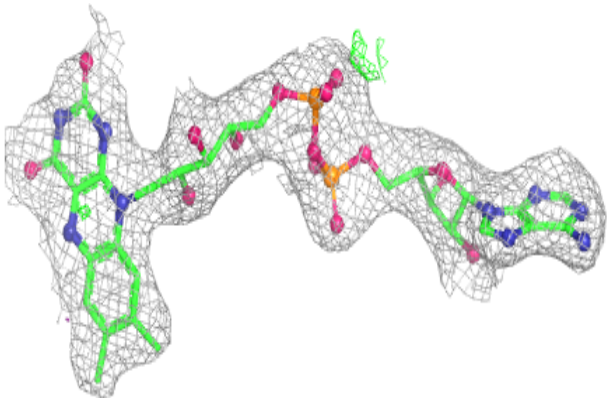
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

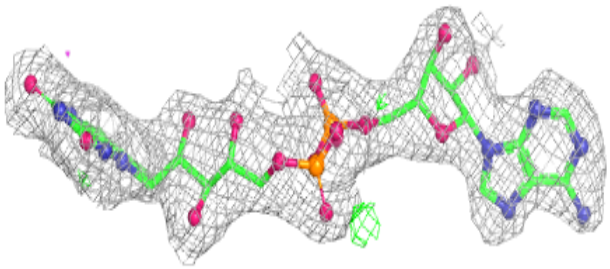
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	3LD	C	402	16/16	0.91	0.20	27,32,47,49	0
3	3LD	D	402	16/16	0.91	0.24	27,32,47,49	0
3	3LD	B	402	16/16	0.92	0.19	32,41,44,44	0
3	3LD	A	402	16/16	0.95	0.19	27,32,47,49	0
2	FAD	C	401	53/53	0.96	0.17	22,30,37,44	0
2	FAD	D	401	53/53	0.96	0.15	20,36,44,47	0
2	FAD	A	401	53/53	0.96	0.16	19,29,38,41	0
2	FAD	B	401	53/53	0.97	0.17	10,30,36,37	0

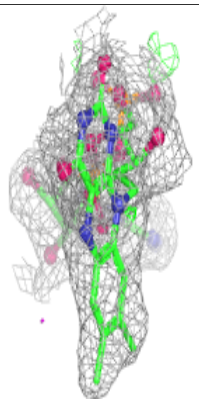
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 401:

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

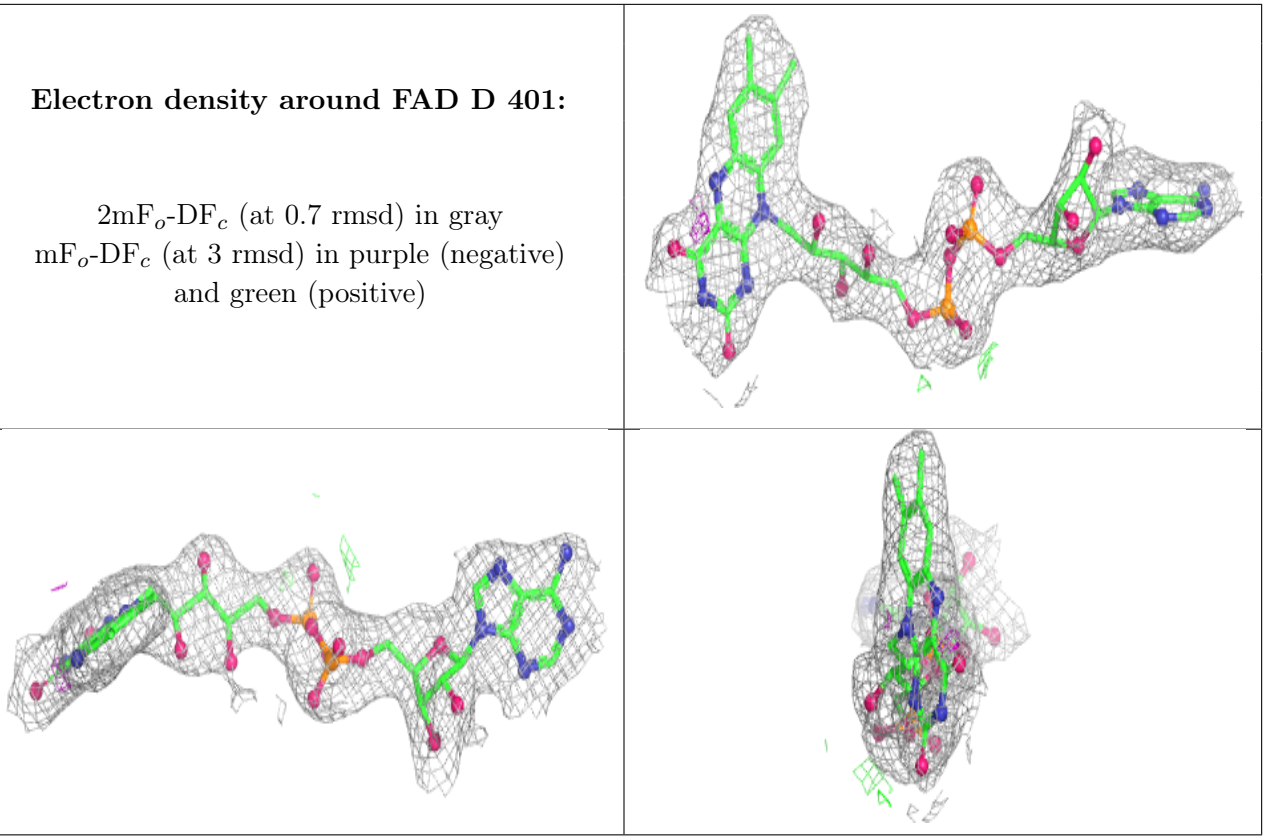






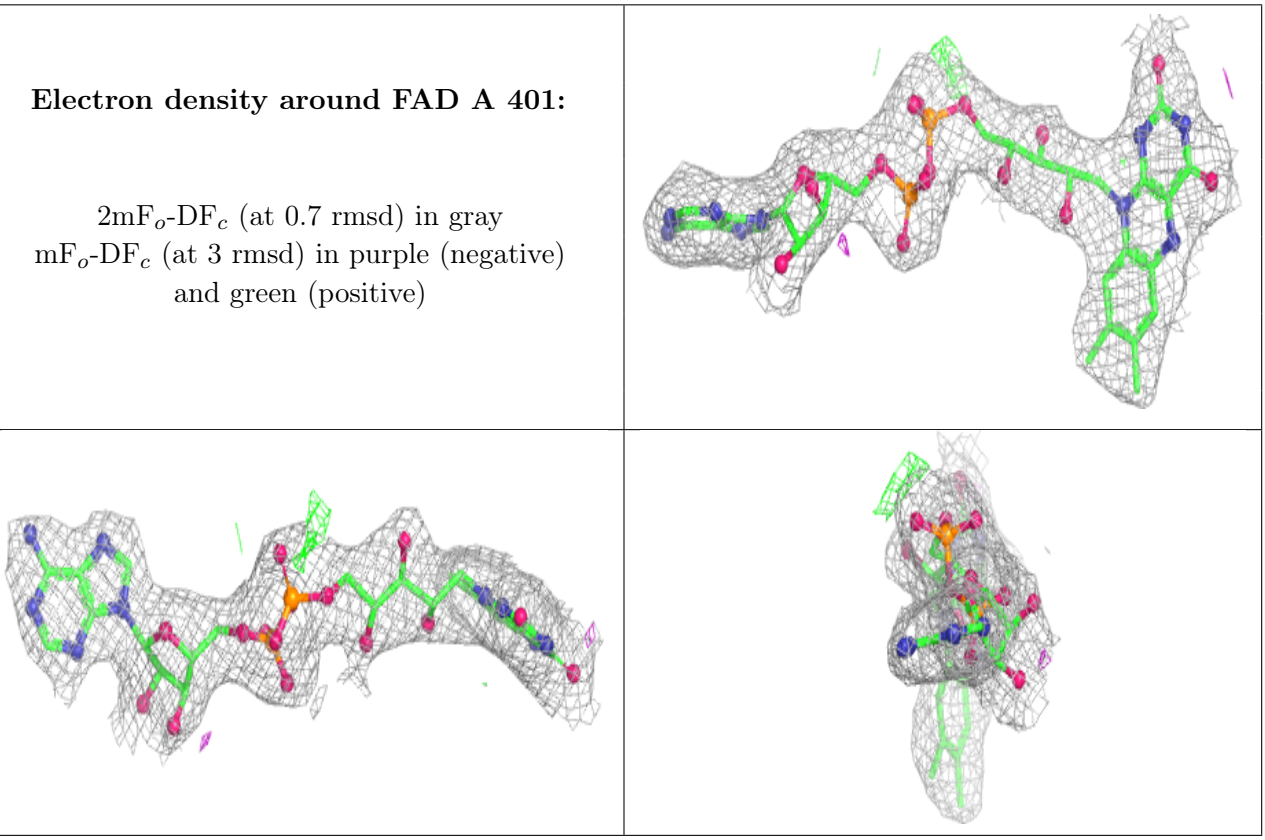
Electron density around FAD D 401:

$2mF_o$-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 401:

$2mF_o$-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 401:

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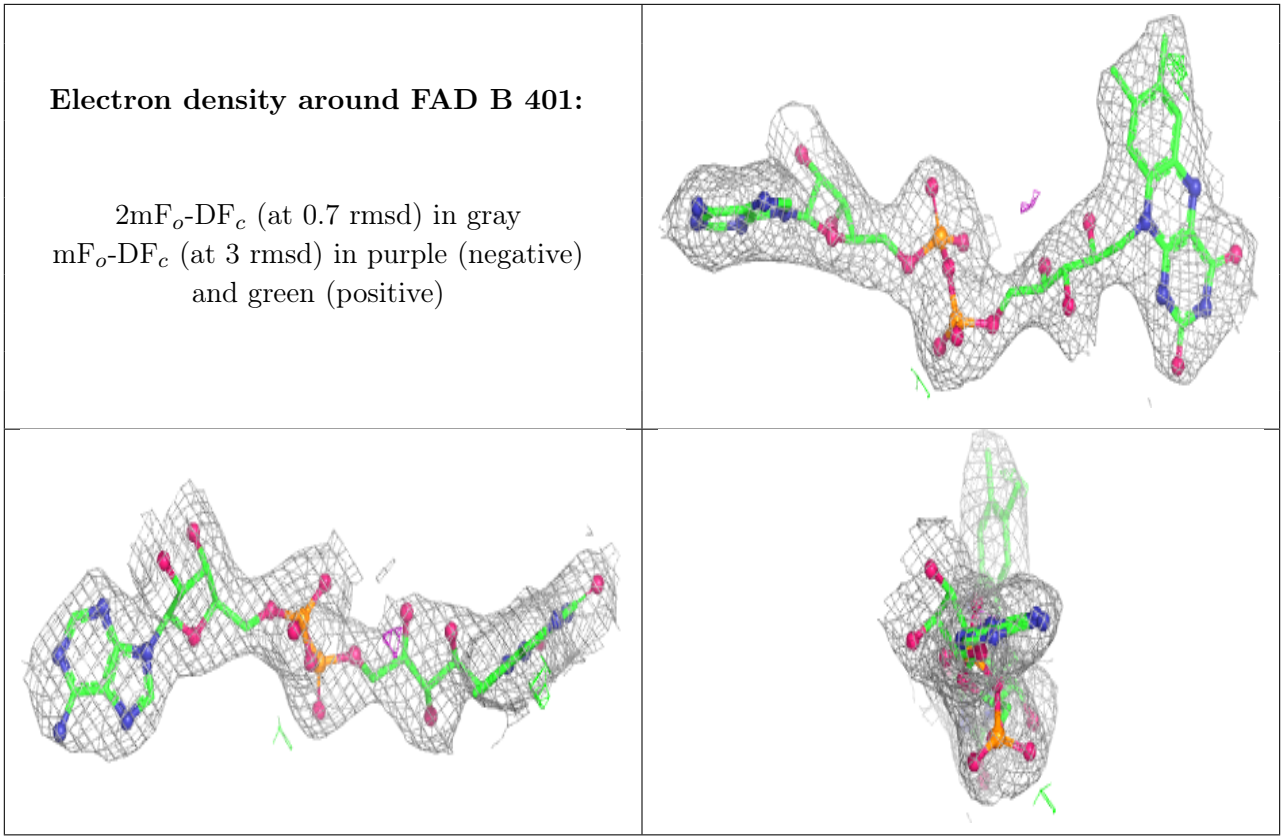
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.