Full wwPDB X-ray Structure Validation Report (i)

Nov 12, 2024 – 04:22 PM EST

PDB ID	:	3T59
Title	:	C76A/C455S mutant of mouse QSOX1 containing an interdomain disulfide
Authors	:	Fass, D.; Alon, A.; Gat, Y.
Deposited on	:	2011-07-27
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

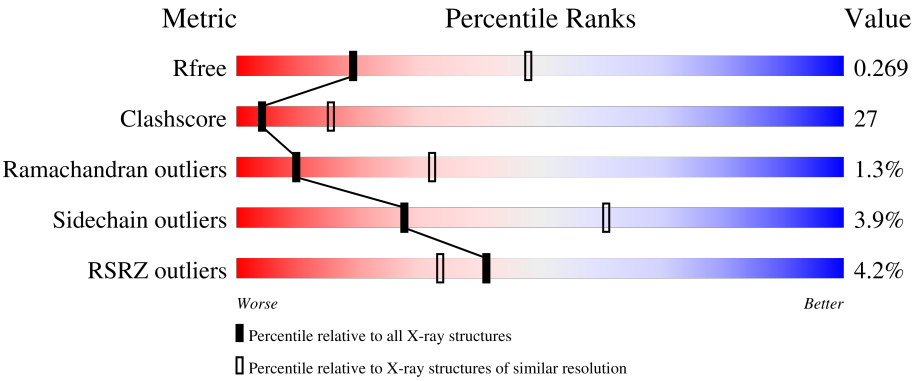
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	519	56% 38%
1	B	519	55% 40%
1	C	519	57% 35%
1	D	519	12% 45% 47%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16478 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 Sulfhydryl oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3979	2551	693	720	15			
1	B	504	Total	C	N	O	S	0	0	0
			4003	2566	697	725	15			
1	C	500	Total	C	N	O	S	0	0	0
			3972	2547	692	718	15			
1	D	498	Total	C	N	O	S	0	0	0
			3959	2539	690	715	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	expression tag	UNP Q8BND5
A	33	SER	-	expression tag	UNP Q8BND5
A	34	HIS	-	expression tag	UNP Q8BND5
A	35	MET	-	expression tag	UNP Q8BND5
A	76	ALA	CYS	engineered mutation	UNP Q8BND5
A	455	SER	CYS	engineered mutation	UNP Q8BND5
B	32	GLY	-	expression tag	UNP Q8BND5
B	33	SER	-	expression tag	UNP Q8BND5
B	34	HIS	-	expression tag	UNP Q8BND5
B	35	MET	-	expression tag	UNP Q8BND5
B	76	ALA	CYS	engineered mutation	UNP Q8BND5
B	455	SER	CYS	engineered mutation	UNP Q8BND5
C	32	GLY	-	expression tag	UNP Q8BND5
C	33	SER	-	expression tag	UNP Q8BND5
C	34	HIS	-	expression tag	UNP Q8BND5
C	35	MET	-	expression tag	UNP Q8BND5
C	76	ALA	CYS	engineered mutation	UNP Q8BND5
C	455	SER	CYS	engineered mutation	UNP Q8BND5
D	32	GLY	-	expression tag	UNP Q8BND5
D	33	SER	-	expression tag	UNP Q8BND5
D	34	HIS	-	expression tag	UNP Q8BND5

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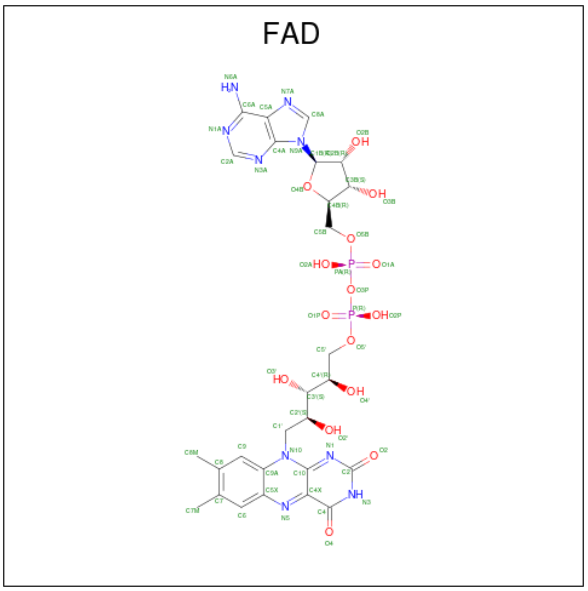
Chain	Residue	Modelled	Actual	Comment	Reference
D	35	MET	-	expression tag	UNP Q8BND5
D	76	ALA	CYS	engineered mutation	UNP Q8BND5
D	455	SER	CYS	engineered mutation	UNP Q8BND5

- 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		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	95	Total	O	0	0
			95	95		
3	C	93	Total	O	0	0
			93	93		

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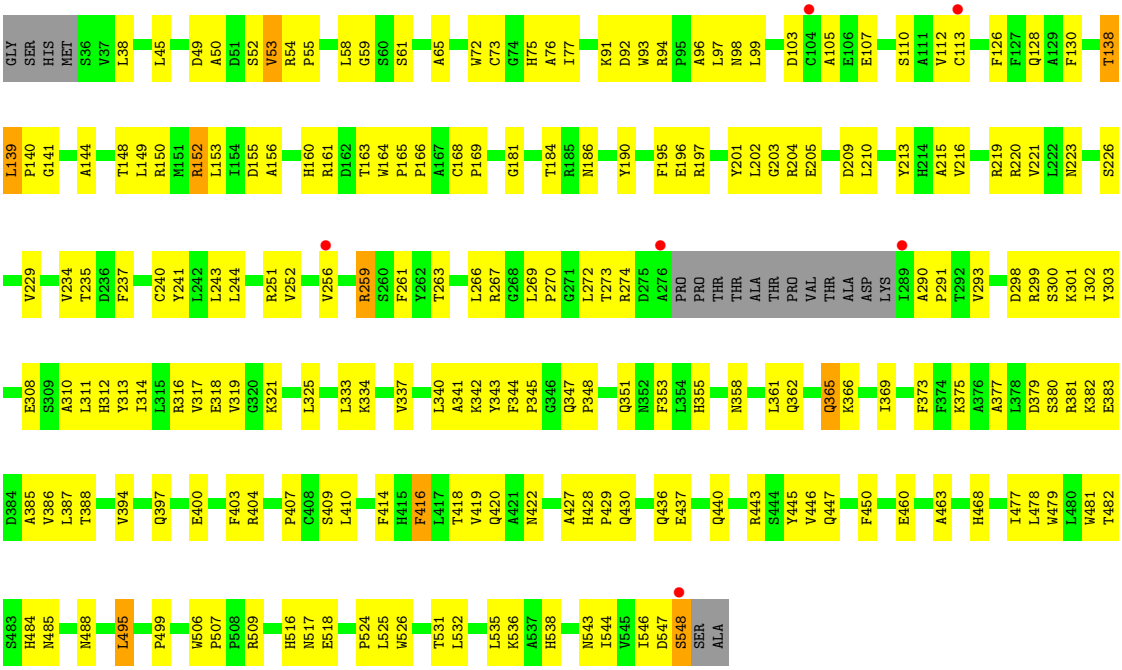
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	58	Total	O	0	0
			58	58		

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.

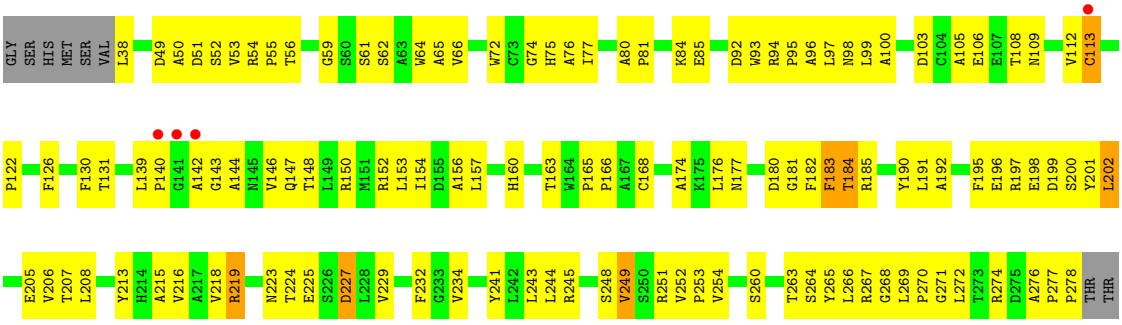
• Molecule 1: Sulfhydryl oxidase 1

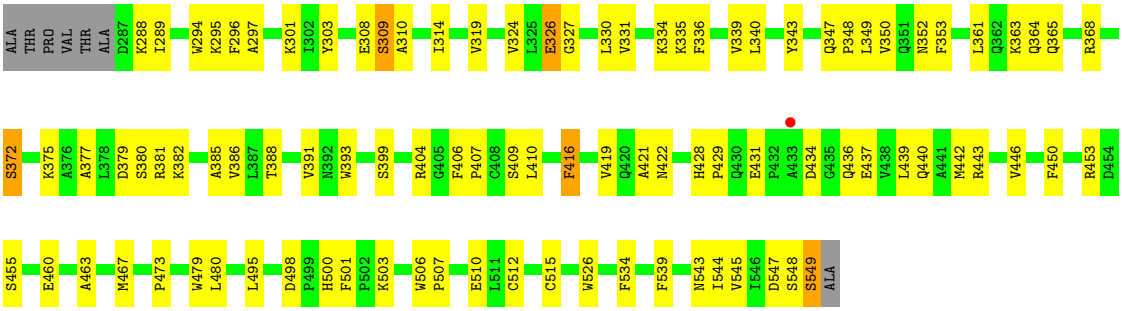
Chain A:



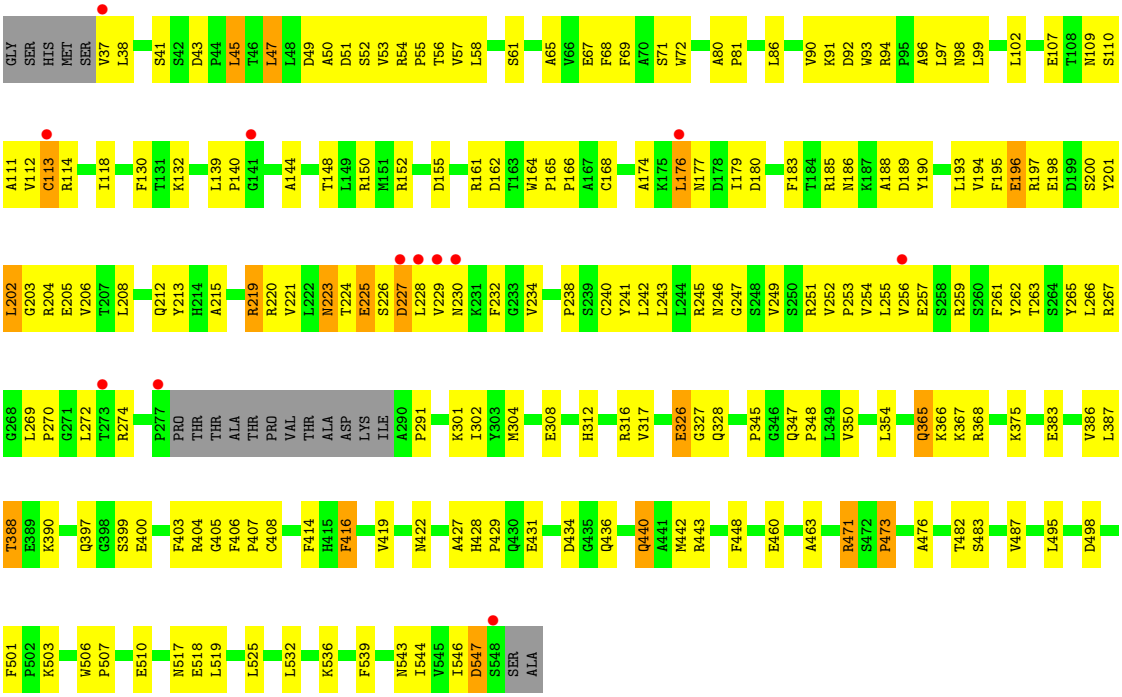
• Molecule 1: Sulfhydryl oxidase 1

Chain B:

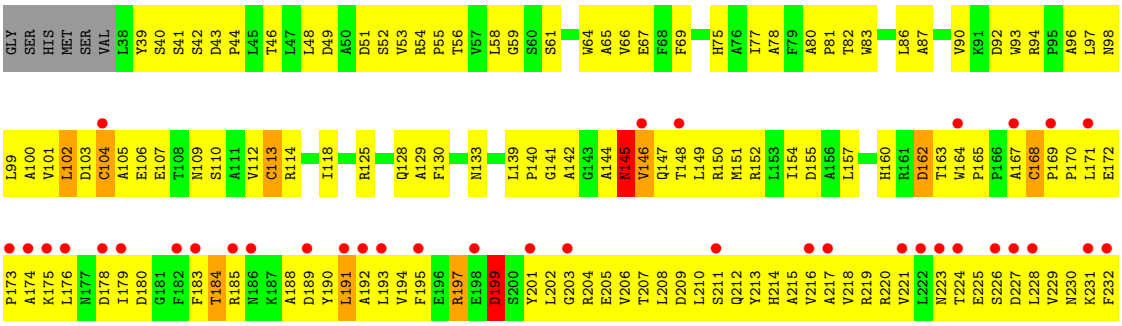


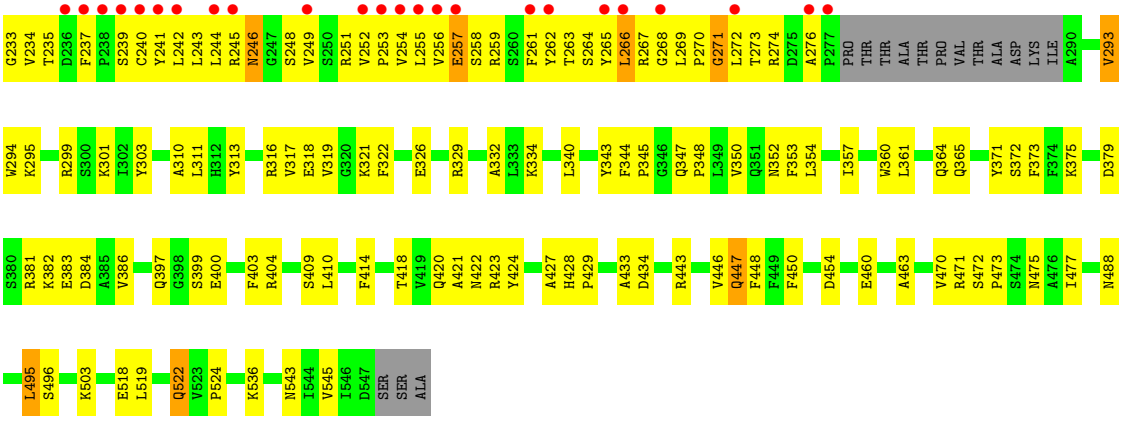


• Molecule 1: Sulfhydryl oxidase 1



• Molecule 1: Sulfhydryl oxidase 1




G233 V234 T235 D236 F237 P238 S239 C240 Y241 L242 L243 L244 R245 N246 G247 S248 V249 S250 R251 V252 P253 V254 L255 V256 E257 S258 R259 S260 F261 Y262 T263 S264 Y265 L266 R267 G268 L269 P270 G271 L272 T273 R274 D275 A276 P277 PRO THR THR ALA THR PRO VAL THR ALA ASP LYS ILE A290 V293
W294 K295 R299 S300 K301 I302 Y303 A310 L311 H312 Y313 R316 V317 E318 V319 G320 K321 F322 E326 R329 A332 L333 K334 L340 Y343 F344 P345 G346 Q347 P348 L349 V350 Q351 N352 F353 L354 I357 W360 L361 Q364 Q365 Y371 S372 F373 F374 K375 D379
S380 R381 K382 E383 D384 A385 V386 Q397 G398 S399 E400 F403 R404 S409 L410 F414 T418 V419 Q420 A421 N422 R423 Y424 A427 H428 P429 A433 D434 R443 V446 Q447 F448 F449 F450 D454 E460 A463 V470 R471 S472 P473 S474 N475 A476 I477 N488
L495 S496 K503 E518 L519 Q522 V523 P524 K536 N543 I544 V545 I546 D547 SER SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.70Å 212.14Å 148.48Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.80) 97.5 (50.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.271 0.210 , 0.269	Depositor DCC
R_{free} test set	4457 reflections (7.09%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16478	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/4091	0.62	0/5569
1	B	0.43	0/4117	0.64	0/5605
1	C	0.43	0/4085	0.62	0/5562
1	D	0.41	0/4072	0.65	1/5544 (0.0%)
All	All	0.42	0/16365	0.63	1/22280 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	145	ASN	N-CA-C	-7.10	91.82	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3979	0	3877	176	0
1	B	4003	0	3899	191	0
1	C	3972	0	3868	187	0
1	D	3959	0	3854	300	0
2	A	53	0	31	2	0
2	B	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	107	0	0	9	0
3	B	95	0	0	13	0
3	C	93	0	0	7	0
3	D	58	0	0	2	0
All	All	16478	0	15622	851	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 27.

All (851) 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:197:ARG:HH21	1:D:223:ASN:HB2	1.07	1.09
1:A:546:ILE:HG22	1:A:547:ASP:H	1.13	1.06
1:A:152:ARG:HA	1:A:152:ARG:HH11	1.24	1.03
1:B:139:LEU:HD12	1:B:140:PRO:HD2	1.35	1.03
1:D:179:ILE:HD12	1:D:193:LEU:HD22	1.37	1.02
1:D:206:VAL:HG13	1:D:263:THR:HG22	1.42	1.02
1:B:244:LEU:HB2	1:B:248:SER:HB2	1.42	0.99
1:D:197:ARG:NH2	1:D:223:ASN:HB2	1.81	0.95
1:D:267:ARG:HG3	1:D:268:GLY:H	1.32	0.94
1:A:316:ARG:HH21	1:A:383:GLU:HG3	1.33	0.94
1:B:65:ALA:HB3	1:B:99:LEU:HD22	1.50	0.94
1:A:546:ILE:HG22	1:A:547:ASP:N	1.86	0.89
1:A:65:ALA:HB3	1:A:99:LEU:HD22	1.54	0.87
1:A:140:PRO:HB2	1:A:152:ARG:HD2	1.56	0.87
1:D:201:TYR:O	1:D:205:GLU:HG3	1.75	0.86
1:A:152:ARG:HA	1:A:152:ARG:NH1	1.89	0.86
1:A:495:LEU:H	1:A:495:LEU:HD12	1.41	0.84
1:C:150:ARG:HD3	1:C:259:ARG:HH12	1.42	0.84
1:D:174:ALA:HB3	1:D:221:VAL:HG22	1.60	0.84
1:D:267:ARG:HG3	1:D:268:GLY:N	1.92	0.84
1:C:316:ARG:HH21	1:C:383:GLU:HG3	1.43	0.83
1:C:347:GLN:HB3	1:C:348:PRO:HD2	1.59	0.83
1:A:546:ILE:CG2	1:A:547:ASP:H	1.91	0.83
1:D:192:ALA:HA	1:D:241:TYR:O	1.77	0.83
1:A:316:ARG:HH21	1:A:383:GLU:CG	1.91	0.83
1:A:416:PHE:HE1	1:A:420:GLN:HE21	1.27	0.81
1:B:382:LYS:O	1:B:386:VAL:HG23	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:HB2	1:D:248:SER:OG	1.80	0.81
1:A:256:VAL:HG13	1:A:261:PHE:CE2	2.16	0.80
1:D:194:VAL:HG22	1:D:240:CYS:SG	2.22	0.80
1:C:183:PHE:HB3	1:C:245:ARG:HH12	1.45	0.80
1:D:179:ILE:HB	1:D:228:LEU:HD22	1.62	0.80
1:D:253:PRO:HG2	1:D:265:TYR:OH	1.81	0.80
1:B:108:THR:HG23	3:B:715:HOH:O	1.81	0.80
1:B:213:TYR:CE2	1:B:274:ARG:HB2	2.16	0.80
1:D:66:VAL:HG22	1:D:100:ALA:HB3	1.62	0.80
1:D:139:LEU:HD12	1:D:140:PRO:HD2	1.63	0.79
1:B:197:ARG:HG2	1:B:223:ASN:ND2	1.98	0.78
1:C:174:ALA:HB2	1:C:219:ARG:HG3	1.65	0.78
1:C:176:LEU:HA	1:C:228:LEU:HD21	1.62	0.78
1:B:106:GLU:HB2	1:B:109:ASN:HD22	1.47	0.78
1:C:243:LEU:HD22	1:C:249:VAL:HG22	1.67	0.77
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.47	0.77
1:B:201:TYR:O	1:B:205:GLU:HG3	1.84	0.77
1:C:201:TYR:O	1:C:205:GLU:HG3	1.86	0.76
1:C:366:LYS:HG3	1:C:368:ARG:O	1.85	0.76
1:C:148:THR:O	1:C:152:ARG:HG2	1.86	0.76
1:D:49:ASP:O	1:D:53:VAL:HG23	1.85	0.76
1:D:179:ILE:HG13	1:D:228:LEU:HD13	1.66	0.76
1:D:242:LEU:HD21	1:D:269:LEU:HD21	1.68	0.76
1:D:144:ALA:HB1	1:D:149:LEU:HG	1.67	0.75
1:B:197:ARG:HG2	1:B:223:ASN:HD22	1.50	0.75
1:D:197:ARG:HE	1:D:223:ASN:CB	2.00	0.74
1:D:316:ARG:HH21	1:D:383:GLU:HG3	1.52	0.74
1:C:223:ASN:HD22	1:C:224:THR:N	1.86	0.74
1:D:400:GLU:HB2	1:D:403:PHE:CD2	2.22	0.74
1:D:264:SER:HA	1:D:267:ARG:HH21	1.53	0.74
1:D:80:ALA:HB3	1:D:81:PRO:HD3	1.70	0.73
1:D:293:VAL:HG13	1:D:397:GLN:OE1	1.89	0.73
1:A:347:GLN:HB3	1:A:348:PRO:HD2	1.68	0.73
1:C:546:ILE:HG22	1:C:547:ASP:H	1.54	0.73
1:D:495:LEU:HD12	1:D:495:LEU:H	1.54	0.73
1:D:443:ARG:HD2	1:D:460:GLU:OE1	1.89	0.72
1:D:433:ALA:O	1:D:472:SER:HA	1.90	0.72
1:B:334:LYS:HG2	1:B:361:LEU:HG	1.72	0.71
1:D:233:GLY:O	1:D:235:THR:HG23	1.90	0.71
1:A:337:VAL:HA	1:A:340:LEU:HD12	1.73	0.71
1:A:130:PHE:HB2	1:A:163:THR:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:HG11	1:B:368:ARG:NH1	2.06	0.71
1:D:240:CYS:HG	1:D:262:TYR:HE2	1.37	0.71
1:A:298:ASP:OD2	1:A:301:LYS:HG2	1.90	0.70
1:D:146:VAL:O	1:D:149:LEU:HB2	1.92	0.70
1:D:212:GLN:O	1:D:274:ARG:HA	1.91	0.70
1:B:241:TYR:HE1	1:B:251:ARG:HD2	1.56	0.70
1:D:229:VAL:HG13	1:D:234:VAL:HB	1.74	0.70
1:C:400:GLU:HB2	1:C:403:PHE:CD2	2.26	0.70
1:B:140:PRO:HD3	3:B:781:HOH:O	1.91	0.70
1:B:453:ARG:HD3	3:B:768:HOH:O	1.90	0.70
1:D:113:CYS:HB3	1:D:118:ILE:HB	1.72	0.69
1:B:335:LYS:HD3	3:B:764:HOH:O	1.91	0.69
1:D:210:LEU:HA	1:D:213:TYR:HD2	1.58	0.69
1:A:382:LYS:HB3	1:A:385:ALA:HB3	1.74	0.69
1:A:443:ARG:HD2	1:A:460:GLU:OE1	1.92	0.69
1:D:382:LYS:O	1:D:386:VAL:HG23	1.92	0.69
1:A:495:LEU:HD12	1:A:495:LEU:N	2.08	0.69
1:C:52:SER:O	1:C:56:THR:HG23	1.92	0.69
1:C:183:PHE:HB3	1:C:245:ARG:NH1	2.07	0.69
1:A:410:LEU:HD23	2:A:601:FAD:HM83	1.76	0.68
1:B:160:HIS:CD2	1:B:165:PRO:HD3	2.29	0.68
1:C:150:ARG:HD3	1:C:259:ARG:NH1	2.08	0.68
1:D:179:ILE:HB	1:D:228:LEU:CD2	2.24	0.68
1:D:316:ARG:NH2	1:D:383:GLU:HG3	2.08	0.68
1:B:216:VAL:HG23	1:B:272:LEU:HD21	1.75	0.68
1:A:256:VAL:HG22	1:A:261:PHE:CD2	2.29	0.68
1:A:201:TYR:O	1:A:205:GLU:HG3	1.94	0.67
1:D:334:LYS:HE2	1:D:361:LEU:O	1.94	0.67
1:A:210:LEU:HD21	1:A:266:LEU:HB3	1.76	0.67
1:A:310:ALA:HB2	1:A:409:SER:HB2	1.75	0.67
1:B:150:ARG:NH1	1:B:205:GLU:OE2	2.27	0.67
1:B:270:PRO:HA	3:B:775:HOH:O	1.94	0.67
1:D:264:SER:HA	1:D:267:ARG:NH2	2.10	0.67
1:C:266:LEU:O	1:C:269:LEU:HG	1.95	0.67
1:D:427:ALA:C	1:D:429:PRO:HD3	2.15	0.67
1:B:66:VAL:HG22	1:B:100:ALA:HB3	1.75	0.67
1:C:223:ASN:H	1:C:223:ASN:ND2	1.93	0.66
1:D:53:VAL:O	1:D:56:THR:HG22	1.95	0.66
1:D:171:LEU:O	1:D:220:ARG:HD3	1.95	0.66
1:D:519:LEU:O	1:D:522:GLN:HG2	1.96	0.66
1:C:223:ASN:HD22	1:C:224:THR:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ALA:HB3	1:C:99:LEU:HD22	1.76	0.66
1:D:193:LEU:O	1:D:240:CYS:HA	1.96	0.66
1:B:225:GLU:O	1:B:229:VAL:HG23	1.97	0.65
1:B:241:TYR:CE1	1:B:251:ARG:HD2	2.32	0.65
1:D:206:VAL:O	1:D:210:LEU:HD23	1.97	0.65
1:A:190:TYR:CG	1:A:269:LEU:HD13	2.32	0.65
1:C:176:LEU:HD22	1:C:227:ASP:OD2	1.96	0.65
1:D:94:ARG:HD2	1:D:98:ASN:OD1	1.97	0.64
1:D:213:TYR:HA	1:D:273:THR:O	1.97	0.64
1:A:256:VAL:HG22	1:A:261:PHE:HD2	1.62	0.64
1:B:195:PHE:CE2	1:B:234:VAL:HG21	2.32	0.64
1:D:243:LEU:HD23	1:D:243:LEU:H	1.63	0.64
1:C:174:ALA:HB2	1:C:219:ARG:CG	2.27	0.64
1:A:144:ALA:HB1	1:A:148:THR:HB	1.80	0.64
1:C:400:GLU:HB2	1:C:403:PHE:HD2	1.63	0.64
1:D:194:VAL:HA	1:D:239:SER:O	1.97	0.64
1:D:350:VAL:HG22	1:D:386:VAL:HG12	1.80	0.63
1:D:201:TYR:O	1:D:205:GLU:CG	2.46	0.63
1:C:91:LYS:HB2	1:C:94:ARG:NH2	2.13	0.63
1:C:399:SER:O	1:C:400:GLU:HG2	1.98	0.63
1:A:333:LEU:O	1:A:337:VAL:HG23	1.99	0.63
1:C:132:LYS:HB2	1:C:132:LYS:NZ	2.13	0.63
1:D:257:GLU:HA	1:D:262:TYR:CE1	2.33	0.63
1:C:316:ARG:HH21	1:C:383:GLU:CG	2.09	0.63
1:D:495:LEU:H	1:D:495:LEU:CD1	2.10	0.63
1:A:38:LEU:HD12	1:A:38:LEU:N	2.14	0.62
1:C:245:ARG:HG3	1:C:245:ARG:NH1	2.12	0.62
1:C:139:LEU:HD12	1:C:140:PRO:HD2	1.82	0.62
1:D:179:ILE:HD12	1:D:193:LEU:CD2	2.22	0.62
1:B:510:GLU:H	1:B:510:GLU:CD	2.03	0.62
1:C:195:PHE:O	1:C:238:PRO:HA	2.00	0.62
1:B:62:SER:HB2	1:B:95:PRO:O	2.00	0.62
1:D:59:GLY:HA2	1:D:130:PHE:HA	1.82	0.62
1:C:190:TYR:CG	1:C:269:LEU:HD13	2.35	0.62
1:A:416:PHE:HE1	1:A:420:GLN:NE2	1.97	0.62
1:B:92:ASP:OD1	1:B:274:ARG:NH2	2.33	0.62
1:D:53:VAL:HG21	1:D:102:LEU:CD1	2.29	0.62
1:D:433:ALA:HB1	1:D:473:PRO:HD3	1.81	0.62
1:D:195:PHE:CD1	1:D:221:VAL:HB	2.34	0.62
1:D:254:VAL:HG21	1:D:262:TYR:CE1	2.35	0.62
1:A:443:ARG:HD3	1:A:463:ALA:CB	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASP:OD2	1:B:436:GLN:HB2	2.00	0.61
1:A:375:LYS:HG2	1:A:379:ASP:OD2	1.99	0.61
1:C:50:ALA:HB2	1:C:109:ASN:HA	1.81	0.61
1:C:206:VAL:HG13	1:C:263:THR:CG2	2.31	0.61
1:A:130:PHE:CD1	1:B:372:SER:HB2	2.36	0.61
1:D:78:ALA:O	1:D:81:PRO:HD2	2.01	0.61
1:D:267:ARG:CG	1:D:268:GLY:H	2.10	0.61
1:A:165:PRO:HB2	1:A:168:CYS:HB3	1.81	0.61
1:C:96:ALA:HB1	1:C:168:CYS:HB2	1.83	0.61
1:D:102:LEU:CD1	1:D:112:VAL:HG11	2.31	0.61
1:D:495:LEU:HD12	1:D:495:LEU:N	2.15	0.61
1:D:94:ARG:HG2	1:D:97:LEU:O	2.01	0.61
1:A:495:LEU:H	1:A:495:LEU:CD1	2.13	0.60
1:D:214:HIS:HD2	1:D:273:THR:HG21	1.66	0.60
1:D:301:LYS:HD3	1:D:543:ASN:OD1	2.01	0.60
1:A:314:ILE:HG23	1:A:445:TYR:OH	2.00	0.60
1:D:41:SER:C	1:D:43:ASP:H	2.04	0.60
1:A:400:GLU:HB2	1:A:403:PHE:CD2	2.36	0.60
1:C:225:GLU:HB2	1:C:229:VAL:HG23	1.83	0.60
1:C:213:TYR:CZ	1:C:274:ARG:HD2	2.37	0.60
1:D:210:LEU:HD12	1:D:216:VAL:HG11	1.84	0.60
1:D:92:ASP:HA	1:D:212:GLN:HE21	1.66	0.60
1:B:365:GLN:H	1:B:365:GLN:CD	2.05	0.60
1:B:202:LEU:O	1:B:206:VAL:HG23	2.00	0.60
1:D:160:HIS:HB3	1:D:163:THR:O	2.02	0.60
1:D:240:CYS:HB3	1:D:252:VAL:HG21	1.83	0.60
1:B:440:GLN:HA	1:B:467:MET:HE1	1.83	0.59
1:C:196:GLU:OE1	1:C:203:GLY:N	2.35	0.59
1:D:48:LEU:HB3	1:D:53:VAL:HG22	1.83	0.59
1:D:61:SER:HA	1:D:130:PHE:CZ	2.37	0.59
1:D:106:GLU:HB2	1:D:109:ASN:HD22	1.68	0.59
1:B:365:GLN:OE1	1:B:365:GLN:N	2.30	0.59
1:B:207:THR:HG23	1:B:218:VAL:HB	1.85	0.59
1:B:288:LYS:O	1:B:289:ILE:HG12	2.03	0.59
1:D:164:TRP:CZ2	1:D:168:CYS:SG	2.96	0.59
1:A:150:ARG:HD2	1:A:205:GLU:OE2	2.02	0.59
1:D:170:PRO:HB2	1:D:219:ARG:HH12	1.66	0.59
1:D:204:ARG:CZ	1:D:220:ARG:HH12	2.16	0.59
1:D:310:ALA:HB2	1:D:409:SER:HB2	1.85	0.59
1:B:268:GLY:O	1:B:269:LEU:HD23	2.03	0.59
1:C:38:LEU:HD13	1:C:69:PHE:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:SER:O	1:C:55:PRO:HG2	2.03	0.59
1:A:72:TRP:CE3	1:A:407:PRO:HG3	2.37	0.58
1:A:190:TYR:OH	1:A:270:PRO:O	2.19	0.58
1:B:50:ALA:HB2	1:B:109:ASN:HA	1.84	0.58
1:C:68:PHE:HE1	1:C:102:LEU:HD23	1.67	0.58
1:C:92:ASP:HA	1:C:212:GLN:NE2	2.19	0.58
1:C:190:TYR:HB3	1:C:242:LEU:HD11	1.85	0.58
1:C:225:GLU:OE1	1:C:225:GLU:HA	2.04	0.58
1:D:174:ALA:H	1:D:221:VAL:HA	1.69	0.58
1:B:177:ASN:O	1:B:185:ARG:NH2	2.37	0.58
1:D:176:LEU:HB2	1:D:227:ASP:CG	2.24	0.58
1:A:50:ALA:HA	1:A:112:VAL:HG21	1.85	0.58
1:B:336:PHE:CE2	1:B:340:LEU:HD11	2.39	0.58
1:C:68:PHE:CE1	1:C:102:LEU:HD23	2.38	0.58
1:C:189:ASP:HA	1:C:245:ARG:HD2	1.85	0.58
1:C:256:VAL:HG12	1:C:261:PHE:CE2	2.38	0.58
1:A:482:THR:HA	3:A:761:HOH:O	2.03	0.57
1:C:41:SER:C	1:C:43:ASP:H	2.08	0.57
1:C:107:GLU:O	1:C:110:SER:HB3	2.04	0.57
1:C:164:TRP:O	1:C:166:PRO:HD3	2.04	0.57
1:D:174:ALA:HB3	1:D:221:VAL:CG2	2.32	0.57
1:D:101:VAL:HG23	1:D:101:VAL:O	2.04	0.57
1:A:365:GLN:H	1:A:365:GLN:CD	2.07	0.57
1:A:485:ASN:HA	1:A:488:ASN:HD22	1.69	0.57
1:C:241:TYR:CE1	1:C:251:ARG:HB2	2.40	0.57
1:A:38:LEU:HD12	1:A:38:LEU:H	1.69	0.57
1:B:54:ARG:HG3	3:B:707:HOH:O	2.04	0.57
1:B:301:LYS:HD3	1:B:543:ASN:OD1	2.05	0.57
1:C:240:CYS:HB2	1:C:262:TYR:CE2	2.39	0.57
1:D:240:CYS:SG	1:D:262:TYR:HE2	2.26	0.57
1:C:427:ALA:C	1:C:429:PRO:HD3	2.25	0.57
1:D:179:ILE:CG1	1:D:228:LEU:HD13	2.33	0.57
1:D:206:VAL:CG1	1:D:263:THR:HG22	2.26	0.57
1:D:242:LEU:O	1:D:242:LEU:HG	2.04	0.57
1:B:216:VAL:CG2	1:B:272:LEU:HD21	2.35	0.57
1:C:366:LYS:HE3	1:C:368:ARG:HB3	1.86	0.57
1:C:267:ARG:CZ	1:C:267:ARG:HB3	2.35	0.56
1:D:146:VAL:HA	1:D:149:LEU:HD12	1.86	0.56
1:A:75:HIS:ND1	1:A:76:ALA:N	2.53	0.56
1:C:443:ARG:HD2	1:C:460:GLU:OE1	2.04	0.56
1:B:183:PHE:HZ	1:B:243:LEU:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:HIS:N	1:B:429:PRO:HD3	2.19	0.56
1:B:443:ARG:HD3	1:B:463:ALA:CB	2.35	0.56
1:B:443:ARG:HD2	1:B:460:GLU:OE1	2.06	0.56
1:C:443:ARG:HD3	1:C:463:ALA:HB1	1.86	0.56
1:A:311:LEU:HD21	1:A:340:LEU:HD22	1.87	0.56
1:B:95:PRO:HD3	1:B:277:PRO:HB3	1.87	0.56
1:A:381:ARG:HH11	1:A:381:ARG:HG3	1.70	0.56
1:B:252:VAL:HG13	1:B:265:TYR:CD2	2.40	0.56
1:C:252:VAL:HG22	1:C:265:TYR:CE2	2.40	0.56
1:D:169:PRO:HG2	1:D:207:THR:HG22	1.86	0.56
1:A:234:VAL:HG22	1:A:241:TYR:CE1	2.41	0.56
1:D:427:ALA:O	1:D:429:PRO:HD3	2.05	0.56
1:A:96:ALA:HB1	1:A:168:CYS:HB2	1.87	0.56
1:A:243:LEU:N	1:A:243:LEU:HD12	2.20	0.56
1:A:353:PHE:CB	1:A:386:VAL:HG11	2.36	0.56
1:C:223:ASN:HD22	1:C:223:ASN:N	2.03	0.56
1:D:350:VAL:HA	1:D:386:VAL:CG1	2.36	0.56
1:A:164:TRP:O	1:A:166:PRO:HD3	2.06	0.55
1:B:181:GLY:O	1:B:184:THR:HB	2.06	0.55
1:D:271:GLY:O	1:D:272:LEU:HG	2.07	0.55
1:D:434:ASP:HB2	1:D:471:ARG:NH2	2.21	0.55
1:C:72:TRP:CE3	1:C:407:PRO:HG3	2.42	0.55
1:C:252:VAL:HG12	1:C:254:VAL:HG13	1.87	0.55
1:D:82:THR:HG23	1:D:146:VAL:HG22	1.87	0.55
1:B:213:TYR:OH	1:B:274:ARG:HD2	2.06	0.55
1:D:244:LEU:HD13	1:D:246:ASN:HD21	1.70	0.55
1:A:140:PRO:HB2	1:A:152:ARG:CD	2.32	0.55
1:B:266:LEU:O	1:B:269:LEU:HG	2.06	0.55
1:B:382:LYS:HG2	1:B:385:ALA:HB3	1.88	0.55
1:C:350:VAL:HA	1:C:386:VAL:CG1	2.36	0.55
1:D:265:TYR:O	1:D:267:ARG:N	2.39	0.55
1:C:431:GLU:HG2	3:C:786:HOH:O	2.07	0.55
1:D:433:ALA:HB1	1:D:473:PRO:CD	2.37	0.55
1:B:215:ALA:HB3	1:B:272:LEU:HD23	1.89	0.55
1:C:80:ALA:HB3	1:C:81:PRO:HD3	1.88	0.55
1:D:184:THR:HG22	1:D:184:THR:O	2.07	0.55
1:A:422:ASN:ND2	1:A:536:LYS:HE2	2.21	0.55
1:D:61:SER:HA	1:D:130:PHE:CE2	2.42	0.55
1:D:227:ASP:O	1:D:228:LEU:HD23	2.07	0.55
1:A:342:LYS:HE2	1:A:343:TYR:OH	2.06	0.54
1:C:471:ARG:NH1	1:C:471:ARG:HG2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HG3	1:B:197:ARG:HH11	1.71	0.54
1:C:546:ILE:HG22	1:C:547:ASP:N	2.20	0.54
1:D:322:PHE:CE2	1:D:329:ARG:NH2	2.76	0.54
1:D:107:GLU:HG3	1:D:317:VAL:HG22	1.90	0.54
1:D:141:GLY:O	1:D:144:ALA:HB2	2.08	0.54
1:D:209:ASP:CG	1:D:259:ARG:HH21	2.11	0.54
1:D:252:VAL:HG12	1:D:254:VAL:HG13	1.90	0.54
1:B:192:ALA:HB3	1:B:218:VAL:HG22	1.90	0.54
1:C:404:ARG:HD2	1:C:501:PHE:CD2	2.42	0.54
1:D:102:LEU:HD13	1:D:112:VAL:HG11	1.89	0.54
1:B:503:LYS:HE2	2:B:601:FAD:O5'	2.07	0.54
1:B:547:ASP:HB2	3:B:759:HOH:O	2.06	0.54
1:C:223:ASN:HD22	1:C:223:ASN:H	1.56	0.54
1:C:365:GLN:H	1:C:365:GLN:CD	2.10	0.54
1:D:197:ARG:HE	1:D:223:ASN:HB3	1.73	0.54
1:A:479:TRP:O	1:A:482:THR:HG22	2.07	0.54
1:D:86:LEU:O	1:D:90:VAL:HG22	2.08	0.54
1:A:517:ASN:HB2	1:A:525:LEU:O	2.08	0.54
1:D:433:ALA:HB1	1:D:473:PRO:CG	2.37	0.54
1:A:186:ASN:ND2	3:A:762:HOH:O	2.40	0.53
1:B:75:HIS:CE1	1:B:122:PRO:HD3	2.43	0.53
1:B:93:TRP:CE3	1:B:208:LEU:HD13	2.43	0.53
1:C:90:VAL:O	1:C:93:TRP:HB2	2.07	0.53
1:C:267:ARG:HA	1:C:272:LEU:HD23	1.89	0.53
1:A:256:VAL:HG13	1:A:261:PHE:HE2	1.73	0.53
1:C:37:VAL:HG21	1:C:400:GLU:OE1	2.08	0.53
1:C:113:CYS:HB3	1:C:118:ILE:HB	1.90	0.53
1:A:94:ARG:HG2	1:A:97:LEU:O	2.07	0.53
1:B:59:GLY:HA2	1:B:130:PHE:HA	1.91	0.53
1:B:160:HIS:NE2	1:B:165:PRO:HD3	2.24	0.53
1:B:215:ALA:HB3	1:B:272:LEU:CD2	2.39	0.53
1:D:318:GLU:O	1:D:321:LYS:HB2	2.08	0.53
1:B:180:ASP:O	1:B:185:ARG:NH2	2.40	0.53
1:B:512:CYS:HB2	1:B:534:PHE:CD1	2.44	0.53
1:C:45:LEU:HD12	1:C:45:LEU:O	2.08	0.53
1:A:52:SER:O	1:A:55:PRO:HG2	2.09	0.53
1:B:309:SER:HB3	1:B:393:TRP:CZ3	2.44	0.53
1:D:360:TRP:O	1:D:364:GLN:HG2	2.08	0.53
1:C:197:ARG:HG3	1:C:198:GLU:N	2.23	0.53
1:C:532:LEU:O	1:C:536:LYS:HG3	2.09	0.53
1:D:410:LEU:HD23	2:D:601:FAD:HM83	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:TYR:CD1	1:B:545:VAL:HB	2.43	0.53
1:C:132:LYS:HB2	1:C:132:LYS:HZ2	1.74	0.53
1:D:344:PHE:CD1	1:D:345:PRO:HD2	2.44	0.53
1:D:422:ASN:ND2	1:D:536:LYS:HE2	2.24	0.53
1:A:436:GLN:O	1:A:440:GLN:HB2	2.09	0.52
1:B:498:ASP:HB3	1:B:501:PHE:HB2	1.90	0.52
1:D:173:PRO:HA	1:D:220:ARG:HG3	1.90	0.52
1:C:471:ARG:HG2	1:C:471:ARG:HH11	1.74	0.52
1:D:174:ALA:O	1:D:221:VAL:HG13	2.10	0.52
1:D:215:ALA:CB	1:D:272:LEU:HD23	2.39	0.52
1:A:204:ARG:HD3	1:A:220:ARG:NH1	2.24	0.52
1:B:223:ASN:O	1:B:229:VAL:HG21	2.10	0.52
1:C:328:GLN:HB3	1:C:448:PHE:CZ	2.44	0.52
1:D:211:SER:C	1:D:213:TYR:H	2.12	0.52
1:D:420:GLN:OE1	1:D:423:ARG:HD3	2.10	0.52
1:B:52:SER:O	1:B:56:THR:HG23	2.09	0.52
1:B:243:LEU:CD2	1:B:249:VAL:HG13	2.39	0.52
1:D:39:TYR:OH	1:D:80:ALA:HA	2.08	0.52
1:A:140:PRO:HA	3:A:710:HOH:O	2.09	0.52
1:D:147:GLN:HG2	1:D:150:ARG:NH2	2.24	0.52
1:D:443:ARG:HD3	1:D:463:ALA:HB1	1.92	0.52
1:C:215:ALA:HB3	1:C:272:LEU:HD12	1.92	0.52
1:D:257:GLU:HA	1:D:262:TYR:HE1	1.72	0.52
1:A:92:ASP:CG	1:A:274:ARG:HH21	2.13	0.52
1:B:140:PRO:HG3	1:B:152:ARG:HD2	1.91	0.52
1:C:267:ARG:HB3	1:C:267:ARG:NH1	2.24	0.52
1:C:267:ARG:NH1	1:C:267:ARG:CB	2.72	0.52
1:D:254:VAL:HG21	1:D:262:TYR:HE1	1.71	0.52
1:B:310:ALA:HB2	1:B:409:SER:HB2	1.91	0.52
1:C:443:ARG:HD3	1:C:463:ALA:CB	2.39	0.52
1:B:85:GLU:CD	1:B:146:VAL:HG21	2.29	0.52
1:B:547:ASP:OD1	1:B:549:SER:HB3	2.09	0.52
1:C:206:VAL:HG13	1:C:263:THR:HG22	1.91	0.52
1:C:223:ASN:O	1:C:229:VAL:HG21	2.09	0.52
1:D:215:ALA:HB3	1:D:272:LEU:HD23	1.92	0.52
1:D:256:VAL:HG13	1:D:258:SER:OG	2.09	0.52
1:C:213:TYR:CE1	1:C:274:ARG:HD2	2.44	0.51
1:D:130:PHE:HB2	1:D:163:THR:HG21	1.91	0.51
1:D:267:ARG:HH11	1:D:267:ARG:HB2	1.75	0.51
1:A:148:THR:O	1:A:152:ARG:HG2	2.10	0.51
1:C:246:ASN:OD1	1:C:247:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:PHE:CE1	1:D:245:ARG:HA	2.44	0.51
1:D:447:GLN:HG2	1:D:448:PHE:CE2	2.44	0.51
1:B:377:ALA:O	1:B:381:ARG:NH1	2.41	0.51
1:C:102:LEU:HD21	1:C:112:VAL:HG11	1.91	0.51
1:A:54:ARG:N	1:A:55:PRO:HD2	2.26	0.51
1:A:181:GLY:O	1:A:184:THR:HB	2.09	0.51
1:A:209:ASP:OD2	1:A:263:THR:HG21	2.11	0.51
1:D:519:LEU:HB2	1:D:522:GLN:OE1	2.09	0.51
1:B:59:GLY:N	1:B:131:THR:O	2.38	0.51
1:B:253:PRO:O	1:B:254:VAL:HG13	2.10	0.51
1:C:503:LYS:HE2	2:C:601:FAD:O5'	2.10	0.51
1:D:92:ASP:HA	1:D:212:GLN:NE2	2.26	0.51
1:D:157:LEU:O	1:D:160:HIS:ND1	2.41	0.51
1:D:75:HIS:CD2	1:D:454:ASP:HB2	2.46	0.51
1:D:82:THR:HG23	1:D:146:VAL:CG2	2.41	0.51
1:B:309:SER:OG	1:B:391:VAL:HA	2.11	0.51
1:A:334:LYS:HD2	3:A:739:HOH:O	2.10	0.51
1:D:53:VAL:HG21	1:D:102:LEU:HD11	1.92	0.51
1:D:113:CYS:HA	1:D:118:ILE:HB	1.93	0.51
1:D:221:VAL:HG11	1:D:228:LEU:HD12	1.93	0.51
1:A:308:GLU:HB3	1:A:387:LEU:HD22	1.93	0.50
1:A:538:HIS:HA	1:A:543:ASN:ND2	2.26	0.50
1:C:302:ILE:O	1:C:544:ILE:HA	2.11	0.50
1:D:113:CYS:CB	1:D:118:ILE:HB	2.41	0.50
1:D:194:VAL:HG13	1:D:240:CYS:SG	2.51	0.50
1:D:365:GLN:HA	3:D:749:HOH:O	2.11	0.50
1:B:62:SER:CB	1:B:95:PRO:O	2.58	0.50
1:D:83:TRP:O	1:D:86:LEU:HB3	2.10	0.50
1:D:171:LEU:HB3	1:D:204:ARG:HG2	1.93	0.50
1:B:126:PHE:CD2	1:B:156:ALA:HB1	2.46	0.50
1:D:223:ASN:HA	1:D:237:PHE:CZ	2.46	0.50
1:A:197:ARG:NH1	1:A:237:PHE:HB2	2.26	0.50
1:C:206:VAL:HG13	1:C:263:THR:HG23	1.93	0.50
1:B:190:TYR:HE1	1:B:244:LEU:HD21	1.77	0.50
1:B:213:TYR:CZ	1:B:274:ARG:HB2	2.46	0.50
1:D:183:PHE:C	1:D:185:ARG:H	2.15	0.50
1:A:73:CYS:O	1:A:76:ALA:HB3	2.12	0.50
1:A:318:GLU:HA	1:A:321:LYS:NZ	2.26	0.50
1:B:375:LYS:NZ	1:B:379:ASP:OD2	2.44	0.50
1:B:428:HIS:HB3	1:B:431:GLU:CG	2.42	0.50
1:C:86:LEU:O	1:C:90:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:CZ	1:D:223:ASN:HB2	2.40	0.50
1:A:443:ARG:HD3	1:A:463:ALA:HB1	1.92	0.50
1:B:182:PHE:CG	1:B:191:LEU:HD22	2.46	0.50
1:C:254:VAL:HG23	1:C:257:GLU:OE1	2.12	0.50
1:D:303:TYR:CD1	1:D:545:VAL:HB	2.46	0.50
1:A:128:GLN:HG3	3:A:726:HOH:O	2.11	0.50
1:C:47:LEU:HD23	1:C:47:LEU:N	2.27	0.50
1:D:149:LEU:O	1:D:152:ARG:N	2.45	0.50
1:D:253:PRO:HG2	1:D:265:TYR:CZ	2.47	0.50
1:B:64:TRP:CZ3	1:B:98:ASN:HB3	2.46	0.50
1:B:440:GLN:NE2	1:B:467:MET:HE2	2.27	0.50
1:D:162:ASP:N	1:D:162:ASP:OD1	2.44	0.50
1:A:152:ARG:NH1	1:A:155:ASP:OD2	2.39	0.49
1:B:350:VAL:O	1:B:353:PHE:HB3	2.11	0.49
1:A:422:ASN:HD22	1:A:536:LYS:HE2	1.77	0.49
1:C:38:LEU:HD13	1:C:69:PHE:CE2	2.47	0.49
1:C:405:GLY:O	1:C:408:CYS:HB3	2.12	0.49
1:D:174:ALA:O	1:D:225:GLU:HG2	2.12	0.49
1:B:80:ALA:HB3	1:B:81:PRO:HD3	1.95	0.49
1:C:144:ALA:HB1	1:C:148:THR:HB	1.94	0.49
1:D:261:PHE:O	1:D:264:SER:HB3	2.12	0.49
1:A:314:ILE:O	1:A:319:VAL:HG23	2.12	0.49
1:B:147:GLN:HB2	3:B:702:HOH:O	2.12	0.49
1:B:363:LYS:O	1:B:364:GLN:C	2.50	0.49
1:C:213:TYR:CE1	1:C:274:ARG:HB2	2.48	0.49
1:C:365:GLN:OE1	1:C:365:GLN:N	2.36	0.49
1:D:174:ALA:HB1	1:D:178:ASP:HB2	1.92	0.49
1:B:72:TRP:CE3	1:B:407:PRO:HG3	2.47	0.49
1:C:215:ALA:HB3	1:C:272:LEU:CD1	2.43	0.49
1:D:243:LEU:HB2	1:D:248:SER:O	2.12	0.49
1:C:38:LEU:CD1	1:C:69:PHE:HE2	2.25	0.49
1:A:126:PHE:HB2	1:A:139:LEU:HD23	1.95	0.49
1:A:325:LEU:HD13	1:A:333:LEU:CD2	2.43	0.49
1:B:326:GLU:HA	1:B:330:LEU:CB	2.43	0.49
1:B:439:LEU:C	1:B:467:MET:HE1	2.33	0.49
1:C:436:GLN:O	1:C:440:GLN:HB2	2.12	0.49
1:D:44:PRO:HG2	1:D:87:ALA:CB	2.42	0.49
1:D:175:LYS:O	1:D:228:LEU:HD11	2.12	0.49
1:B:139:LEU:HD21	1:B:153:LEU:HD23	1.94	0.49
1:B:223:ASN:OD1	1:B:224:THR:HG23	2.13	0.49
1:B:277:PRO:N	1:B:278:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:HD13	1:D:496:SER:HA	1.94	0.49
1:A:213:TYR:N	1:A:213:TYR:CD1	2.80	0.49
1:B:140:PRO:CD	3:B:781:HOH:O	2.56	0.49
1:D:213:TYR:CD1	1:D:273:THR:O	2.66	0.49
1:B:334:LYS:HE2	1:B:361:LEU:O	2.13	0.48
1:D:354:LEU:HA	1:D:357:ILE:HG22	1.94	0.48
1:B:38:LEU:O	1:B:84:LYS:CE	2.61	0.48
1:D:348:PRO:O	1:D:352:ASN:ND2	2.47	0.48
1:B:53:VAL:HG11	1:B:112:VAL:HG22	1.95	0.48
1:C:38:LEU:HD11	1:C:71:SER:CB	2.42	0.48
1:D:171:LEU:HD11	1:D:208:LEU:HD21	1.96	0.48
1:D:179:ILE:CB	1:D:228:LEU:HD22	2.40	0.48
1:D:422:ASN:OD1	1:D:473:PRO:HB2	2.12	0.48
1:A:91:LYS:HG3	1:A:92:ASP:OD1	2.12	0.48
1:C:53:VAL:O	1:C:57:VAL:HG22	2.13	0.48
1:C:253:PRO:HD2	1:C:265:TYR:CE1	2.49	0.48
1:D:44:PRO:HG2	1:D:87:ALA:HB1	1.95	0.48
1:D:150:ARG:HD3	1:D:259:ARG:HH12	1.78	0.48
1:D:229:VAL:HA	1:D:234:VAL:CG2	2.43	0.48
1:B:49:ASP:OD1	1:B:51:ASP:N	2.44	0.48
1:B:196:GLU:HB2	1:B:200:SER:HB3	1.95	0.48
1:B:419:VAL:HG21	1:B:539:PHE:HB2	1.95	0.48
1:C:416:PHE:CZ	1:C:544:ILE:HD11	2.48	0.48
1:D:199:ASP:OD1	1:D:199:ASP:N	2.47	0.48
1:C:495:LEU:HD22	1:C:495:LEU:H	1.79	0.48
1:D:267:ARG:NH1	1:D:267:ARG:CB	2.77	0.48
1:B:53:VAL:HG11	1:B:112:VAL:CG2	2.44	0.48
1:D:195:PHE:CD1	1:D:229:VAL:HG22	2.48	0.48
1:B:144:ALA:HB1	1:B:148:THR:HB	1.95	0.48
1:B:174:ALA:HB2	1:B:219:ARG:HG3	1.96	0.48
1:B:190:TYR:CE1	1:B:244:LEU:HD21	2.48	0.48
1:C:204:ARG:HG3	1:C:220:ARG:HD2	1.96	0.47
1:D:41:SER:O	1:D:43:ASP:N	2.47	0.47
1:D:169:PRO:CG	1:D:207:THR:HG22	2.43	0.47
1:A:65:ALA:HB3	1:A:99:LEU:CD2	2.37	0.47
1:A:293:VAL:HG12	1:A:397:GLN:OE1	2.14	0.47
1:A:303:TYR:CD1	1:A:303:TYR:N	2.83	0.47
1:A:404:ARG:O	1:A:407:PRO:HD2	2.12	0.47
1:C:150:ARG:HD2	1:C:205:GLU:OE2	2.14	0.47
1:D:488:ASN:OD1	1:D:503:LYS:HD2	2.14	0.47
1:A:126:PHE:CD2	1:A:156:ALA:HB1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD21	1:A:266:LEU:CB	2.44	0.47
1:A:403:PHE:CZ	1:A:499:PRO:HD3	2.49	0.47
1:C:50:ALA:HA	1:C:112:VAL:HG21	1.97	0.47
1:D:421:ALA:O	1:D:424:TYR:HB3	2.13	0.47
1:C:91:LYS:O	1:C:94:ARG:NE	2.46	0.47
1:D:41:SER:C	1:D:43:ASP:N	2.68	0.47
1:B:74:GLY:HA3	2:B:601:FAD:O2	2.14	0.47
1:B:182:PHE:CD1	1:B:191:LEU:HD22	2.50	0.47
1:B:404:ARG:HD2	1:B:501:PHE:CD2	2.49	0.47
1:B:510:GLU:CD	1:B:510:GLU:N	2.66	0.47
1:B:294:TRP:CZ2	1:B:295:LYS:HE3	2.50	0.47
1:C:49:ASP:OD1	1:C:51:ASP:N	2.47	0.47
1:D:40:SER:O	1:D:43:ASP:HB2	2.14	0.47
1:D:213:TYR:HD1	1:D:273:THR:O	1.97	0.47
1:A:344:PHE:CD1	1:A:345:PRO:HD2	2.48	0.47
1:C:194:VAL:HG13	1:C:262:TYR:HE2	1.80	0.47
1:C:506:TRP:CG	1:C:507:PRO:HA	2.50	0.47
1:D:202:LEU:C	1:D:202:LEU:HD23	2.35	0.47
1:D:206:VAL:HG22	1:D:263:THR:HG23	1.96	0.47
1:D:210:LEU:HA	1:D:213:TYR:CD2	2.44	0.47
1:A:419:VAL:O	1:A:422:ASN:N	2.48	0.47
1:D:190:TYR:HE2	1:D:272:LEU:HD21	1.80	0.47
1:D:206:VAL:HG12	1:D:210:LEU:HD23	1.97	0.47
1:D:267:ARG:HH11	1:D:267:ARG:CB	2.28	0.47
1:B:422:ASN:OD1	1:B:473:PRO:HB2	2.14	0.47
1:D:64:TRP:CZ3	1:D:98:ASN:HB3	2.50	0.47
1:D:129:ALA:CB	1:D:165:PRO:HG3	2.45	0.47
1:D:252:VAL:HG12	1:D:254:VAL:CG1	2.45	0.47
1:A:477:ILE:HG22	1:A:535:LEU:HD13	1.97	0.47
1:B:139:LEU:HD11	1:B:152:ARG:HB3	1.96	0.47
1:C:267:ARG:HH11	1:C:267:ARG:HB2	1.80	0.47
1:D:106:GLU:HB2	1:D:109:ASN:ND2	2.29	0.47
1:A:436:GLN:HE22	1:A:468:HIS:HA	1.79	0.46
1:B:142:ALA:O	1:B:144:ALA:N	2.48	0.46
1:B:326:GLU:HA	1:B:330:LEU:HB2	1.97	0.46
1:D:470:VAL:HG13	1:D:475:ASN:HB3	1.97	0.46
1:A:509:ARG:HA	1:A:516:HIS:CD2	2.51	0.46
1:C:196:GLU:HB2	1:C:200:SER:HB3	1.97	0.46
1:C:510:GLU:CD	1:C:510:GLU:H	2.18	0.46
1:D:172:GLU:HG3	1:D:173:PRO:HD2	1.96	0.46
1:D:371:TYR:O	1:D:373:PHE:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:VAL:HA	1:D:450:PHE:HB2	1.97	0.46
1:B:148:THR:O	1:B:152:ARG:HG2	2.16	0.46
1:B:184:THR:HG22	1:B:185:ARG:N	2.30	0.46
1:B:308:GLU:OE2	1:B:350:VAL:HG21	2.15	0.46
1:B:503:LYS:HE2	2:B:601:FAD:P	2.54	0.46
1:C:301:LYS:HE2	3:C:757:HOH:O	2.14	0.46
1:C:304:MET:O	1:C:308:GLU:HG3	2.15	0.46
1:A:316:ARG:HH21	1:A:383:GLU:HG2	1.79	0.46
1:B:442:MET:O	1:B:446:VAL:HG23	2.16	0.46
1:C:422:ASN:ND2	3:C:728:HOH:O	2.48	0.46
1:C:428:HIS:N	1:C:429:PRO:HD3	2.30	0.46
1:A:202:LEU:HD11	1:A:259:ARG:N	2.30	0.46
1:A:244:LEU:HB3	3:A:735:HOH:O	2.14	0.46
1:C:257:GLU:HA	1:C:262:TYR:HE1	1.81	0.46
1:D:96:ALA:HB2	1:D:167:ALA:O	2.16	0.46
1:D:197:ARG:NE	1:D:223:ASN:CB	2.76	0.46
1:D:206:VAL:HG13	1:D:263:THR:CG2	2.29	0.46
1:D:316:ARG:HE	1:D:383:GLU:CD	2.19	0.46
1:D:360:TRP:CD1	1:D:381:ARG:NH2	2.83	0.46
1:A:149:LEU:O	1:A:153:LEU:HG	2.16	0.46
1:B:314:ILE:O	1:B:319:VAL:HG23	2.16	0.46
1:D:211:SER:C	1:D:213:TYR:N	2.69	0.46
1:D:243:LEU:HB3	1:D:249:VAL:HA	1.95	0.46
1:A:160:HIS:CD2	1:A:165:PRO:HD3	2.51	0.46
1:B:450:PHE:HE2	1:B:455:SER:HB2	1.81	0.46
1:B:479:TRP:HD1	1:C:519:LEU:HD12	1.81	0.46
1:A:460:GLU:OE1	1:A:460:GLU:HA	2.15	0.46
1:C:195:PHE:CD1	1:C:221:VAL:HB	2.51	0.46
1:C:291:PRO:HB2	1:C:397:GLN:NE2	2.31	0.46
1:D:75:HIS:HD2	1:D:454:ASP:HB2	1.80	0.46
1:D:213:TYR:HE1	1:D:274:ARG:HD2	1.80	0.46
1:D:375:LYS:HG2	1:D:379:ASP:OD2	2.16	0.46
1:A:414:PHE:O	1:A:418:THR:HG23	2.16	0.46
1:C:37:VAL:HG12	1:C:37:VAL:O	2.14	0.46
1:D:164:TRP:O	1:D:165:PRO:C	2.54	0.46
1:D:192:ALA:O	1:D:218:VAL:HG13	2.16	0.46
1:A:59:GLY:HA2	1:A:130:PHE:HA	1.97	0.46
1:B:197:ARG:HA	1:B:223:ASN:HD22	1.81	0.46
1:C:54:ARG:NH1	1:C:58:LEU:HD12	2.31	0.46
1:D:174:ALA:CB	1:D:221:VAL:HG22	2.38	0.46
1:D:179:ILE:HG13	1:D:221:VAL:HG21	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:O	1:A:110:SER:HB3	2.16	0.45
1:A:365:GLN:OE1	1:A:366:LYS:HG3	2.16	0.45
1:A:509:ARG:NH1	3:A:774:HOH:O	2.48	0.45
1:A:518:GLU:CD	1:A:524:PRO:HA	2.36	0.45
1:B:197:ARG:HB2	1:B:199:ASP:OD1	2.16	0.45
1:C:267:ARG:HA	1:C:272:LEU:CD2	2.45	0.45
1:D:473:PRO:O	1:D:477:ILE:HG13	2.16	0.45
1:A:49:ASP:O	1:A:53:VAL:HG23	2.16	0.45
1:A:54:ARG:O	1:A:58:LEU:HB2	2.16	0.45
1:C:326:GLU:HG2	1:C:327:GLY:N	2.31	0.45
1:C:388:THR:OG1	1:C:390:LYS:O	2.31	0.45
1:D:174:ALA:HB2	1:D:219:ARG:HE	1.82	0.45
1:A:341:ALA:O	1:A:351:GLN:NE2	2.49	0.45
1:C:132:LYS:NZ	1:C:132:LYS:CB	2.79	0.45
1:C:189:ASP:HA	1:C:245:ARG:HB2	1.99	0.45
1:C:517:ASN:HB2	1:C:525:LEU:O	2.16	0.45
1:D:212:GLN:OE1	1:D:276:ALA:HB2	2.16	0.45
1:D:215:ALA:HB3	1:D:272:LEU:CD2	2.46	0.45
1:D:232:PHE:HB2	1:D:234:VAL:CG2	2.46	0.45
1:D:244:LEU:HB2	1:D:248:SER:HG	1.78	0.45
1:D:404:ARG:HA	2:D:601:FAD:H5'2	1.98	0.45
1:A:312:HIS:CE1	1:A:316:ARG:HG3	2.51	0.45
1:B:335:LYS:O	1:B:339:VAL:HG23	2.16	0.45
1:D:216:VAL:HG21	1:D:266:LEU:HD13	1.98	0.45
1:A:195:PHE:HA	1:A:221:VAL:O	2.17	0.45
1:D:185:ARG:HG2	1:D:185:ARG:HH11	1.82	0.45
1:C:165:PRO:HB2	1:C:168:CYS:CB	2.47	0.45
1:D:148:THR:O	1:D:152:ARG:HG2	2.16	0.45
1:D:205:GLU:HB3	1:D:259:ARG:HD2	1.98	0.45
1:D:253:PRO:HG2	1:D:265:TYR:HH	1.76	0.45
1:D:318:GLU:HA	1:D:321:LYS:NZ	2.31	0.45
1:D:414:PHE:O	1:D:418:THR:HG23	2.17	0.45
1:B:440:GLN:HA	1:B:467:MET:CE	2.47	0.45
1:C:518:GLU:OE1	1:C:518:GLU:N	2.45	0.45
1:B:296:PHE:O	1:B:297:ALA:C	2.55	0.45
1:D:343:TYR:O	1:D:420:GLN:HG3	2.17	0.45
1:D:422:ASN:HD22	1:D:536:LYS:HE2	1.82	0.45
1:A:50:ALA:HA	1:A:112:VAL:CG2	2.47	0.45
1:A:168:CYS:HA	1:A:169:PRO:HD3	1.86	0.45
1:B:241:TYR:HD1	1:B:251:ARG:HA	1.82	0.45
1:D:90:VAL:O	1:D:93:TRP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD23	1:A:77:ILE:HA	1.99	0.45
1:B:112:VAL:HG12	1:B:113:CYS:N	2.32	0.45
1:D:128:GLN:O	1:D:129:ALA:C	2.54	0.45
1:D:176:LEU:HB2	1:D:227:ASP:CB	2.47	0.45
1:D:256:VAL:O	1:D:258:SER:N	2.50	0.45
1:A:481:TRP:HH2	1:A:526:TRP:CG	2.35	0.44
1:C:202:LEU:O	1:C:206:VAL:HG23	2.17	0.44
1:A:428:HIS:N	1:A:429:PRO:HD3	2.33	0.44
1:A:538:HIS:HA	1:A:543:ASN:HD22	1.82	0.44
1:C:93:TRP:CE3	1:C:208:LEU:HD13	2.53	0.44
1:C:139:LEU:CD1	1:C:140:PRO:HD2	2.46	0.44
1:D:205:GLU:CB	1:D:259:ARG:HD2	2.47	0.44
1:D:251:ARG:HG3	1:D:252:VAL:H	1.81	0.44
1:B:547:ASP:O	1:B:549:SER:N	2.50	0.44
1:C:97:LEU:HD12	1:C:98:ASN:N	2.32	0.44
1:C:188:ALA:HA	1:C:215:ALA:O	2.17	0.44
1:C:205:GLU:CB	1:C:259:ARG:HD2	2.47	0.44
1:C:345:PRO:HG3	1:C:416:PHE:CE1	2.53	0.44
1:C:387:LEU:O	1:C:388:THR:HG22	2.17	0.44
1:D:264:SER:O	1:D:267:ARG:NE	2.51	0.44
1:D:319:VAL:C	1:D:321:LYS:H	2.19	0.44
1:D:381:ARG:HG3	1:D:381:ARG:HH11	1.83	0.44
1:A:103:ASP:C	1:A:105:ALA:H	2.20	0.44
1:A:144:ALA:HB1	1:A:148:THR:CG2	2.47	0.44
1:B:197:ARG:HG3	1:B:197:ARG:NH1	2.32	0.44
1:B:197:ARG:HA	1:B:223:ASN:ND2	2.31	0.44
1:C:102:LEU:CD2	1:C:112:VAL:HG11	2.47	0.44
1:A:302:ILE:HD12	1:A:538:HIS:O	2.17	0.44
1:A:355:HIS:CE1	1:D:185:ARG:HH22	2.36	0.44
1:B:506:TRP:CG	1:B:507:PRO:HA	2.52	0.44
1:D:190:TYR:OH	1:D:270:PRO:HG2	2.17	0.44
1:D:195:PHE:HB3	1:D:237:PHE:CZ	2.53	0.44
1:B:336:PHE:CZ	1:B:340:LEU:HD11	2.52	0.44
1:D:175:LYS:O	1:D:228:LEU:HD21	2.18	0.44
1:A:195:PHE:CE2	1:A:234:VAL:HG21	2.53	0.44
1:B:245:ARG:N	3:B:721:HOH:O	2.51	0.44
1:D:255:LEU:HD12	1:D:261:PHE:CZ	2.52	0.44
1:A:196:GLU:OE1	1:A:203:GLY:HA3	2.18	0.44
1:A:223:ASN:O	1:A:229:VAL:HG21	2.18	0.44
1:B:399:SER:HB3	1:B:498:ASP:OD1	2.17	0.44
1:C:304:MET:HG3	1:C:308:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:HD22	1:D:133:ASN:HA	2.00	0.44
1:D:215:ALA:CB	1:D:272:LEU:HA	2.48	0.44
1:D:243:LEU:HD23	1:D:243:LEU:N	2.30	0.44
1:B:219:ARG:HG3	1:B:219:ARG:HH11	1.83	0.44
1:B:446:VAL:O	1:B:453:ARG:NH2	2.51	0.44
1:C:139:LEU:HD12	1:C:139:LEU:HA	1.79	0.44
1:C:197:ARG:NH2	3:C:770:HOH:O	2.51	0.44
1:D:65:ALA:HB3	1:D:99:LEU:HD22	1.99	0.44
1:D:188:ALA:O	1:D:245:ARG:HD2	2.17	0.44
1:A:381:ARG:HG3	1:A:381:ARG:NH1	2.33	0.43
1:B:382:LYS:HG2	1:B:385:ALA:CB	2.47	0.43
1:B:507:PRO:HD2	1:B:526:TRP:CZ3	2.53	0.43
1:D:129:ALA:HB2	1:D:165:PRO:HG3	2.00	0.43
1:D:185:ARG:HG2	1:D:185:ARG:NH1	2.33	0.43
1:D:347:GLN:HB3	1:D:348:PRO:HD2	1.98	0.43
1:A:130:PHE:HB2	1:A:163:THR:CG2	2.45	0.43
1:B:75:HIS:ND1	1:B:76:ALA:N	2.65	0.43
1:B:150:ARG:O	1:B:154:ILE:HG13	2.17	0.43
1:C:312:HIS:CE1	1:C:316:ARG:HG3	2.53	0.43
1:D:94:ARG:CD	1:D:98:ASN:OD1	2.66	0.43
1:D:203:GLY:O	1:D:204:ARG:C	2.56	0.43
1:D:223:ASN:OD1	1:D:224:THR:HG23	2.18	0.43
1:D:352:ASN:OD1	1:D:353:PHE:N	2.52	0.43
1:A:313:TYR:CZ	1:A:317:VAL:HG11	2.53	0.43
1:B:176:LEU:HD22	1:B:227:ASP:HB3	2.00	0.43
1:C:375:LYS:HE3	3:C:743:HOH:O	2.18	0.43
1:D:205:GLU:HB3	1:D:259:ARG:NE	2.32	0.43
1:A:387:LEU:O	1:A:388:THR:HG23	2.19	0.43
1:B:480:LEU:HB3	3:B:729:HOH:O	2.18	0.43
1:C:54:ARG:HB3	1:C:55:PRO:CD	2.47	0.43
1:C:252:VAL:HG13	1:C:265:TYR:CG	2.54	0.43
1:C:498:ASP:HB3	1:C:501:PHE:HB2	2.00	0.43
1:D:144:ALA:CB	1:D:149:LEU:HG	2.43	0.43
1:A:138:THR:O	1:A:138:THR:HG22	2.17	0.43
1:A:263:THR:O	1:A:267:ARG:N	2.50	0.43
1:A:273:THR:HG22	1:A:274:ARG:O	2.19	0.43
1:A:377:ALA:O	1:A:381:ARG:NH1	2.52	0.43
1:B:54:ARG:N	1:B:55:PRO:HD2	2.33	0.43
1:B:106:GLU:CG	3:B:714:HOH:O	2.66	0.43
1:D:150:ARG:O	1:D:154:ILE:HG13	2.17	0.43
1:D:256:VAL:HG22	1:D:257:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:HIS:N	1:D:429:PRO:HD3	2.33	0.43
1:A:144:ALA:HB1	1:A:148:THR:CB	2.46	0.43
1:A:478:LEU:HD23	1:A:478:LEU:HA	1.84	0.43
1:C:152:ARG:NH1	1:C:155:ASP:OD2	2.52	0.43
1:B:53:VAL:HG13	1:B:54:ARG:H	1.82	0.43
1:C:61:SER:HA	1:C:130:PHE:CZ	2.53	0.43
1:C:152:ARG:HA	1:C:152:ARG:HD3	1.72	0.43
1:C:190:TYR:OH	1:C:270:PRO:HG2	2.18	0.43
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.80	0.43
1:A:351:GLN:HG3	1:A:355:HIS:CE1	2.54	0.43
1:B:77:ILE:CD1	1:B:495:LEU:HB3	2.49	0.43
1:C:213:TYR:OH	1:C:274:ARG:NH1	2.52	0.43
1:D:67:GLU:OE2	1:D:69:PHE:HB3	2.18	0.43
1:A:38:LEU:H	1:A:38:LEU:CD1	2.31	0.43
1:A:443:ARG:HD3	1:A:463:ALA:HB3	1.99	0.43
1:A:506:TRP:CG	1:A:507:PRO:HA	2.54	0.43
1:B:343:TYR:CE1	1:B:421:ALA:HA	2.53	0.43
1:B:512:CYS:O	1:B:515:CYS:HB2	2.18	0.43
1:D:322:PHE:CZ	1:D:329:ARG:NH2	2.87	0.43
1:A:302:ILE:O	1:A:544:ILE:HA	2.19	0.43
1:A:369:ILE:HG23	1:A:373:PHE:HD2	1.84	0.43
1:B:216:VAL:HG23	1:B:272:LEU:CD2	2.45	0.43
1:B:327:GLY:O	1:B:331:VAL:HG23	2.19	0.43
1:C:532:LEU:HG	1:C:536:LYS:HE3	2.00	0.43
1:D:78:ALA:HA	1:D:495:LEU:HD22	2.01	0.43
1:D:197:ARG:HE	1:D:223:ASN:HB2	1.82	0.43
1:D:267:ARG:NH1	1:D:267:ARG:HB3	2.33	0.43
1:A:404:ARG:NH2	2:A:601:FAD:O3B	2.52	0.42
1:B:219:ARG:HG3	1:B:219:ARG:NH1	2.34	0.42
1:B:352:ASN:OD1	1:B:353:PHE:N	2.52	0.42
1:B:443:ARG:HD3	1:B:463:ALA:HB1	2.00	0.42
1:C:483:SER:O	1:C:487:VAL:HG23	2.19	0.42
1:D:176:LEU:HB2	1:D:227:ASP:HB3	2.01	0.42
1:D:518:GLU:CD	1:D:524:PRO:HA	2.39	0.42
1:B:49:ASP:HB2	1:B:109:ASN:OD1	2.19	0.42
1:B:160:HIS:HB3	1:B:163:THR:O	2.19	0.42
1:C:387:LEU:C	1:C:388:THR:HG22	2.39	0.42
1:D:180:ASP:OD2	1:D:231:LYS:HE2	2.19	0.42
1:D:322:PHE:CE2	1:D:329:ARG:CZ	3.02	0.42
1:A:215:ALA:HB3	1:A:272:LEU:HD23	2.01	0.42
1:A:446:VAL:HA	1:A:450:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:SER:O	1:D:230:ASN:HB2	2.19	0.42
1:B:53:VAL:HG13	1:B:54:ARG:N	2.35	0.42
1:B:428:HIS:HB3	1:B:431:GLU:HG3	2.01	0.42
1:C:354:LEU:HD23	1:C:354:LEU:HA	1.87	0.42
1:C:473:PRO:O	1:C:476:ALA:HB3	2.18	0.42
1:D:125:ARG:HG3	1:D:125:ARG:HH11	1.84	0.42
1:D:206:VAL:HG22	1:D:263:THR:CG2	2.49	0.42
1:D:294:TRP:CE2	1:D:399:SER:HA	2.54	0.42
1:D:294:TRP:CZ3	1:D:295:LYS:HG2	2.54	0.42
1:A:152:ARG:HH11	1:A:152:ARG:CA	2.12	0.42
1:B:96:ALA:HB1	1:B:168:CYS:HB2	2.02	0.42
1:B:399:SER:HB2	1:B:500:HIS:CD2	2.55	0.42
1:C:190:TYR:CD1	1:C:269:LEU:HD13	2.55	0.42
1:C:301:LYS:HD3	1:C:543:ASN:OD1	2.19	0.42
1:C:434:ASP:OD2	1:C:436:GLN:HB2	2.20	0.42
1:D:110:SER:OG	1:D:114:ARG:NH2	2.51	0.42
1:D:259:ARG:CZ	3:D:710:HOH:O	2.67	0.42
1:A:93:TRP:O	1:A:96:ALA:HB3	2.20	0.42
1:A:547:ASP:OD1	1:A:548:SER:N	2.52	0.42
1:B:103:ASP:OD1	1:B:105:ALA:CB	2.67	0.42
1:C:406:PHE:HB3	1:C:407:PRO:HD3	2.01	0.42
1:D:53:VAL:HG21	1:D:102:LEU:HD12	2.02	0.42
1:D:151:MET:O	1:D:155:ASP:OD2	2.37	0.42
1:A:318:GLU:HA	1:A:321:LYS:HZ3	1.85	0.42
1:C:414:PHE:CE2	1:C:442:MET:HG3	2.55	0.42
1:C:419:VAL:HG21	1:C:539:PHE:HB2	2.02	0.42
1:D:103:ASP:C	1:D:105:ALA:H	2.23	0.42
1:D:204:ARG:HD3	1:D:220:ARG:NH1	2.34	0.42
1:D:232:PHE:HB2	1:D:234:VAL:HG23	2.02	0.42
1:A:139:LEU:O	1:A:141:GLY:N	2.53	0.42
1:A:366:LYS:HA	3:A:722:HOH:O	2.20	0.42
1:C:223:ASN:ND2	1:C:224:THR:HG23	2.34	0.42
1:D:221:VAL:HG21	1:D:228:LEU:HD13	2.02	0.42
1:D:360:TRP:HD1	1:D:381:ARG:HH22	1.67	0.42
1:B:431:GLU:H	1:B:431:GLU:HG2	1.57	0.42
1:C:107:GLU:O	1:C:110:SER:CB	2.67	0.42
1:D:205:GLU:CD	1:D:259:ARG:HD2	2.41	0.42
1:B:54:ARG:HB2	1:B:55:PRO:CD	2.50	0.42
1:B:263:THR:O	1:B:267:ARG:HB2	2.19	0.42
1:B:440:GLN:CD	1:B:467:MET:HE2	2.39	0.42
1:D:142:ALA:O	1:D:144:ALA:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ASN:ND2	1:D:148:THR:OG1	2.53	0.42
1:D:223:ASN:O	1:D:229:VAL:HG11	2.20	0.42
1:B:94:ARG:HG2	1:B:97:LEU:O	2.20	0.41
1:B:271:GLY:N	3:B:775:HOH:O	2.50	0.41
1:C:262:TYR:O	1:C:265:TYR:HB3	2.20	0.41
1:D:165:PRO:HB2	1:D:168:CYS:HB3	2.02	0.41
1:D:191:LEU:HA	1:D:217:ALA:O	2.19	0.41
1:D:197:ARG:NH2	1:D:237:PHE:CE1	2.88	0.41
1:A:73:CYS:HB3	1:A:75:HIS:CD2	2.56	0.41
1:A:161:ARG:HB2	3:A:789:HOH:O	2.19	0.41
1:A:379:ASP:C	1:A:381:ARG:H	2.23	0.41
1:B:243:LEU:HD22	1:B:249:VAL:HG22	2.02	0.41
1:B:260:SER:O	1:B:264:SER:HB2	2.21	0.41
1:B:347:GLN:HB3	1:B:348:PRO:HD2	2.02	0.41
1:B:440:GLN:CA	1:B:467:MET:HE1	2.50	0.41
1:C:109:ASN:O	1:C:112:VAL:HB	2.20	0.41
1:B:61:SER:O	1:B:166:PRO:HD2	2.20	0.41
1:B:77:ILE:HD13	1:B:495:LEU:O	2.21	0.41
1:B:198:GLU:OE2	1:B:198:GLU:N	2.54	0.41
1:B:512:CYS:O	1:B:512:CYS:SG	2.78	0.41
1:C:503:LYS:HE3	3:C:741:HOH:O	2.20	0.41
1:D:195:PHE:HB2	1:D:239:SER:OG	2.20	0.41
1:B:232:PHE:HE2	1:B:243:LEU:HD21	1.85	0.41
1:C:176:LEU:HD12	1:C:176:LEU:C	2.39	0.41
1:C:185:ARG:HG2	1:C:185:ARG:HH11	1.86	0.41
1:D:202:LEU:O	1:D:206:VAL:HG23	2.20	0.41
1:B:196:GLU:HB2	1:B:200:SER:CB	2.49	0.41
1:B:277:PRO:N	1:B:278:PRO:HD2	2.35	0.41
1:C:267:ARG:CB	1:C:267:ARG:HH11	2.33	0.41
1:D:223:ASN:O	1:D:229:VAL:HG21	2.21	0.41
1:D:242:LEU:O	1:D:242:LEU:CG	2.69	0.41
1:D:259:ARG:HA	1:D:262:TYR:HB2	2.02	0.41
1:A:240:CYS:O	1:A:251:ARG:HD2	2.20	0.41
1:A:334:LYS:NZ	1:A:361:LEU:O	2.47	0.41
1:A:428:HIS:C	1:A:430:GLN:N	2.73	0.41
1:C:176:LEU:HG	1:C:177:ASN:N	2.36	0.41
1:C:229:VAL:O	1:C:234:VAL:HG23	2.20	0.41
1:D:329:ARG:O	1:D:332:ALA:HB3	2.20	0.41
1:D:343:TYR:CE1	1:D:421:ALA:HA	2.56	0.41
1:A:347:GLN:OE1	1:A:546:ILE:HD12	2.21	0.41
1:B:439:LEU:O	1:B:467:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:GLU:HG3	1:C:317:VAL:HG22	2.03	0.41
1:C:179:ILE:CD1	1:C:193:LEU:HD21	2.50	0.41
1:D:52:SER:O	1:D:55:PRO:HD2	2.21	0.41
1:D:197:ARG:NE	1:D:223:ASN:HB2	2.36	0.41
1:A:38:LEU:N	1:A:38:LEU:CD1	2.83	0.41
1:A:139:LEU:HA	1:A:139:LEU:HD22	1.85	0.41
1:A:204:ARG:HD3	1:A:220:ARG:HH11	1.85	0.41
1:D:54:ARG:N	1:D:55:PRO:HD2	2.35	0.41
1:A:94:ARG:HD2	1:A:98:ASN:OD1	2.20	0.41
1:A:152:ARG:NH1	1:A:152:ARG:CA	2.74	0.41
1:A:298:ASP:C	1:A:300:SER:H	2.23	0.41
1:B:276:ALA:C	1:B:278:PRO:HD2	2.41	0.41
1:B:406:PHE:O	1:B:407:PRO:C	2.58	0.41
1:B:503:LYS:HE2	2:B:601:FAD:O1P	2.19	0.41
1:C:110:SER:O	1:C:112:VAL:N	2.53	0.41
1:C:291:PRO:HB2	1:C:397:GLN:HE22	1.85	0.41
1:C:312:HIS:HE1	3:C:751:HOH:O	2.04	0.41
1:D:175:LYS:C	1:D:228:LEU:HD11	2.42	0.41
1:D:311:LEU:HD21	1:D:340:LEU:HD22	2.02	0.41
1:D:313:TYR:CE1	1:D:317:VAL:HG21	2.56	0.41
1:A:290:ALA:HA	1:A:291:PRO:HD3	1.89	0.41
1:B:406:PHE:CE2	1:B:410:LEU:HD22	2.56	0.41
1:C:205:GLU:HB3	1:C:259:ARG:HD2	2.03	0.41
1:A:61:SER:HA	1:A:130:PHE:CZ	2.56	0.40
1:A:303:TYR:CD2	1:A:394:VAL:HG11	2.56	0.40
1:A:427:ALA:C	1:A:429:PRO:HD3	2.40	0.40
1:A:484:HIS:HD2	1:A:484:HIS:O	2.05	0.40
1:B:349:LEU:O	1:B:352:ASN:OD1	2.38	0.40
1:B:416:PHE:CZ	1:B:544:ILE:HD11	2.56	0.40
1:D:243:LEU:CB	1:D:249:VAL:HA	2.51	0.40
1:D:353:PHE:O	1:D:357:ILE:HG22	2.21	0.40
1:A:358:ASN:O	1:A:362:GLN:HG2	2.21	0.40
1:A:531:THR:O	1:A:532:LEU:C	2.58	0.40
1:C:254:VAL:CG2	1:C:257:GLU:OE1	2.69	0.40
1:D:172:GLU:O	1:D:219:ARG:CZ	2.68	0.40
1:B:157:LEU:O	1:B:160:HIS:ND1	2.52	0.40
1:C:230:ASN:O	1:C:232:PHE:N	2.54	0.40
1:D:49:ASP:OD1	1:D:51:ASP:HB2	2.21	0.40
1:D:205:GLU:HB3	1:D:259:ARG:CD	2.51	0.40
1:A:210:LEU:CD2	1:A:266:LEU:HB3	2.50	0.40
1:A:382:LYS:O	1:A:386:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD11	1:B:334:LYS:HE3	2.03	0.40
1:C:112:VAL:C	1:C:114:ARG:H	2.24	0.40
1:A:546:ILE:CG2	1:A:547:ASP:N	2.57	0.40
1:D:214:HIS:CD2	1:D:273:THR:HG21	2.52	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	497/519 (96%)	441 (89%)	50 (10%)	6 (1%)	11	34
1	B	500/519 (96%)	457 (91%)	37 (7%)	6 (1%)	11	34
1	C	496/519 (96%)	434 (88%)	60 (12%)	2 (0%)	30	61
1	D	494/519 (95%)	402 (81%)	80 (16%)	12 (2%)	5	18
All	All	1987/2076 (96%)	1734 (87%)	227 (11%)	26 (1%)	10	32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	111	ALA
1	D	42	SER
1	D	372	SER
1	A	299	ARG
1	B	227	ASP
1	C	255	LEU
1	D	184	THR
1	D	266	LEU
1	D	299	ARG
1	A	53	VAL
1	A	259	ARG

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Mol	Chain	Res	Type
1	A	380	SER
1	B	437	GLU
1	B	548	SER
1	D	146	VAL
1	D	199	ASP
1	D	257	GLU
1	A	226	SER
1	A	437	GLU
1	D	104	CYS
1	D	191	LEU
1	D	246	ASN
1	B	143	GLY
1	B	183	PHE
1	D	271	GLY
1	B	249	VAL

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	427/441 (97%)	414 (97%)	13 (3%)	36	70
1	B	430/441 (98%)	419 (97%)	11 (3%)	41	75
1	C	426/441 (97%)	400 (94%)	26 (6%)	15	43
1	D	424/441 (96%)	408 (96%)	16 (4%)	28	62
All	All	1707/1764 (97%)	1641 (96%)	66 (4%)	27	61

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	113	CYS
1	A	138	THR
1	A	139	LEU
1	A	152	ARG
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	235	THR
1	A	252	VAL
1	A	365	GLN
1	A	416	PHE
1	A	447	GLN
1	A	495	LEU
1	A	548	SER
1	B	113	CYS
1	B	184	THR
1	B	202	LEU
1	B	219	ARG
1	B	309	SER
1	B	326	GLU
1	B	372	SER
1	B	380	SER
1	B	388	THR
1	B	416	PHE
1	B	549	SER
1	C	45	LEU
1	C	47	LEU
1	C	67	GLU
1	C	113	CYS
1	C	161	ARG
1	C	162	ASP
1	C	176	LEU
1	C	180	ASP
1	C	186	ASN
1	C	196	GLU
1	C	202	LEU
1	C	219	ARG
1	C	223	ASN
1	C	225	GLU
1	C	226	SER
1	C	227	ASP
1	C	326	GLU
1	C	365	GLN
1	C	367	LYS
1	C	388	THR
1	C	416	PHE
1	C	440	GLN
1	C	471	ARG
1	C	473	PRO

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Mol	Chain	Res	Type
1	C	482	THR
1	C	547	ASP
1	D	46	THR
1	D	102	LEU
1	D	104	CYS
1	D	113	CYS
1	D	145	ASN
1	D	162	ASP
1	D	168	CYS
1	D	189	ASP
1	D	197	ARG
1	D	199	ASP
1	D	293	VAL
1	D	326	GLU
1	D	384	ASP
1	D	447	GLN
1	D	495	LEU
1	D	522	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	B	500	HIS
1	C	223	ASN
1	C	447	GLN
1	D	212	GLN
1	D	214	HIS
1	D	538	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	601	-	54,58,58	2.18	12 (22%)	71,89,89	1.23	7 (9%)
2	FAD	B	601	-	54,58,58	2.18	12 (22%)	71,89,89	1.23	7 (9%)
2	FAD	D	601	-	54,58,58	2.30	14 (25%)	71,89,89	1.20	7 (9%)
2	FAD	C	601	-	54,58,58	2.33	15 (27%)	71,89,89	1.19	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	8/30/50/50	0/6/6/6
2	FAD	B	601	-	-	8/30/50/50	0/6/6/6
2	FAD	D	601	-	-	8/30/50/50	0/6/6/6
2	FAD	C	601	-	-	4/30/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C4X-N5	7.29	1.46	1.30
2	C	601	FAD	C4X-N5	7.24	1.46	1.30
2	A	601	FAD	C4X-N5	7.17	1.46	1.30
2	B	601	FAD	C4X-N5	7.15	1.46	1.30
2	D	601	FAD	C2A-N3A	6.33	1.41	1.32
2	C	601	FAD	C2A-N3A	6.10	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4A-N3A	6.06	1.43	1.35
2	D	601	FAD	C4A-N3A	5.92	1.43	1.35
2	A	601	FAD	C2A-N3A	5.77	1.41	1.32
2	B	601	FAD	C2A-N3A	5.74	1.41	1.32
2	A	601	FAD	C9A-N10	5.41	1.50	1.41
2	B	601	FAD	C9A-N10	5.40	1.50	1.41
2	D	601	FAD	C9A-N10	5.31	1.50	1.41
2	B	601	FAD	C4A-N3A	5.21	1.42	1.35
2	A	601	FAD	C4A-N3A	5.20	1.42	1.35
2	C	601	FAD	C9A-N10	5.18	1.50	1.41
2	C	601	FAD	C9A-C5X	4.96	1.49	1.41
2	D	601	FAD	C9A-C5X	4.75	1.48	1.41
2	A	601	FAD	C9A-C5X	4.63	1.48	1.41
2	B	601	FAD	C9A-C5X	4.63	1.48	1.41
2	C	601	FAD	C10-N1	3.33	1.40	1.33
2	C	601	FAD	C5X-N5	3.25	1.45	1.39
2	B	601	FAD	C10-N1	3.12	1.39	1.33
2	A	601	FAD	C10-N1	3.11	1.39	1.33
2	D	601	FAD	C10-N1	3.09	1.39	1.33
2	C	601	FAD	C6-C7	3.08	1.43	1.39
2	D	601	FAD	C6-C7	3.06	1.43	1.39
2	D	601	FAD	C2B-C3B	-2.93	1.45	1.53
2	D	601	FAD	C5X-N5	2.89	1.44	1.39
2	A	601	FAD	C6-C7	2.78	1.43	1.39
2	B	601	FAD	C6-C7	2.77	1.43	1.39
2	A	601	FAD	C8A-N7A	-2.75	1.29	1.34
2	B	601	FAD	C8A-N7A	-2.72	1.29	1.34
2	A	601	FAD	O4B-C1B	2.70	1.44	1.40
2	B	601	FAD	O4B-C1B	2.66	1.44	1.40
2	C	601	FAD	C4-N3	2.57	1.43	1.38
2	D	601	FAD	C4-N3	2.51	1.43	1.38
2	C	601	FAD	O4B-C1B	2.50	1.44	1.40
2	C	601	FAD	C2B-C3B	-2.45	1.46	1.53
2	A	601	FAD	C5X-N5	2.45	1.43	1.39
2	B	601	FAD	C5X-N5	2.45	1.43	1.39
2	C	601	FAD	C8A-N7A	-2.44	1.30	1.34
2	C	601	FAD	O4-C4	2.43	1.28	1.23
2	A	601	FAD	C1B-N9A	-2.43	1.43	1.49
2	B	601	FAD	C1B-N9A	-2.42	1.43	1.49
2	D	601	FAD	C8A-N7A	-2.30	1.30	1.34
2	D	601	FAD	O4-C4	2.28	1.27	1.23
2	B	601	FAD	C9-C9A	2.22	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9-C9A	2.19	1.43	1.39
2	C	601	FAD	C9-C9A	2.18	1.43	1.39
2	D	601	FAD	C9-C9A	2.06	1.43	1.39
2	C	601	FAD	C1B-N9A	-2.03	1.44	1.49
2	D	601	FAD	C2'-C3'	-2.02	1.49	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	FAD	C5X-C9A-N10	-3.76	114.57	117.97
2	D	601	FAD	C5X-C9A-N10	-3.73	114.60	117.97
2	A	601	FAD	C5X-C9A-N10	-3.60	114.71	117.97
2	B	601	FAD	C5X-C9A-N10	-3.57	114.74	117.97
2	A	601	FAD	N3A-C2A-N1A	-2.67	125.05	128.67
2	B	601	FAD	N3A-C2A-N1A	-2.66	125.06	128.67
2	C	601	FAD	N3A-C2A-N1A	-2.64	125.08	128.67
2	B	601	FAD	C1'-C2'-C3'	2.58	116.67	109.66
2	D	601	FAD	C9-C9A-N10	2.57	125.31	121.85
2	A	601	FAD	C1'-C2'-C3'	2.57	116.62	109.66
2	B	601	FAD	C5'-C4'-C3'	2.57	117.06	112.22
2	A	601	FAD	C5'-C4'-C3'	2.55	117.03	112.22
2	A	601	FAD	C9-C9A-N10	2.54	125.27	121.85
2	B	601	FAD	C9-C9A-N10	2.54	125.27	121.85
2	C	601	FAD	C9-C9A-N10	2.50	125.22	121.85
2	A	601	FAD	O2B-C2B-C3B	2.46	119.72	111.82
2	B	601	FAD	O2B-C2B-C3B	2.46	119.71	111.82
2	D	601	FAD	N3A-C2A-N1A	-2.46	125.33	128.67
2	C	601	FAD	C5'-C4'-C3'	2.31	116.58	112.22
2	C	601	FAD	O2B-C2B-C3B	2.30	119.19	111.82
2	C	601	FAD	C1'-C2'-C3'	2.23	115.70	109.66
2	A	601	FAD	C4X-C10-N10	2.22	119.66	116.48
2	B	601	FAD	C4X-C10-N10	2.22	119.65	116.48
2	D	601	FAD	C1'-C2'-C3'	2.16	115.52	109.66
2	C	601	FAD	C6-C5X-C9A	-2.10	116.16	119.05
2	D	601	FAD	C4X-C10-N10	2.07	119.45	116.48
2	C	601	FAD	C4X-C10-N10	2.03	119.39	116.48
2	D	601	FAD	C5'-C4'-C3'	2.02	116.03	112.22
2	D	601	FAD	O3'-C3'-C4'	-2.02	104.35	108.93

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	C5'-O5'-P-O1P
2	C	601	FAD	C5'-O5'-P-O2P
2	C	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5'-O5'-P-O1P
2	D	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	PA-O3P-P-O1P
2	B	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	P-O3P-PA-O1A
2	D	601	FAD	P-O3P-PA-O2A

There are no ring outliers.

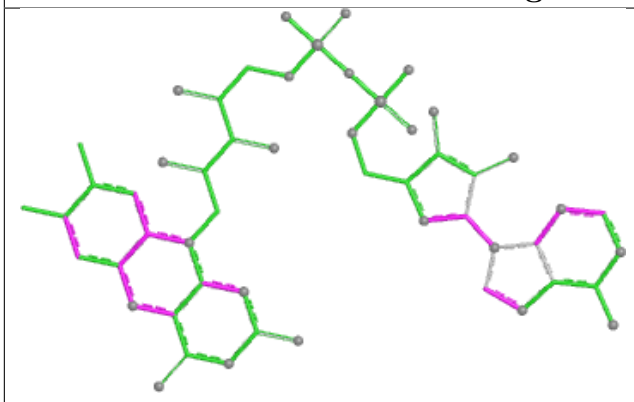
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	2	0
2	B	601	FAD	4	0
2	D	601	FAD	2	0
2	C	601	FAD	1	0

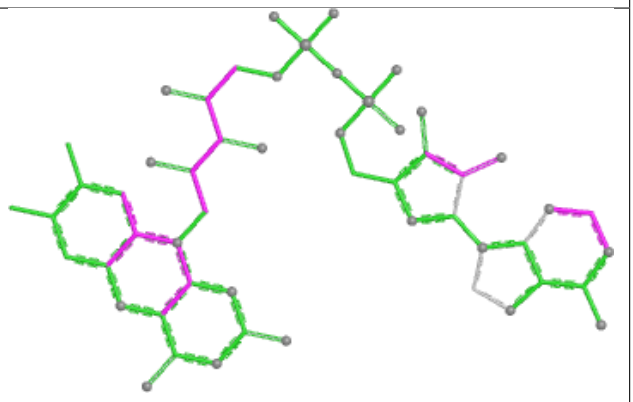
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

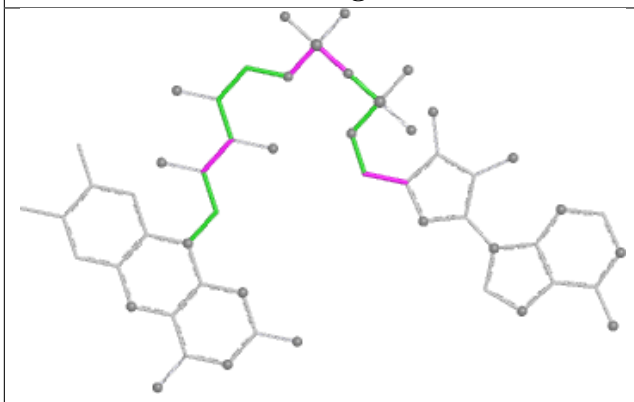
Ligand FAD A 601



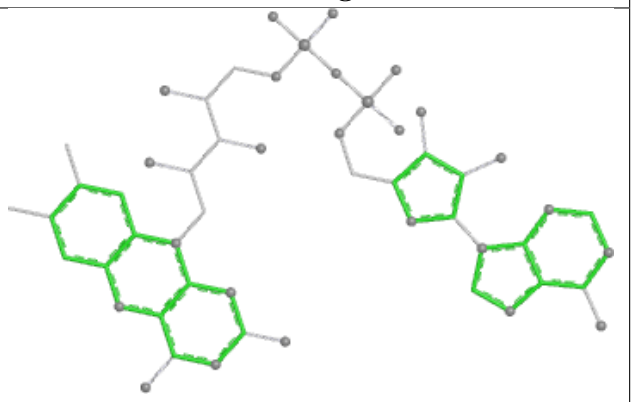
Bond lengths



Bond angles

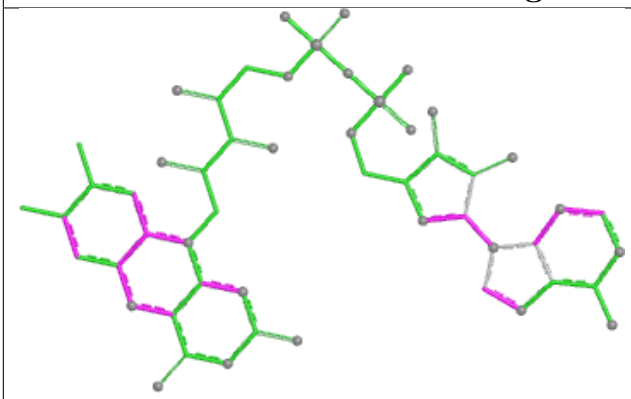


Torsions



Rings

Ligand FAD B 601



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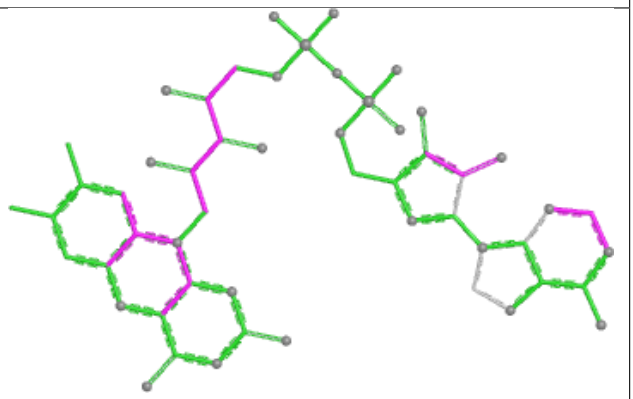
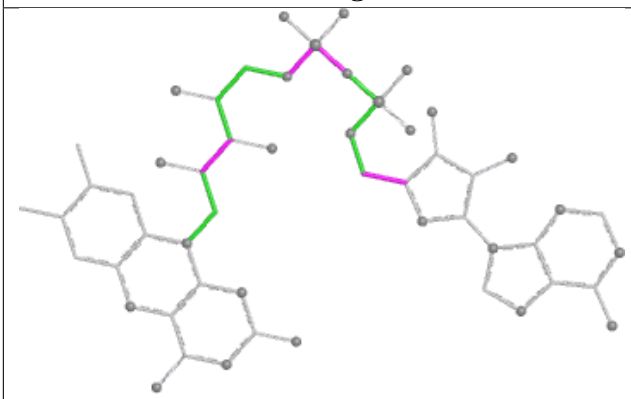
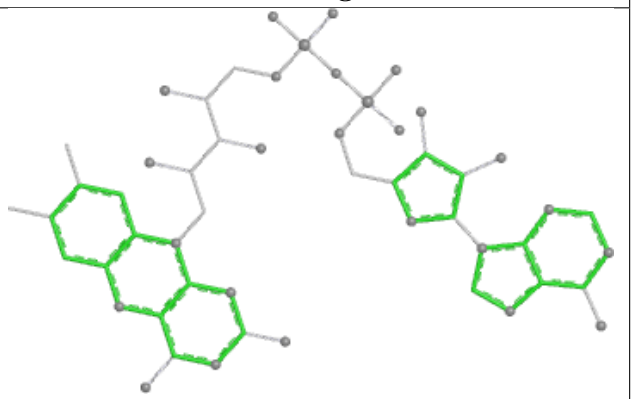


Bond angles

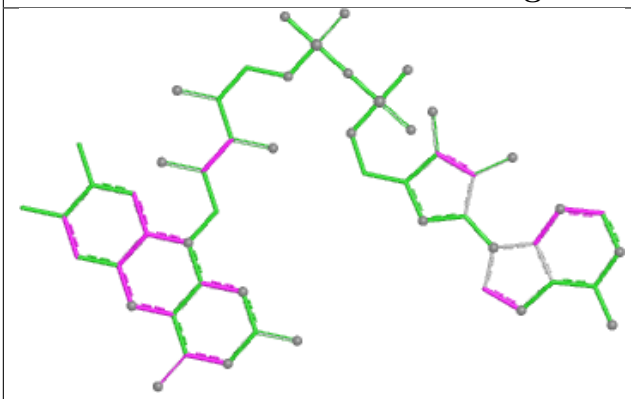


Torsions

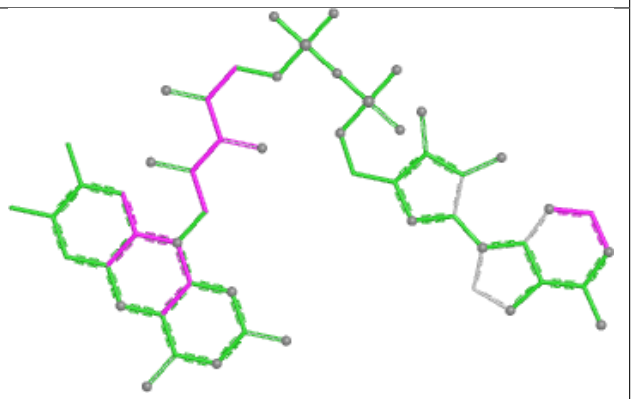


Rings

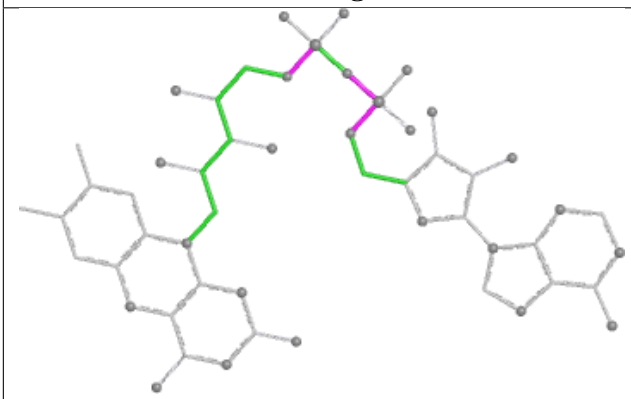
Ligand FAD D 601



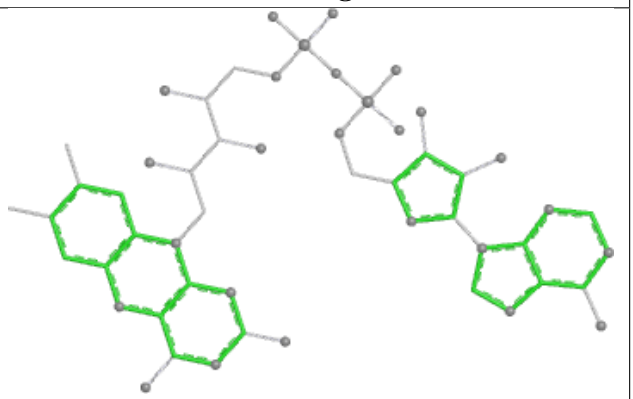
Bond lengths



Bond angles

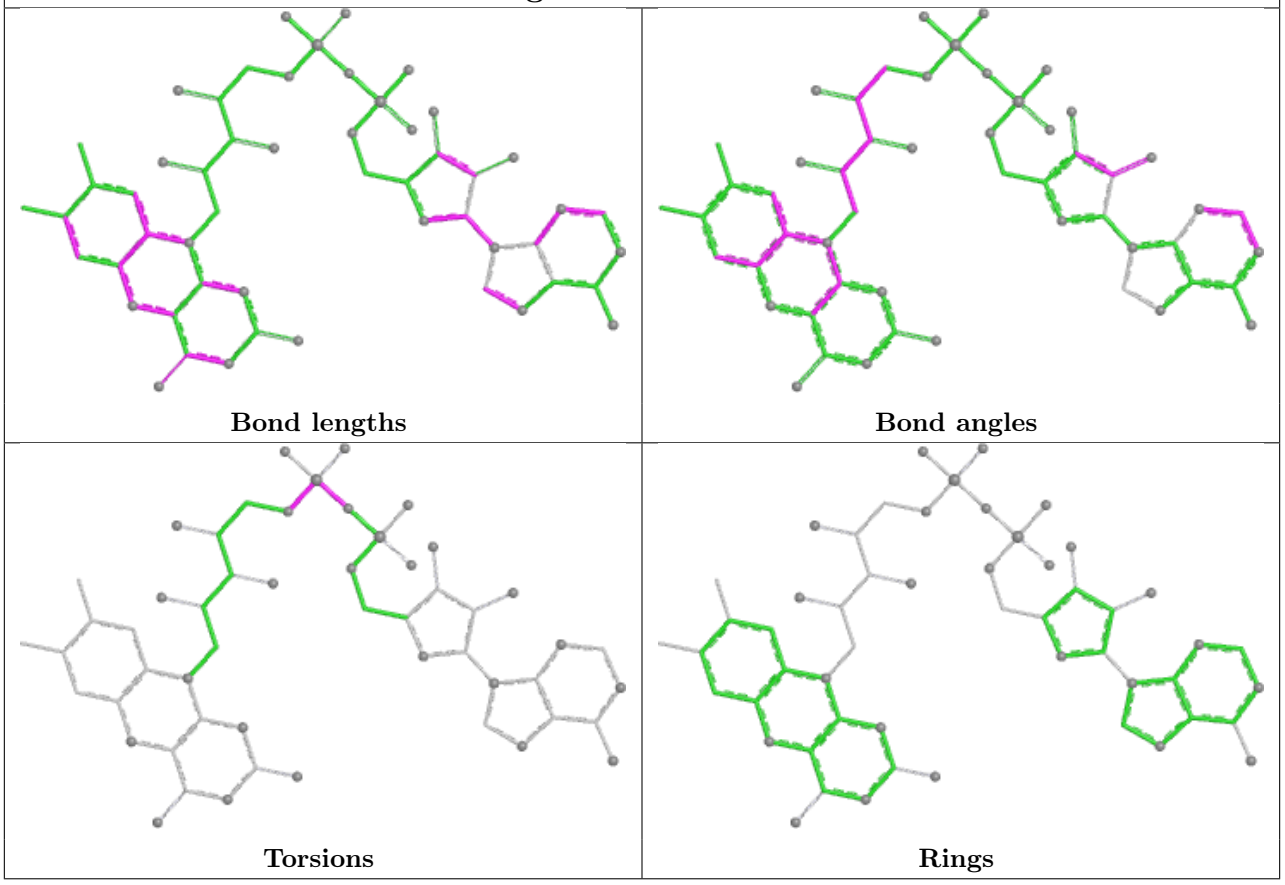


Torsions



Rings

Ligand FAD C 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	501/519 (96%)	-0.16	6 (1%) 76 69	32, 52, 71, 84	1 (0%)
1	B	504/519 (97%)	-0.20	5 (0%) 79 73	24, 49, 79, 94	1 (0%)
1	C	500/519 (96%)	-0.14	12 (2%) 59 51	21, 48, 90, 115	1 (0%)
1	D	498/519 (95%)	0.48	61 (12%) 10 8	34, 63, 144, 151	1 (0%)
All	All	2003/2076 (96%)	-0.01	84 (4%) 41 33	21, 52, 118, 151	4 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	PRO	6.0
1	D	193	LEU	6.0
1	B	433	ALA	5.6
1	D	241	TYR	5.5
1	C	113	CYS	5.0
1	D	191	LEU	4.5
1	D	232	PHE	4.4
1	D	256	VAL	4.2
1	D	239	SER	4.1
1	D	277	PRO	4.0
1	D	266	LEU	4.0
1	D	174	ALA	3.9
1	D	222	LEU	3.9
1	D	192	ALA	3.8
1	D	221	VAL	3.6
1	D	240	CYS	3.6
1	D	244	LEU	3.5
1	D	265	TYR	3.2
1	D	167	ALA	3.2
1	C	227	ASP	3.1
1	D	268	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	255	LEU	3.1
1	B	141	GLY	3.1
1	D	261	PHE	3.0
1	D	178	ASP	2.9
1	C	273	THR	2.9
1	D	217	ALA	2.9
1	D	216	VAL	2.8
1	D	262	TYR	2.8
1	C	256	VAL	2.8
1	D	231	LYS	2.8
1	B	140	PRO	2.7
1	D	237	PHE	2.7
1	D	171	LEU	2.7
1	D	242	LEU	2.7
1	C	548	SER	2.7
1	D	201	TYR	2.7
1	A	276	ALA	2.6
1	D	227	ASP	2.6
1	C	141	GLY	2.5
1	D	146	VAL	2.5
1	A	113	CYS	2.5
1	D	228	LEU	2.5
1	A	289	ILE	2.4
1	D	183	PHE	2.4
1	D	189	ASP	2.4
1	D	203	GLY	2.4
1	D	254	VAL	2.4
1	D	182	PHE	2.4
1	C	277	PRO	2.3
1	C	37	VAL	2.3
1	C	229	VAL	2.3
1	C	176	LEU	2.3
1	D	164	TRP	2.3
1	D	257	GLU	2.3
1	A	548	SER	2.3
1	D	185	ARG	2.3
1	D	173	PRO	2.3
1	D	211	SER	2.3
1	D	272	LEU	2.3
1	D	223	ASN	2.2
1	D	179	ILE	2.2
1	D	198	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	176	LEU	2.2
1	D	169	PRO	2.2
1	D	249	VAL	2.2
1	D	104	CYS	2.2
1	B	142	ALA	2.2
1	B	113	CYS	2.2
1	D	245	ARG	2.2
1	D	148	THR	2.2
1	D	276	ALA	2.2
1	A	256	VAL	2.2
1	D	253	PRO	2.1
1	D	236	ASP	2.1
1	D	186	ASN	2.1
1	A	104	CYS	2.1
1	D	175	LYS	2.1
1	D	252	VAL	2.0
1	D	224	THR	2.0
1	D	226	SER	2.0
1	C	230	ASN	2.0
1	C	228	LEU	2.0
1	D	195	PHE	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
2	FAD	A	601	53/53	0.93	0.11	36,52,57,58	0
2	FAD	B	601	53/53	0.95	0.09	26,45,54,56	0

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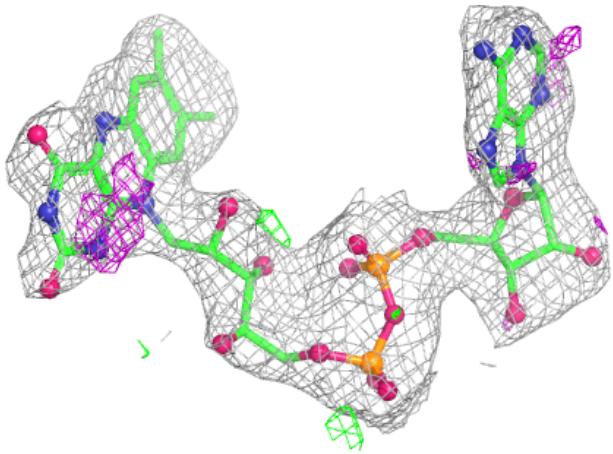
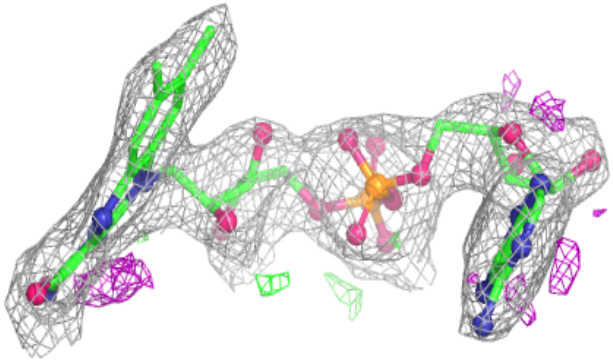
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	C	601	53/53	0.96	0.08	28,42,53,55	0
2	FAD	D	601	53/53	0.96	0.09	34,56,65,66	0

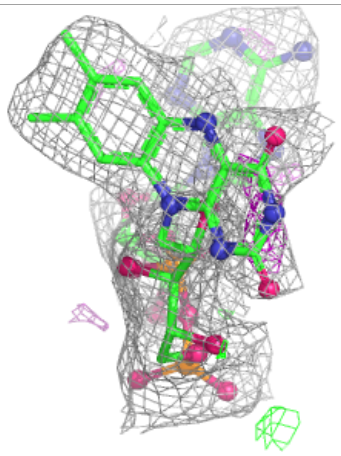
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 601:

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

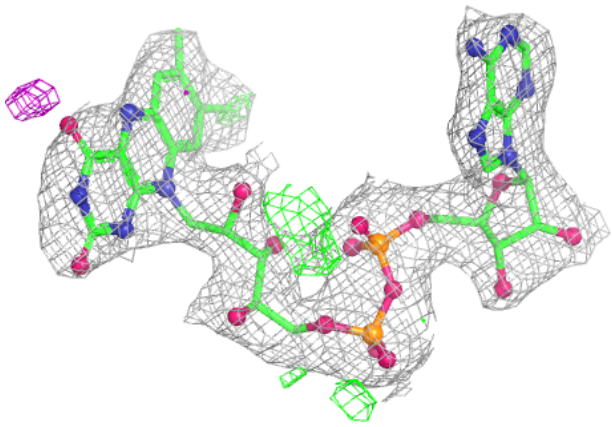


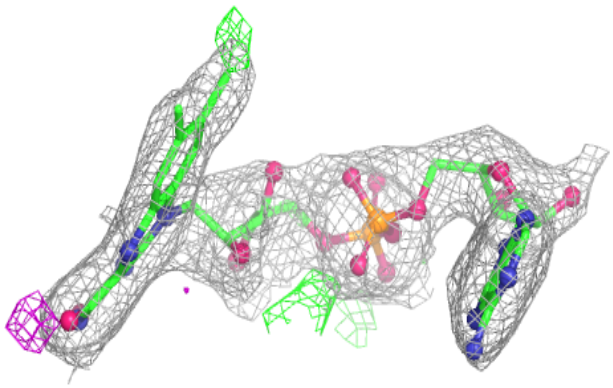


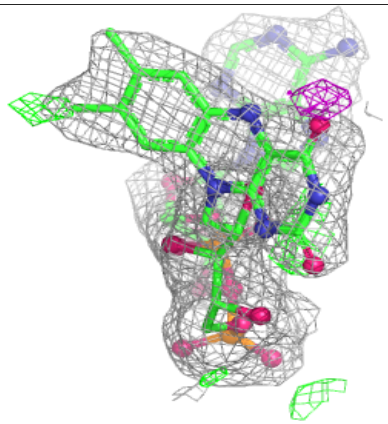


Electron density around FAD B 601:

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

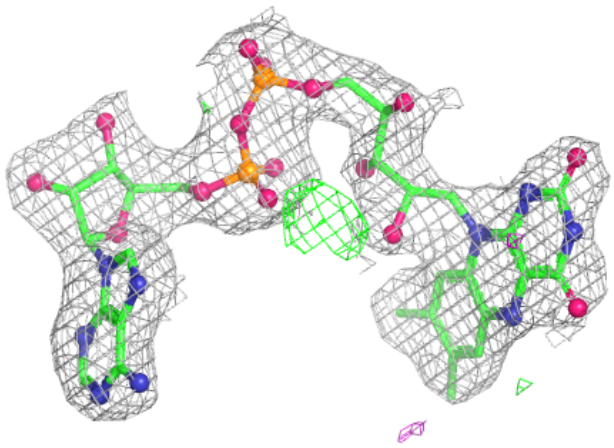


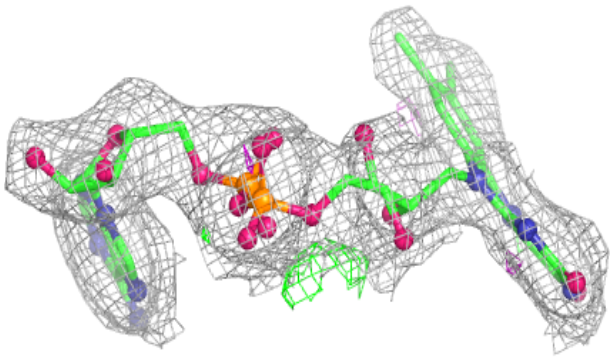


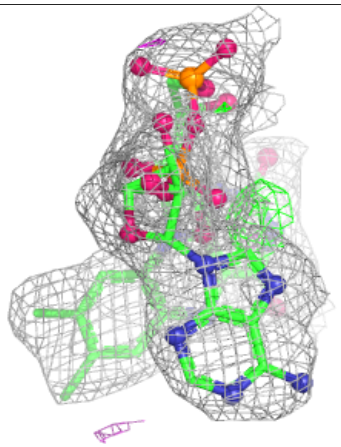


Electron density around FAD C 601:

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

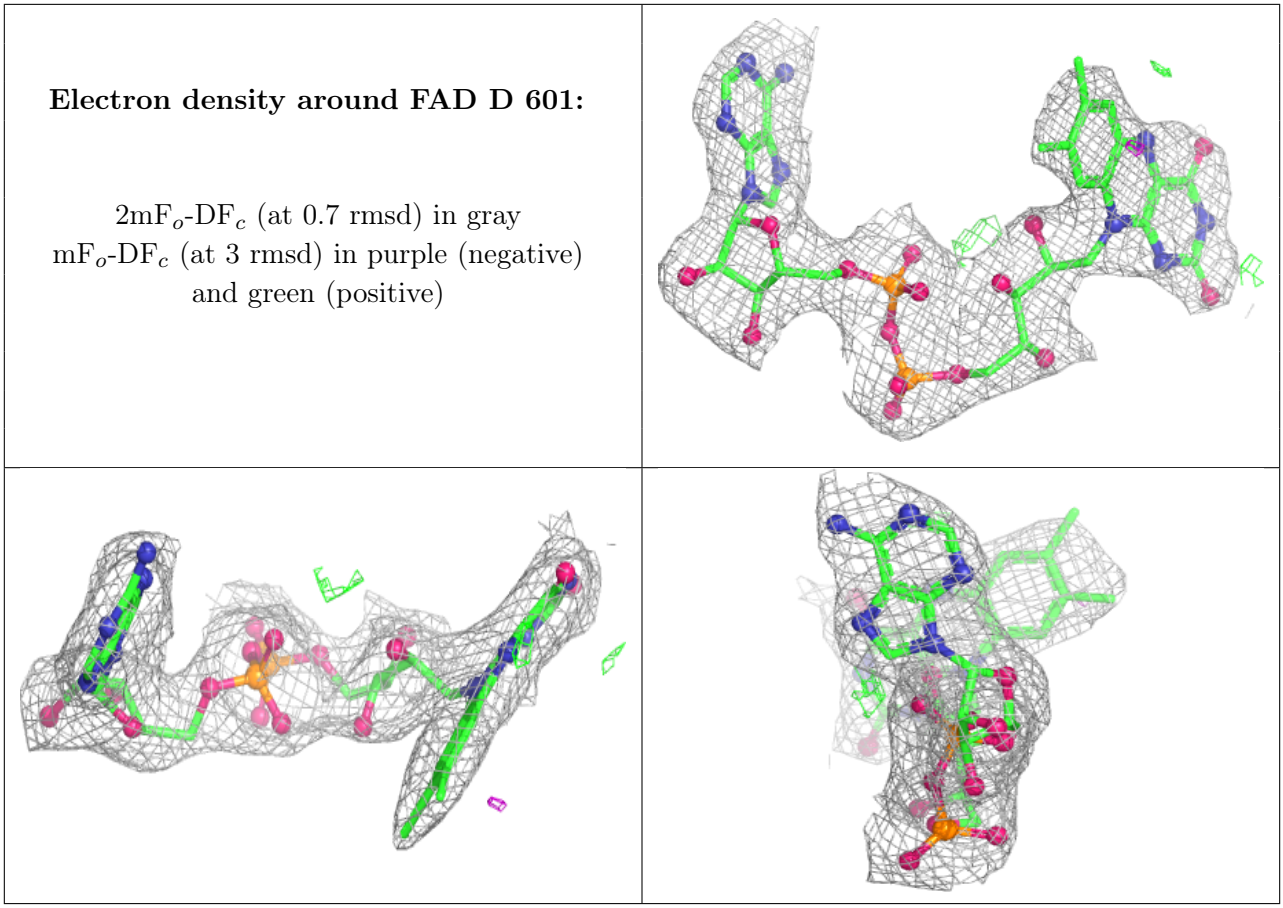






Electron density around FAD D 601:

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



6.5 Other polymers

There are no such residues in this entry.