



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

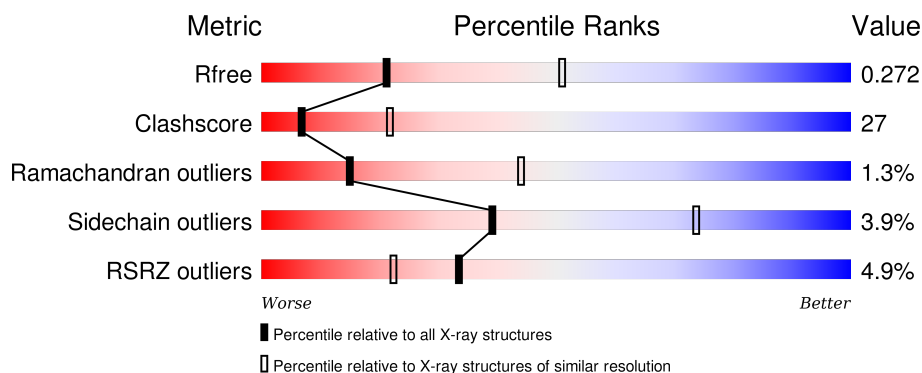
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div></div> <div>56%38% . .</div> </div>
1	B	519	<div> <div>%</div> <div>55%40% . .</div> </div>
1	C	519	<div> <div>4%</div> <div>57%35% . .</div> </div>
1	D	519	<div> <div>14%</div> <div>45%47% . .</div> </div>

2 Entry composition

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:

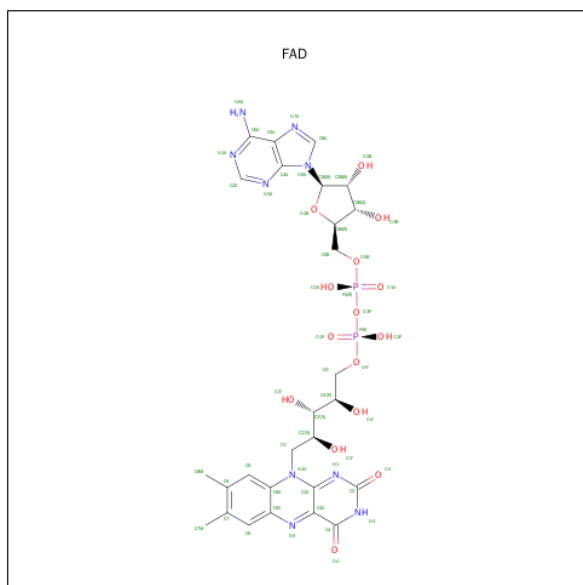
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	EXPRESSION TAG	UNP Q8BND5
A	33	SER	-	EXPRESSION TAG	UNP Q8BND5
A	34	HIS	-	EXPRESSION TAG	UNP Q8BND5
A	35	MET	-	EXPRESSION TAG	UNP Q8BND5
A	76	ALA	CYS	ENGINEERED MUTATION	UNP Q8BND5
A	455	SER	CYS	ENGINEERED MUTATION	UNP Q8BND5
B	32	GLY	-	EXPRESSION 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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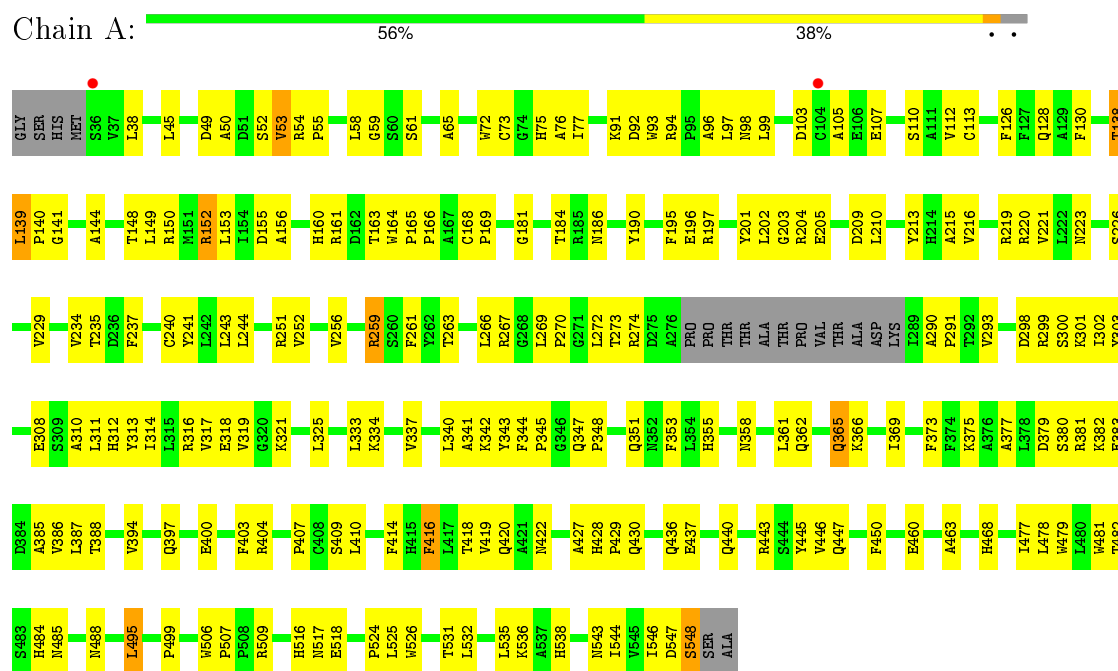
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	58	Total	O	0	0
			58	58		

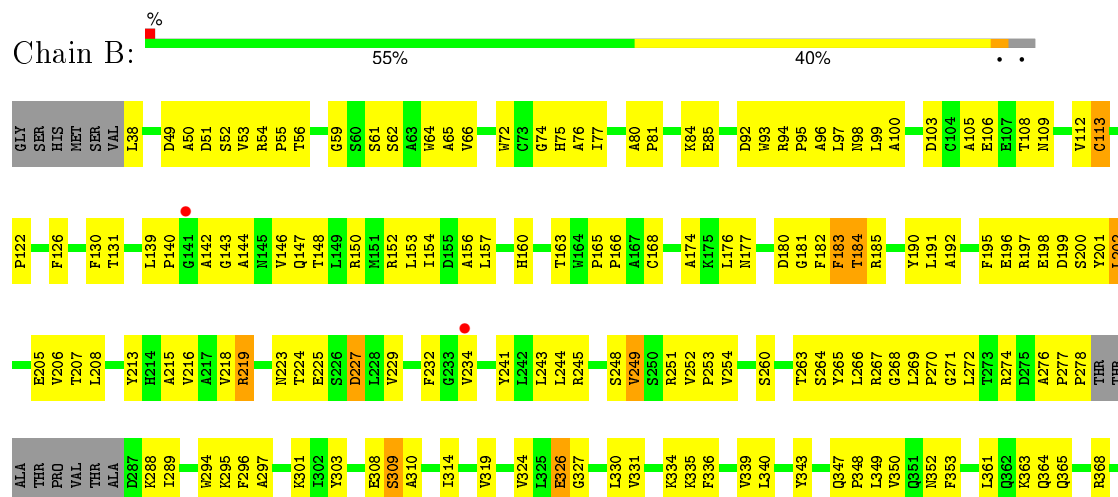
3 Residue-property plots

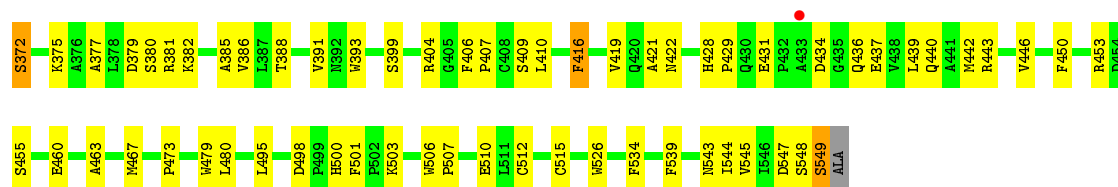
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

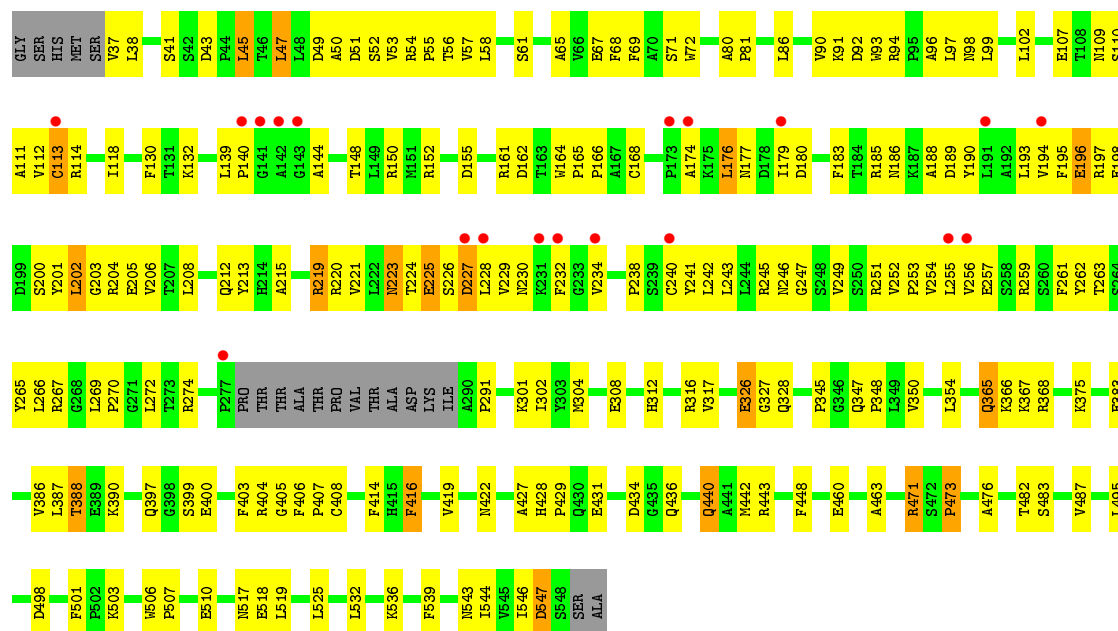


• Molecule 1: Sulfhydryl oxidase 1

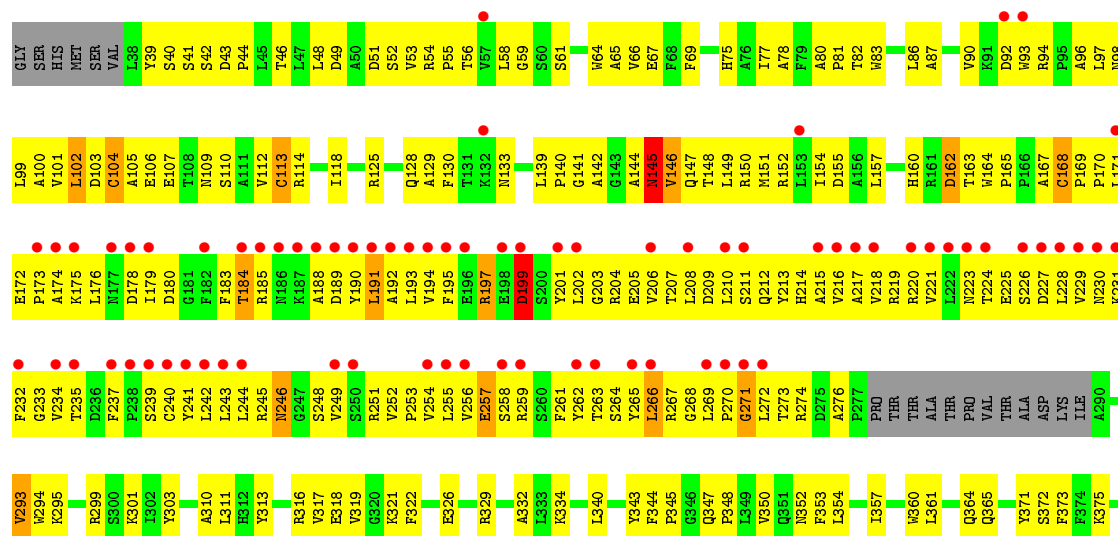


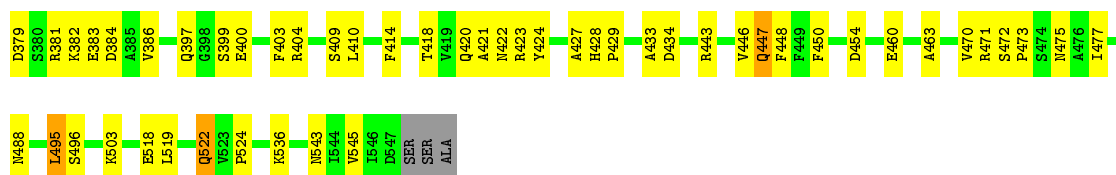


● Molecule 1: Sulfhydryl oxidase 1



● Molecule 1: Sulfhydryl oxidase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70 Å 212.14 Å 148.48 Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.17 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.80) 97.0 (49.17-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.77 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.271 0.218 , 0.272	Depositor DCC
R_{free} test set	4455 reflections (7.09%)	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63776 reflections	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(°)	Ideal(°)
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 [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	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:B:65:ALA:HB3	1:B:99:LEU:HD22	1.50	0.94
1:A:316:ARG:HH21	1:A:383:GLU:HG3	1.33	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:NH1	1:A:152:ARG:HA	1.89	0.86
1:D:174:ALA:HB3	1:D:221:VAL:HG22	1.60	0.84
1:A:495:LEU:HD12	1:A:495:LEU:H	1.41	0.84
1:C:150:ARG:HD3	1:C:259:ARG:HH12	1.42	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:B:382:LYS:O	1:B:386:VAL:HG23	1.79	0.81
1:A:416:PHE:HE1	1:A:420:GLN:HE21	1.27	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:D:179:ILE:HB	1:D:228:LEU:HD22	1.62	0.80
1:C:183:PHE:HB3	1:C:245:ARG:HH12	1.45	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:C:174:ALA:HB2	1:C:219:ARG:HG3	1.65	0.78
1:B:197:ARG:HG2	1:B:223:ASN:ND2	1.98	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:245:ARG:HG3	1:C:245:ARG:HH11	1.47	0.77
1:C:243:LEU:HD22	1:C:249:VAL:HG22	1.67	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: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:49:ASP:O	1:D:53:VAL:HG23	1.85	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:H	1:D:495:LEU:HD12	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:B:324:VAL:HG11	1:B:368:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:HB2	1:A:163:THR:HG21	1.72	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:183:PHE:HB3	1:C:245:ARG:NH1	2.07	0.69
1:C:52:SER:O	1:C:56:THR:HG23	1.92	0.69
1:A:410:LEU:HD23	2:A:601:FAD:HM83	1.76	0.68
1:C:150:ARG:HD3	1:C:259:ARG:NH1	2.08	0.68
1:B:160:HIS:CD2	1:B:165:PRO:HD3	2.29	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:D:264:SER:HA	1:D:267:ARG:NH2	2.10	0.67
1:B:150:ARG:NH1	1:B:205:GLU:OE2	2.27	0.67
1:A:210:LEU:HD21	1:A:266:LEU:HB3	1.76	0.67
1:B:270:PRO:HA	3:B:775:HOH:O	1.94	0.67
1:A:310:ALA:HB2	1:A:409:SER:HB2	1.75	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:D:53:VAL:O	1:D:56:THR:HG22	1.95	0.66
1:C:223:ASN:H	1:C:223:ASN:ND2	1.93	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:D:193:LEU:O	1:D:240:CYS:HA	1.96	0.66
1:C:65:ALA:HB3	1:C:99:LEU:HD22	1.76	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:D:194:VAL:HA	1:D:239:SER:O	1.97	0.64
1:C:400:GLU:HB2	1:C:403:PHE:HD2	1.63	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:399:SER:O	1:C:400:GLU:HG2	1.98	0.63
1:C:91:LYS:HB2	1:C:94:ARG:NH2	2.13	0.63
1:D:257:GLU:HA	1:D:262:TYR:CE1	2.33	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: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:C:245:ARG:NH1	1:C:245:ARG:HG3	2.12	0.62
1:A:38:LEU:HD12	1:A:38:LEU:N	2.14	0.62
1:D:179:ILE:HD12	1:D:193:LEU:CD2	2.22	0.62
1:C:139:LEU:HD12	1:C:140:PRO:HD2	1.82	0.62
1:C:195:PHE:O	1:C:238:PRO:HA	2.00	0.62
1:B:510:GLU:H	1:B:510:GLU:CD	2.03	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:D:267:ARG:CG	1:D:268:GLY:H	2.10	0.61
1:D:78:ALA:O	1:D:81:PRO:HD2	2.01	0.61
1:A:130:PHE:CD1	1:B:372:SER:HB2	2.36	0.61
1:A:165:PRO:HB2	1:A:168:CYS:HB3	1.81	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:C:96:ALA:HB1	1:C:168:CYS:HB2	1.83	0.61
1:D:94:ARG:HG2	1:D:97:LEU:O	2.01	0.61
1:D:214:HIS:HD2	1:D:273:THR:HG21	1.66	0.60
1:A:495:LEU:CD1	1:A:495:LEU:H	2.13	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:C:225:GLU:HB2	1:C:229:VAL:HG23	1.83	0.60
1:A:400:GLU:HB2	1:A:403:PHE:CD2	2.36	0.60
1:D:210:LEU:HD12	1:D:216:VAL:HG11	1.84	0.60
1:C:213:TYR:CZ	1:C:274:ARG:HD2	2.37	0.60
1:D:92:ASP:HA	1:D:212:GLN:HE21	1.66	0.60
1:B:365:GLN:CD	1:B:365:GLN:H	2.05	0.60
1:D:240:CYS:HB3	1:D:252:VAL:HG21	1.83	0.60
1:D:160:HIS:HB3	1:D:163:THR:O	2.02	0.60
1:B:202:LEU:O	1:B:206:VAL:HG23	2.00	0.60
1:B:440:GLN:HA	1:B:467:MET:HE1	1.83	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:C:196:GLU:OE1	1:C:203:GLY:N	2.35	0.59
1:B:365:GLN:N	1:B:365:GLN:OE1	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: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:A:150:ARG:HD2	1:A:205:GLU:OE2	2.02	0.59
1:D:310:ALA:HB2	1:D:409:SER:HB2	1.85	0.59
1:C:52:SER:O	1:C:55:PRO:HG2	2.03	0.59
1:B:268:GLY:O	1:B:269:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:HD13	1:C:69:PHE:HE2	1.67	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:225:GLU:HA	1:C:225:GLU:OE1	2.04	0.58
1:C:190:TYR:HB3	1:C:242:LEU:HD11	1.85	0.58
1:D:174:ALA:H	1:D:221:VAL:HA	1.69	0.58
1:D:176:LEU:HB2	1:D:227:ASP:CG	2.24	0.58
1:B:177:ASN:O	1:B:185:ARG:NH2	2.37	0.58
1:A:50:ALA:HA	1:A:112:VAL:HG21	1.85	0.58
1:C:189:ASP:HA	1:C:245:ARG:HD2	1.85	0.58
1:C:68:PHE:CE1	1:C:102:LEU:HD23	2.38	0.58
1:B:336:PHE:CE2	1:B:340:LEU:HD11	2.39	0.58
1:C:256:VAL:HG12	1:C:261:PHE:CE2	2.38	0.58
1:D:174:ALA:HB3	1:D:221:VAL:CG2	2.32	0.57
1:C:107:GLU:O	1:C:110:SER:HB3	2.04	0.57
1:C:41:SER:C	1:C:43:ASP:H	2.08	0.57
1:C:164:TRP:O	1:C:166:PRO:HD3	2.04	0.57
1:A:482:THR:HA	3:A:761:HOH:O	2.03	0.57
1:D:101:VAL:O	1:D:101:VAL:HG23	2.04	0.57
1:A:365:GLN:CD	1:A:365:GLN:H	2.07	0.57
1:C:241:TYR:CE1	1:C:251:ARG:HB2	2.40	0.57
1:A:485:ASN:HA	1:A:488:ASN:HD22	1.69	0.57
1:D:240:CYS:SG	1:D:262:TYR:HE2	2.26	0.57
1:A:38:LEU:H	1:A:38:LEU:HD12	1.69	0.57
1:C:240:CYS:HB2	1:C:262:TYR:CE2	2.39	0.57
1:B:301:LYS:HD3	1:B:543:ASN:OD1	2.05	0.57
1:B:54:ARG:HG3	3:B:707:HOH:O	2.04	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:C:366:LYS:HE3	1:C:368:ARG:HB3	1.86	0.57
1:B:216:VAL:CG2	1:B:272:LEU:HD21	2.35	0.57
1:D:146:VAL:HA	1:D:149:LEU:HD12	1.86	0.56
1:C:267:ARG:CZ	1:C:267:ARG:HB3	2.35	0.56
1:C:443:ARG:HD2	1:C:460:GLU:OE1	2.04	0.56
1:A:75:HIS:ND1	1:A:76:ALA:N	2.53	0.56
1:C:443:ARG:HD3	1:C:463:ALA:HB1	1.86	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:B:183:PHE:HZ	1:B:243:LEU:O	1.88	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:C:252:VAL:HG22	1:C:265:TYR:CE2	2.40	0.56
1:B:252:VAL:HG13	1:B:265:TYR:CD2	2.40	0.56
1:D:169:PRO:HG2	1:D:207:THR:HG22	1.86	0.56
1:D:427:ALA:O	1:D:429:PRO:HD3	2.05	0.56
1:A:234:VAL:HG22	1:A:241:TYR:CE1	2.41	0.56
1:C:223:ASN:N	1:C:223:ASN:HD22	2.03	0.56
1:A:353:PHE:CB	1:A:386:VAL:HG11	2.36	0.56
1:D:350:VAL:HA	1:D:386:VAL:CG1	2.36	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:B:181:GLY:O	1:B:184:THR:HB	2.06	0.55
1:A:164:TRP:O	1:A:166:PRO:HD3	2.06	0.55
1:D:434:ASP:HB2	1:D:471:ARG:NH2	2.21	0.55
1:D:271:GLY:O	1:D:272:LEU:HG	2.07	0.55
1:D:82:THR:HG23	1:D:146:VAL:HG22	1.87	0.55
1:C:252:VAL:HG12	1:C:254:VAL:HG13	1.87	0.55
1:C:72:TRP:CE3	1:C:407:PRO:HG3	2.42	0.55
1:D:244:LEU:HD13	1:D:246:ASN:HD21	1.70	0.55
1:B:213:TYR:OH	1:B:274:ARG:HD2	2.06	0.55
1:A:140:PRO:HB2	1:A:152:ARG:CD	2.32	0.55
1:D:265:TYR:O	1:D:267:ARG:N	2.39	0.55
1:B:382:LYS:HG2	1:B:385:ALA:HB3	1.88	0.55
1:B:266:LEU:O	1:B:269:LEU:HG	2.06	0.55
1:C:350:VAL:HA	1:C:386:VAL:CG1	2.36	0.55
1:D:433:ALA:HB1	1:D:473:PRO:CD	2.37	0.55
1:C:431:GLU:HG2	3:C:786:HOH:O	2.07	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:O	1:D:184:THR:HG22	2.07	0.55
1:A:422:ASN:ND2	1:A:536:LYS:HE2	2.21	0.55
1:D:227:ASP:O	1:D:228:LEU:HD23	2.07	0.55
1:D:61:SER:HA	1:D:130:PHE:CE2	2.42	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:252:VAL:HG12	1:D:254:VAL:HG13	1.90	0.54
1:D:209:ASP:CG	1:D:259:ARG:HH21	2.11	0.54
1:D:141:GLY:O	1:D:144:ALA:HB2	2.08	0.54
1:D:107:GLU:HG3	1:D:317:VAL:HG22	1.90	0.54
1:D:102:LEU:HD13	1:D:112:VAL:HG11	1.89	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:C:223:ASN:H	1:C:223:ASN:HD22	1.56	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: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:D:433:ALA:HB1	1:D:473:PRO:CG	2.37	0.54
1:A:517:ASN:HB2	1:A:525:LEU:O	2.08	0.54
1:B:93:TRP:CE3	1:B:208:LEU:HD13	2.43	0.53
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:C:267:ARG:HA	1:C:272:LEU:HD23	1.89	0.53
1:C:90:VAL:O	1:C:93:TRP:HB2	2.07	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: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: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: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:O	1:C:45:LEU:HD12	2.08	0.53
1:B:309:SER:HB3	1:B:393:TRP:CZ3	2.44	0.53
1:A:52:SER:O	1:A:55:PRO:HG2	2.09	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:D:410:LEU:HD23	2:D:601:FAD:HM83	1.91	0.53
1:C:532:LEU:O	1:C:536:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ASN:ND2	1:D:536:LYS:HE2	2.24	0.53
1:C:132:LYS:HZ2	1:C:132:LYS:HB2	1.74	0.53
1:D:344:PHE:CD1	1:D:345:PRO:HD2	2.44	0.53
1:B:303:TYR:CD1	1:B:545:VAL:HB	2.43	0.53
1:D:173:PRO:HA	1:D:220:ARG:HG3	1.90	0.52
1:B:498:ASP:HB3	1:B:501:PHE:HB2	1.90	0.52
1:A:436:GLN:O	1:A:440:GLN:HB2	2.09	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:C:471:ARG:HH11	1:C:471:ARG:HG2	1.74	0.52
1:D:211:SER:C	1:D:213:TYR:H	2.12	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:420:GLN:OE1	1:D:423:ARG:HD3	2.10	0.52
1:A:204:ARG:HD3	1:A:220:ARG:NH1	2.24	0.52
1:D:39:TYR:OH	1:D:80:ALA:HA	2.08	0.52
1:B:243:LEU:CD2	1:B:249:VAL:HG13	2.39	0.52
1:B:52:SER:O	1:B:56:THR:HG23	2.09	0.52
1:D:147:GLN:HG2	1:D:150:ARG:NH2	2.24	0.52
1:A:140:PRO:HA	3:A:710:HOH:O	2.09	0.52
1:D:443:ARG:HD3	1:D:463:ALA:HB1	1.92	0.52
1:D:257:GLU:HA	1:D:262:TYR:HE1	1.72	0.52
1:C:215:ALA:HB3	1:C:272:LEU:HD12	1.92	0.52
1:B:140:PRO:HG3	1:B:152:ARG:HD2	1.91	0.52
1:A:92:ASP:CG	1:A:274:ARG:HH21	2.13	0.52
1:D:254:VAL:HG21	1:D:262:TYR:HE1	1.71	0.52
1:C:267:ARG:NH1	1:C:267:ARG:CB	2.72	0.52
1:C:267:ARG:NH1	1:C:267:ARG:HB3	2.24	0.52
1:C:443:ARG:HD3	1:C:463:ALA:CB	2.39	0.52
1:B:310:ALA:HB2	1:B:409:SER:HB2	1.91	0.52
1:D:256:VAL:HG13	1:D:258:SER:OG	2.09	0.52
1:C:223:ASN:O	1:C:229:VAL:HG21	2.09	0.52
1:C:206:VAL:HG13	1:C:263:THR:HG22	1.91	0.52
1:D:215:ALA:HB3	1:D:272:LEU:HD23	1.92	0.52
1:B:547:ASP:OD1	1:B:549:SER:HB3	2.09	0.52
1:B:85:GLU:CD	1:B:146:VAL:HG21	2.29	0.52
1:D:267:ARG:HH11	1:D:267:ARG:HB2	1.75	0.51
1:D:130:PHE:HB2	1:D:163:THR:HG21	1.91	0.51
1:C:213:TYR:CE1	1:C:274:ARG:HD2	2.44	0.51
1:A:148:THR:O	1:A:152:ARG:HG2	2.10	0.51
1:D:183:PHE:CE1	1:D:245:ARG:HA	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ASN:OD1	1:C:247:GLY:N	2.43	0.51
1:D:447:GLN:HG2	1:D:448:PHE:CE2	2.44	0.51
1:C:102:LEU:HD21	1:C:112:VAL:HG11	1.91	0.51
1:B:377:ALA:O	1:B:381:ARG:NH1	2.41	0.51
1:D:519:LEU:HB2	1:D:522:GLN:OE1	2.09	0.51
1:A:54:ARG:N	1:A:55:PRO:HD2	2.26	0.51
1:A:209:ASP:OD2	1:A:263:THR:HG21	2.11	0.51
1:A:181:GLY:O	1:A:184:THR:HB	2.09	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: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: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:D:221:VAL:HG11	1:D:228:LEU:HD12	1.93	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:A:334:LYS:HD2	3:A:739:HOH:O	2.10	0.51
1:D:194:VAL:HG13	1:D:240:CYS:SG	2.51	0.50
1:D:113:CYS:CB	1:D:118:ILE:HB	2.41	0.50
1:A:538:HIS:HA	1:A:543:ASN:ND2	2.26	0.50
1:A:308:GLU:HB3	1:A:387:LEU:HD22	1.93	0.50
1:C:302:ILE:O	1:C:544:ILE:HA	2.11	0.50
1:D:365:GLN:HA	3:D:749:HOH:O	2.11	0.50
1:D:171:LEU:HB3	1:D:204:ARG:HG2	1.93	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:223:ASN:HA	1:D:237:PHE:CZ	2.46	0.50
1:B:126:PHE:CD2	1:B:156:ALA:HB1	2.46	0.50
1:C:206:VAL:HG13	1:C:263:THR:HG23	1.93	0.50
1:A:197:ARG:NH1	1:A:237:PHE:HB2	2.26	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:D:197:ARG:CZ	1:D:223:ASN:HB2	2.40	0.50
1:A:73:CYS:O	1:A:76:ALA:HB3	2.12	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
1:B:375:LYS:NZ	1:B:379:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HA	1:A:321:LYS:NZ	2.26	0.50
1:A:443:ARG:HD3	1:A:463:ALA:HB1	1.92	0.50
1:C:254:VAL:HG23	1:C:257:GLU:OE1	2.12	0.50
1:B:182:PHE:CG	1:B:191:LEU:HD22	2.46	0.50
1:D:303:TYR:CD1	1:D:545:VAL:HB	2.46	0.50
1:D:253:PRO:HG2	1:D:265:TYR:CZ	2.47	0.50
1:D:149:LEU:O	1:D:152:ARG:N	2.45	0.50
1:A:128:GLN:HG3	3:A:726:HOH:O	2.11	0.50
1:C:47:LEU:N	1:C:47:LEU:HD23	2.27	0.50
1:B:440:GLN:NE2	1:B:467:MET:HE2	2.27	0.50
1:B:64:TRP:CZ3	1:B:98:ASN:HB3	2.46	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:D:174:ALA:O	1:D:225:GLU:HG2	2.12	0.49
1:C:38:LEU:HD13	1:C:69:PHE:CE2	2.47	0.49
1:A:422:ASN:HD22	1:A:536:LYS:HE2	1.77	0.49
1:C:405:GLY:O	1:C:408:CYS:HB3	2.12	0.49
1:D:261:PHE:O	1:D:264:SER:HB3	2.12	0.49
1:C:144:ALA:HB1	1:C:148:THR:HB	1.94	0.49
1:B:80:ALA:HB3	1:B:81:PRO:HD3	1.95	0.49
1:D:174:ALA:HB1	1:D:178:ASP:HB2	1.92	0.49
1:A:314:ILE:O	1:A:319:VAL:HG23	2.12	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: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:D:243:LEU:HB2	1:D:248:SER:O	2.12	0.49
1:C:215:ALA:HB3	1:C:272:LEU:CD1	2.43	0.49
1:B:72:TRP:CE3	1:B:407:PRO:HG3	2.47	0.49
1:C:38:LEU:CD1	1:C:69:PHE:HE2	2.25	0.49
1:A:325:LEU:HD13	1:A:333:LEU:CD2	2.43	0.49
1:A:126:PHE:HB2	1:A:139:LEU:HD23	1.95	0.49
1:D:175:LYS:O	1:D:228:LEU:HD11	2.12	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: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: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:A:213:TYR:CD1	1:A:213:TYR:N	2.80	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:D:348:PRO:O	1:D:352:ASN:ND2	2.47	0.48
1:B:38:LEU:O	1:B:84:LYS:CE	2.61	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:C:38:LEU:HD11	1:C:71:SER:CB	2.42	0.48
1:B:53:VAL:HG11	1:B:112:VAL:HG22	1.95	0.48
1:C:253:PRO:HD2	1:C:265:TYR:CE1	2.49	0.48
1:A:91:LYS:HG3	1:A:92:ASP:OD1	2.12	0.48
1:D:44:PRO:HG2	1:D:87:ALA:HB1	1.95	0.48
1:C:53:VAL:O	1:C:57:VAL:HG22	2.13	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:C:416:PHE:CZ	1:C:544:ILE:HD11	2.48	0.48
1:B:419:VAL:HG21	1:B:539:PHE:HB2	1.95	0.48
1:B:196:GLU:HB2	1:B:200:SER:HB3	1.95	0.48
1:D:199:ASP:N	1:D:199:ASP:OD1	2.47	0.48
1:D:267:ARG:CB	1:D:267:ARG:NH1	2.77	0.48
1:C:495:LEU:HD22	1:C:495:LEU:H	1.79	0.48
1:D:195:PHE:CD1	1:D:229:VAL:HG22	2.48	0.48
1:B:53:VAL:HG11	1:B:112:VAL:CG2	2.44	0.48
1:B:144:ALA:HB1	1:B:148:THR:HB	1.95	0.48
1:B:190:TYR:CE1	1:B:244:LEU:HD21	2.48	0.48
1:B:174:ALA:HB2	1:B:219:ARG:HG3	1.96	0.48
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:C:204:ARG:HG3	1:C:220:ARG:HD2	1.96	0.47
1:A:65:ALA:HB3	1:A:99:LEU:CD2	2.37	0.47
1:C:150:ARG:HD2	1:C:205:GLU:OE2	2.14	0.47
1:A:404:ARG:O	1:A:407:PRO:HD2	2.12	0.47
1:D:488:ASN:OD1	1:D:503:LYS:HD2	2.14	0.47
1:A:303:TYR:CD1	1:A:303:TYR:N	2.83	0.47
1:A:293:VAL:HG12	1:A:397:GLN:OE1	2.14	0.47
1:A:210:LEU:HD21	1:A:266:LEU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ALA:HA	1:C:112:VAL:HG21	1.97	0.47
1:A:403:PHE:CZ	1:A:499:PRO:HD3	2.49	0.47
1:D:421:ALA:O	1:D:424:TYR:HB3	2.13	0.47
1:A:126:PHE:CD2	1:A:156:ALA:HB1	2.50	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:510:GLU:N	1:B:510:GLU:CD	2.66	0.47
1:B:74:GLY:HA3	2:B:601:FAD:O2	2.14	0.47
1:B:404:ARG:HD2	1:B:501:PHE:CD2	2.49	0.47
1:B:182:PHE:CD1	1:B:191:LEU:HD22	2.50	0.47
1:D:213:TYR:HD1	1:D:273:THR:O	1.97	0.47
1:D:40:SER:O	1:D:43:ASP:HB2	2.14	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:202:LEU:C	1:D:202:LEU:HD23	2.35	0.47
1:D:210:LEU:HA	1:D:213:TYR:CD2	2.44	0.47
1:D:206:VAL:HG22	1:D:263:THR:HG23	1.96	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:A:344:PHE:CD1	1:A:345:PRO:HD2	2.48	0.47
1:D:206:VAL:HG12	1:D:210:LEU:HD23	1.97	0.47
1:D:267:ARG:CB	1:D:267:ARG:HH11	2.28	0.47
1:D:190:TYR:HE2	1:D:272:LEU:HD21	1.80	0.47
1:A:419:VAL:O	1:A:422:ASN:N	2.48	0.47
1:D:252:VAL:HG12	1:D:254:VAL:CG1	2.45	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:B:422:ASN:OD1	1:B:473:PRO:HB2	2.14	0.47
1:B:139:LEU:HD11	1:B:152:ARG:HB3	1.96	0.47
1:D:106:GLU:HB2	1:D:109:ASN:ND2	2.29	0.47
1:C:267:ARG:HB2	1:C:267:ARG:HH11	1.80	0.47
1:A:477:ILE:HG22	1:A:535:LEU:HD13	1.97	0.47
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:A:436:GLN:HE22	1:A:468:HIS:HA	1.79	0.46
1:D:470:VAL:HG13	1:D:475:ASN:HB3	1.97	0.46
1:D:172:GLU:HG3	1:D:173:PRO:HD2	1.96	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:446:VAL:HA	1:D:450:PHE:HB2	1.97	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:A:509:ARG:HA	1:A:516:HIS:CD2	2.51	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:503:LYS:HE2	2:B:601:FAD:P	2.54	0.46
1:B:308:GLU:OE2	1:B:350:VAL:HG21	2.15	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:428:HIS:N	1:C:429:PRO:HD3	2.30	0.46
1:C:422:ASN:ND2	3:C:728:HOH:O	2.48	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:C:257:GLU:HA	1:C:262:TYR:HE1	1.81	0.46
1:D:360:TRP:CD1	1:D:381:ARG:NH2	2.83	0.46
1:A:244:LEU:HB3	3:A:735:HOH:O	2.14	0.46
1:D:96:ALA:HB2	1:D:167:ALA:O	2.16	0.46
1:A:202:LEU:HD11	1:A:259:ARG:N	2.30	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: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: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:D:213:TYR:HE1	1:D:274:ARG:HD2	1.80	0.46
1:A:460:GLU:HA	1:A:460:GLU:OE1	2.15	0.46
1:C:195:PHE:CD1	1:C:221:VAL:HB	2.51	0.46
1:D:75:HIS:HD2	1:D:454:ASP:HB2	1.80	0.46
1:C:291:PRO:HB2	1:C:397:GLN:NE2	2.31	0.46
1:D:375:LYS:HG2	1:D:379:ASP:OD2	2.16	0.46
1:D:192:ALA:O	1:D:218:VAL:HG13	2.16	0.46
1:C:37:VAL:O	1:C:37:VAL:HG12	2.14	0.46
1:D:164:TRP:O	1:D:165:PRO:C	2.54	0.46
1:A:414:PHE:O	1:A:418:THR:HG23	2.16	0.46
1:D:179:ILE:HG13	1:D:221:VAL:HG21	1.99	0.46
1:D:174:ALA:CB	1:D:221:VAL:HG22	2.38	0.46
1:B:197:ARG:HA	1:B:223:ASN:HD22	1.81	0.46
1:A:59:GLY:HA2	1:A:130:PHE:HA	1.97	0.46
1:C:54:ARG:NH1	1:C:58:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HB2	1:B:199:ASP:OD1	2.16	0.45
1:D:473:PRO:O	1:D:477:ILE:HG13	2.16	0.45
1:A:365:GLN:OE1	1:A:366:LYS:HG3	2.16	0.45
1:C:267:ARG:HA	1:C:272:LEU:CD2	2.45	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:A:107:GLU:O	1:A:110:SER:HB3	2.16	0.45
1:D:174:ALA:HB2	1:D:219:ARG:HE	1.82	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:A:49:ASP:O	1:A:53:VAL:HG23	2.16	0.45
1:C:388:THR:OG1	1:C:390:LYS:O	2.31	0.45
1:D:232:PHE:HB2	1:D:234:VAL:CG2	2.46	0.45
1:D:212:GLN:OE1	1:D:276:ALA:HB2	2.16	0.45
1:D:244:LEU:HB2	1:D:248:SER:HG	1.78	0.45
1:C:189:ASP:HA	1:C:245:ARG:HB2	1.99	0.45
1:C:132:LYS:NZ	1:C:132:LYS:CB	2.79	0.45
1:D:215:ALA:HB3	1:D:272:LEU:CD2	2.46	0.45
1:D:404:ARG:HA	2:D:601:FAD:H5'2	1.98	0.45
1:A:341:ALA:O	1:A:351:GLN:NE2	2.49	0.45
1:C:517:ASN:HB2	1:C:525:LEU:O	2.16	0.45
1:D:216:VAL:HG21	1:D:266:LEU:HD13	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:A:195:PHE:HA	1:A:221:VAL:O	2.17	0.45
1:D:185:ARG:HH11	1:D:185:ARG:HG2	1.82	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:148:THR:O	1:D:152:ARG:HG2	2.16	0.45
1:C:165:PRO:HB2	1:C:168:CYS:CB	2.47	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:D:422:ASN:HD22	1:D:536:LYS:HE2	1.82	0.45
1:D:343:TYR:O	1:D:420:GLN:HG3	2.17	0.45
1:B:296:PHE:O	1:B:297:ALA:C	2.55	0.45
1:B:241:TYR:HD1	1:B:251:ARG:HA	1.82	0.45
1:A:168:CYS:HA	1:A:169:PRO:HD3	1.86	0.45
1:A:50:ALA:HA	1:A:112:VAL:CG2	2.47	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: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:38:LEU:HD23	1:A:77:ILE:HA	1.99	0.45
1:D:128:GLN:O	1:D:129:ALA:C	2.54	0.45
1:B:112:VAL:HG12	1:B:113:CYS:N	2.32	0.45
1:C:202:LEU:O	1:C:206:VAL:HG23	2.17	0.44
1:A:481:TRP:HH2	1:A:526:TRP:CG	2.35	0.44
1:D:251:ARG:HG3	1:D:252:VAL:H	1.81	0.44
1:D:205:GLU:CB	1:D:259:ARG:HD2	2.47	0.44
1:C:139:LEU:CD1	1:C:140:PRO:HD2	2.46	0.44
1:C:93:TRP:CE3	1:C:208:LEU:HD13	2.53	0.44
1:A:538:HIS:HA	1:A:543:ASN:HD22	1.82	0.44
1:A:428:HIS:N	1:A:429:PRO:HD3	2.33	0.44
1:D:264:SER:O	1:D:267:ARG:NE	2.51	0.44
1:C:205:GLU:CB	1:C:259:ARG:HD2	2.47	0.44
1:C:188:ALA:HA	1:C:215:ALA:O	2.17	0.44
1:B:547:ASP:O	1:B:549:SER:N	2.50	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: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:C:97:LEU:HD12	1:C:98:ASN:N	2.32	0.44
1:A:144:ALA:HB1	1:A:148:THR:CG2	2.47	0.44
1:B:197:ARG:HA	1:B:223:ASN:ND2	2.31	0.44
1:B:197:ARG:NH1	1:B:197:ARG:HG3	2.32	0.44
1:C:102:LEU:CD2	1:C:112:VAL:HG11	2.47	0.44
1:A:103:ASP:C	1:A:105:ALA:H	2.20	0.44
1:D:195:PHE:HB3	1:D:237:PHE:CZ	2.53	0.44
1:D:190:TYR:OH	1:D:270:PRO:HG2	2.17	0.44
1:A:355:HIS:CE1	1:D:185:ARG:HH22	2.36	0.44
1:A:302:ILE:HD12	1:A:538:HIS:O	2.17	0.44
1:B:506:TRP:CG	1:B:507:PRO:HA	2.52	0.44
1:D:175:LYS:O	1:D:228:LEU:HD21	2.18	0.44
1:B:336:PHE:CZ	1:B:340:LEU:HD11	2.52	0.44
1:D:255:LEU:HD12	1:D:261:PHE:CZ	2.52	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:243:LEU:HD23	1:D:243:LEU:N	2.30	0.44
1:D:215:ALA:CB	1:D:272:LEU:HA	2.48	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: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:D:58:LEU:HD22	1:D:133:ASN:HA	2.00	0.44
1:B:446:VAL:O	1:B:453:ARG:NH2	2.51	0.44
1:C:139:LEU:HA	1:C:139:LEU:HD12	1.79	0.44
1:C:197:ARG:NH2	3:C:770:HOH:O	2.51	0.44
1:D:188:ALA:O	1:D:245:ARG:HD2	2.17	0.44
1:B:219:ARG:HH11	1:B:219:ARG:HG3	1.83	0.44
1:D:65:ALA:HB3	1:D:99:LEU:HD22	1.99	0.44
1:B:382:LYS:HG2	1:B:385:ALA:CB	2.47	0.43
1:A:381:ARG:HG3	1:A:381:ARG:NH1	2.33	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:B:507:PRO:HD2	1:B:526:TRP:CZ3	2.53	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:C:312:HIS:CE1	1:C:316:ARG:HG3	2.53	0.43
1:B:150:ARG:O	1:B:154:ILE:HG13	2.17	0.43
1:A:130:PHE:HB2	1:A:163:THR:CG2	2.45	0.43
1:D:94:ARG:CD	1:D:98:ASN:OD1	2.66	0.43
1:B:75:HIS:ND1	1:B:76:ALA:N	2.65	0.43
1:D:352:ASN:OD1	1:D:353:PHE:N	2.52	0.43
1:D:205:GLU:HB3	1:D:259:ARG:NE	2.32	0.43
1:C:375:LYS:HE3	3:C:743:HOH:O	2.18	0.43
1:B:176:LEU:HD22	1:B:227:ASP:HB3	2.00	0.43
1:A:313:TYR:CZ	1:A:317:VAL:HG11	2.53	0.43
1:D:144:ALA:CB	1:D:149:LEU:HG	2.43	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: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: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
1:B:106:GLU:CG	3:B:714:HOH:O	2.66	0.43
1:D:428:HIS:N	1:D:429:PRO:HD3	2.33	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:A:273:THR:HG22	1:A:274:ARG:O	2.19	0.43
1:A:263:THR:O	1:A:267:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG22	1:A:138:THR:O	2.17	0.43
1:A:144:ALA:HB1	1:A:148:THR:CB	2.46	0.43
1:C:152:ARG:NH1	1:C:155:ASP:OD2	2.52	0.43
1:A:478:LEU:HA	1:A:478:LEU:HD23	1.84	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: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:213:TYR:OH	1:C:274:ARG:NH1	2.52	0.43
1:A:351:GLN:HG3	1:A:355:HIS:CE1	2.54	0.43
1:D:67:GLU:OE2	1:D:69:PHE:HB3	2.18	0.43
1:A:219:ARG:HD2	1:A:219:ARG:HA	1.80	0.43
1:B:77:ILE:CD1	1:B:495:LEU:HB3	2.49	0.43
1:A:443:ARG:HD3	1:A:463:ALA:HB3	1.99	0.43
1:A:38:LEU:H	1:A:38:LEU:CD1	2.31	0.43
1:D:322:PHE:CZ	1:D:329:ARG:NH2	2.87	0.43
1:B:512:CYS:O	1:B:515:CYS:HB2	2.18	0.43
1:B:343:TYR:CE1	1:B:421:ALA:HA	2.53	0.43
1:A:506:TRP:CG	1:A:507:PRO:HA	2.54	0.43
1:D:197:ARG:HE	1:D:223:ASN:HB2	1.82	0.43
1:D:267:ARG:HB3	1:D:267:ARG:NH1	2.33	0.43
1:D:78:ALA:HA	1:D:495:LEU:HD22	2.01	0.43
1:B:216:VAL:HG23	1:B:272:LEU:CD2	2.45	0.43
1:C:532:LEU:HG	1:C:536:LYS:HE3	2.00	0.43
1:A:302:ILE:O	1:A:544:ILE:HA	2.19	0.43
1:B:327:GLY:O	1:B:331:VAL:HG23	2.19	0.43
1:A:369:ILE:HG23	1:A:373:PHE:HD2	1.84	0.43
1:D:176:LEU:HB2	1:D:227:ASP:HB3	2.01	0.42
1:A:404:ARG:NH2	2:A:601:FAD:O3B	2.52	0.42
1:B:443:ARG:HD3	1:B:463:ALA:HB1	2.00	0.42
1:B:352:ASN:OD1	1:B:353:PHE:N	2.52	0.42
1:B:219:ARG:HG3	1:B:219:ARG:NH1	2.34	0.42
1:D:518:GLU:CD	1:D:524:PRO:HA	2.39	0.42
1:C:483:SER:O	1:C:487:VAL:HG23	2.19	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:D:322:PHE:CE2	1:D:329:ARG:CZ	3.02	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: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:D:206:VAL:HG22	1:D:263:THR:CG2	2.49	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:D:125:ARG:HG3	1:D:125:ARG:HH11	1.84	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:294:TRP:CZ3	1:D:295:LYS:HG2	2.54	0.42
1:D:294:TRP:CE2	1:D:399:SER:HA	2.54	0.42
1:D:259:ARG:CZ	3:D:710:HOH:O	2.67	0.42
1:A:152:ARG:CA	1:A:152:ARG:HH11	2.12	0.42
1:C:190:TYR:CD1	1:C:269:LEU:HD13	2.55	0.42
1:B:399:SER:HB2	1:B:500:HIS:CD2	2.55	0.42
1:C:434:ASP:OD2	1:C:436:GLN:HB2	2.20	0.42
1:C:301:LYS:HD3	1:C:543:ASN:OD1	2.19	0.42
1:B:96:ALA:HB1	1:B:168:CYS:HB2	2.02	0.42
1:D:110:SER:OG	1:D:114:ARG:NH2	2.51	0.42
1:A:547:ASP:OD1	1:A:548:SER:N	2.52	0.42
1:D:53:VAL:HG21	1:D:102:LEU:HD12	2.02	0.42
1:A:93:TRP:O	1:A:96:ALA:HB3	2.20	0.42
1:C:406:PHE:HB3	1:C:407:PRO:HD3	2.01	0.42
1:D:151:MET:O	1:D:155:ASP:OD2	2.37	0.42
1:B:103:ASP:OD1	1:B:105:ALA:CB	2.67	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:318:GLU:HA	1:A:321:LYS:HZ3	1.85	0.42
1:D:103:ASP:C	1:D:105:ALA:H	2.23	0.42
1:C:419:VAL:HG21	1:C:539:PHE:HB2	2.02	0.42
1:C:414:PHE:CE2	1:C:442:MET:HG3	2.55	0.42
1:D:221:VAL:HG21	1:D:228:LEU:HD13	2.02	0.42
1:C:223:ASN:ND2	1:C:224:THR:HG23	2.34	0.42
1:A:366:LYS:HA	3:A:722:HOH:O	2.20	0.42
1:D:360:TRP:HD1	1:D:381:ARG:HH22	1.67	0.42
1:A:139:LEU:O	1:A:141:GLY:N	2.53	0.42
1:D:205:GLU:CD	1:D:259:ARG:HD2	2.41	0.42
1:C:107:GLU:O	1:C:110:SER:CB	2.67	0.42
1:B:431:GLU:H	1:B:431:GLU:HG2	1.57	0.42
1:D:223:ASN:O	1:D:229:VAL:HG11	2.20	0.42
1:D:142:ALA:O	1:D:144:ALA:N	2.50	0.42
1:D:145:ASN:ND2	1:D:148:THR:OG1	2.53	0.42
1:B:440:GLN:CD	1:B:467:MET:HE2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:197:ARG:NH2	1:D:237:PHE:CE1	2.88	0.41
1:B:271:GLY:N	3:B:775:HOH:O	2.50	0.41
1:D:165:PRO:HB2	1:D:168:CYS:HB3	2.02	0.41
1:C:262:TYR:O	1:C:265:TYR:HB3	2.20	0.41
1:B:94:ARG:HG2	1:B:97:LEU:O	2.20	0.41
1:D:191:LEU:HA	1:D:217:ALA:O	2.19	0.41
1:A:379:ASP:C	1:A:381:ARG:H	2.23	0.41
1:C:109:ASN:O	1:C:112:VAL:HB	2.20	0.41
1:B:440:GLN:CA	1:B:467:MET:HE1	2.50	0.41
1:A:73:CYS:HB3	1:A:75:HIS:CD2	2.56	0.41
1:B:243:LEU:HD22	1:B:249:VAL:HG22	2.02	0.41
1:A:161:ARG:HB2	3:A:789:HOH:O	2.19	0.41
1:B:347:GLN:HB3	1:B:348:PRO:HD2	2.02	0.41
1:B:260:SER:O	1:B:264:SER:HB2	2.21	0.41
1:D:195:PHE:HB2	1:D:239:SER:OG	2.20	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:B:77:ILE:HD13	1:B:495:LEU:O	2.21	0.41
1:B:61:SER:O	1:B:166:PRO:HD2	2.20	0.41
1:B:198:GLU:OE2	1:B:198:GLU:N	2.54	0.41
1:D:202:LEU:O	1:D:206:VAL:HG23	2.20	0.41
1:C:176:LEU:HD12	1:C:176:LEU:C	2.39	0.41
1:B:232:PHE:HE2	1:B:243:LEU:HD21	1.85	0.41
1:C:185:ARG:HG2	1:C:185:ARG:HH11	1.86	0.41
1:D:223:ASN:O	1:D:229:VAL:HG21	2.21	0.41
1:D:259:ARG:HA	1:D:262:TYR:HB2	2.02	0.41
1:D:242:LEU:O	1:D:242:LEU:CG	2.69	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:B:196:GLU:HB2	1:B:200:SER:CB	2.49	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: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:A:240:CYS:O	1:A:251:ARG:HD2	2.20	0.41
1:D:197:ARG:NE	1:D:223:ASN:HB2	2.36	0.41
1:A:347:GLN:OE1	1:A:546:ILE:HD12	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:B:439:LEU:O	1:B:467:MET:HE1	2.21	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:A:38:LEU:N	1:A:38:LEU:CD1	2.83	0.41
1:A:204:ARG:HD3	1:A:220:ARG:HH11	1.85	0.41
1:A:139:LEU:HD22	1:A:139:LEU:HA	1.85	0.41
1:D:54:ARG:N	1:D:55:PRO:HD2	2.35	0.41
1:D:175:LYS:C	1:D:228:LEU:HD11	2.42	0.41
1:A:152:ARG:CA	1:A:152:ARG:NH1	2.74	0.41
1:C:312:HIS:HE1	3:C:751:HOH:O	2.04	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:C:110:SER:O	1:C:112:VAL:N	2.53	0.41
1:D:313:TYR:CE1	1:D:317:VAL:HG21	2.56	0.41
1:B:503:LYS:HE2	2:B:601:FAD:O1P	2.19	0.41
1:A:94:ARG:HD2	1:A:98:ASN:OD1	2.20	0.41
1:B:406:PHE:O	1:B:407:PRO:C	2.58	0.41
1:C:291:PRO:HB2	1:C:397:GLN:HE22	1.85	0.41
1:D:311:LEU:HD21	1:D:340:LEU:HD22	2.02	0.41
1:C:205:GLU:HB3	1:C:259:ARG:HD2	2.03	0.41
1:B:406:PHE:CE2	1:B:410:LEU:HD22	2.56	0.41
1:A:290:ALA:HA	1:A:291:PRO:HD3	1.89	0.41
1:D:243:LEU:CB	1:D:249:VAL:HA	2.51	0.40
1:A:61:SER:HA	1:A:130:PHE:CZ	2.56	0.40
1:B:349:LEU:O	1:B:352:ASN:OD1	2.38	0.40
1:D:353:PHE:O	1:D:357:ILE:HG22	2.21	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:B:416:PHE:CZ	1:B:544:ILE:HD11	2.56	0.40
1:A:484:HIS:O	1:A:484:HIS:HD2	2.05	0.40
1:D:172:GLU:O	1:D:219:ARG:CZ	2.68	0.40
1:C:254:VAL:CG2	1:C:257:GLU:OE1	2.69	0.40
1:A:531:THR:O	1:A:532:LEU:C	2.58	0.40
1:A:358:ASN:O	1:A:362:GLN:HG2	2.21	0.40
1:D:205:GLU:HB3	1:D:259:ARG:CD	2.51	0.40
1:D:49:ASP:OD1	1:D:51:ASP:HB2	2.21	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:B:330:LEU:HD11	1:B:334:LYS:HE3	2.03	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:A:210:LEU:CD2	1:A:266:LEU:HB3	2.50	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%)	16	47
1	B	500/519 (96%)	457 (91%)	37 (7%)	6 (1%)	16	47
1	C	496/519 (96%)	434 (88%)	60 (12%)	2 (0%)	39	74
1	D	494/519 (95%)	402 (81%)	80 (16%)	12 (2%)	7	25
All	All	1987/2076 (96%)	1734 (87%)	227 (11%)	26 (1%)	15	44

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 ⓘ

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%)	48	82
1	B	430/441 (98%)	419 (97%)	11 (3%)	54	86
1	C	426/441 (97%)	400 (94%)	26 (6%)	23	55
1	D	424/441 (96%)	408 (96%)	16 (4%)	40	74
All	All	1707/1764 (97%)	1641 (96%)	66 (4%)	39	74

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

Some 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 carbohydrates 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	-	48,58,58	2.62	13 (27%)	54,89,89	2.28	7 (12%)
2	FAD	B	601	-	48,58,58	2.62	13 (27%)	54,89,89	2.27	7 (12%)
2	FAD	C	601	-	48,58,58	2.79	14 (29%)	54,89,89	2.31	8 (14%)
2	FAD	D	601	-	48,58,58	2.77	13 (27%)	54,89,89	2.28	5 (9%)

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	-	-	0/30/50/50	0/6/6/6
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
2	FAD	D	601	-	-	0/30/50/50	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	C1'-N10	-4.55	1.43	1.48
2	C	601	FAD	C1'-N10	-4.48	1.43	1.48
2	A	601	FAD	C5A-C4A	-4.06	1.31	1.40
2	B	601	FAD	C5A-C4A	-4.03	1.31	1.40
2	D	601	FAD	C5A-C4A	-3.72	1.32	1.40
2	C	601	FAD	C5A-C4A	-3.68	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C1'-N10	-3.19	1.45	1.48
2	A	601	FAD	C1'-N10	-3.14	1.45	1.48
2	D	601	FAD	C2B-C3B	-2.93	1.45	1.53
2	A	601	FAD	C8A-N7A	-2.58	1.29	1.34
2	B	601	FAD	C8A-N7A	-2.55	1.29	1.34
2	C	601	FAD	C2B-C3B	-2.45	1.46	1.53
2	C	601	FAD	C8A-N7A	-2.28	1.30	1.34
2	D	601	FAD	C8A-N7A	-2.15	1.30	1.34
2	B	601	FAD	C6-C7	2.04	1.43	1.37
2	A	601	FAD	C6-C7	2.05	1.43	1.37
2	D	601	FAD	C6-C7	2.18	1.43	1.37
2	C	601	FAD	C6-C7	2.20	1.43	1.37
2	D	601	FAD	C10-N1	2.31	1.39	1.35
2	A	601	FAD	C10-N1	2.33	1.39	1.35
2	C	601	FAD	O4B-C1B	2.35	1.44	1.41
2	B	601	FAD	C10-N1	2.35	1.39	1.35
2	B	601	FAD	O4B-C1B	2.51	1.44	1.41
2	A	601	FAD	O4B-C1B	2.56	1.44	1.41
2	C	601	FAD	C10-N1	2.60	1.40	1.35
2	B	601	FAD	C9A-C5X	2.94	1.48	1.42
2	A	601	FAD	C9A-C5X	2.95	1.48	1.42
2	D	601	FAD	C9A-C5X	3.04	1.48	1.42
2	C	601	FAD	C9A-C5X	3.20	1.49	1.42
2	A	601	FAD	C4A-N3A	4.77	1.42	1.35
2	B	601	FAD	C4A-N3A	4.78	1.42	1.35
2	B	601	FAD	C2A-N3A	4.98	1.41	1.32
2	A	601	FAD	C2A-N3A	5.00	1.41	1.32
2	A	601	FAD	C4-N3	5.02	1.42	1.33
2	B	601	FAD	C4-N3	5.06	1.42	1.33
2	C	601	FAD	C2A-N3A	5.29	1.41	1.32
2	B	601	FAD	C5X-N5	5.36	1.43	1.35
2	A	601	FAD	C5X-N5	5.36	1.43	1.35
2	D	601	FAD	C4A-N3A	5.43	1.43	1.35
2	D	601	FAD	C2A-N3A	5.50	1.41	1.32
2	C	601	FAD	C4A-N3A	5.55	1.43	1.35
2	D	601	FAD	C4-N3	5.63	1.43	1.33
2	C	601	FAD	C4-N3	5.69	1.43	1.33
2	D	601	FAD	C5X-N5	5.87	1.44	1.35
2	C	601	FAD	C5X-N5	6.27	1.45	1.35
2	B	601	FAD	C4X-N5	8.18	1.46	1.33
2	A	601	FAD	C4X-N5	8.20	1.46	1.33
2	C	601	FAD	C9A-N10	8.22	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4X-N5	8.30	1.46	1.33
2	D	601	FAD	C4X-N5	8.37	1.46	1.33
2	D	601	FAD	C9A-N10	8.38	1.50	1.38
2	B	601	FAD	C9A-N10	8.50	1.50	1.38
2	A	601	FAD	C9A-N10	8.51	1.50	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C4X-C4-N3	-6.79	114.30	123.59
2	D	601	FAD	C4X-C4-N3	-6.67	114.47	123.59
2	B	601	FAD	C4X-C4-N3	-6.48	114.73	123.59
2	A	601	FAD	C4X-C4-N3	-6.47	114.74	123.59
2	A	601	FAD	N3A-C2A-N1A	-5.02	125.05	128.89
2	B	601	FAD	N3A-C2A-N1A	-5.01	125.06	128.89
2	C	601	FAD	N3A-C2A-N1A	-4.98	125.08	128.89
2	D	601	FAD	N3A-C2A-N1A	-4.65	125.33	128.89
2	C	601	FAD	C5X-C9A-N10	-4.01	114.57	117.62
2	D	601	FAD	C5X-C9A-N10	-3.97	114.60	117.62
2	A	601	FAD	C5X-C9A-N10	-3.82	114.71	117.62
2	B	601	FAD	C5X-C9A-N10	-3.78	114.74	117.62
2	C	601	FAD	C6-C5X-C9A	-2.15	116.16	118.98
2	C	601	FAD	C1'-C2'-C3'	2.06	115.70	109.82
2	C	601	FAD	O2B-C2B-C3B	2.27	119.19	111.83
2	B	601	FAD	C2B-C1B-N9A	2.33	117.86	114.29
2	A	601	FAD	C2B-C1B-N9A	2.36	117.90	114.29
2	A	601	FAD	C1'-C2'-C3'	2.38	116.62	109.82
2	B	601	FAD	C1'-C2'-C3'	2.39	116.67	109.82
2	B	601	FAD	O2B-C2B-C3B	2.42	119.71	111.83
2	A	601	FAD	O2B-C2B-C3B	2.43	119.72	111.83
2	C	601	FAD	C2B-C1B-N9A	2.77	118.53	114.29
2	D	601	FAD	C2B-C1B-N9A	2.83	118.62	114.29
2	B	601	FAD	C4-N3-C2	11.90	125.53	115.25
2	A	601	FAD	C4-N3-C2	11.91	125.54	115.25
2	D	601	FAD	C4-N3-C2	11.94	125.56	115.25
2	C	601	FAD	C4-N3-C2	12.06	125.67	115.25

There are no chirality outliers.

There are no torsion outliers.

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	C	601	FAD	1	0
2	D	601	FAD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	501/519 (96%)	0.01	2 (0%) 93 90	32, 52, 71, 84	1 (0%)
1	B	504/519 (97%)	0.02	3 (0%) 90 86	24, 49, 79, 94	1 (0%)
1	C	500/519 (96%)	0.14	19 (3%) 44 32	21, 48, 90, 115	1 (0%)
1	D	498/519 (95%)	0.80	75 (15%) 3 2	34, 63, 144, 151	1 (0%)
All	All	2003/2076 (96%)	0.24	99 (4%) 33 22	21, 52, 118, 151	4 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	241	TYR	10.9
1	D	193	LEU	8.8
1	D	174	ALA	7.0
1	D	191	LEU	6.8
1	D	222	LEU	6.8
1	D	221	VAL	6.8
1	D	177	ASN	6.7
1	D	272	LEU	6.6
1	D	254	VAL	6.2
1	D	239	SER	6.0
1	D	231	LYS	6.0
1	D	227	ASP	5.9
1	D	217	ALA	5.8
1	D	249	VAL	5.7
1	D	238	PRO	5.7
1	D	242	LEU	5.5
1	D	235	THR	5.4
1	D	263	THR	5.4
1	D	262	TYR	5.2
1	D	195	PHE	5.1
1	C	228	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	265	TYR	5.0
1	D	240	CYS	4.9
1	D	224	THR	4.9
1	D	226	SER	4.8
1	D	228	LEU	4.7
1	D	250	SER	4.6
1	D	232	PHE	4.6
1	D	178	ASP	4.5
1	C	277	PRO	4.3
1	D	269	LEU	4.3
1	B	433	ALA	4.2
1	D	258	SER	4.2
1	D	271	GLY	4.1
1	C	143	GLY	4.1
1	D	201	TYR	3.9
1	A	36	SER	3.9
1	D	266	LEU	3.8
1	D	173	PRO	3.8
1	D	210	LEU	3.7
1	D	175	LYS	3.6
1	D	229	VAL	3.6
1	D	192	ALA	3.6
1	C	227	ASP	3.5
1	D	237	PHE	3.5
1	D	208	LEU	3.4
1	D	270	PRO	3.4
1	D	194	VAL	3.3
1	D	211	SER	3.3
1	D	220	ARG	3.3
1	D	171	LEU	3.3
1	C	179	ILE	3.1
1	D	186	ASN	3.1
1	D	259	ARG	3.1
1	D	185	ARG	3.1
1	D	198	GLU	3.1
1	D	189	ASP	3.0
1	D	202	LEU	2.9
1	D	215	ALA	2.9
1	D	234	VAL	2.9
1	D	182	PHE	2.9
1	D	188	ALA	2.8
1	D	218	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	223	ASN	2.7
1	C	231	LYS	2.7
1	D	93	TRP	2.7
1	B	141	GLY	2.7
1	C	113	CYS	2.6
1	D	256	VAL	2.6
1	D	243	LEU	2.5
1	C	141	GLY	2.5
1	C	232	PHE	2.5
1	C	256	VAL	2.5
1	D	216	VAL	2.4
1	D	199	ASP	2.4
1	C	142	ALA	2.4
1	C	234	VAL	2.4
1	D	92	ASP	2.3
1	D	132	LYS	2.3
1	D	187	LYS	2.3
1	B	234	VAL	2.3
1	D	206	VAL	2.3
1	D	184	THR	2.3
1	D	244	LEU	2.2
1	D	230	ASN	2.2
1	D	196	GLU	2.2
1	C	174	ALA	2.2
1	D	179	ILE	2.2
1	C	140	PRO	2.2
1	D	57	VAL	2.1
1	D	255	LEU	2.1
1	A	104	CYS	2.1
1	C	173	PRO	2.1
1	C	191	LEU	2.1
1	D	153	LEU	2.0
1	C	240	CYS	2.0
1	C	255	LEU	2.0
1	C	194	VAL	2.0
1	D	190	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	B	601	53/53	0.96	0.22	1.26	26,45,54,56	0
2	FAD	A	601	53/53	0.95	0.24	0.75	36,52,57,58	0
2	FAD	C	601	53/53	0.97	0.22	0.50	28,42,53,55	0
2	FAD	D	601	53/53	0.96	0.21	0.28	34,56,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.