



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 12:37 PM EST

PDB ID : 3N70  
Title : The Crystal Structure of the P-loop NTPase domain of the Sigma-54 transport activator from E. coli to 2.8Å  
Authors : Stein, A.J.; Mulligan, R.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-05-26  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

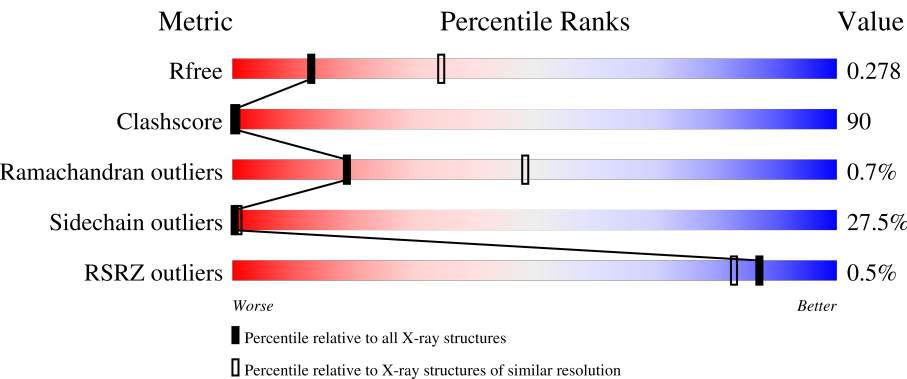
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	145	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>32%53%13%.</div></div>
1	B	145	<div><div></div><div></div><div></div><div></div><div></div></div> <div>19%46%10%26%</div>
1	C	145	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>30%50%10%9%</div></div>
1	D	145	<div><div></div><div></div><div></div><div></div><div></div></div> <div>30%39%11%20%</div>
1	E	145	<div><div></div><div></div><div></div><div></div><div></div></div> <div>31%48%14%. 6%</div>

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Mol	Chain	Length	Quality of chain
1	F	145	
1	G	145	
1	H	145	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	2	-	-	X	-
2	SO4	D	4	-	-	X	-
2	SO4	F	7	-	-	X	-
2	SO4	G	6	-	-	X	-
2	SO4	H	8	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7146 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 Transport activator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	Se	0	0	0
			1060	672	190	195	2	1			
1	B	108	Total	C	N	O	S	Se	0	0	0
			734	464	129	138	1	2			
1	C	132	Total	C	N	O	S	Se	0	0	0
			959	615	169	171	2	2			
1	D	116	Total	C	N	O	S	Se	0	0	0
			833	535	149	148	1				
1	E	137	Total	C	N	O	S	Se	0	0	0
			1026	659	183	180	2	2			
1	F	105	Total	C	N	O	S	Se	0	0	0
			719	455	128	133	2	1			
1	G	128	Total	C	N	O	S	Se	0	0	0
			936	591	170	171	2	2			
1	H	122	Total	C	N	O	S	Se	0	0	0
			834	526	154	152	1	1			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

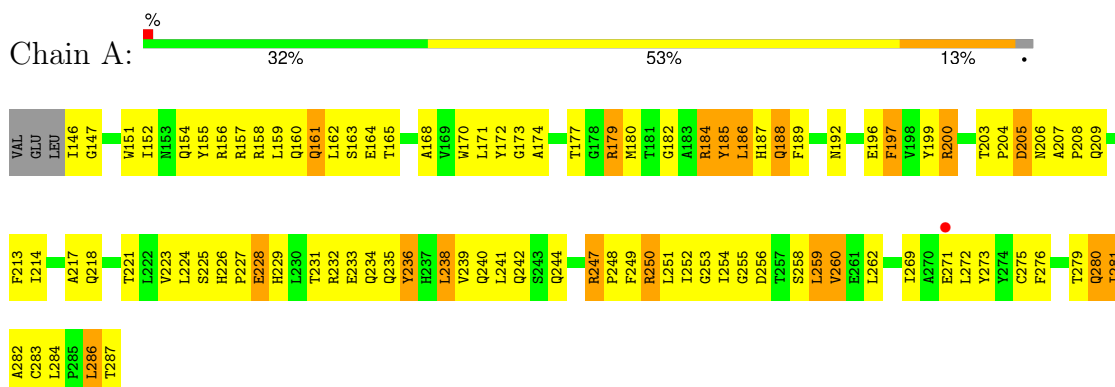
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	E	2	Total	O	0	0
			2	2		

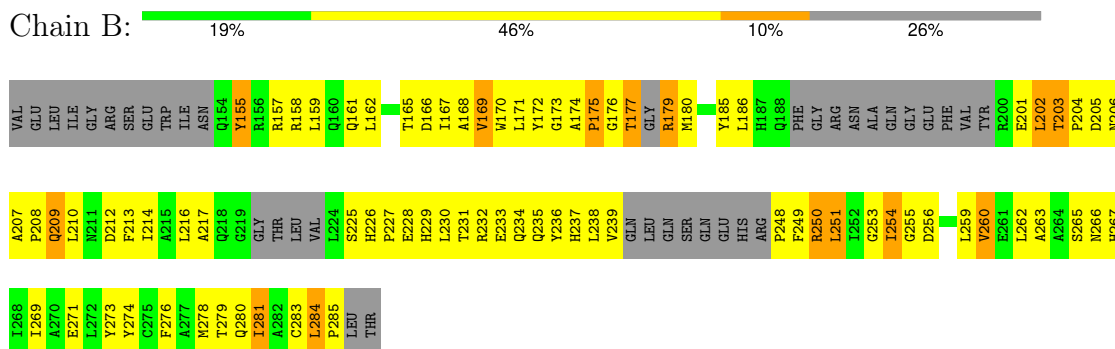
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

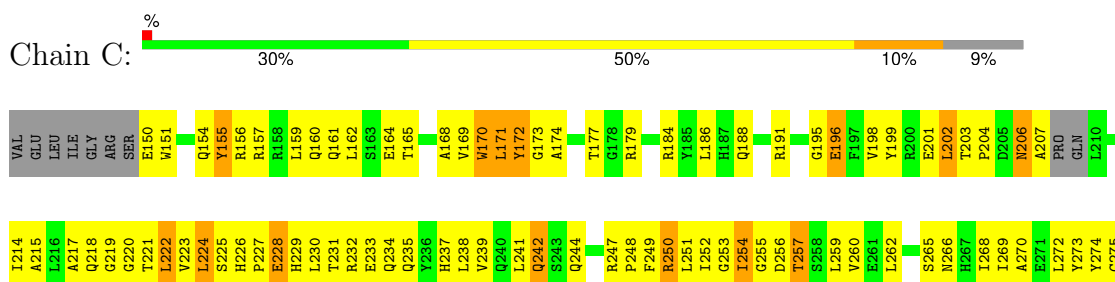
#### • Molecule 1: Transport activator

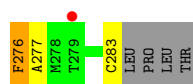


#### • Molecule 1: Transport activator

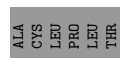
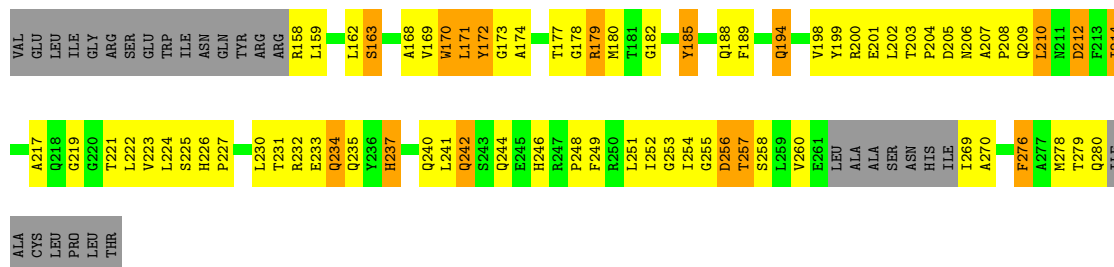


#### • Molecule 1: Transport activator

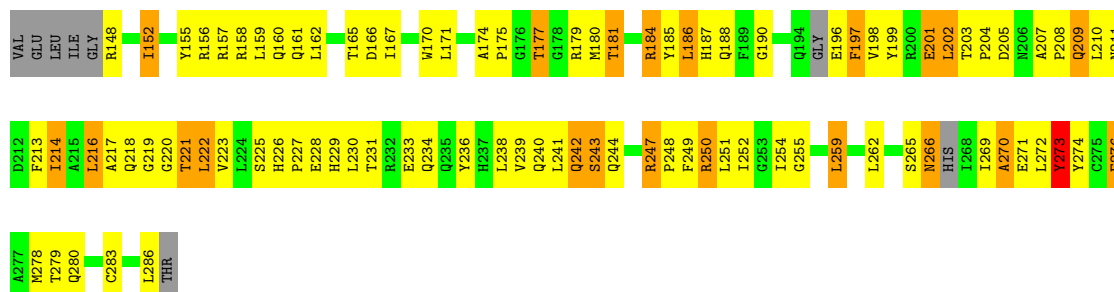




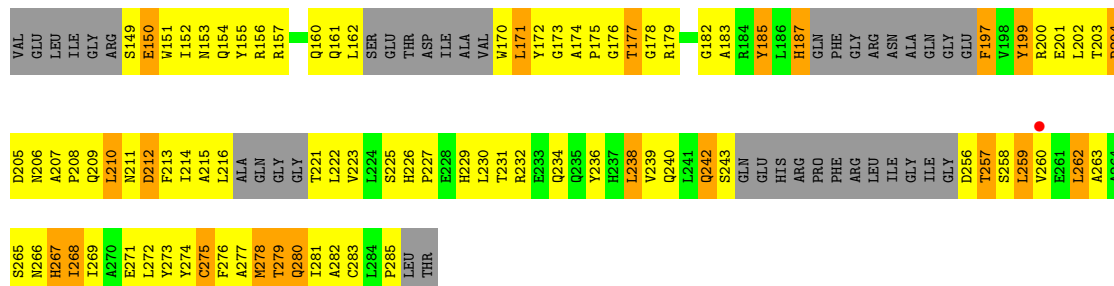
- Molecule 1: Transport activator



- Molecule 1: Transport activator

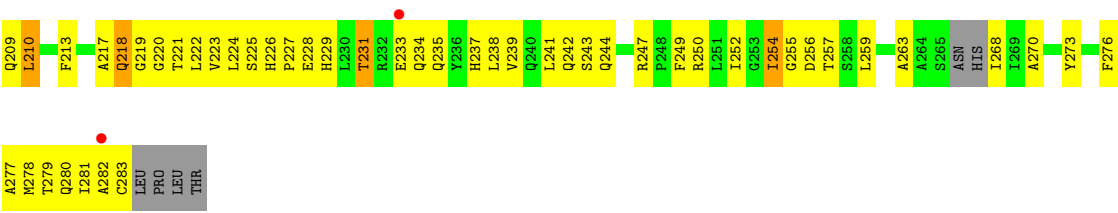


- Molecule 1: Transport activator

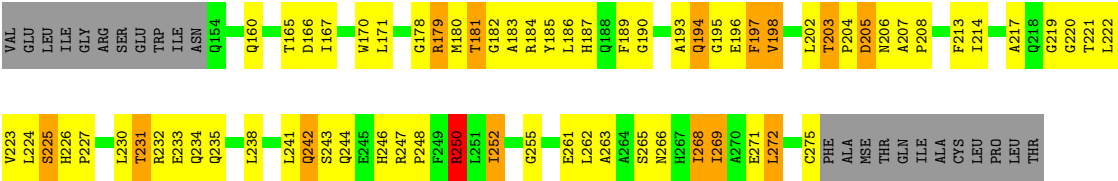
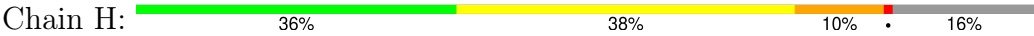


- Molecule 1: Transport activator





● Molecule 1: Transport activator





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.61Å 77.61Å 215.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.80 48.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (48.88-2.80) 99.9 (48.88-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.229 , 0.280 0.260 , 0.278	Depositor DCC
$R_{free}$ test set	1572 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 88.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.496 for h,-k,-l	Depositor
Outliers	0 of 31209 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.50	0/1082	0.58	1/1474 (0.1%)
1	B	0.55	0/744	0.55	0/1014
1	C	0.47	0/978	0.57	0/1331
1	D	0.39	0/850	0.49	0/1158
1	E	0.47	0/1048	0.50	0/1426
1	F	0.55	0/731	0.54	0/998
1	G	0.49	0/953	0.49	0/1294
1	H	0.49	0/850	0.55	0/1162
All	All	0.49	0/7236	0.53	1/9857 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	238	LEU	CA-CB-CG	-5.17	103.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	250	ARG	Sidechain

## 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	1060	0	975	124	1
1	B	734	0	611	166	0
1	C	959	0	861	161	4
1	D	833	0	740	152	3
1	E	1026	0	936	165	2
1	F	719	0	575	213	0
1	G	936	0	843	161	2
1	H	834	0	710	129	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	0	0
2	F	5	0	0	4	0
2	G	5	0	0	3	0
2	H	5	0	0	3	0
3	A	3	0	0	0	0
3	E	2	0	0	0	0
All	All	7146	0	6251	1203	6

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 90.

All (1203) 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:F:199:TYR:HB2	1:F:223:VAL:CG1	1.31	1.55
1:F:187:HIS:CD2	1:F:197:PHE:HB2	1.54	1.42
1:F:278:MSE:HE1	1:G:263:ALA:CB	1.47	1.42
1:A:204:PRO:HD2	1:B:267:HIS:ND1	1.38	1.38
1:C:195:GLY:HA3	1:C:219:GLY:C	1.42	1.36
1:F:239:VAL:CG2	1:G:278:MSE:CE	2.10	1.30
1:F:239:VAL:CG2	1:G:278:MSE:HE1	1.60	1.30
1:F:239:VAL:CG2	1:G:278:MSE:SE	2.30	1.30
1:B:174:ALA:O	1:B:177:THR:HG22	1.28	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:THR:HB	1:H:204:PRO:CD	1.60	1.26
1:B:210:LEU:O	1:B:214:ILE:HD12	1.14	1.25
1:C:172:TYR:HA	1:C:255:GLY:O	1.34	1.25
1:E:156:ARG:O	1:E:160:GLN:HG3	1.36	1.25
1:G:202:LEU:HD12	1:G:227:PRO:CA	1.65	1.25
1:G:202:LEU:CD1	1:G:227:PRO:HA	1.66	1.24
1:D:172:TYR:HA	1:D:255:GLY:O	1.37	1.23
1:D:237:HIS:CE1	1:D:241:LEU:HD11	1.75	1.20
1:F:259:LEU:HB3	1:F:280:GLN:NE2	1.56	1.20
1:F:199:TYR:CB	1:F:223:VAL:CG1	2.20	1.20
1:C:262:LEU:HD23	1:C:262:LEU:O	1.40	1.20
1:A:204:PRO:HD2	1:B:267:HIS:CE1	1.76	1.19
1:F:239:VAL:HG23	1:G:278:MSE:HE1	1.23	1.18
1:B:210:LEU:O	1:B:214:ILE:CD1	1.92	1.17
1:B:202:LEU:HD23	1:B:202:LEU:N	1.55	1.17
1:F:239:VAL:HG22	1:G:278:MSE:SE	1.95	1.17
1:F:239:VAL:HG23	1:G:278:MSE:CE	1.70	1.16
1:F:187:HIS:NE2	1:F:197:PHE:HB2	1.60	1.16
1:G:170:TRP:CH2	1:G:172:TYR:HB3	1.79	1.16
1:B:210:LEU:HG	1:B:214:ILE:HD11	1.29	1.15
1:B:262:LEU:HD12	1:B:266:ASN:HD22	1.03	1.15
1:C:241:LEU:HA	1:C:244:GLN:HE21	1.10	1.15
1:D:168:ALA:HB1	1:D:276:PHE:CE1	1.82	1.15
1:D:170:TRP:C	1:D:171:LEU:CD1	2.16	1.14
1:D:210:LEU:HD22	1:D:234:GLN:HG2	1.19	1.14
1:C:262:LEU:HD21	1:C:266:ASN:CB	1.78	1.13
1:F:278:MSE:HE1	1:G:263:ALA:HB1	1.17	1.13
1:G:171:LEU:N	1:G:171:LEU:HD12	1.64	1.13
1:B:166:ASP:O	1:B:250:ARG:HG3	1.48	1.12
1:F:239:VAL:HG23	1:G:278:MSE:SE	1.97	1.12
1:F:187:HIS:HD2	1:F:197:PHE:CD1	1.68	1.11
1:B:158:ARG:O	1:B:162:LEU:CB	1.98	1.11
1:H:262:LEU:HB3	1:H:268:ILE:HG21	1.16	1.11
1:B:174:ALA:HB1	1:B:175:PRO:HD2	1.28	1.10
1:C:226:HIS:N	1:C:227:PRO:HD3	1.58	1.10
1:C:230:LEU:HA	1:C:234:GLN:OE1	1.49	1.09
1:E:231:THR:HG22	1:E:234:GLN:HG3	1.11	1.09
1:D:170:TRP:C	1:D:171:LEU:HD12	1.72	1.09
1:A:179:ARG:HA	1:A:283:CYS:SG	1.94	1.08
1:F:259:LEU:CB	1:F:280:GLN:HE21	1.66	1.08
1:H:203:THR:HB	1:H:204:PRO:HD2	1.20	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HE21	1:A:188:GLN:HA	1.19	1.08
1:B:170:TRP:HB3	1:B:280:GLN:HB3	1.15	1.08
1:F:199:TYR:HB2	1:F:223:VAL:HG13	1.33	1.08
1:F:199:TYR:HB2	1:F:223:VAL:HG11	1.08	1.08
1:F:221:THR:HG22	1:F:222:LEU:N	1.64	1.08
1:D:169:VAL:HG12	1:D:171:LEU:HD11	1.33	1.08
1:F:171:LEU:HB3	1:F:283:CYS:SG	1.94	1.07
1:D:210:LEU:CD2	1:D:234:GLN:HG2	1.83	1.07
1:G:217:ALA:HB2	1:G:222:LEU:HD13	1.36	1.07
1:G:231:THR:HG22	1:G:234:GLN:N	1.70	1.06
1:D:170:TRP:O	1:D:171:LEU:HD12	1.55	1.06
1:D:172:TYR:CA	1:D:255:GLY:O	2.01	1.06
1:E:157:ARG:O	1:E:161:GLN:HG3	1.53	1.06
1:F:187:HIS:CD2	1:F:197:PHE:CB	2.38	1.06
1:C:235:GLN:NE2	1:C:269:ILE:H	1.53	1.05
1:B:262:LEU:CD1	1:B:266:ASN:HD22	1.68	1.05
1:E:226:HIS:N	1:E:227:PRO:HD3	1.69	1.05
1:F:151:TRP:O	1:F:155:TYR:CB	2.04	1.05
1:F:221:THR:CG2	1:F:222:LEU:H	1.67	1.05
1:E:247:ARG:CG	1:E:247:ARG:HH11	1.70	1.05
1:F:157:ARG:O	1:F:161:GLN:CB	2.04	1.05
1:G:231:THR:CG2	1:G:234:GLN:H	1.70	1.05
1:C:195:GLY:HA3	1:C:220:GLY:N	1.71	1.04
1:F:171:LEU:CB	1:F:283:CYS:SG	2.45	1.04
1:H:195:GLY:HA3	1:H:219:GLY:O	1.56	1.04
1:F:239:VAL:HG21	1:G:278:MSE:CE	1.87	1.04
1:H:196:GLU:O	1:H:220:GLY:HA3	1.55	1.04
1:F:259:LEU:HB3	1:F:280:GLN:HE21	0.88	1.04
1:E:152:ILE:CD1	1:E:152:ILE:H	1.70	1.03
1:A:174:ALA:O	1:A:177:THR:HG23	1.59	1.03
1:B:235:GLN:HE22	1:B:269:ILE:H	1.06	1.03
1:B:169:VAL:HG11	1:B:186:LEU:CD1	1.87	1.02
1:A:155:TYR:HE2	1:A:286:LEU:HD11	1.24	1.02
1:G:223:VAL:C	1:G:224:LEU:HD23	1.79	1.02
1:A:204:PRO:CD	1:B:267:HIS:ND1	2.24	1.01
1:F:278:MSE:CE	1:G:263:ALA:CB	2.37	1.01
1:A:226:HIS:N	1:A:227:PRO:HD3	1.74	1.01
1:C:195:GLY:CA	1:C:219:GLY:C	2.29	1.01
1:E:152:ILE:N	1:E:152:ILE:HD12	1.74	1.01
1:G:170:TRP:HH2	1:G:257:THR:O	1.44	1.01
1:F:226:HIS:N	1:F:227:PRO:HD3	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:THR:HG22	1:G:234:GLN:H	0.84	1.01
1:B:165:THR:CG2	1:B:167:ILE:HG13	1.91	1.01
1:D:221:THR:CG2	1:D:252:ILE:CD1	2.37	1.01
1:F:278:MSE:HG3	1:G:270:ALA:CB	1.91	1.00
1:C:155:TYR:HE1	1:C:159:LEU:HD13	1.26	1.00
1:H:204:PRO:HD2	1:H:205:ASP:H	1.26	0.99
1:F:238:LEU:O	1:F:242:GLN:HB2	1.62	0.99
1:C:173:GLY:O	1:C:256:ASP:HA	1.62	0.99
1:G:177:THR:CG2	1:G:179:ARG:HG2	1.91	0.99
1:G:170:TRP:CZ3	1:G:172:TYR:HB3	1.98	0.98
1:E:247:ARG:HH11	1:E:247:ARG:HG3	1.27	0.98
1:F:221:THR:HG22	1:F:222:LEU:H	0.85	0.98
1:A:172:TYR:HA	1:A:255:GLY:O	1.62	0.98
1:F:178:GLY:O	1:F:182:GLY:HA3	1.63	0.98
1:F:197:PHE:HD2	1:F:197:PHE:O	1.46	0.98
1:D:226:HIS:N	1:D:227:PRO:HD3	1.77	0.98
1:F:199:TYR:CB	1:F:223:VAL:HG13	1.89	0.97
1:F:262:LEU:O	1:F:262:LEU:HD12	1.62	0.97
1:D:221:THR:CG2	1:D:252:ILE:HD12	1.94	0.97
1:E:226:HIS:CE1	1:F:265:SER:O	2.17	0.97
1:F:187:HIS:CD2	1:F:197:PHE:CD1	2.52	0.97
1:B:235:GLN:NE2	1:B:269:ILE:H	1.63	0.97
1:G:210:LEU:HD12	1:G:210:LEU:O	1.64	0.97
1:E:231:THR:CG2	1:E:234:GLN:HG3	1.95	0.96
1:F:239:VAL:HG21	1:G:278:MSE:HE1	1.38	0.96
1:G:170:TRP:CH2	1:G:257:THR:O	2.17	0.96
1:B:174:ALA:N	1:B:177:THR:HG21	1.80	0.96
1:F:278:MSE:CE	1:G:263:ALA:HB1	1.94	0.96
1:C:226:HIS:N	1:C:227:PRO:CD	2.29	0.96
1:D:170:TRP:C	1:D:171:LEU:HD13	1.86	0.96
1:F:278:MSE:HE1	1:G:263:ALA:HB3	1.47	0.96
1:D:171:LEU:CD1	1:D:171:LEU:N	2.29	0.95
1:G:170:TRP:HZ3	1:G:172:TYR:CD2	1.84	0.95
1:B:170:TRP:O	1:B:280:GLN:HA	1.63	0.95
1:C:203:THR:CB	1:C:206:ASN:HB2	1.96	0.95
1:C:222:LEU:HD11	1:C:224:LEU:HD21	1.48	0.95
1:D:232:ARG:HB3	1:D:269:ILE:HD11	1.48	0.95
1:D:172:TYR:CB	1:D:255:GLY:O	2.14	0.95
1:H:203:THR:CB	1:H:204:PRO:CD	2.35	0.95
1:H:262:LEU:HA	1:H:266:ASN:CB	1.95	0.95
1:F:187:HIS:CD2	1:F:197:PHE:HD1	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:HD1	1:A:223:VAL:HG12	1.28	0.94
1:C:242:GLN:HA	1:C:242:GLN:NE2	1.82	0.94
1:C:214:ILE:HG23	1:C:249:PHE:HE2	1.33	0.94
1:E:208:PRO:HB2	1:E:209:GLN:NE2	1.83	0.94
1:G:177:THR:HG22	1:G:179:ARG:HG2	1.50	0.94
1:C:235:GLN:HE22	1:C:269:ILE:N	1.64	0.94
1:B:203:THR:HG23	1:B:206:ASN:CB	1.98	0.93
1:C:235:GLN:HE22	1:C:269:ILE:H	0.95	0.93
1:B:202:LEU:N	1:B:202:LEU:CD2	2.30	0.93
1:D:205:ASP:O	1:D:208:PRO:HD2	1.69	0.93
1:D:221:THR:HG21	1:D:252:ILE:CD1	1.97	0.93
1:F:177:THR:O	1:F:285:PRO:HD3	1.67	0.93
1:E:152:ILE:CD1	1:E:152:ILE:N	2.30	0.93
1:B:170:TRP:HB3	1:B:280:GLN:CB	1.99	0.93
1:A:152:ILE:O	1:A:156:ARG:HG3	1.69	0.92
1:H:226:HIS:N	1:H:227:PRO:HD3	1.82	0.92
1:E:204:PRO:CG	1:F:229:HIS:O	2.18	0.92
1:A:259:LEU:HD23	1:A:276:PHE:CB	1.99	0.92
1:E:202:LEU:HB2	1:E:225:SER:O	1.68	0.92
1:E:211:ASN:HA	1:E:214:ILE:HG13	1.49	0.92
1:E:214:ILE:HG21	1:E:241:LEU:CD1	1.99	0.92
1:F:199:TYR:C	1:F:199:TYR:CD2	2.41	0.92
1:H:262:LEU:O	1:H:266:ASN:CB	2.18	0.91
1:E:231:THR:HG22	1:E:234:GLN:CG	2.00	0.91
1:G:177:THR:HG22	1:G:179:ARG:H	1.35	0.91
1:F:259:LEU:HD23	1:F:276:PHE:HB2	1.51	0.91
1:F:199:TYR:HD2	1:F:199:TYR:O	1.52	0.91
1:H:242:GLN:OE1	1:H:242:GLN:HA	1.68	0.91
1:G:223:VAL:O	1:G:224:LEU:HD23	1.71	0.90
1:D:203:THR:CG2	1:D:204:PRO:HD2	2.01	0.90
1:E:226:HIS:N	1:E:227:PRO:CD	2.34	0.90
1:H:231:THR:HG22	1:H:234:GLN:H	1.36	0.90
1:D:223:VAL:O	1:D:224:LEU:HD23	1.70	0.90
1:B:169:VAL:HG11	1:B:186:LEU:HD13	1.50	0.89
1:G:170:TRP:CZ3	1:G:172:TYR:CD2	2.60	0.89
1:H:170:TRP:CZ2	1:H:255:GLY:HA3	2.07	0.89
1:D:171:LEU:HD13	1:D:171:LEU:N	1.87	0.89
1:F:203:THR:O	1:F:206:ASN:N	2.05	0.89
1:D:168:ALA:CB	1:D:276:PHE:CE1	2.55	0.89
1:H:203:THR:HB	1:H:204:PRO:HD3	1.55	0.89
1:C:172:TYR:CA	1:C:255:GLY:O	2.18	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:VAL:HG21	1:H:217:ALA:HA	1.52	0.88
1:E:220:GLY:O	1:E:249:PHE:HB2	1.73	0.88
1:B:262:LEU:HD12	1:B:266:ASN:ND2	1.89	0.88
1:H:203:THR:CB	1:H:204:PRO:HD3	2.00	0.88
1:C:195:GLY:HA3	1:C:219:GLY:O	1.72	0.87
1:E:197:PHE:CE2	1:H:193:ALA:HB3	2.08	0.87
1:B:165:THR:HG22	1:B:167:ILE:H	1.37	0.87
1:E:197:PHE:HD2	1:E:197:PHE:O	1.57	0.87
1:G:171:LEU:HD12	1:G:171:LEU:H	1.33	0.87
1:A:204:PRO:HD2	1:B:267:HIS:HD1	1.38	0.87
1:F:187:HIS:HD2	1:F:197:PHE:HB2	1.39	0.87
1:B:262:LEU:O	1:B:266:ASN:HB2	1.75	0.87
1:C:241:LEU:O	1:C:244:GLN:HG3	1.75	0.87
1:D:219:GLY:N	1:D:248:PRO:O	2.07	0.86
1:B:170:TRP:CB	1:B:280:GLN:HB3	2.04	0.86
1:C:221:THR:HG23	1:C:250:ARG:HB3	1.55	0.86
1:F:187:HIS:HD2	1:F:197:PHE:CG	1.94	0.86
1:H:180:MSE:O	1:H:184:ARG:HG3	1.75	0.86
1:D:221:THR:HG23	1:D:252:ILE:HD12	1.58	0.86
1:E:196:GLU:O	1:E:220:GLY:HA3	1.76	0.86
1:G:181:THR:HG23	1:G:184:ARG:NH2	1.91	0.85
1:D:172:TYR:H	1:D:172:TYR:HD2	1.22	0.85
1:G:171:LEU:N	1:G:171:LEU:CD1	2.39	0.85
1:D:170:TRP:CH2	1:D:255:GLY:HA3	2.11	0.85
1:F:171:LEU:HB2	1:F:283:CYS:SG	2.14	0.85
1:A:155:TYR:CE2	1:A:286:LEU:HD11	2.13	0.84
1:D:203:THR:HG22	1:D:204:PRO:HD2	1.58	0.84
1:C:231:THR:HG22	1:C:233:GLU:H	1.42	0.84
1:B:177:THR:OG1	1:B:283:CYS:O	1.96	0.84
1:F:197:PHE:O	1:F:197:PHE:CD2	2.30	0.84
1:C:202:LEU:CD1	1:C:207:ALA:HB2	2.07	0.84
1:E:226:HIS:HE1	1:F:265:SER:O	1.59	0.84
1:B:203:THR:HG23	1:B:206:ASN:HB3	1.58	0.83
1:B:213:PHE:O	1:B:217:ALA:N	2.11	0.83
1:F:178:GLY:O	1:F:182:GLY:CA	2.25	0.83
1:B:174:ALA:O	1:B:177:THR:CG2	2.22	0.83
1:C:155:TYR:CE1	1:C:159:LEU:HD13	2.13	0.83
1:F:201:GLU:HG2	1:F:225:SER:OG	1.78	0.83
1:E:181:THR:HA	1:E:184:ARG:HG3	1.60	0.83
1:C:228:GLU:CD	1:C:228:GLU:H	1.79	0.82
1:B:170:TRP:N	1:B:279:THR:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:HIS:CE1	1:D:241:LEU:CD1	2.61	0.82
1:C:276:PHE:HD2	1:C:276:PHE:N	1.75	0.82
1:B:174:ALA:N	1:B:177:THR:CG2	2.43	0.82
1:C:241:LEU:HA	1:C:244:GLN:NE2	1.93	0.82
1:B:262:LEU:CD1	1:B:266:ASN:ND2	2.42	0.82
1:C:214:ILE:HG23	1:C:249:PHE:CE2	2.14	0.82
1:C:195:GLY:CA	1:C:220:GLY:N	2.43	0.81
1:D:172:TYR:CD1	1:D:258:SER:HA	2.15	0.81
1:A:226:HIS:N	1:A:227:PRO:CD	2.43	0.81
1:E:247:ARG:HG3	1:E:247:ARG:NH1	1.89	0.81
1:F:226:HIS:N	1:F:227:PRO:CD	2.43	0.81
1:F:278:MSE:HG3	1:G:270:ALA:HB2	1.62	0.81
1:B:235:GLN:HE22	1:B:269:ILE:N	1.79	0.81
1:C:276:PHE:N	1:C:276:PHE:CD2	2.44	0.81
1:E:236:TYR:CE2	1:E:240:GLN:NE2	2.47	0.81
1:C:276:PHE:HD2	1:C:276:PHE:H	1.26	0.81
1:H:262:LEU:O	1:H:266:ASN:CA	2.28	0.81
1:A:236:TYR:CE2	1:A:240:GLN:NE2	2.49	0.81
1:F:242:GLN:HE21	1:F:242:GLN:CA	1.93	0.81
1:C:222:LEU:HD11	1:C:224:LEU:CD2	2.11	0.80
1:B:165:THR:HG22	1:B:167:ILE:HG13	1.61	0.80
1:E:156:ARG:O	1:E:160:GLN:CG	2.26	0.80
1:F:278:MSE:HG3	1:G:270:ALA:HB1	1.60	0.80
1:A:203:THR:OG1	1:B:267:HIS:CE1	2.33	0.80
1:B:201:GLU:C	1:B:202:LEU:HD23	2.01	0.80
1:B:276:PHE:O	1:B:280:GLN:HG2	1.81	0.80
1:C:228:GLU:HG2	1:C:229:HIS:HD2	1.47	0.80
1:B:202:LEU:HD23	1:B:202:LEU:H	1.46	0.79
1:D:203:THR:HB	1:D:206:ASN:HB3	1.64	0.79
1:D:221:THR:HG23	1:D:252:ILE:CD1	2.09	0.79
1:F:276:PHE:O	1:F:279:THR:N	2.12	0.79
1:D:170:TRP:HD1	1:D:280:GLN:HA	1.46	0.79
1:D:226:HIS:N	1:D:227:PRO:CD	2.44	0.79
1:D:231:THR:H	1:D:234:GLN:HE21	1.29	0.79
1:D:170:TRP:CZ2	1:D:172:TYR:HB3	2.17	0.79
1:H:204:PRO:CD	1:H:205:ASP:H	1.96	0.79
1:E:177:THR:CG2	1:E:177:THR:O	2.30	0.79
1:H:262:LEU:CB	1:H:268:ILE:HG21	2.05	0.79
1:H:198:VAL:CG2	1:H:217:ALA:HA	2.12	0.79
1:E:166:ASP:OD2	1:E:247:ARG:NH1	2.17	0.79
1:C:226:HIS:H	1:C:227:PRO:HD3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:PRO:HA	1:F:179:ARG:HH21	1.48	0.78
1:F:259:LEU:HG	1:F:273:TYR:HD1	1.47	0.78
1:G:166:ASP:HA	1:G:250:ARG:HH21	1.47	0.78
1:B:168:ALA:O	1:B:279:THR:CB	2.30	0.78
1:G:201:GLU:HA	1:G:225:SER:OG	1.83	0.78
1:G:217:ALA:HB1	1:G:222:LEU:HB2	1.64	0.78
1:C:202:LEU:HD13	1:C:207:ALA:HB2	1.65	0.77
1:C:221:THR:HG23	1:C:250:ARG:CB	2.13	0.77
1:B:157:ARG:O	1:B:161:GLN:CB	2.33	0.77
1:B:174:ALA:H	1:B:177:THR:HG21	1.46	0.77
1:E:202:LEU:HD12	1:E:227:PRO:HA	1.66	0.77
1:B:158:ARG:O	1:B:162:LEU:N	2.16	0.77
1:A:199:TYR:HD1	1:A:223:VAL:CG1	1.97	0.77
1:C:177:THR:CB	2:C:2:SO4:O3	2.33	0.77
1:E:152:ILE:H	1:E:152:ILE:HD13	1.48	0.77
1:E:197:PHE:O	1:E:197:PHE:CD2	2.37	0.77
1:E:208:PRO:HB2	1:E:209:GLN:HE21	1.47	0.77
1:C:150:GLU:O	1:C:154:GLN:N	2.16	0.76
1:E:197:PHE:CD2	1:E:197:PHE:C	2.58	0.76
1:C:203:THR:O	1:C:207:ALA:N	2.19	0.76
1:B:210:LEU:HG	1:B:214:ILE:CD1	2.14	0.76
1:B:170:TRP:HB2	1:B:276:PHE:CD1	2.21	0.76
1:F:171:LEU:HD23	1:F:281:ILE:HG21	1.67	0.76
1:B:259:LEU:H	1:B:280:GLN:NE2	1.84	0.76
1:D:203:THR:O	1:D:207:ALA:N	2.19	0.76
1:E:214:ILE:HG21	1:E:241:LEU:HD11	1.69	0.75
1:A:241:LEU:O	1:A:244:GLN:NE2	2.18	0.75
1:A:158:ARG:O	1:A:162:LEU:HB2	1.87	0.75
1:B:177:THR:HA	1:E:270:ALA:HB1	1.66	0.75
1:E:241:LEU:HD23	1:E:244:GLN:NE2	2.02	0.75
1:A:259:LEU:N	1:A:280:GLN:OE1	2.19	0.75
1:C:169:VAL:HG12	1:C:171:LEU:CD1	2.16	0.75
1:E:225:SER:C	1:E:227:PRO:HD3	2.05	0.75
1:C:230:LEU:CA	1:C:234:GLN:OE1	2.32	0.75
1:D:221:THR:CG2	1:D:252:ILE:HD11	2.15	0.75
1:D:210:LEU:HD22	1:D:234:GLN:CG	2.10	0.75
1:E:177:THR:O	1:E:177:THR:HG22	1.87	0.74
1:F:201:GLU:CG	1:F:225:SER:OG	2.34	0.74
1:A:205:ASP:OD1	1:B:232:ARG:HD2	1.86	0.74
1:C:184:ARG:O	1:C:188:GLN:HB2	1.87	0.74
1:D:185:TYR:CD2	1:D:189:PHE:CE2	2.74	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLY:O	1:F:182:GLY:N	2.21	0.74
1:E:219:GLY:N	1:E:248:PRO:O	2.18	0.74
1:C:196:GLU:O	1:C:220:GLY:HA3	1.87	0.74
1:D:207:ALA:N	1:D:208:PRO:CD	2.51	0.74
1:H:222:LEU:HD12	1:H:223:VAL:N	2.03	0.74
1:H:262:LEU:CA	1:H:266:ASN:CB	2.65	0.74
1:A:225:SER:C	1:A:227:PRO:HD3	2.07	0.74
1:D:221:THR:HG21	1:D:252:ILE:HD11	1.68	0.74
1:D:203:THR:CG2	1:D:204:PRO:CD	2.66	0.74
1:F:225:SER:C	1:F:227:PRO:HD3	2.08	0.74
1:H:196:GLU:O	1:H:220:GLY:CA	2.35	0.74
1:A:152:ILE:O	1:A:156:ARG:N	2.18	0.73
1:A:172:TYR:CA	1:A:255:GLY:O	2.36	0.73
1:D:185:TYR:CD1	1:D:185:TYR:C	2.61	0.73
1:E:226:HIS:HA	1:E:228:GLU:OE2	1.88	0.73
1:G:177:THR:CG2	1:G:283:CYS:HB2	2.18	0.73
1:F:199:TYR:CB	1:F:223:VAL:HG11	2.03	0.73
1:B:173:GLY:HA3	1:B:177:THR:HG21	1.69	0.73
1:H:226:HIS:N	1:H:227:PRO:CD	2.51	0.73
1:E:204:PRO:CB	1:F:229:HIS:O	2.36	0.73
1:E:242:GLN:HA	1:E:242:GLN:NE2	2.03	0.73
1:A:232:ARG:HG2	1:A:232:ARG:HH11	1.54	0.72
1:F:199:TYR:CD2	1:F:199:TYR:O	2.38	0.72
1:F:199:TYR:O	1:F:200:ARG:NH1	2.21	0.72
1:B:271:GLU:HA	1:B:274:TYR:CD2	2.24	0.72
1:C:235:GLN:HB2	1:C:269:ILE:HD13	1.71	0.72
1:C:274:TYR:HA	1:C:277:ALA:HB2	1.71	0.72
1:G:221:THR:HG21	1:G:252:ILE:HD13	1.71	0.72
1:G:166:ASP:HA	1:G:250:ARG:NH2	2.04	0.72
1:A:179:ARG:CA	1:A:283:CYS:SG	2.75	0.72
1:B:259:LEU:CD2	1:B:276:PHE:HB2	2.19	0.72
1:F:170:TRP:HB2	1:F:276:PHE:CD1	2.25	0.72
1:D:203:THR:HG23	1:D:204:PRO:HD2	1.72	0.72
1:B:259:LEU:O	1:B:263:ALA:N	2.19	0.72
1:F:278:MSE:CG	1:G:270:ALA:CB	2.68	0.72
1:G:158:ARG:HG2	1:G:281:ILE:HD12	1.70	0.72
1:B:233:GLU:O	1:B:237:HIS:N	2.22	0.72
1:G:174:ALA:O	1:G:177:THR:HB	1.89	0.71
1:G:177:THR:HG22	1:G:179:ARG:N	2.04	0.71
1:G:187:HIS:CE1	1:G:195:GLY:O	2.42	0.71
1:B:173:GLY:HA2	1:E:273:TYR:OH	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ALA:CB	1:B:175:PRO:HD2	2.00	0.71
1:F:260:VAL:HG22	1:F:273:TYR:CZ	2.25	0.71
1:G:155:TYR:HD1	1:G:155:TYR:O	1.73	0.71
1:G:177:THR:HG21	1:G:283:CYS:HB2	1.70	0.71
1:H:203:THR:CG2	1:H:204:PRO:HD3	2.21	0.71
1:C:169:VAL:HG12	1:C:171:LEU:HD11	1.72	0.71
1:E:165:THR:CB	1:E:167:ILE:CD1	2.69	0.71
1:G:167:ILE:HG22	1:G:247:ARG:HH22	1.55	0.71
1:H:196:GLU:HG3	1:H:198:VAL:HG22	1.71	0.71
1:A:168:ALA:O	1:A:279:THR:CB	2.39	0.71
1:G:170:TRP:CZ3	1:G:172:TYR:CB	2.73	0.71
1:G:181:THR:HG23	1:G:184:ARG:HH22	1.55	0.71
1:G:210:LEU:HD12	1:G:210:LEU:C	2.09	0.71
1:G:241:LEU:HD23	1:G:244:GLN:NE2	2.04	0.71
1:F:259:LEU:CD2	1:F:276:PHE:HB2	2.21	0.71
1:C:239:VAL:HG22	1:C:272:LEU:HA	1.74	0.70
1:F:242:GLN:HA	1:F:242:GLN:NE2	2.06	0.70
1:H:223:VAL:HG13	1:H:252:ILE:HG22	1.73	0.70
1:H:262:LEU:HB3	1:H:268:ILE:CG2	2.10	0.70
1:A:174:ALA:O	1:A:177:THR:CG2	2.38	0.70
1:D:203:THR:HG22	1:D:204:PRO:CD	2.21	0.70
1:A:203:THR:OG1	1:B:267:HIS:HE1	1.71	0.70
1:F:260:VAL:CG2	1:F:273:TYR:OH	2.40	0.70
1:A:199:TYR:CD1	1:A:223:VAL:HG12	2.19	0.70
1:C:162:LEU:HB2	1:C:186:LEU:HD21	1.73	0.70
1:E:265:SER:C	1:E:266:ASN:OD1	2.30	0.70
1:E:148:ARG:O	1:E:152:ILE:CD1	2.40	0.69
1:E:230:LEU:HD22	1:E:234:GLN:OE1	1.91	0.69
1:F:201:GLU:HA	1:F:225:SER:OG	1.92	0.69
1:C:170:TRP:CZ3	1:C:257:THR:O	2.46	0.69
1:D:168:ALA:HB1	1:D:276:PHE:HE1	1.50	0.69
1:C:262:LEU:O	1:C:262:LEU:CD2	2.30	0.69
1:E:216:LEU:HD12	1:E:216:LEU:O	1.92	0.69
1:F:278:MSE:CG	1:G:270:ALA:HB1	2.21	0.69
1:D:232:ARG:HG2	1:D:269:ILE:CD1	2.23	0.69
1:F:210:LEU:HD22	1:F:234:GLN:HE21	1.58	0.69
1:H:262:LEU:O	1:H:266:ASN:N	2.26	0.69
1:A:188:GLN:HA	1:A:188:GLN:NE2	2.01	0.69
1:C:215:ALA:O	1:C:218:GLN:HB3	1.92	0.69
1:C:231:THR:N	1:C:234:GLN:HB2	2.08	0.69
1:D:172:TYR:HD2	1:D:172:TYR:N	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:SER:C	1:D:227:PRO:HD3	2.13	0.69
1:G:221:THR:CG2	1:G:252:ILE:HD13	2.22	0.69
1:H:262:LEU:C	1:H:268:ILE:CG2	2.60	0.69
1:B:201:GLU:CA	1:B:202:LEU:HD23	2.23	0.69
1:C:262:LEU:HD23	1:C:262:LEU:C	2.12	0.69
1:C:198:VAL:HB	1:C:221:THR:O	1.93	0.69
1:D:202:LEU:HD13	1:D:230:LEU:HG	1.74	0.69
1:G:165:THR:OG1	1:G:167:ILE:HG12	1.93	0.69
1:A:184:ARG:O	1:A:188:GLN:HG2	1.93	0.69
1:B:173:GLY:CA	1:B:177:THR:HG21	2.23	0.69
1:B:232:ARG:O	1:B:236:TYR:N	2.20	0.69
1:F:199:TYR:HB2	1:F:223:VAL:HG12	1.62	0.69
1:G:155:TYR:CE1	1:G:159:LEU:HD22	2.28	0.69
1:A:229:HIS:O	1:B:204:PRO:HB3	1.92	0.68
1:B:165:THR:O	1:B:250:ARG:NH2	2.26	0.68
1:H:202:LEU:HD12	1:H:227:PRO:HA	1.75	0.68
1:D:172:TYR:HB2	1:D:255:GLY:O	1.93	0.68
1:A:236:TYR:HD2	1:A:236:TYR:O	1.77	0.68
1:C:238:LEU:O	1:C:242:GLN:HB2	1.93	0.68
1:D:231:THR:HG22	1:D:233:GLU:N	2.07	0.68
1:E:188:GLN:HA	1:E:188:GLN:OE1	1.92	0.68
1:B:201:GLU:HA	1:B:225:SER:OG	1.93	0.68
1:D:232:ARG:CB	1:D:269:ILE:CD1	2.71	0.68
1:D:232:ARG:HG2	1:D:269:ILE:HD12	1.74	0.68
1:C:170:TRP:HD1	1:C:276:PHE:CE1	2.11	0.68
1:F:262:LEU:HD12	1:F:262:LEU:C	2.14	0.68
1:B:203:THR:HG23	1:B:206:ASN:HB2	1.76	0.68
1:C:151:TRP:O	1:C:156:ARG:N	2.23	0.68
1:D:232:ARG:HB3	1:D:269:ILE:CD1	2.21	0.68
1:D:205:ASP:O	1:D:208:PRO:CD	2.41	0.68
1:E:269:ILE:HG13	1:E:272:LEU:H	1.58	0.68
1:G:201:GLU:HG3	1:G:225:SER:OG	1.93	0.68
1:B:259:LEU:H	1:B:280:GLN:HE22	1.39	0.68
1:D:231:THR:HG22	1:D:233:GLU:H	1.58	0.68
1:G:177:THR:HG21	1:G:179:ARG:HG2	1.74	0.68
1:H:196:GLU:CG	1:H:198:VAL:HG22	2.24	0.68
1:H:203:THR:OG1	1:H:206:ASN:CB	2.42	0.68
1:E:218:GLN:HA	1:E:249:PHE:HB3	1.76	0.67
1:F:272:LEU:O	1:F:276:PHE:CD2	2.47	0.67
1:F:187:HIS:HD2	1:F:197:PHE:CB	1.89	0.67
1:E:214:ILE:CG2	1:E:241:LEU:HD13	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:PRO:HG2	1:F:229:HIS:O	1.93	0.67
1:F:171:LEU:HB3	1:F:281:ILE:HG23	1.75	0.67
1:F:199:TYR:C	1:F:199:TYR:HD2	1.90	0.67
1:B:168:ALA:HA	1:B:251:LEU:O	1.95	0.67
1:D:159:LEU:O	1:D:163:SER:N	2.26	0.67
1:D:170:TRP:HH2	1:D:255:GLY:HA3	1.58	0.67
1:G:171:LEU:HD11	1:G:252:ILE:HG23	1.77	0.67
1:F:177:THR:O	1:F:285:PRO:CD	2.41	0.67
1:A:207:ALA:N	1:A:208:PRO:CD	2.58	0.67
1:D:232:ARG:CB	1:D:269:ILE:HD11	2.23	0.67
1:F:268:ILE:CG2	1:F:269:ILE:N	2.58	0.67
1:G:170:TRP:HZ3	1:G:172:TYR:CG	2.13	0.67
1:B:278:MSE:HE2	1:C:270:ALA:HB2	1.77	0.67
1:C:262:LEU:CD2	1:C:266:ASN:CB	2.67	0.67
1:H:194:GLN:HG2	1:H:195:GLY:N	2.08	0.67
1:E:214:ILE:HG21	1:E:241:LEU:HD13	1.76	0.66
1:F:197:PHE:CD2	1:F:197:PHE:C	2.67	0.66
1:E:247:ARG:HH11	1:E:247:ARG:HG2	1.57	0.66
1:G:170:TRP:CZ3	1:G:172:TYR:CG	2.83	0.66
1:H:204:PRO:HD2	1:H:205:ASP:N	2.07	0.66
1:H:262:LEU:HD13	1:H:266:ASN:CB	2.24	0.66
1:C:225:SER:C	1:C:227:PRO:HD3	2.15	0.66
1:C:242:GLN:OE1	1:C:247:ARG:HD3	1.96	0.66
1:H:261:GLU:O	1:H:265:SER:N	2.27	0.66
1:B:173:GLY:C	1:B:177:THR:HG21	2.15	0.66
1:E:167:ILE:O	1:E:250:ARG:NH2	2.21	0.66
1:B:259:LEU:N	1:B:280:GLN:HE22	1.93	0.66
1:C:226:HIS:HA	1:C:228:GLU:OE1	1.96	0.66
1:D:168:ALA:C	1:D:276:PHE:HE1	1.98	0.66
1:G:171:LEU:H	1:G:171:LEU:CD1	2.02	0.66
1:D:237:HIS:HE1	1:D:241:LEU:HD21	1.60	0.66
1:D:231:THR:H	1:D:234:GLN:NE2	1.94	0.66
1:E:165:THR:CB	1:E:167:ILE:HD13	2.26	0.66
1:B:174:ALA:H	1:B:177:THR:CG2	2.06	0.66
1:F:210:LEU:O	1:F:214:ILE:N	2.29	0.66
1:E:207:ALA:N	1:E:208:PRO:CD	2.59	0.65
1:F:170:TRP:O	1:F:281:ILE:HG22	1.96	0.65
1:F:177:THR:C	1:F:285:PRO:HD3	2.16	0.65
1:F:260:VAL:HG22	1:F:273:TYR:OH	1.97	0.65
1:H:203:THR:HG22	1:H:204:PRO:HD3	1.78	0.65
1:C:228:GLU:HG2	1:C:229:HIS:CD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ARG:O	1:G:160:GLN:HB2	1.97	0.65
1:D:185:TYR:CD2	1:D:189:PHE:HE2	2.14	0.65
1:C:173:GLY:O	1:C:256:ASP:CA	2.44	0.65
1:F:187:HIS:NE2	1:F:197:PHE:CB	2.50	0.65
1:H:195:GLY:CA	1:H:219:GLY:O	2.41	0.65
1:E:209:GLN:HE21	1:E:209:GLN:N	1.94	0.65
1:F:203:THR:O	1:F:205:ASP:N	2.30	0.65
1:A:173:GLY:O	1:A:256:ASP:HA	1.97	0.65
1:C:195:GLY:HA3	1:C:220:GLY:CA	2.26	0.65
1:H:231:THR:O	1:H:235:GLN:OE1	2.14	0.65
1:A:259:LEU:HB2	1:A:280:GLN:OE1	1.97	0.65
1:C:242:GLN:NE2	1:C:242:GLN:CA	2.56	0.65
1:A:286:LEU:HD12	1:A:286:LEU:N	2.10	0.64
1:E:197:PHE:CE2	1:H:193:ALA:CB	2.80	0.64
1:C:214:ILE:HG12	1:C:249:PHE:CE2	2.30	0.64
1:F:171:LEU:HA	1:F:281:ILE:HG23	1.79	0.64
1:A:155:TYR:HE2	1:A:286:LEU:CD1	2.06	0.64
1:B:159:LEU:O	1:B:185:TYR:HE2	1.80	0.64
1:G:166:ASP:OD1	1:G:166:ASP:N	2.30	0.64
1:G:172:TYR:HA	1:G:255:GLY:O	1.98	0.64
1:H:204:PRO:CD	1:H:205:ASP:N	2.60	0.64
1:A:172:TYR:CD2	1:A:281:ILE:O	2.51	0.64
1:C:235:GLN:NE2	1:C:269:ILE:HG23	2.12	0.64
1:F:187:HIS:O	1:F:187:HIS:ND1	2.30	0.64
1:F:242:GLN:HE21	1:F:242:GLN:HA	1.63	0.64
1:H:262:LEU:O	1:H:268:ILE:CG2	2.45	0.64
1:A:259:LEU:O	1:A:262:LEU:N	2.30	0.64
1:B:170:TRP:CE3	1:B:253:GLY:HA3	2.32	0.64
1:B:177:THR:O	1:B:285:PRO:HD3	1.97	0.64
1:B:210:LEU:CG	1:B:214:ILE:HD11	2.17	0.64
1:D:169:VAL:HG12	1:D:171:LEU:CD1	2.21	0.64
1:E:196:GLU:O	1:E:220:GLY:CA	2.46	0.64
1:H:231:THR:C	1:H:235:GLN:OE1	2.35	0.64
1:A:155:TYR:HB2	1:A:284:LEU:HD12	1.79	0.64
1:B:177:THR:O	1:B:285:PRO:CD	2.45	0.64
1:E:197:PHE:HE2	1:H:193:ALA:HB3	1.62	0.64
1:E:202:LEU:CD1	1:E:230:LEU:HG	2.28	0.64
1:B:253:GLY:C	1:B:254:ILE:HD13	2.18	0.63
1:D:201:GLU:HA	1:D:225:SER:OG	1.98	0.63
1:E:186:LEU:O	1:E:190:GLY:N	2.31	0.63
1:F:242:GLN:CA	1:F:242:GLN:NE2	2.58	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:CYS:O	1:B:284:LEU:HD23	1.98	0.63
1:C:201:GLU:O	1:C:206:ASN:ND2	2.30	0.63
1:A:179:ARG:HB3	1:A:283:CYS:SG	2.38	0.63
1:F:203:THR:O	1:F:204:PRO:C	2.37	0.63
1:G:205:ASP:OD2	1:G:205:ASP:N	2.30	0.63
1:F:207:ALA:O	1:F:210:LEU:HB3	1.98	0.63
1:E:204:PRO:HB3	1:F:229:HIS:O	1.99	0.63
1:E:214:ILE:CG2	1:E:241:LEU:CD1	2.77	0.63
1:A:188:GLN:HE21	1:A:188:GLN:CA	2.02	0.63
1:D:185:TYR:CD1	1:D:189:PHE:HD2	2.16	0.63
1:E:241:LEU:HD23	1:E:244:GLN:HE21	1.63	0.63
1:C:231:THR:HG22	1:C:233:GLU:N	2.14	0.63
1:F:171:LEU:HA	1:F:281:ILE:CG2	2.29	0.63
1:A:170:TRP:HB3	1:A:280:GLN:HA	1.81	0.63
1:B:269:ILE:O	1:B:273:TYR:N	2.32	0.63
1:D:204:PRO:O	1:D:208:PRO:HD3	1.98	0.62
1:F:176:GLY:O	2:F:7:SO4:O2	2.16	0.62
1:H:223:VAL:HA	1:H:252:ILE:O	1.99	0.62
1:A:152:ILE:HG22	1:A:156:ARG:HG3	1.81	0.62
1:A:239:VAL:HG22	1:A:272:LEU:HA	1.80	0.62
1:E:197:PHE:HE2	1:H:193:ALA:CB	2.12	0.62
1:A:286:LEU:N	1:A:286:LEU:CD1	2.62	0.62
1:D:168:ALA:CB	1:D:276:PHE:HE1	2.06	0.62
1:F:259:LEU:HG	1:F:273:TYR:CD1	2.33	0.62
1:B:260:VAL:HB	1:B:273:TYR:OH	1.99	0.62
1:F:199:TYR:CG	1:F:223:VAL:HG13	2.34	0.62
1:A:229:HIS:O	1:B:204:PRO:CG	2.48	0.62
1:E:165:THR:CB	1:E:167:ILE:HD12	2.29	0.62
1:C:203:THR:HA	1:C:229:HIS:CE1	2.35	0.62
1:F:273:TYR:O	1:F:277:ALA:N	2.33	0.62
1:F:161:GLN:O	1:F:162:LEU:C	2.37	0.62
1:F:157:ARG:O	1:F:161:GLN:N	2.32	0.61
1:H:187:HIS:CD2	1:H:197:PHE:HB2	2.35	0.61
1:A:204:PRO:CD	1:B:267:HIS:CE1	2.70	0.61
1:G:226:HIS:N	1:G:227:PRO:CD	2.63	0.61
1:G:226:HIS:N	1:G:227:PRO:HD3	2.16	0.61
1:B:278:MSE:CE	1:C:270:ALA:HB2	2.28	0.61
1:C:202:LEU:HB2	1:C:225:SER:O	2.00	0.61
1:E:231:THR:CG2	1:E:234:GLN:H	2.14	0.61
1:G:155:TYR:O	1:G:155:TYR:CD1	2.54	0.61
1:C:198:VAL:O	1:C:223:VAL:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:O	1:A:158:ARG:HG2	1.99	0.61
1:B:207:ALA:N	1:B:208:PRO:CD	2.62	0.61
1:C:203:THR:HA	1:C:229:HIS:ND1	2.16	0.61
1:C:214:ILE:HG12	1:C:249:PHE:CZ	2.35	0.61
1:D:171:LEU:O	1:D:254:ILE:HA	2.00	0.61
1:A:284:LEU:O	1:A:286:LEU:HD12	2.00	0.61
1:B:172:TYR:HA	1:B:255:GLY:O	2.01	0.61
1:A:236:TYR:O	1:A:236:TYR:CD2	2.54	0.61
1:C:242:GLN:HA	1:C:242:GLN:HE21	1.65	0.61
1:D:159:LEU:CB	1:D:185:TYR:CZ	2.84	0.61
1:D:169:VAL:CG1	1:D:171:LEU:HD11	2.23	0.60
1:F:278:MSE:HB2	1:G:273:TYR:CD2	2.35	0.60
1:G:238:LEU:O	1:G:242:GLN:N	2.30	0.60
1:B:170:TRP:O	1:B:280:GLN:CA	2.43	0.60
1:E:231:THR:HG23	1:E:234:GLN:H	1.66	0.60
1:A:229:HIS:O	1:B:204:PRO:CB	2.49	0.60
1:D:248:PRO:HG2	1:D:249:PHE:HD2	1.65	0.60
1:E:207:ALA:N	1:E:208:PRO:HD2	2.17	0.60
1:F:199:TYR:CA	1:F:223:VAL:CG1	2.78	0.60
1:H:262:LEU:O	1:H:268:ILE:HG23	2.02	0.60
1:H:167:ILE:O	1:H:250:ARG:NH2	2.34	0.60
1:D:207:ALA:N	1:D:208:PRO:HD3	2.16	0.60
1:H:186:LEU:O	1:H:190:GLY:CA	2.50	0.60
1:H:198:VAL:HG21	1:H:217:ALA:CA	2.29	0.60
1:B:259:LEU:HB3	1:B:280:GLN:NE2	2.17	0.60
1:F:151:TRP:O	1:F:155:TYR:N	2.35	0.60
1:C:222:LEU:HD12	1:C:223:VAL:N	2.17	0.60
1:D:223:VAL:C	1:D:224:LEU:HD23	2.22	0.60
1:A:231:THR:HG22	1:A:233:GLU:N	2.17	0.60
1:D:172:TYR:N	1:D:172:TYR:CD2	2.59	0.60
1:F:234:GLN:O	1:F:238:LEU:HD12	2.01	0.60
1:G:169:VAL:N	1:G:276:PHE:HE1	2.00	0.60
1:F:272:LEU:O	1:F:276:PHE:CE2	2.55	0.59
1:D:168:ALA:HA	1:D:251:LEU:O	2.02	0.59
1:H:185:TYR:CD2	1:H:189:PHE:CD2	2.90	0.59
1:F:210:LEU:HA	1:F:213:PHE:CB	2.33	0.59
1:B:170:TRP:CD2	1:B:259:LEU:HB2	2.38	0.59
1:E:241:LEU:HD22	1:E:248:PRO:HG2	1.85	0.59
1:A:205:ASP:OD2	1:A:205:ASP:N	2.36	0.59
1:F:171:LEU:HA	1:F:281:ILE:O	2.03	0.59
1:D:237:HIS:ND1	1:D:241:LEU:HD11	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:PRO:CB	1:E:209:GLN:NE2	2.64	0.59
1:E:222:LEU:O	1:E:252:ILE:N	2.32	0.59
1:F:176:GLY:HA2	2:F:7:SO4:S	2.43	0.59
1:C:169:VAL:CG1	1:C:171:LEU:HD11	2.31	0.58
1:E:188:GLN:NE2	1:H:194:GLN:HG3	2.17	0.58
1:E:239:VAL:O	1:E:243:SER:N	2.35	0.58
1:C:170:TRP:HZ3	1:C:257:THR:O	1.85	0.58
1:H:222:LEU:HD12	1:H:223:VAL:H	1.68	0.58
1:A:152:ILE:O	1:A:156:ARG:CG	2.49	0.58
1:D:217:ALA:O	1:D:249:PHE:HB3	2.03	0.58
1:G:179:ARG:HG3	2:G:6:SO4:O3	2.03	0.58
1:D:170:TRP:HZ2	1:D:257:THR:O	1.87	0.58
1:F:202:LEU:CB	1:F:225:SER:O	2.51	0.58
1:G:207:ALA:O	1:G:210:LEU:HB3	2.03	0.58
1:C:156:ARG:O	1:C:160:GLN:HG3	2.04	0.58
1:F:259:LEU:HD12	1:F:259:LEU:O	2.04	0.58
1:H:231:THR:HG22	1:H:233:GLU:N	2.19	0.58
1:C:222:LEU:CD1	1:C:224:LEU:HD21	2.27	0.58
1:D:185:TYR:C	1:D:185:TYR:HD1	2.07	0.58
1:A:232:ARG:HG2	1:A:232:ARG:NH1	2.19	0.58
1:F:209:GLN:O	1:F:213:PHE:N	2.37	0.58
1:H:185:TYR:CD2	1:H:189:PHE:HD2	2.22	0.58
1:C:242:GLN:CA	1:C:242:GLN:HE21	2.16	0.57
1:H:167:ILE:O	1:H:250:ARG:CZ	2.52	0.57
1:A:236:TYR:CD2	1:A:236:TYR:C	2.78	0.57
1:G:195:GLY:HA3	1:G:219:GLY:O	2.03	0.57
1:E:202:LEU:HD11	1:E:230:LEU:HG	1.86	0.57
1:E:217:ALA:O	1:E:220:GLY:O	2.23	0.57
1:F:171:LEU:CB	1:F:281:ILE:HG23	2.34	0.57
1:G:177:THR:HG22	1:G:179:ARG:CG	2.30	0.57
1:C:150:GLU:O	1:C:154:GLN:CB	2.53	0.57
1:H:165:THR:O	1:H:250:ARG:NH1	2.37	0.57
1:H:170:TRP:CH2	1:H:255:GLY:HA3	2.39	0.57
1:B:170:TRP:N	1:B:276:PHE:HD1	2.02	0.57
1:F:212:ASP:OD2	1:F:212:ASP:N	2.37	0.57
1:C:170:TRP:CH2	1:C:255:GLY:HA3	2.39	0.57
1:A:147:GLY:HA2	1:H:184:ARG:NH1	2.20	0.57
1:D:159:LEU:CB	1:D:185:TYR:CE1	2.87	0.57
1:D:172:TYR:CE1	1:D:258:SER:HA	2.40	0.57
1:D:209:GLN:O	1:D:212:ASP:OD2	2.22	0.57
1:G:156:ARG:O	1:G:160:GLN:N	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:LEU:HB2	1:G:226:HIS:O	2.05	0.57
1:H:182:GLY:O	1:H:186:LEU:HG	2.04	0.57
1:F:149:SER:OG	1:F:150:GLU:N	2.33	0.57
1:H:225:SER:C	1:H:227:PRO:HD3	2.25	0.57
1:A:221:THR:HG23	1:A:250:ARG:HB3	1.86	0.57
1:E:181:THR:CA	1:E:184:ARG:HG3	2.33	0.57
1:D:178:GLY:N	2:D:4:SO4:O1	2.37	0.56
1:A:159:LEU:HB3	1:A:185:TYR:CE2	2.40	0.56
1:F:210:LEU:HD22	1:F:234:GLN:NE2	2.20	0.56
1:A:204:PRO:O	1:A:208:PRO:HD3	2.06	0.56
1:B:158:ARG:O	1:B:162:LEU:CA	2.52	0.56
1:F:151:TRP:O	1:F:155:TYR:CA	2.53	0.56
1:F:230:LEU:HB3	1:F:234:GLN:HB2	1.87	0.56
1:F:242:GLN:HE21	1:F:242:GLN:C	2.08	0.56
1:H:185:TYR:CE2	1:H:189:PHE:CD2	2.93	0.56
1:H:217:ALA:HB1	1:H:222:LEU:HB2	1.87	0.56
1:B:169:VAL:HA	1:B:279:THR:O	2.05	0.56
1:D:249:PHE:HE1	1:D:251:LEU:HD13	1.70	0.56
1:G:231:THR:HB	1:G:234:GLN:HB2	1.88	0.56
1:E:272:LEU:O	1:E:274:TYR:N	2.39	0.56
1:F:262:LEU:O	1:F:262:LEU:CD1	2.45	0.56
1:F:187:HIS:CD2	1:F:197:PHE:CG	2.80	0.56
1:A:259:LEU:CD2	1:A:276:PHE:CB	2.81	0.56
1:B:170:TRP:HE3	1:B:253:GLY:HA3	1.70	0.56
1:B:253:GLY:O	1:B:254:ILE:HD13	2.06	0.56
1:C:231:THR:CG2	1:C:232:ARG:N	2.68	0.56
1:E:272:LEU:O	1:E:273:TYR:C	2.43	0.56
1:G:170:TRP:CH2	1:G:172:TYR:CB	2.73	0.56
1:C:235:GLN:HE22	1:C:268:ILE:HA	1.71	0.56
1:E:188:GLN:OE1	1:E:188:GLN:CA	2.53	0.56
1:E:247:ARG:CG	1:E:247:ARG:NH1	2.41	0.56
1:H:186:LEU:O	1:H:190:GLY:HA3	2.05	0.56
1:A:171:LEU:O	1:A:254:ILE:HA	2.05	0.56
1:A:187:HIS:CG	1:A:197:PHE:HD1	2.24	0.56
1:A:231:THR:HG22	1:A:233:GLU:H	1.70	0.56
1:C:202:LEU:HD12	1:C:229:HIS:HB2	1.88	0.56
1:G:158:ARG:O	1:G:162:LEU:HG	2.06	0.56
1:A:185:TYR:O	1:A:189:PHE:HD2	1.88	0.55
1:E:228:GLU:OE1	1:E:262:LEU:HD21	2.06	0.55
1:A:199:TYR:CD1	1:A:223:VAL:CG1	2.85	0.55
1:F:232:ARG:O	1:F:236:TYR:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:HA	1:B:274:TYR:CE2	2.40	0.55
1:H:181:THR:O	1:H:185:TYR:N	2.31	0.55
1:B:259:LEU:HD22	1:B:276:PHE:HB2	1.89	0.55
1:D:199:TYR:HD1	1:D:223:VAL:HG12	1.70	0.55
1:E:259:LEU:H	1:E:280:GLN:NE2	2.04	0.55
1:F:239:VAL:O	1:F:243:SER:CB	2.54	0.55
1:C:221:THR:CG2	1:C:250:ARG:HG2	2.37	0.55
1:G:179:ARG:CG	2:G:6:SO4:O3	2.54	0.55
1:C:229:HIS:CD2	1:C:229:HIS:H	2.25	0.55
1:H:262:LEU:C	1:H:266:ASN:CB	2.75	0.55
1:A:204:PRO:CD	1:B:267:HIS:HD1	2.07	0.55
1:C:195:GLY:C	1:C:220:GLY:CA	2.75	0.55
1:F:263:ALA:O	1:F:266:ASN:O	2.25	0.55
1:C:231:THR:HG22	1:C:232:ARG:N	2.20	0.55
1:F:150:GLU:O	1:F:154:GLN:N	2.40	0.55
1:F:172:TYR:CE1	1:F:282:ALA:HB2	2.41	0.55
1:G:169:VAL:C	1:G:276:PHE:CE1	2.81	0.55
1:A:236:TYR:HE2	1:A:240:GLN:NE2	2.04	0.55
1:D:203:THR:CB	1:D:206:ASN:HB3	2.35	0.55
1:F:209:GLN:HA	1:F:212:ASP:OD1	2.06	0.55
1:F:221:THR:CG2	1:F:222:LEU:N	2.38	0.55
1:G:170:TRP:HB2	1:G:276:PHE:CG	2.41	0.55
1:A:185:TYR:C	1:A:185:TYR:CD2	2.81	0.54
1:A:242:GLN:O	1:A:247:ARG:HD2	2.07	0.54
1:A:207:ALA:N	1:A:208:PRO:HD2	2.22	0.54
1:D:232:ARG:CG	1:D:269:ILE:CD1	2.85	0.54
1:F:199:TYR:CA	1:F:223:VAL:HG13	2.37	0.54
1:D:232:ARG:HA	1:D:269:ILE:HD13	1.90	0.54
1:F:210:LEU:HD23	1:F:211:ASN:N	2.22	0.54
1:G:206:ASN:O	1:G:209:GLN:HB2	2.08	0.54
1:H:269:ILE:HG22	1:H:271:GLU:N	2.21	0.54
1:C:164:GLU:O	1:C:191:ARG:NH2	2.39	0.54
1:E:186:LEU:O	1:E:190:GLY:CA	2.55	0.54
1:F:172:TYR:HB3	1:F:257:THR:O	2.08	0.54
1:H:166:ASP:OD2	1:H:247:ARG:HD2	2.07	0.54
1:F:176:GLY:HA2	2:F:7:SO4:O4	2.07	0.54
1:G:155:TYR:CD1	1:G:155:TYR:C	2.80	0.54
1:H:187:HIS:CE1	1:H:197:PHE:HB2	2.42	0.54
1:C:241:LEU:HD22	1:C:244:GLN:NE2	2.22	0.54
1:F:271:GLU:O	1:F:275:CYS:SG	2.62	0.54
1:F:273:TYR:O	1:F:277:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:ALA:CB	1:G:222:LEU:HB2	2.34	0.54
1:E:170:TRP:CZ2	1:E:255:GLY:HA3	2.42	0.54
1:E:197:PHE:CD2	1:H:193:ALA:HB3	2.42	0.54
1:F:268:ILE:HG23	1:F:269:ILE:N	2.23	0.54
1:G:224:LEU:HD23	1:G:224:LEU:N	2.16	0.54
1:H:262:LEU:C	1:H:268:ILE:HG23	2.28	0.54
1:B:228:GLU:O	1:B:267:HIS:HB3	2.06	0.54
1:F:173:GLY:H	1:F:256:ASP:HA	1.73	0.54
1:F:267:HIS:O	1:F:267:HIS:CD2	2.61	0.54
1:A:197:PHE:C	1:A:197:PHE:CD2	2.80	0.54
1:C:174:ALA:O	1:C:177:THR:CB	2.55	0.54
1:C:237:HIS:O	1:C:241:LEU:HG	2.08	0.54
1:C:262:LEU:CD2	1:C:262:LEU:C	2.74	0.54
1:F:259:LEU:HD21	1:F:276:PHE:CD2	2.42	0.54
1:G:170:TRP:CZ2	1:G:255:GLY:HA3	2.42	0.53
1:G:238:LEU:O	1:G:242:GLN:HG2	2.08	0.53
1:E:148:ARG:O	1:E:152:ILE:HD13	2.08	0.53
1:E:186:LEU:O	1:E:190:GLY:HA3	2.08	0.53
1:E:242:GLN:O	1:E:247:ARG:HD3	2.08	0.53
1:A:179:ARG:CB	1:A:283:CYS:SG	2.96	0.53
1:B:177:THR:C	1:B:285:PRO:HD3	2.28	0.53
1:B:281:ILE:HD13	1:B:281:ILE:H	1.72	0.53
1:C:204:PRO:HD3	1:C:229:HIS:CE1	2.43	0.53
1:H:243:SER:O	1:H:244:GLN:HG2	2.09	0.53
1:A:259:LEU:CB	1:A:280:GLN:OE1	2.56	0.53
1:B:165:THR:HG21	1:B:167:ILE:HG13	1.87	0.53
1:B:170:TRP:HD1	1:B:280:GLN:HB2	1.73	0.53
1:E:148:ARG:O	1:E:152:ILE:HD11	2.07	0.53
1:H:231:THR:CG2	1:H:233:GLU:H	2.21	0.53
1:B:179:ARG:HG3	1:B:283:CYS:HB2	1.91	0.53
1:F:152:ILE:O	1:F:156:ARG:CB	2.56	0.53
1:D:199:TYR:HD1	1:D:223:VAL:CG1	2.22	0.53
1:H:179:ARG:CG	2:H:8:SO4:O1	2.57	0.53
1:B:165:THR:CG2	1:B:167:ILE:CG1	2.78	0.52
1:C:239:VAL:CG2	1:C:272:LEU:HA	2.40	0.52
1:G:155:TYR:CZ	1:G:159:LEU:HD22	2.45	0.52
1:A:147:GLY:CA	1:H:184:ARG:NH1	2.72	0.52
1:B:259:LEU:HD23	1:B:276:PHE:HB2	1.89	0.52
1:E:207:ALA:HB3	1:E:208:PRO:HD3	1.91	0.52
1:A:235:GLN:HB2	1:A:269:ILE:HD13	1.91	0.52
1:B:172:TYR:CB	1:B:255:GLY:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:CB	1:B:229:HIS:HD2	2.22	0.52
1:C:170:TRP:O	1:C:171:LEU:HD12	2.09	0.52
1:E:170:TRP:HB3	1:E:280:GLN:HG2	1.91	0.52
1:F:272:LEU:O	1:F:276:PHE:HD2	1.90	0.52
1:B:170:TRP:CZ2	1:B:255:GLY:HA3	2.45	0.52
1:D:231:THR:O	1:D:235:GLN:HG3	2.10	0.52
1:E:240:GLN:O	1:E:243:SER:N	2.42	0.52
1:F:231:THR:HG23	1:F:234:GLN:OE1	2.09	0.52
1:H:262:LEU:CD1	1:H:266:ASN:CB	2.87	0.52
1:A:236:TYR:HD2	1:A:236:TYR:C	2.11	0.52
1:D:203:THR:HG23	1:D:204:PRO:CD	2.36	0.52
1:E:177:THR:CG2	1:E:179:ARG:HG3	2.40	0.52
1:E:217:ALA:C	1:E:249:PHE:HB3	2.30	0.52
1:G:169:VAL:O	1:G:252:ILE:HA	2.09	0.52
1:E:177:THR:HG22	1:E:179:ARG:HG3	1.92	0.52
1:B:174:ALA:C	1:B:177:THR:HG22	2.20	0.52
1:C:235:GLN:NE2	1:C:269:ILE:N	2.34	0.52
1:A:239:VAL:CG2	1:A:272:LEU:HA	2.39	0.52
1:B:155:TYR:OH	1:B:283:CYS:SG	2.68	0.52
1:B:235:GLN:OE1	1:B:267:HIS:O	2.28	0.52
1:D:231:THR:HG21	1:D:233:GLU:OE1	2.11	0.52
1:E:187:HIS:CD2	1:E:197:PHE:HB2	2.45	0.52
1:G:166:ASP:HA	1:G:250:ARG:HD2	1.91	0.52
1:B:232:ARG:O	1:B:236:TYR:CB	2.59	0.51
1:D:217:ALA:O	1:D:249:PHE:CB	2.58	0.51
1:E:217:ALA:O	1:E:249:PHE:HB3	2.10	0.51
1:B:170:TRP:CE2	1:B:259:LEU:HB2	2.44	0.51
1:C:217:ALA:O	1:C:218:GLN:C	2.49	0.51
1:D:206:ASN:OD1	1:D:206:ASN:C	2.47	0.51
1:D:240:GLN:O	1:D:244:GLN:HG3	2.11	0.51
1:E:238:LEU:O	1:E:242:GLN:N	2.35	0.51
1:E:276:PHE:CD2	1:E:276:PHE:N	2.78	0.51
1:C:203:THR:CA	1:C:229:HIS:ND1	2.74	0.51
1:D:185:TYR:CD1	1:D:189:PHE:CD2	2.98	0.51
1:B:212:ASP:O	1:B:216:LEU:CB	2.59	0.51
1:B:225:SER:C	1:B:227:PRO:HD3	2.31	0.51
1:E:203:THR:HA	1:E:229:HIS:HD1	1.76	0.51
1:F:210:LEU:HD13	1:F:230:LEU:HD22	1.91	0.51
1:F:276:PHE:O	1:F:277:ALA:C	2.48	0.51
1:G:210:LEU:HA	1:G:213:PHE:CD2	2.46	0.51
1:G:254:ILE:O	1:G:254:ILE:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:PRO:HA	1:E:179:ARG:HH21	1.76	0.51
1:E:242:GLN:O	1:E:247:ARG:CD	2.59	0.51
1:H:213:PHE:CD1	1:H:213:PHE:N	2.76	0.51
1:B:177:THR:O	1:B:285:PRO:HG3	2.11	0.51
1:F:156:ARG:O	1:F:160:GLN:CB	2.59	0.51
1:G:177:THR:HG23	1:G:283:CYS:HB2	1.92	0.51
1:H:231:THR:HG22	1:H:234:GLN:N	2.16	0.51
1:C:162:LEU:O	1:C:165:THR:O	2.29	0.51
1:C:170:TRP:CD1	1:C:253:GLY:HA3	2.46	0.51
1:H:213:PHE:O	1:H:217:ALA:HB2	2.11	0.51
1:E:174:ALA:O	1:E:177:THR:HB	2.11	0.50
1:F:260:VAL:CG2	1:F:273:TYR:CE1	2.94	0.50
1:G:170:TRP:CZ3	1:G:172:TYR:HD2	2.24	0.50
1:B:170:TRP:HB2	1:B:276:PHE:CG	2.45	0.50
1:B:171:LEU:N	1:B:253:GLY:O	2.36	0.50
1:F:207:ALA:HB3	1:F:208:PRO:HD3	1.93	0.50
1:F:239:VAL:CG1	1:F:240:GLN:N	2.75	0.50
1:F:262:LEU:C	1:F:262:LEU:CD1	2.79	0.50
1:H:187:HIS:CG	1:H:197:PHE:HB2	2.46	0.50
1:G:170:TRP:O	1:G:280:GLN:HA	2.11	0.50
1:G:174:ALA:O	1:G:177:THR:CB	2.59	0.50
1:B:284:LEU:HD21	1:E:274:TYR:HB2	1.93	0.50
1:C:235:GLN:O	1:C:239:VAL:HG23	2.11	0.50
1:D:174:ALA:O	1:D:177:THR:CB	2.59	0.50
1:G:231:THR:CB	1:G:234:GLN:HB2	2.42	0.50
1:G:270:ALA:O	1:G:273:TYR:HB3	2.11	0.50
1:H:182:GLY:O	1:H:186:LEU:N	2.38	0.50
1:H:263:ALA:HA	1:H:268:ILE:HG23	1.92	0.50
1:H:269:ILE:HG22	1:H:271:GLU:H	1.76	0.50
1:D:210:LEU:HD23	1:D:234:GLN:HG2	1.84	0.50
1:F:176:GLY:C	1:F:178:GLY:H	2.14	0.50
1:A:213:PHE:O	1:A:217:ALA:CB	2.60	0.50
1:B:206:ASN:OD1	1:B:206:ASN:O	2.30	0.50
1:B:170:TRP:O	1:B:281:ILE:N	2.44	0.50
1:D:214:ILE:HG23	1:D:249:PHE:CE2	2.46	0.50
1:E:203:THR:HA	1:E:229:HIS:ND1	2.27	0.50
1:E:209:GLN:NE2	1:E:209:GLN:N	2.58	0.50
1:F:171:LEU:CA	1:F:281:ILE:HG23	2.41	0.50
1:F:230:LEU:HD22	1:F:234:GLN:NE2	2.26	0.50
1:H:262:LEU:C	1:H:268:ILE:HG21	2.30	0.50
1:C:228:GLU:OE2	1:C:266:ASN:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:HIS:CD2	1:G:192:ASN:O	2.65	0.50
1:G:237:HIS:O	1:G:241:LEU:N	2.34	0.50
1:C:155:TYR:CE2	1:C:283:CYS:HA	2.47	0.49
1:E:210:LEU:HA	1:E:213:PHE:CD2	2.46	0.49
1:C:201:GLU:OE1	1:C:226:HIS:CD2	2.65	0.49
1:C:214:ILE:CG2	1:C:249:PHE:HE2	2.12	0.49
1:D:178:GLY:O	1:D:182:GLY:N	2.39	0.49
1:G:195:GLY:HA3	1:G:220:GLY:CA	2.42	0.49
1:G:202:LEU:HD21	1:G:224:LEU:HD13	1.93	0.49
1:C:235:GLN:HB3	1:C:272:LEU:HD22	1.95	0.49
1:E:157:ARG:O	1:E:161:GLN:CG	2.43	0.49
1:E:214:ILE:HG23	1:E:249:PHE:CE2	2.47	0.49
1:F:239:VAL:HG13	1:F:240:GLN:N	2.28	0.49
1:G:199:TYR:HE1	1:G:225:SER:HB3	1.77	0.49
1:A:284:LEU:O	1:A:286:LEU:CD1	2.59	0.49
1:C:172:TYR:N	1:C:172:TYR:CD2	2.79	0.49
1:D:269:ILE:CG2	1:D:270:ALA:N	2.75	0.49
1:F:173:GLY:N	1:F:256:ASP:HA	2.26	0.49
1:H:187:HIS:CB	1:H:197:PHE:HD1	2.25	0.49
1:A:179:ARG:HG3	2:A:1:SO4:O3	2.13	0.49
1:A:242:GLN:HE22	1:A:247:ARG:HG2	1.78	0.49
1:D:194:GLN:H	1:D:194:GLN:HE21	1.61	0.49
1:E:220:GLY:O	1:E:249:PHE:CB	2.55	0.49
1:F:236:TYR:C	1:F:238:LEU:N	2.66	0.49
1:F:260:VAL:HG22	1:F:273:TYR:CE1	2.47	0.49
1:F:269:ILE:O	1:F:269:ILE:HG13	2.11	0.49
1:H:221:THR:HG22	1:H:222:LEU:N	2.28	0.49
1:C:151:TRP:O	1:C:156:ARG:CB	2.60	0.49
1:E:236:TYR:CZ	1:E:240:GLN:NE2	2.79	0.49
1:F:202:LEU:O	1:F:226:HIS:HB2	2.13	0.49
1:G:157:ARG:O	1:G:161:GLN:N	2.41	0.49
1:H:262:LEU:O	1:H:266:ASN:C	2.50	0.49
1:A:241:LEU:HA	1:A:244:GLN:NE2	2.27	0.49
1:D:206:ASN:C	1:D:208:PRO:HD2	2.33	0.49
1:D:232:ARG:CA	1:D:269:ILE:HD13	2.42	0.49
1:F:175:PRO:CA	1:F:179:ARG:HH21	2.23	0.49
1:G:200:ARG:HG3	1:G:213:PHE:CD2	2.48	0.49
1:A:260:VAL:CG1	1:A:273:TYR:OH	2.61	0.48
1:H:180:MSE:O	1:H:184:ARG:CG	2.55	0.48
1:B:202:LEU:HD12	1:B:226:HIS:O	2.13	0.48
1:E:201:GLU:H	1:H:189:PHE:HE1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:TRP:HZ2	1:G:255:GLY:HA3	1.78	0.48
1:B:159:LEU:O	1:B:185:TYR:CE2	2.63	0.48
1:G:223:VAL:O	1:G:224:LEU:CD2	2.53	0.48
1:A:248:PRO:HB2	1:A:249:PHE:HD2	1.78	0.48
1:D:203:THR:N	1:D:206:ASN:HB3	2.28	0.48
1:F:215:ALA:O	1:F:216:LEU:C	2.50	0.48
1:F:256:ASP:OD2	1:F:256:ASP:C	2.52	0.48
1:G:231:THR:HG22	1:G:234:GLN:HB2	1.95	0.48
1:D:203:THR:HB	1:D:206:ASN:CB	2.39	0.48
1:F:203:THR:C	1:F:205:ASP:N	2.65	0.48
1:F:260:VAL:CG2	1:F:273:TYR:CZ	2.93	0.48
1:D:185:TYR:CE1	1:D:189:PHE:CD2	3.01	0.48
1:G:220:GLY:O	1:G:249:PHE:HB2	2.14	0.48
1:B:260:VAL:HA	1:B:273:TYR:HE1	1.78	0.48
1:C:254:ILE:HG22	1:C:254:ILE:O	2.12	0.48
1:A:177:THR:OG1	1:A:179:ARG:HG2	2.13	0.48
1:B:284:LEU:HD21	1:E:274:TYR:CD1	2.48	0.48
1:G:241:LEU:HD23	1:G:244:GLN:HE22	1.77	0.48
1:F:171:LEU:CA	1:F:281:ILE:CG2	2.92	0.48
1:F:278:MSE:HG2	1:G:270:ALA:HA	1.96	0.48
1:C:235:GLN:CB	1:C:269:ILE:HD13	2.42	0.47
1:H:231:THR:CG2	1:H:233:GLU:N	2.77	0.47
1:H:261:GLU:O	1:H:265:SER:CA	2.62	0.47
1:A:168:ALA:HA	1:A:251:LEU:O	2.14	0.47
1:B:260:VAL:HA	1:B:273:TYR:CE1	2.49	0.47
1:C:225:SER:O	1:C:226:HIS:HB2	2.14	0.47
1:D:248:PRO:HG2	1:D:249:PHE:CD2	2.46	0.47
1:H:197:PHE:C	1:H:197:PHE:CD2	2.87	0.47
1:D:222:LEU:HB3	1:D:249:PHE:HD1	1.79	0.47
1:E:226:HIS:NE2	1:F:265:SER:O	2.45	0.47
1:F:157:ARG:O	1:F:161:GLN:CA	2.62	0.47
1:F:278:MSE:CE	1:G:263:ALA:HB2	2.41	0.47
1:G:273:TYR:O	1:G:277:ALA:N	2.47	0.47
1:B:172:TYR:CA	1:B:255:GLY:O	2.62	0.47
1:C:229:HIS:CD2	1:C:229:HIS:N	2.83	0.47
1:E:177:THR:O	1:E:177:THR:HG23	2.12	0.47
1:E:236:TYR:O	1:E:240:GLN:HG2	2.13	0.47
1:G:201:GLU:HG3	1:G:225:SER:HG	1.78	0.47
1:F:178:GLY:C	1:F:182:GLY:H	2.17	0.47
1:F:199:TYR:HA	1:F:223:VAL:CG1	2.44	0.47
1:D:169:VAL:N	1:D:276:PHE:HE1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLY:O	1:D:256:ASP:HA	2.14	0.47
1:E:228:GLU:CD	1:E:228:GLU:H	2.18	0.47
1:G:231:THR:HG23	1:G:233:GLU:H	1.80	0.47
1:H:230:LEU:HD22	1:H:234:GLN:OE1	2.14	0.47
1:A:171:LEU:N	1:A:253:GLY:O	2.39	0.47
1:C:195:GLY:CA	1:C:220:GLY:CA	2.90	0.47
1:C:218:GLN:OE1	1:C:248:PRO:HB3	2.13	0.47
1:D:205:ASP:C	1:D:208:PRO:HD2	2.34	0.47
1:B:157:ARG:O	1:B:161:GLN:N	2.47	0.47
1:B:165:THR:O	1:B:250:ARG:CZ	2.63	0.47
1:C:235:GLN:HA	1:C:238:LEU:HD12	1.96	0.47
1:D:158:ARG:O	1:D:159:LEU:C	2.52	0.47
1:D:185:TYR:CG	1:D:189:PHE:CE2	3.03	0.47
1:E:266:ASN:OD1	1:E:266:ASN:N	2.48	0.47
1:F:231:THR:OG1	1:F:234:GLN:HG3	2.15	0.47
1:H:207:ALA:N	1:H:208:PRO:CD	2.78	0.47
1:E:204:PRO:HG3	1:F:229:HIS:O	2.10	0.47
1:G:166:ASP:CA	1:G:250:ARG:NH2	2.76	0.47
1:D:202:LEU:HB2	1:D:225:SER:O	2.14	0.47
1:D:222:LEU:HB3	1:D:249:PHE:CD1	2.50	0.47
1:F:171:LEU:CB	1:F:281:ILE:CG2	2.93	0.47
1:B:185:TYR:C	1:B:185:TYR:CD2	2.88	0.46
1:B:207:ALA:N	1:B:208:PRO:HD3	2.29	0.46
1:E:198:VAL:HG21	1:E:216:LEU:HG	1.97	0.46
1:A:180:MSE:O	1:A:184:ARG:HG3	2.14	0.46
1:D:231:THR:CG2	1:D:233:GLU:H	2.27	0.46
1:F:267:HIS:O	1:F:268:ILE:HG12	2.15	0.46
1:B:262:LEU:HD11	1:B:266:ASN:ND2	2.26	0.46
1:D:203:THR:H	1:D:206:ASN:HB3	1.80	0.46
1:G:170:TRP:C	1:G:171:LEU:HD12	2.29	0.46
1:C:199:TYR:HA	1:C:223:VAL:HB	1.97	0.46
1:C:269:ILE:HG12	1:C:272:LEU:HB3	1.97	0.46
1:D:185:TYR:CE2	1:D:189:PHE:CE2	3.03	0.46
1:E:272:LEU:C	1:E:274:TYR:N	2.66	0.46
1:F:150:GLU:H	1:F:150:GLU:HG2	1.55	0.46
1:F:263:ALA:HA	1:F:268:ILE:HB	1.97	0.46
1:H:186:LEU:O	1:H:190:GLY:N	2.48	0.46
1:H:262:LEU:O	1:H:266:ASN:O	2.33	0.46
1:B:168:ALA:CA	1:B:251:LEU:O	2.61	0.46
1:E:221:THR:OG1	1:E:250:ARG:HG2	2.16	0.46
1:F:174:ALA:HB1	1:F:175:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:PHE:HA	1:F:279:THR:HG23	1.96	0.46
1:G:179:ARG:HB3	1:G:283:CYS:SG	2.55	0.46
1:C:221:THR:CG2	1:C:250:ARG:HB3	2.38	0.46
1:C:170:TRP:HD1	1:C:276:PHE:CD1	2.34	0.46
1:D:168:ALA:C	1:D:276:PHE:CE1	2.86	0.46
1:G:231:THR:CG2	1:G:234:GLN:HB2	2.44	0.46
1:E:180:MSE:O	1:E:184:ARG:HG2	2.16	0.46
1:B:170:TRP:N	1:B:276:PHE:CD1	2.83	0.46
1:D:185:TYR:CD1	1:D:185:TYR:O	2.69	0.46
1:E:240:GLN:O	1:E:241:LEU:C	2.53	0.46
1:H:187:HIS:NE2	1:H:197:PHE:HB2	2.31	0.46
1:E:229:HIS:O	1:F:204:PRO:HG3	2.16	0.46
1:G:235:GLN:HE22	1:G:268:ILE:HA	1.81	0.46
1:B:169:VAL:CA	1:B:279:THR:O	2.64	0.45
1:D:242:GLN:OE1	1:D:242:GLN:HA	2.15	0.45
1:E:259:LEU:HD21	1:E:276:PHE:CD2	2.51	0.45
1:H:272:LEU:HD23	1:H:272:LEU:HA	1.71	0.45
1:A:206:ASN:C	1:A:208:PRO:HD2	2.36	0.45
1:F:199:TYR:C	1:F:200:ARG:HH11	2.20	0.45
1:F:199:TYR:CD1	1:F:223:VAL:HG13	2.51	0.45
1:C:170:TRP:C	1:C:171:LEU:HD12	2.37	0.45
1:D:170:TRP:HZ2	1:D:172:TYR:HB3	1.79	0.45
1:E:226:HIS:H	1:E:227:PRO:HD3	1.73	0.45
1:G:273:TYR:CE2	1:G:277:ALA:HB2	2.52	0.45
1:H:266:ASN:CB	1:H:268:ILE:HG22	2.47	0.45
1:C:179:ARG:N	2:C:2:SO4:O1	2.49	0.45
1:D:199:TYR:C	1:D:200:ARG:HG2	2.36	0.45
1:D:256:ASP:OD1	1:D:256:ASP:N	2.48	0.45
1:E:180:MSE:O	1:E:184:ARG:CG	2.65	0.45
1:G:207:ALA:HB3	1:G:208:PRO:HD3	1.99	0.45
1:H:179:ARG:H	1:H:179:ARG:HG2	1.14	0.45
1:H:202:LEU:CD1	1:H:227:PRO:HA	2.44	0.45
1:D:170:TRP:CA	1:D:171:LEU:HD13	2.47	0.45
1:G:187:HIS:HE1	1:G:195:GLY:O	1.96	0.45
1:A:152:ILE:C	1:A:156:ARG:HG3	2.35	0.45
1:C:156:ARG:O	1:C:160:GLN:CG	2.64	0.45
1:F:176:GLY:CA	2:F:7:SO4:S	3.04	0.45
1:F:185:TYR:CD1	1:F:185:TYR:C	2.90	0.45
1:G:187:HIS:NE2	1:G:195:GLY:O	2.49	0.45
1:B:177:THR:O	1:B:285:PRO:CG	2.65	0.45
1:B:201:GLU:HA	1:B:202:LEU:HD23	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ILE:HG23	1:F:269:ILE:H	1.81	0.45
1:G:199:TYR:HA	1:G:223:VAL:O	2.16	0.45
1:G:202:LEU:HD12	1:G:227:PRO:HA	0.72	0.45
1:G:259:LEU:H	1:G:280:GLN:NE2	2.15	0.45
1:C:168:ALA:HA	1:C:251:LEU:O	2.17	0.45
1:G:168:ALA:HB1	1:G:276:PHE:CE1	2.51	0.45
1:B:202:LEU:HG	1:B:226:HIS:H	1.81	0.45
1:B:278:MSE:SE	1:C:270:ALA:HB2	2.67	0.45
1:D:203:THR:HG22	1:D:204:PRO:N	2.30	0.45
1:D:210:LEU:CD2	1:D:234:GLN:CG	2.76	0.45
1:A:157:ARG:O	1:A:161:GLN:HG2	2.17	0.45
1:A:228:GLU:H	1:A:228:GLU:HG3	1.36	0.45
1:C:272:LEU:O	1:C:275:CYS:HB2	2.17	0.45
1:D:202:LEU:CD1	1:D:230:LEU:HG	2.45	0.45
1:E:217:ALA:HB2	1:E:222:LEU:HG	1.98	0.45
1:F:201:GLU:CG	1:F:225:SER:HG	2.28	0.45
1:G:221:THR:CG2	1:G:252:ILE:CD1	2.95	0.45
1:H:179:ARG:HG2	2:H:8:SO4:O1	2.17	0.45
1:E:276:PHE:HA	1:E:279:THR:OG1	2.16	0.44
1:B:169:VAL:HA	1:B:279:THR:CB	2.48	0.44
1:E:265:SER:O	1:E:266:ASN:OD1	2.34	0.44
1:B:203:THR:H	1:B:206:ASN:HB3	1.82	0.44
1:B:251:LEU:HD23	1:B:251:LEU:HA	1.78	0.44
1:C:259:LEU:HG	1:C:273:TYR:HD1	1.82	0.44
1:D:221:THR:HG23	1:D:252:ILE:HD11	1.87	0.44
1:F:279:THR:O	1:F:279:THR:OG1	2.30	0.44
1:D:180:MSE:N	2:D:4:SO4:O3	2.51	0.44
1:A:239:VAL:HG11	1:A:271:GLU:HB3	2.00	0.44
1:A:242:GLN:O	1:A:247:ARG:NE	2.51	0.44
1:A:249:PHE:N	1:A:249:PHE:CD2	2.84	0.44
1:C:235:GLN:HE22	1:C:268:ILE:CA	2.31	0.44
1:E:170:TRP:HZ2	1:E:255:GLY:HA3	1.81	0.44
1:H:187:HIS:CG	1:H:197:PHE:HD1	2.36	0.44
1:C:171:LEU:CD1	1:C:171:LEU:N	2.81	0.44
1:D:170:TRP:CH2	1:D:255:GLY:CA	2.93	0.44
1:D:237:HIS:ND1	1:D:241:LEU:CD1	2.79	0.44
1:E:155:TYR:O	1:E:159:LEU:HB2	2.17	0.44
1:E:269:ILE:O	1:E:272:LEU:N	2.51	0.44
1:A:203:THR:HG23	1:A:206:ASN:H	1.82	0.44
1:B:230:LEU:HD22	1:B:234:GLN:HG2	2.00	0.44
1:C:157:ARG:O	1:C:161:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:CB	1:C:179:ARG:HG3	2.47	0.44
1:C:195:GLY:HA3	1:C:220:GLY:HA2	1.99	0.44
1:F:274:TYR:O	1:G:273:TYR:OH	2.36	0.44
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.79	0.44
1:B:170:TRP:HB2	1:B:276:PHE:HB3	1.99	0.44
1:F:274:TYR:O	1:G:273:TYR:CE2	2.71	0.44
1:G:167:ILE:HA	1:G:247:ARG:NH2	2.33	0.44
1:G:218:GLN:O	1:G:218:GLN:HG3	2.13	0.44
1:G:270:ALA:O	1:G:273:TYR:N	2.51	0.44
1:A:269:ILE:HG13	1:A:272:LEU:H	1.83	0.44
1:F:281:ILE:HG23	1:F:281:ILE:O	2.17	0.44
1:H:202:LEU:HD21	1:H:224:LEU:HD22	2.00	0.44
1:E:188:GLN:HE22	1:H:194:GLN:HG3	1.79	0.43
1:E:208:PRO:CB	1:E:209:GLN:HE21	2.23	0.43
1:G:167:ILE:HG22	1:G:247:ARG:NH2	2.26	0.43
1:C:195:GLY:C	1:C:220:GLY:N	2.71	0.43
1:D:231:THR:CG2	1:D:232:ARG:N	2.80	0.43
1:D:237:HIS:CE1	1:D:241:LEU:CG	3.01	0.43
1:E:230:LEU:HD23	1:E:230:LEU:HA	1.87	0.43
1:B:165:THR:HG21	1:B:167:ILE:CG1	2.48	0.43
1:E:218:GLN:HA	1:E:248:PRO:O	2.19	0.43
1:H:178:GLY:N	2:H:8:SO4:O1	2.49	0.43
1:H:230:LEU:CD1	1:H:238:LEU:HD12	2.48	0.43
1:A:200:ARG:HH21	1:D:189:PHE:HB3	1.83	0.43
1:F:173:GLY:O	1:F:256:ASP:CB	2.66	0.43
1:G:207:ALA:N	1:G:208:PRO:CD	2.81	0.43
1:G:228:GLU:HG2	1:G:229:HIS:N	2.33	0.43
1:A:182:GLY:O	1:A:186:LEU:HB2	2.19	0.43
1:A:187:HIS:CE1	1:A:197:PHE:HB2	2.54	0.43
1:B:209:GLN:H	1:B:209:GLN:HG3	1.65	0.43
1:B:248:PRO:HB2	1:B:249:PHE:H	1.59	0.43
1:H:183:ALA:HB2	1:H:252:ILE:HG21	2.00	0.43
1:H:231:THR:HG23	1:H:232:ARG:N	2.34	0.43
1:E:187:HIS:ND1	1:E:221:THR:HB	2.33	0.43
1:F:276:PHE:CD2	1:F:276:PHE:N	2.86	0.43
1:H:196:GLU:HG2	1:H:198:VAL:HG22	2.01	0.43
1:A:223:VAL:HG22	1:A:252:ILE:HB	2.01	0.43
1:B:169:VAL:HG11	1:B:186:LEU:HD11	1.93	0.43
1:C:155:TYR:HD1	1:C:155:TYR:O	2.01	0.43
1:C:223:VAL:HG22	1:C:252:ILE:HB	2.00	0.43
1:D:198:VAL:HG12	1:D:198:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:PRO:HG3	1:F:229:HIS:HA	2.00	0.43
1:G:239:VAL:O	1:G:243:SER:HB3	2.18	0.43
1:A:152:ILE:HD12	1:A:152:ILE:H	1.83	0.43
1:E:218:GLN:CA	1:E:249:PHE:HB3	2.46	0.43
1:C:170:TRP:C	1:C:171:LEU:CD1	2.86	0.43
1:D:185:TYR:CG	1:D:189:PHE:CD2	3.07	0.43
1:E:239:VAL:O	1:E:240:GLN:C	2.56	0.43
1:G:179:ARG:HG2	2:G:6:SO4:O3	2.19	0.43
1:C:168:ALA:HB2	1:C:251:LEU:HB3	2.01	0.43
1:C:173:GLY:H	1:C:256:ASP:HA	1.84	0.43
1:C:222:LEU:CD1	1:C:224:LEU:CD2	2.91	0.43
1:C:247:ARG:HA	1:C:248:PRO:HD3	1.91	0.43
1:G:172:TYR:O	1:G:282:ALA:HA	2.19	0.43
1:D:194:GLN:H	1:D:194:GLN:NE2	2.16	0.42
1:G:169:VAL:O	1:G:276:PHE:CE1	2.72	0.42
1:H:231:THR:HG23	1:H:233:GLU:H	1.84	0.42
1:A:231:THR:HG22	1:A:234:GLN:H	1.85	0.42
1:B:176:GLY:O	1:B:285:PRO:HG3	2.18	0.42
1:E:170:TRP:O	1:E:280:GLN:HA	2.19	0.42
1:C:186:LEU:HD23	1:C:186:LEU:HA	1.83	0.42
1:D:237:HIS:CE1	1:D:241:LEU:HD21	2.47	0.42
1:E:162:LEU:HD23	1:E:162:LEU:HA	1.85	0.42
1:F:199:TYR:CA	1:F:223:VAL:HG12	2.49	0.42
1:F:274:TYR:O	1:G:273:TYR:HE2	2.02	0.42
1:G:210:LEU:C	1:G:210:LEU:CD1	2.76	0.42
1:A:235:GLN:O	1:A:239:VAL:HG23	2.19	0.42
1:B:169:VAL:CG1	1:B:186:LEU:CD1	2.78	0.42
1:C:221:THR:HG23	1:C:250:ARG:CG	2.50	0.42
1:C:231:THR:H	1:C:234:GLN:HB2	1.83	0.42
1:E:217:ALA:O	1:E:220:GLY:N	2.51	0.42
1:H:231:THR:CG2	1:H:232:ARG:N	2.80	0.42
1:H:241:LEU:O	1:H:244:GLN:HG3	2.18	0.42
1:A:172:TYR:CZ	1:A:282:ALA:HB2	2.55	0.42
1:G:199:TYR:CE1	1:G:225:SER:HB3	2.55	0.42
1:A:179:ARG:NH1	1:A:255:GLY:C	2.73	0.42
1:D:185:TYR:CE1	1:D:189:PHE:HD2	2.35	0.42
1:F:268:ILE:HG22	1:F:269:ILE:N	2.32	0.42
1:G:223:VAL:HG13	1:G:252:ILE:HG22	2.01	0.42
1:H:230:LEU:HD23	1:H:230:LEU:HA	1.88	0.42
1:H:269:ILE:HG22	1:H:272:LEU:H	1.84	0.42
1:F:199:TYR:OH	1:F:201:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:PHE:O	1:H:217:ALA:CB	2.66	0.42
1:H:230:LEU:HD13	1:H:238:LEU:HD12	2.01	0.42
1:A:231:THR:CG2	1:A:232:ARG:N	2.81	0.42
1:B:228:GLU:OE1	1:B:262:LEU:HD11	2.18	0.42
1:C:269:ILE:HG13	1:C:272:LEU:H	1.84	0.42
1:E:248:PRO:HB2	1:E:249:PHE:HD2	1.84	0.42
1:B:260:VAL:HG12	1:B:280:GLN:OE1	2.20	0.42
1:B:170:TRP:CD1	1:B:280:GLN:HB2	2.54	0.42
1:B:254:ILE:HD13	1:B:254:ILE:N	2.35	0.42
1:H:181:THR:O	1:H:185:TYR:CB	2.68	0.42
1:A:151:TRP:O	1:A:155:TYR:N	2.39	0.41
1:A:155:TYR:CG	1:A:284:LEU:HB2	2.55	0.41
1:B:203:THR:O	1:B:207:ALA:N	2.53	0.41
1:C:221:THR:HG21	1:C:250:ARG:HG2	2.01	0.41
1:C:241:LEU:HD22	1:C:244:GLN:HE22	1.84	0.41
1:F:149:SER:O	1:F:153:ASN:CB	2.68	0.41
1:G:187:HIS:CD2	1:G:221:THR:OG1	2.73	0.41
1:C:272:LEU:O	1:C:273:TYR:C	2.55	0.41
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.89	0.41
1:E:202:LEU:O	1:E:229:HIS:ND1	2.52	0.41
1:F:153:ASN:O	1:F:157:ARG:CB	2.68	0.41
1:F:199:TYR:C	1:F:200:ARG:NH1	2.73	0.41
1:G:157:ARG:O	1:G:161:GLN:CB	2.68	0.41
1:H:247:ARG:HA	1:H:248:PRO:HD3	1.88	0.41
1:A:260:VAL:HG13	1:A:273:TYR:OH	2.19	0.41
1:A:281:ILE:HG23	1:A:282:ALA:N	2.35	0.41
1:E:171:LEU:HD22	1:E:283:CYS:SG	2.60	0.41
1:C:222:LEU:HD12	1:C:222:LEU:C	2.39	0.41
1:C:231:THR:N	1:C:234:GLN:OE1	2.53	0.41
1:C:231:THR:O	1:C:234:GLN:N	2.54	0.41
1:E:229:HIS:O	1:F:204:PRO:CG	2.68	0.41
1:E:259:LEU:CD2	1:E:276:PHE:CD2	3.04	0.41
1:B:238:LEU:O	1:B:239:VAL:CB	2.68	0.41
1:E:239:VAL:HA	1:E:242:GLN:HB2	2.01	0.41
1:E:251:LEU:HD12	1:E:252:ILE:N	2.36	0.41
1:E:269:ILE:C	1:E:271:GLU:N	2.74	0.41
1:G:276:PHE:O	1:G:280:GLN:HG3	2.20	0.41
1:B:203:THR:CG2	1:B:206:ASN:HB3	2.41	0.41
1:B:281:ILE:HD13	1:B:281:ILE:N	2.33	0.41
1:F:276:PHE:O	1:F:278:MSE:N	2.54	0.41
1:G:231:THR:O	1:G:235:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ILE:HD13	1:C:241:LEU:CD1	2.51	0.41
1:E:175:PRO:HA	1:E:179:ARG:NH2	2.35	0.41
1:A:172:TYR:CD1	1:A:172:TYR:C	2.93	0.41
1:B:259:LEU:HD22	1:B:276:PHE:CB	2.49	0.41
1:B:271:GLU:HA	1:B:274:TYR:HD2	1.82	0.41
1:D:179:ARG:CG	1:D:179:ARG:HH11	2.33	0.41
1:E:199:TYR:HB2	1:E:223:VAL:HB	2.03	0.41
1:G:239:VAL:O	1:G:243:SER:N	2.52	0.41
1:C:195:GLY:CA	1:C:219:GLY:CA	2.96	0.41
1:D:206:ASN:C	1:D:208:PRO:CD	2.90	0.41
1:E:185:TYR:CD2	1:E:185:TYR:C	2.94	0.41
1:E:202:LEU:HD23	1:E:202:LEU:HA	1.81	0.41
1:E:239:VAL:O	1:E:243:SER:HB2	2.21	0.41
1:H:230:LEU:CD2	1:H:234:GLN:OE1	2.69	0.41
1:B:162:LEU:CB	1:B:186:LEU:HD21	2.51	0.41
1:B:206:ASN:C	1:B:208:PRO:HD2	2.42	0.41
1:D:199:TYR:HB2	1:D:223:VAL:HB	2.02	0.41
1:D:231:THR:CG2	1:D:233:GLU:OE1	2.69	0.41
1:F:260:VAL:HG23	1:F:273:TYR:CE1	2.56	0.41
1:H:268:ILE:O	1:H:268:ILE:HG12	2.16	0.41
1:H:269:ILE:HD12	1:H:269:ILE:HA	1.82	0.41
1:A:173:GLY:N	1:A:255:GLY:O	2.53	0.40
1:A:258:SER:O	1:A:259:LEU:C	2.59	0.40
1:C:231:THR:HB	1:C:234:GLN:HG3	2.02	0.40
1:D:172:TYR:CD1	1:D:258:SER:CA	2.96	0.40
1:F:274:TYR:HA	1:G:273:TYR:OH	2.21	0.40
1:A:204:PRO:CD	1:B:267:HIS:CG	3.01	0.40
1:C:221:THR:HG21	1:C:252:ILE:HG13	2.03	0.40
1:D:202:LEU:HB2	1:D:226:HIS:O	2.21	0.40
1:E:222:LEU:HB2	1:E:249:PHE:CD1	2.56	0.40
1:F:199:TYR:HA	1:F:223:VAL:HG13	2.03	0.40
1:G:187:HIS:NE2	1:G:192:ASN:O	2.54	0.40
1:H:269:ILE:N	1:H:269:ILE:HD13	2.37	0.40
1:A:286:LEU:CD1	1:A:286:LEU:H	2.31	0.40
1:F:179:ARG:O	1:F:183:ALA:HB2	2.20	0.40
1:A:242:GLN:NE2	1:A:247:ARG:HG2	2.37	0.40
1:C:228:GLU:O	1:C:229:HIS:C	2.60	0.40
1:D:171:LEU:N	1:D:253:GLY:O	2.34	0.40
1:E:202:LEU:HD13	1:E:230:LEU:HG	2.04	0.40
1:H:217:ALA:O	1:H:220:GLY:O	2.40	0.40
1:A:152:ILE:HG22	1:A:156:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:C	1:B:179:ARG:HD3	2.42	0.40
1:B:210:LEU:C	1:B:214:ILE:HD12	2.16	0.40
1:F:236:TYR:C	1:F:238:LEU:H	2.24	0.40
1:G:186:LEU:O	1:G:190:GLY:HA3	2.22	0.40
1:H:221:THR:HA	1:H:250:ARG:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLU:OE1	1:D:200:ARG:NH2[3_554]	0.86	1.34
1:A:160:GLN:NE2	1:C:164:GLU:OE2[4_555]	1.51	0.69
1:C:196:GLU:CD	1:D:200:ARG:NH2[3_554]	1.92	0.28
1:E:185:TYR:OH	1:G:160:GLN:CG[3_544]	1.95	0.25
1:C:196:GLU:OE1	1:D:200:ARG:CZ[3_554]	2.06	0.14
1:E:185:TYR:OH	1:G:160:GLN:CD[3_544]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
1	B	98/145 (68%)	92 (94%)	5 (5%)	1 (1%)	13	39
1	C	128/145 (88%)	121 (94%)	6 (5%)	1 (1%)	16	44
1	D	112/145 (77%)	109 (97%)	2 (2%)	1 (1%)	14	42
1	E	131/145 (90%)	123 (94%)	6 (5%)	2 (2%)	8	29
1	F	95/145 (66%)	90 (95%)	3 (3%)	2 (2%)	5	20
1	G	124/145 (86%)	123 (99%)	1 (1%)	0	100	100
1	H	120/145 (83%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	948/1160 (82%)	910 (96%)	31 (3%)	7 (1%)	19	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	265	SER
1	E	273	TYR
1	F	177	THR
1	B	175	PRO
1	E	270	ALA
1	D	260	VAL
1	F	204	PRO

### 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	98/120 (82%)	67 (68%)	31 (32%)	0	0
1	B	57/120 (48%)	39 (68%)	18 (32%)	0	0
1	C	83/120 (69%)	67 (81%)	16 (19%)	1	4
1	D	70/120 (58%)	50 (71%)	20 (29%)	0	1
1	E	92/120 (77%)	65 (71%)	27 (29%)	0	1
1	F	55/120 (46%)	35 (64%)	20 (36%)	0	0
1	G	83/120 (69%)	69 (83%)	14 (17%)	1	5
1	H	65/120 (54%)	45 (69%)	20 (31%)	0	0
All	All	603/960 (63%)	437 (72%)	166 (28%)	0	1

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ILE
1	A	161	GLN
1	A	163	SER

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Mol	Chain	Res	Type
1	A	164	GLU
1	A	165	THR
1	A	179	ARG
1	A	184	ARG
1	A	185	TYR
1	A	186	LEU
1	A	188	GLN
1	A	192	ASN
1	A	196	GLU
1	A	197	PHE
1	A	200	ARG
1	A	205	ASP
1	A	209	GLN
1	A	214	ILE
1	A	218	GLN
1	A	224	LEU
1	A	228	GLU
1	A	236	TYR
1	A	238	LEU
1	A	247	ARG
1	A	250	ARG
1	A	259	LEU
1	A	260	VAL
1	A	275	CYS
1	A	280	GLN
1	A	281	ILE
1	A	286	LEU
1	A	287	THR
1	B	155	TYR
1	B	169	VAL
1	B	177	THR
1	B	179	ARG
1	B	180	MSE
1	B	202	LEU
1	B	203	THR
1	B	205	ASP
1	B	209	GLN
1	B	231	THR
1	B	250	ARG
1	B	251	LEU
1	B	254	ILE
1	B	256	ASP

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Mol	Chain	Res	Type
1	B	260	VAL
1	B	265	SER
1	B	281	ILE
1	B	284	LEU
1	C	155	TYR
1	C	170	TRP
1	C	171	LEU
1	C	172	TYR
1	C	196	GLU
1	C	202	LEU
1	C	206	ASN
1	C	222	LEU
1	C	224	LEU
1	C	228	GLU
1	C	242	GLN
1	C	250	ARG
1	C	254	ILE
1	C	257	THR
1	C	260	VAL
1	C	276	PHE
1	D	163	SER
1	D	170	TRP
1	D	171	LEU
1	D	172	TYR
1	D	179	ARG
1	D	185	TYR
1	D	188	GLN
1	D	194	GLN
1	D	210	LEU
1	D	212	ASP
1	D	214	ILE
1	D	234	GLN
1	D	237	HIS
1	D	242	GLN
1	D	246	HIS
1	D	256	ASP
1	D	257	THR
1	D	276	PHE
1	D	278	MSE
1	D	279	THR
1	E	152	ILE
1	E	158	ARG

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Mol	Chain	Res	Type
1	E	177	THR
1	E	181	THR
1	E	184	ARG
1	E	186	LEU
1	E	197	PHE
1	E	201	GLU
1	E	202	LEU
1	E	205	ASP
1	E	209	GLN
1	E	214	ILE
1	E	216	LEU
1	E	221	THR
1	E	222	LEU
1	E	233	GLU
1	E	242	GLN
1	E	243	SER
1	E	247	ARG
1	E	250	ARG
1	E	254	ILE
1	E	259	LEU
1	E	266	ASN
1	E	273	TYR
1	E	276	PHE
1	E	278	MSE
1	E	286	LEU
1	F	150	GLU
1	F	171	LEU
1	F	185	TYR
1	F	187	HIS
1	F	197	PHE
1	F	199	TYR
1	F	210	LEU
1	F	212	ASP
1	F	238	LEU
1	F	242	GLN
1	F	257	THR
1	F	258	SER
1	F	259	LEU
1	F	262	LEU
1	F	267	HIS
1	F	268	ILE
1	F	275	CYS

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Mol	Chain	Res	Type
1	F	278	MSE
1	F	279	THR
1	F	280	GLN
1	G	155	TYR
1	G	158	ARG
1	G	171	LEU
1	G	177	THR
1	G	188	GLN
1	G	191	ARG
1	G	196	GLU
1	G	205	ASP
1	G	210	LEU
1	G	218	GLN
1	G	231	THR
1	G	254	ILE
1	G	256	ASP
1	G	279	THR
1	H	160	GLN
1	H	171	LEU
1	H	179	ARG
1	H	181	THR
1	H	194	GLN
1	H	197	PHE
1	H	198	VAL
1	H	203	THR
1	H	205	ASP
1	H	214	ILE
1	H	225	SER
1	H	231	THR
1	H	242	GLN
1	H	246	HIS
1	H	250	ARG
1	H	252	ILE
1	H	268	ILE
1	H	269	ILE
1	H	272	LEU
1	H	275	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	229	HIS
1	A	240	GLN
1	A	242	GLN
1	A	244	GLN
1	B	206	ASN
1	B	229	HIS
1	B	235	GLN
1	B	266	ASN
1	B	267	HIS
1	B	280	GLN
1	C	226	HIS
1	C	235	GLN
1	C	237	HIS
1	C	242	GLN
1	C	244	GLN
1	D	192	ASN
1	D	194	GLN
1	D	234	GLN
1	D	235	GLN
1	E	153	ASN
1	E	209	GLN
1	E	237	HIS
1	E	242	GLN
1	E	244	GLN
1	E	280	GLN
1	F	187	HIS
1	F	211	ASN
1	F	242	GLN
1	F	280	GLN
1	G	187	HIS
1	G	209	GLN
1	G	244	GLN
1	G	280	GLN
1	H	237	HIS
1	H	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	F	7	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	E	5	-	4,4,4	0.34	0	6,6,6	0.42	0
2	SO4	G	6	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	D	4	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	C	2	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	H	8	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	B	3	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	A	1	-	4,4,4	0.24	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	7	SO4	4	0
2	G	6	SO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	SO4	2	0
2	C	2	SO4	2	0
2	H	8	SO4	3	0
2	A	1	SO4	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	140/145 (96%)	-0.74	1 (0%) 84 79	49, 59, 68, 76	0
1	B	106/145 (73%)	-0.93	0 100 100	55, 68, 75, 78	0
1	C	130/145 (89%)	-0.73	1 (0%) 82 77	52, 65, 84, 89	0
1	D	114/145 (78%)	-0.68	0 100 100	56, 66, 86, 95	0
1	E	135/145 (93%)	-0.84	0 100 100	45, 59, 72, 83	0
1	F	103/145 (71%)	-0.77	1 (0%) 79 73	60, 69, 99, 106	0
1	G	126/145 (86%)	-0.83	2 (1%) 70 63	50, 60, 77, 86	0
1	H	121/145 (83%)	-0.91	0 100 100	52, 63, 83, 89	0
All	All	975/1160 (84%)	-0.80	5 (0%) 87 83	45, 64, 83, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	279	THR	4.3
1	A	271	GLU	2.5
1	G	282	ALA	2.5
1	G	233	GLU	2.3
1	F	260	VAL	2.1

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	3	5/5	0.98	0.04	71,73,77,78	0
2	SO4	C	2	5/5	0.98	0.05	80,80,83,86	0
2	SO4	F	7	5/5	0.98	0.03	83,86,92,95	0
2	SO4	D	4	5/5	0.99	0.03	70,73,75,77	0
2	SO4	E	5	5/5	0.99	0.04	45,45,48,49	0
2	SO4	A	1	5/5	0.99	0.04	56,57,60,61	0
2	SO4	G	6	5/5	0.99	0.03	62,62,64,67	0
2	SO4	H	8	5/5	0.99	0.04	81,82,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.