



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VFJ  
Title : STRUCTURE OF THE A20 OVARIAN TUMOUR (OTU) DOMAIN  
Authors : Komander, D.; Barford, D.  
Deposited on : 2007-11-04  
Resolution : 3.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 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

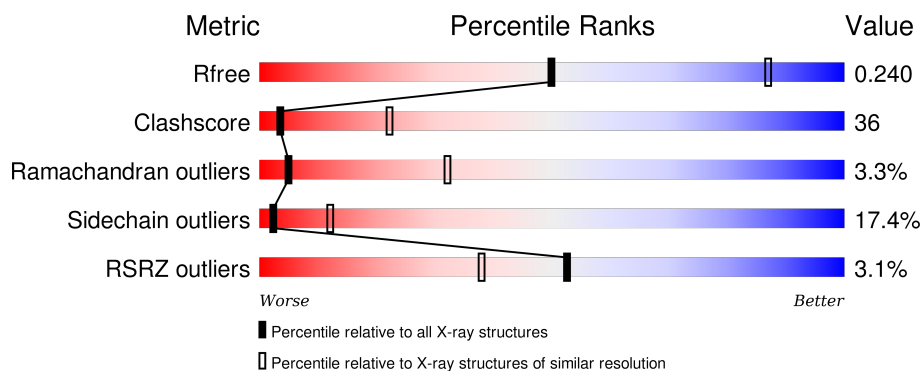
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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	366	<div> <div>2%</div> <div>43% 37% 10% 10%</div> </div>
1	B	366	<div> <div>6%</div> <div>43% 35% 9% 13%</div> </div>
1	C	366	<div> <div>2%</div> <div>41% 38% 10% 11%</div> </div>
1	D	366	<div> <div>%</div> <div>41% 38% 10% 10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	1364	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10203 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 TUMOR NECROSIS FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2566	1652	435	465	14			
1	B	317	Total	C	N	O	S	0	0	0
			2476	1597	419	446	14			
1	C	327	Total	C	N	O	S	0	0	0
			2557	1645	437	461	14			
1	D	329	Total	C	N	O	S	0	0	0
			2583	1659	443	467	14			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

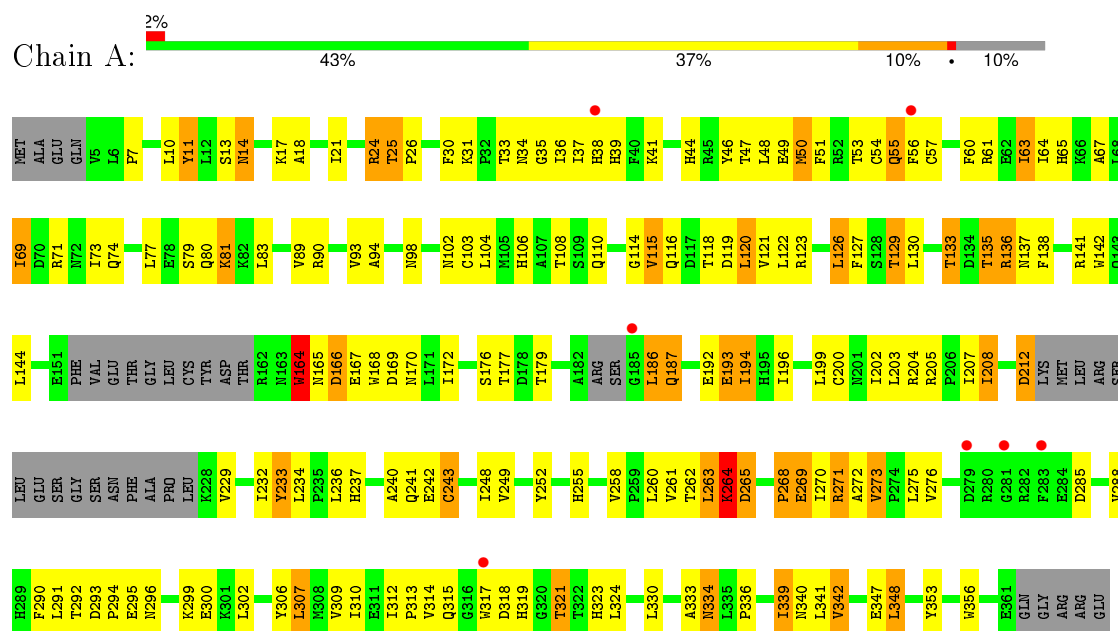
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

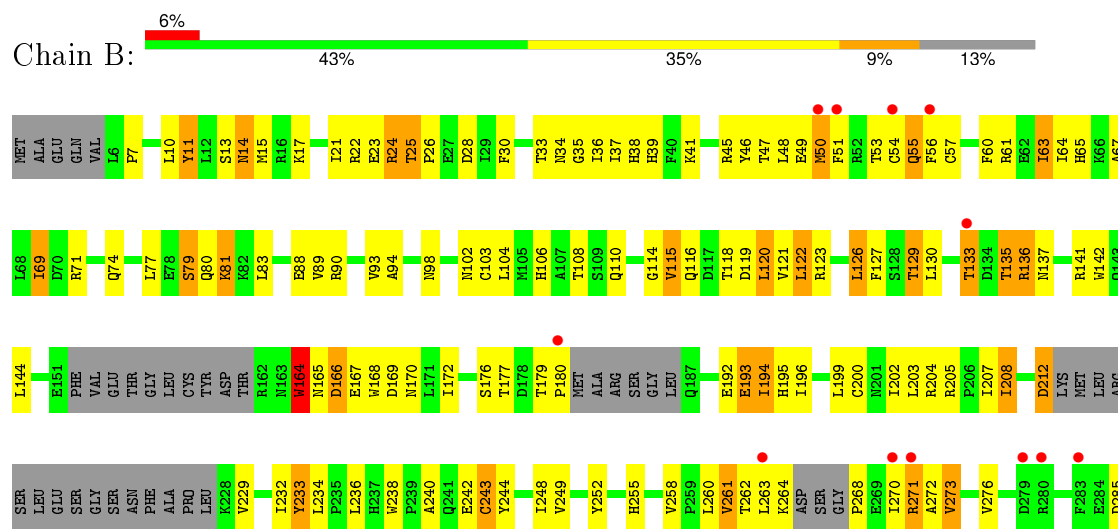
### 3 Residue-property plots

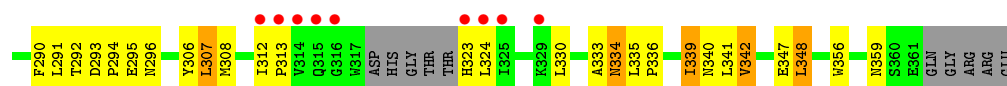
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

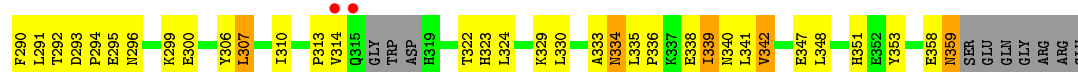
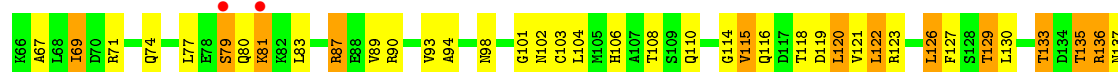


#### • Molecule 1: TUMOR NECROSIS FACTOR

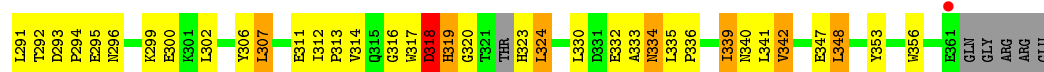
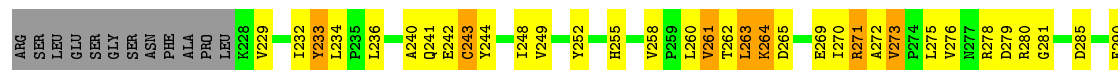
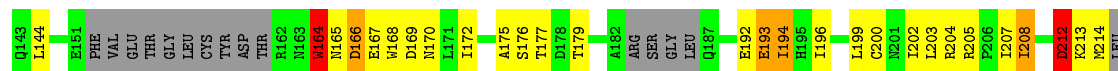
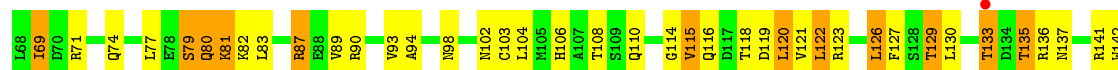
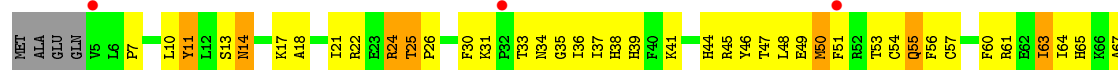




### • Molecule 1: TUMOR NECROSIS FACTOR



### • Molecule 1: TUMOR NECROSIS FACTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.96 Å 83.02 Å 164.94 Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	50.29 – 3.20 50.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (50.29-3.20) 95.7 (50.29-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.204 , 0.243 0.198 , 0.240	Depositor DCC
$R_{free}$ test set	1848 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.9	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 120.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 36216 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 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	0.47	0/2629	0.63	0/3586
1	B	0.49	0/2535	0.69	4/3454 (0.1%)
1	C	0.46	0/2618	0.64	0/3568
1	D	0.52	0/2646	0.74	3/3604 (0.1%)
All	All	0.49	0/10428	0.68	7/14212 (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	D	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	212	ASP	CB-CA-C	-14.90	80.60	110.40
1	D	212	ASP	N-CA-C	9.75	137.33	111.00
1	B	180	PRO	N-CA-C	-8.75	89.35	112.10
1	D	214	MET	N-CA-C	-7.78	89.98	111.00
1	B	180	PRO	CA-C-O	7.75	138.80	120.20
1	B	264	LYS	N-CA-C	6.22	127.80	111.00
1	B	268	PRO	N-CA-C	-5.07	98.91	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	213	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2401	195	0
1	B	2476	0	2319	160	0
1	C	2557	0	2414	190	0
1	D	2583	0	2423	183	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	D	1	0	0	0	0
All	All	10203	0	9557	714	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 36.

All (714) 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:A:292:THR:HG23	1:A:294:PRO:HD2	1.25	1.13
1:B:292:THR:HG23	1:B:294:PRO:HD2	1.33	1.09
1:C:292:THR:HG23	1:C:294:PRO:HD2	1.36	1.07
1:D:292:THR:HG23	1:D:294:PRO:HD2	1.37	1.05
1:C:49:GLU:HB2	1:C:333:ALA:HB2	1.39	1.03
1:B:194:ILE:HD12	1:B:194:ILE:H	1.20	1.03
1:D:194:ILE:H	1:D:194:ILE:HD12	1.24	1.02
1:A:74:GLN:NE2	1:A:93:VAL:HA	1.76	1.01
1:A:194:ILE:H	1:A:194:ILE:HD12	1.26	1.00
1:D:87:ARG:HH22	1:D:314:VAL:HG13	1.24	0.99
1:B:49:GLU:HB2	1:B:333:ALA:HB2	1.43	0.99
1:D:49:GLU:HB2	1:D:333:ALA:HB2	1.44	0.99
1:C:194:ILE:H	1:C:194:ILE:HD12	1.24	0.98
1:A:49:GLU:HB2	1:A:333:ALA:HB2	1.45	0.98
1:B:74:GLN:NE2	1:B:93:VAL:HA	1.79	0.97
1:C:74:GLN:NE2	1:C:93:VAL:HA	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:HD12	1:A:339:ILE:C	1.88	0.94
1:B:339:ILE:HD12	1:B:339:ILE:C	1.88	0.93
1:D:74:GLN:NE2	1:D:93:VAL:HA	1.84	0.93
1:D:339:ILE:C	1:D:339:ILE:HD12	1.90	0.92
1:C:339:ILE:C	1:C:339:ILE:HD12	1.91	0.90
1:B:102:ASN:HD22	1:B:123:ARG:HH11	1.19	0.88
1:D:278:ARG:HD3	1:D:317:TRP:CH2	2.11	0.86
1:C:102:ASN:HD22	1:C:123:ARG:HH11	1.24	0.85
1:A:102:ASN:HD22	1:A:123:ARG:HH11	1.20	0.85
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.40	0.85
1:A:317:TRP:HE1	1:A:323:HIS:CD2	1.95	0.84
1:D:205:ARG:HE	1:D:248:ILE:HG13	1.45	0.82
1:A:205:ARG:HE	1:A:248:ILE:HG13	1.45	0.82
1:D:80:GLN:HB3	1:D:82:LYS:HZ2	1.43	0.81
1:D:204:ARG:O	1:D:243:CYS:HB2	1.81	0.81
1:A:204:ARG:HB3	1:A:243:CYS:HB3	1.61	0.81
1:A:47:THR:H	1:A:334:ASN:HD21	1.27	0.81
1:C:47:THR:H	1:C:334:ASN:HD21	1.28	0.81
1:D:102:ASN:HD22	1:D:123:ARG:HH11	1.25	0.81
1:B:49:GLU:CB	1:B:333:ALA:HB2	2.11	0.80
1:B:24:ARG:HH11	1:B:24:ARG:HG2	1.45	0.80
1:C:49:GLU:CB	1:C:333:ALA:HB2	2.12	0.80
1:B:205:ARG:HE	1:B:248:ILE:HG13	1.48	0.80
1:D:49:GLU:CB	1:D:333:ALA:HB2	2.11	0.79
1:C:205:ARG:HE	1:C:248:ILE:HG13	1.48	0.79
1:A:292:THR:CG2	1:A:294:PRO:HD2	2.10	0.79
1:C:338:GLU:OE1	1:D:324:LEU:HD13	1.82	0.78
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.46	0.78
1:C:24:ARG:HG2	1:C:24:ARG:HH11	1.47	0.78
1:A:10:LEU:HD11	1:A:342:VAL:HG13	1.65	0.78
1:D:94:ALA:HB1	1:D:258:VAL:HG11	1.64	0.77
1:B:194:ILE:HD12	1:B:194:ILE:N	1.96	0.77
1:C:194:ILE:HD12	1:C:194:ILE:N	1.99	0.77
1:A:49:GLU:CB	1:A:333:ALA:HB2	2.14	0.77
1:B:10:LEU:HD11	1:B:342:VAL:HG13	1.65	0.77
1:D:47:THR:H	1:D:334:ASN:HD21	1.29	0.77
1:B:47:THR:H	1:B:334:ASN:HD21	1.28	0.77
1:D:318:ASP:O	1:D:320:GLY:HA2	1.86	0.76
1:D:47:THR:H	1:D:334:ASN:ND2	1.84	0.75
1:D:194:ILE:N	1:D:194:ILE:HD12	2.01	0.75
1:B:94:ALA:HB1	1:B:258:VAL:HG11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:HG23	1:A:294:PRO:CD	2.11	0.75
1:C:94:ALA:HB1	1:C:258:VAL:HG11	1.67	0.74
1:A:194:ILE:HD12	1:A:194:ILE:N	2.02	0.74
1:B:292:THR:CG2	1:B:294:PRO:HD2	2.17	0.74
1:D:10:LEU:HD11	1:D:342:VAL:HG13	1.68	0.74
1:A:25:THR:HG22	1:A:26:PRO:CD	2.18	0.74
1:A:94:ALA:HB1	1:A:258:VAL:HG11	1.69	0.73
1:A:74:GLN:HE22	1:A:93:VAL:HA	1.52	0.73
1:C:47:THR:H	1:C:334:ASN:ND2	1.87	0.73
1:A:240:ALA:HB2	1:A:306:TYR:CD2	2.23	0.73
1:C:74:GLN:HE21	1:C:94:ALA:H	1.37	0.73
1:C:169:ASP:O	1:C:172:ILE:HG13	1.89	0.72
1:B:47:THR:H	1:B:334:ASN:ND2	1.87	0.72
1:C:87:ARG:HH12	1:C:314:VAL:HG13	1.54	0.72
1:B:292:THR:HG23	1:B:294:PRO:CD	2.17	0.72
1:C:10:LEU:HD11	1:C:342:VAL:HG13	1.71	0.72
1:A:74:GLN:HE21	1:A:94:ALA:H	1.34	0.72
1:A:74:GLN:HE21	1:A:93:VAL:HA	1.54	0.72
1:B:169:ASP:O	1:B:172:ILE:HG13	1.90	0.72
1:B:37:ILE:H	1:B:37:ILE:HD12	1.55	0.72
1:A:47:THR:H	1:A:334:ASN:ND2	1.87	0.71
1:D:25:THR:CG2	1:D:121:VAL:HG11	2.19	0.71
1:B:74:GLN:HE21	1:B:93:VAL:HA	1.54	0.71
1:A:204:ARG:O	1:A:243:CYS:HB2	1.91	0.71
1:A:102:ASN:ND2	1:A:123:ARG:HH11	1.87	0.71
1:A:25:THR:CG2	1:A:121:VAL:HG11	2.20	0.71
1:C:25:THR:CG2	1:C:121:VAL:HG11	2.20	0.70
1:D:37:ILE:H	1:D:37:ILE:HD12	1.56	0.70
1:A:292:THR:HG22	1:A:295:GLU:CG	2.21	0.70
1:C:234:LEU:HD12	1:C:234:LEU:N	2.06	0.70
1:D:130:LEU:HG	1:D:172:ILE:HG22	1.72	0.70
1:B:102:ASN:ND2	1:B:123:ARG:HH11	1.89	0.70
1:B:25:THR:CG2	1:B:121:VAL:HG11	2.21	0.70
1:A:50:MET:HG3	1:A:51:PHE:N	2.06	0.70
1:B:74:GLN:HE21	1:B:94:ALA:H	1.37	0.70
1:C:204:ARG:O	1:C:243:CYS:HB2	1.92	0.70
1:C:74:GLN:HE22	1:C:93:VAL:HA	1.56	0.70
1:C:276:VAL:HA	1:C:285:ASP:HA	1.73	0.70
1:A:25:THR:HG22	1:A:26:PRO:HD3	1.73	0.69
1:A:115:VAL:HG22	1:A:116:GLN:H	1.57	0.69
1:B:339:ILE:HD12	1:B:340:ASN:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLN:HB3	1:D:82:LYS:NZ	2.07	0.69
1:A:241:GLN:O	1:C:329:LYS:HE3	1.92	0.69
1:A:242:GLU:HB3	1:C:310:ILE:HG22	1.76	0.69
1:B:273:VAL:HG22	1:B:330:LEU:HD21	1.75	0.68
1:C:292:THR:HG23	1:C:294:PRO:CD	2.20	0.68
1:C:74:GLN:HE21	1:C:93:VAL:HA	1.59	0.68
1:B:276:VAL:HA	1:B:285:ASP:HA	1.76	0.68
1:D:276:VAL:HA	1:D:285:ASP:HA	1.75	0.68
1:B:74:GLN:HE22	1:B:93:VAL:HA	1.58	0.68
1:D:30:PHE:HB2	1:D:41:LYS:HD2	1.75	0.68
1:C:338:GLU:OE1	1:D:311:GLU:CD	2.31	0.68
1:A:276:VAL:HA	1:A:285:ASP:HA	1.76	0.68
1:D:292:THR:HG22	1:D:295:GLU:CG	2.24	0.68
1:A:37:ILE:H	1:A:37:ILE:HD12	1.57	0.68
1:D:25:THR:HG22	1:D:121:VAL:HG11	1.77	0.67
1:D:102:ASN:ND2	1:D:123:ARG:HH11	1.91	0.67
1:C:25:THR:HG22	1:C:26:PRO:CD	2.24	0.67
1:B:192:GLU:HG2	1:B:193:GLU:HG2	1.76	0.67
1:B:292:THR:HG22	1:B:295:GLU:CG	2.24	0.67
1:C:194:ILE:HA	1:C:290:PHE:CE1	2.28	0.67
1:C:115:VAL:HG22	1:C:116:GLN:H	1.59	0.67
1:A:169:ASP:O	1:A:172:ILE:HG13	1.94	0.67
1:A:194:ILE:HA	1:A:290:PHE:CE1	2.29	0.67
1:D:336:PRO:O	1:D:340:ASN:HB2	1.95	0.67
1:A:186:LEU:H	1:A:186:LEU:HD22	1.59	0.67
1:A:292:THR:HG22	1:A:295:GLU:HG3	1.75	0.66
1:B:25:THR:HG22	1:B:26:PRO:CD	2.25	0.66
1:A:98:ASN:H	1:A:116:GLN:NE2	1.94	0.66
1:C:37:ILE:HD12	1:C:37:ILE:H	1.60	0.66
1:D:194:ILE:HA	1:D:290:PHE:CE1	2.31	0.66
1:C:273:VAL:HG22	1:C:330:LEU:HD21	1.78	0.66
1:D:74:GLN:HE21	1:D:93:VAL:HA	1.58	0.66
1:C:25:THR:HG22	1:C:121:VAL:HG11	1.77	0.66
1:D:25:THR:HG22	1:D:26:PRO:CD	2.26	0.66
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.60	0.66
1:B:102:ASN:ND2	1:B:123:ARG:HD3	2.11	0.66
1:C:102:ASN:ND2	1:C:123:ARG:HH11	1.95	0.66
1:B:240:ALA:HB2	1:B:306:TYR:CD2	2.31	0.66
1:C:102:ASN:ND2	1:C:123:ARG:HD3	2.11	0.65
1:C:291:LEU:HD22	1:C:295:GLU:HB3	1.77	0.65
1:A:339:ILE:HD12	1:A:340:ASN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ILE:CD1	1:C:339:ILE:C	2.64	0.65
1:C:183:ARG:HH11	1:C:183:ARG:HB2	1.60	0.65
1:D:339:ILE:HD12	1:D:340:ASN:N	2.12	0.65
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.61	0.65
1:D:50:MET:HG3	1:D:51:PHE:N	2.10	0.65
1:D:115:VAL:HG22	1:D:116:GLN:H	1.61	0.65
1:D:234:LEU:HD12	1:D:234:LEU:N	2.11	0.65
1:B:234:LEU:N	1:B:234:LEU:HD12	2.12	0.65
1:C:339:ILE:HD12	1:C:340:ASN:N	2.11	0.65
1:A:30:PHE:HB2	1:A:41:LYS:HD2	1.79	0.65
1:A:130:LEU:HG	1:A:172:ILE:HG22	1.78	0.65
1:B:25:THR:HG22	1:B:121:VAL:HG11	1.79	0.65
1:C:240:ALA:HB2	1:C:306:TYR:CD2	2.31	0.64
1:D:292:THR:CG2	1:D:294:PRO:HD2	2.22	0.64
1:A:273:VAL:HG22	1:A:330:LEU:HD21	1.80	0.64
1:B:65:HIS:CD2	1:B:69:ILE:HD13	2.33	0.64
1:D:292:THR:HG23	1:D:294:PRO:CD	2.23	0.64
1:C:192:GLU:HG2	1:C:193:GLU:HG2	1.79	0.64
1:A:336:PRO:O	1:A:340:ASN:HB2	1.98	0.64
1:C:50:MET:HG3	1:C:51:PHE:N	2.12	0.64
1:A:25:THR:HG22	1:A:121:VAL:HG11	1.80	0.64
1:C:194:ILE:H	1:C:194:ILE:CD1	1.97	0.64
1:B:336:PRO:O	1:B:340:ASN:HB2	1.97	0.64
1:C:292:THR:HG22	1:C:295:GLU:CG	2.27	0.63
1:D:102:ASN:ND2	1:D:123:ARG:HD3	2.13	0.63
1:D:65:HIS:CD2	1:D:69:ILE:HD13	2.32	0.63
1:D:71:ARG:HH11	1:D:71:ARG:HG3	1.62	0.63
1:B:25:THR:HG22	1:B:26:PRO:HD3	1.81	0.63
1:B:204:ARG:HB3	1:B:243:CYS:HB3	1.79	0.63
1:A:232:ILE:HG22	1:A:234:LEU:HD11	1.81	0.63
1:A:324:LEU:HD11	1:D:81:LYS:NZ	2.14	0.63
1:A:102:ASN:ND2	1:A:123:ARG:HD3	2.13	0.63
1:C:204:ARG:HB3	1:C:243:CYS:HB3	1.80	0.63
1:D:169:ASP:O	1:D:172:ILE:HG13	1.99	0.62
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.64	0.62
1:D:208:ILE:HD11	1:D:273:VAL:HG11	1.81	0.62
1:A:194:ILE:CD1	1:A:194:ILE:H	1.98	0.62
1:A:291:LEU:HD22	1:A:295:GLU:HB3	1.79	0.62
1:D:292:THR:HG22	1:D:295:GLU:HG3	1.81	0.62
1:B:194:ILE:HA	1:B:290:PHE:CE1	2.35	0.62
1:B:102:ASN:HD21	1:B:123:ARG:HD3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASN:H	1:C:116:GLN:NE2	1.96	0.62
1:D:98:ASN:H	1:D:116:GLN:NE2	1.98	0.62
1:D:129:THR:O	1:D:133:THR:HG22	2.00	0.62
1:D:47:THR:N	1:D:334:ASN:HD21	1.98	0.62
1:B:204:ARG:O	1:B:243:CYS:HB2	1.98	0.62
1:D:194:ILE:CD1	1:D:194:ILE:H	1.97	0.62
1:D:74:GLN:HE21	1:D:94:ALA:H	1.46	0.62
1:C:87:ARG:HH22	1:C:314:VAL:HG13	1.64	0.62
1:D:232:ILE:HG22	1:D:234:LEU:HD11	1.82	0.62
1:B:30:PHE:HB2	1:B:41:LYS:HD2	1.82	0.62
1:A:339:ILE:C	1:A:339:ILE:CD1	2.60	0.61
1:D:204:ARG:HB3	1:D:243:CYS:HB3	1.82	0.61
1:B:130:LEU:HG	1:B:172:ILE:HG22	1.82	0.61
1:A:252:TYR:OH	1:A:255:HIS:HA	2.00	0.61
1:A:102:ASN:HD21	1:A:123:ARG:HD3	1.65	0.61
1:C:25:THR:HG22	1:C:26:PRO:HD3	1.80	0.61
1:B:292:THR:HG22	1:B:295:GLU:HG3	1.82	0.61
1:A:317:TRP:O	1:A:319:HIS:N	2.32	0.61
1:B:169:ASP:HA	1:B:172:ILE:HD11	1.83	0.61
1:A:192:GLU:HG2	1:A:193:GLU:HG2	1.81	0.61
1:A:234:LEU:HD12	1:A:234:LEU:N	2.16	0.61
1:C:169:ASP:HA	1:C:172:ILE:HD11	1.82	0.61
1:C:127:PHE:CD2	1:C:176:SER:HA	2.36	0.61
1:A:47:THR:N	1:A:334:ASN:HD21	1.98	0.61
1:B:98:ASN:H	1:B:116:GLN:NE2	1.99	0.61
1:C:130:LEU:HG	1:C:172:ILE:HG22	1.82	0.60
1:A:65:HIS:CD2	1:A:69:ILE:HD13	2.35	0.60
1:D:291:LEU:HD22	1:D:295:GLU:HB3	1.83	0.60
1:C:102:ASN:HD21	1:C:123:ARG:HD3	1.67	0.60
1:D:53:THR:O	1:D:61:ARG:HG3	2.01	0.60
1:C:292:THR:CG2	1:C:294:PRO:HD2	2.21	0.60
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.14	0.60
1:C:65:HIS:CD2	1:C:69:ILE:HD13	2.36	0.60
1:B:164:TRP:CE3	1:B:164:TRP:HA	2.37	0.60
1:D:115:VAL:HG13	1:D:116:GLN:N	2.16	0.60
1:D:192:GLU:HG2	1:D:193:GLU:HG2	1.84	0.60
1:D:278:ARG:NH2	1:D:316:GLY:HA2	2.17	0.59
1:C:47:THR:N	1:C:334:ASN:HD21	2.00	0.59
1:A:129:THR:O	1:A:133:THR:HG22	2.01	0.59
1:C:129:THR:O	1:C:133:THR:HG22	2.03	0.59
1:D:240:ALA:HB2	1:D:306:TYR:CD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG22	1:B:116:GLN:H	1.66	0.59
1:A:89:VAL:HG23	1:A:270:ILE:O	2.03	0.59
1:D:48:LEU:HD23	1:D:49:GLU:N	2.17	0.59
1:A:229:VAL:HG13	1:A:233:TYR:OH	2.02	0.59
1:B:48:LEU:HD23	1:B:49:GLU:N	2.18	0.59
1:B:252:TYR:OH	1:B:255:HIS:HA	2.02	0.59
1:C:164:TRP:CE3	1:C:164:TRP:HA	2.37	0.59
1:B:129:THR:O	1:B:133:THR:HG22	2.03	0.59
1:D:55:GLN:C	1:D:56:PHE:HD1	2.07	0.59
1:B:137:ASN:O	1:B:141:ARG:HG3	2.03	0.59
1:B:127:PHE:CD2	1:B:176:SER:HA	2.38	0.59
1:D:164:TRP:CE3	1:D:164:TRP:HA	2.38	0.59
1:D:74:GLN:HE22	1:D:93:VAL:HA	1.64	0.58
1:C:336:PRO:O	1:C:340:ASN:HB2	2.02	0.58
1:C:137:ASN:O	1:C:141:ARG:HG3	2.03	0.58
1:C:292:THR:HG22	1:C:295:GLU:HG3	1.86	0.58
1:C:30:PHE:HB2	1:C:41:LYS:HD2	1.85	0.58
1:B:232:ILE:HG22	1:B:234:LEU:HD11	1.84	0.58
1:B:272:ALA:HA	1:B:330:LEU:HG	1.85	0.58
1:D:319:HIS:N	1:D:319:HIS:CD2	2.72	0.58
1:B:17:LYS:HE2	1:B:340:ASN:H	1.69	0.58
1:D:339:ILE:CD1	1:D:339:ILE:C	2.63	0.58
1:C:115:VAL:HG13	1:C:116:GLN:N	2.18	0.58
1:D:229:VAL:HG13	1:D:233:TYR:OH	2.04	0.58
1:D:87:ARG:NH2	1:D:314:VAL:HG13	2.08	0.58
1:A:21:ILE:HG12	1:A:339:ILE:HG12	1.86	0.58
1:A:17:LYS:HE2	1:A:340:ASN:H	1.69	0.58
1:A:317:TRP:C	1:A:319:HIS:H	2.07	0.58
1:B:339:ILE:CD1	1:B:339:ILE:C	2.60	0.58
1:C:252:TYR:OH	1:C:255:HIS:HA	2.04	0.58
1:A:167:GLU:O	1:A:170:ASN:HB3	2.04	0.58
1:B:291:LEU:HD22	1:B:295:GLU:HB3	1.86	0.57
1:A:74:GLN:HE21	1:A:94:ALA:N	2.02	0.57
1:D:273:VAL:HG22	1:D:330:LEU:HD21	1.87	0.57
1:D:278:ARG:HH22	1:D:316:GLY:HA2	1.69	0.57
1:D:25:THR:HG22	1:D:26:PRO:HD3	1.85	0.57
1:A:25:THR:CB	1:A:26:PRO:HD3	2.35	0.57
1:B:55:GLN:C	1:B:56:PHE:HD1	2.07	0.57
1:B:47:THR:N	1:B:334:ASN:HD21	1.99	0.57
1:C:55:GLN:C	1:C:56:PHE:HD1	2.08	0.57
1:B:229:VAL:HG13	1:B:233:TYR:OH	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:VAL:HG13	1:C:233:TYR:OH	2.05	0.57
1:A:240:ALA:HB2	1:A:306:TYR:CE2	2.38	0.57
1:A:53:THR:O	1:A:61:ARG:HG3	2.04	0.57
1:B:50:MET:HG3	1:B:51:PHE:N	2.19	0.57
1:D:137:ASN:O	1:D:141:ARG:HG3	2.04	0.57
1:D:127:PHE:CD2	1:D:176:SER:HA	2.40	0.57
1:D:17:LYS:HE2	1:D:340:ASN:H	1.70	0.57
1:A:164:TRP:HA	1:A:164:TRP:CE3	2.40	0.57
1:D:102:ASN:HD21	1:D:123:ARG:HD3	1.68	0.56
1:A:98:ASN:H	1:A:116:GLN:HE22	1.53	0.56
1:A:25:THR:CG2	1:A:26:PRO:HD3	2.34	0.56
1:D:279:ASP:O	1:D:280:ARG:C	2.43	0.56
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.17	0.56
1:A:169:ASP:HA	1:A:172:ILE:HD11	1.86	0.56
1:A:77:LEU:HB3	1:A:83:LEU:HB2	1.86	0.56
1:B:17:LYS:HD3	1:B:341:LEU:HD22	1.88	0.56
1:D:236:LEU:HD23	1:D:306:TYR:CE1	2.40	0.56
1:C:7:PRO:HD3	1:C:348:LEU:HD21	1.87	0.56
1:A:137:ASN:O	1:A:141:ARG:HG3	2.06	0.56
1:A:264:LYS:NZ	1:A:264:LYS:HB2	2.21	0.56
1:C:48:LEU:HD23	1:C:49:GLU:N	2.20	0.56
1:B:167:GLU:O	1:B:170:ASN:HB3	2.05	0.56
1:D:135:THR:HG23	1:D:168:TRP:CZ2	2.41	0.56
1:C:208:ILE:HD11	1:C:273:VAL:HG11	1.87	0.56
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.17	0.56
1:B:89:VAL:HG23	1:B:270:ILE:O	2.06	0.56
1:C:11:TYR:CE2	1:C:12:LEU:HG	2.41	0.55
1:B:7:PRO:HD3	1:B:348:LEU:HD21	1.87	0.55
1:D:169:ASP:HA	1:D:172:ILE:HD11	1.89	0.55
1:D:106:HIS:ND1	1:D:116:GLN:O	2.37	0.55
1:C:54:CYS:O	1:C:55:GLN:HG3	2.07	0.55
1:A:127:PHE:CD2	1:A:176:SER:HA	2.41	0.55
1:D:46:TYR:HA	1:D:334:ASN:HD21	1.72	0.55
1:A:236:LEU:HD23	1:A:306:TYR:CE1	2.42	0.55
1:C:212:ASP:N	1:C:212:ASP:OD2	2.40	0.55
1:A:7:PRO:HD3	1:A:348:LEU:HD21	1.87	0.55
1:A:317:TRP:HB2	1:A:321:THR:HG23	1.89	0.55
1:C:232:ILE:HG22	1:C:234:LEU:HD11	1.88	0.55
1:B:115:VAL:HG13	1:B:116:GLN:N	2.22	0.55
1:A:55:GLN:C	1:A:56:PHE:HD1	2.10	0.55
1:C:135:THR:HG23	1:C:168:TRP:CZ2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:HIS:ND1	1:C:116:GLN:O	2.39	0.54
1:B:53:THR:O	1:B:61:ARG:HG3	2.07	0.54
1:A:17:LYS:HD3	1:A:341:LEU:HD22	1.90	0.54
1:D:60:PHE:HD1	1:D:63:ILE:HD11	1.73	0.54
1:C:240:ALA:HB2	1:C:306:TYR:CE2	2.43	0.54
1:D:54:CYS:O	1:D:55:GLN:HG3	2.08	0.54
1:D:49:GLU:OE1	1:D:271:ARG:NH2	2.40	0.54
1:B:74:GLN:HE21	1:B:94:ALA:N	2.06	0.54
1:B:48:LEU:HD12	1:B:114:GLY:HA2	1.89	0.54
1:A:54:CYS:O	1:A:55:GLN:HG3	2.08	0.54
1:B:135:THR:HG23	1:B:168:TRP:CZ2	2.42	0.54
1:D:167:GLU:O	1:D:170:ASN:HB3	2.08	0.53
1:C:98:ASN:H	1:C:116:GLN:HE22	1.55	0.53
1:A:60:PHE:HD1	1:A:63:ILE:HD11	1.73	0.53
1:C:24:ARG:HH11	1:C:24:ARG:CG	2.20	0.53
1:C:87:ARG:NH1	1:C:314:VAL:HG13	2.23	0.53
1:D:252:TYR:OH	1:D:255:HIS:HA	2.08	0.53
1:D:39:HIS:HD2	1:D:204:ARG:HH11	1.55	0.53
1:D:98:ASN:H	1:D:116:GLN:HE22	1.56	0.53
1:B:65:HIS:HD2	1:B:69:ILE:HD13	1.73	0.53
1:D:65:HIS:HD2	1:D:69:ILE:HD13	1.72	0.53
1:C:167:GLU:O	1:C:170:ASN:HB3	2.08	0.53
1:C:48:LEU:HD12	1:C:114:GLY:HA2	1.91	0.53
1:A:135:THR:HG23	1:A:168:TRP:CZ2	2.43	0.53
1:B:313:PRO:HA	1:B:324:LEU:HD23	1.91	0.53
1:B:106:HIS:ND1	1:B:116:GLN:O	2.39	0.53
1:B:45:ARG:HB3	1:B:244:TYR:CE2	2.44	0.53
1:C:49:GLU:OE1	1:C:271:ARG:NH2	2.42	0.53
1:C:11:TYR:HA	1:C:341:LEU:HD13	1.91	0.53
1:B:54:CYS:O	1:B:55:GLN:HG3	2.09	0.53
1:A:115:VAL:HG13	1:A:116:GLN:N	2.23	0.52
1:A:48:LEU:HD23	1:A:49:GLU:N	2.24	0.52
1:A:25:THR:HG22	1:A:26:PRO:N	2.24	0.52
1:B:15:MET:CE	1:C:7:PRO:HG3	2.39	0.52
1:A:38:HIS:O	1:A:202:ILE:HG23	2.09	0.52
1:D:25:THR:HG22	1:D:26:PRO:N	2.24	0.52
1:C:77:LEU:HB3	1:C:83:LEU:HB2	1.91	0.52
1:D:48:LEU:HD12	1:D:114:GLY:HA2	1.91	0.52
1:C:340:ASN:OD1	1:C:342:VAL:HG23	2.09	0.52
1:D:25:THR:CB	1:D:26:PRO:HD3	2.40	0.52
1:A:264:LYS:O	1:A:265:ASP:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:C	1:A:265:ASP:H	2.13	0.52
1:B:212:ASP:N	1:B:212:ASP:OD2	2.42	0.52
1:C:53:THR:O	1:C:61:ARG:HG3	2.09	0.52
1:D:7:PRO:HD3	1:D:348:LEU:HD21	1.91	0.51
1:A:64:ILE:O	1:A:67:ALA:HB3	2.10	0.51
1:B:11:TYR:HA	1:B:341:LEU:HD13	1.91	0.51
1:C:338:GLU:OE2	1:D:324:LEU:HB3	2.11	0.51
1:D:212:ASP:OD2	1:D:212:ASP:N	2.43	0.51
1:B:98:ASN:H	1:B:116:GLN:HE22	1.58	0.51
1:A:65:HIS:HD2	1:A:69:ILE:HD13	1.74	0.51
1:C:60:PHE:HD1	1:C:63:ILE:HD11	1.74	0.51
1:C:46:TYR:HA	1:C:334:ASN:HD21	1.76	0.51
1:B:77:LEU:HB3	1:B:83:LEU:HB2	1.93	0.51
1:A:115:VAL:HG22	1:A:116:GLN:N	2.24	0.51
1:B:25:THR:CB	1:B:26:PRO:HD3	2.41	0.51
1:C:338:GLU:CD	1:D:324:LEU:HD13	2.31	0.51
1:C:183:ARG:HB2	1:C:183:ARG:NH1	2.24	0.51
1:D:291:LEU:HD13	1:D:296:ASN:HA	1.93	0.51
1:A:106:HIS:ND1	1:A:116:GLN:O	2.43	0.50
1:B:208:ILE:HD11	1:B:273:VAL:HG11	1.93	0.50
1:B:240:ALA:HB2	1:B:306:TYR:CE2	2.45	0.50
1:B:60:PHE:HD1	1:B:63:ILE:HD11	1.74	0.50
1:B:334:ASN:C	1:B:334:ASN:HD22	2.15	0.50
1:A:252:TYR:CZ	1:A:255:HIS:HA	2.46	0.50
1:C:45:ARG:HB3	1:C:244:TYR:CE2	2.46	0.50
1:A:49:GLU:OE1	1:A:271:ARG:NH2	2.45	0.50
1:D:232:ILE:HD11	1:D:275:LEU:HD22	1.93	0.50
1:C:236:LEU:HD23	1:C:306:TYR:CE1	2.46	0.50
1:B:23:GLU:OE2	1:C:351:HIS:ND1	2.41	0.50
1:C:115:VAL:HG22	1:C:116:GLN:N	2.25	0.50
1:C:25:THR:HG22	1:C:26:PRO:N	2.24	0.50
1:C:164:TRP:HE3	1:C:164:TRP:HA	1.76	0.50
1:C:264:LYS:O	1:C:264:LYS:HG3	2.11	0.50
1:B:7:PRO:HG3	1:C:15:MET:CE	2.42	0.50
1:C:203:LEU:O	1:C:204:ARG:HB2	2.11	0.50
1:B:236:LEU:HD23	1:B:306:TYR:CE1	2.47	0.50
1:A:340:ASN:OD1	1:A:342:VAL:HG23	2.12	0.50
1:A:334:ASN:C	1:A:334:ASN:HD22	2.15	0.49
1:A:240:ALA:C	1:A:242:GLU:H	2.14	0.49
1:D:60:PHE:HA	1:D:63:ILE:HD11	1.94	0.49
1:D:17:LYS:HD3	1:D:341:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:HIS:HD2	1:C:69:ILE:HD13	1.76	0.49
1:B:13:SER:O	1:B:14:ASN:HB2	2.12	0.49
1:A:199:LEU:HD12	1:A:207:ILE:HD11	1.93	0.49
1:A:212:ASP:OD2	1:A:212:ASP:N	2.46	0.49
1:B:46:TYR:HA	1:B:334:ASN:HD21	1.77	0.49
1:C:25:THR:CB	1:C:26:PRO:HD3	2.42	0.49
1:D:208:ILE:HD13	1:D:273:VAL:HG21	1.93	0.49
1:A:119:ASP:O	1:A:120:LEU:HB2	2.11	0.49
1:B:199:LEU:HD12	1:B:207:ILE:HD11	1.94	0.49
1:D:53:THR:HG21	1:D:65:HIS:CE1	2.47	0.49
1:B:108:THR:HG21	1:B:199:LEU:HD11	1.94	0.49
1:A:48:LEU:HD12	1:A:114:GLY:HA2	1.94	0.49
1:D:126:LEU:HD13	1:D:175:ALA:HB1	1.94	0.49
1:D:110:GLN:HG2	1:D:115:VAL:O	2.13	0.49
1:B:164:TRP:HE3	1:B:164:TRP:HA	1.76	0.49
1:C:263:LEU:C	1:C:265:ASP:H	2.16	0.49
1:C:64:ILE:O	1:C:67:ALA:HB3	2.13	0.49
1:A:57:CYS:HG	1:A:356:TRP:HZ3	1.61	0.49
1:C:334:ASN:C	1:C:334:ASN:HD22	2.16	0.49
1:D:57:CYS:HG	1:D:356:TRP:HZ3	1.61	0.49
1:C:89:VAL:HG23	1:C:270:ILE:O	2.12	0.49
1:B:49:GLU:OE1	1:B:271:ARG:NH2	2.46	0.48
1:A:89:VAL:HG21	1:A:272:ALA:O	2.13	0.48
1:B:126:LEU:HD11	1:B:195:HIS:HB3	1.95	0.48
1:C:17:LYS:HD3	1:C:341:LEU:HD22	1.96	0.48
1:A:108:THR:HG21	1:A:199:LEU:HD11	1.94	0.48
1:A:110:GLN:HG2	1:A:115:VAL:O	2.13	0.48
1:C:135:THR:O	1:C:136:ARG:C	2.51	0.48
1:B:292:THR:HG22	1:B:295:GLU:CD	2.34	0.48
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.18	0.48
1:B:192:GLU:HG2	1:B:193:GLU:N	2.27	0.48
1:B:252:TYR:CZ	1:B:255:HIS:HA	2.48	0.48
1:A:73:ILE:HD11	1:A:258:VAL:HG21	1.95	0.48
1:D:164:TRP:O	1:D:166:ASP:N	2.46	0.48
1:C:74:GLN:HE21	1:C:94:ALA:N	2.06	0.48
1:B:79:SER:C	1:B:81:LYS:H	2.17	0.48
1:B:340:ASN:OD1	1:B:342:VAL:HG23	2.14	0.48
1:B:25:THR:CG2	1:B:26:PRO:HD3	2.43	0.48
1:C:240:ALA:C	1:C:242:GLU:H	2.16	0.48
1:A:299:LYS:O	1:A:300:GLU:C	2.52	0.48
1:B:307:LEU:HA	1:B:307:LEU:HD22	1.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:PRO:HA	1:C:324:LEU:HD23	1.96	0.48
1:C:127:PHE:CE2	1:C:176:SER:HB2	2.49	0.48
1:D:64:ILE:O	1:D:67:ALA:HB3	2.14	0.48
1:B:102:ASN:HD22	1:B:123:ARG:NH1	2.00	0.47
1:C:249:VAL:HG12	1:C:260:LEU:HB2	1.96	0.47
1:B:110:GLN:HG2	1:B:115:VAL:O	2.14	0.47
1:B:64:ILE:O	1:B:67:ALA:HB3	2.14	0.47
1:B:291:LEU:HD13	1:B:296:ASN:HA	1.96	0.47
1:D:278:ARG:HD3	1:D:317:TRP:CZ2	2.49	0.47
1:C:39:HIS:HD2	1:C:204:ARG:HH11	1.61	0.47
1:D:119:ASP:O	1:D:120:LEU:HB2	2.14	0.47
1:C:25:THR:CG2	1:C:26:PRO:HD3	2.43	0.47
1:D:193:GLU:HG2	1:D:193:GLU:H	1.38	0.47
1:C:268:PRO:HD2	1:C:269:GLU:H	1.79	0.47
1:A:291:LEU:HD13	1:A:296:ASN:HA	1.96	0.47
1:D:340:ASN:OD1	1:D:342:VAL:HG23	2.14	0.47
1:C:108:THR:HG21	1:C:199:LEU:HD11	1.97	0.47
1:D:77:LEU:CB	1:D:83:LEU:HB2	2.44	0.47
1:A:240:ALA:C	1:A:242:GLU:N	2.67	0.47
1:A:39:HIS:HD2	1:A:204:ARG:HH11	1.63	0.47
1:B:119:ASP:O	1:B:120:LEU:HB2	2.15	0.47
1:D:299:LYS:O	1:D:300:GLU:C	2.52	0.47
1:B:17:LYS:HB3	1:B:341:LEU:HD21	1.95	0.47
1:C:240:ALA:C	1:C:242:GLU:N	2.68	0.47
1:D:45:ARG:HB3	1:D:244:TYR:CE2	2.50	0.47
1:A:79:SER:C	1:A:81:LYS:H	2.19	0.47
1:D:307:LEU:HA	1:D:307:LEU:HD22	1.80	0.47
1:D:49:GLU:OE2	1:D:264:LYS:HE3	2.15	0.47
1:B:348:LEU:C	1:B:348:LEU:HD23	2.36	0.47
1:A:74:GLN:HG2	1:A:94:ALA:HB3	1.97	0.46
1:C:17:LYS:HB3	1:C:341:LEU:HD21	1.97	0.46
1:D:53:THR:HG21	1:D:65:HIS:HE1	1.80	0.46
1:D:192:GLU:HG2	1:D:193:GLU:N	2.30	0.46
1:D:164:TRP:HE3	1:D:164:TRP:HA	1.79	0.46
1:D:108:THR:HG21	1:D:199:LEU:HD11	1.97	0.46
1:C:79:SER:C	1:C:81:LYS:H	2.19	0.46
1:A:17:LYS:HB3	1:A:341:LEU:HD21	1.97	0.46
1:A:21:ILE:HG12	1:A:339:ILE:CG1	2.45	0.46
1:D:48:LEU:C	1:D:48:LEU:HD23	2.36	0.46
1:D:204:ARG:O	1:D:243:CYS:CB	2.58	0.46
1:D:25:THR:CG2	1:D:26:PRO:HD3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PRO:HA	1:A:324:LEU:HD23	1.98	0.46
1:C:252:TYR:CZ	1:C:255:HIS:HA	2.50	0.46
1:C:186:LEU:HD23	1:C:188:TYR:H	1.80	0.46
1:D:30:PHE:HD2	1:D:39:HIS:CE1	2.34	0.46
1:A:164:TRP:HA	1:A:164:TRP:HE3	1.80	0.46
1:C:77:LEU:CB	1:C:83:LEU:HB2	2.45	0.46
1:C:199:LEU:HD12	1:C:207:ILE:HD11	1.98	0.46
1:A:74:GLN:HE21	1:A:93:VAL:CA	2.26	0.46
1:B:48:LEU:HD22	1:B:261:VAL:HG11	1.96	0.46
1:A:241:GLN:HG3	1:A:241:GLN:H	1.61	0.46
1:C:9:ALA:O	1:C:12:LEU:HB2	2.16	0.46
1:C:193:GLU:HG2	1:C:193:GLU:H	1.50	0.46
1:C:348:LEU:HD23	1:C:348:LEU:C	2.36	0.46
1:D:77:LEU:HB3	1:D:83:LEU:HB2	1.97	0.46
1:A:232:ILE:HG22	1:A:234:LEU:CD1	2.44	0.45
1:B:233:TYR:N	1:B:233:TYR:CD1	2.83	0.45
1:D:252:TYR:CZ	1:D:255:HIS:HA	2.50	0.45
1:C:313:PRO:HA	1:C:323:HIS:O	2.16	0.45
1:B:57:CYS:HG	1:B:356:TRP:HZ3	1.62	0.45
1:B:38:HIS:O	1:B:202:ILE:HG23	2.16	0.45
1:B:36:ILE:HG22	1:B:37:ILE:N	2.31	0.45
1:C:110:GLN:HG2	1:C:115:VAL:O	2.17	0.45
1:D:115:VAL:HG22	1:D:116:GLN:N	2.28	0.45
1:B:293:ASP:N	1:B:294:PRO:CD	2.79	0.45
1:A:17:LYS:HD3	1:A:341:LEU:CD2	2.46	0.45
1:A:204:ARG:O	1:A:243:CYS:CB	2.63	0.45
1:C:119:ASP:O	1:C:120:LEU:HB2	2.15	0.45
1:A:11:TYR:HA	1:A:341:LEU:HD13	1.99	0.45
1:D:21:ILE:HG12	1:D:339:ILE:HG12	1.99	0.45
1:C:87:ARG:NE	1:C:87:ARG:H	2.13	0.45
1:C:292:THR:HG22	1:C:295:GLU:CD	2.37	0.45
1:B:48:LEU:HD23	1:B:48:LEU:C	2.36	0.45
1:C:87:ARG:N	1:C:87:ARG:CD	2.80	0.45
1:B:23:GLU:HG3	1:C:351:HIS:CE1	2.51	0.45
1:D:241:GLN:H	1:D:241:GLN:HG3	1.55	0.45
1:A:249:VAL:HG12	1:A:260:LEU:HB2	1.98	0.45
1:B:88:GLU:HG3	1:B:313:PRO:O	2.17	0.45
1:D:89:VAL:HG23	1:D:270:ILE:O	2.16	0.45
1:D:249:VAL:HG12	1:D:260:LEU:HB2	1.98	0.45
1:C:291:LEU:HD13	1:C:296:ASN:HA	1.99	0.45
1:A:46:TYR:HA	1:A:334:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ALA:HA	1:C:330:LEU:HG	1.98	0.45
1:A:53:THR:HG21	1:A:65:HIS:CE1	2.52	0.45
1:D:240:ALA:HB2	1:D:306:TYR:CE2	2.52	0.45
1:D:279:ASP:O	1:D:281:GLY:N	2.50	0.45
1:C:101:GLY:HA3	1:C:186:LEU:HD21	1.98	0.45
1:A:314:VAL:HG12	1:A:315:GLN:O	2.16	0.45
1:C:358:GLU:O	1:C:359:ASN:CB	2.65	0.45
1:B:122:LEU:HA	1:B:122:LEU:HD22	1.77	0.45
1:B:249:VAL:HG12	1:B:260:LEU:HB2	1.98	0.45
1:A:317:TRP:HB2	1:A:321:THR:CG2	2.46	0.45
1:C:87:ARG:HH22	1:C:314:VAL:CG1	2.30	0.45
1:A:272:ALA:HA	1:A:330:LEU:HG	1.99	0.45
1:C:199:LEU:HD12	1:C:207:ILE:CD1	2.47	0.45
1:C:74:GLN:HG2	1:C:94:ALA:HB3	1.97	0.45
1:D:334:ASN:C	1:D:334:ASN:HD22	2.19	0.45
1:C:192:GLU:HG2	1:C:193:GLU:N	2.32	0.45
1:B:39:HIS:HD2	1:B:204:ARG:HH11	1.65	0.45
1:C:263:LEU:HA	1:C:263:LEU:HD22	1.63	0.45
1:C:87:ARG:NH2	1:C:314:VAL:HG13	2.29	0.44
1:B:25:THR:HG22	1:B:26:PRO:N	2.29	0.44
1:C:299:LYS:O	1:C:300:GLU:C	2.53	0.44
1:A:293:ASP:N	1:A:294:PRO:CD	2.80	0.44
1:D:194:ILE:HA	1:D:290:PHE:HE1	1.82	0.44
1:D:24:ARG:NH1	1:D:24:ARG:CG	2.79	0.44
1:A:208:ILE:HD11	1:A:273:VAL:HG11	1.98	0.44
1:A:33:THR:C	1:A:35:GLY:H	2.21	0.44
1:D:203:LEU:O	1:D:204:ARG:HB2	2.17	0.44
1:B:203:LEU:O	1:B:204:ARG:HB2	2.17	0.44
1:A:264:LYS:HZ2	1:A:264:LYS:HB2	1.82	0.44
1:B:142:TRP:CD1	1:B:168:TRP:HE3	2.35	0.44
1:B:199:LEU:HD12	1:B:207:ILE:CD1	2.48	0.44
1:B:115:VAL:HG22	1:B:116:GLN:N	2.31	0.44
1:A:299:LYS:O	1:A:302:LEU:N	2.50	0.44
1:D:199:LEU:HD12	1:D:207:ILE:HD11	1.98	0.44
1:A:25:THR:HB	1:A:26:PRO:HD3	1.99	0.44
1:D:79:SER:C	1:D:81:LYS:H	2.21	0.44
1:A:348:LEU:HD23	1:A:348:LEU:C	2.38	0.44
1:D:292:THR:HG22	1:D:295:GLU:CD	2.37	0.44
1:C:33:THR:C	1:C:35:GLY:H	2.21	0.44
1:A:288:VAL:O	1:A:288:VAL:HG12	2.18	0.44
1:D:30:PHE:HB2	1:D:41:LYS:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:H	1:C:87:ARG:CD	2.31	0.44
1:A:135:THR:O	1:A:136:ARG:C	2.55	0.44
1:D:312:ILE:HA	1:D:313:PRO:HD3	1.90	0.44
1:C:122:LEU:HA	1:C:122:LEU:HD22	1.78	0.44
1:B:232:ILE:HG22	1:B:234:LEU:CD1	2.48	0.44
1:C:139:LYS:O	1:C:143:GLN:HG3	2.18	0.44
1:D:293:ASP:N	1:D:294:PRO:CD	2.80	0.43
1:A:193:GLU:HG2	1:A:193:GLU:H	1.47	0.43
1:A:229:VAL:HG12	1:A:229:VAL:O	2.18	0.43
1:A:164:TRP:O	1:A:166:ASP:N	2.51	0.43
1:C:293:ASP:N	1:C:294:PRO:CD	2.82	0.43
1:C:53:THR:HG21	1:C:65:HIS:CE1	2.53	0.43
1:D:33:THR:C	1:D:35:GLY:H	2.22	0.43
1:A:116:GLN:O	1:A:116:GLN:CG	2.66	0.43
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.84	0.43
1:A:192:GLU:HG2	1:A:193:GLU:N	2.34	0.43
1:B:135:THR:O	1:B:136:ARG:C	2.56	0.43
1:A:63:ILE:H	1:A:63:ILE:HG12	1.56	0.43
1:A:199:LEU:HD12	1:A:207:ILE:CD1	2.47	0.43
1:A:73:ILE:CD1	1:A:258:VAL:HG21	2.49	0.43
1:A:275:LEU:HA	1:A:275:LEU:HD23	1.85	0.43
1:D:348:LEU:HD23	1:D:348:LEU:C	2.39	0.43
1:D:299:LYS:O	1:D:302:LEU:N	2.52	0.43
1:C:17:LYS:HE2	1:C:340:ASN:H	1.83	0.43
1:C:24:ARG:HG2	1:C:24:ARG:NH1	2.26	0.43
1:D:25:THR:HB	1:D:26:PRO:HD3	2.01	0.43
1:B:193:GLU:HG2	1:B:193:GLU:H	1.46	0.43
1:C:182:ALA:O	1:C:183:ARG:C	2.57	0.43
1:B:28:ASP:O	1:B:41:LYS:HD3	2.18	0.43
1:D:142:TRP:CD1	1:D:168:TRP:HE3	2.36	0.43
1:B:74:GLN:HG2	1:B:94:ALA:HB3	1.99	0.43
1:C:60:PHE:CD2	1:C:353:TYR:CD2	3.07	0.43
1:B:335:LEU:HA	1:B:335:LEU:HD23	1.81	0.43
1:C:11:TYR:CE2	1:C:12:LEU:CD2	3.01	0.43
1:A:30:PHE:HB2	1:A:41:LYS:CD	2.48	0.43
1:C:338:GLU:CD	1:D:324:LEU:HB3	2.39	0.43
1:A:36:ILE:HG22	1:A:37:ILE:N	2.33	0.43
1:D:60:PHE:CD2	1:D:353:TYR:CD2	3.07	0.43
1:A:317:TRP:HE1	1:A:323:HIS:CG	2.35	0.43
1:D:272:ALA:HA	1:D:330:LEU:HG	2.00	0.43
1:D:126:LEU:O	1:D:129:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:PHE:CE2	1:D:176:SER:HB2	2.54	0.43
1:D:199:LEU:HD12	1:D:207:ILE:CD1	2.48	0.43
1:D:240:ALA:C	1:D:242:GLU:H	2.21	0.43
1:A:127:PHE:CE2	1:A:176:SER:HB2	2.54	0.43
1:D:240:ALA:C	1:D:242:GLU:N	2.71	0.43
1:B:263:LEU:HA	1:B:263:LEU:HD23	1.75	0.43
1:A:13:SER:O	1:A:14:ASN:HB2	2.19	0.43
1:A:21:ILE:HG12	1:A:339:ILE:CD1	2.48	0.42
1:D:11:TYR:HA	1:D:341:LEU:HD13	2.01	0.42
1:D:232:ILE:HG22	1:D:234:LEU:CD1	2.49	0.42
1:C:13:SER:O	1:C:14:ASN:HB2	2.19	0.42
1:D:122:LEU:HD22	1:D:122:LEU:HA	1.79	0.42
1:C:74:GLN:NE2	1:C:94:ALA:H	2.12	0.42
1:C:21:ILE:HG12	1:C:339:ILE:HD13	2.01	0.42
1:A:186:LEU:N	1:A:186:LEU:HD22	2.29	0.42
1:A:60:PHE:CD2	1:A:353:TYR:CD2	3.07	0.42
1:D:21:ILE:H	1:D:21:ILE:HG13	1.66	0.42
1:B:53:THR:HG21	1:B:65:HIS:CE1	2.54	0.42
1:B:240:ALA:C	1:B:242:GLU:N	2.72	0.42
1:A:233:TYR:CD1	1:A:233:TYR:N	2.87	0.42
1:C:164:TRP:O	1:C:166:ASP:N	2.52	0.42
1:B:60:PHE:HA	1:B:63:ILE:HD11	2.01	0.42
1:A:268:PRO:O	1:A:269:GLU:C	2.57	0.42
1:A:309:VAL:HG12	1:A:310:ILE:N	2.35	0.42
1:A:17:LYS:O	1:A:18:ALA:C	2.57	0.42
1:A:341:LEU:HA	1:A:341:LEU:HD22	1.83	0.42
1:D:74:GLN:HG2	1:D:94:ALA:HB3	2.01	0.42
1:A:102:ASN:HD22	1:A:123:ARG:NH1	2.00	0.42
1:C:205:ARG:HE	1:C:248:ILE:CG1	2.23	0.42
1:B:164:TRP:O	1:B:166:ASP:N	2.52	0.42
1:A:229:VAL:CG1	1:A:229:VAL:O	2.67	0.42
1:A:77:LEU:CB	1:A:83:LEU:HB2	2.49	0.42
1:C:335:LEU:HA	1:C:335:LEU:HD23	1.80	0.42
1:B:194:ILE:H	1:B:194:ILE:CD1	1.93	0.42
1:D:116:GLN:O	1:D:116:GLN:CG	2.68	0.42
1:C:126:LEU:HD13	1:C:175:ALA:HB1	2.02	0.42
1:D:263:LEU:HA	1:D:263:LEU:HD22	1.61	0.42
1:C:307:LEU:HA	1:C:307:LEU:HD22	1.69	0.42
1:A:138:PHE:CE2	1:A:237:HIS:CE1	3.07	0.42
1:D:87:ARG:HH22	1:D:314:VAL:CG1	2.12	0.42
1:B:21:ILE:H	1:B:21:ILE:HG13	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HB	1:A:233:TYR:CE2	2.55	0.42
1:C:233:TYR:N	1:C:233:TYR:CD1	2.88	0.42
1:B:89:VAL:CG2	1:B:270:ILE:O	2.68	0.42
1:A:89:VAL:CG2	1:A:270:ILE:O	2.67	0.42
1:D:44:HIS:CD2	1:D:44:HIS:H	2.37	0.42
1:C:197:PHE:HB2	1:C:290:PHE:CD1	2.55	0.42
1:C:31:LYS:HA	1:C:38:HIS:HD2	1.84	0.42
1:B:229:VAL:CG1	1:B:229:VAL:O	2.68	0.42
1:D:335:LEU:HA	1:D:335:LEU:HD23	1.79	0.42
1:A:292:THR:HG22	1:A:295:GLU:CD	2.40	0.41
1:B:240:ALA:C	1:B:242:GLU:H	2.23	0.41
1:C:236:LEU:HA	1:C:236:LEU:HD23	1.92	0.41
1:C:240:ALA:O	1:C:242:GLU:N	2.52	0.41
1:B:33:THR:C	1:B:35:GLY:H	2.23	0.41
1:A:50:MET:HA	1:A:50:MET:HE2	2.02	0.41
1:B:236:LEU:C	1:B:238:TRP:H	2.23	0.41
1:D:229:VAL:CG1	1:D:229:VAL:O	2.68	0.41
1:C:17:LYS:O	1:C:18:ALA:C	2.59	0.41
1:A:317:TRP:C	1:A:319:HIS:N	2.72	0.41
1:D:36:ILE:HG22	1:D:37:ILE:N	2.35	0.41
1:C:142:TRP:CD1	1:C:168:TRP:HE3	2.37	0.41
1:B:14:ASN:HA	1:C:14:ASN:HA	2.02	0.41
1:A:232:ILE:HD11	1:A:275:LEU:HD22	2.02	0.41
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.33	0.41
1:B:196:ILE:HB	1:B:233:TYR:CE2	2.54	0.41
1:A:142:TRP:CD1	1:A:168:TRP:HE3	2.39	0.41
1:B:312:ILE:HA	1:B:313:PRO:HD3	1.86	0.41
1:A:203:LEU:O	1:A:204:ARG:HB2	2.20	0.41
1:A:240:ALA:O	1:A:242:GLU:N	2.53	0.41
1:C:235:PRO:HG2	1:C:243:CYS:SG	2.61	0.41
1:A:264:LYS:O	1:A:264:LYS:HG3	2.20	0.41
1:B:77:LEU:CB	1:B:83:LEU:HB2	2.50	0.41
1:A:307:LEU:HA	1:A:307:LEU:HD22	1.73	0.41
1:D:17:LYS:O	1:D:18:ALA:C	2.59	0.41
1:B:208:ILE:HD13	1:B:273:VAL:HG21	2.01	0.41
1:C:186:LEU:N	1:C:186:LEU:HD13	2.35	0.41
1:D:31:LYS:HA	1:D:38:HIS:HD2	1.86	0.41
1:D:271:ARG:NH1	1:D:332:GLU:CB	2.84	0.41
1:D:37:ILE:H	1:D:37:ILE:CD1	2.23	0.41
1:A:186:LEU:HB2	1:A:187:GLN:H	1.69	0.41
1:D:233:TYR:CD1	1:D:233:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:HE3	1:C:81:LYS:HA	2.03	0.41
1:A:194:ILE:HA	1:A:290:PHE:HE1	1.81	0.41
1:C:11:TYR:CZ	1:C:12:LEU:CD2	3.04	0.41
1:C:21:ILE:CD1	1:C:339:ILE:CD1	2.99	0.41
1:A:30:PHE:HD2	1:A:39:HIS:CE1	2.39	0.41
1:A:334:ASN:C	1:A:334:ASN:ND2	2.74	0.41
1:C:30:PHE:HD2	1:C:39:HIS:CE1	2.39	0.41
1:D:71:ARG:NH1	1:D:71:ARG:HG3	2.31	0.41
1:A:31:LYS:HA	1:A:38:HIS:HD2	1.86	0.41
1:C:268:PRO:CD	1:C:269:GLU:H	2.33	0.41
1:C:126:LEU:HD11	1:C:195:HIS:HB3	2.03	0.41
1:D:13:SER:O	1:D:14:ASN:HB2	2.21	0.41
1:A:21:ILE:HD11	1:A:339:ILE:HD13	2.03	0.41
1:C:21:ILE:HG12	1:C:339:ILE:CD1	2.51	0.41
1:B:30:PHE:HD2	1:B:39:HIS:CE1	2.38	0.41
1:A:53:THR:HG21	1:A:65:HIS:HE1	1.86	0.41
1:A:126:LEU:O	1:A:129:THR:HG22	2.21	0.41
1:B:126:LEU:O	1:B:129:THR:HG22	2.21	0.41
1:B:15:MET:HE1	1:C:7:PRO:HG3	2.03	0.41
1:A:60:PHE:HA	1:A:63:ILE:HD11	2.03	0.41
1:C:264:LYS:O	1:C:265:ASP:C	2.60	0.41
1:C:21:ILE:HG12	1:C:339:ILE:HG12	2.04	0.40
1:C:36:ILE:HG22	1:C:37:ILE:N	2.35	0.40
1:A:273:VAL:CG2	1:A:330:LEU:HD21	2.51	0.40
1:B:81:LYS:HE3	1:B:81:LYS:HA	2.03	0.40
1:B:21:ILE:HG12	1:B:339:ILE:HG12	2.02	0.40
1:D:110:GLN:HA	1:D:115:VAL:O	2.21	0.40
1:B:110:GLN:HA	1:B:115:VAL:O	2.21	0.40
1:B:323:HIS:CG	1:B:324:LEU:H	2.39	0.40
1:D:38:HIS:O	1:D:202:ILE:HG23	2.21	0.40
1:D:48:LEU:HD22	1:D:261:VAL:HG11	2.04	0.40
1:D:21:ILE:CD1	1:D:339:ILE:CD1	2.99	0.40
1:D:196:ILE:HB	1:D:233:TYR:CE2	2.55	0.40
1:B:229:VAL:O	1:B:229:VAL:HG12	2.19	0.40
1:A:81:LYS:HE3	1:A:81:LYS:HA	2.03	0.40
1:A:44:HIS:H	1:A:44:HIS:CD2	2.38	0.40
1:D:264:LYS:HB2	1:D:264:LYS:HZ2	1.86	0.40
1:B:21:ILE:HG12	1:B:339:ILE:HD13	2.03	0.40
1:A:240:ALA:CB	1:A:306:TYR:CD2	3.02	0.40
1:C:234:LEU:CD1	1:C:234:LEU:N	2.77	0.40
1:C:71:ARG:HG3	1:C:71:ARG:NH1	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LYS:HB3	1:D:341:LEU:HD21	2.03	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	322/366 (88%)	268 (83%)	42 (13%)	12 (4%)	4	29
1	B	305/366 (83%)	260 (85%)	36 (12%)	9 (3%)	5	35
1	C	319/366 (87%)	266 (83%)	42 (13%)	11 (3%)	5	31
1	D	319/366 (87%)	264 (83%)	45 (14%)	10 (3%)	5	34
All	All	1265/1464 (86%)	1058 (84%)	165 (13%)	42 (3%)	5	32

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	A	318	ASP
1	B	14	ASN
1	C	14	ASN
1	A	14	ASN
1	A	34	ASN
1	A	136	ARG
1	A	164	TRP
1	A	269	GLU
1	B	34	ASN
1	B	136	ARG
1	B	164	TRP
1	C	34	ASN
1	C	136	ARG

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Mol	Chain	Res	Type
1	C	164	TRP
1	D	14	ASN
1	D	34	ASN
1	D	136	ARG
1	D	164	TRP
1	D	165	ASN
1	A	80	GLN
1	A	165	ASN
1	B	22	ARG
1	B	80	GLN
1	B	165	ASN
1	C	22	ARG
1	C	80	GLN
1	C	165	ASN
1	D	318	ASP
1	C	265	ASP
1	D	22	ARG
1	D	80	GLN
1	A	55	GLN
1	A	264	LYS
1	C	55	GLN
1	C	264	LYS
1	D	55	GLN
1	B	55	GLN
1	A	115	VAL
1	B	115	VAL
1	C	115	VAL
1	D	115	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	261/335 (78%)	216 (83%)	45 (17%)	2	12
1	B	253/335 (76%)	211 (83%)	42 (17%)	3	13
1	C	262/335 (78%)	217 (83%)	45 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	265/335 (79%)	216 (82%)	49 (18%)	2	10
All	All	1041/1340 (78%)	860 (83%)	181 (17%)	2	12

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	24	ARG
1	A	25	THR
1	A	50	MET
1	A	63	ILE
1	A	69	ILE
1	A	81	LYS
1	A	90	ARG
1	A	103	CYS
1	A	104	LEU
1	A	118	THR
1	A	120	LEU
1	A	122	LEU
1	A	126	LEU
1	A	129	THR
1	A	133	THR
1	A	135	THR
1	A	144	LEU
1	A	164	TRP
1	A	166	ASP
1	A	177	THR
1	A	179	THR
1	A	186	LEU
1	A	187	GLN
1	A	193	GLU
1	A	194	ILE
1	A	200	CYS
1	A	208	ILE
1	A	212	ASP
1	A	233	TYR
1	A	243	CYS
1	A	261	VAL
1	A	262	THR
1	A	263	LEU
1	A	264	LYS
1	A	268	PRO

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Mol	Chain	Res	Type
1	A	271	ARG
1	A	273	VAL
1	A	307	LEU
1	A	321	THR
1	A	334	ASN
1	A	339	ILE
1	A	342	VAL
1	A	347	GLU
1	A	348	LEU
1	B	11	TYR
1	B	24	ARG
1	B	25	THR
1	B	50	MET
1	B	63	ILE
1	B	69	ILE
1	B	79	SER
1	B	81	LYS
1	B	90	ARG
1	B	103	CYS
1	B	104	LEU
1	B	118	THR
1	B	120	LEU
1	B	122	LEU
1	B	126	LEU
1	B	129	THR
1	B	133	THR
1	B	135	THR
1	B	144	LEU
1	B	164	TRP
1	B	166	ASP
1	B	177	THR
1	B	179	THR
1	B	193	GLU
1	B	194	ILE
1	B	200	CYS
1	B	208	ILE
1	B	212	ASP
1	B	233	TYR
1	B	243	CYS
1	B	261	VAL
1	B	262	THR
1	B	271	ARG

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	307	LEU
1	B	308	MET
1	B	334	ASN
1	B	339	ILE
1	B	342	VAL
1	B	347	GLU
1	B	348	LEU
1	B	359	ASN
1	C	24	ARG
1	C	25	THR
1	C	50	MET
1	C	63	ILE
1	C	69	ILE
1	C	79	SER
1	C	81	LYS
1	C	87	ARG
1	C	90	ARG
1	C	103	CYS
1	C	104	LEU
1	C	118	THR
1	C	120	LEU
1	C	122	LEU
1	C	126	LEU
1	C	129	THR
1	C	133	THR
1	C	135	THR
1	C	144	LEU
1	C	164	TRP
1	C	166	ASP
1	C	177	THR
1	C	179	THR
1	C	183	ARG
1	C	186	LEU
1	C	193	GLU
1	C	194	ILE
1	C	200	CYS
1	C	208	ILE
1	C	212	ASP
1	C	233	TYR
1	C	243	CYS
1	C	261	VAL

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Mol	Chain	Res	Type
1	C	262	THR
1	C	263	LEU
1	C	264	LYS
1	C	271	ARG
1	C	273	VAL
1	C	307	LEU
1	C	322	THR
1	C	334	ASN
1	C	339	ILE
1	C	342	VAL
1	C	347	GLU
1	C	359	ASN
1	D	11	TYR
1	D	24	ARG
1	D	25	THR
1	D	50	MET
1	D	63	ILE
1	D	69	ILE
1	D	79	SER
1	D	81	LYS
1	D	87	ARG
1	D	90	ARG
1	D	103	CYS
1	D	104	LEU
1	D	118	THR
1	D	120	LEU
1	D	122	LEU
1	D	126	LEU
1	D	129	THR
1	D	133	THR
1	D	135	THR
1	D	144	LEU
1	D	164	TRP
1	D	166	ASP
1	D	177	THR
1	D	179	THR
1	D	193	GLU
1	D	194	ILE
1	D	200	CYS
1	D	208	ILE
1	D	212	ASP
1	D	233	TYR

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Mol	Chain	Res	Type
1	D	243	CYS
1	D	261	VAL
1	D	262	THR
1	D	263	LEU
1	D	264	LYS
1	D	265	ASP
1	D	269	GLU
1	D	271	ARG
1	D	273	VAL
1	D	307	LEU
1	D	318	ASP
1	D	319	HIS
1	D	323	HIS
1	D	324	LEU
1	D	334	ASN
1	D	339	ILE
1	D	342	VAL
1	D	347	GLU
1	D	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	44	HIS
1	A	65	HIS
1	A	74	GLN
1	A	102	ASN
1	A	110	GLN
1	A	116	GLN
1	A	143	GLN
1	A	187	GLN
1	A	237	HIS
1	A	255	HIS
1	A	256	HIS
1	A	323	HIS
1	A	334	ASN
1	A	359	ASN
1	B	39	HIS
1	B	44	HIS
1	B	65	HIS
1	B	74	GLN

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	110	GLN
1	B	116	GLN
1	B	143	GLN
1	B	237	HIS
1	B	255	HIS
1	B	256	HIS
1	B	334	ASN
1	B	359	ASN
1	C	38	HIS
1	C	39	HIS
1	C	44	HIS
1	C	65	HIS
1	C	74	GLN
1	C	102	ASN
1	C	110	GLN
1	C	116	GLN
1	C	143	GLN
1	C	237	HIS
1	C	255	HIS
1	C	256	HIS
1	C	334	ASN
1	C	357	GLN
1	C	359	ASN
1	D	39	HIS
1	D	44	HIS
1	D	65	HIS
1	D	74	GLN
1	D	102	ASN
1	D	110	GLN
1	D	116	GLN
1	D	143	GLN
1	D	255	HIS
1	D	256	HIS
1	D	296	ASN
1	D	319	HIS
1	D	334	ASN
1	D	359	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	C	1360	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	C	1361	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	D	1362	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	D	1363	-	4,4,4	0.13	0	6,6,6	0.17	0

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	SO4	C	1360	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1361	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1362	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1363	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	330/366 (90%)	0.07	7 (2%) 67 52	57, 109, 173, 230	0
1	B	317/366 (86%)	0.18	21 (6%) 22 12	74, 125, 180, 294	0
1	C	327/366 (89%)	0.03	8 (2%) 62 47	50, 109, 175, 223	0
1	D	329/366 (89%)	-0.07	5 (1%) 76 63	61, 113, 177, 256	0
All	All	1303/1464 (89%)	0.05	41 (3%) 52 38	50, 114, 176, 294	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	ASP	5.5
1	A	185	GLY	4.2
1	B	323	HIS	4.2
1	A	281	GLY	4.1
1	B	325	ILE	3.8
1	B	283	PHE	3.7
1	B	263	LEU	3.7
1	D	5	VAL	3.4
1	B	50	MET	3.3
1	A	283	PHE	3.2
1	B	314	VAL	3.2
1	C	266	SER	3.1
1	D	361	GLU	3.0
1	B	313	PRO	2.9
1	D	51	PHE	2.7
1	C	151	GLU	2.7
1	A	279	ASP	2.6
1	B	324	LEU	2.5
1	C	314	VAL	2.5
1	B	180	PRO	2.4
1	C	315	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	312	ILE	2.3
1	B	51	PHE	2.3
1	B	315	GLN	2.2
1	C	56	PHE	2.2
1	B	329	LYS	2.2
1	C	81	LYS	2.2
1	B	133	THR	2.2
1	C	58	PRO	2.1
1	B	54	CYS	2.1
1	B	270	ILE	2.1
1	A	56	PHE	2.1
1	A	317	TRP	2.1
1	C	79	SER	2.1
1	B	56	PHE	2.1
1	B	271	ARG	2.1
1	B	316	GLY	2.1
1	D	32	PRO	2.1
1	A	38	HIS	2.0
1	D	133	THR	2.0
1	B	280	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	1364	1/1	0.76	0.47	4.02	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	1360	5/5	0.72	0.39	1.42	196,208,211,222	0
2	SO4	D	1363	5/5	0.86	0.15	-0.48	134,165,176,202	0
2	SO4	D	1362	5/5	0.94	0.15	-	145,156,164,183	0
2	SO4	C	1361	5/5	0.62	0.68	-	223,235,249,257	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.