



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:20 PM GMT

PDB ID : 1OHG  
Title : STRUCTURE OF THE DSDNA BACTERIOPHAGE HK97 MATURE  
EMPTY CAPSID  
Authors : Helgstrand, C.; Wikoff, W.R.; Duda, R.L.; Hendrix, R.W.; Johnson, J.E.;  
Liljas, L.  
Deposited on : 2003-05-26  
Resolution : 3.45 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 : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

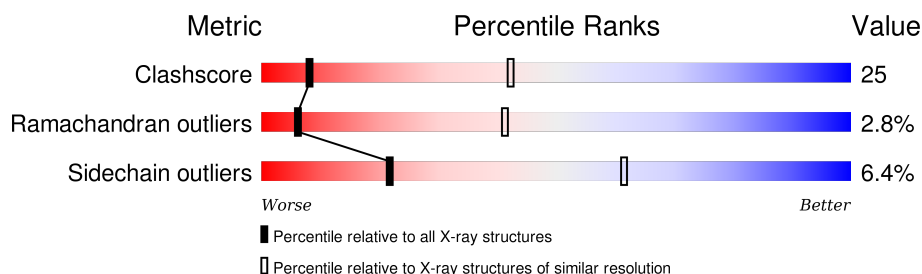
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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))
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	
1	F	282	
1	G	282	

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	A	1384	-	X	-	-

## 2 Entry composition [i](#)

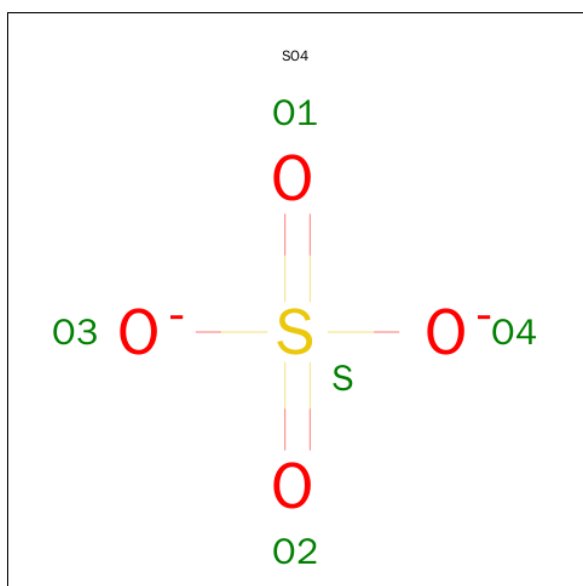
There are 3 unique types of molecules in this entry. The entry contains 15070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAJOR CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	B	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	C	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	D	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	E	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	F	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			
1	G	281	Total	C	N	O	S	0	0	1
			2152	1344	376	422	10			

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

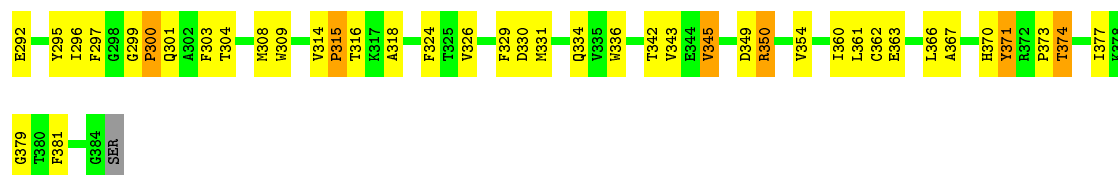


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

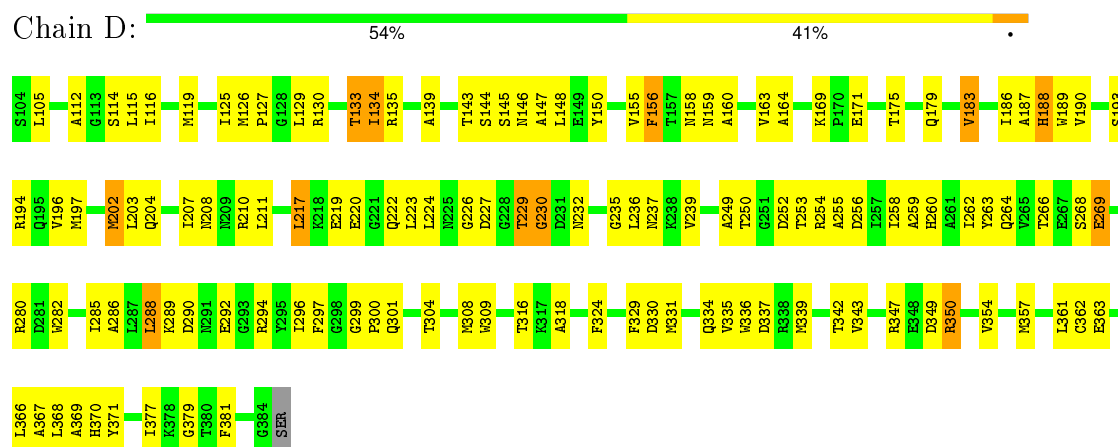
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		

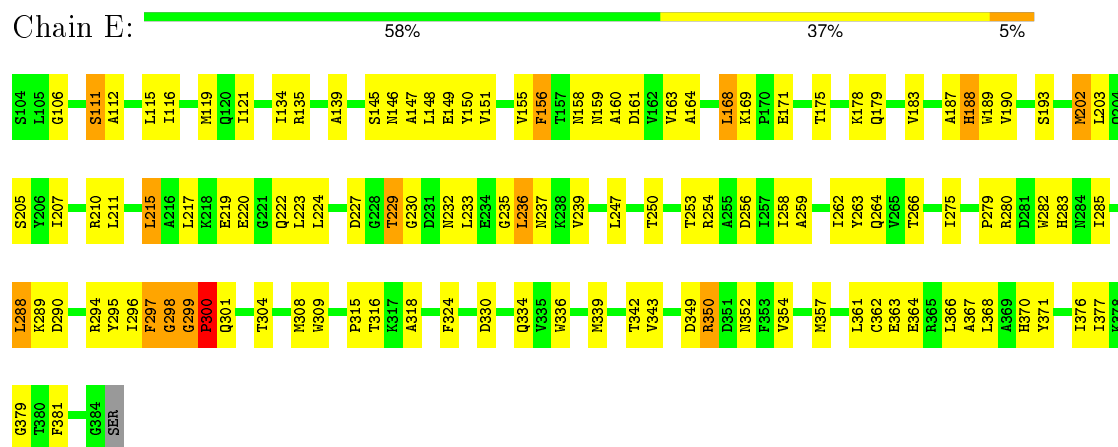




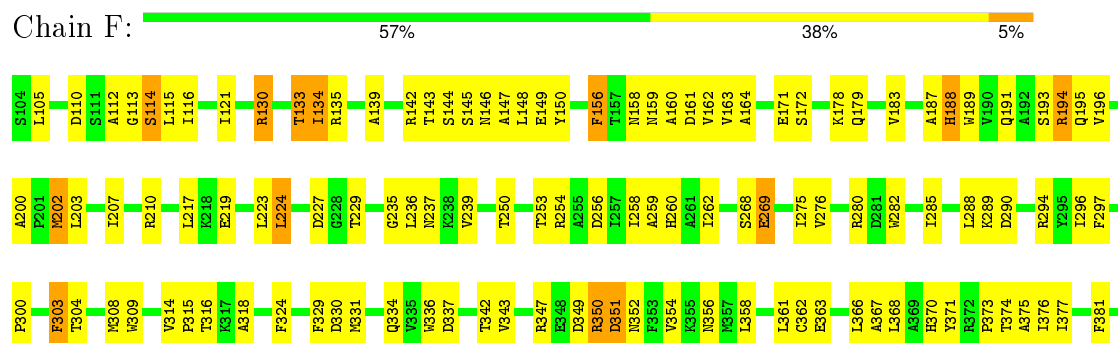
• Molecule 1: MAJOR CAPSID PROTEIN



• Molecule 1: MAJOR CAPSID PROTEIN



• Molecule 1: MAJOR CAPSID PROTEIN



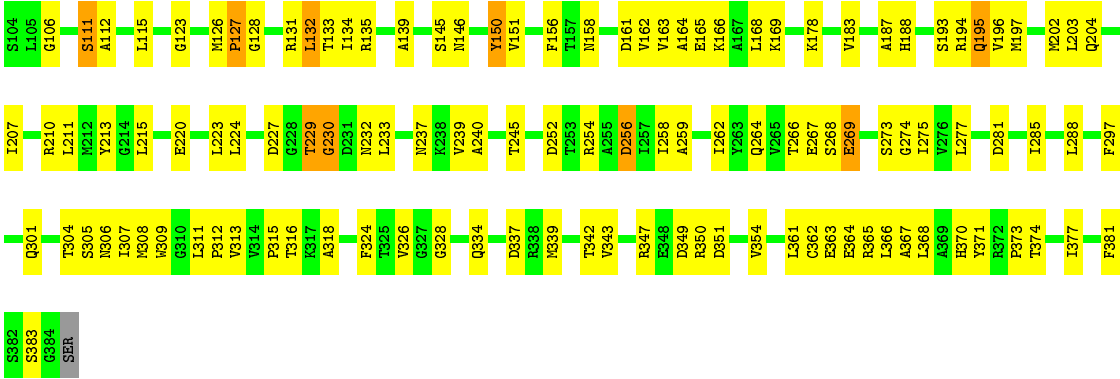
S104  
SER

● Molecule 1: MAJOR CAPSID PROTEIN

Chain G: 

58%

38%





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	579.70 Å 626.65 Å 787.20 Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	190.13 – 3.45	Depositor
% Data completeness (in resolution range)	65.2 (190.13-3.45)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.41 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.373 , 0.374	Depositor
Wilson B-factor (Å <sup>2</sup> )	97.5	Xtriage
Anisotropy	0.326	Xtriage
Estimated twinning fraction	0.003 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 4797606 reflections (0.000%)	Xtriage
Total number of atoms	15070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: SO4, CL

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	0.44	0/2189	0.68	1/2971 (0.0%)
1	B	0.44	0/2189	0.67	0/2971
1	C	0.45	0/2189	0.68	0/2971
1	D	0.48	0/2189	0.67	0/2971
1	E	0.46	0/2189	0.69	2/2971 (0.1%)
1	F	0.44	0/2189	0.68	0/2971
1	G	0.46	0/2189	0.69	1/2971 (0.0%)
All	All	0.45	0/15323	0.68	4/20797 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLY	N-CA-C	5.27	126.28	113.10
1	E	298	GLY	N-CA-C	5.18	126.05	113.10
1	E	299	GLY	C-N-CD	-5.09	109.40	120.60
1	G	132	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2152	0	2119	107	0
1	B	2152	0	2119	119	0
1	C	2152	0	2119	121	0
1	D	2152	0	2119	138	0
1	E	2152	0	2119	118	0
1	F	2152	0	2119	109	0
1	G	2152	0	2119	99	0
2	A	5	0	0	0	0
3	G	1	0	0	0	0
All	All	15070	0	14833	733	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 25.

All (733) 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:B:316:THR:HG22	1:B:318:ALA:H	1.11	1.09
1:D:316:THR:HG22	1:D:318:ALA:H	1.13	1.09
1:E:316:THR:HG22	1:E:318:ALA:H	1.13	1.09
1:C:316:THR:HG22	1:C:318:ALA:H	1.17	1.06
1:G:316:THR:HG22	1:G:318:ALA:H	1.21	1.05
1:A:316:THR:HG22	1:A:318:ALA:H	1.21	1.02
1:E:116:ILE:HG21	1:F:146:ASN:HB2	1.38	1.01
1:F:316:THR:HG22	1:F:318:ALA:H	1.27	0.97
1:G:133:THR:HG22	1:G:135:ARG:H	1.34	0.91
1:D:194:ARG:NH2	1:D:347:ARG:HH22	1.72	0.88
1:E:295:TYR:HB2	1:E:299:GLY:H	1.39	0.87
1:D:188:HIS:HB3	1:E:160:ALA:HA	1.58	0.85
1:E:316:THR:HG22	1:E:318:ALA:N	1.90	0.85
1:A:258:ILE:HG21	1:A:308:MET:HE3	1.59	0.83
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.58	0.83
1:F:193:SER:OG	1:F:196:VAL:HG23	1.78	0.83
1:B:188:HIS:HB3	1:C:160:ALA:HA	1.60	0.82
1:D:316:THR:HG22	1:D:318:ALA:N	1.95	0.81
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.62	0.81
1:G:254:ARG:HB3	1:G:381:PHE:CE2	2.16	0.80
1:E:207:ILE:O	1:E:211:LEU:HD13	1.80	0.80
1:F:297:PHE:HB3	1:F:304:THR:HG21	1.66	0.78
1:E:258:ILE:HD13	1:E:308:MET:HE1	1.64	0.78
1:A:285:ILE:O	1:A:288:LEU:HB2	1.84	0.77
1:A:160:ALA:HA	1:F:188:HIS:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:THR:CG2	1:G:232:ASN:HD22	1.98	0.77
1:D:285:ILE:O	1:D:288:LEU:HB2	1.84	0.77
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.65	0.77
1:C:316:THR:HG22	1:C:318:ALA:N	1.99	0.77
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.20	0.76
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.67	0.76
1:G:254:ARG:HB3	1:G:381:PHE:HE2	1.50	0.76
1:B:258:ILE:HG21	1:B:308:MET:HE3	1.67	0.76
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.67	0.75
1:G:150:TYR:HD2	1:G:150:TYR:H	1.34	0.75
1:G:193:SER:HB3	1:G:196:VAL:HG23	1.69	0.74
1:B:215:LEU:HD21	1:B:364:GLU:HB2	1.70	0.74
1:D:258:ILE:O	1:D:262:ILE:HG13	1.88	0.74
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.69	0.73
1:D:116:ILE:HG21	1:E:146:ASN:CB	2.18	0.73
1:A:316:THR:HG22	1:A:318:ALA:N	2.02	0.73
1:A:297:PHE:HB3	1:A:304:THR:HG21	1.71	0.72
1:F:112:ALA:C	1:F:114:SER:H	1.91	0.72
1:F:258:ILE:O	1:F:262:ILE:HG13	1.89	0.72
1:A:342:THR:HG22	1:A:343:VAL:N	2.04	0.72
1:G:197:MET:HE3	1:G:204:GLN:HB2	1.72	0.72
1:G:339:MET:CE	1:G:363:GLU:HG3	2.20	0.72
1:B:116:ILE:HG21	1:C:146:ASN:HD22	1.55	0.71
1:G:258:ILE:HB	1:G:308:MET:HE1	1.71	0.71
1:C:361:LEU:HD12	1:C:362:CYS:H	1.55	0.71
1:G:195:GLN:H	1:G:195:GLN:HE21	1.39	0.71
1:E:295:TYR:CD1	1:E:300:PRO:HD3	2.26	0.70
1:G:264:GLN:HB3	1:G:377:ILE:HD13	1.73	0.70
1:G:229:THR:HG23	1:G:230:GLY:N	2.06	0.70
1:F:361:LEU:HD12	1:F:362:CYS:H	1.55	0.70
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.74	0.70
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.72	0.70
1:D:297:PHE:HB3	1:D:304:THR:HG21	1.72	0.70
1:B:133:THR:O	1:B:135:ARG:N	2.25	0.70
1:C:244:ASP:OD1	1:C:246:SER:HB3	1.92	0.69
1:B:303:PHE:HE1	1:C:309:TRP:HB3	1.57	0.69
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.74	0.69
1:C:224:LEU:HD13	1:C:237:ASN:ND2	2.07	0.69
1:D:183:VAL:HG23	1:D:366:LEU:O	1.93	0.69
1:A:258:ILE:HD12	1:A:258:ILE:H	1.57	0.68
1:B:239:VAL:HG12	1:B:373:PRO:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:O	1:A:262:ILE:HG13	1.94	0.68
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.75	0.68
1:G:229:THR:HG23	1:G:230:GLY:H	1.59	0.68
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.28	0.68
1:C:258:ILE:O	1:C:262:ILE:HG13	1.94	0.68
1:C:254:ARG:HB3	1:C:381:PHE:CE2	2.29	0.68
1:C:285:ILE:O	1:C:288:LEU:HB2	1.94	0.67
1:E:210:ARG:NH2	1:F:156:PHE:HD2	1.93	0.67
1:C:258:ILE:HG21	1:C:308:MET:HE3	1.77	0.67
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.30	0.67
1:B:316:THR:HG22	1:B:318:ALA:N	1.97	0.67
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.77	0.67
1:D:202:MET:H	1:D:202:MET:HE3	1.59	0.67
1:A:133:THR:O	1:A:135:ARG:N	2.28	0.66
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.29	0.66
1:C:258:ILE:HG21	1:C:308:MET:CE	2.25	0.66
1:B:254:ARG:HB3	1:B:381:PHE:CE2	2.31	0.66
1:C:334:GLN:NE2	1:C:371:TYR:OH	2.28	0.66
1:B:297:PHE:HB3	1:B:304:THR:HG21	1.78	0.65
1:A:258:ILE:HD12	1:A:258:ILE:N	2.10	0.65
1:F:258:ILE:HB	1:F:308:MET:HE1	1.77	0.65
1:E:361:LEU:HD12	1:E:362:CYS:H	1.62	0.65
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.32	0.65
1:E:295:TYR:HB2	1:E:299:GLY:N	2.10	0.65
1:D:258:ILE:HD13	1:D:308:MET:HE1	1.78	0.65
1:G:339:MET:HE1	1:G:363:GLU:HG3	1.78	0.65
1:F:112:ALA:O	1:F:114:SER:N	2.29	0.65
1:D:342:THR:HG22	1:D:343:VAL:N	2.12	0.64
1:G:361:LEU:HD12	1:G:362:CYS:H	1.62	0.64
1:B:258:ILE:HG21	1:B:308:MET:CE	2.28	0.64
1:E:339:MET:HE2	1:E:363:GLU:HG3	1.80	0.64
1:D:219:GLU:HG3	1:D:366:LEU:HD11	1.80	0.64
1:C:193:SER:OG	1:C:196:VAL:HG23	1.97	0.64
1:B:254:ARG:HB3	1:B:381:PHE:HE2	1.60	0.64
1:F:258:ILE:HB	1:F:308:MET:CE	2.27	0.63
1:B:202:MET:HE3	1:B:202:MET:H	1.63	0.63
1:D:207:ILE:O	1:D:211:LEU:HD23	1.98	0.63
1:G:223:LEU:HD22	1:G:368:LEU:HD22	1.80	0.63
1:B:288:LEU:O	1:B:296:ILE:HG12	1.99	0.63
1:E:258:ILE:HG21	1:E:308:MET:CE	2.29	0.63
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:THR:HG23	1:D:232:ASN:HD22	1.64	0.62
1:D:229:THR:HG23	1:D:230:GLY:N	2.13	0.62
1:C:371:TYR:N	1:C:371:TYR:HD1	1.98	0.62
1:G:259:ALA:HB2	1:G:309:TRP:NE1	2.15	0.62
1:F:105:LEU:HD12	1:F:105:LEU:O	2.00	0.62
1:A:187:ALA:HB2	1:A:363:GLU:CB	2.29	0.62
1:E:119:MET:HB3	1:F:148:LEU:HD22	1.81	0.62
1:B:116:ILE:CG2	1:C:146:ASN:HD22	2.13	0.62
1:C:361:LEU:HD12	1:C:362:CYS:N	2.15	0.62
1:D:361:LEU:HD12	1:D:362:CYS:H	1.65	0.62
1:G:131:ARG:HG3	1:G:132:LEU:O	2.00	0.62
1:D:334:GLN:NE2	1:D:371:TYR:OH	2.33	0.61
1:E:258:ILE:O	1:E:262:ILE:HG13	2.00	0.61
1:A:107:SER:HB2	1:C:165:GLU:OE2	2.01	0.61
1:B:361:LEU:HD12	1:B:362:CYS:H	1.64	0.61
1:F:334:GLN:NE2	1:F:371:TYR:OH	2.34	0.61
1:A:135:ARG:NH1	1:A:219:GLU:OE2	2.33	0.61
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.35	0.61
1:C:124:ILE:HD12	1:C:124:ILE:N	2.15	0.61
1:C:342:THR:HG22	1:C:343:VAL:N	2.16	0.61
1:E:134:ILE:CD1	1:E:224:LEU:HB2	2.30	0.61
1:D:256:ASP:O	1:D:259:ALA:HB3	2.01	0.61
1:G:233:LEU:HD11	1:G:366:LEU:CD1	2.31	0.61
1:F:290:ASP:OD2	1:F:294:ARG:HB2	2.01	0.60
1:F:115:LEU:HD23	1:G:151:VAL:HG21	1.83	0.60
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.65	0.60
1:C:297:PHE:HB3	1:C:304:THR:HG21	1.82	0.60
1:D:194:ARG:CZ	1:D:347:ARG:NH2	2.65	0.60
1:A:258:ILE:HG21	1:A:308:MET:CE	2.30	0.60
1:C:371:TYR:CD1	1:C:371:TYR:N	2.68	0.60
1:C:288:LEU:O	1:C:296:ILE:HG12	2.01	0.60
1:E:116:ILE:CG2	1:F:146:ASN:HB2	2.24	0.59
1:G:223:LEU:CD2	1:G:368:LEU:HD22	2.32	0.59
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.37	0.59
1:C:254:ARG:HB3	1:C:381:PHE:HE2	1.66	0.59
1:C:135:ARG:NH2	1:C:219:GLU:OE2	2.36	0.59
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.36	0.59
1:G:183:VAL:HA	1:G:367:ALA:HB2	1.84	0.59
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.31	0.59
1:B:349:ASP:OD1	1:B:350:ARG:HG2	2.03	0.59
1:G:227:ASP:OD1	1:G:229:THR:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:HB2	1:A:309:TRP:NE1	2.18	0.59
1:A:258:ILE:CD1	1:A:258:ILE:H	2.16	0.59
1:B:197:MET:CE	1:B:204:GLN:HB2	2.32	0.59
1:E:264:GLN:HB3	1:E:377:ILE:CD1	2.33	0.58
1:B:349:ASP:O	1:B:350:ARG:HG3	2.03	0.58
1:E:112:ALA:HB1	1:E:115:LEU:HD12	1.84	0.58
1:G:194:ARG:CZ	1:G:347:ARG:NH2	2.66	0.58
1:G:307:ILE:HA	1:G:311:LEU:O	2.03	0.58
1:E:354:VAL:O	1:E:354:VAL:HG12	2.04	0.58
1:D:258:ILE:HG21	1:D:308:MET:CE	2.33	0.58
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.86	0.58
1:D:259:ALA:HB2	1:D:309:TRP:NE1	2.18	0.58
1:F:239:VAL:HG12	1:F:373:PRO:HB3	1.86	0.58
1:G:239:VAL:HG12	1:G:373:PRO:HB3	1.86	0.58
1:C:354:VAL:O	1:C:354:VAL:HG12	2.04	0.58
1:G:193:SER:HB3	1:G:196:VAL:CG2	2.33	0.58
1:G:354:VAL:O	1:G:354:VAL:HG12	2.03	0.58
1:G:112:ALA:HB1	1:G:115:LEU:HD12	1.85	0.58
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.39	0.58
1:A:354:VAL:O	1:A:354:VAL:HG12	2.03	0.58
1:A:342:THR:HG22	1:A:343:VAL:H	1.66	0.57
1:G:339:MET:HB3	1:G:365:ARG:HG2	1.84	0.57
1:F:156:PHE:CD1	1:F:156:PHE:C	2.77	0.57
1:B:135:ARG:NH1	1:B:219:GLU:OE2	2.38	0.57
1:B:285:ILE:O	1:B:288:LEU:HB2	2.04	0.57
1:F:200:ALA:HB1	1:F:202:MET:HE1	1.87	0.57
1:G:229:THR:HG22	1:G:232:ASN:HD22	1.69	0.57
1:F:259:ALA:HB2	1:F:309:TRP:NE1	2.19	0.57
1:E:223:LEU:O	1:E:236:LEU:HD22	2.05	0.57
1:E:187:ALA:HB2	1:E:363:GLU:CB	2.35	0.57
1:D:349:ASP:O	1:D:350:ARG:C	2.42	0.57
1:B:292:GLU:HA	1:B:292:GLU:OE2	2.05	0.57
1:B:334:GLN:NE2	1:B:371:TYR:OH	2.38	0.57
1:F:194:ARG:NH2	1:F:347:ARG:HH21	2.03	0.57
1:A:200:ALA:C	1:A:202:MET:HE3	2.25	0.57
1:F:147:ALA:HA	1:F:183:VAL:HG23	1.87	0.56
1:A:254:ARG:HB3	1:A:381:PHE:HE2	1.69	0.56
1:A:334:GLN:NE2	1:A:371:TYR:OH	2.38	0.56
1:B:303:PHE:CE1	1:C:309:TRP:HB3	2.38	0.56
1:F:223:LEU:HD23	1:F:368:LEU:HD22	1.88	0.56
1:F:254:ARG:HB3	1:F:381:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ALA:HB2	1:C:309:TRP:NE1	2.19	0.56
1:D:197:MET:CE	1:D:204:GLN:HB2	2.35	0.56
1:B:256:ASP:O	1:B:259:ALA:HB3	2.05	0.56
1:B:342:THR:HG22	1:B:343:VAL:N	2.19	0.56
1:C:244:ASP:HB2	1:C:264:GLN:HE22	1.71	0.56
1:E:339:MET:CE	1:E:363:GLU:HG3	2.36	0.56
1:C:156:PHE:CE1	1:C:158:ASN:HB2	2.41	0.56
1:F:156:PHE:HD1	1:F:156:PHE:C	2.08	0.56
1:A:168:LEU:HD22	1:A:169:LYS:O	2.05	0.56
1:A:295:TYR:HB2	1:A:299:GLY:H	1.70	0.56
1:A:288:LEU:O	1:A:296:ILE:HG12	2.05	0.56
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.20	0.56
1:D:183:VAL:HB	1:D:367:ALA:HB2	1.87	0.56
1:G:168:LEU:HD12	1:G:169:LYS:N	2.20	0.56
1:B:163:VAL:HG12	1:B:164:ALA:O	2.04	0.56
1:D:227:ASP:OD1	1:D:229:THR:HB	2.05	0.56
1:B:134:ILE:HD13	1:B:224:LEU:HB2	1.87	0.56
1:D:342:THR:HG22	1:D:343:VAL:H	1.70	0.56
1:G:361:LEU:HD12	1:G:362:CYS:N	2.20	0.56
1:E:227:ASP:OD1	1:E:229:THR:HB	2.05	0.56
1:B:354:VAL:O	1:B:354:VAL:HG12	2.06	0.56
1:D:194:ARG:CZ	1:D:347:ARG:HH22	2.19	0.56
1:A:339:MET:CE	1:A:363:GLU:HG3	2.35	0.56
1:E:224:LEU:HG	1:E:237:ASN:ND2	2.21	0.56
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.50	0.55
1:C:150:TYR:CE1	1:C:179:GLN:HB2	2.40	0.55
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.72	0.55
1:C:349:ASP:O	1:C:350:ARG:C	2.44	0.55
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.19	0.55
1:G:316:THR:HG22	1:G:318:ALA:N	2.06	0.55
1:F:361:LEU:HD12	1:F:362:CYS:N	2.22	0.55
1:G:258:ILE:HG21	1:G:275:ILE:HD13	1.89	0.55
1:A:256:ASP:O	1:A:259:ALA:HB3	2.06	0.55
1:G:165:GLU:O	1:G:166:LYS:HB2	2.06	0.55
1:A:324:PHE:HB3	1:A:381:PHE:HE1	1.71	0.55
1:E:342:THR:HG22	1:E:343:VAL:N	2.22	0.55
1:C:256:ASP:O	1:C:259:ALA:HB3	2.06	0.55
1:F:276:VAL:HA	1:F:314:VAL:HG23	1.89	0.55
1:G:139:ALA:HB3	1:G:334:GLN:HB3	1.88	0.55
1:B:258:ILE:HG21	1:B:275:ILE:HD13	1.89	0.55
1:C:133:THR:O	1:C:134:ILE:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD13	1:B:237:ASN:ND2	2.21	0.55
1:A:193:SER:HB3	1:A:196:VAL:CG2	2.36	0.55
1:F:143:THR:OG1	1:F:144:SER:N	2.40	0.55
1:E:259:ALA:HB2	1:E:309:TRP:NE1	2.22	0.55
1:B:289:LYS:HZ1	1:C:253:THR:HG23	1.72	0.55
1:C:299:GLY:O	1:C:301:GLN:N	2.39	0.55
1:E:156:PHE:C	1:E:156:PHE:CD2	2.79	0.55
1:G:227:ASP:HB3	1:G:229:THR:HG22	1.88	0.54
1:A:239:VAL:HG21	1:A:370:HIS:CG	2.41	0.54
1:D:292:GLU:HA	1:D:292:GLU:OE1	2.06	0.54
1:A:134:ILE:HD13	1:A:224:LEU:HB2	1.89	0.54
1:A:223:LEU:HD23	1:A:368:LEU:HD22	1.90	0.54
1:G:127:PRO:HB2	1:G:210:ARG:HH12	1.72	0.54
1:C:224:LEU:HD13	1:C:237:ASN:HD21	1.72	0.54
1:D:135:ARG:NH1	1:D:219:GLU:OE2	2.40	0.54
1:F:376:ILE:O	1:F:377:ILE:HD13	2.07	0.54
1:G:264:GLN:HB3	1:G:377:ILE:CD1	2.38	0.54
1:G:366:LEU:HD12	1:G:366:LEU:C	2.27	0.54
1:F:324:PHE:HD2	1:F:381:PHE:CE1	2.26	0.54
1:C:187:ALA:HB2	1:C:363:GLU:CB	2.38	0.54
1:D:188:HIS:ND1	1:E:160:ALA:HB2	2.23	0.54
1:D:229:THR:HG23	1:D:230:GLY:H	1.71	0.54
1:C:156:PHE:HD1	1:C:156:PHE:C	2.11	0.54
1:D:329:PHE:O	1:D:331:MET:N	2.40	0.54
1:F:183:VAL:HG13	1:F:366:LEU:O	2.08	0.54
1:B:263:TYR:O	1:B:266:THR:N	2.40	0.54
1:F:135:ARG:NH1	1:F:219:GLU:OE2	2.41	0.54
1:G:197:MET:HE1	1:G:204:GLN:HG3	1.90	0.54
1:E:163:VAL:HG12	1:E:164:ALA:O	2.07	0.54
1:E:334:GLN:NE2	1:E:371:TYR:OH	2.40	0.54
1:C:197:MET:CE	1:C:204:GLN:HB2	2.38	0.54
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.23	0.54
1:A:226:GLY:HA3	1:A:235:GLY:H	1.72	0.54
1:C:156:PHE:CD1	1:C:156:PHE:C	2.81	0.53
1:F:189:TRP:HZ3	1:F:191:GLN:HG2	1.73	0.53
1:E:299:GLY:O	1:E:301:GLN:N	2.41	0.53
1:D:229:THR:CG2	1:D:232:ASN:ND2	2.71	0.53
1:A:155:VAL:H	1:A:175:THR:HB	1.74	0.53
1:B:258:ILE:O	1:B:262:ILE:HG13	2.07	0.53
1:F:227:ASP:CG	1:F:229:THR:HG22	2.29	0.53
1:G:305:SER:OG	1:G:306:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:TRP:CZ2	1:F:171:GLU:HB2	2.43	0.53
1:G:252:ASP:HB2	1:G:256:ASP:CG	2.29	0.53
1:D:155:VAL:H	1:D:175:THR:HB	1.74	0.53
1:A:342:THR:CG2	1:A:343:VAL:N	2.71	0.53
1:D:187:ALA:HB2	1:D:363:GLU:HA	1.91	0.53
1:F:145:SER:O	1:F:183:VAL:HG21	2.08	0.53
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.23	0.53
1:B:143:THR:OG1	1:B:144:SER:N	2.42	0.53
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.43	0.53
1:B:197:MET:HE3	1:B:204:GLN:HB2	1.91	0.53
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.23	0.53
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.23	0.53
1:A:226:GLY:HA3	1:A:235:GLY:N	2.24	0.53
1:D:290:ASP:OD2	1:D:294:ARG:HB2	2.09	0.53
1:C:188:HIS:HB3	1:D:160:ALA:CA	2.36	0.52
1:F:256:ASP:O	1:F:259:ALA:HB3	2.08	0.52
1:C:183:VAL:HG13	1:C:366:LEU:O	2.09	0.52
1:E:361:LEU:HD12	1:E:362:CYS:N	2.23	0.52
1:E:106:GLY:O	1:E:111:SER:HB3	2.09	0.52
1:G:215:LEU:HD21	1:G:364:GLU:HB3	1.90	0.52
1:G:324:PHE:HB3	1:G:381:PHE:HE1	1.73	0.52
1:G:163:VAL:HG12	1:G:164:ALA:O	2.09	0.52
1:D:354:VAL:O	1:D:354:VAL:HG12	2.09	0.52
1:C:133:THR:O	1:C:136:ASP:N	2.43	0.52
1:D:112:ALA:HB1	1:D:115:LEU:HD12	1.90	0.52
1:E:254:ARG:HB3	1:E:381:PHE:CE2	2.45	0.52
1:D:119:MET:HB3	1:E:148:LEU:CD2	2.39	0.52
1:E:258:ILE:HG21	1:E:308:MET:HE1	1.90	0.52
1:G:258:ILE:CB	1:G:308:MET:HE1	2.37	0.52
1:A:187:ALA:CB	1:A:363:GLU:HB3	2.39	0.52
1:D:361:LEU:HD12	1:D:362:CYS:N	2.25	0.52
1:D:339:MET:CE	1:D:363:GLU:HG3	2.40	0.52
1:A:361:LEU:HD12	1:A:362:CYS:H	1.73	0.52
1:C:263:TYR:O	1:C:266:THR:N	2.40	0.52
1:G:197:MET:CE	1:G:204:GLN:HB2	2.39	0.52
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.90	0.52
1:C:297:PHE:HB3	1:C:304:THR:CG2	2.39	0.52
1:E:193:SER:HA	1:E:357:MET:SD	2.50	0.52
1:D:207:ILE:O	1:D:211:LEU:CD2	2.57	0.52
1:F:258:ILE:HD12	1:F:308:MET:HE1	1.92	0.52
1:D:135:ARG:NH2	1:D:337:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:MET:HB3	1:C:148:LEU:CD2	2.40	0.52
1:A:119:MET:HB3	1:B:148:LEU:CD2	2.40	0.52
1:E:295:TYR:HD1	1:E:300:PRO:HD3	1.72	0.51
1:C:239:VAL:HG12	1:C:373:PRO:HB3	1.92	0.51
1:D:197:MET:HE1	1:D:204:GLN:HB2	1.92	0.51
1:G:194:ARG:CZ	1:G:347:ARG:HH21	2.23	0.51
1:A:260:HIS:O	1:A:263:TYR:HB3	2.10	0.51
1:D:289:LYS:NZ	1:E:253:THR:HG23	2.25	0.51
1:F:200:ALA:HB1	1:F:202:MET:CE	2.39	0.51
1:C:268:SER:O	1:C:269:GLU:HB2	2.09	0.51
1:B:371:TYR:CD1	1:B:371:TYR:N	2.77	0.51
1:E:290:ASP:OD2	1:E:294:ARG:HB2	2.11	0.51
1:D:263:TYR:O	1:D:266:THR:N	2.39	0.51
1:G:150:TYR:N	1:G:150:TYR:CD2	2.79	0.51
1:E:134:ILE:HD12	1:E:224:LEU:HB2	1.93	0.51
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.26	0.51
1:A:112:ALA:HB1	1:A:115:LEU:HD12	1.92	0.51
1:A:125:ILE:HG22	1:A:125:ILE:O	2.09	0.51
1:C:303:PHE:HE1	1:D:309:TRP:HB3	1.76	0.51
1:E:139:ALA:O	1:E:334:GLN:HG3	2.11	0.51
1:G:313:VAL:O	1:G:315:PRO:HD3	2.11	0.51
1:F:187:ALA:HB2	1:F:363:GLU:CB	2.41	0.51
1:F:133:THR:O	1:F:134:ILE:C	2.49	0.51
1:D:253:THR:HB	1:D:288:LEU:HD11	1.92	0.51
1:A:297:PHE:HB3	1:A:304:THR:CG2	2.39	0.51
1:C:258:ILE:N	1:C:258:ILE:HD12	2.25	0.51
1:F:105:LEU:HD12	1:F:105:LEU:C	2.31	0.51
1:A:187:ALA:HB2	1:A:363:GLU:HB3	1.92	0.51
1:B:187:ALA:HB2	1:B:363:GLU:HA	1.92	0.51
1:A:272:ALA:HB3	1:A:311:LEU:HD11	1.93	0.51
1:G:258:ILE:HD12	1:G:308:MET:HE1	1.94	0.50
1:F:135:ARG:NH2	1:F:337:ASP:OD1	2.44	0.50
1:F:349:ASP:C	1:F:350:ARG:HG3	2.31	0.50
1:E:190:VAL:HG22	1:F:172:SER:O	2.11	0.50
1:B:295:TYR:HD1	1:B:300:PRO:HD3	1.76	0.50
1:D:219:GLU:HG3	1:D:366:LEU:CD1	2.41	0.50
1:A:197:MET:HE3	1:A:204:GLN:HB2	1.92	0.50
1:E:236:LEU:HD13	1:E:370:HIS:HE1	1.76	0.50
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.41	0.50
1:D:156:PHE:C	1:D:156:PHE:CD2	2.83	0.50
1:A:156:PHE:CD1	1:A:156:PHE:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:HG12	1:A:308:MET:HE1	1.94	0.50
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.77	0.50
1:E:285:ILE:O	1:E:288:LEU:HB2	2.12	0.50
1:E:145:SER:OG	1:E:146:ASN:N	2.44	0.50
1:C:303:PHE:CE1	1:D:309:TRP:HB3	2.46	0.50
1:F:163:VAL:HG12	1:F:164:ALA:O	2.11	0.50
1:C:275:ILE:HG23	1:C:326:VAL:HG22	1.92	0.50
1:D:202:MET:H	1:D:202:MET:CE	2.22	0.50
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.45	0.50
1:E:324:PHE:HD2	1:E:381:PHE:CE1	2.29	0.50
1:D:260:HIS:O	1:D:263:TYR:HB3	2.12	0.50
1:F:297:PHE:HB3	1:F:304:THR:CG2	2.40	0.50
1:F:235:GLY:O	1:F:236:LEU:C	2.48	0.50
1:C:244:ASP:CG	1:C:246:SER:HB3	2.32	0.49
1:F:288:LEU:O	1:F:296:ILE:HG12	2.12	0.49
1:A:258:ILE:CG2	1:A:275:ILE:HD13	2.42	0.49
1:B:289:LYS:NZ	1:C:253:THR:HG23	2.26	0.49
1:A:156:PHE:CE1	1:A:158:ASN:HB2	2.47	0.49
1:G:268:SER:O	1:G:269:GLU:HB2	2.12	0.49
1:E:297:PHE:CB	1:E:304:THR:HG21	2.42	0.49
1:A:339:MET:HE3	1:A:363:GLU:HG3	1.93	0.49
1:F:316:THR:HG22	1:F:318:ALA:N	2.11	0.49
1:F:297:PHE:CB	1:F:304:THR:HG21	2.40	0.49
1:C:133:THR:O	1:C:135:ARG:N	2.46	0.49
1:G:128:GLY:HA2	1:G:213:TYR:CZ	2.48	0.49
1:A:263:TYR:O	1:A:266:THR:N	2.35	0.49
1:A:163:VAL:HG12	1:A:164:ALA:O	2.12	0.49
1:C:145:SER:OG	1:C:146:ASN:N	2.45	0.49
1:C:258:ILE:HD11	1:C:381:PHE:CZ	2.48	0.49
1:D:119:MET:HB3	1:E:148:LEU:HD22	1.94	0.49
1:B:297:PHE:HB3	1:B:304:THR:CG2	2.42	0.49
1:D:187:ALA:HB2	1:D:363:GLU:CB	2.42	0.49
1:G:224:LEU:HG	1:G:237:ASN:ND2	2.27	0.49
1:F:112:ALA:C	1:F:114:SER:N	2.62	0.48
1:A:193:SER:CB	1:A:196:VAL:HG23	2.43	0.48
1:D:146:ASN:C	1:D:183:VAL:HG12	2.33	0.48
1:B:295:TYR:OH	1:C:256:ASP:OD1	2.31	0.48
1:G:161:ASP:CG	1:G:162:VAL:H	2.15	0.48
1:D:299:GLY:O	1:D:301:GLN:N	2.46	0.48
1:B:219:GLU:HG3	1:B:366:LEU:HD11	1.94	0.48
1:D:125:ILE:HD13	1:E:371:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:THR:OG1	1:B:255:ALA:HB3	2.13	0.48
1:B:210:ARG:NH2	1:C:156:PHE:HD2	2.11	0.48
1:E:349:ASP:O	1:E:352:ASN:HB2	2.13	0.48
1:D:133:THR:O	1:D:134:ILE:C	2.51	0.48
1:F:276:VAL:HG22	1:F:314:VAL:CG2	2.44	0.48
1:A:156:PHE:HD1	1:A:156:PHE:C	2.17	0.48
1:G:342:THR:HG22	1:G:343:VAL:N	2.28	0.48
1:F:224:LEU:HD22	1:F:237:ASN:ND2	2.28	0.48
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.29	0.48
1:E:224:LEU:HG	1:E:237:ASN:HD22	1.79	0.48
1:D:193:SER:OG	1:D:196:VAL:HG23	2.13	0.48
1:D:297:PHE:CB	1:D:304:THR:HG21	2.41	0.48
1:F:347:ARG:HH11	1:F:347:ARG:HG3	1.77	0.48
1:C:268:SER:HB2	1:C:374:THR:HB	1.96	0.48
1:C:163:VAL:HG12	1:C:164:ALA:O	2.14	0.48
1:B:193:SER:HB3	1:B:196:VAL:HG23	1.96	0.48
1:E:202:MET:N	1:E:202:MET:SD	2.86	0.48
1:G:133:THR:C	1:G:135:ARG:N	2.65	0.48
1:F:148:LEU:HD12	1:F:336:TRP:CD1	2.49	0.48
1:D:258:ILE:HG21	1:D:308:MET:HE1	1.95	0.47
1:A:371:TYR:CD2	1:A:371:TYR:N	2.81	0.47
1:B:369:ALA:HB1	1:B:371:TYR:HE1	1.79	0.47
1:D:339:MET:HE1	1:D:363:GLU:HG3	1.96	0.47
1:D:223:LEU:HD23	1:D:368:LEU:HD22	1.96	0.47
1:B:316:THR:HG22	1:B:317:LYS:N	2.29	0.47
1:D:190:VAL:CG2	1:D:211:LEU:HD11	2.44	0.47
1:E:258:ILE:HG21	1:E:308:MET:HE3	1.95	0.47
1:E:258:ILE:CD1	1:E:308:MET:HE1	2.40	0.47
1:D:324:PHE:HB3	1:D:381:PHE:HE1	1.79	0.47
1:B:275:ILE:HD13	1:B:308:MET:HE3	1.96	0.47
1:C:324:PHE:HD2	1:C:381:PHE:CE1	2.32	0.47
1:B:239:VAL:HG21	1:B:370:HIS:CG	2.49	0.47
1:F:187:ALA:HB2	1:F:363:GLU:HB3	1.96	0.47
1:A:282:TRP:HA	1:A:282:TRP:HE3	1.80	0.47
1:A:258:ILE:CD1	1:A:258:ILE:N	2.76	0.47
1:C:188:HIS:CG	1:D:160:ALA:HB2	2.48	0.47
1:A:342:THR:CG2	1:A:343:VAL:H	2.27	0.47
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.79	0.47
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.45	0.47
1:B:187:ALA:HB2	1:B:363:GLU:CB	2.45	0.47
1:G:123:GLY:H	1:G:202:MET:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:O	1:B:207:ILE:HG13	2.14	0.47
1:E:295:TYR:CB	1:E:299:GLY:H	2.18	0.47
1:E:135:ARG:NH1	1:E:219:GLU:OE2	2.48	0.47
1:B:197:MET:HE1	1:B:204:GLN:HB2	1.96	0.47
1:D:163:VAL:HG12	1:D:164:ALA:O	2.15	0.47
1:F:354:VAL:O	1:F:354:VAL:HG12	2.12	0.47
1:E:211:LEU:HD12	1:E:211:LEU:N	2.29	0.47
1:D:268:SER:O	1:D:269:GLU:HB2	2.15	0.47
1:E:210:ARG:HH21	1:F:156:PHE:HD2	1.63	0.47
1:D:139:ALA:O	1:D:334:GLN:HG3	2.14	0.47
1:G:347:ARG:HB3	1:G:347:ARG:CZ	2.45	0.47
1:G:135:ARG:NH2	1:G:337:ASP:OD1	2.47	0.46
1:D:282:TRP:HE3	1:D:282:TRP:HA	1.81	0.46
1:D:188:HIS:NE2	1:D:211:LEU:HD12	2.30	0.46
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.31	0.46
1:E:236:LEU:HD12	1:E:376:ILE:HD13	1.97	0.46
1:B:150:TYR:CE1	1:B:179:GLN:HB2	2.51	0.46
1:G:134:ILE:CD1	1:G:224:LEU:HB2	2.44	0.46
1:D:371:TYR:CD2	1:D:371:TYR:N	2.83	0.46
1:A:282:TRP:HA	1:A:282:TRP:CE3	2.50	0.46
1:E:146:ASN:O	1:E:183:VAL:HG23	2.16	0.46
1:F:373:PRO:C	1:F:375:ALA:H	2.19	0.46
1:G:139:ALA:O	1:G:334:GLN:HB2	2.16	0.46
1:A:280:ARG:CZ	1:B:247:LEU:HD21	2.46	0.46
1:E:159:ASN:O	1:E:160:ALA:C	2.54	0.46
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.80	0.46
1:C:189:TRP:HB3	1:C:361:LEU:HD13	1.98	0.46
1:E:235:GLY:O	1:E:236:LEU:C	2.54	0.46
1:D:335:VAL:HG22	1:D:368:LEU:HD13	1.97	0.46
1:E:155:VAL:H	1:E:175:THR:HB	1.79	0.46
1:F:161:ASP:CG	1:F:162:VAL:H	2.18	0.46
1:B:258:ILE:HD12	1:B:258:ILE:N	2.31	0.46
1:E:297:PHE:HB3	1:E:304:THR:HG21	1.98	0.46
1:D:148:LEU:HD11	1:D:336:TRP:CG	2.49	0.46
1:F:156:PHE:CE1	1:F:158:ASN:HB2	2.50	0.46
1:A:150:TYR:HB3	1:F:121:ILE:HD12	1.98	0.46
1:F:282:TRP:CE3	1:F:282:TRP:HA	2.51	0.46
1:C:168:LEU:HD22	1:C:169:LYS:O	2.16	0.46
1:E:263:TYR:O	1:E:266:THR:N	2.46	0.46
1:E:149:GLU:CD	1:E:178:LYS:HE2	2.36	0.46
1:B:183:VAL:HG13	1:B:366:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASN:O	1:D:147:ALA:HB2	2.16	0.46
1:E:227:ASP:CG	1:E:229:THR:HB	2.36	0.46
1:D:189:TRP:HD1	1:E:169:LYS:HB3	1.81	0.46
1:E:116:ILE:HG21	1:F:146:ASN:CB	2.28	0.46
1:E:156:PHE:C	1:E:156:PHE:HD2	2.20	0.46
1:F:142:ARG:NH1	1:F:142:ARG:HB3	2.31	0.46
1:B:361:LEU:HD12	1:B:362:CYS:N	2.30	0.45
1:F:329:PHE:O	1:F:331:MET:N	2.49	0.45
1:B:235:GLY:O	1:B:236:LEU:C	2.53	0.45
1:D:156:PHE:CE2	1:D:158:ASN:HB2	2.51	0.45
1:C:292:GLU:HA	1:C:292:GLU:OE2	2.15	0.45
1:F:159:ASN:O	1:F:160:ALA:C	2.54	0.45
1:C:125:ILE:HD13	1:D:371:TYR:HB3	1.98	0.45
1:B:260:HIS:O	1:B:263:TYR:HB3	2.16	0.45
1:D:280:ARG:CZ	1:E:247:LEU:HD21	2.46	0.45
1:A:188:HIS:CG	1:B:160:ALA:HB2	2.52	0.45
1:B:329:PHE:O	1:B:331:MET:N	2.49	0.45
1:A:148:LEU:CD1	1:A:336:TRP:CG	2.99	0.45
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.98	0.45
1:E:336:TRP:HB2	1:E:367:ALA:HB3	1.98	0.45
1:E:215:LEU:HD21	1:E:364:GLU:HB3	1.99	0.45
1:E:156:PHE:CE2	1:E:158:ASN:HB2	2.51	0.45
1:D:282:TRP:CE3	1:D:282:TRP:HA	2.51	0.45
1:D:189:TRP:CZ2	1:E:171:GLU:HB2	2.51	0.45
1:C:121:ILE:HA	1:C:122:PRO:HD3	1.80	0.45
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.82	0.45
1:G:187:ALA:HB2	1:G:363:GLU:CB	2.46	0.45
1:D:229:THR:CG2	1:D:230:GLY:H	2.28	0.45
1:F:336:TRP:HB2	1:F:367:ALA:HB3	1.98	0.45
1:A:295:TYR:HB2	1:A:299:GLY:N	2.32	0.45
1:F:314:VAL:O	1:F:314:VAL:HG23	2.17	0.45
1:G:266:THR:C	1:G:268:SER:H	2.20	0.45
1:D:193:SER:HA	1:D:357:MET:SD	2.57	0.45
1:A:188:HIS:CE1	1:B:160:ALA:HB2	2.52	0.45
1:B:132:LEU:HD22	1:B:220:GLU:HG3	1.99	0.45
1:F:196:VAL:HG12	1:F:203:LEU:HD22	1.98	0.45
1:A:135:ARG:NH2	1:A:337:ASP:OD1	2.46	0.45
1:G:339:MET:HE3	1:G:363:GLU:HG3	1.99	0.45
1:C:235:GLY:O	1:C:236:LEU:C	2.55	0.45
1:E:334:GLN:O	1:E:368:LEU:HD12	2.17	0.45
1:D:163:VAL:HG21	1:D:169:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:HD3	1:B:316:THR:O	2.15	0.45
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.98	0.45
1:B:148:LEU:HD11	1:B:336:TRP:CG	2.51	0.45
1:C:148:LEU:HD12	1:C:336:TRP:CD1	2.52	0.45
1:D:143:THR:OG1	1:D:144:SER:N	2.49	0.45
1:F:145:SER:OG	1:F:146:ASN:N	2.50	0.44
1:D:288:LEU:O	1:D:296:ILE:HG12	2.18	0.44
1:A:258:ILE:HD11	1:A:381:PHE:CZ	2.52	0.44
1:B:189:TRP:HB3	1:B:361:LEU:HD13	2.00	0.44
1:F:139:ALA:O	1:F:334:GLN:HG3	2.17	0.44
1:E:134:ILE:HD13	1:E:224:LEU:HB2	1.97	0.44
1:C:161:ASP:CG	1:C:162:VAL:H	2.21	0.44
1:D:239:VAL:HG21	1:D:370:HIS:CG	2.52	0.44
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.84	0.44
1:B:156:PHE:C	1:B:156:PHE:CD2	2.88	0.44
1:F:193:SER:HG	1:F:196:VAL:HG23	1.78	0.44
1:E:324:PHE:CZ	1:E:379:GLY:HA3	2.52	0.44
1:A:361:LEU:HD12	1:A:362:CYS:N	2.32	0.44
1:E:350:ARG:O	1:E:352:ASN:N	2.49	0.44
1:B:299:GLY:O	1:B:301:GLN:N	2.50	0.44
1:A:300:PRO:HG2	1:B:296:ILE:HG22	2.00	0.44
1:F:347:ARG:HD2	1:F:358:LEU:HD11	2.00	0.44
1:C:189:TRP:CZ2	1:D:171:GLU:HB2	2.53	0.44
1:D:133:THR:O	1:D:135:ARG:N	2.51	0.44
1:D:146:ASN:HA	1:D:183:VAL:CG1	2.48	0.44
1:E:134:ILE:HD13	1:E:224:LEU:HD13	1.99	0.44
1:D:197:MET:HE3	1:D:204:GLN:HB2	2.00	0.44
1:E:168:LEU:HD22	1:E:169:LYS:O	2.17	0.44
1:B:329:PHE:C	1:B:331:MET:H	2.21	0.44
1:A:107:SER:HB2	1:C:165:GLU:CD	2.38	0.44
1:C:197:MET:HE3	1:C:204:GLN:HB2	1.99	0.44
1:D:289:LYS:HZ1	1:E:253:THR:HG23	1.83	0.44
1:A:146:ASN:O	1:A:147:ALA:HB2	2.18	0.44
1:F:149:GLU:CD	1:F:178:LYS:HE2	2.38	0.44
1:F:282:TRP:HA	1:F:282:TRP:HE3	1.81	0.44
1:C:345:VAL:HG13	1:C:360:ILE:HG12	1.98	0.44
1:E:239:VAL:HG21	1:E:370:HIS:CG	2.53	0.43
1:G:123:GLY:H	1:G:202:MET:CE	2.29	0.43
1:D:146:ASN:HA	1:D:183:VAL:HG11	1.99	0.43
1:D:208:ASN:OD1	1:D:343:VAL:HG11	2.19	0.43
1:F:376:ILE:C	1:F:377:ILE:HD13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASN:O	1:C:160:ALA:C	2.55	0.43
1:F:114:SER:HB3	1:G:178:LYS:HB2	2.00	0.43
1:D:229:THR:HG23	1:D:232:ASN:ND2	2.31	0.43
1:E:134:ILE:HD11	1:E:224:LEU:HD22	2.00	0.43
1:G:233:LEU:HD11	1:G:366:LEU:HD11	1.99	0.43
1:B:283:HIS:NE2	1:C:260:HIS:HA	2.34	0.43
1:A:254:ARG:HB3	1:A:381:PHE:CE2	2.50	0.43
1:G:275:ILE:HG12	1:G:326:VAL:HG22	2.01	0.43
1:D:369:ALA:HB1	1:D:371:TYR:HE2	1.83	0.43
1:F:350:ARG:HB2	1:F:351:ASP:H	1.52	0.43
1:E:288:LEU:O	1:E:296:ILE:HG12	2.19	0.43
1:G:349:ASP:O	1:G:350:ARG:C	2.56	0.43
1:G:133:THR:HG22	1:G:134:ILE:N	2.32	0.43
1:D:159:ASN:O	1:D:160:ALA:C	2.56	0.43
1:C:208:ASN:OD1	1:C:343:VAL:HG11	2.19	0.43
1:B:134:ILE:HD11	1:B:224:LEU:HG	2.00	0.43
1:B:224:LEU:HD22	1:B:237:ASN:ND2	2.33	0.43
1:B:280:ARG:CZ	1:C:247:LEU:HD21	2.48	0.43
1:C:155:VAL:H	1:C:175:THR:HB	1.82	0.43
1:B:314:VAL:HA	1:B:315:PRO:HD3	1.74	0.43
1:B:295:TYR:HE1	1:B:300:PRO:HG3	1.84	0.43
1:A:253:THR:HG23	1:F:289:LYS:NZ	2.34	0.43
1:F:276:VAL:HG22	1:F:314:VAL:HG21	2.00	0.43
1:A:119:MET:HE3	1:B:336:TRP:CZ3	2.53	0.43
1:A:145:SER:OG	1:A:146:ASN:N	2.51	0.43
1:G:196:VAL:HG12	1:G:203:LEU:CD2	2.48	0.43
1:B:371:TYR:HD1	1:B:371:TYR:N	2.17	0.43
1:E:289:LYS:NZ	1:F:253:THR:HG23	2.34	0.43
1:D:186:ILE:HA	1:E:161:ASP:O	2.18	0.43
1:G:274:GLY:HA2	1:G:312:PRO:HD2	2.00	0.43
1:A:275:ILE:HD13	1:A:308:MET:HE3	1.99	0.43
1:D:235:GLY:O	1:D:236:LEU:C	2.58	0.43
1:C:139:ALA:O	1:C:334:GLN:HG3	2.19	0.43
1:B:134:ILE:CD1	1:B:224:LEU:HG	2.49	0.43
1:A:119:MET:HB3	1:B:148:LEU:HD22	2.01	0.43
1:C:148:LEU:CD1	1:C:336:TRP:CG	3.02	0.43
1:G:277:LEU:HD13	1:G:285:ILE:HD12	2.01	0.43
1:B:155:VAL:H	1:B:175:THR:HB	1.82	0.43
1:C:342:THR:CG2	1:C:343:VAL:N	2.82	0.43
1:E:148:LEU:HD11	1:E:336:TRP:CG	2.54	0.43
1:D:368:LEU:HA	1:D:368:LEU:HD12	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:LEU:HA	1:G:211:LEU:HD23	1.88	0.43
1:D:129:LEU:HD12	1:D:129:LEU:HA	1.77	0.43
1:G:134:ILE:HB	1:G:220:GLU:HG3	2.00	0.42
1:A:183:VAL:HG13	1:A:366:LEU:O	2.19	0.42
1:D:253:THR:OG1	1:D:255:ALA:HB3	2.18	0.42
1:A:183:VAL:HG22	1:A:367:ALA:HB2	2.01	0.42
1:C:224:LEU:CD1	1:C:237:ASN:HD21	2.31	0.42
1:A:339:MET:HE1	1:A:363:GLU:HG3	2.01	0.42
1:B:210:ARG:HA	1:B:210:ARG:HD2	1.89	0.42
1:A:235:GLY:O	1:A:236:LEU:C	2.57	0.42
1:C:207:ILE:O	1:C:211:LEU:HG	2.18	0.42
1:B:159:ASN:O	1:B:160:ALA:C	2.56	0.42
1:C:275:ILE:HD13	1:C:308:MET:HE3	2.01	0.42
1:F:148:LEU:HD11	1:F:336:TRP:CD2	2.54	0.42
1:C:329:PHE:O	1:C:331:MET:N	2.52	0.42
1:E:275:ILE:HD13	1:E:308:MET:CE	2.50	0.42
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.42
1:G:334:GLN:HG2	1:G:371:TYR:OH	2.19	0.42
1:D:297:PHE:HB3	1:D:304:THR:CG2	2.46	0.42
1:E:121:ILE:HG13	1:F:150:TYR:HB3	2.02	0.42
1:A:294:ARG:H	1:A:294:ARG:HG2	1.42	0.42
1:F:203:LEU:HG	1:F:207:ILE:HD11	2.01	0.42
1:C:289:LYS:HZ2	1:D:253:THR:HG23	1.84	0.42
1:D:146:ASN:C	1:D:183:VAL:CG1	2.87	0.42
1:E:256:ASP:O	1:E:259:ALA:HB3	2.19	0.42
1:C:268:SER:O	1:C:269:GLU:CB	2.67	0.42
1:E:297:PHE:CD1	1:E:297:PHE:N	2.87	0.42
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.34	0.42
1:E:203:LEU:HG	1:E:207:ILE:HD11	2.02	0.42
1:C:258:ILE:HG21	1:C:275:ILE:HD13	2.01	0.42
1:D:342:THR:CG2	1:D:343:VAL:N	2.80	0.42
1:B:286:ALA:C	1:B:288:LEU:H	2.23	0.42
1:F:373:PRO:C	1:F:375:ALA:N	2.72	0.42
1:B:349:ASP:C	1:B:350:ARG:CG	2.88	0.42
1:B:224:LEU:HD13	1:B:237:ASN:HD22	1.85	0.42
1:A:283:HIS:NE2	1:B:260:HIS:HA	2.34	0.42
1:E:371:TYR:CD2	1:E:371:TYR:N	2.87	0.42
1:B:146:ASN:O	1:B:147:ALA:HB2	2.19	0.42
1:C:148:LEU:HD11	1:C:336:TRP:CG	2.54	0.42
1:C:143:THR:OG1	1:C:144:SER:N	2.52	0.42
1:F:342:THR:HG22	1:F:343:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:THR:O	1:F:135:ARG:N	2.52	0.42
1:D:148:LEU:HD11	1:D:336:TRP:CD2	2.54	0.42
1:D:249:ALA:N	1:D:252:ASP:OD2	2.46	0.42
1:A:245:THR:HG22	1:A:245:THR:O	2.19	0.42
1:F:268:SER:O	1:F:269:GLU:HB2	2.18	0.42
1:F:258:ILE:HG21	1:F:275:ILE:HD13	2.00	0.42
1:D:145:SER:OG	1:D:146:ASN:N	2.52	0.42
1:B:342:THR:CG2	1:B:343:VAL:N	2.83	0.42
1:E:146:ASN:C	1:E:183:VAL:HG23	2.40	0.41
1:C:254:ARG:O	1:C:258:ILE:HD13	2.19	0.41
1:C:258:ILE:CD1	1:C:258:ILE:H	2.33	0.41
1:E:254:ARG:HB3	1:E:381:PHE:HE2	1.83	0.41
1:C:148:LEU:HD11	1:C:336:TRP:CD2	2.55	0.41
1:G:106:GLY:O	1:G:111:SER:HB3	2.20	0.41
1:D:258:ILE:HD13	1:D:308:MET:CE	2.48	0.41
1:E:290:ASP:C	1:E:290:ASP:OD1	2.58	0.41
1:D:222:GLN:O	1:D:223:LEU:C	2.59	0.41
1:B:335:VAL:HG22	1:B:368:LEU:HD13	2.02	0.41
1:C:243:TYR:HA	1:C:264:GLN:OE1	2.20	0.41
1:C:342:THR:HG22	1:C:343:VAL:H	1.83	0.41
1:D:189:TRP:CD1	1:E:169:LYS:HB3	2.55	0.41
1:B:272:ALA:HB3	1:B:311:LEU:HD11	2.02	0.41
1:G:156:PHE:CZ	1:G:158:ASN:HB2	2.54	0.41
1:B:188:HIS:CE1	1:C:160:ALA:HB2	2.55	0.41
1:G:254:ARG:HB3	1:G:381:PHE:CD2	2.55	0.41
1:G:229:THR:CG2	1:G:230:GLY:H	2.20	0.41
1:D:324:PHE:CE1	1:D:379:GLY:HA3	2.56	0.41
1:B:350:ARG:HB2	1:B:351:ASP:H	1.62	0.41
1:B:280:ARG:NH1	1:C:247:LEU:HD23	2.34	0.41
1:G:350:ARG:HB2	1:G:351:ASP:H	1.61	0.41
1:G:281:ASP:O	1:G:285:ILE:HG13	2.20	0.41
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.41
1:D:286:ALA:C	1:D:288:LEU:H	2.23	0.41
1:C:119:MET:HB3	1:D:148:LEU:CD2	2.50	0.41
1:G:128:GLY:HA2	1:G:213:TYR:CE1	2.56	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.82	0.41
1:D:130:ARG:CZ	1:D:217:LEU:HD21	2.51	0.41
1:C:295:TYR:HD1	1:C:300:PRO:HD3	1.86	0.41
1:A:324:PHE:CE1	1:A:379:GLY:HA3	2.54	0.41
1:B:129:LEU:HA	1:B:129:LEU:HD12	1.83	0.41
1:G:197:MET:HE1	1:G:204:GLN:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:VAL:HG23	1:C:377:ILE:HD12	2.03	0.41
1:C:224:LEU:HD12	1:C:225:ASN:ND2	2.36	0.41
1:G:239:VAL:HG21	1:G:370:HIS:CD2	2.56	0.41
1:E:229:THR:HG22	1:E:232:ASN:HD22	1.86	0.41
1:C:187:ALA:HB2	1:C:363:GLU:HA	2.02	0.41
1:C:187:ALA:HB2	1:C:363:GLU:HB3	2.02	0.41
1:B:148:LEU:HD11	1:B:336:TRP:CD2	2.56	0.41
1:F:285:ILE:O	1:F:288:LEU:HB2	2.21	0.41
1:A:146:ASN:CG	1:F:116:ILE:HG21	2.42	0.41
1:A:120:GLN:O	1:A:122:PRO:HD3	2.19	0.41
1:E:222:GLN:HB3	1:E:233:LEU:HB2	2.03	0.41
1:G:133:THR:O	1:G:134:ILE:C	2.57	0.41
1:G:203:LEU:HD11	1:G:207:ILE:HD11	2.03	0.41
1:C:124:ILE:N	1:C:124:ILE:CD1	2.84	0.41
1:B:147:ALA:O	1:B:148:LEU:HD23	2.21	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.83	0.41
1:D:224:LEU:HG	1:D:237:ASN:ND2	2.36	0.41
1:A:206:TYR:CZ	1:A:210:ARG:HD3	2.56	0.41
1:F:303:PHE:HD2	1:F:303:PHE:HA	1.77	0.41
1:D:255:ALA:HA	1:D:258:ILE:HD12	2.02	0.40
1:B:349:ASP:O	1:B:350:ARG:C	2.58	0.40
1:G:258:ILE:O	1:G:262:ILE:HG13	2.21	0.40
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.85	0.40
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.03	0.40
1:G:194:ARG:NH1	1:G:347:ARG:NH2	2.69	0.40
1:G:126:MET:HA	1:G:127:PRO:HD3	1.85	0.40
1:E:147:ALA:O	1:E:148:LEU:HD23	2.21	0.40
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.85	0.40
1:B:268:SER:HB2	1:B:374:THR:CG2	2.51	0.40
1:A:376:ILE:C	1:A:377:ILE:HD13	2.41	0.40
1:E:282:TRP:CE3	1:E:282:TRP:HA	2.56	0.40
1:F:210:ARG:HD2	1:F:210:ARG:HA	1.82	0.40
1:A:314:VAL:HA	1:A:315:PRO:HD3	1.78	0.40
1:D:196:VAL:HG12	1:D:203:LEU:CD2	2.52	0.40
1:B:126:MET:HA	1:B:127:PRO:HD3	1.84	0.40
1:F:356:ASN:OD1	1:G:363:GLU:OE2	2.40	0.40
1:B:259:ALA:HB2	1:B:309:TRP:NE1	2.36	0.40
1:G:306:ASN:HB3	1:G:313:VAL:HB	2.03	0.40
1:A:119:MET:HE1	1:B:143:THR:HB	2.02	0.40
1:B:145:SER:OG	1:B:146:ASN:N	2.55	0.40
1:B:223:LEU:HD23	1:B:368:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:HG2	1:F:130:ARG:HA	2.03	0.40
1:A:130:ARG:HG2	1:A:131:ARG:N	2.36	0.40
1:G:273:SER:H	1:G:328:GLY:HA2	1.86	0.40
1:E:211:LEU:CD1	1:E:211:LEU:N	2.85	0.40
1:C:371:TYR:H	1:C:371:TYR:HD1	1.64	0.40
1:F:347:ARG:NH1	1:F:347:ARG:HG3	2.35	0.40
1:B:148:LEU:CD1	1:B:336:TRP:CG	3.05	0.40
1:E:282:TRP:HA	1:E:282:TRP:HE3	1.86	0.40
1:C:314:VAL:HA	1:C:315:PRO:HD3	1.78	0.40
1:B:282:TRP:HA	1:B:282:TRP:CE3	2.56	0.40
1:G:145:SER:OG	1:G:146:ASN:N	2.54	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	279/282 (99%)	237 (85%)	36 (13%)	6 (2%)	8	47
1	B	279/282 (99%)	229 (82%)	43 (15%)	7 (2%)	7	44
1	C	279/282 (99%)	236 (85%)	34 (12%)	9 (3%)	5	38
1	D	279/282 (99%)	232 (83%)	39 (14%)	8 (3%)	6	40
1	E	279/282 (99%)	240 (86%)	32 (12%)	7 (2%)	7	44
1	F	279/282 (99%)	231 (83%)	40 (14%)	8 (3%)	6	40
1	G	279/282 (99%)	232 (83%)	38 (14%)	9 (3%)	5	38
All	All	1953/1974 (99%)	1637 (84%)	262 (13%)	54 (3%)	6	41

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	PRO
1	B	352	ASN
1	C	134	ILE
1	C	300	PRO
1	D	229	THR
1	E	300	PRO
1	F	352	ASN
1	G	127	PRO
1	G	229	THR
1	G	297	PHE
1	A	226	GLY
1	C	269	GLU
1	D	134	ILE
1	D	230	GLY
1	D	300	PRO
1	D	330	ASP
1	D	350	ARG
1	E	230	GLY
1	E	298	GLY
1	E	350	ARG
1	F	113	GLY
1	F	134	ILE
1	F	300	PRO
1	F	330	ASP
1	G	301	GLN
1	A	227	ASP
1	B	230	GLY
1	B	330	ASP
1	C	330	ASP
1	D	269	GLU
1	E	236	LEU
1	F	269	GLU
1	G	230	GLY
1	G	240	ALA
1	G	267	GLU
1	G	269	GLU
1	A	240	ALA
1	B	134	ILE
1	B	329	PHE
1	C	226	GLY
1	C	227	ASP
1	C	350	ARG
1	E	330	ASP

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Mol	Chain	Res	Type
1	F	351	ASP
1	B	315	PRO
1	A	315	PRO
1	E	315	PRO
1	G	304	THR
1	A	230	GLY
1	D	226	GLY
1	A	134	ILE
1	C	315	PRO
1	C	196	VAL
1	F	315	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	230/231 (100%)	211 (92%)	19 (8%)	14	49
1	B	230/231 (100%)	216 (94%)	14 (6%)	23	63
1	C	230/231 (100%)	211 (92%)	19 (8%)	14	49
1	D	230/231 (100%)	220 (96%)	10 (4%)	35	74
1	E	230/231 (100%)	214 (93%)	16 (7%)	19	58
1	F	230/231 (100%)	214 (93%)	16 (7%)	19	58
1	G	230/231 (100%)	221 (96%)	9 (4%)	39	75
All	All	1610/1617 (100%)	1507 (94%)	103 (6%)	22	61

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	108	ASP
1	A	114	SER
1	A	124	ILE
1	A	133	THR
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	156	PHE
1	A	157	THR
1	A	168	LEU
1	A	188	HIS
1	A	202	MET
1	A	217	LEU
1	A	220	GLU
1	A	224	LEU
1	A	250	THR
1	A	288	LEU
1	A	292	GLU
1	A	301	GLN
1	A	374	THR
1	B	133	THR
1	B	151	VAL
1	B	156	PHE
1	B	169	LYS
1	B	188	HIS
1	B	191	GLN
1	B	194	ARG
1	B	202	MET
1	B	220	GLU
1	B	224	LEU
1	B	250	THR
1	B	268	SER
1	B	288	LEU
1	B	374	THR
1	C	114	SER
1	C	133	THR
1	C	135	ARG
1	C	156	PHE
1	C	168	LEU
1	C	188	HIS
1	C	195	GLN
1	C	202	MET
1	C	210	ARG
1	C	215	LEU
1	C	224	LEU
1	C	234	GLU
1	C	250	THR
1	C	256	ASP
1	C	280	ARG

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Mol	Chain	Res	Type
1	C	288	LEU
1	C	345	VAL
1	C	371	TYR
1	C	374	THR
1	D	114	SER
1	D	133	THR
1	D	156	PHE
1	D	183	VAL
1	D	188	HIS
1	D	202	MET
1	D	210	ARG
1	D	217	LEU
1	D	250	THR
1	D	288	LEU
1	E	111	SER
1	E	151	VAL
1	E	156	PHE
1	E	168	LEU
1	E	188	HIS
1	E	202	MET
1	E	205	SER
1	E	215	LEU
1	E	217	LEU
1	E	229	THR
1	E	250	THR
1	E	279	PRO
1	E	280	ARG
1	E	288	LEU
1	E	297	PHE
1	E	300	PRO
1	F	110	ASP
1	F	114	SER
1	F	130	ARG
1	F	133	THR
1	F	156	PHE
1	F	188	HIS
1	F	194	ARG
1	F	195	GLN
1	F	202	MET
1	F	217	LEU
1	F	224	LEU
1	F	250	THR

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Mol	Chain	Res	Type
1	F	280	ARG
1	F	303	PHE
1	F	350	ARG
1	F	374	THR
1	G	111	SER
1	G	150	TYR
1	G	188	HIS
1	G	195	GLN
1	G	245	THR
1	G	256	ASP
1	G	288	LEU
1	G	374	THR
1	G	383	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	225	ASN
1	A	237	ASN
1	A	291	ASN
1	A	334	GLN
1	B	191	GLN
1	B	225	ASN
1	B	237	ASN
1	B	334	GLN
1	C	146	ASN
1	C	225	ASN
1	C	237	ASN
1	C	334	GLN
1	D	232	ASN
1	D	291	ASN
1	D	334	GLN
1	E	191	GLN
1	E	208	ASN
1	E	232	ASN
1	E	237	ASN
1	E	334	GLN
1	E	352	ASN
1	F	225	ASN
1	F	232	ASN
1	F	237	ASN

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Mol	Chain	Res	Type
1	F	334	GLN
1	G	195	GLN
1	G	232	ASN
1	G	334	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	A	1384	-	4,4,4	3.18	4 (100%)	6,6,6	0.14	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	A	1384	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1384	SO4	O3-S	2.79	1.57	1.47
2	A	1384	SO4	O4-S	2.94	1.58	1.47
2	A	1384	SO4	O1-S	3.45	1.59	1.47
2	A	1384	SO4	O2-S	3.45	1.59	1.47

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.