



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:07 AM GMT

PDB ID : 1ZT2  
Title : Heterodimeric structure of the core primase.  
Authors : Lao-Sirieix, S.H.; Nookala, R.K.; Roversi, P.; Bell, S.D.; Pellegrini, L.  
Deposited on : 2005-05-26  
Resolution : 3.33 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

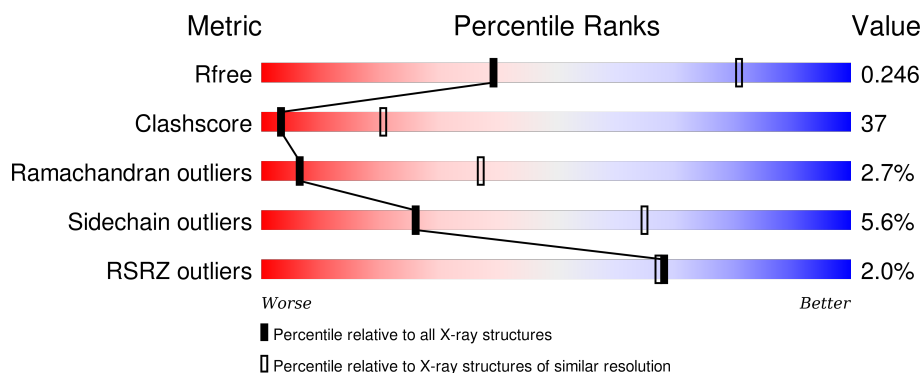
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.33 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	330	<div> <div>2%</div> <div>50%44%5%</div> </div>
1	C	330	<div> <div>%</div> <div>44%47%6%</div> </div>
2	B	212	<div> <div></div> <div>41%50%8%</div> </div>
2	D	212	<div> <div>5%</div> <div>43%50%5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1005	-	-	X	-
4	SO4	A	1009	-	-	-	X
4	SO4	C	1004	-	-	-	X
4	SO4	C	1006	-	-	-	X
4	SO4	C	1012	-	-	X	-
4	SO4	D	215	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8799 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 DNA primase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2629	1674	451	492	12			
1	C	320	Total	C	N	O	S	0	1	0
			2579	1641	444	482	12			

- Molecule 2 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1717	1117	284	313	3			
2	D	202	Total	C	N	O	S	0	0	0
			1665	1085	271	306	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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

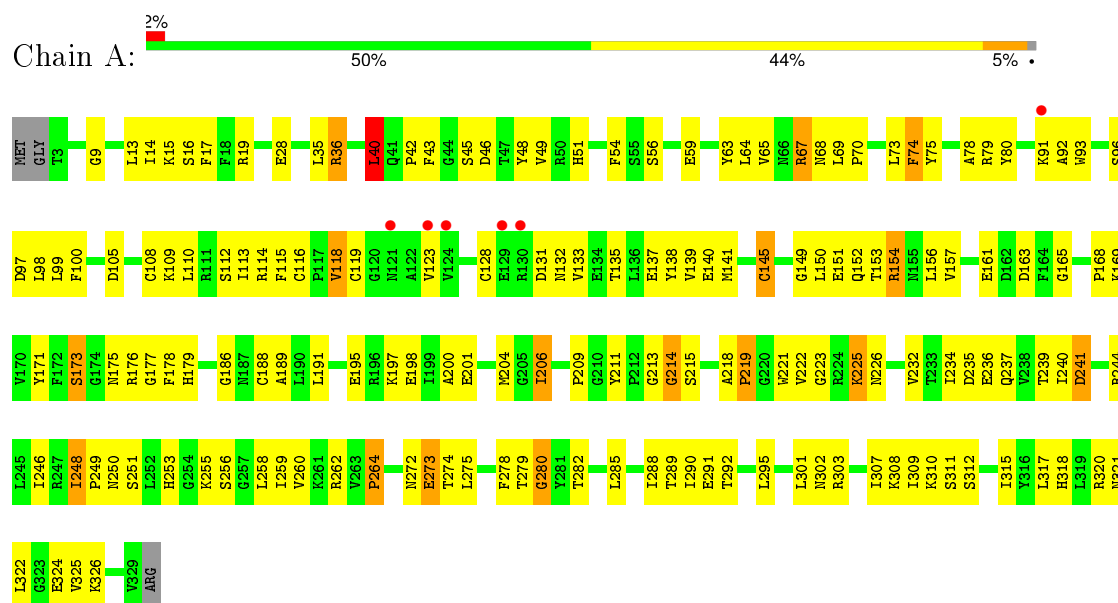
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	3	Total	O	0	0
			3	3		
5	C	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

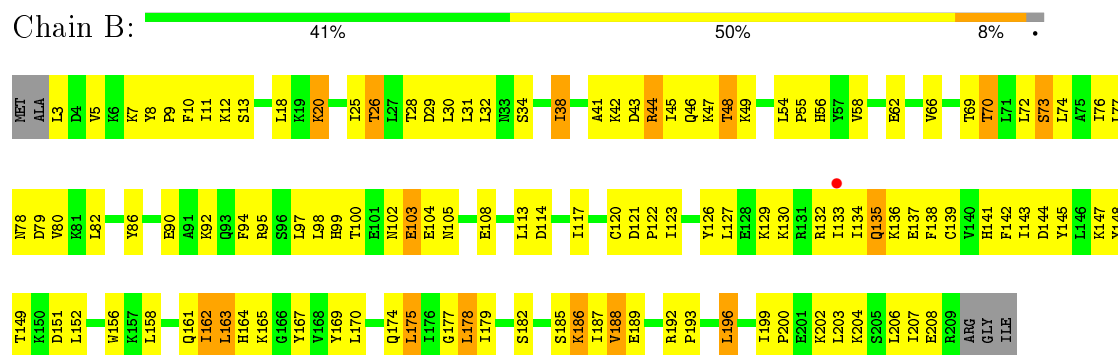
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: DNA primase small subunit

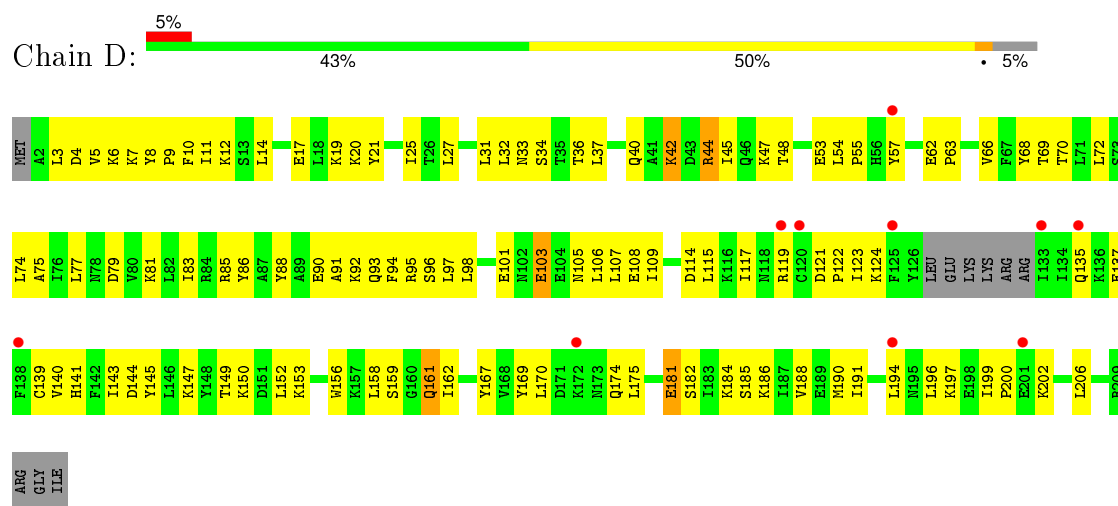




• Molecule 2: DNA primase large subunit



• Molecule 2: DNA primase large subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.29 Å   193.29 Å   213.03 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.12 – 3.33 39.12 – 3.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.12-3.33) 99.7 (39.12-3.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 3.32 Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.236   ,   0.243 0.236   ,   0.246	Depositor DCC
$R_{free}$ test set	2994 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 78.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 59249 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.36	0/2689	0.64	1/3635 (0.0%)
1	C	0.38	0/2633	0.60	3/3558 (0.1%)
2	B	0.31	0/1746	0.54	0/2348
2	D	0.29	0/1693	0.50	0/2279
All	All	0.35	0/8761	0.58	4/11820 (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	40	LEU	CA-CB-CG	6.62	130.53	115.30
1	C	271	PHE	CB-CG-CD1	5.74	124.81	120.80
1	C	263	VAL	C-N-CD	-5.69	108.08	120.60
1	C	271	PHE	CB-CG-CD2	-5.32	117.07	120.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2600	199	0
1	C	2579	0	2557	202	0
2	B	1717	0	1809	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1665	0	1744	129	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	65	0	0	5	0
4	B	40	0	0	1	0
4	C	75	0	0	7	0
4	D	15	0	0	3	0
5	A	5	0	0	1	0
5	B	3	0	0	1	0
5	C	4	0	0	0	0
All	All	8799	0	8710	649	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 37.

All (649) 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)
2:D:74:LEU:HD23	2:D:77:LEU:HD12	1.38	1.04
1:C:201:GLU:HA	1:C:204:MET:HE2	1.44	1.00
1:C:78:ALA:HA	1:C:96:SER:HB3	1.43	0.97
1:A:141:MET:HE3	1:A:176:ARG:HG2	1.42	0.96
1:A:141:MET:CE	1:A:176:ARG:HG2	1.95	0.95
1:A:43:PHE:CE1	1:A:69:LEU:HD23	2.02	0.93
2:B:5:VAL:HG21	2:B:12:LYS:HE2	1.51	0.90
1:A:42:PRO:HG2	1:A:45:SER:HB3	1.54	0.90
1:A:110:LEU:HD11	1:A:141:MET:HE2	1.54	0.89
2:D:31:LEU:HD21	2:D:69:THR:CG2	2.02	0.89
1:A:43:PHE:HE1	1:A:69:LEU:HD23	1.34	0.88
2:D:152:LEU:HD21	2:D:181:GLU:HG2	1.55	0.88
2:D:124:LYS:HG2	2:D:135:GLN:HB3	1.52	0.87
1:C:218:ALA:HB3	1:C:223:GLY:N	1.90	0.86
1:C:218:ALA:HB1	1:C:219:PRO:HD2	1.58	0.86
1:A:218:ALA:HB3	1:A:223:GLY:N	1.91	0.86
1:C:232:VAL:HG12	1:C:234:ILE:HG13	1.55	0.86
1:A:28:GLU:HB2	1:A:249:PRO:HB2	1.59	0.85
2:B:66:VAL:O	2:B:70:THR:HG23	1.77	0.85
1:C:280:GLY:HA3	1:C:328:TYR:HE1	1.42	0.85
1:C:253:HIS:CE1	1:C:255:LYS:HB2	2.12	0.85
2:D:8:TYR:HB2	2:D:11:ILE:CD1	2.07	0.84
2:D:47:LYS:NZ	2:D:55:PRO:HG3	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TRP:CE3	1:A:225:LYS:HD3	2.11	0.84
1:C:141:MET:CE	1:C:176:ARG:HG2	2.08	0.84
1:C:310:LYS:HB2	1:C:310:LYS:NZ	1.92	0.84
1:A:289:THR:HG22	1:A:302:ASN:HA	1.58	0.84
1:C:22:TYR:CE1	1:C:70:PRO:HG2	2.13	0.84
1:C:201:GLU:HA	1:C:204:MET:CE	2.07	0.83
2:D:31:LEU:HD21	2:D:69:THR:HG22	1.60	0.82
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.42	0.82
2:D:45:ILE:HD13	2:D:77:LEU:HD11	1.62	0.81
1:C:73:LEU:HG	1:C:248:ILE:HD12	1.60	0.81
2:B:31:LEU:HD21	2:B:69:THR:CG2	2.10	0.81
2:D:4:ASP:OD2	2:D:6:LYS:HB2	1.80	0.80
1:C:192:ASP:HB2	1:C:195:GLU:HG3	1.63	0.80
1:C:218:ALA:HB3	1:C:223:GLY:CA	2.11	0.80
1:C:288:ILE:HG22	1:C:290:ILE:HG13	1.64	0.79
2:D:62:GLU:O	2:D:66:VAL:HG23	1.82	0.79
2:D:21:TYR:O	2:D:25:ILE:HG13	1.82	0.79
2:B:95:ARG:HH12	2:B:177:GLY:HA2	1.48	0.79
1:C:210:GLY:O	1:C:212:PRO:HD3	1.83	0.78
2:B:62:GLU:O	2:B:66:VAL:HG23	1.84	0.78
1:C:253:HIS:HE1	1:C:255:LYS:HB2	1.48	0.78
1:C:288:ILE:CG2	1:C:290:ILE:HG13	2.14	0.77
1:C:161:GLU:O	1:C:165:GLY:HA2	1.82	0.77
2:D:66:VAL:O	2:D:70:THR:HG23	1.84	0.77
1:A:110:LEU:CD1	1:A:141:MET:HE2	2.14	0.77
1:A:318:HIS:ND1	1:A:324:GLU:HA	1.99	0.77
1:C:141:MET:HG3	1:C:271:PHE:HZ	1.49	0.76
1:A:258:LEU:HD22	1:A:275:LEU:HB2	1.66	0.76
2:B:199:ILE:HG23	2:B:200:PRO:HD2	1.65	0.76
1:C:74:PHE:HB3	1:C:247:ARG:HA	1.66	0.76
1:C:218:ALA:HB1	1:C:219:PRO:CD	2.16	0.75
1:C:311:SER:O	1:C:315:ILE:HD12	1.87	0.74
1:C:141:MET:HE1	1:C:176:ARG:HG2	1.69	0.74
2:B:158:LEU:HD11	2:B:163:LEU:HD22	1.70	0.74
1:A:307:ILE:HG22	1:A:309:ILE:HG13	1.69	0.74
1:C:78:ALA:CA	1:C:96:SER:HB3	2.17	0.74
1:C:28:GLU:HB2	1:C:249:PRO:HB2	1.70	0.74
1:A:119:CYS:HA	1:A:303:ARG:NH2	2.03	0.73
2:B:44:ARG:O	2:B:48:THR:HG23	1.87	0.73
2:B:31:LEU:HD21	2:B:69:THR:HG21	1.70	0.73
2:D:115:LEU:HD11	2:D:182:SER:OG	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD13	1:C:94:MET:HE1	1.69	0.73
1:C:141:MET:HG3	1:C:271:PHE:CZ	2.24	0.72
1:C:74:PHE:HA	1:C:248:ILE:HG13	1.71	0.72
2:D:141:HIS:CD2	2:D:143:ILE:HG13	2.24	0.72
1:C:78:ALA:HA	1:C:96:SER:CB	2.18	0.72
2:D:8:TYR:HB2	2:D:11:ILE:HD11	1.71	0.71
2:B:102:ASN:HB2	2:B:105:ASN:ND2	2.06	0.71
1:C:248:ILE:O	1:C:251:SER:HB3	1.90	0.71
1:A:197:LYS:HB2	1:A:240:ILE:HG12	1.73	0.71
1:C:112:SER:O	1:C:113:ILE:HG13	1.90	0.71
2:D:124:LYS:HE2	2:D:135:GLN:NE2	2.05	0.71
1:A:262:ARG:HH11	1:A:262:ARG:HG2	1.55	0.70
1:A:73:LEU:CD2	1:A:248:ILE:HD12	2.20	0.70
2:D:186:LYS:O	2:D:190:MET:HG3	1.92	0.70
2:B:76:ILE:HD11	2:B:199:ILE:HD13	1.72	0.70
1:C:289:THR:HG22	1:C:302:ASN:HA	1.72	0.70
1:A:175:ASN:HB3	4:A:1000:SO4:O4	1.91	0.70
1:A:54:PHE:HD2	1:A:59:GLU:HB3	1.57	0.70
2:D:27:LEU:O	2:D:27:LEU:HD12	1.91	0.69
1:C:289:THR:HA	1:C:301:LEU:O	1.92	0.69
2:B:202:LYS:O	2:B:206:LEU:HG	1.92	0.69
2:B:193:PRO:HA	2:B:196:LEU:HG	1.73	0.69
1:C:93:TRP:CZ2	1:C:95:GLY:HA2	2.27	0.69
2:D:44:ARG:HD3	2:D:70:THR:HG21	1.74	0.69
2:D:145:TYR:CZ	2:D:149:THR:HG21	2.27	0.69
2:B:175:LEU:O	2:B:175:LEU:HD12	1.92	0.69
2:B:78:ASN:HB3	2:D:36:THR:CG2	2.23	0.69
2:B:72:LEU:HD11	2:B:199:ILE:HD11	1.75	0.69
1:C:287:TYR:CD1	1:C:323:GLY:HA2	2.28	0.69
1:A:51:HIS:HE1	1:A:91:LYS:HE2	1.58	0.68
2:B:56:HIS:HD2	2:B:97:LEU:HG	1.59	0.68
1:A:218:ALA:HB3	1:A:223:GLY:CA	2.24	0.68
1:A:309:ILE:HG22	1:A:310:LYS:N	2.07	0.68
1:C:40:LEU:CD2	1:C:49:VAL:HB	2.24	0.68
2:D:47:LYS:HZ3	2:D:55:PRO:HG3	1.55	0.68
2:D:17:GLU:O	2:D:20:LYS:HG2	1.95	0.68
2:B:192:ARG:HD2	2:D:32:LEU:CD1	2.24	0.68
1:C:236:GLU:O	1:C:240:ILE:HD12	1.95	0.67
1:A:93:TRP:HE1	1:A:96:SER:HB3	1.59	0.67
2:D:9:PRO:HG2	2:D:57:TYR:CD1	2.29	0.67
2:B:132:ARG:HG2	2:B:133:ILE:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:HD13	2:D:156:TRP:CE2	2.30	0.67
1:A:73:LEU:HD21	1:A:248:ILE:HD12	1.77	0.67
2:B:56:HIS:CD2	2:B:97:LEU:HG	2.30	0.67
1:A:288:ILE:HG22	1:A:290:ILE:HG13	1.76	0.67
1:C:294:VAL:HG21	1:C:317:LEU:HD21	1.76	0.67
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.06	0.67
1:A:115:PHE:HB2	1:A:288:ILE:HD11	1.76	0.66
1:A:289:THR:CG2	1:A:303:ARG:H	2.07	0.66
1:C:81:GLN:O	1:C:82:LEU:HD23	1.95	0.66
2:B:31:LEU:HD21	2:B:69:THR:HG22	1.77	0.66
1:C:138:TYR:CG	1:C:322:LEU:HD21	2.30	0.66
1:C:133:VAL:HG12	1:C:134:GLU:N	2.10	0.66
1:C:118:VAL:O	1:C:303:ARG:NH2	2.28	0.66
2:D:74:LEU:HA	2:D:77:LEU:HD12	1.76	0.66
2:B:185:SER:O	2:B:189:GLU:HG3	1.95	0.66
2:D:97:LEU:O	2:D:101:GLU:HG2	1.96	0.66
1:A:64:LEU:HD22	1:A:70:PRO:HG3	1.79	0.65
1:A:260:VAL:HG12	1:A:260:VAL:O	1.95	0.65
2:B:151:ASP:HA	2:D:19:LYS:NZ	2.11	0.65
1:C:110:LEU:CD1	1:C:141:MET:HE2	2.26	0.65
1:A:171:TYR:CE2	1:A:262:ARG:HB2	2.31	0.65
2:B:192:ARG:HD2	2:D:32:LEU:HD12	1.78	0.65
1:A:157:VAL:HG13	1:A:168:PRO:HG2	1.77	0.65
2:D:31:LEU:HD21	2:D:69:THR:HG21	1.76	0.65
1:C:173:SER:HA	1:C:179[B]:HIS:CD2	2.32	0.65
1:A:115:PHE:CB	1:A:288:ILE:HD11	2.26	0.65
1:C:284:PHE:CZ	1:C:323:GLY:HA3	2.33	0.64
1:A:139:VAL:O	1:A:320:ARG:NH1	2.31	0.64
1:A:110:LEU:HD11	1:A:141:MET:CE	2.24	0.64
1:C:307:ILE:HG22	1:C:309:ILE:HG13	1.80	0.64
1:C:74:PHE:HB3	1:C:247:ARG:CA	2.27	0.64
2:B:192:ARG:N	2:B:193:PRO:HD2	2.13	0.64
1:A:249:PRO:O	1:A:250:ASN:HB2	1.96	0.64
2:B:7:LYS:HG2	2:B:58:VAL:CG2	2.28	0.63
2:B:151:ASP:HB3	2:D:19:LYS:HG3	1.78	0.63
2:D:117:ILE:HG23	2:D:140:VAL:HG22	1.79	0.63
1:A:51:HIS:HE1	1:A:91:LYS:CE	2.11	0.63
2:B:18:LEU:HD22	2:B:25:ILE:HG22	1.80	0.63
1:A:309:ILE:HG22	1:A:310:LYS:H	1.61	0.63
1:C:56:SER:HA	4:C:1006:SO4:O2	1.97	0.63
2:D:83:ILE:HD13	2:D:191:ILE:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:MET:HE1	1:A:176:ARG:HG2	1.79	0.63
1:A:51:HIS:CE1	1:A:91:LYS:HE2	2.33	0.63
1:A:234:ILE:HG22	1:A:235:ASP:N	2.13	0.63
1:C:310:LYS:HB2	1:C:310:LYS:HZ2	1.63	0.62
2:D:114:ASP:O	2:D:115:LEU:HD23	1.98	0.62
1:A:188:CYS:O	1:A:191:LEU:HG	1.99	0.62
1:C:219:PRO:HD2	1:C:222:VAL:HB	1.82	0.62
1:A:236:GLU:HB2	1:A:240:ILE:CD1	2.30	0.62
1:C:196:ARG:HE	1:C:242:VAL:HG22	1.65	0.61
2:D:47:LYS:HZ2	2:D:55:PRO:HG3	1.62	0.61
1:C:318:HIS:ND1	1:C:324:GLU:HA	2.14	0.61
1:A:221:TRP:HE3	1:A:225:LYS:HD3	1.60	0.61
2:B:92:LYS:O	2:B:95:ARG:HB2	2.00	0.61
2:D:72:LEU:HA	2:D:194:LEU:HD13	1.82	0.61
2:B:170:LEU:HA	2:B:174:GLN:OE1	2.00	0.61
1:C:156:LEU:HD13	1:C:234:ILE:HD11	1.82	0.61
1:C:140:GLU:HG3	1:C:292:THR:HB	1.81	0.61
1:A:200:ALA:O	1:A:204:MET:HG3	2.01	0.61
1:C:317:LEU:CD2	1:C:322:LEU:HD12	2.31	0.61
1:A:17:PHE:CE1	1:A:315:ILE:HD11	2.35	0.61
1:A:209:PRO:HG2	1:A:211:TYR:CZ	2.36	0.61
1:A:289:THR:O	1:A:290:ILE:HG13	2.01	0.61
1:C:320:ARG:O	1:C:321:ASN:HB2	2.01	0.60
2:B:7:LYS:O	2:B:9:PRO:HD3	2.01	0.60
2:D:200:PRO:HA	4:D:215:SO4:O4	2.01	0.60
1:A:17:PHE:CD1	1:A:315:ILE:HD11	2.36	0.60
1:A:317:LEU:HD23	1:A:322:LEU:HD12	1.83	0.60
1:C:110:LEU:HD11	1:C:141:MET:HE2	1.84	0.60
1:C:290:ILE:CG2	1:C:292:THR:HG23	2.32	0.60
2:B:48:THR:HG21	2:B:86:TYR:HD1	1.66	0.60
1:C:76:SER:HA	1:C:245:LEU:HD23	1.84	0.59
1:C:75:TYR:HD2	1:C:248:ILE:HG12	1.66	0.59
1:C:40:LEU:O	1:C:40:LEU:HD23	2.01	0.59
1:A:219:PRO:HG3	2:B:123:ILE:HG21	1.84	0.59
1:A:195:GLU:O	1:A:198:GLU:HB2	2.01	0.59
1:C:219:PRO:HG2	1:C:220:GLY:H	1.67	0.59
2:B:185:SER:HB3	2:D:25:ILE:HD11	1.83	0.59
1:C:88:MET:HE3	1:C:243:LYS:HD2	1.83	0.59
1:C:141:MET:HE3	1:C:176:ARG:HG2	1.83	0.59
2:D:44:ARG:HH11	2:D:44:ARG:HG3	1.68	0.59
1:C:112:SER:C	1:C:113:ILE:HG13	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:NH1	4:A:1005:SO4:O3	2.35	0.59
1:C:317:LEU:HD22	1:C:322:LEU:HD12	1.85	0.59
1:A:131:ASP:O	1:A:133:VAL:HG23	2.02	0.59
1:A:113:ILE:O	1:A:137:GLU:HA	2.02	0.59
1:C:110:LEU:HD11	1:C:141:MET:CE	2.33	0.59
1:C:143:SER:HA	1:C:271:PHE:CD2	2.38	0.59
1:A:149:GLY:O	1:A:153:THR:HG23	2.02	0.59
2:D:27:LEU:HD11	2:D:31:LEU:HD11	1.83	0.59
1:C:201:GLU:CA	1:C:204:MET:HE2	2.27	0.59
2:B:79:ASP:HB3	2:B:82:LEU:HB3	1.83	0.59
2:D:119:ARG:HD2	2:D:137:GLU:OE2	2.02	0.59
1:A:213:GLY:HA3	2:B:126:TYR:CD2	2.38	0.58
1:C:309:ILE:HG22	1:C:310:LYS:N	2.18	0.58
1:A:288:ILE:CG2	1:A:290:ILE:CD1	2.81	0.58
1:A:288:ILE:CG2	1:A:290:ILE:HD11	2.32	0.58
1:A:253:HIS:CE1	1:A:255:LYS:HB2	2.37	0.58
2:D:20:LYS:HG3	2:D:21:TYR:CE1	2.37	0.58
1:A:78:ALA:HB1	1:A:93:TRP:CD1	2.39	0.58
1:A:288:ILE:HG21	1:A:290:ILE:HD11	1.86	0.58
1:C:156:LEU:HD23	1:C:180:VAL:HG21	1.85	0.58
1:C:192:ASP:HB2	1:C:195:GLU:CG	2.31	0.58
1:A:307:ILE:HG21	1:A:309:ILE:HD11	1.86	0.58
1:C:35:LEU:HD13	1:C:94:MET:CE	2.34	0.58
1:C:197:LYS:HB2	1:C:240:ILE:HG12	1.86	0.57
2:B:38:ILE:HD13	2:B:207:ILE:HG12	1.86	0.57
1:C:290:ILE:HG22	1:C:292:THR:HG23	1.85	0.57
2:D:90:GLU:O	2:D:94:PHE:HD1	1.88	0.57
2:B:175:LEU:C	2:B:175:LEU:HD12	2.23	0.57
2:D:74:LEU:HD23	2:D:77:LEU:CD1	2.23	0.57
1:C:74:PHE:HB3	1:C:246:ILE:C	2.25	0.57
1:A:290:ILE:HG22	1:A:292:THR:HG23	1.86	0.57
1:C:309:ILE:HG22	1:C:310:LYS:H	1.70	0.57
2:B:18:LEU:HD13	2:B:25:ILE:O	2.04	0.57
1:A:49:VAL:HG12	1:A:49:VAL:O	2.04	0.57
2:D:27:LEU:CD1	2:D:31:LEU:HD11	2.35	0.57
1:A:282:THR:HG23	1:A:311:SER:HA	1.87	0.57
1:C:290:ILE:HG22	1:C:291:GLU:N	2.20	0.56
1:C:22:TYR:HE1	1:C:70:PRO:HG2	1.69	0.56
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.18	0.56
1:A:9:GLY:HA2	4:A:1007:SO4:O1	2.05	0.56
1:A:100:PHE:HA	5:A:1015:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LEU:HD11	2:B:199:ILE:CD1	2.34	0.56
1:C:265:ASN:HB3	1:C:268:ASP:HB2	1.85	0.56
2:D:48:THR:HG21	2:D:86:TYR:HD1	1.69	0.56
2:D:57:TYR:O	2:D:63:PRO:HB3	2.05	0.56
1:C:77:SER:HB3	1:C:99:LEU:HD11	1.87	0.56
1:A:73:LEU:HG	1:A:248:ILE:CD1	2.36	0.56
1:A:289:THR:HG23	1:A:303:ARG:H	1.69	0.56
1:C:75:TYR:CD2	1:C:248:ILE:HG12	2.41	0.56
1:A:51:HIS:HE1	1:A:91:LYS:NZ	2.03	0.56
2:B:133:ILE:C	2:B:134:ILE:HD13	2.26	0.56
1:A:211:TYR:CD1	1:A:222:VAL:HA	2.41	0.56
1:C:80:TYR:HB3	1:C:91:LYS:O	2.05	0.56
2:B:95:ARG:NH1	2:B:177:GLY:HA2	2.19	0.56
2:D:8:TYR:HB2	2:D:11:ILE:HD12	1.87	0.55
1:A:307:ILE:CG2	1:A:309:ILE:HG13	2.35	0.55
1:A:128:CYS:O	1:A:132:ASN:N	2.39	0.55
1:A:289:THR:HG22	1:A:302:ASN:CA	2.35	0.55
1:C:188:CYS:O	1:C:191:LEU:HG	2.06	0.55
1:A:169:LYS:HG2	1:A:262:ARG:NH2	2.22	0.55
1:C:289:THR:CG2	1:C:303:ARG:H	2.20	0.55
2:B:152:LEU:N	2:B:152:LEU:HD23	2.20	0.55
1:C:208:VAL:HG21	1:C:221:TRP:CD1	2.42	0.55
1:C:247:ARG:NE	4:C:1004:SO4:O4	2.32	0.55
2:B:7:LYS:C	2:B:9:PRO:HD3	2.27	0.55
1:C:111:ARG:HH21	1:C:292:THR:HG22	1.72	0.54
2:D:123:ILE:HD12	2:D:169:TYR:CE2	2.42	0.54
1:C:15:LYS:HE2	1:C:43:PHE:HB2	1.89	0.54
2:B:94:PHE:O	2:B:98:LEU:HD12	2.07	0.54
2:B:104:GLU:O	2:B:108:GLU:HG3	2.08	0.54
2:D:152:LEU:HD13	2:D:156:TRP:NE1	2.23	0.54
1:C:133:VAL:HG12	1:C:134:GLU:H	1.71	0.54
2:B:73:SER:HB3	2:B:207:ILE:HG21	1.89	0.54
1:A:289:THR:HA	1:A:301:LEU:O	2.07	0.54
2:B:151:ASP:CB	2:D:19:LYS:HG3	2.38	0.54
1:A:248:ILE:O	1:A:251:SER:HB3	2.08	0.54
1:C:279:THR:O	1:C:280:GLY:O	2.25	0.54
1:C:115:PHE:O	1:C:135:THR:HB	2.08	0.54
1:C:282:THR:HB	1:C:325:VAL:HG13	1.89	0.54
1:C:12:ASN:ND2	1:C:15:LYS:NZ	2.55	0.54
1:C:208:VAL:HG21	1:C:221:TRP:NE1	2.23	0.54
1:C:40:LEU:C	1:C:40:LEU:HD23	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:HB2	2:B:105:ASN:HD22	1.73	0.54
1:C:99:LEU:HB3	1:C:179[A]:HIS:HE1	1.73	0.54
1:A:64:LEU:HA	1:A:68:ASN:O	2.08	0.53
1:C:141:MET:CG	1:C:271:PHE:HZ	2.17	0.53
2:D:170:LEU:HA	2:D:174:GLN:OE1	2.08	0.53
1:C:42:PRO:HG2	1:C:45:SER:HB3	1.90	0.53
2:B:151:ASP:C	2:B:152:LEU:HD23	2.29	0.53
2:B:151:ASP:HA	2:D:19:LYS:HZ1	1.72	0.53
2:D:79:ASP:O	2:D:83:ILE:HG13	2.08	0.53
1:C:197:LYS:O	1:C:201:GLU:HG3	2.09	0.53
1:C:175:ASN:HB3	4:C:1001:SO4:O4	2.08	0.53
2:B:204:LYS:HE2	2:B:208:GLU:OE2	2.09	0.53
1:A:237:GLN:O	1:A:241:ASP:HB2	2.08	0.53
1:A:80:TYR:CD2	1:A:91:LYS:HB3	2.44	0.53
2:D:7:LYS:O	2:D:9:PRO:HD3	2.09	0.53
1:A:279:THR:O	1:A:280:GLY:O	2.26	0.53
1:A:221:TRP:O	1:A:225:LYS:HG2	2.09	0.53
1:C:74:PHE:HB3	1:C:246:ILE:O	2.08	0.53
1:C:131:ASP:O	1:C:133:VAL:HG23	2.09	0.53
1:A:112:SER:HB3	1:A:139:VAL:HG22	1.91	0.53
1:A:115:PHE:HZ	1:A:321:ASN:O	1.91	0.52
2:B:113:LEU:O	2:B:114:ASP:HB2	2.07	0.52
1:A:74:PHE:CD2	1:A:74:PHE:N	2.76	0.52
1:A:123:VAL:HB	1:A:135:THR:HG21	1.91	0.52
2:D:3:LEU:HD11	2:D:108:GLU:HG3	1.92	0.52
1:C:202:TYR:HD1	2:D:159:SER:HA	1.74	0.52
1:A:317:LEU:CD2	1:A:322:LEU:HD12	2.39	0.52
1:A:19:ARG:NH1	1:A:65:VAL:O	2.40	0.52
2:B:76:ILE:HD11	2:B:199:ILE:CD1	2.38	0.52
2:B:5:VAL:CG1	2:B:12:LYS:HG2	2.40	0.52
1:A:140:GLU:HG3	1:A:292:THR:HB	1.91	0.52
1:A:73:LEU:O	1:A:248:ILE:HG13	2.10	0.52
1:C:75:TYR:HD1	1:C:76:SER:O	1.93	0.52
1:A:290:ILE:CG2	1:A:292:THR:HG23	2.39	0.52
2:B:156:TRP:CH2	2:B:178:LEU:HD23	2.44	0.52
1:C:156:LEU:CD1	1:C:203:VAL:HG11	2.40	0.51
2:B:149:THR:HA	2:B:152:LEU:HG	1.92	0.51
2:B:8:TYR:HB2	2:B:11:ILE:HD12	1.91	0.51
2:B:5:VAL:CG2	2:B:12:LYS:HE2	2.34	0.51
1:C:289:THR:HG22	1:C:303:ARG:H	1.75	0.51
1:C:249:PRO:O	1:C:250:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:LYS:O	2:B:208:GLU:HG3	2.10	0.51
2:D:196:LEU:O	2:D:197:LYS:HB2	2.09	0.51
1:A:13:LEU:O	1:A:16:SER:HB2	2.10	0.51
2:B:73:SER:O	2:B:77:LEU:HG	2.11	0.51
2:B:7:LYS:HG2	2:B:58:VAL:HG21	1.92	0.51
2:B:80:VAL:HG22	2:D:34:SER:OG	2.11	0.51
1:A:40:LEU:HG	1:A:70:PRO:HB3	1.93	0.51
2:D:81:LYS:O	2:D:85:ARG:HG3	2.11	0.51
1:A:272:ASN:HB2	1:A:274:THR:OG1	2.10	0.51
2:D:95:ARG:HA	2:D:98:LEU:HD12	1.92	0.51
2:D:95:ARG:O	2:D:98:LEU:HB2	2.11	0.51
2:B:43:ASP:O	2:B:46:GLN:HB2	2.11	0.51
1:C:171:TYR:CE2	1:C:262:ARG:HB2	2.46	0.51
2:D:74:LEU:CD2	2:D:77:LEU:HD12	2.26	0.51
1:C:221:TRP:CE3	1:C:224:ARG:HB3	2.46	0.51
2:D:141:HIS:HD2	2:D:143:ILE:HG13	1.76	0.51
1:A:112:SER:HA	1:A:138:TYR:O	2.11	0.51
1:A:232:VAL:HG12	1:A:234:ILE:HG13	1.93	0.51
1:A:311:SER:O	1:A:315:ILE:HG12	2.10	0.51
2:B:7:LYS:HB3	2:B:97:LEU:HD13	1.93	0.50
2:D:45:ILE:CD1	2:D:77:LEU:HD11	2.36	0.50
1:C:138:TYR:CE1	1:C:322:LEU:HD11	2.47	0.50
2:B:134:ILE:N	2:B:134:ILE:HD13	2.26	0.50
2:D:5:VAL:CG2	2:D:12:LYS:HG2	2.40	0.50
1:A:14:ILE:HD11	1:A:318:HIS:CD2	2.46	0.50
1:A:213:GLY:O	1:A:214:GLY:O	2.29	0.50
1:C:232:VAL:HG12	1:C:234:ILE:CG1	2.35	0.50
2:D:20:LYS:HG3	2:D:21:TYR:CD1	2.47	0.50
1:A:258:LEU:HD22	1:A:275:LEU:CB	2.37	0.50
1:C:18:PHE:CD2	1:C:43:PHE:HZ	2.29	0.50
1:A:35:LEU:HD22	1:A:80:TYR:O	2.12	0.50
1:C:80:TYR:CD2	1:C:91:LYS:HB3	2.47	0.50
1:C:78:ALA:HB1	1:C:93:TRP:CD1	2.47	0.50
1:A:318:HIS:CE1	1:A:324:GLU:HA	2.46	0.50
1:C:220:GLY:C	1:C:222:VAL:H	2.14	0.50
1:A:288:ILE:HA	1:A:303:ARG:HB2	1.92	0.50
1:C:318:HIS:HB2	1:C:325:VAL:HG23	1.94	0.50
1:C:40:LEU:HB3	1:C:73:LEU:HD12	1.94	0.50
1:A:285:LEU:HD23	1:A:326:LYS:HE3	1.93	0.50
2:D:37:LEU:O	2:D:40:GLN:HB2	2.11	0.50
2:B:11:ILE:HG22	2:B:12:LYS:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:SER:HB3	1:C:177:GLY:O	2.11	0.49
1:A:213:GLY:HA3	2:B:126:TYR:CE2	2.47	0.49
1:C:148:ARG:NH2	4:C:1012:SO4:O2	2.43	0.49
2:B:78:ASN:HB3	2:D:36:THR:HG21	1.94	0.49
2:B:78:ASN:ND2	2:D:36:THR:HG23	2.28	0.49
1:C:150:LEU:HD21	1:C:266:LEU:O	2.11	0.49
1:C:216:GLU:HG2	1:C:226:ASN:O	2.11	0.49
2:B:132:ARG:CG	2:B:133:ILE:N	2.75	0.49
1:C:173:SER:HB3	1:C:177:GLY:C	2.32	0.49
2:D:108:GLU:OE1	2:D:108:GLU:HA	2.11	0.49
1:A:246:ILE:O	1:A:246:ILE:HG22	2.12	0.49
1:A:105:ASP:OD1	1:A:176:ARG:NH1	2.42	0.49
1:A:307:ILE:CG2	1:A:309:ILE:HD11	2.43	0.49
2:B:136:LYS:NZ	2:B:174:GLN:HE22	2.10	0.49
2:D:5:VAL:HG21	2:D:12:LYS:HG2	1.95	0.49
1:C:19:ARG:O	1:C:23:LEU:HB2	2.13	0.49
2:B:103:GLU:N	4:B:219:SO4:O1	2.40	0.49
1:C:125:SER:HB2	4:C:1011:SO4:O4	2.12	0.49
1:C:224:ARG:O	1:C:227:ARG:N	2.44	0.49
2:B:74:LEU:HD11	2:B:86:TYR:CD2	2.48	0.49
2:D:139:CYS:HB2	2:D:167:TYR:HB3	1.95	0.49
2:B:3:LEU:HD13	2:B:11:ILE:HD11	1.94	0.49
1:A:197:LYS:HA	1:A:240:ILE:CG1	2.42	0.49
1:A:78:ALA:HB1	1:A:93:TRP:HD1	1.76	0.49
2:D:123:ILE:HD12	2:D:169:TYR:CD2	2.48	0.49
1:A:123:VAL:CB	1:A:135:THR:HG21	2.43	0.49
1:A:91:LYS:O	1:A:92:ALA:HB3	2.13	0.49
1:C:98:LEU:HD13	1:C:196:ARG:NH1	2.27	0.49
2:B:151:ASP:CG	2:D:19:LYS:HG3	2.34	0.48
2:D:200:PRO:HB3	4:D:215:SO4:O2	2.13	0.48
2:D:48:THR:HG21	2:D:86:TYR:CD1	2.47	0.48
2:D:92:LYS:HA	2:D:95:ARG:HD3	1.94	0.48
1:A:201:GLU:HB3	1:A:206:ILE:HB	1.95	0.48
1:A:289:THR:HG22	1:A:303:ARG:H	1.76	0.48
2:B:44:ARG:HH12	2:B:55:PRO:HG2	1.77	0.48
2:B:103:GLU:HG2	2:B:138:PHE:HZ	1.78	0.48
1:C:133:VAL:CG1	1:C:134:GLU:N	2.76	0.48
1:A:278:PHE:CD1	1:A:315:ILE:HG13	2.48	0.48
1:C:88:MET:CE	1:C:243:LYS:HD2	2.43	0.48
2:B:41:ALA:HA	2:B:70:THR:HG22	1.95	0.48
1:A:169:LYS:HG2	1:A:262:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:C	2:B:100:THR:H	2.16	0.48
1:C:218:ALA:CB	1:C:222:VAL:HG12	2.44	0.48
1:C:208:VAL:HG12	1:C:225:LYS:HE3	1.95	0.48
2:B:127:LEU:HD23	2:B:130:LYS:HG2	1.95	0.48
2:D:144:ASP:O	2:D:147:LYS:HB3	2.13	0.48
2:B:162:ILE:O	2:B:162:ILE:HG22	2.13	0.48
1:C:40:LEU:HD22	1:C:49:VAL:HB	1.96	0.48
1:A:119:CYS:HA	1:A:303:ARG:HH22	1.78	0.48
1:C:196:ARG:NE	1:C:242:VAL:HG22	2.29	0.48
2:D:107:LEU:HD21	2:D:119:ARG:HG3	1.95	0.48
1:A:15:LYS:HE2	1:A:43:PHE:CB	2.44	0.48
2:B:8:TYR:O	2:B:11:ILE:HB	2.14	0.48
1:A:197:LYS:CB	1:A:240:ILE:HG12	2.42	0.48
2:D:199:ILE:HG22	2:D:200:PRO:N	2.28	0.48
1:C:232:VAL:HG11	1:C:234:ILE:HD11	1.96	0.47
2:D:103:GLU:HG3	4:D:214:SO4:O1	2.14	0.47
2:D:3:LEU:CD1	2:D:108:GLU:HG3	2.44	0.47
1:A:218:ALA:CB	1:A:222:VAL:HG12	2.43	0.47
1:A:14:ILE:HG13	1:A:318:HIS:CD2	2.49	0.47
2:B:42:LYS:O	2:B:46:GLN:HG2	2.14	0.47
1:A:253:HIS:HE1	1:A:255:LYS:HB2	1.78	0.47
2:B:69:THR:O	2:B:73:SER:OG	2.28	0.47
1:A:288:ILE:CG2	1:A:289:THR:N	2.76	0.47
2:B:192:ARG:HD2	2:D:32:LEU:HD13	1.93	0.47
1:C:12:ASN:HB3	1:C:15:LYS:HB2	1.96	0.47
2:B:78:ASN:HB3	2:D:36:THR:HG23	1.96	0.47
1:C:143:SER:HA	1:C:271:PHE:HD2	1.78	0.47
1:C:115:PHE:CG	1:C:288:ILE:CD1	2.98	0.47
1:C:74:PHE:CB	1:C:247:ARG:HA	2.42	0.47
2:B:144:ASP:HB3	2:B:148:TYR:CE1	2.50	0.47
2:D:45:ILE:HD13	2:D:77:LEU:CD1	2.41	0.47
1:C:208:VAL:N	2:D:159:SER:HB2	2.29	0.47
2:B:45:ILE:HD12	2:B:77:LEU:HD11	1.95	0.47
2:D:8:TYR:O	2:D:11:ILE:HG13	2.15	0.47
2:B:123:ILE:HD11	2:B:169:TYR:CZ	2.50	0.47
2:B:170:LEU:HD22	2:B:174:GLN:HB3	1.96	0.47
2:B:144:ASP:O	2:B:147:LYS:HB3	2.14	0.47
2:B:164:HIS:NE2	2:B:165:LYS:HD2	2.30	0.47
1:C:310:LYS:HZ3	1:C:310:LYS:HB2	1.78	0.47
2:B:123:ILE:HD12	2:B:169:TYR:CE2	2.50	0.47
1:A:249:PRO:HA	1:A:260:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:THR:HG22	2:B:54:LEU:HD21	1.97	0.47
1:C:67:ARG:O	1:C:68:ASN:ND2	2.48	0.47
2:B:77:LEU:O	2:B:78:ASN:HB2	2.15	0.46
1:C:218:ALA:HB3	1:C:223:GLY:H	1.78	0.46
1:C:74:PHE:CD1	1:C:247:ARG:HA	2.50	0.46
1:C:138:TYR:HE2	1:C:292:THR:HG21	1.80	0.46
1:C:149:GLY:O	1:C:153:THR:HG23	2.15	0.46
2:D:161:GLN:HA	2:D:161:GLN:NE2	2.29	0.46
2:B:127:LEU:CB	2:B:134:ILE:HG12	2.45	0.46
2:B:134:ILE:HG22	2:B:135:GLN:N	2.30	0.46
1:C:77:SER:CB	1:C:99:LEU:HD11	2.46	0.46
2:D:152:LEU:HB3	2:D:156:TRP:CD1	2.50	0.46
2:D:9:PRO:O	2:D:11:ILE:N	2.49	0.46
2:B:47:LYS:NZ	2:B:55:PRO:HG3	2.29	0.46
1:A:236:GLU:HB2	1:A:240:ILE:HD12	1.97	0.46
1:A:234:ILE:CG2	1:A:235:ASP:N	2.78	0.46
2:D:175:LEU:HD12	2:D:175:LEU:O	2.15	0.46
1:A:259:ILE:HG22	1:A:260:VAL:N	2.29	0.46
2:B:199:ILE:CG2	2:B:200:PRO:HD2	2.43	0.46
1:C:258:LEU:HD22	1:C:275:LEU:HB2	1.97	0.46
1:A:273:GLU:CD	1:A:273:GLU:H	2.18	0.46
2:B:199:ILE:CG2	2:B:200:PRO:N	2.79	0.46
1:A:273:GLU:HA	1:A:295:LEU:HD13	1.97	0.46
1:C:61:ARG:O	1:C:63:TYR:N	2.48	0.46
1:A:116:CYS:SG	1:A:118:VAL:HB	2.56	0.45
1:A:290:ILE:HG22	1:A:291:GLU:N	2.30	0.45
1:C:74:PHE:N	1:C:74:PHE:CD2	2.84	0.45
1:C:223:GLY:O	1:C:227:ARG:HG3	2.16	0.45
1:C:290:ILE:CG2	1:C:291:GLU:N	2.79	0.45
2:B:192:ARG:N	2:B:193:PRO:CD	2.79	0.45
2:D:107:LEU:HD11	2:D:119:ARG:NE	2.31	0.45
2:B:120:CYS:O	2:B:122:PRO:N	2.49	0.45
1:A:213:GLY:HA3	2:B:126:TYR:HD2	1.82	0.45
2:B:188:VAL:O	2:D:33:ASN:ND2	2.48	0.45
2:D:106:LEU:HA	2:D:109:ILE:HD12	1.98	0.45
2:D:152:LEU:HD13	2:D:156:TRP:CD1	2.51	0.45
2:D:20:LYS:HB3	2:D:20:LYS:HE3	1.72	0.45
1:C:284:PHE:CZ	1:C:323:GLY:CA	3.00	0.45
2:B:123:ILE:HD12	2:B:169:TYR:CD2	2.51	0.45
2:D:5:VAL:HG21	2:D:12:LYS:CG	2.46	0.45
1:A:262:ARG:CG	1:A:262:ARG:NH1	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLU:HG2	2:B:187:ILE:CD1	2.46	0.45
1:C:156:LEU:HD13	1:C:203:VAL:HG11	1.98	0.45
1:A:288:ILE:HG22	1:A:290:ILE:CG1	2.45	0.45
1:C:74:PHE:HB3	1:C:247:ARG:N	2.32	0.45
2:B:43:ASP:OD1	2:B:47:LYS:HE3	2.17	0.45
1:C:33:MET:HG3	1:C:54:PHE:O	2.17	0.45
1:C:62:ASP:O	1:C:66:ASN:HB2	2.17	0.45
1:A:309:ILE:CG2	1:A:310:LYS:N	2.76	0.45
1:C:198:GLU:OE2	2:D:158:LEU:HB2	2.17	0.45
1:A:248:ILE:HA	1:A:249:PRO:HD2	1.77	0.45
2:B:199:ILE:HG22	2:B:200:PRO:N	2.30	0.45
1:A:161:GLU:HG2	1:A:168:PRO:HD3	1.99	0.45
1:A:309:ILE:CG2	1:A:310:LYS:H	2.28	0.45
1:A:197:LYS:HA	1:A:240:ILE:HG13	1.99	0.45
1:A:153:THR:HG21	1:A:178:PHE:HB2	1.98	0.45
2:B:10:PHE:HE2	2:B:94:PHE:CE2	2.35	0.45
1:A:236:GLU:O	1:A:239:THR:N	2.50	0.44
2:D:103:GLU:OE1	2:D:119:ARG:NH1	2.50	0.44
1:C:258:LEU:HA	1:C:258:LEU:HD23	1.87	0.44
1:C:60:LEU:O	1:C:63:TYR:HB3	2.17	0.44
1:C:104:ALA:HA	1:C:107:LEU:HB3	1.99	0.44
2:D:14:LEU:HB2	2:D:68:TYR:CD1	2.52	0.44
1:A:36:ARG:NH2	1:A:97:ASP:OD2	2.50	0.44
1:C:115:PHE:CG	1:C:288:ILE:HD12	2.52	0.44
1:C:72:HIS:CE1	1:C:254:GLY:HA3	2.51	0.44
1:C:280:GLY:HA3	1:C:328:TYR:CE1	2.34	0.44
2:B:135:GLN:HG3	2:B:135:GLN:O	2.15	0.44
1:A:73:LEU:HG	1:A:248:ILE:HD12	1.98	0.44
1:C:260:VAL:O	1:C:260:VAL:HG12	2.17	0.44
2:B:20:LYS:HG3	2:B:20:LYS:H	1.46	0.44
2:B:207:ILE:HG22	2:B:207:ILE:O	2.18	0.44
2:B:44:ARG:NH1	2:B:55:PRO:HG2	2.32	0.44
2:B:127:LEU:HB2	2:B:134:ILE:HG12	1.99	0.44
2:D:5:VAL:HG12	2:D:5:VAL:O	2.17	0.44
1:A:14:ILE:CD1	1:A:318:HIS:CD2	3.01	0.44
1:A:241:ASP:HB3	1:A:244:ARG:HG3	1.99	0.44
1:A:79:ARG:HH22	1:A:189:ALA:CB	2.31	0.44
1:C:201:GLU:CA	1:C:204:MET:CE	2.89	0.44
2:D:27:LEU:CD1	2:D:31:LEU:CD1	2.96	0.44
1:C:110:LEU:HD13	1:C:141:MET:HE2	1.97	0.44
1:A:288:ILE:HG22	1:A:289:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:THR:HB	2:B:203:LEU:HD22	2.00	0.44
1:A:289:THR:C	1:A:290:ILE:HG13	2.39	0.44
1:C:273:GLU:H	1:C:273:GLU:CD	2.22	0.44
1:A:161:GLU:O	1:A:165:GLY:HA2	2.18	0.43
2:D:122:PRO:HB3	2:D:137:GLU:HB2	1.99	0.43
2:B:186:LYS:HD3	2:B:186:LYS:HA	1.63	0.43
2:B:5:VAL:HG11	2:B:12:LYS:CG	2.47	0.43
1:A:288:ILE:CG2	1:A:290:ILE:HG13	2.45	0.43
2:B:127:LEU:HG	2:B:129:LYS:H	1.83	0.43
2:B:123:ILE:CD1	2:B:169:TYR:CZ	3.01	0.43
2:B:113:LEU:HD12	2:B:179:ILE:HG23	2.00	0.43
1:A:114:ARG:HG2	1:A:123:VAL:O	2.16	0.43
1:A:256:SER:OG	1:A:258:LEU:HB2	2.19	0.43
2:B:199:ILE:HG23	2:B:200:PRO:CD	2.42	0.43
2:D:140:VAL:HG23	2:D:170:LEU:HD12	1.99	0.43
1:C:285:LEU:HD11	1:C:304:GLY:O	2.19	0.43
2:B:32:LEU:HA	2:B:32:LEU:HD23	1.71	0.43
1:C:39:ALA:HA	1:C:49:VAL:O	2.19	0.43
1:A:171:TYR:CD2	1:A:262:ARG:HB2	2.54	0.43
2:D:199:ILE:CG2	2:D:200:PRO:N	2.81	0.43
1:C:172:PHE:CD1	1:C:269:PHE:CZ	3.06	0.43
2:B:141:HIS:HB2	2:B:167:TYR:CE2	2.54	0.43
1:A:222:VAL:O	1:A:226:ASN:ND2	2.44	0.43
1:A:163:ASP:O	2:B:163:LEU:HD12	2.18	0.43
1:C:256:SER:OG	1:C:258:LEU:HB2	2.19	0.43
1:A:108:CYS:HB3	1:A:145:CYS:HB2	1.96	0.43
2:D:27:LEU:HG	2:D:31:LEU:HD11	2.01	0.43
1:A:156:LEU:HD22	1:A:234:ILE:HD11	2.00	0.43
1:A:258:LEU:HD11	1:A:295:LEU:HD21	2.01	0.43
1:A:219:PRO:HG3	2:B:123:ILE:CG2	2.48	0.43
1:C:108:CYS:HA	1:C:148:ARG:HH11	1.84	0.43
1:C:184:CYS:O	1:C:184:CYS:SG	2.76	0.43
1:A:118:VAL:HG12	1:A:119:CYS:N	2.33	0.43
1:A:290:ILE:CG2	1:A:291:GLU:N	2.82	0.43
2:D:54:LEU:O	2:D:93:GLN:HG3	2.19	0.43
1:A:48:TYR:HD1	4:A:1004:SO4:O3	2.02	0.43
2:D:27:LEU:C	2:D:27:LEU:HD12	2.39	0.42
1:A:73:LEU:CG	1:A:248:ILE:HD12	2.49	0.42
1:A:119:CYS:CA	1:A:303:ARG:NH2	2.79	0.42
1:C:138:TYR:CD2	1:C:322:LEU:HD21	2.54	0.42
2:B:48:THR:HG21	2:B:86:TYR:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PRO:CG	2:B:123:ILE:HG21	2.47	0.42
2:D:88:TYR:O	2:D:91:ALA:HB3	2.20	0.42
2:D:170:LEU:HD22	2:D:174:GLN:HB3	2.00	0.42
2:D:75:ALA:CB	2:D:194:LEU:CB	2.98	0.42
1:C:109:LYS:HD2	4:C:1012:SO4:O1	2.19	0.42
1:A:173:SER:HB2	1:A:179[B]:HIS:CE1	2.54	0.42
2:B:161:GLN:NE2	5:B:1009:HOH:O	2.52	0.42
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.88	0.42
1:A:215:SER:O	1:A:223:GLY:HA2	2.19	0.42
1:C:287:TYR:CD1	1:C:323:GLY:CA	3.00	0.42
2:B:130:LYS:CG	2:B:134:ILE:HD11	2.49	0.42
1:A:222:VAL:CG2	2:B:162:ILE:HD11	2.49	0.42
1:A:40:LEU:HD23	1:A:40:LEU:C	2.40	0.42
2:D:162:ILE:HG22	2:D:162:ILE:O	2.18	0.42
2:B:145:TYR:CZ	2:B:149:THR:HG21	2.55	0.42
2:D:83:ILE:HG23	2:D:191:ILE:HD12	2.01	0.42
2:D:191:ILE:HG22	2:D:191:ILE:O	2.18	0.42
2:D:5:VAL:HG21	2:D:12:LYS:CE	2.50	0.42
1:C:247:ARG:HG2	1:C:260:VAL:HG21	2.02	0.42
1:C:191:LEU:HD23	1:C:195:GLU:OE1	2.20	0.42
1:C:317:LEU:HD23	1:C:322:LEU:HD12	2.01	0.42
1:A:262:ARG:O	1:A:264:PRO:HD3	2.20	0.42
2:B:139:CYS:HB2	2:B:167:TYR:HB3	2.01	0.42
2:D:27:LEU:CG	2:D:31:LEU:HD11	2.49	0.42
2:B:78:ASN:ND2	2:D:36:THR:CG2	2.82	0.42
1:A:307:ILE:HG22	1:A:308:LYS:N	2.34	0.42
2:D:91:ALA:O	2:D:95:ARG:HG3	2.18	0.42
1:C:170:VAL:HG22	1:C:180:VAL:HG22	2.02	0.42
1:C:115:PHE:CB	1:C:288:ILE:HD11	2.49	0.42
1:C:61:ARG:C	1:C:63:TYR:H	2.23	0.42
1:A:40:LEU:C	1:A:40:LEU:CD2	2.88	0.41
1:A:244:ARG:NH1	4:A:1005:SO4:S	2.93	0.41
2:B:196:LEU:HD13	2:D:202:LYS:HZ2	1.86	0.41
1:C:80:TYR:OH	1:C:243:LYS:HG3	2.20	0.41
1:C:215:SER:HB2	4:C:1007:SO4:O2	2.20	0.41
2:D:11:ILE:O	2:D:11:ILE:HG22	2.20	0.41
1:C:98:LEU:HD13	1:C:196:ARG:HH11	1.85	0.41
1:A:17:PHE:CD1	1:A:315:ILE:CD1	3.02	0.41
1:A:63:TYR:CD1	1:A:67:ARG:HD2	2.56	0.41
2:D:184:LYS:O	2:D:188:VAL:HG23	2.20	0.41
1:A:288:ILE:HB	1:A:290:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:HG22	1:A:290:ILE:CD1	2.50	0.41
1:C:133:VAL:CG1	1:C:134:GLU:H	2.32	0.41
1:A:152:GLN:OE1	1:A:232:VAL:HA	2.21	0.41
2:B:141:HIS:HB2	2:B:167:TYR:HE2	1.86	0.41
1:C:218:ALA:CB	1:C:219:PRO:CD	2.88	0.41
1:A:222:VAL:HG21	2:B:162:ILE:HD11	2.02	0.41
1:A:307:ILE:CG2	1:A:309:ILE:CG1	2.98	0.41
1:C:220:GLY:O	1:C:222:VAL:N	2.52	0.41
2:B:170:LEU:HD23	2:B:174:GLN:OE1	2.21	0.41
1:A:173:SER:HB3	1:A:177:GLY:C	2.41	0.41
1:A:151:GLU:O	1:A:154:ARG:N	2.52	0.41
1:A:110:LEU:HD13	1:A:141:MET:HA	2.02	0.41
1:C:156:LEU:HD13	1:C:234:ILE:CD1	2.50	0.41
2:B:199:ILE:CG2	2:B:200:PRO:CD	2.99	0.41
1:A:307:ILE:CG2	1:A:309:ILE:CD1	2.99	0.41
1:A:282:THR:CG2	1:A:311:SER:HA	2.51	0.41
2:B:141:HIS:HA	2:B:167:TYR:CD2	2.56	0.41
1:C:283:ILE:HD12	1:C:327:ALA:HB3	2.03	0.41
2:B:66:VAL:HA	2:B:69:THR:OG1	2.21	0.41
1:A:318:HIS:CG	1:A:325:VAL:HG23	2.56	0.41
1:A:64:LEU:HD22	1:A:70:PRO:CG	2.50	0.41
1:C:72:HIS:CE1	1:C:254:GLY:CA	3.04	0.41
2:B:141:HIS:HD2	2:B:143:ILE:HB	1.86	0.41
1:A:108:CYS:O	1:A:109:LYS:HB2	2.21	0.41
1:C:238:VAL:HG22	1:C:244:ARG:CZ	2.50	0.41
1:A:75:TYR:CD1	1:A:75:TYR:C	2.95	0.41
1:A:259:ILE:CG2	1:A:260:VAL:N	2.84	0.41
2:B:73:SER:HB3	2:B:207:ILE:CG2	2.51	0.41
1:C:141:MET:CG	1:C:271:PHE:CZ	2.97	0.41
2:D:105:ASN:O	2:D:108:GLU:HB3	2.21	0.41
1:C:276:SER:HA	1:C:277:PRO:HD3	1.98	0.41
1:C:78:ALA:CB	1:C:96:SER:HB3	2.49	0.40
1:C:224:ARG:O	1:C:227:ARG:HB2	2.20	0.40
1:C:316:TYR:CE2	1:C:320:ARG:HG2	2.55	0.40
1:C:15:LYS:HE2	1:C:43:PHE:CB	2.51	0.40
1:C:57:SER:O	1:C:60:LEU:HB3	2.21	0.40
2:B:26:THR:O	2:B:29:ASP:HB2	2.21	0.40
1:A:218:ALA:HB1	1:A:222:VAL:HB	2.03	0.40
1:A:115:PHE:CG	1:A:288:ILE:HD11	2.56	0.40
1:C:172:PHE:CD2	1:C:174:GLY:HA2	2.57	0.40
1:A:15:LYS:HE2	1:A:43:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ARG:CG	2:D:44:ARG:HH11	2.31	0.40
2:B:136:LYS:HZ1	2:B:174:GLN:HE22	1.70	0.40
2:D:107:LEU:HD11	2:D:119:ARG:CZ	2.51	0.40
1:A:98:LEU:O	1:A:99:LEU:HD23	2.21	0.40
2:D:42:LYS:HE2	2:D:206:LEU:O	2.20	0.40
2:B:78:ASN:CG	2:D:36:THR:HG23	2.42	0.40
2:D:44:ARG:NH2	2:D:90:GLU:OE2	2.54	0.40
2:B:130:LYS:C	2:B:132:ARG:N	2.74	0.40
1:C:115:PHE:CG	1:C:288:ILE:HD11	2.57	0.40
2:B:130:LYS:CB	2:B:134:ILE:HD11	2.51	0.40
2:B:30:LEU:O	2:B:34:SER:N	2.47	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	326/330 (99%)	285 (87%)	33 (10%)	8 (2%)	7	39
1	C	319/330 (97%)	272 (85%)	37 (12%)	10 (3%)	5	34
2	B	205/212 (97%)	184 (90%)	18 (9%)	3 (2%)	13	50
2	D	198/212 (93%)	168 (85%)	23 (12%)	7 (4%)	4	31
All	All	1048/1084 (97%)	909 (87%)	111 (11%)	28 (3%)	6	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLY
1	A	219	PRO
1	A	280	GLY
1	C	218	ALA

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Mol	Chain	Res	Type
1	C	219	PRO
1	C	280	GLY
1	A	186	GLY
1	C	221	TRP
2	D	10	PHE
1	C	62	ASP
1	C	175	ASN
1	C	264	PRO
2	D	103	GLU
1	A	67	ARG
1	C	97	ASP
2	D	53	GLU
2	D	161	GLN
2	B	99	HIS
2	B	196	LEU
2	D	150	LYS
2	D	153	LYS
1	A	206	ILE
1	C	260	VAL
2	B	121	ASP
1	A	118	VAL
1	A	264	PRO
1	C	304	GLY
2	D	121	ASP

### 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	292/293 (100%)	279 (96%)	13 (4%)	34	72
1	C	286/293 (98%)	271 (95%)	15 (5%)	29	67
2	B	194/197 (98%)	173 (89%)	21 (11%)	8	32
2	D	188/197 (95%)	183 (97%)	5 (3%)	52	82
All	All	960/980 (98%)	906 (94%)	54 (6%)	26	65

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	40	LEU
1	A	46	ASP
1	A	56	SER
1	A	74	PHE
1	A	145	CYS
1	A	154	ARG
1	A	173	SER
1	A	225	LYS
1	A	241	ASP
1	A	248	ILE
1	A	273	GLU
1	A	312	SER
1	C	33	MET
1	C	40	LEU
1	C	56	SER
1	C	74	PHE
1	C	88	MET
1	C	108	CYS
1	C	181	GLN
1	C	188	CYS
1	C	192	ASP
1	C	221	TRP
1	C	251	SER
1	C	262	ARG
1	C	267	ASP
1	C	310	LYS
1	C	320	ARG
2	B	13	SER
2	B	20	LYS
2	B	26	THR
2	B	38	ILE
2	B	44	ARG
2	B	48	THR
2	B	49	LYS
2	B	70	THR
2	B	73	SER
2	B	103	GLU
2	B	117	ILE
2	B	135	GLN
2	B	137	GLU
2	B	142	PHE

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Mol	Chain	Res	Type
2	B	162	ILE
2	B	163	LEU
2	B	175	LEU
2	B	178	LEU
2	B	182	SER
2	B	186	LYS
2	B	188	VAL
2	D	42	LYS
2	D	44	ARG
2	D	96	SER
2	D	181	GLU
2	D	185	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	C	12	ASN
1	C	68	ASN
1	C	72	HIS
1	C	106	HIS
1	C	226	ASN
2	B	56	HIS
2	B	78	ASN
2	B	105	ASN
2	B	141	HIS
2	B	174	GLN
2	D	135	GLN
2	D	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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	$\# Z  > 2$
4	SO4	A	1000	-	4,4,4	0.63	0	6,6,6	0.77	0
4	SO4	A	1001	-	4,4,4	0.56	0	6,6,6	0.72	0
4	SO4	A	1002	-	4,4,4	0.55	0	6,6,6	0.72	0
4	SO4	A	1003	-	4,4,4	0.57	0	6,6,6	0.73	0
4	SO4	A	1004	-	4,4,4	0.57	0	6,6,6	0.73	0
4	SO4	A	1005	-	4,4,4	0.59	0	6,6,6	0.73	0
4	SO4	A	1006	-	4,4,4	0.57	0	6,6,6	0.74	0
4	SO4	A	1007	-	4,4,4	0.56	0	6,6,6	0.73	0
4	SO4	A	1008	-	4,4,4	0.60	0	6,6,6	0.73	0
4	SO4	A	1009	-	4,4,4	0.57	0	6,6,6	0.73	0
4	SO4	A	1010	-	4,4,4	0.57	0	6,6,6	0.73	0
4	SO4	A	1011	-	4,4,4	0.58	0	6,6,6	0.72	0
4	SO4	A	1012	-	4,4,4	0.57	0	6,6,6	0.74	0
4	SO4	B	213	-	4,4,4	0.57	0	6,6,6	0.73	0
4	SO4	B	214	-	4,4,4	0.58	0	6,6,6	0.74	0
4	SO4	B	215	-	4,4,4	0.56	0	6,6,6	0.72	0
4	SO4	B	216	-	4,4,4	0.58	0	6,6,6	0.72	0
4	SO4	B	217	-	4,4,4	0.56	0	6,6,6	0.73	0
4	SO4	B	218	-	4,4,4	0.56	0	6,6,6	0.74	0
4	SO4	B	219	-	4,4,4	0.57	0	6,6,6	0.72	0
4	SO4	B	220	-	4,4,4	0.55	0	6,6,6	0.56	0
4	SO4	C	1000	-	4,4,4	0.61	0	6,6,6	0.77	0
4	SO4	C	1001	-	4,4,4	0.58	0	6,6,6	0.77	0
4	SO4	C	1002	-	4,4,4	0.56	0	6,6,6	0.74	0
4	SO4	C	1003	-	4,4,4	0.55	0	6,6,6	0.72	0
4	SO4	C	1004	-	4,4,4	0.56	0	6,6,6	0.75	0
4	SO4	C	1005	-	4,4,4	0.56	0	6,6,6	0.73	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	1006	-	4,4,4	0.57	0	6,6,6	0.72	0
4	SO4	C	1007	-	4,4,4	0.56	0	6,6,6	0.72	0
4	SO4	C	1008	-	4,4,4	0.62	0	6,6,6	0.71	0
4	SO4	C	1009	-	4,4,4	0.56	0	6,6,6	0.73	0
4	SO4	C	1010	-	4,4,4	0.58	0	6,6,6	0.72	0
4	SO4	C	1011	-	4,4,4	0.59	0	6,6,6	0.72	0
4	SO4	C	1012	-	4,4,4	0.56	0	6,6,6	0.70	0
4	SO4	C	1013	-	4,4,4	0.60	0	6,6,6	0.71	0
4	SO4	C	1014	-	4,4,4	1.49	0	6,6,6	1.71	1 (16%)
4	SO4	D	213	-	4,4,4	0.56	0	6,6,6	0.72	0
4	SO4	D	214	-	4,4,4	0.53	0	6,6,6	0.71	0
4	SO4	D	215	-	4,4,4	0.56	0	6,6,6	0.72	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
4	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1009	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1010	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1011	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1012	-	-	0/0/0/0	0/0/0/0
4	SO4	B	213	-	-	0/0/0/0	0/0/0/0
4	SO4	B	214	-	-	0/0/0/0	0/0/0/0
4	SO4	B	215	-	-	0/0/0/0	0/0/0/0
4	SO4	B	216	-	-	0/0/0/0	0/0/0/0
4	SO4	B	217	-	-	0/0/0/0	0/0/0/0
4	SO4	B	218	-	-	0/0/0/0	0/0/0/0
4	SO4	B	219	-	-	0/0/0/0	0/0/0/0
4	SO4	B	220	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1000	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1008	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1009	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1010	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1011	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1012	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1013	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1014	-	-	0/0/0/0	0/0/0/0
4	SO4	D	213	-	-	0/0/0/0	0/0/0/0
4	SO4	D	214	-	-	0/0/0/0	0/0/0/0
4	SO4	D	215	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1014	SO4	O4-S-O3	4.04	125.39	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	SO4	1	0
4	A	1004	SO4	1	0
4	A	1005	SO4	2	0
4	A	1007	SO4	1	0
4	B	219	SO4	1	0
4	C	1001	SO4	1	0
4	C	1004	SO4	1	0
4	C	1006	SO4	1	0
4	C	1007	SO4	1	0
4	C	1011	SO4	1	0
4	C	1012	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	214	SO4	1	0
4	D	215	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	327/330 (99%)	0.02	6 (1%) 71 70	44, 70, 118, 148	1 (0%)
1	C	320/330 (96%)	-0.04	4 (1%) 79 80	29, 80, 117, 138	0
2	B	207/212 (97%)	-0.07	1 (0%) 91 92	55, 86, 117, 132	0
2	D	202/212 (95%)	0.26	10 (4%) 32 32	74, 111, 144, 155	0
All	All	1056/1084 (97%)	0.03	21 (1%) 68 67	29, 85, 131, 155	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	3.4
2	D	119	ARG	3.2
1	A	124	VAL	2.9
2	D	172	LYS	2.9
1	A	121	ASN	2.8
2	D	194	LEU	2.7
1	A	91	LYS	2.7
1	A	129	GLU	2.6
2	D	133	ILE	2.6
1	A	130	ARG	2.4
2	D	125	PHE	2.3
1	C	130	ARG	2.3
1	C	11	THR	2.3
2	D	135	GLN	2.2
2	D	120	CYS	2.2
1	C	12	ASN	2.2
1	C	46	ASP	2.2
2	B	133	ILE	2.2
1	A	123	VAL	2.1
2	D	201	GLU	2.1
2	D	57	TYR	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
4	SO4	C	1006	5/5	0.64	0.41	4.94	188,188,188,188	0
4	SO4	C	1004	5/5	0.74	0.40	4.56	172,172,172,172	5
4	SO4	A	1009	5/5	0.75	0.39	3.58	182,182,182,182	5
4	SO4	A	1000	5/5	0.82	0.28	1.54	107,107,107,107	0
4	SO4	C	1000	5/5	0.85	0.28	1.27	130,130,130,130	5
4	SO4	C	1001	5/5	0.89	0.21	-0.29	112,112,113,113	0
4	SO4	B	218	5/5	0.79	0.20	-0.80	171,171,171,171	0
3	ZN	C	999	1/1	0.97	0.06	-1.31	88,88,88,88	0
3	ZN	A	999	1/1	0.97	0.03	-2.23	104,104,104,104	0
4	SO4	A	1006	5/5	0.73	0.20	-	160,160,160,160	0
4	SO4	A	1004	5/5	0.70	0.48	-	179,179,180,180	0
4	SO4	D	214	5/5	0.54	0.39	-	194,194,194,194	0
4	SO4	B	217	5/5	0.92	0.25	-	169,169,169,169	0
4	SO4	C	1007	5/5	0.76	0.34	-	201,201,201,201	0
4	SO4	A	1007	5/5	0.66	0.59	-	197,197,197,197	5
4	SO4	C	1010	5/5	0.88	0.29	-	161,161,161,161	0
4	SO4	A	1003	5/5	0.86	0.24	-	156,156,156,156	0
4	SO4	B	216	5/5	0.75	0.44	-	188,188,188,188	0
4	SO4	C	1011	5/5	0.88	0.28	-	159,159,159,159	5
4	SO4	C	1005	5/5	0.79	0.32	-	180,180,180,180	0
4	SO4	C	1013	5/5	0.83	0.20	-	158,158,158,158	0
4	SO4	C	1012	5/5	0.51	0.37	-	157,157,157,158	5
4	SO4	A	1008	5/5	0.85	0.15	-	153,153,153,153	0
4	SO4	B	220	5/5	0.74	0.35	-	155,155,155,155	5
4	SO4	B	213	5/5	0.78	0.29	-	172,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	214	5/5	0.73	0.34	-	162,162,162,162	0
4	SO4	A	1002	5/5	0.84	0.42	-	153,153,153,153	0
4	SO4	D	213	5/5	0.82	0.32	-	162,162,162,162	5
4	SO4	A	1011	5/5	0.89	0.42	-	153,153,153,153	0
4	SO4	C	1009	5/5	0.62	0.44	-	186,186,186,186	0
4	SO4	A	1012	5/5	0.72	0.50	-	161,161,161,161	5
4	SO4	A	1005	5/5	0.39	0.56	-	186,186,186,186	5
4	SO4	C	1014	5/5	0.78	0.40	-	152,152,152,152	5
4	SO4	C	1003	5/5	0.81	0.21	-	170,170,170,170	0
4	SO4	B	215	5/5	0.72	0.41	-	179,179,179,179	5
4	SO4	A	1010	5/5	0.83	0.28	-	175,175,175,175	0
4	SO4	B	219	5/5	0.70	0.30	-	179,179,179,179	0
4	SO4	C	1002	5/5	0.84	0.28	-	151,151,151,151	0
4	SO4	C	1008	5/5	0.87	0.33	-	171,171,171,171	0
4	SO4	D	215	5/5	0.75	0.29	-	164,164,164,164	5
4	SO4	A	1001	5/5	0.93	0.21	-	138,138,138,138	0

## 6.5 Other polymers

There are no such residues in this entry.