



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:03 pm BST

PDB ID : 3BL5  
Title : Crystal structure of QueC from Bacillus subtilis: an enzyme involved in preQ1 biosynthesis  
Authors : Cicmil, N.; Huang, R.H.  
Deposited on : 2007-12-10  
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

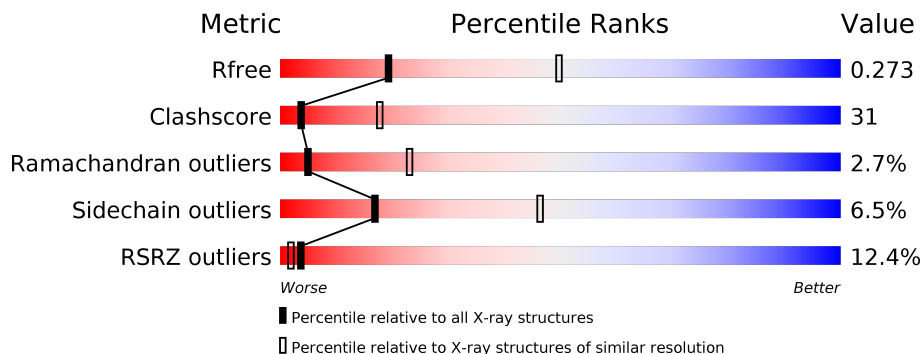
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">49% 35% 5% 11%</div> </div>
1	B	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">47% 37% • 11%</div> </div>
1	C	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">10%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">43% 41% 5% 11%</div> </div>
1	D	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">44% 41% • 11%</div> </div>
1	E	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">10%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">48% 36% 7% 9%</div> </div>
1	F	219	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">28%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">42% 43% 5% 9%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9341 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 Queuosine biosynthesis protein queC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1527	975	254	285	13	0	0	0
1	B	195	1527	975	254	285	13	0	0	0
1	C	195	1527	975	254	285	13	0	0	0
1	D	195	1527	975	254	285	13	0	0	0
1	E	199	1559	995	258	293	13	0	0	0
1	F	199	1559	995	258	293	13	0	0	0

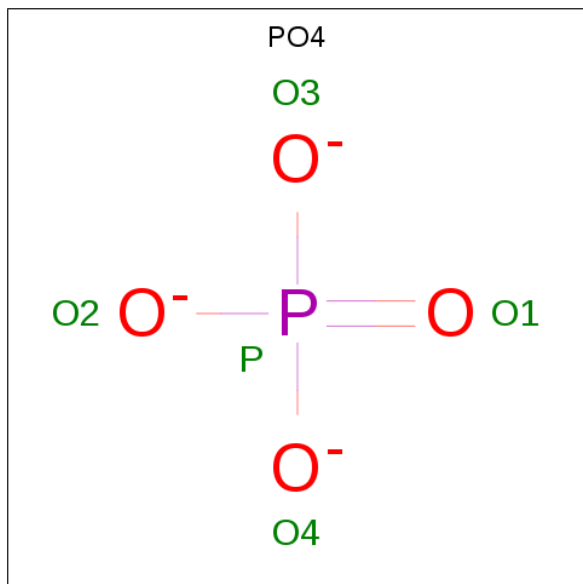
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

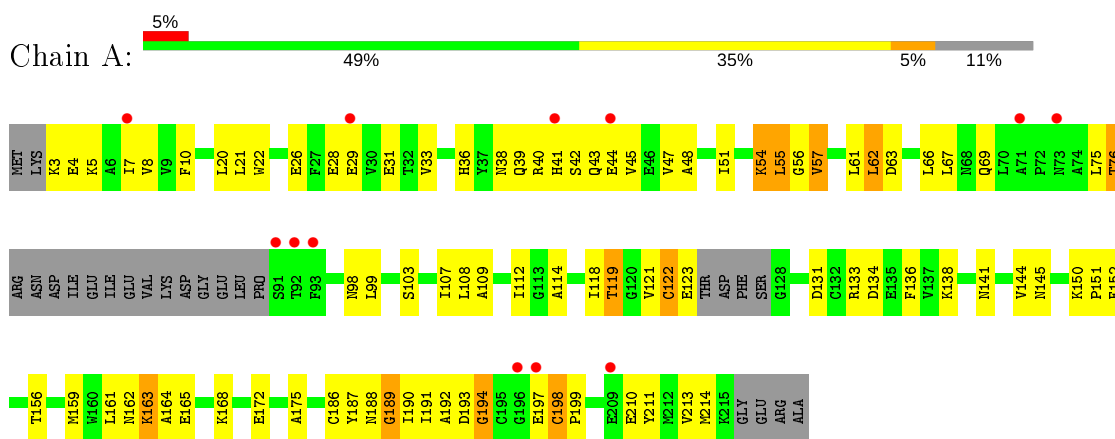
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	13	Total 13	O 13	0	0
5	B	16	Total 16	O 16	0	0
5	C	11	Total 11	O 11	0	0
5	D	9	Total 9	O 9	0	0
5	E	14	Total 14	O 14	0	0
5	F	10	Total 10	O 10	0	0

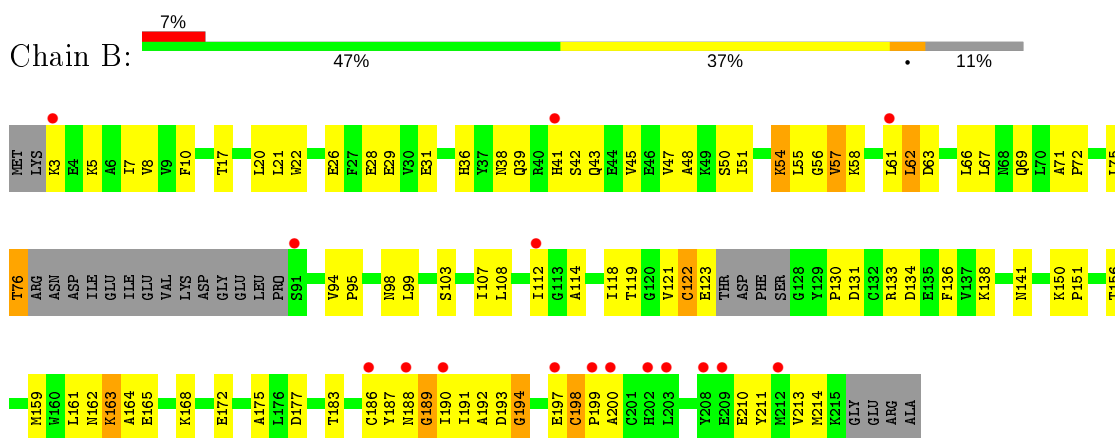
### 3 Residue-property plots [i](#)

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

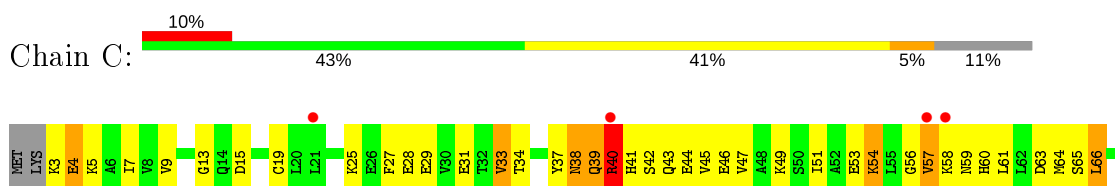
- Molecule 1: Queuosine biosynthesis protein queC

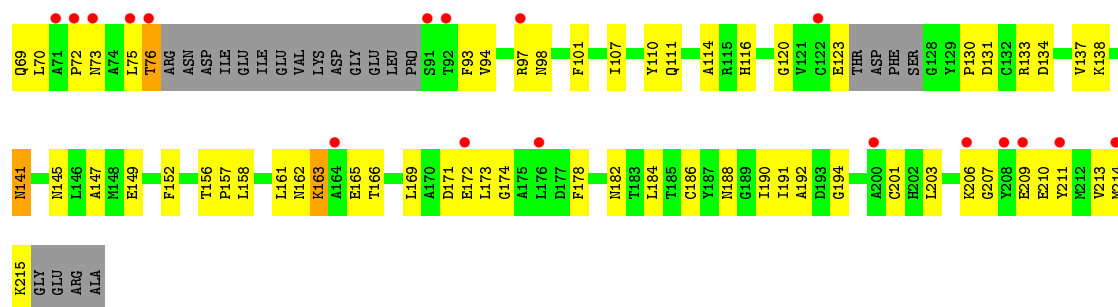


- Molecule 1: Queuosine biosynthesis protein queC

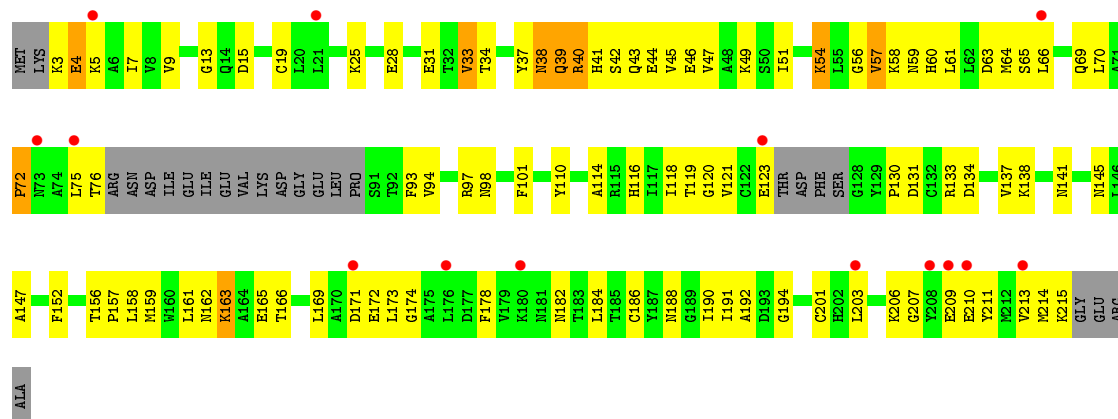


- Molecule 1: Queuosine biosynthesis protein queC

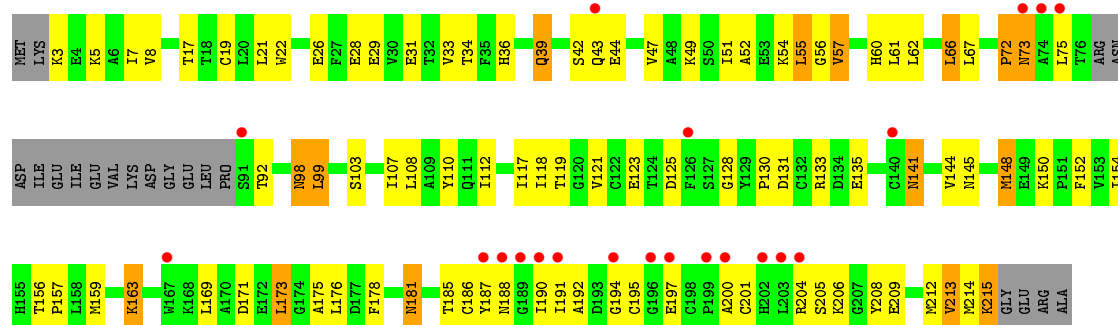




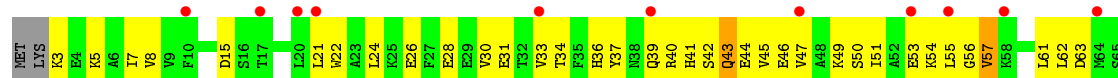
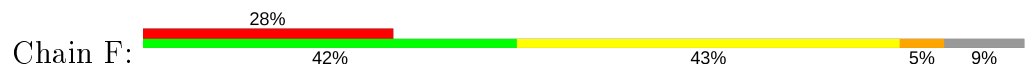
- Molecule 1: Queuosine biosynthesis protein queC

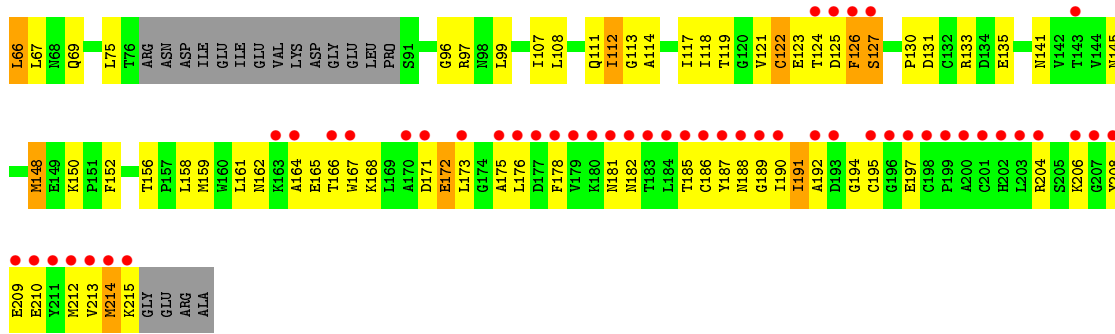


- Molecule 1: Queuosine biosynthesis protein queC



- Molecule 1: Queuosine biosynthesis protein queC







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.06Å 75.54Å 131.02Å 90.00° 94.73° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 48.27 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.95) 95.9 (48.27-2.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.00 (at 2.96Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.272 0.228 , 0.273	Depositor DCC
$R_{free}$ test set	2835 reflections (8.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtrriage
Anisotropy	0.491	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ZN

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	0/1557	0.65	0/2106
1	B	0.42	0/1557	0.65	0/2106
1	C	0.42	0/1557	0.64	0/2106
1	D	0.44	0/1557	0.64	0/2106
1	E	0.44	0/1591	0.64	0/2154
1	F	0.43	0/1591	0.63	0/2154
All	All	0.43	0/9410	0.64	0/12732

There are no bond length outliers.

There are no bond angle outliers.

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	1527	0	1510	100	0
1	B	1527	0	1510	113	0
1	C	1527	0	1510	116	0
1	D	1527	0	1510	101	0
1	E	1559	0	1536	93	0
1	F	1559	0	1538	97	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	13	0	0	5	0
5	B	16	0	0	6	0
5	C	11	0	0	7	0
5	D	9	0	0	2	0
5	E	14	0	0	3	0
5	F	10	0	0	1	0
All	All	9341	0	9114	572	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 31.

All (572) 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:69:GLN:NE2	1:C:63:ASP:H	1.45	1.14
1:B:69:GLN:HE22	1:C:63:ASP:N	1.48	1.10
1:F:8:VAL:HG22	1:F:118:ILE:HB	1.35	1.03
1:A:123:GLU:HG2	1:A:159:MET:HE2	1.42	1.01
1:A:123:GLU:H	1:A:159:MET:HE1	1.26	0.96
1:F:130:PRO:HA	1:F:133:ARG:HD2	1.48	0.95
1:B:63:ASP:H	1:C:69:GLN:HE22	0.94	0.91
1:A:42:SER:HB3	1:A:45:VAL:HG12	1.53	0.91
1:E:190:ILE:HB	1:E:194:GLY:HA2	1.52	0.91
1:B:123:GLU:HG2	1:B:159:MET:HE2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:H	1:D:69:GLN:HE22	0.94	0.90
1:E:47:VAL:O	1:E:51:ILE:HG22	1.73	0.89
1:E:213:VAL:HG23	1:E:214:MET:H	1.36	0.89
1:B:42:SER:HB3	1:B:45:VAL:HG12	1.53	0.88
1:A:69:GLN:HE22	1:D:63:ASP:H	0.92	0.88
1:B:66:LEU:HD13	1:C:66:LEU:HD22	1.53	0.88
1:E:39:GLN:HB3	1:E:42:SER:HB3	1.55	0.87
1:B:123:GLU:H	1:B:159:MET:HE1	1.37	0.87
1:A:123:GLU:H	1:A:159:MET:CE	1.87	0.87
1:F:171:ASP:HB2	1:F:176:LEU:HD22	1.56	0.86
1:F:7:ILE:HD11	1:F:33:VAL:HG23	1.56	0.86
1:B:123:GLU:H	1:B:159:MET:CE	1.88	0.85
1:B:186:CYS:HB2	1:B:194:GLY:HA3	1.60	0.83
1:A:66:LEU:HD13	1:D:66:LEU:HD22	1.61	0.82
1:B:66:LEU:HB3	1:C:66:LEU:HD13	1.62	0.81
1:E:61:LEU:O	1:E:62:LEU:HD13	1.80	0.81
1:F:5:LYS:HB3	1:F:114:ALA:HA	1.61	0.81
1:B:3:LYS:HB3	1:B:28:GLU:HG2	1.64	0.80
1:D:210:GLU:O	1:D:213:VAL:HG22	1.81	0.80
1:A:186:CYS:HB2	1:A:194:GLY:HA3	1.62	0.79
1:A:69:GLN:NE2	1:D:63:ASP:H	1.76	0.79
1:B:94:VAL:HG22	5:C:511:HOH:O	1.81	0.79
1:E:7:ILE:HD11	1:E:33:VAL:CG2	2.12	0.79
1:A:69:GLN:HE22	1:D:63:ASP:N	1.77	0.79
1:C:38:ASN:ND2	1:C:39:GLN:HG3	1.98	0.79
1:A:7:ILE:HD11	1:A:112:ILE:HG21	1.63	0.78
1:C:210:GLU:O	1:C:213:VAL:HG22	1.83	0.77
1:A:3:LYS:HB3	1:A:28:GLU:HG2	1.66	0.76
1:B:66:LEU:CD1	1:C:66:LEU:HD22	2.15	0.76
1:B:7:ILE:HD11	1:B:112:ILE:HG21	1.66	0.76
1:D:37:TYR:HD1	1:D:65:SER:HA	1.50	0.76
1:F:212:MET:SD	1:F:215:LYS:HD3	2.26	0.76
1:F:213:VAL:HG23	1:F:214:MET:SD	2.26	0.76
1:C:37:TYR:HD1	1:C:65:SER:HA	1.50	0.75
1:A:63:ASP:H	1:D:69:GLN:NE2	1.79	0.75
1:C:38:ASN:HD22	1:C:39:GLN:HG3	1.52	0.75
1:A:123:GLU:HG2	1:A:159:MET:CE	2.15	0.75
1:A:66:LEU:HB3	1:D:66:LEU:HD13	1.68	0.75
1:B:71:ALA:HA	5:C:511:HOH:O	1.85	0.75
1:F:191:ILE:HG22	1:F:192:ALA:H	1.52	0.74
1:C:42:SER:HB3	1:C:45:VAL:HG12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LYS:HB2	1:F:152:PHE:CE1	2.23	0.74
1:E:141:ASN:ND2	1:E:154:ILE:HG13	2.03	0.74
1:D:42:SER:HB3	1:D:45:VAL:HG12	1.71	0.73
1:E:213:VAL:O	1:E:215:LYS:HD3	1.88	0.73
1:B:63:ASP:N	1:C:69:GLN:HE22	1.79	0.73
1:A:63:ASP:N	1:D:69:GLN:HE22	1.80	0.73
1:E:125:ASP:OD1	1:E:128:GLY:HA2	1.89	0.73
1:E:60:HIS:HB2	5:E:510:HOH:O	1.88	0.73
1:D:163:LYS:HA	1:D:163:LYS:HE3	1.71	0.73
1:D:38:ASN:ND2	1:D:39:GLN:HG3	2.03	0.73
1:B:123:GLU:HG2	1:B:159:MET:CE	2.17	0.72
1:F:171:ASP:HA	1:F:176:LEU:HB2	1.70	0.72
1:D:158:LEU:HD22	1:D:166:THR:HG23	1.72	0.72
1:C:9:VAL:HA	1:C:33:VAL:HG23	1.71	0.72
1:B:66:LEU:HD23	1:B:67:LEU:H	1.55	0.71
1:F:39:GLN:HB3	1:F:42:SER:HB3	1.73	0.71
1:D:9:VAL:HA	1:D:33:VAL:HG23	1.72	0.71
1:B:168:LYS:O	1:B:172:GLU:HG3	1.92	0.70
1:E:130:PRO:HA	1:E:133:ARG:HD2	1.72	0.70
1:E:66:LEU:HD23	1:E:67:LEU:N	2.05	0.70
1:C:163:LYS:HA	1:C:163:LYS:HE3	1.73	0.70
1:F:206:LYS:O	1:F:210:GLU:HG3	1.92	0.69
1:F:21:LEU:HD13	1:F:175:ALA:HB3	1.74	0.69
1:C:45:VAL:O	1:C:49:LYS:HG3	1.92	0.69
1:E:213:VAL:HG23	1:E:214:MET:N	2.06	0.69
1:C:158:LEU:HD22	1:C:166:THR:HG23	1.74	0.69
1:B:190:ILE:CG2	1:B:194:GLY:HA2	2.21	0.69
1:B:66:LEU:HD23	1:B:67:LEU:N	2.08	0.69
1:C:130:PRO:HA	1:C:133:ARG:HD3	1.74	0.69
1:A:190:ILE:CG2	1:A:194:GLY:HA2	2.23	0.69
1:A:66:LEU:HD23	1:A:67:LEU:H	1.57	0.68
1:D:45:VAL:O	1:D:49:LYS:HG3	1.93	0.68
1:A:36:HIS:CD2	1:A:61:LEU:HD22	2.28	0.68
1:D:130:PRO:HA	1:D:133:ARG:HD3	1.75	0.68
1:A:56:GLY:O	1:A:57:VAL:HG22	1.94	0.68
1:D:38:ASN:HD22	1:D:39:GLN:HG3	1.59	0.68
1:F:181:ASN:HA	1:F:192:ALA:HB2	1.75	0.68
1:C:94:VAL:HA	5:C:503:HOH:O	1.93	0.68
1:D:213:VAL:O	1:D:215:LYS:HD3	1.94	0.68
1:F:55:LEU:HD11	1:F:178:PHE:HE2	1.58	0.67
1:B:20:LEU:HB2	5:B:512:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD13	1:C:66:LEU:HB3	1.76	0.67
1:B:75:LEU:O	1:B:76:THR:HG23	1.95	0.67
1:A:66:LEU:HD23	1:A:67:LEU:N	2.10	0.67
1:F:66:LEU:HD23	1:F:67:LEU:N	2.10	0.67
1:F:122:CYS:SG	1:F:124:THR:HG23	2.35	0.67
1:C:111:GLN:NE2	5:C:511:HOH:O	2.28	0.67
1:D:134:ASP:OD2	1:D:138:LYS:HE3	1.95	0.67
1:B:56:GLY:O	1:B:57:VAL:HG22	1.95	0.66
1:A:36:HIS:HD2	1:A:61:LEU:HD22	1.59	0.66
1:A:75:LEU:O	1:A:76:THR:HG23	1.96	0.66
1:A:66:LEU:CD1	1:D:66:LEU:HD22	2.25	0.66
1:B:7:ILE:HD13	1:B:31:GLU:HB2	1.78	0.66
1:C:162:ASN:OD1	1:C:165:GLU:HG3	1.96	0.66
1:D:34:THR:HB	1:D:61:LEU:HD23	1.78	0.66
1:C:66:LEU:HD23	1:C:66:LEU:O	1.96	0.65
1:F:96:GLY:HA2	1:F:131:ASP:OD2	1.96	0.65
1:C:213:VAL:O	1:C:215:LYS:HD3	1.97	0.65
1:E:33:VAL:HG22	1:E:108:LEU:HD13	1.79	0.65
1:B:48:ALA:HB1	5:B:504:HOH:O	1.97	0.65
1:E:33:VAL:HG13	5:E:510:HOH:O	1.96	0.65
1:F:8:VAL:HG22	1:F:118:ILE:CB	2.21	0.65
1:E:98:ASN:HB2	1:E:131:ASP:OD2	1.98	0.64
1:B:72:PRO:HD3	5:C:511:HOH:O	1.96	0.64
1:E:56:GLY:O	1:E:57:VAL:HG22	1.97	0.64
1:C:134:ASP:OD2	1:C:138:LYS:HE3	1.97	0.64
1:E:103:SER:O	1:E:107:ILE:HG12	1.97	0.64
1:A:66:LEU:HD13	1:D:66:LEU:HB3	1.80	0.64
1:E:7:ILE:HD11	1:E:33:VAL:HG23	1.78	0.63
1:B:98:ASN:HB2	1:B:131:ASP:OD2	1.99	0.63
1:C:34:THR:HB	1:C:61:LEU:HD23	1.80	0.63
1:E:119:THR:HG23	1:E:156:THR:HG22	1.79	0.62
1:B:63:ASP:H	1:C:69:GLN:NE2	1.80	0.62
1:F:212:MET:HA	1:F:215:LYS:HG3	1.81	0.62
1:C:54:LYS:HE2	1:C:178:PHE:HE1	1.63	0.62
1:E:3:LYS:HB3	1:E:28:GLU:N	2.14	0.62
1:F:119:THR:HG23	1:F:121:VAL:HG22	1.81	0.62
1:A:168:LYS:O	1:A:172:GLU:HG3	1.99	0.62
1:D:54:LYS:HE2	1:D:178:PHE:HE1	1.65	0.62
1:D:130:PRO:HA	1:D:133:ARG:CD	2.30	0.61
1:C:206:LYS:O	1:C:210:GLU:HG3	2.00	0.61
1:B:36:HIS:CD2	1:B:61:LEU:HD22	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:HIS:CD2	1:E:61:LEU:HG	2.36	0.61
1:A:7:ILE:HD13	1:A:31:GLU:HB2	1.83	0.61
1:F:47:VAL:O	1:F:51:ILE:HG22	2.01	0.61
1:C:130:PRO:HA	1:C:133:ARG:CD	2.30	0.60
1:E:190:ILE:CB	1:E:194:GLY:HA2	2.29	0.60
1:B:190:ILE:HG22	1:B:194:GLY:HA2	1.82	0.60
1:B:66:LEU:HD22	1:C:66:LEU:HD22	1.82	0.60
1:E:73:ASN:HD21	1:E:92:THR:HG22	1.66	0.60
1:E:34:THR:O	1:E:61:LEU:HD12	2.02	0.60
1:F:208:TYR:O	1:F:212:MET:HG2	2.01	0.60
1:B:36:HIS:HD2	1:B:61:LEU:HD22	1.66	0.60
1:D:206:LYS:O	1:D:210:GLU:HG3	2.00	0.60
1:B:21:LEU:HD13	1:B:175:ALA:CB	2.31	0.59
1:E:213:VAL:CG2	1:E:214:MET:H	2.13	0.59
1:A:48:ALA:O	1:A:51:ILE:HG22	2.02	0.59
1:F:3:LYS:HA	1:F:28:GLU:CD	2.22	0.59
1:D:191:ILE:HG22	1:D:192:ALA:N	2.17	0.59
1:F:43:GLN:O	1:F:47:VAL:HG23	2.02	0.59
1:B:119:THR:HG23	1:B:156:THR:HG22	1.84	0.59
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.67	0.59
1:A:163:LYS:HE3	1:A:163:LYS:HA	1.85	0.59
1:A:190:ILE:HG22	1:A:194:GLY:HA2	1.85	0.59
1:A:42:SER:HB3	1:A:45:VAL:CG1	2.30	0.59
1:B:48:ALA:O	1:B:51:ILE:HG22	2.03	0.59
1:B:103:SER:O	1:B:107:ILE:HG12	2.04	0.58
1:C:37:TYR:O	1:C:38:ASN:HB3	2.01	0.58
1:C:40:ARG:N	1:C:40:ARG:HD3	2.18	0.58
1:D:162:ASN:OD1	1:D:165:GLU:HG3	2.03	0.58
1:D:3:LYS:HB2	1:D:28:GLU:HG2	1.85	0.58
1:A:211:TYR:HA	1:A:214:MET:HE3	1.86	0.58
1:B:66:LEU:HD13	1:C:66:LEU:CD2	2.29	0.58
1:A:66:LEU:HD22	1:D:66:LEU:HD13	1.86	0.58
1:B:163:LYS:HA	1:B:163:LYS:HE3	1.86	0.58
1:D:43:GLN:O	1:D:47:VAL:HG23	2.04	0.58
1:B:42:SER:CB	1:B:45:VAL:HG12	2.32	0.58
1:D:37:TYR:O	1:D:38:ASN:HB3	2.03	0.57
1:A:123:GLU:N	1:A:159:MET:CE	2.65	0.57
1:F:185:THR:OG1	1:F:204:ARG:HD2	2.03	0.57
1:B:123:GLU:N	1:B:159:MET:CE	2.65	0.57
1:C:43:GLN:O	1:C:47:VAL:HG23	2.04	0.57
1:A:39:GLN:O	1:A:45:VAL:HG11	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ARG:N	1:D:40:ARG:HD3	2.19	0.57
1:B:22:TRP:CZ2	1:B:26:GLU:HG3	2.40	0.57
1:B:61:LEU:O	1:B:62:LEU:HD12	2.05	0.57
1:B:39:GLN:O	1:B:45:VAL:HG11	2.04	0.57
1:A:22:TRP:CZ2	1:A:26:GLU:HG3	2.40	0.57
1:E:31:GLU:OE2	1:E:112:ILE:HG12	2.04	0.57
1:B:95:PRO:HG2	1:C:107:ILE:HG23	1.86	0.56
1:C:163:LYS:HG2	1:C:203:LEU:O	2.04	0.56
1:E:49:LYS:O	1:E:52:ALA:HB3	2.05	0.56
1:C:169:LEU:O	1:C:173:LEU:HD23	2.05	0.56
1:A:118:ILE:HD12	1:A:118:ILE:N	2.21	0.56
1:F:40:ARG:O	1:F:41:HIS:HB2	2.06	0.56
1:C:191:ILE:HG22	1:C:192:ALA:N	2.21	0.56
1:B:66:LEU:HD22	1:C:66:LEU:CD2	2.36	0.56
1:E:169:LEU:O	1:E:173:LEU:HB2	2.05	0.56
1:C:3:LYS:HB2	1:C:28:GLU:HG2	1.87	0.56
1:D:40:ARG:HH11	1:D:40:ARG:HG3	1.71	0.56
1:F:42:SER:OG	1:F:45:VAL:HG12	2.06	0.56
1:B:118:ILE:N	1:B:118:ILE:HD12	2.21	0.55
1:B:45:VAL:HG23	1:B:61:LEU:HD21	1.87	0.55
1:A:21:LEU:HD13	1:A:175:ALA:CB	2.35	0.55
1:D:39:GLN:C	1:D:41:HIS:H	2.10	0.55
1:B:66:LEU:CD2	1:C:66:LEU:HD22	2.37	0.55
1:E:117:ILE:N	1:E:117:ILE:HD12	2.21	0.55
1:B:121:VAL:O	1:B:122:CYS:HB3	2.06	0.55
1:D:66:LEU:HD23	1:D:66:LEU:O	2.05	0.55
1:C:39:GLN:C	1:C:41:HIS:H	2.09	0.55
1:E:99:LEU:HD22	1:E:99:LEU:O	2.07	0.55
1:A:42:SER:CB	1:A:45:VAL:HG12	2.32	0.55
1:F:22:TRP:CZ2	1:F:26:GLU:HG3	2.41	0.55
1:B:66:LEU:HD22	1:C:66:LEU:HD13	1.88	0.55
1:E:130:PRO:HA	1:E:133:ARG:CD	2.35	0.55
1:C:54:LYS:NZ	1:C:182:ASN:ND2	2.55	0.55
1:E:186:CYS:HB2	1:E:194:GLY:HA3	1.89	0.55
1:E:52:ALA:O	1:E:56:GLY:O	2.25	0.55
1:B:42:SER:HB3	1:B:45:VAL:CG1	2.31	0.54
1:E:73:ASN:ND2	1:E:92:THR:HG22	2.21	0.54
1:C:66:LEU:HD23	1:C:66:LEU:C	2.27	0.54
1:B:5:LYS:HB3	1:B:114:ALA:HA	1.89	0.54
1:A:103:SER:O	1:A:107:ILE:HG12	2.08	0.54
1:A:61:LEU:O	1:A:62:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:HD23	1:D:66:LEU:C	2.28	0.54
1:A:63:ASP:O	1:D:66:LEU:HD11	2.07	0.54
1:A:45:VAL:HG23	1:A:61:LEU:HD21	1.90	0.54
1:A:98:ASN:HB2	1:A:131:ASP:OD2	2.07	0.54
1:D:130:PRO:O	1:D:133:ARG:HD3	2.08	0.54
1:A:119:THR:HG23	1:A:156:THR:HG22	1.89	0.54
1:C:163:LYS:HB3	1:C:207:GLY:HA3	1.90	0.54
1:E:17:THR:HG23	1:E:51:ILE:HD11	1.90	0.54
1:E:43:GLN:HG2	1:E:44:GLU:OE2	2.08	0.54
1:B:63:ASP:O	1:C:66:LEU:HD11	2.07	0.53
1:C:3:LYS:CB	1:C:28:GLU:HG2	2.39	0.53
1:C:188:ASN:O	1:C:190:ILE:HG12	2.08	0.53
1:D:3:LYS:CB	1:D:28:GLU:HG2	2.37	0.53
1:E:121:VAL:O	1:E:121:VAL:HG23	2.08	0.53
1:F:22:TRP:HA	1:F:173:LEU:HD21	1.91	0.53
1:B:186:CYS:CB	1:B:194:GLY:HA3	2.35	0.53
1:B:69:GLN:HE22	1:C:63:ASP:H	0.67	0.53
1:E:163:LYS:HA	1:E:163:LYS:NZ	2.24	0.53
1:E:54:LYS:HD2	1:E:178:PHE:HE1	1.73	0.53
1:F:190:ILE:HB	1:F:194:GLY:HA2	1.89	0.53
1:B:210:GLU:O	1:B:213:VAL:HG22	2.08	0.53
1:F:171:ASP:CB	1:F:176:LEU:HD22	2.35	0.53
1:F:181:ASN:HA	1:F:192:ALA:CB	2.38	0.53
1:B:177:ASP:HB3	1:E:181:ASN:ND2	2.24	0.53
1:F:7:ILE:CD1	1:F:33:VAL:HG23	2.32	0.53
1:A:121:VAL:O	1:A:122:CYS:HB3	2.09	0.52
1:D:56:GLY:O	1:D:57:VAL:O	2.27	0.52
1:E:47:VAL:CG2	1:E:191:ILE:HD11	2.40	0.52
1:C:49:LYS:HB3	1:C:49:LYS:NZ	2.24	0.52
1:E:57:VAL:O	1:E:57:VAL:HG23	2.09	0.52
1:F:186:CYS:C	1:F:188:ASN:H	2.12	0.52
1:B:10:PHE:HZ	1:B:51:ILE:HG21	1.73	0.52
1:E:108:LEU:HD23	1:E:108:LEU:O	2.09	0.52
1:E:3:LYS:HB3	1:E:28:GLU:H	1.74	0.52
1:F:54:LYS:HE3	1:F:182:ASN:HD22	1.75	0.52
1:D:163:LYS:HG2	1:D:203:LEU:O	2.10	0.52
1:F:162:ASN:OD1	1:F:164:ALA:HB3	2.09	0.52
1:B:66:LEU:CB	1:C:66:LEU:HD13	2.37	0.52
1:D:42:SER:O	1:D:46:GLU:HB2	2.10	0.52
1:B:66:LEU:HD22	1:C:66:LEU:CD1	2.39	0.52
1:B:130:PRO:HB3	1:C:149:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:CYS:HA	1:B:159:MET:HE3	1.91	0.51
1:B:39:GLN:HG2	1:B:41:HIS:CE1	2.46	0.51
1:C:56:GLY:O	1:C:57:VAL:O	2.27	0.51
1:D:13:GLY:HA2	1:D:184:LEU:O	2.11	0.51
1:E:21:LEU:HD13	1:E:175:ALA:HB3	1.91	0.51
1:A:39:GLN:HG2	1:A:41:HIS:CE1	2.46	0.51
1:B:98:ASN:CB	1:B:131:ASP:OD2	2.58	0.51
1:C:40:ARG:H	1:C:40:ARG:HD3	1.75	0.51
1:C:75:LEU:O	1:C:76:THR:HG23	2.10	0.51
1:A:66:LEU:HD22	1:D:66:LEU:CD1	2.40	0.51
1:F:43:GLN:HB2	5:F:507:HOH:O	2.10	0.51
1:A:47:VAL:HG13	1:A:48:ALA:N	2.26	0.51
1:C:42:SER:O	1:C:46:GLU:HB2	2.10	0.51
1:E:171:ASP:HA	1:E:176:LEU:HB2	1.92	0.51
1:E:209:GLU:O	1:E:213:VAL:HG22	2.11	0.51
1:D:49:LYS:HB3	1:D:49:LYS:NZ	2.26	0.51
1:E:171:ASP:OD1	1:E:176:LEU:HD22	2.11	0.51
1:F:5:LYS:NZ	1:F:31:GLU:OE1	2.38	0.51
1:B:66:LEU:H	1:C:66:LEU:HD13	1.76	0.51
1:D:4:GLU:HG3	1:D:116:HIS:HE2	1.76	0.51
1:D:186:CYS:HB2	1:D:201:CYS:SG	2.50	0.51
1:F:126:PHE:O	1:F:127:SER:HB3	2.11	0.51
1:F:171:ASP:CA	1:F:176:LEU:HB2	2.37	0.51
1:B:136:PHE:CE1	1:C:147:ALA:HB2	2.46	0.51
1:D:169:LEU:O	1:D:173:LEU:HD23	2.11	0.51
1:D:75:LEU:O	1:D:76:THR:HG23	2.11	0.51
1:A:5:LYS:HG3	1:A:29:GLU:HB3	1.92	0.50
1:B:193:ASP:O	1:B:194:GLY:O	2.30	0.50
1:B:211:TYR:HA	1:B:214:MET:HE3	1.93	0.50
1:D:190:ILE:HB	1:D:194:GLY:HA2	1.92	0.50
1:F:43:GLN:OE1	1:F:44:GLU:HG2	2.11	0.50
1:E:150:LYS:HG2	1:E:152:PHE:CZ	2.46	0.50
1:A:193:ASP:O	1:A:194:GLY:O	2.30	0.50
1:C:130:PRO:O	1:C:133:ARG:HD3	2.11	0.50
1:C:4:GLU:HG3	1:C:116:HIS:HE2	1.77	0.50
1:C:7:ILE:O	1:C:7:ILE:HG23	2.12	0.50
1:B:188:ASN:O	1:B:190:ILE:HG13	2.11	0.50
1:C:19:CYS:SG	1:C:120:GLY:HA2	2.52	0.50
1:D:57:VAL:O	1:D:57:VAL:HG23	2.11	0.50
1:D:94:VAL:HG23	1:D:97:ARG:HH11	1.77	0.50
1:C:57:VAL:O	1:C:57:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:CYS:HB2	1:F:158:LEU:O	2.11	0.49
1:B:122:CYS:SG	1:B:122:CYS:O	2.71	0.49
1:E:22:TRP:HA	1:E:173:LEU:HD21	1.94	0.49
1:C:27:PHE:HD2	5:C:507:HOH:O	1.94	0.49
1:A:134:ASP:OD2	1:A:138:LYS:NZ	2.45	0.49
1:B:133:ARG:HH11	1:B:133:ARG:CB	2.25	0.49
1:F:61:LEU:C	1:F:61:LEU:HD12	2.32	0.49
1:F:111:GLN:O	1:F:113:GLY:N	2.45	0.49
1:C:190:ILE:HB	1:C:194:GLY:HA2	1.94	0.49
1:C:94:VAL:HG23	1:C:97:ARG:HH11	1.78	0.49
1:D:191:ILE:CG2	1:D:192:ALA:N	2.76	0.49
1:E:22:TRP:CZ2	1:E:26:GLU:HG3	2.48	0.49
1:C:49:LYS:HE2	1:C:59:ASN:HD22	1.76	0.49
1:C:163:LYS:HA	1:C:163:LYS:CE	2.42	0.49
1:B:57:VAL:O	1:B:57:VAL:HG23	2.13	0.49
1:D:163:LYS:HA	1:D:163:LYS:CE	2.41	0.49
1:E:107:ILE:O	1:E:110:TYR:HB3	2.13	0.48
1:B:134:ASP:OD2	1:B:138:LYS:NZ	2.46	0.48
1:C:123:GLU:O	1:C:123:GLU:HG2	2.12	0.48
1:A:191:ILE:HG22	1:A:192:ALA:N	2.28	0.48
1:A:188:ASN:O	1:A:190:ILE:HG13	2.13	0.48
1:B:51:ILE:HB	5:B:505:HOH:O	2.13	0.48
1:E:22:TRP:CE2	1:E:26:GLU:HG3	2.48	0.48
1:B:58:LYS:HG3	5:B:510:HOH:O	2.13	0.48
1:D:188:ASN:O	1:D:190:ILE:HG12	2.14	0.48
1:F:209:GLU:O	1:F:212:MET:HB2	2.14	0.48
1:A:186:CYS:CB	1:A:194:GLY:HA3	2.38	0.48
1:D:19:CYS:SG	1:D:120:GLY:HA2	2.54	0.48
1:D:121:VAL:HB	5:D:503:HOH:O	2.13	0.47
1:D:213:VAL:CG2	1:D:214:MET:N	2.77	0.47
1:F:121:VAL:O	1:F:121:VAL:HG23	2.14	0.47
1:B:3:LYS:HB3	1:B:28:GLU:CG	2.41	0.47
1:B:5:LYS:HG3	1:B:29:GLU:HB3	1.95	0.47
1:D:49:LYS:HE2	1:D:59:ASN:HD22	1.79	0.47
1:B:38:ASN:HA	1:B:63:ASP:OD2	2.14	0.47
1:F:15:ASP:OD1	1:F:166:THR:HG21	2.14	0.47
1:A:48:ALA:HA	1:A:51:ILE:HG22	1.97	0.47
1:B:10:PHE:CZ	1:B:51:ILE:CG2	2.98	0.47
1:D:159:MET:HE1	5:D:503:HOH:O	2.13	0.47
1:E:17:THR:CG2	1:E:51:ILE:HD11	2.44	0.47
1:F:37:TYR:O	1:F:63:ASP:OD1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:CYS:O	1:A:122:CYS:SG	2.73	0.47
1:B:47:VAL:HG13	1:B:48:ALA:N	2.29	0.47
1:A:5:LYS:HB3	1:A:114:ALA:HA	1.97	0.47
1:B:48:ALA:HA	1:B:51:ILE:HG22	1.97	0.47
1:E:186:CYS:HB2	1:E:201:CYS:SG	2.55	0.47
1:A:136:PHE:CE1	1:D:147:ALA:HB2	2.50	0.47
1:A:33:VAL:HG22	5:A:510:HOH:O	2.15	0.47
1:C:40:ARG:HG3	1:C:40:ARG:NH1	2.30	0.47
1:D:163:LYS:HB3	1:D:207:GLY:HA3	1.96	0.47
1:A:210:GLU:O	1:A:213:VAL:HG22	2.15	0.47
1:C:94:VAL:HG23	1:C:97:ARG:NH1	2.30	0.47
1:D:40:ARG:HD3	1:D:40:ARG:H	1.79	0.47
1:E:163:LYS:HA	1:E:163:LYS:HZ2	1.78	0.47
1:A:7:ILE:HD12	5:A:510:HOH:O	2.15	0.47
1:B:10:PHE:HZ	1:B:51:ILE:CG2	2.27	0.47
1:C:13:GLY:HA2	1:C:184:LEU:O	2.15	0.47
1:C:5:LYS:HE2	1:C:31:GLU:OE2	2.15	0.46
1:B:43:GLN:HB2	5:B:503:HOH:O	2.16	0.46
5:A:508:HOH:O	1:D:72:PRO:HG3	2.15	0.46
1:D:94:VAL:HG23	1:D:97:ARG:NH1	2.30	0.46
1:C:172:GLU:C	1:C:174:GLY:H	2.19	0.46
1:D:213:VAL:HG23	1:D:214:MET:N	2.31	0.46
1:F:3:LYS:HA	1:F:28:GLU:HG3	1.97	0.46
1:A:4:GLU:HA	5:A:501:HOH:O	2.16	0.46
1:D:7:ILE:HG23	1:D:7:ILE:O	2.14	0.46
1:A:144:VAL:HG23	1:A:145:ASN:N	2.30	0.46
1:B:191:ILE:HG22	1:B:192:ALA:N	2.31	0.46
1:B:187:TYR:HD2	1:B:198:CYS:HB2	1.81	0.46
1:B:8:VAL:HG22	1:B:118:ILE:HB	1.97	0.46
1:D:51:ILE:HG23	1:D:178:PHE:CZ	2.51	0.46
1:E:107:ILE:HA	1:E:148:MET:HE3	1.97	0.46
1:C:64:MET:HG3	1:C:101:PHE:HE1	1.80	0.45
1:C:60:HIS:CD2	1:C:60:HIS:H	2.34	0.45
1:E:185:THR:CB	1:E:204:ARG:HD2	2.45	0.45
1:F:42:SER:O	1:F:46:GLU:HG2	2.16	0.45
1:A:10:PHE:HZ	1:A:51:ILE:HG21	1.80	0.45
1:B:69:GLN:HE22	1:C:63:ASP:CB	2.29	0.45
1:C:191:ILE:CG2	1:C:192:ALA:N	2.79	0.45
1:A:66:LEU:HD22	1:D:66:LEU:HD22	1.98	0.45
1:E:188:ASN:ND2	1:E:195:CYS:SG	2.89	0.45
1:E:5:LYS:NZ	1:E:31:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:HG3	1:C:29:GLU:HB3	1.98	0.45
1:D:63:ASP:OD2	1:D:65:SER:OG	2.32	0.45
1:E:31:GLU:OE2	1:E:60:HIS:NE2	2.46	0.45
1:B:119:THR:OG1	1:B:121:VAL:HG13	2.15	0.45
1:B:123:GLU:N	1:B:159:MET:HE3	2.32	0.45
1:D:4:GLU:HG3	1:D:116:HIS:NE2	2.32	0.45
1:A:38:ASN:HA	1:A:63:ASP:OD2	2.16	0.45
1:C:145:ASN:OD1	1:C:152:PHE:HB2	2.16	0.45
1:E:19:CYS:SG	1:E:157:PRO:HG2	2.57	0.45
1:A:119:THR:OG1	1:A:121:VAL:HG13	2.16	0.45
1:D:145:ASN:OD1	1:D:152:PHE:HB2	2.16	0.45
1:E:123:GLU:HB2	1:E:159:MET:SD	2.56	0.45
1:E:21:LEU:HD13	1:E:175:ALA:CB	2.47	0.45
1:F:161:LEU:HA	1:F:165:GLU:OE1	2.16	0.45
1:C:54:LYS:HZ1	1:C:182:ASN:ND2	2.14	0.45
1:F:195:CYS:C	1:F:197:GLU:H	2.19	0.45
1:F:39:GLN:OE1	1:F:42:SER:HB2	2.16	0.45
1:F:67:LEU:HD21	1:F:97:ARG:HB2	1.99	0.45
1:F:123:GLU:C	1:F:125:ASP:H	2.20	0.45
1:C:40:ARG:H	1:C:40:ARG:CD	2.26	0.45
1:F:212:MET:C	1:F:214:MET:H	2.21	0.45
1:B:168:LYS:HE2	1:B:172:GLU:OE2	2.17	0.45
1:C:137:VAL:HG11	1:C:156:THR:HG21	1.98	0.45
1:E:212:MET:O	1:E:215:LYS:CD	2.65	0.45
1:F:34:THR:O	1:F:61:LEU:HA	2.16	0.45
1:C:47:VAL:O	1:C:51:ILE:HG13	2.18	0.44
1:C:98:ASN:HB2	1:C:131:ASP:OD2	2.16	0.44
1:A:133:ARG:CB	1:A:133:ARG:HH11	2.30	0.44
1:B:163:LYS:HA	1:B:163:LYS:CE	2.47	0.44
1:E:47:VAL:HG21	1:E:191:ILE:HD11	1.99	0.44
1:E:72:PRO:O	1:E:75:LEU:HB2	2.17	0.44
1:B:8:VAL:HG11	5:B:512:HOH:O	2.18	0.44
1:E:5:LYS:NZ	1:E:112:ILE:HG13	2.32	0.44
1:F:51:ILE:HG13	1:F:178:PHE:CZ	2.52	0.44
1:F:161:LEU:HB3	1:F:165:GLU:HB2	1.99	0.44
1:C:4:GLU:HG3	1:C:116:HIS:NE2	2.32	0.44
1:D:40:ARG:H	1:D:40:ARG:CD	2.28	0.44
1:E:33:VAL:HG13	1:E:62:LEU:CD2	2.47	0.44
1:F:34:THR:HG23	1:F:61:LEU:HA	2.00	0.44
1:A:118:ILE:CD1	1:A:118:ILE:N	2.80	0.44
1:C:39:GLN:C	1:C:41:HIS:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLU:OE2	1:F:145:ASN:HB3	2.17	0.44
1:E:171:ASP:HB2	1:E:176:LEU:HD13	1.99	0.44
1:F:186:CYS:SG	1:F:188:ASN:HB2	2.57	0.44
1:A:10:PHE:CZ	1:A:51:ILE:CG2	3.01	0.44
1:A:187:TYR:HD2	1:A:198:CYS:HB2	1.83	0.44
1:E:22:TRP:CA	1:E:173:LEU:HD21	2.48	0.44
1:F:125:ASP:C	1:F:127:SER:N	2.71	0.44
1:F:209:GLU:OE2	1:F:212:MET:HB2	2.18	0.44
1:C:171:ASP:OD2	1:C:211:TYR:OH	2.36	0.43
1:E:123:GLU:HG3	1:E:133:ARG:HA	1.99	0.43
1:E:144:VAL:HG23	1:E:145:ASN:N	2.33	0.43
1:E:33:VAL:HA	5:E:510:HOH:O	2.17	0.43
1:E:135:GLU:CD	1:F:145:ASN:HD22	2.20	0.43
1:F:3:LYS:HA	1:F:28:GLU:CG	2.48	0.43
1:F:56:GLY:O	1:F:57:VAL:O	2.36	0.43
1:F:118:ILE:N	1:F:118:ILE:HD12	2.33	0.43
1:F:212:MET:HA	1:F:215:LYS:CG	2.47	0.43
1:A:20:LEU:HD21	1:A:55:LEU:HD11	1.98	0.43
1:B:10:PHE:CZ	1:B:51:ILE:HG21	2.52	0.43
1:C:171:ASP:O	1:C:174:GLY:N	2.41	0.43
1:B:107:ILE:HG21	1:C:70:LEU:HD13	1.99	0.43
1:D:161:LEU:HD22	1:D:165:GLU:HB3	2.00	0.43
1:F:39:GLN:HB3	1:F:42:SER:CB	2.43	0.43
1:B:164:ALA:HB1	1:B:214:MET:HE3	2.01	0.43
1:C:213:VAL:CG2	1:C:214:MET:N	2.82	0.43
1:A:107:ILE:HB	1:D:70:LEU:HD13	1.99	0.43
1:F:107:ILE:HA	1:F:148:MET:HE3	2.01	0.43
1:A:107:ILE:HG21	1:D:70:LEU:HD13	1.99	0.43
1:D:211:TYR:HD1	1:D:214:MET:HE3	1.82	0.43
1:E:212:MET:O	1:E:215:LYS:HD2	2.19	0.43
1:F:167:TRP:CD1	1:F:208:TYR:HA	2.52	0.43
1:A:57:VAL:HG23	1:A:57:VAL:O	2.18	0.43
1:C:5:LYS:HB3	1:C:114:ALA:HA	2.00	0.43
1:E:108:LEU:HD23	1:E:108:LEU:C	2.39	0.43
1:D:42:SER:H	1:D:45:VAL:CG1	2.31	0.43
1:E:213:VAL:O	1:E:215:LYS:N	2.46	0.43
1:F:123:GLU:HB3	1:F:159:MET:SD	2.59	0.43
1:A:44:GLU:O	1:A:47:VAL:HG12	2.19	0.43
1:B:123:GLU:H	1:B:159:MET:HE3	1.77	0.43
1:C:211:TYR:HD1	1:C:214:MET:HE3	1.84	0.43
1:F:190:ILE:O	1:F:194:GLY:HA2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLN:C	1:D:41:HIS:N	2.73	0.43
1:D:44:GLU:N	1:D:44:GLU:OE1	2.52	0.43
1:F:168:LYS:O	1:F:172:GLU:HB2	2.18	0.43
1:F:24:LEU:CD2	1:F:30:VAL:HB	2.49	0.43
1:A:164:ALA:HB1	1:A:214:MET:HE3	2.01	0.43
1:B:211:TYR:HA	1:B:214:MET:HG2	2.01	0.43
1:A:211:TYR:HA	1:A:214:MET:HG2	2.01	0.42
1:D:64:MET:HG3	1:D:101:PHE:HE1	1.84	0.42
1:D:54:LYS:NZ	1:D:182:ASN:ND2	2.67	0.42
1:D:5:LYS:HE2	1:D:31:GLU:OE2	2.19	0.42
1:D:60:HIS:H	1:D:60:HIS:CD2	2.37	0.42
1:A:145:ASN:OD1	1:A:152:PHE:HB2	2.18	0.42
1:A:3:LYS:HB3	1:A:28:GLU:CG	2.45	0.42
1:B:162:ASN:N	1:B:165:GLU:OE1	2.46	0.42
1:C:186:CYS:HB2	1:C:201:CYS:SG	2.59	0.42
1:D:118:ILE:HD12	1:D:118:ILE:N	2.34	0.42
1:E:205:SER:O	1:E:208:TYR:HB3	2.19	0.42
1:A:10:PHE:HZ	1:A:51:ILE:CG2	2.32	0.42
1:D:34:THR:HB	1:D:61:LEU:CD2	2.48	0.42
1:F:7:ILE:O	1:F:117:ILE:HA	2.19	0.42
1:A:3:LYS:HE3	1:A:28:GLU:OE2	2.20	0.42
1:E:55:LEU:HD22	1:E:55:LEU:H	1.84	0.42
1:C:209:GLU:O	1:C:210:GLU:C	2.58	0.42
1:F:33:VAL:HG21	1:F:108:LEU:HD22	2.02	0.42
1:D:209:GLU:O	1:D:210:GLU:C	2.57	0.42
1:E:145:ASN:ND2	1:F:135:GLU:HG3	2.34	0.42
1:F:186:CYS:HB2	1:F:194:GLY:HA3	2.02	0.42
1:F:212:MET:HA	1:F:215:LYS:CD	2.50	0.42
1:A:161:LEU:HA	1:A:165:GLU:OE1	2.19	0.42
1:A:40:ARG:HB2	5:A:504:HOH:O	2.19	0.42
1:B:47:VAL:O	1:B:50:SER:HB3	2.20	0.42
1:D:98:ASN:HB2	1:D:131:ASP:OD2	2.20	0.42
1:E:212:MET:O	1:E:215:LYS:HB3	2.20	0.42
1:E:8:VAL:HG13	1:E:118:ILE:HG22	2.02	0.42
1:A:5:LYS:NZ	1:A:31:GLU:OE1	2.53	0.42
1:A:98:ASN:CB	1:A:131:ASP:OD2	2.68	0.42
1:B:118:ILE:N	1:B:118:ILE:CD1	2.83	0.42
1:B:133:ARG:NH1	1:B:133:ARG:CB	2.83	0.42
1:C:40:ARG:N	1:C:40:ARG:CD	2.82	0.42
1:D:171:ASP:O	1:D:174:GLY:N	2.43	0.42
1:A:43:GLN:HE21	1:A:189:GLY:HA3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLU:C	1:C:174:GLY:N	2.73	0.41
1:C:51:ILE:HG23	1:C:178:PHE:CZ	2.55	0.41
1:C:31:GLU:HG2	1:C:58:LYS:HB2	2.01	0.41
1:D:119:THR:CG2	1:D:156:THR:HG22	2.50	0.41
1:D:137:VAL:HG11	1:D:156:THR:HG21	2.01	0.41
1:A:10:PHE:CZ	1:A:51:ILE:HG21	2.55	0.41
1:D:31:GLU:HG2	1:D:58:LYS:HB2	2.02	0.41
1:B:199:PRO:O	1:B:200:ALA:C	2.58	0.41
1:B:3:LYS:HE3	1:B:28:GLU:OE2	2.21	0.41
1:C:141:ASN:HD22	1:C:141:ASN:C	2.21	0.41
1:D:172:GLU:C	1:D:174:GLY:H	2.24	0.41
1:D:94:VAL:CG2	1:D:97:ARG:HH11	2.32	0.41
1:E:125:ASP:O	1:E:128:GLY:N	2.53	0.41
1:F:191:ILE:HG22	1:F:192:ALA:N	2.26	0.41
1:A:107:ILE:CG2	1:D:70:LEU:HD13	2.50	0.41
1:B:133:ARG:HH11	1:B:133:ARG:HB3	1.84	0.41
1:C:94:VAL:CG2	1:C:97:ARG:HH11	2.33	0.41
1:D:40:ARG:NH1	1:D:40:ARG:HG3	2.34	0.41
1:E:187:TYR:CZ	1:E:200:ALA:HB2	2.54	0.41
1:E:33:VAL:HG13	1:E:62:LEU:HD23	2.03	0.41
1:F:145:ASN:OD1	1:F:152:PHE:HB2	2.20	0.41
1:F:62:LEU:HA	1:F:62:LEU:HD12	1.93	0.41
1:C:34:THR:HB	1:C:61:LEU:CD2	2.49	0.41
1:F:49:LYS:O	1:F:53:GLU:HB2	2.21	0.41
1:A:61:LEU:O	1:A:62:LEU:CD1	2.68	0.41
1:C:42:SER:H	1:C:45:VAL:CG1	2.33	0.41
1:C:53:GLU:O	1:C:54:LYS:C	2.58	0.41
1:D:5:LYS:HB3	1:D:114:ALA:HA	2.02	0.41
1:E:191:ILE:CG2	1:E:192:ALA:N	2.83	0.41
1:F:50:SER:O	1:F:53:GLU:HB3	2.20	0.41
1:B:133:ARG:HB2	1:B:133:ARG:NH1	2.36	0.41
1:B:95:PRO:HG3	1:C:110:TYR:CD1	2.55	0.41
1:E:56:GLY:O	1:E:57:VAL:CG2	2.68	0.41
1:A:162:ASN:ND2	1:A:165:GLU:HG3	2.36	0.41
1:A:198:CYS:HB2	1:A:199:PRO:CD	2.51	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.88	0.41
1:A:40:ARG:HE	1:A:61:LEU:HD13	1.85	0.41
1:B:61:LEU:O	1:B:62:LEU:CD1	2.67	0.41
1:C:44:GLU:OE1	1:C:44:GLU:N	2.54	0.41
1:D:123:GLU:O	1:D:123:GLU:HG2	2.21	0.41
1:E:141:ASN:CG	1:E:154:ILE:HG13	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:GLN:O	1:F:75:LEU:HG	2.20	0.41
1:C:3:LYS:HE2	1:C:3:LYS:HB2	1.92	0.41
1:A:66:LEU:HD22	1:D:66:LEU:CD2	2.50	0.41
1:E:112:ILE:O	1:E:112:ILE:HG13	2.21	0.41
1:F:40:ARG:C	1:F:42:SER:H	2.24	0.41
1:A:150:LYS:HA	1:A:151:PRO:HD3	1.85	0.41
1:B:150:LYS:HA	1:B:151:PRO:HD3	1.86	0.41
1:C:161:LEU:HD22	1:C:165:GLU:HB3	2.02	0.41
1:C:161:LEU:HA	1:C:165:GLU:OE1	2.21	0.41
1:C:3:LYS:HG2	5:C:507:HOH:O	2.20	0.41
1:C:63:ASP:OD2	1:C:65:SER:OG	2.37	0.41
1:F:195:CYS:C	1:F:197:GLU:N	2.75	0.41
1:A:162:ASN:N	1:A:165:GLU:OE1	2.49	0.40
1:C:4:GLU:HG3	1:C:116:HIS:CD2	2.57	0.40
1:F:126:PHE:HA	1:F:126:PHE:HD2	1.80	0.40
1:F:175:ALA:HB1	1:F:178:PHE:HB3	2.03	0.40
1:B:161:LEU:HA	1:B:165:GLU:OE1	2.21	0.40
1:D:110:TYR:CD1	1:D:110:TYR:C	2.94	0.40
1:A:8:VAL:HG22	1:A:118:ILE:HB	2.04	0.40
1:B:17:THR:OG1	1:B:183:THR:HG22	2.22	0.40
1:C:213:VAL:HG23	1:C:214:MET:N	2.37	0.40
1:E:141:ASN:O	1:E:144:VAL:HG22	2.21	0.40
1:F:168:LYS:HE2	1:F:172:GLU:OE1	2.21	0.40
1:F:36:HIS:NE2	1:F:61:LEU:HD13	2.36	0.40
1:A:109:ALA:HA	1:A:112:ILE:HG22	2.04	0.40
1:B:43:GLN:HE21	1:B:189:GLY:HA3	1.87	0.40
1:F:119:THR:CG2	1:F:156:THR:HG22	2.51	0.40
1:F:22:TRP:CE2	1:F:26:GLU:HG3	2.56	0.40
1:F:24:LEU:HD23	1:F:30:VAL:HB	2.04	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	189/219 (86%)	166 (88%)	17 (9%)	6 (3%)	4	19
1	B	189/219 (86%)	162 (86%)	21 (11%)	6 (3%)	4	19
1	C	189/219 (86%)	164 (87%)	19 (10%)	6 (3%)	4	19
1	D	189/219 (86%)	167 (88%)	18 (10%)	4 (2%)	7	29
1	E	195/219 (89%)	169 (87%)	23 (12%)	3 (2%)	10	38
1	F	195/219 (89%)	157 (80%)	32 (16%)	6 (3%)	4	19
All	All	1146/1314 (87%)	985 (86%)	130 (11%)	31 (3%)	5	23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	B	194	GLY
1	C	57	VAL
1	C	72	PRO
1	D	57	VAL
1	D	72	PRO
1	F	57	VAL
1	F	112	ILE
1	F	127	SER
1	A	54	LYS
1	A	57	VAL
1	B	57	VAL
1	E	57	VAL
1	B	54	LYS
1	C	38	ASN
1	D	38	ASN
1	F	187	TYR
1	B	122	CYS
1	C	157	PRO
1	A	122	CYS
1	D	157	PRO
1	F	189	GLY
1	C	40	ARG
1	C	73	ASN
1	F	191	ILE
1	A	189	GLY
1	A	198	CYS
1	B	189	GLY
1	E	213	VAL
1	B	198	CYS

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Mol	Chain	Res	Type
1	E	72	PRO

### 5.3.2 Protein sidechains [i](#)

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	168/189 (89%)	158 (94%)	10 (6%)	19	50
1	B	168/189 (89%)	159 (95%)	9 (5%)	22	54
1	C	168/189 (89%)	156 (93%)	12 (7%)	14	43
1	D	168/189 (89%)	158 (94%)	10 (6%)	19	50
1	E	172/189 (91%)	157 (91%)	15 (9%)	10	33
1	F	172/189 (91%)	162 (94%)	10 (6%)	20	51
All	All	1016/1134 (90%)	950 (94%)	66 (6%)	17	46

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	55	LEU
1	A	62	LEU
1	A	76	THR
1	A	99	LEU
1	A	108	LEU
1	A	119	THR
1	A	141	ASN
1	A	163	LYS
1	A	197	GLU
1	B	54	LYS
1	B	55	LEU
1	B	62	LEU
1	B	76	THR
1	B	99	LEU
1	B	108	LEU
1	B	141	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	163	LYS
1	B	197	GLU
1	C	4	GLU
1	C	15	ASP
1	C	25	LYS
1	C	33	VAL
1	C	39	GLN
1	C	40	ARG
1	C	54	LYS
1	C	66	LEU
1	C	76	THR
1	C	93	PHE
1	C	141	ASN
1	C	163	LYS
1	D	4	GLU
1	D	15	ASP
1	D	25	LYS
1	D	33	VAL
1	D	39	GLN
1	D	40	ARG
1	D	54	LYS
1	D	93	PHE
1	D	141	ASN
1	D	163	LYS
1	E	29	GLU
1	E	39	GLN
1	E	55	LEU
1	E	66	LEU
1	E	73	ASN
1	E	98	ASN
1	E	99	LEU
1	E	141	ASN
1	E	148	MET
1	E	163	LYS
1	E	173	LEU
1	E	181	ASN
1	E	197	GLU
1	E	206	LYS
1	E	215	LYS
1	F	43	GLN
1	F	66	LEU
1	F	99	LEU

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Mol	Chain	Res	Type
1	F	112	ILE
1	F	122	CYS
1	F	126	PHE
1	F	141	ASN
1	F	148	MET
1	F	172	GLU
1	F	214	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	69	GLN
1	A	73	ASN
1	B	59	ASN
1	B	69	GLN
1	B	73	ASN
1	B	98	ASN
1	B	181	ASN
1	C	38	ASN
1	C	41	HIS
1	C	43	GLN
1	C	59	ASN
1	C	69	GLN
1	C	182	ASN
1	D	38	ASN
1	D	41	HIS
1	D	43	GLN
1	D	59	ASN
1	D	69	GLN
1	D	182	ASN
1	E	38	ASN
1	E	59	ASN
1	E	69	GLN
1	E	73	ASN
1	E	141	ASN
1	E	145	ASN
1	E	181	ASN
1	E	188	ASN
1	F	98	ASN
1	F	188	ASN

### 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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	PO4	E	500	-	4,4,4	1.59	0	6,6,6	0.48	0
4	PO4	C	500	-	4,4,4	1.64	0	6,6,6	0.43	0
4	PO4	B	500	-	4,4,4	1.73	1 (25%)	6,6,6	0.43	0
4	PO4	F	500	-	4,4,4	1.44	0	6,6,6	0.43	0
4	PO4	D	500	-	4,4,4	1.56	0	6,6,6	0.43	0
4	PO4	A	500	-	4,4,4	1.78	1 (25%)	6,6,6	0.44	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	PO4	P-O2	-2.05	1.48	1.54
4	B	500	PO4	P-O4	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	195/219 (89%)	0.65	12 (6%) 20 12	46, 66, 99, 102	0
1	B	195/219 (89%)	0.70	16 (8%) 11 6	44, 67, 100, 102	0
1	C	195/219 (89%)	0.81	22 (11%) 5 3	46, 71, 100, 102	0
1	D	195/219 (89%)	0.66	14 (7%) 15 8	49, 72, 101, 102	0
1	E	199/219 (90%)	0.75	21 (10%) 6 3	53, 73, 101, 102	0
1	F	199/219 (90%)	1.54	61 (30%) 0 0	51, 87, 102, 102	0
All	All	1178/1314 (89%)	0.85	146 (12%) 4 2	44, 73, 101, 102	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	124	THR	6.2
1	C	91	SER	6.0
1	F	208	TYR	5.7
1	F	207	GLY	5.7
1	D	73	ASN	5.6
1	F	178	PHE	5.5
1	F	184	LEU	5.5
1	F	210	GLU	5.2
1	F	211	TYR	5.1
1	F	209	GLU	4.8
1	F	179	VAL	4.8
1	E	73	ASN	4.7
1	F	189	GLY	4.7
1	F	203	LEU	4.6
1	A	92	THR	4.6
1	F	188	ASN	4.6
1	F	214	MET	4.6
1	F	180	LYS	4.5
1	E	188	ASN	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	92	THR	4.4
1	F	21	LEU	4.4
1	F	200	ALA	4.4
1	F	204	ARG	4.4
1	F	182	ASN	4.3
1	F	173	LEU	4.3
1	E	91	SER	4.3
1	F	176	LEU	4.2
1	F	213	VAL	4.2
1	A	91	SER	4.0
1	F	215	LYS	4.0
1	A	73	ASN	4.0
1	F	185	THR	4.0
1	F	197	GLU	3.9
1	F	212	MET	3.9
1	B	41	HIS	3.9
1	F	181	ASN	3.9
1	F	175	ALA	3.8
1	F	186	CYS	3.8
1	F	201	CYS	3.8
1	B	199	PRO	3.8
1	C	76	THR	3.8
1	D	209	GLU	3.8
1	F	167	TRP	3.7
1	C	73	ASN	3.7
1	F	55	LEU	3.6
1	E	200	ALA	3.6
1	E	199	PRO	3.6
1	C	21	LEU	3.6
1	A	196	GLY	3.5
1	E	187	TYR	3.5
1	F	190	ILE	3.5
1	F	171	ASP	3.4
1	F	187	TYR	3.4
1	E	203	LEU	3.4
1	E	189	GLY	3.3
1	F	125	ASP	3.3
1	B	61	LEU	3.3
1	F	202	HIS	3.3
1	C	176	LEU	3.3
1	F	198	CYS	3.2
1	E	126	PHE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	197	GLU	3.2
1	A	197	GLU	3.2
1	B	209	GLU	3.0
1	F	192	ALA	3.0
1	C	71	ALA	3.0
1	E	75	LEU	3.0
1	E	74	ALA	3.0
1	F	206	LYS	2.9
1	F	39	GLN	2.9
1	F	193	ASP	2.9
1	D	210	GLU	2.9
1	B	202	HIS	2.8
1	D	171	ASP	2.8
1	B	190	ILE	2.8
1	F	126	PHE	2.8
1	B	208	TYR	2.8
1	F	163	LYS	2.8
1	E	43	GLN	2.8
1	F	183	THR	2.8
1	C	58	LYS	2.7
1	C	75	LEU	2.7
1	B	200	ALA	2.7
1	D	5	LYS	2.7
1	D	75	LEU	2.7
1	A	44	GLU	2.7
1	D	176	LEU	2.7
1	A	41	HIS	2.6
1	F	177	ASP	2.6
1	F	195	CYS	2.6
1	C	200	ALA	2.6
1	F	164	ALA	2.6
1	F	166	THR	2.6
1	C	214	MET	2.6
1	C	209	GLU	2.5
1	B	212	MET	2.5
1	C	97	ARG	2.5
1	A	93	PHE	2.5
1	F	196	GLY	2.5
1	C	122	CYS	2.5
1	F	58	LYS	2.5
1	D	21	LEU	2.5
1	B	186	CYS	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	47	VAL	2.5
1	E	190	ILE	2.5
1	F	20	LEU	2.5
1	D	208	TYR	2.5
1	E	196	GLY	2.5
1	B	197	GLU	2.4
1	C	164	ALA	2.4
1	B	112	ILE	2.4
1	C	208	TYR	2.3
1	F	143	THR	2.3
1	B	188	ASN	2.3
1	F	170	ALA	2.3
1	C	57	VAL	2.3
1	B	203	LEU	2.3
1	C	211	TYR	2.3
1	E	194	GLY	2.3
1	D	180	LYS	2.3
1	F	10	PHE	2.3
1	E	140	CYS	2.2
1	B	3	LYS	2.2
1	E	204	ARG	2.2
1	C	72	PRO	2.2
1	C	206	LYS	2.2
1	E	191	ILE	2.2
1	C	40	ARG	2.2
1	A	71	ALA	2.2
1	D	203	LEU	2.2
1	D	213	VAL	2.2
1	F	127	SER	2.1
1	D	123	GLU	2.1
1	E	202	HIS	2.1
1	F	53	GLU	2.1
1	F	199	PRO	2.1
1	A	209	GLU	2.1
1	D	66	LEU	2.1
1	A	29	GLU	2.1
1	F	33	VAL	2.1
1	F	17	THR	2.1
1	C	172	GLU	2.0
1	A	7	ILE	2.0
1	E	167	TRP	2.0
1	F	64	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	91	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	E	400	1/1	0.12	0.33	69,69,69,69	0
3	MG	A	400	1/1	0.44	0.33	65,65,65,65	0
3	MG	F	400	1/1	0.46	0.09	73,73,73,73	0
3	MG	D	400	1/1	0.61	0.25	62,62,62,62	0
3	MG	B	400	1/1	0.66	0.25	63,63,63,63	0
3	MG	C	400	1/1	0.70	0.22	59,59,59,59	0
2	ZN	F	300	1/1	0.88	0.13	101,101,101,101	0
4	PO4	F	500	5/5	0.90	0.22	101,101,101,101	0
4	PO4	D	500	5/5	0.91	0.16	98,99,100,100	0
4	PO4	B	500	5/5	0.92	0.16	86,88,89,90	0
4	PO4	C	500	5/5	0.94	0.14	92,93,94,94	0
4	PO4	E	500	5/5	0.94	0.14	89,90,91,92	0
4	PO4	A	500	5/5	0.95	0.15	84,85,86,86	0
2	ZN	B	300	1/1	0.98	0.04	96,96,96,96	0
2	ZN	E	300	1/1	0.99	0.03	101,101,101,101	0
2	ZN	C	300	1/1	0.99	0.15	63,63,63,63	0
2	ZN	A	300	1/1	1.00	0.08	101,101,101,101	0
2	ZN	D	300	1/1	1.00	0.14	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.