



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 06:30 am GMT

PDB ID : 1R4A  
Title : Crystal Structure of GTP-bound ADP-ribosylation Factor Like Protein 1 (Arl1) and GRIP Domain of Golgin245 COMPLEX  
Authors : Wu, M.; Lu, L.; Hong, W.; Song, H.  
Deposited on : 2003-10-04  
Resolution : 2.30 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

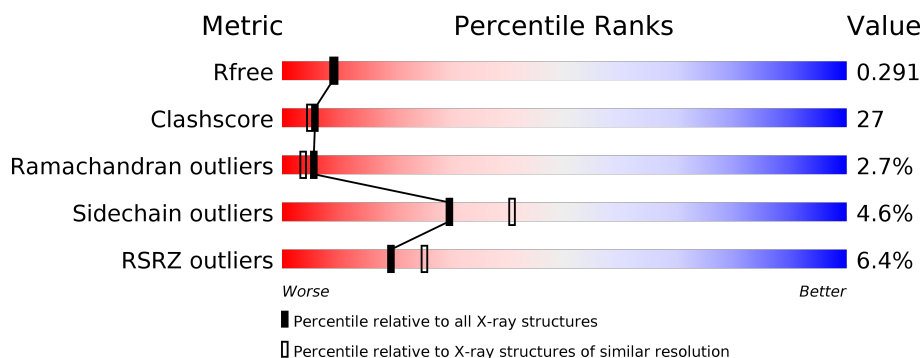
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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	165	<div> <div>10%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>5%</div> </div> </div>
1	B	165	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>6%</div> </div> </div>
1	C	165	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>6%</div> </div> </div>
1	D	165	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>6%</div> </div> </div>
2	E	51	<div> <div>10%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>6%</div> </div> </div>
2	F	51	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	51	<div><div></div><div>71%</div><div>25%</div><div></div></div>
2	H	51	<div><div>2%</div><div></div><div>67%</div><div>29%</div><div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7380 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 ADP-ribosylation factor-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1312	835	221	248	8			
1	B	165	Total	C	N	O	S	0	0	0
			1312	835	221	248	8			
1	C	165	Total	C	N	O	S	0	0	0
			1312	835	221	248	8			
1	D	165	Total	C	N	O	S	0	0	0
			1312	835	221	248	8			

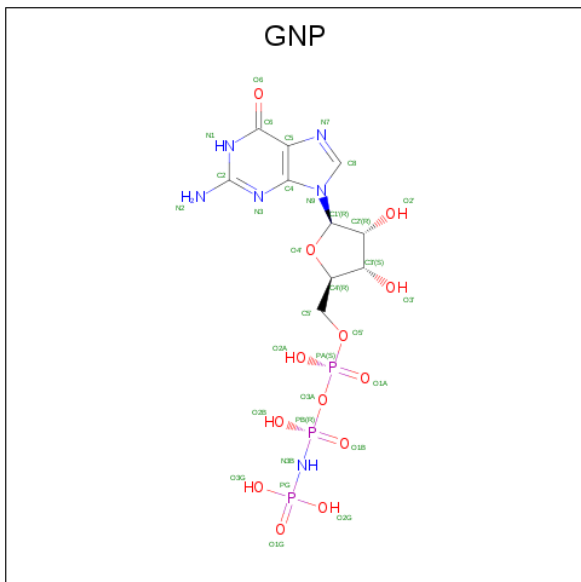
- Molecule 2 is a protein called Golgi autoantigen, golgin subfamily A member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	51	Total	C	N	O	S	0	0	0
			433	279	70	80	4			
2	F	51	Total	C	N	O	S	0	0	0
			433	279	70	80	4			
2	G	51	Total	C	N	O	S	0	0	0
			433	279	70	80	4			
2	H	51	Total	C	N	O	S	0	0	0
			433	279	70	80	4			

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

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	E	14	Total O 14 14	0	0
5	B	46	Total O 46 46	0	0
5	F	13	Total O 13 13	0	0
5	C	64	Total O 64 64	0	0
5	G	11	Total O 11 11	0	0

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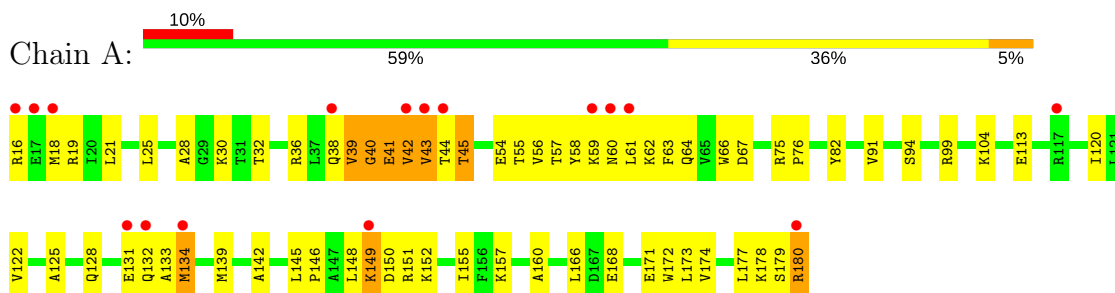
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	64	Total 64	O 64	0	0
5	H	18	Total 18	O 18	0	0

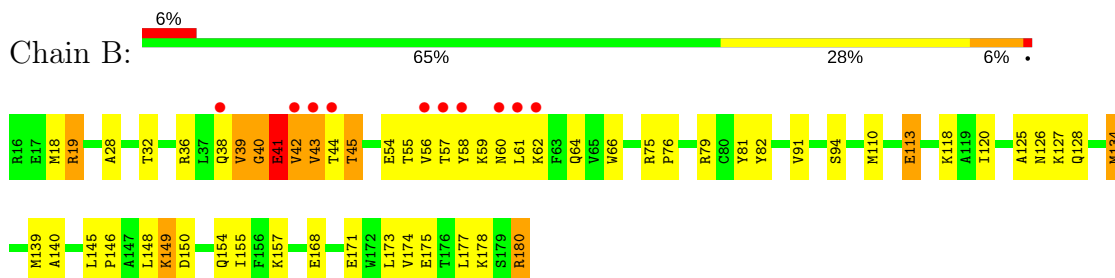
### 3 Residue-property plots [i](#)

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.

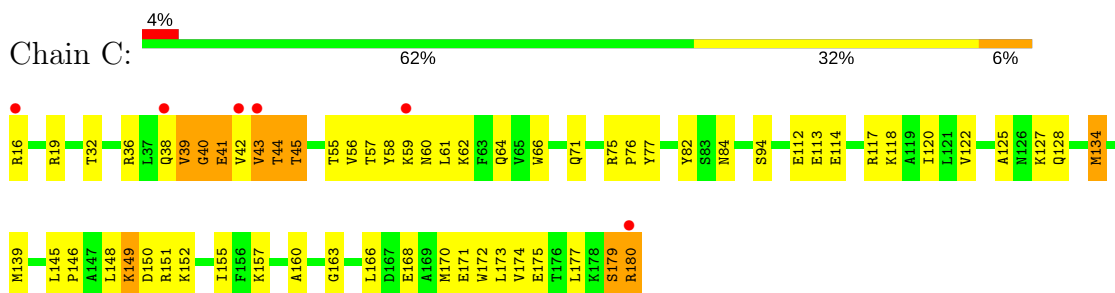
#### • Molecule 1: ADP-ribosylation factor-like protein 1



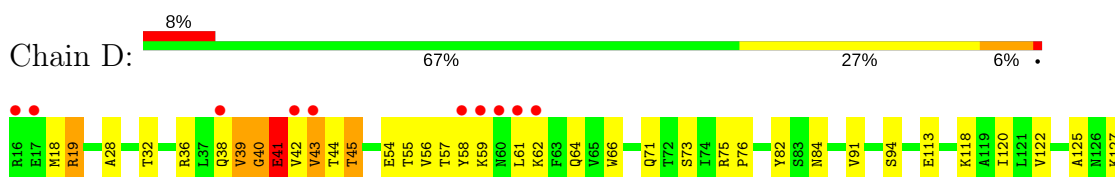
#### • Molecule 1: ADP-ribosylation factor-like protein 1

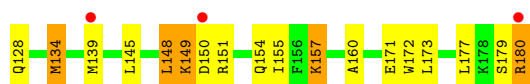


#### • Molecule 1: ADP-ribosylation factor-like protein 1



#### • Molecule 1: ADP-ribosylation factor-like protein 1





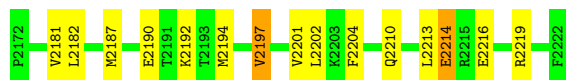
- Molecule 2: Golgi autoantigen, golgin subfamily A member 4



- Molecule 2: Golgi autoantigen, golgin subfamily A member 4



- Molecule 2: Golgi autoantigen, golgin subfamily A member 4



- Molecule 2: Golgi autoantigen, golgin subfamily A member 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.08Å 86.92Å 86.25Å 118.11° 99.65° 95.47°	Depositor
Resolution (Å)	20.00 – 2.30 39.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.30) 91.0 (39.19-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.246 , 0.260 0.278 , 0.291	Depositor DCC
$R_{free}$ test set	2806 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: GNP, MG

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	0.38	0/1333	0.65	0/1802
1	B	0.39	0/1333	0.67	0/1802
1	C	0.42	0/1333	0.69	0/1802
1	D	0.43	0/1333	0.71	0/1802
2	E	0.41	0/440	0.62	0/586
2	F	0.42	0/440	0.60	0/586
2	G	0.42	0/440	0.62	0/586
2	H	0.46	0/440	0.62	0/586
All	All	0.41	0/7092	0.66	0/9552

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	1312	0	1337	82	0
1	B	1312	0	1337	79	0
1	C	1312	0	1337	85	0
1	D	1312	0	1337	78	0
2	E	433	0	444	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	433	0	444	20	0
2	G	433	0	444	14	0
2	H	433	0	444	18	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
4	A	32	0	13	1	0
4	B	32	0	13	2	0
4	C	32	0	13	4	0
4	D	32	0	13	3	0
5	A	38	0	0	15	0
5	B	46	0	0	14	1
5	C	64	0	0	14	0
5	D	64	0	0	23	1
5	E	14	0	0	8	0
5	F	13	0	0	5	0
5	G	11	0	0	1	0
5	H	18	0	0	3	0
All	All	7380	0	7176	385	1

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 27.

All (385) 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:E:2222:PHE:HA	5:E:138:HOH:O	1.20	1.34
1:C:175:GLU:HG2	5:C:1261:HOH:O	1.23	1.29
1:B:149:LYS:HA	5:B:1210:HOH:O	1.26	1.25
1:D:19:ARG:HB2	5:D:1227:HOH:O	1.38	1.20
1:A:128:GLN:HG3	1:A:157:LYS:HB2	1.23	1.18
1:D:151:ARG:HD2	5:D:1251:HOH:O	1.43	1.14
1:D:151:ARG:CD	5:D:1251:HOH:O	1.95	1.14
1:C:128:GLN:HG3	1:C:157:LYS:HB2	1.25	1.14
1:D:19:ARG:CD	5:D:1227:HOH:O	1.96	1.13
1:B:44:THR:HA	5:B:1228:HOH:O	1.58	1.04
1:B:128:GLN:HG3	1:B:157:LYS:HB2	1.39	1.03
1:C:113:GLU:HG3	5:C:1235:HOH:O	1.60	1.01
1:B:60:ASN:HB2	1:C:60:ASN:HD21	1.23	1.00
1:A:16:ARG:O	5:A:1212:HOH:O	1.81	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLN:HB2	1:D:56:VAL:HG13	1.43	0.99
1:B:120:ILE:HD11	1:B:173:LEU:HD12	1.46	0.97
1:B:149:LYS:CA	5:B:1210:HOH:O	1.90	0.96
1:C:112:GLU:OE2	5:C:1224:HOH:O	1.83	0.95
1:B:149:LYS:HD2	5:B:1229:HOH:O	1.64	0.95
1:A:64:GLN:HE21	1:A:66:TRP:HE1	1.14	0.95
1:B:150:ASP:N	5:B:1210:HOH:O	1.90	0.94
1:C:145:LEU:HA	1:C:148:LEU:HD23	1.50	0.94
1:B:145:LEU:HA	1:B:148:LEU:HD23	1.50	0.94
1:D:120:ILE:HD11	1:D:173:LEU:HD12	1.47	0.93
1:D:19:ARG:HD2	5:D:1227:HOH:O	1.62	0.93
1:D:180:ARG:N	5:D:1223:HOH:O	2.01	0.92
4:B:1202:GNP:O2G	5:B:1203:HOH:O	1.85	0.92
1:B:60:ASN:HB2	5:C:1209:HOH:O	1.69	0.91
1:A:36:ARG:HH11	1:A:41:GLU:HG3	1.36	0.90
2:F:2213:LEU:O	2:F:2214:GLU:HG3	1.71	0.90
1:A:120:ILE:HD11	1:A:173:LEU:HD12	1.52	0.89
1:D:179:SER:HB3	5:D:1223:HOH:O	1.71	0.89
1:C:36:ARG:HH11	1:C:41:GLU:HG3	1.37	0.89
1:D:179:SER:CB	5:D:1223:HOH:O	2.20	0.89
1:C:38:GLN:HB2	1:C:56:VAL:HG13	1.53	0.89
1:D:150:ASP:N	5:D:1232:HOH:O	1.80	0.88
4:D:1204:GNP:O1G	5:D:1207:HOH:O	1.89	0.88
1:D:19:ARG:HD3	1:D:84:ASN:O	1.73	0.88
1:A:134:MET:SD	1:A:139:MET:HB2	2.13	0.88
1:B:120:ILE:HD11	1:B:173:LEU:CD1	2.03	0.87
1:B:43:VAL:O	5:B:1206:HOH:O	1.92	0.87
1:C:59:LYS:HE3	5:C:1209:HOH:O	1.74	0.87
1:D:149:LYS:HA	5:D:1232:HOH:O	1.74	0.87
1:A:38:GLN:HB2	1:A:56:VAL:HG13	1.58	0.84
1:D:134:MET:SD	1:D:139:MET:HB2	2.19	0.82
1:B:55:THR:HG21	1:B:62:LYS:HE3	1.63	0.81
1:D:57:THR:HG22	1:D:62:LYS:HD2	1.63	0.80
1:B:125:ALA:HB2	1:B:139:MET:HE2	1.64	0.80
1:A:16:ARG:HG3	5:A:1225:HOH:O	1.82	0.79
1:C:16:ARG:O	5:C:1262:HOH:O	2.00	0.78
1:D:151:ARG:HD3	5:D:1251:HOH:O	1.73	0.78
1:A:64:GLN:NE2	1:A:66:TRP:HE1	1.81	0.77
1:D:120:ILE:HD11	1:D:173:LEU:CD1	2.14	0.77
1:D:19:ARG:CG	5:D:1227:HOH:O	2.21	0.77
1:A:60:ASN:HA	5:A:1233:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLN:NE2	1:D:66:TRP:HE1	1.83	0.75
1:A:59:LYS:HG2	5:A:1235:HOH:O	1.86	0.74
1:B:61:LEU:HB2	5:B:1227:HOH:O	1.86	0.74
1:D:145:LEU:HA	1:D:148:LEU:HD23	1.69	0.74
2:F:2182:LEU:HG	2:F:2186:MET:CE	2.17	0.74
1:B:145:LEU:HA	1:B:148:LEU:CD2	2.17	0.73
1:D:128:GLN:HG3	1:D:157:LYS:HB2	1.69	0.73
1:C:57:THR:HA	1:C:61:LEU:O	1.88	0.73
1:C:120:ILE:HD11	1:C:173:LEU:CD1	2.19	0.72
1:C:66:TRP:CH2	2:G:2190:GLU:HG2	2.25	0.72
1:D:128:GLN:HG3	1:D:157:LYS:CB	2.19	0.72
2:F:2222:PHE:CB	5:F:172:HOH:O	2.37	0.71
1:A:55:THR:HG21	1:A:62:LYS:HE3	1.71	0.71
1:B:60:ASN:CB	5:C:1209:HOH:O	2.34	0.71
1:A:120:ILE:HG22	1:A:152:LYS:HD2	1.71	0.71
1:C:120:ILE:HD11	1:C:173:LEU:HD12	1.71	0.71
1:A:57:THR:HG22	1:A:62:LYS:HD2	1.72	0.71
1:A:125:ALA:HB2	1:A:139:MET:HE2	1.73	0.71
2:G:2219:ARG:HG2	5:G:164:HOH:O	1.90	0.71
1:C:163:GLY:O	5:C:1208:HOH:O	2.09	0.70
1:A:36:ARG:NH1	1:A:41:GLU:HG3	2.07	0.70
1:C:66:TRP:HH2	2:G:2190:GLU:HG2	1.57	0.69
2:F:2182:LEU:HG	2:F:2186:MET:HE2	1.72	0.69
1:B:60:ASN:CB	1:C:60:ASN:HD21	2.02	0.69
1:D:55:THR:HG21	1:D:62:LYS:HE3	1.74	0.69
1:C:58:TYR:CD2	1:C:174:VAL:HG21	2.27	0.69
1:B:64:GLN:HE21	1:B:66:TRP:HE1	1.41	0.68
1:C:112:GLU:CD	5:C:1224:HOH:O	2.29	0.68
2:G:2192:LYS:HA	2:G:2216:GLU:HG2	1.76	0.68
2:E:2213:LEU:O	2:E:2214:GLU:HG3	1.94	0.68
1:B:66:TRP:HH2	2:F:2190:GLU:HG2	1.59	0.68
1:A:94:SER:O	1:A:134:MET:HG3	1.93	0.67
1:D:44:THR:HA	5:D:1262:HOH:O	1.95	0.67
1:D:122:VAL:HG22	1:D:172:TRP:HZ3	1.60	0.67
1:A:145:LEU:HA	1:A:148:LEU:HD23	1.77	0.66
2:E:2179:ARG:HD2	2:G:2202:LEU:O	1.96	0.66
1:A:18:MET:HE2	1:A:177:LEU:HD22	1.76	0.66
1:C:57:THR:HG22	1:C:62:LYS:HD2	1.78	0.66
1:D:73:SER:O	5:D:1226:HOH:O	2.13	0.66
1:B:82:TYR:HD2	1:B:113:GLU:HG2	1.60	0.65
1:A:55:THR:CG2	1:A:62:LYS:HE3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TRP:HH2	2:E:2190:GLU:HG2	1.60	0.65
1:C:82:TYR:HD2	1:C:113:GLU:HG2	1.61	0.65
1:C:43:VAL:O	1:C:45:THR:N	2.29	0.65
1:B:43:VAL:HG12	5:B:1206:HOH:O	1.97	0.65
1:C:134:MET:SD	1:C:139:MET:HB2	2.37	0.65
1:C:170:MET:O	1:C:174:VAL:HG23	1.96	0.64
1:B:60:ASN:HB2	1:C:60:ASN:ND2	2.06	0.64
1:D:18:MET:HE2	1:D:177:LEU:HD13	1.80	0.64
2:F:2222:PHE:C	5:F:172:HOH:O	2.35	0.64
1:B:64:GLN:NE2	1:B:66:TRP:HE1	1.96	0.64
1:A:148:LEU:HD12	1:A:151:ARG:HG3	1.79	0.63
1:D:82:TYR:HD2	1:D:113:GLU:HG2	1.62	0.63
1:B:36:ARG:HH11	1:B:41:GLU:HG3	1.63	0.63
1:A:180:ARG:NH1	5:A:1221:HOH:O	2.32	0.63
1:D:179:SER:C	5:D:1223:HOH:O	2.33	0.63
1:A:128:GLN:HG3	1:A:157:LYS:CB	2.15	0.63
1:C:38:GLN:O	1:C:39:VAL:HG23	1.99	0.63
1:D:38:GLN:O	1:D:39:VAL:HG23	1.99	0.62
1:A:38:GLN:O	1:A:39:VAL:HG23	1.99	0.62
1:A:66:TRP:CH2	2:E:2190:GLU:HG2	2.33	0.62
1:C:64:GLN:NE2	1:C:66:TRP:HE1	1.97	0.62
1:D:134:MET:SD	1:D:139:MET:SD	2.98	0.62
1:A:19:ARG:HH21	1:A:21:LEU:HD21	1.63	0.62
1:B:82:TYR:CD2	1:B:113:GLU:HG2	2.34	0.62
1:A:43:VAL:HG11	4:A:1201:GNP:O2'	1.99	0.62
1:A:41:GLU:OE1	1:A:43:VAL:HG23	1.99	0.61
1:B:32:THR:HG23	1:B:43:VAL:HG22	1.81	0.61
2:F:2184:GLU:OE2	2:F:2189:ARG:HD2	2.00	0.61
2:H:2213:LEU:O	2:H:2214:GLU:HG3	2.01	0.61
1:A:40:GLY:O	1:A:41:GLU:HB2	2.01	0.60
1:A:179:SER:O	1:A:180:ARG:HD3	2.01	0.60
1:B:173:LEU:O	1:B:177:LEU:HG	2.01	0.60
1:C:145:LEU:HA	1:C:148:LEU:CD2	2.28	0.60
1:A:82:TYR:HD2	1:A:113:GLU:HG2	1.66	0.60
1:D:32:THR:HG23	1:D:43:VAL:HG22	1.83	0.60
1:A:139:MET:HE2	1:A:155:ILE:HD11	1.83	0.60
1:A:120:ILE:HD11	1:A:173:LEU:CD1	2.29	0.59
1:A:16:ARG:CG	5:A:1225:HOH:O	2.45	0.59
2:G:2213:LEU:O	2:G:2214:GLU:HG3	2.02	0.59
1:B:38:GLN:HB2	1:B:56:VAL:HG13	1.84	0.59
1:B:40:GLY:O	1:B:41:GLU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:TYR:OH	1:C:171:GLU:HG2	2.03	0.59
2:F:2216:GLU:O	2:F:2219:ARG:HB3	2.02	0.59
1:A:149:LYS:O	1:A:149:LYS:HD2	2.03	0.59
1:C:43:VAL:HG11	4:C:1203:GNP:O2'	2.02	0.59
1:D:66:TRP:CH2	2:H:2190:GLU:HG2	2.37	0.59
1:D:66:TRP:HH2	2:H:2190:GLU:HG2	1.66	0.59
1:C:149:LYS:HD2	1:C:149:LYS:O	2.04	0.58
1:A:122:VAL:HG21	1:A:173:LEU:HD13	1.85	0.58
1:D:134:MET:CE	1:D:139:MET:SD	2.92	0.58
1:D:64:GLN:HE21	1:D:66:TRP:HE1	1.51	0.58
1:C:120:ILE:HG22	1:C:152:LYS:HD2	1.85	0.58
1:C:36:ARG:NH1	1:C:41:GLU:HG3	2.13	0.58
2:E:2205:PRO:HB2	5:E:132:HOH:O	2.03	0.58
2:E:2181:VAL:HG13	2:E:2194:MET:SD	2.44	0.58
1:A:132:GLN:HG2	5:A:1229:HOH:O	2.02	0.58
1:C:39:VAL:CG1	1:C:40:GLY:N	2.67	0.58
1:C:36:ARG:HD2	1:C:41:GLU:HB2	1.86	0.58
1:A:36:ARG:HD2	1:A:41:GLU:HB2	1.86	0.57
1:D:149:LYS:O	1:D:149:LYS:HD2	2.03	0.57
1:C:45:THR:HA	5:C:1248:HOH:O	2.03	0.57
1:D:179:SER:O	1:D:180:ARG:HD3	2.03	0.57
1:B:55:THR:CG2	1:B:62:LYS:HE3	2.34	0.57
2:E:2216:GLU:O	2:E:2219:ARG:HB3	2.04	0.57
2:F:2222:PHE:OXT	5:F:172:HOH:O	2.17	0.57
5:D:1256:HOH:O	2:H:2180:LYS:HE3	2.04	0.57
1:B:58:TYR:CD2	1:B:174:VAL:HG21	2.40	0.57
1:A:149:LYS:O	1:A:150:ASP:HB2	2.04	0.56
1:C:19:ARG:HD3	1:C:84:ASN:O	2.05	0.56
1:B:66:TRP:CH2	2:F:2190:GLU:HG2	2.40	0.56
1:D:36:ARG:HH11	1:D:41:GLU:HG3	1.68	0.56
1:D:58:TYR:OH	1:D:171:GLU:HG2	2.05	0.56
1:A:99:ARG:HA	5:A:1232:HOH:O	2.06	0.56
1:B:18:MET:HE2	1:B:177:LEU:HD13	1.87	0.56
2:E:2205:PRO:CA	5:E:3:HOH:O	2.54	0.56
2:F:2182:LEU:HG	2:F:2186:MET:HE1	1.87	0.56
1:D:36:ARG:NH1	1:D:41:GLU:HG3	2.21	0.56
1:D:148:LEU:HD12	1:D:151:ARG:HG3	1.87	0.56
1:C:82:TYR:CD2	1:C:113:GLU:HG2	2.41	0.55
1:A:43:VAL:O	1:A:43:VAL:HG12	2.07	0.55
1:C:64:GLN:HE21	1:C:66:TRP:HE1	1.53	0.55
1:D:43:VAL:HG12	1:D:43:VAL:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:THR:CG2	1:D:62:LYS:HE3	2.37	0.55
2:G:2219:ARG:HD3	2:H:2222:PHE:CZ	2.42	0.55
2:F:2211:LYS:HG3	2:H:2187:MET:CE	2.36	0.55
1:C:125:ALA:HB2	1:C:139:MET:HE2	1.89	0.55
1:C:139:MET:HE2	1:C:155:ILE:HD11	1.87	0.55
1:C:179:SER:O	1:C:180:ARG:HD3	2.06	0.55
1:A:122:VAL:CG2	1:A:173:LEU:HD13	2.37	0.54
1:B:41:GLU:OE1	1:B:42:VAL:N	2.40	0.54
1:C:173:LEU:O	1:C:177:LEU:HG	2.07	0.54
2:H:2220:LEU:C	2:H:2222:PHE:H	2.10	0.54
1:B:57:THR:HG21	5:C:1255:HOH:O	2.07	0.54
1:B:145:LEU:CA	1:B:148:LEU:HD23	2.32	0.54
1:B:57:THR:HG22	1:B:62:LYS:CD	2.37	0.54
1:D:45:THR:HG21	4:D:1204:GNP:O2A	2.08	0.54
1:D:36:ARG:HD3	1:D:160:ALA:O	2.07	0.54
1:B:139:MET:HE2	1:B:155:ILE:HD11	1.90	0.54
2:F:2222:PHE:HB2	5:F:172:HOH:O	2.05	0.54
1:B:59:LYS:HG2	5:B:1225:HOH:O	2.08	0.54
1:B:75:ARG:NH2	5:B:1208:HOH:O	2.39	0.54
1:A:58:TYR:CD2	1:A:174:VAL:HG21	2.43	0.53
1:C:43:VAL:O	1:C:43:VAL:HG12	2.07	0.53
1:B:36:ARG:HD2	1:B:41:GLU:HB2	1.90	0.53
1:D:94:SER:HB3	1:D:134:MET:HE3	1.91	0.53
1:B:75:ARG:N	1:B:76:PRO:CD	2.72	0.53
1:C:114:GLU:O	1:C:117:ARG:HG2	2.08	0.53
1:D:32:THR:HG22	1:D:160:ALA:HB1	1.91	0.53
1:D:32:THR:OG1	1:D:43:VAL:HG13	2.08	0.53
2:G:2210:GLN:O	2:G:2213:LEU:O	2.27	0.53
1:C:77:TYR:HB2	5:C:1231:HOH:O	2.09	0.53
1:D:139:MET:HE2	1:D:155:ILE:HD11	1.91	0.53
1:D:19:ARG:CZ	5:D:1227:HOH:O	2.57	0.53
1:B:41:GLU:O	1:B:42:VAL:HG23	2.09	0.53
1:D:134:MET:HE2	1:D:139:MET:SD	2.48	0.53
1:B:134:MET:SD	1:B:139:MET:HB2	2.48	0.52
1:A:28:ALA:HB1	1:A:91:VAL:HG12	1.91	0.52
1:A:16:ARG:NH2	5:A:1216:HOH:O	2.43	0.52
1:B:28:ALA:HB1	1:B:91:VAL:HG12	1.91	0.52
1:B:139:MET:CE	1:B:155:ILE:HD11	2.39	0.52
2:E:2215:ARG:NE	5:E:51:HOH:O	2.12	0.52
2:F:2219:ARG:O	2:F:2219:ARG:HD2	2.10	0.52
1:D:82:TYR:CD2	1:D:113:GLU:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LYS:HG2	4:D:1204:GNP:C6	2.40	0.52
2:E:2222:PHE:CA	5:E:138:HOH:O	2.06	0.52
1:C:75:ARG:N	1:C:76:PRO:CD	2.74	0.51
1:B:58:TYR:HD2	1:B:174:VAL:HG21	1.76	0.51
2:E:2207:ASP:OD2	2:E:2208:GLN:N	2.39	0.51
1:B:61:LEU:HD11	1:B:178:LYS:HE3	1.93	0.51
1:C:122:VAL:HG22	1:C:172:TRP:HZ3	1.75	0.51
1:A:42:VAL:C	1:A:44:THR:H	2.13	0.51
1:A:59:LYS:HE3	5:A:1235:HOH:O	2.10	0.51
1:C:59:LYS:HG2	1:C:59:LYS:O	2.09	0.51
2:F:2222:PHE:HB3	5:F:172:HOH:O	2.05	0.51
1:B:94:SER:O	1:B:134:MET:HG3	2.11	0.51
1:D:19:ARG:NE	5:D:1227:HOH:O	2.29	0.51
2:F:2213:LEU:O	2:F:2214:GLU:CG	2.53	0.51
2:H:2184:GLU:OE2	2:H:2189:ARG:HD2	2.11	0.50
1:A:43:VAL:O	1:A:45:THR:N	2.45	0.50
2:G:2181:VAL:HG13	2:G:2194:MET:SD	2.52	0.50
1:A:122:VAL:HG22	1:A:172:TRP:HZ3	1.76	0.50
1:B:59:LYS:CG	5:B:1225:HOH:O	2.59	0.50
1:D:94:SER:O	1:D:134:MET:HG3	2.11	0.50
1:B:128:GLN:CG	1:B:157:LYS:HB2	2.27	0.49
1:B:168:GLU:N	1:B:168:GLU:OE1	2.37	0.49
1:C:94:SER:O	1:C:134:MET:HG3	2.12	0.49
1:C:57:THR:CG2	1:C:62:LYS:NZ	2.75	0.49
1:A:61:LEU:HD11	1:A:178:LYS:HE3	1.93	0.49
1:C:122:VAL:HG22	1:C:172:TRP:CZ3	2.48	0.49
1:B:126:ASN:O	1:B:127:LYS:HB2	2.12	0.49
2:E:2184:GLU:OE2	2:E:2189:ARG:HD2	2.13	0.49
1:A:82:TYR:CD2	1:A:113:GLU:HG2	2.46	0.49
1:C:55:THR:HG21	1:C:62:LYS:HE3	1.95	0.49
1:A:131:GLU:HB3	5:A:1229:HOH:O	2.12	0.49
2:F:2207:ASP:N	2:F:2207:ASP:OD2	2.44	0.49
1:B:110:MET:O	1:B:113:GLU:HB2	2.13	0.48
2:E:2205:PRO:HA	5:E:3:HOH:O	2.10	0.48
2:G:2197:VAL:O	2:G:2201:VAL:HG23	2.13	0.48
1:A:177:LEU:HD12	1:A:178:LYS:N	2.28	0.48
1:C:45:THR:HG21	4:C:1203:GNP:O2A	2.13	0.48
2:H:2192:LYS:HA	2:H:2216:GLU:HG2	1.95	0.48
1:B:42:VAL:C	1:B:44:THR:H	2.16	0.48
1:D:40:GLY:O	1:D:41:GLU:HB2	2.11	0.48
2:G:2192:LYS:HA	2:G:2216:GLU:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:NE	5:A:1225:HOH:O	2.34	0.48
1:D:41:GLU:OE1	1:D:43:VAL:HG23	2.14	0.48
1:A:58:TYR:OH	1:A:171:GLU:HG2	2.13	0.48
1:B:57:THR:HA	1:B:61:LEU:O	2.14	0.48
1:C:42:VAL:C	1:C:44:THR:H	2.17	0.48
1:A:36:ARG:NH1	1:A:41:GLU:CG	2.77	0.48
1:C:36:ARG:HD3	1:C:160:ALA:O	2.14	0.48
1:D:125:ALA:HB2	1:D:139:MET:HE2	1.96	0.48
1:D:43:VAL:O	1:D:45:THR:N	2.47	0.48
2:E:2215:ARG:NH1	5:E:51:HOH:O	2.46	0.47
1:B:19:ARG:NH2	1:B:81:TYR:O	2.47	0.47
2:H:2181:VAL:HG11	2:H:2197:VAL:HG22	1.96	0.47
1:D:134:MET:SD	1:D:139:MET:CB	2.98	0.47
2:E:2197:VAL:O	2:E:2201:VAL:HG23	2.14	0.47
1:C:149:LYS:O	1:C:150:ASP:HB2	2.14	0.47
1:B:44:THR:CA	5:B:1228:HOH:O	2.37	0.47
1:D:128:GLN:HG3	1:D:157:LYS:HB3	1.93	0.47
1:A:104:LYS:HD2	1:A:142:ALA:O	2.15	0.47
1:C:148:LEU:HD12	1:C:151:ARG:HG3	1.96	0.47
1:D:75:ARG:N	1:D:76:PRO:CD	2.79	0.46
2:E:2180:LYS:O	2:E:2180:LYS:HD3	2.16	0.46
1:D:122:VAL:HG22	1:D:172:TRP:CZ3	2.46	0.46
2:F:2194:MET:O	2:F:2197:VAL:HG13	2.15	0.46
2:H:2211:LYS:NZ	5:H:102:HOH:O	2.49	0.46
1:C:145:LEU:CA	1:C:148:LEU:HD23	2.35	0.46
1:C:36:ARG:HG2	1:C:166:LEU:CD1	2.45	0.46
1:C:59:LYS:O	1:C:60:ASN:CG	2.54	0.46
2:E:2211:LYS:HG3	2:G:2187:MET:CE	2.45	0.46
1:C:38:GLN:O	1:C:39:VAL:CB	2.63	0.46
1:B:180:ARG:C	1:B:180:ARG:HD3	2.36	0.46
1:D:59:LYS:HG2	5:D:1235:HOH:O	2.15	0.45
1:A:38:GLN:HE22	1:A:57:THR:HG23	1.82	0.45
1:C:139:MET:CE	1:C:155:ILE:HD11	2.46	0.45
1:D:19:ARG:NH1	5:D:1227:HOH:O	2.49	0.45
1:D:19:ARG:CD	1:D:84:ASN:O	2.57	0.45
2:H:2222:PHE:HB3	5:H:67:HOH:O	2.16	0.45
1:D:118:LYS:HA	1:D:118:LYS:HD3	1.83	0.45
1:A:64:GLN:NE2	1:A:66:TRP:NE1	2.58	0.45
1:B:154:GLN:HA	1:B:154:GLN:OE1	2.16	0.45
1:B:38:GLN:O	1:B:39:VAL:HB	2.17	0.45
1:C:32:THR:OG1	1:C:43:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:N	1:A:146:PRO:CD	2.79	0.45
1:A:94:SER:HA	1:A:134:MET:HE2	1.99	0.45
1:C:42:VAL:HG12	1:C:44:THR:OG1	2.17	0.44
2:E:2179:ARG:HG2	2:G:2204:PHE:CE1	2.51	0.44
1:B:42:VAL:O	1:B:44:THR:N	2.49	0.44
1:C:38:GLN:O	1:C:39:VAL:CG2	2.64	0.44
1:D:149:LYS:CA	5:D:1232:HOH:O	2.43	0.44
1:B:45:THR:HG21	4:B:1202:GNP:O2A	2.16	0.44
1:A:38:GLN:NE2	1:A:57:THR:HG23	2.33	0.44
1:B:41:GLU:OE1	1:B:43:VAL:N	2.51	0.44
1:B:32:THR:OG1	1:B:43:VAL:HG13	2.17	0.44
2:G:2219:ARG:HD3	2:H:2222:PHE:HZ	1.80	0.44
1:A:94:SER:HB3	1:A:133:ALA:HB1	1.98	0.44
1:A:42:VAL:O	1:A:44:THR:N	2.48	0.44
1:A:25:LEU:O	1:A:30:LYS:NZ	2.50	0.44
1:D:149:LYS:O	1:D:150:ASP:HB2	2.18	0.43
1:A:57:THR:HA	1:A:61:LEU:O	2.18	0.43
1:B:57:THR:HG22	1:B:62:LYS:HD2	1.99	0.43
1:C:36:ARG:NH1	1:C:41:GLU:CG	2.81	0.43
2:E:2208:GLN:O	2:E:2212:ILE:HG13	2.17	0.43
1:A:122:VAL:HG22	1:A:172:TRP:CZ3	2.54	0.43
1:A:39:VAL:CG1	1:A:40:GLY:N	2.82	0.43
2:E:2215:ARG:CZ	5:E:51:HOH:O	2.62	0.43
1:D:71:GLN:HG2	5:D:1248:HOH:O	2.18	0.43
1:D:28:ALA:HB1	1:D:91:VAL:HG12	1.99	0.43
1:A:120:ILE:CG2	1:A:152:LYS:HD2	2.45	0.43
1:C:168:GLU:N	1:C:168:GLU:OE1	2.39	0.43
1:C:175:GLU:CG	5:C:1261:HOH:O	2.09	0.43
1:C:127:LYS:HG2	4:C:1203:GNP:C6	2.49	0.43
1:D:57:THR:HA	1:D:61:LEU:O	2.19	0.43
1:A:75:ARG:N	1:A:76:PRO:CD	2.82	0.43
1:B:145:LEU:N	1:B:146:PRO:CD	2.82	0.42
1:C:179:SER:O	1:C:180:ARG:CD	2.67	0.42
1:C:41:GLU:OE1	1:C:42:VAL:N	2.52	0.42
2:E:2182:LEU:O	2:E:2186:MET:HG3	2.19	0.42
1:A:132:GLN:NE2	5:A:1220:HOH:O	2.51	0.42
1:B:41:GLU:OE1	1:B:43:VAL:HG23	2.19	0.42
1:B:79:ARG:HA	1:B:82:TYR:CD2	2.54	0.42
1:B:38:GLN:O	1:B:39:VAL:CB	2.67	0.42
1:B:58:TYR:O	1:B:60:ASN:N	2.53	0.42
1:B:177:LEU:HD12	1:B:178:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:HG2	1:C:166:LEU:HD12	2.01	0.42
1:B:118:LYS:HA	1:B:118:LYS:HD3	1.75	0.42
1:B:57:THR:CG2	1:B:62:LYS:NZ	2.82	0.42
2:F:2222:PHE:CD1	2:F:2222:PHE:N	2.88	0.42
1:A:59:LYS:C	1:A:61:LEU:H	2.24	0.42
1:D:148:LEU:HA	1:D:148:LEU:HD13	1.89	0.42
1:A:36:ARG:HG2	1:A:166:LEU:CD1	2.49	0.41
2:H:2220:LEU:C	2:H:2222:PHE:N	2.73	0.41
1:A:152:LYS:NZ	5:A:1224:HOH:O	2.53	0.41
1:A:19:ARG:O	1:A:19:ARG:HG3	2.20	0.41
1:B:171:GLU:O	1:B:175:GLU:HG3	2.20	0.41
1:C:32:THR:HG23	1:C:43:VAL:HG22	2.01	0.41
2:E:2222:PHE:N	2:E:2222:PHE:CD1	2.88	0.41
1:C:43:VAL:HG11	4:C:1203:GNP:C2'	2.50	0.41
1:D:43:VAL:O	1:D:45:THR:HB	2.21	0.41
2:E:2192:LYS:HD3	2:E:2216:GLU:HG3	2.03	0.41
1:A:16:ARG:CZ	5:A:1216:HOH:O	2.69	0.41
1:B:140:ALA:O	1:B:146:PRO:HD3	2.20	0.41
1:C:118:LYS:HA	1:C:118:LYS:HD3	1.79	0.41
1:C:128:GLN:CG	1:C:157:LYS:HB2	2.19	0.41
1:D:154:GLN:HA	1:D:154:GLN:OE1	2.21	0.41
1:D:180:ARG:HD3	1:D:180:ARG:C	2.40	0.41
1:B:59:LYS:CD	5:B:1225:HOH:O	2.68	0.41
2:E:2219:ARG:HH22	2:H:2222:PHE:HA	1.85	0.41
2:H:2177:TYR:OH	5:H:92:HOH:O	2.14	0.41
1:C:58:TYR:CD2	1:C:59:LYS:N	2.89	0.41
2:E:2221:MET:C	2:E:2222:PHE:CD1	2.93	0.41
1:C:134:MET:CE	1:C:139:MET:HB2	2.51	0.41
2:F:2211:LYS:HG3	2:H:2187:MET:HE1	2.00	0.41
1:A:18:MET:HB2	1:A:63:PHE:CD2	2.56	0.41
2:H:2221:MET:C	2:H:2222:PHE:CD1	2.94	0.41
1:B:41:GLU:OE1	1:B:42:VAL:CA	2.69	0.40
1:A:32:THR:HG22	1:A:160:ALA:HB1	2.03	0.40
1:A:41:GLU:OE1	1:A:43:VAL:N	2.54	0.40
1:C:32:THR:HG22	1:C:160:ALA:HB1	2.03	0.40
1:C:39:VAL:HG12	1:C:40:GLY:N	2.35	0.40
1:A:168:GLU:N	1:A:168:GLU:OE1	2.50	0.40
1:C:145:LEU:HB2	1:C:146:PRO:HD3	2.02	0.40
1:C:58:TYR:CG	1:C:59:LYS:N	2.89	0.40
1:C:57:THR:HG23	1:C:62:LYS:HZ2	1.87	0.40
1:D:42:VAL:C	1:D:44:THR:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:O	1:A:60:ASN:CG	2.60	0.40
1:C:71:GLN:HG2	5:C:1223:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1223:HOH:O	5:D:1205:HOH:O[1_444]	2.08	0.12

## 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	163/165 (99%)	147 (90%)	11 (7%)	5 (3%)	4	3
1	B	163/165 (99%)	146 (90%)	12 (7%)	5 (3%)	4	3
1	C	163/165 (99%)	148 (91%)	10 (6%)	5 (3%)	4	3
1	D	163/165 (99%)	150 (92%)	9 (6%)	4 (2%)	6	4
2	E	49/51 (96%)	47 (96%)	1 (2%)	1 (2%)	8	7
2	F	49/51 (96%)	47 (96%)	1 (2%)	1 (2%)	8	7
2	G	49/51 (96%)	48 (98%)	0	1 (2%)	8	7
2	H	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	8	7
All	All	848/864 (98%)	779 (92%)	46 (5%)	23 (3%)	5	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	43	VAL
1	B	39	VAL

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Mol	Chain	Res	Type
1	B	43	VAL
2	F	2214	GLU
1	C	39	VAL
2	G	2214	GLU
1	D	39	VAL
1	A	40	GLY
1	A	41	GLU
2	E	2214	GLU
1	B	40	GLY
1	B	42	VAL
1	C	43	VAL
1	C	179	SER
1	D	40	GLY
1	D	41	GLU
1	D	43	VAL
2	H	2214	GLU
1	B	41	GLU
1	C	44	THR
1	C	40	GLY
1	A	42	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/143 (100%)	137 (96%)	6 (4%)	32	45
1	B	143/143 (100%)	135 (94%)	8 (6%)	23	32
1	C	143/143 (100%)	138 (96%)	5 (4%)	39	53
1	D	143/143 (100%)	134 (94%)	9 (6%)	20	26
2	E	48/48 (100%)	46 (96%)	2 (4%)	32	45
2	F	48/48 (100%)	47 (98%)	1 (2%)	56	73
2	G	48/48 (100%)	46 (96%)	2 (4%)	32	45
2	H	48/48 (100%)	46 (96%)	2 (4%)	32	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	764/764 (100%)	729 (95%)	35 (5%)	29	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	54	GLU
1	A	67	ASP
1	A	134	MET
1	A	149	LYS
1	A	180	ARG
2	E	2182	LEU
2	E	2197	VAL
1	B	19	ARG
1	B	41	GLU
1	B	45	THR
1	B	54	GLU
1	B	113	GLU
1	B	134	MET
1	B	149	LYS
1	B	180	ARG
2	F	2197	VAL
1	C	41	GLU
1	C	45	THR
1	C	134	MET
1	C	149	LYS
1	C	180	ARG
2	G	2182	LEU
2	G	2197	VAL
1	D	19	ARG
1	D	41	GLU
1	D	45	THR
1	D	54	GLU
1	D	134	MET
1	D	148	LEU
1	D	149	LYS
1	D	157	LYS
1	D	180	ARG
2	H	2182	LEU
2	H	2197	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	B	64	GLN
1	B	128	GLN
1	C	60	ASN
1	C	64	GLN
1	D	64	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GNP	A	1201	3	27,34,34	2.66	11 (40%)	30,54,54	2.44	7 (23%)
4	GNP	B	1202	3	27,34,34	2.64	13 (48%)	30,54,54	2.31	8 (26%)
4	GNP	C	1203	3	27,34,34	2.61	12 (44%)	30,54,54	2.39	8 (26%)
4	GNP	D	1204	3	27,34,34	2.52	11 (40%)	30,54,54	2.34	7 (23%)

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	GNP	A	1201	3	-	0/16/38/38	0/3/3/3
4	GNP	B	1202	3	-	1/16/38/38	0/3/3/3
4	GNP	C	1203	3	-	1/16/38/38	0/3/3/3
4	GNP	D	1204	3	-	0/16/38/38	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	GNP	C4-N9	-9.20	1.35	1.47
4	C	1203	GNP	C4-N9	-8.58	1.36	1.47
4	A	1201	GNP	C4-N9	-8.51	1.36	1.47
4	D	1204	GNP	C4-N9	-8.07	1.37	1.47
4	D	1204	GNP	C5-C6	-3.36	1.47	1.52
4	A	1201	GNP	C5-C6	-3.17	1.47	1.52
4	C	1203	GNP	C5-C6	-3.02	1.47	1.52
4	B	1202	GNP	C5-C6	-3.01	1.47	1.52
4	C	1203	GNP	O4'-C4'	-2.83	1.38	1.45
4	C	1203	GNP	O6-C6	-2.82	1.17	1.23
4	B	1202	GNP	PG-O3G	-2.79	1.49	1.56
4	C	1203	GNP	PB-O2B	-2.66	1.49	1.56
4	A	1201	GNP	O6-C6	-2.64	1.18	1.23
4	C	1203	GNP	C5-C4	-2.56	1.36	1.52
4	D	1204	GNP	PB-O2B	-2.53	1.49	1.56
4	B	1202	GNP	C5-C4	-2.49	1.37	1.52
4	D	1204	GNP	C5-C4	-2.44	1.37	1.52
4	B	1202	GNP	O6-C6	-2.43	1.18	1.23
4	B	1202	GNP	O4'-C4'	-2.41	1.39	1.45
4	B	1202	GNP	PB-O2B	-2.41	1.50	1.56
4	A	1201	GNP	C5-C4	-2.37	1.37	1.52
4	A	1201	GNP	PG-O3G	-2.37	1.50	1.56
4	D	1204	GNP	O6-C6	-2.34	1.18	1.23
4	B	1202	GNP	PG-O2G	-2.33	1.50	1.56
4	A	1201	GNP	PB-O2B	-2.29	1.50	1.56
4	C	1203	GNP	PG-O3G	-2.28	1.50	1.56
4	D	1204	GNP	PG-O3G	-2.24	1.50	1.56
4	A	1201	GNP	O4'-C4'	-2.08	1.40	1.45
4	D	1204	GNP	O4'-C4'	-2.02	1.40	1.45
4	B	1202	GNP	PB-O3A	2.12	1.61	1.59
4	B	1202	GNP	PB-N3B	2.12	1.68	1.63
4	C	1203	GNP	PB-N3B	2.24	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1204	GNP	PB-O3A	2.32	1.62	1.59
4	C	1203	GNP	PB-O3A	2.43	1.62	1.59
4	B	1202	GNP	PG-O1G	2.54	1.49	1.46
4	D	1204	GNP	PG-O1G	2.89	1.49	1.46
4	B	1202	GNP	C6-N1	3.11	1.38	1.33
4	C	1203	GNP	C6-N1	3.37	1.38	1.33
4	A	1201	GNP	PG-N3B	3.37	1.72	1.63
4	A	1201	GNP	PB-O3A	3.54	1.63	1.59
4	C	1203	GNP	PG-O1G	3.65	1.50	1.46
4	D	1204	GNP	C6-N1	3.88	1.39	1.33
4	C	1203	GNP	PG-N3B	4.25	1.74	1.63
4	A	1201	GNP	C6-N1	4.38	1.40	1.33
4	B	1202	GNP	PG-N3B	4.53	1.75	1.63
4	A	1201	GNP	PG-O1G	4.60	1.51	1.46
4	D	1204	GNP	PG-N3B	4.76	1.75	1.63

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	GNP	O1G-PG-N3B	-6.56	101.97	111.79
4	C	1203	GNP	O1G-PG-N3B	-6.46	102.14	111.79
4	B	1202	GNP	C5-C6-N1	-6.33	110.72	118.27
4	D	1204	GNP	C5-C6-N1	-6.14	110.96	118.27
4	A	1201	GNP	C5-C6-N1	-6.10	111.00	118.27
4	D	1204	GNP	O1G-PG-N3B	-6.08	102.70	111.79
4	C	1203	GNP	C5-C6-N1	-5.98	111.14	118.27
4	B	1202	GNP	O1G-PG-N3B	-5.58	103.44	111.79
4	A	1201	GNP	O1B-PB-N3B	-3.29	106.86	111.79
4	C	1203	GNP	O1B-PB-N3B	-2.50	108.06	111.79
4	C	1203	GNP	O6-C6-N1	-2.45	119.45	122.71
4	B	1202	GNP	O6-C6-N1	-2.28	119.69	122.71
4	D	1204	GNP	O6-C6-N1	-2.18	119.81	122.71
4	B	1202	GNP	O1B-PB-N3B	-2.03	108.76	111.79
4	A	1201	GNP	O4'-C4'-C5'	2.06	116.26	109.39
4	C	1203	GNP	O4'-C4'-C5'	2.08	116.31	109.39
4	B	1202	GNP	O4'-C4'-C5'	2.21	116.75	109.39
4	D	1204	GNP	O4'-C4'-C5'	2.24	116.84	109.39
4	D	1204	GNP	O2B-PB-O1B	3.27	116.65	109.88
4	C	1203	GNP	O2B-PB-O1B	3.50	117.12	109.88
4	B	1202	GNP	O2B-PB-O1B	3.53	117.19	109.88
4	A	1201	GNP	O2B-PB-O1B	4.00	118.16	109.88
4	A	1201	GNP	O6-C6-C5	4.42	128.94	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1204	GNP	O6-C6-C5	4.56	129.23	119.82
4	C	1203	GNP	O6-C6-C5	4.65	129.41	119.82
4	B	1202	GNP	O6-C6-C5	4.74	129.59	119.82
4	B	1202	GNP	C4-C5-N7	5.27	109.45	102.46
4	C	1203	GNP	C4-C5-N7	5.34	109.53	102.46
4	A	1201	GNP	C4-C5-N7	5.41	109.63	102.46
4	D	1204	GNP	C4-C5-N7	5.69	110.00	102.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1203	GNP	O1B-PB-N3B-PG
4	B	1202	GNP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1201	GNP	1	0
4	B	1202	GNP	2	0
4	C	1203	GNP	4	0
4	D	1204	GNP	3	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	165/165 (100%)	0.53	16 (9%) 8 10	14, 21, 30, 33	0
1	B	165/165 (100%)	0.16	10 (6%) 21 27	14, 21, 30, 35	0
1	C	165/165 (100%)	0.23	6 (3%) 42 49	16, 21, 31, 36	0
1	D	165/165 (100%)	0.43	13 (7%) 12 17	15, 21, 33, 38	0
2	E	51/51 (100%)	0.53	5 (9%) 7 10	15, 22, 29, 30	0
2	F	51/51 (100%)	0.13	4 (7%) 13 17	15, 22, 30, 33	0
2	G	51/51 (100%)	-0.02	0 100 100	13, 22, 28, 30	0
2	H	51/51 (100%)	0.01	1 (1%) 65 71	15, 22, 31, 35	0
All	All	864/864 (100%)	0.29	55 (6%) 19 25	13, 21, 31, 38	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	10.0
1	A	42	VAL	9.1
1	D	43	VAL	8.3
1	C	43	VAL	7.7
2	E	2220	LEU	7.3
1	A	16	ARG	6.9
2	H	2222	PHE	5.8
1	D	59	LYS	5.8
2	E	2221	MET	5.6
2	E	2222	PHE	5.5
1	C	42	VAL	5.4
1	D	60	ASN	5.2
1	B	43	VAL	4.7
1	D	16	ARG	4.6
1	B	42	VAL	4.4
1	A	44	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	60	ASN	4.0
1	C	38	GLN	3.9
1	B	60	ASN	3.9
2	F	2222	PHE	3.8
2	F	2220	LEU	3.5
1	A	59	LYS	3.4
1	A	18	MET	3.4
1	D	61	LEU	3.4
1	B	61	LEU	3.3
1	D	42	VAL	3.3
1	A	180	ARG	3.2
1	C	16	ARG	3.2
1	D	180	ARG	3.1
1	D	58	TYR	3.1
1	A	132	GLN	2.9
2	F	2221	MET	2.9
1	A	149	LYS	2.8
2	E	2210	GLN	2.7
2	E	2219	ARG	2.7
1	A	131	GLU	2.7
1	B	44	THR	2.5
1	D	139	MET	2.5
1	A	38	GLN	2.5
1	B	38	GLN	2.5
1	A	17	GLU	2.5
1	A	134	MET	2.4
1	C	180	ARG	2.4
1	B	57	THR	2.4
1	D	17	GLU	2.4
1	B	58	TYR	2.3
1	A	117	ARG	2.3
1	A	61	LEU	2.2
1	C	59	LYS	2.2
1	D	62	LYS	2.2
1	D	38	GLN	2.2
1	D	150	ASP	2.1
2	F	2219	ARG	2.1
1	B	62	LYS	2.1
1	B	56	VAL	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
3	MG	A	901	1/1	0.41	0.14	54,54,54,54	0
3	MG	C	903	1/1	0.76	0.29	38,38,38,38	0
3	MG	D	904	1/1	0.81	0.26	41,41,41,41	0
4	GNP	A	1201	32/32	0.90	0.17	35,47,56,57	0
3	MG	B	902	1/1	0.93	0.20	39,39,39,39	0
4	GNP	C	1203	32/32	0.96	0.19	28,33,39,41	0
4	GNP	D	1204	32/32	0.97	0.22	27,35,40,42	0
4	GNP	B	1202	32/32	0.97	0.18	27,40,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.