



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:54 pm BST

PDB ID : 1WQA  
Title : Crystal Structure of Pyrococcus horikoshii phosphomannomutase/phosphoglucose mutase complexed with Mg<sup>2+</sup>  
Authors : Kawamura, T.; Tsuge, M.; Watanabe, N.; Tanaka, I.  
Deposited on : 2004-09-24  
Resolution : 2.00 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
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

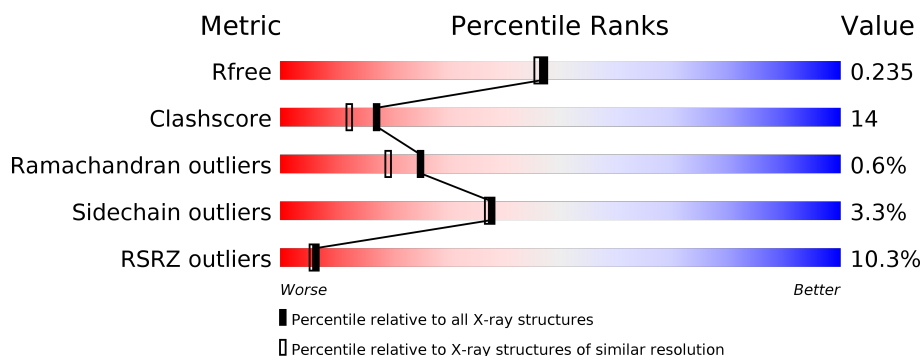
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	455	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>.</div> </div> </div>
1	B	455	<div> <div>15%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	C	455	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	455	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14766 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 phospho-sugar mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	B	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	C	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	D	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

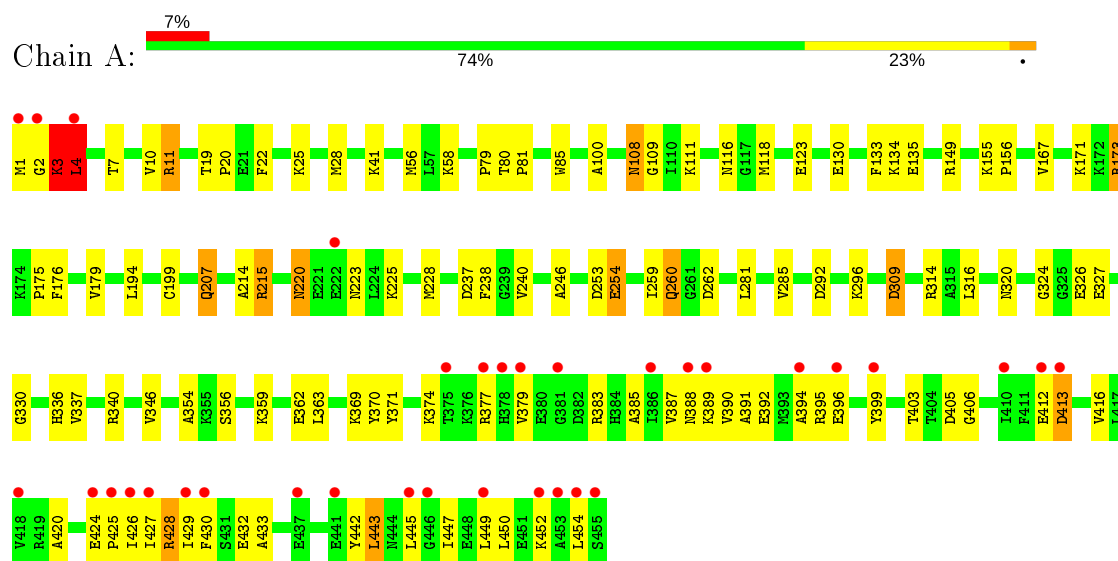
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	192	Total	O	0	0
			192	192		
3	C	186	Total	O	0	0
			186	186		
3	D	165	Total	O	0	0
			165	165		

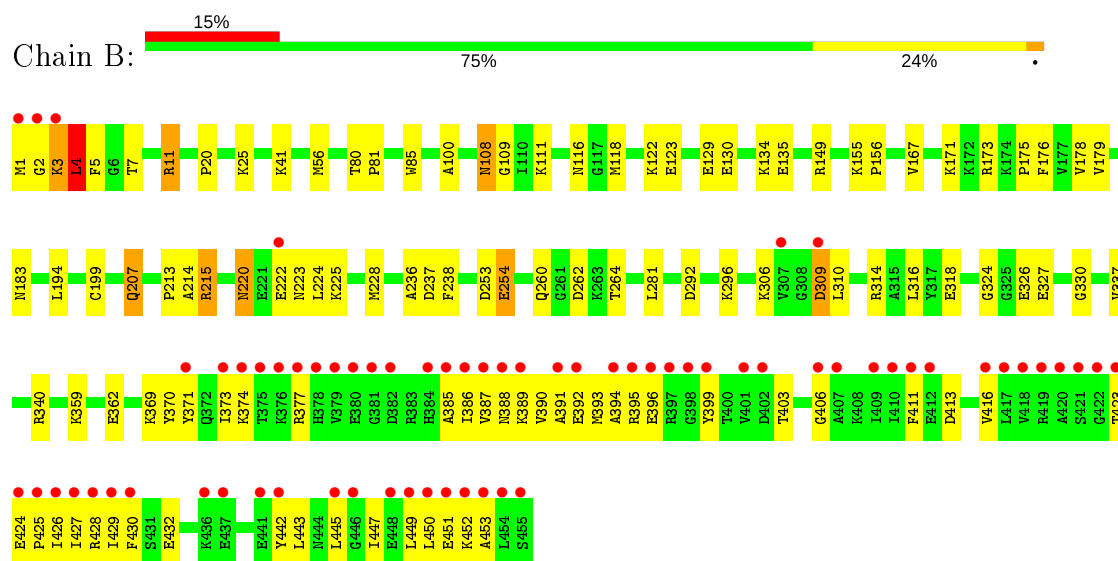
### 3 Residue-property plots [i](#)

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.

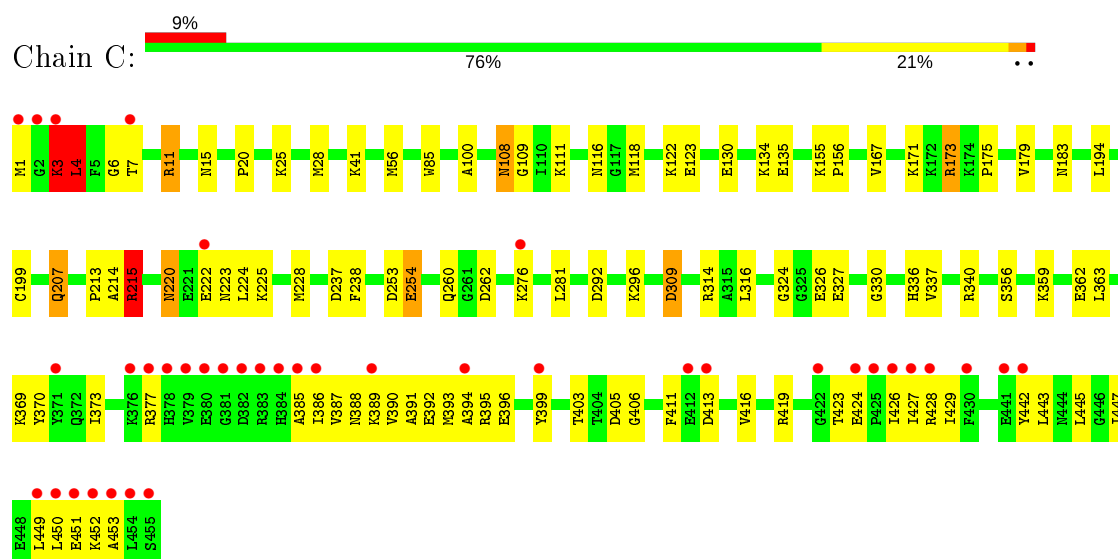
- Molecule 1: phospho-sugar mutase



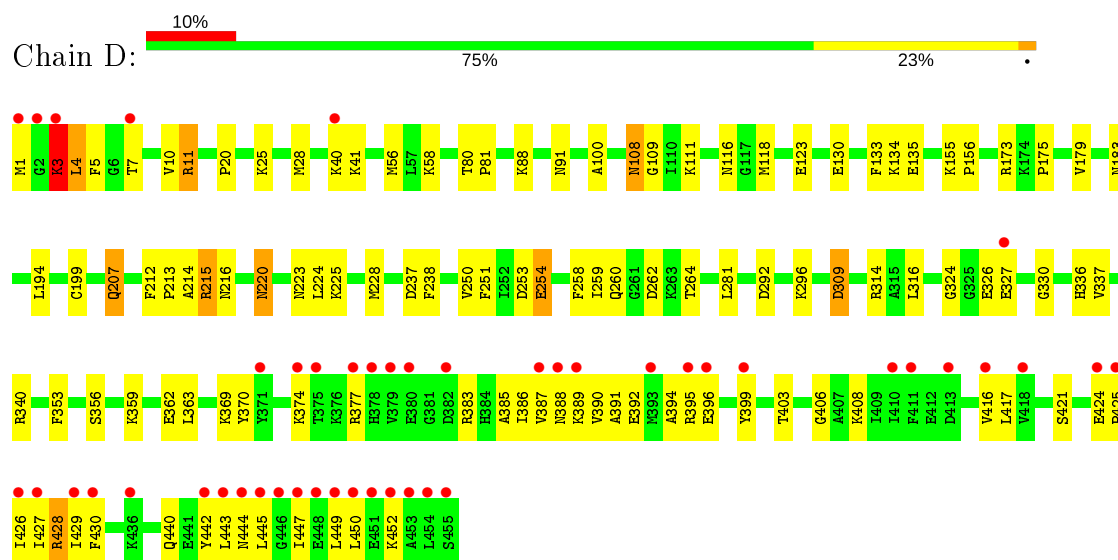
- Molecule 1: phospho-sugar mutase



- Molecule 1: phospho-sugar mutase



- Molecule 1: phospho-sugar mutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.65Å 137.92Å 98.41Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.00) 98.5 (49.12-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.236 0.210 , 0.235	Depositor DCC
$R_{free}$ test set	6883 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: 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	0.49	0/3570	0.70	3/4807 (0.1%)
1	B	0.52	0/3570	0.69	0/4807
1	C	0.50	0/3570	0.69	2/4807 (0.0%)
1	D	0.49	0/3570	0.67	1/4807 (0.0%)
All	All	0.50	0/14280	0.68	6/19228 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	LYS	N-CA-C	-7.71	90.19	111.00
1	A	2	GLY	N-CA-C	-6.95	95.72	113.10
1	A	3	LYS	N-CA-C	-5.90	95.07	111.00
1	D	3	LYS	N-CA-C	-5.80	95.33	111.00
1	C	4	LEU	N-CA-C	5.65	126.27	111.00
1	A	4	LEU	N-CA-C	5.21	125.05	111.00

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	3512	0	3590	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3512	0	3590	106	0
1	C	3512	0	3590	94	0
1	D	3512	0	3591	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	171	0	0	9	0
3	B	192	0	0	7	0
3	C	186	0	0	4	0
3	D	165	0	0	4	0
All	All	14766	0	14361	396	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 14.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HA	1:A:3:LYS:CE	1.56	1.29
1:C:3:LYS:HE3	1:C:3:LYS:HA	1.24	1.15
1:A:416:VAL:HG22	1:A:442:TYR:HB3	1.39	0.99
1:D:416:VAL:HG22	1:D:442:TYR:HB3	1.45	0.98
1:A:3:LYS:HA	1:A:3:LYS:HE3	1.46	0.93
1:A:3:LYS:HE2	1:A:3:LYS:HA	1.48	0.93
1:C:3:LYS:CE	1:C:3:LYS:HA	1.98	0.91
1:C:3:LYS:HE3	1:C:3:LYS:CA	2.03	0.88
1:A:207:GLN:HE21	1:A:207:GLN:H	1.17	0.88
1:A:385:ALA:HA	1:A:388:ASN:HD22	1.39	0.87
1:C:416:VAL:HG22	1:C:442:TYR:HB3	1.58	0.86
1:B:416:VAL:HG22	1:B:442:TYR:HB3	1.58	0.86
1:D:207:GLN:H	1:D:207:GLN:HE21	1.20	0.86
1:B:207:GLN:HE21	1:B:207:GLN:H	1.24	0.84
1:C:207:GLN:HE21	1:C:207:GLN:H	1.22	0.82
1:B:220:ASN:ND2	1:B:223:ASN:H	1.78	0.81
1:D:385:ALA:HA	1:D:388:ASN:HD22	1.43	0.81
1:A:220:ASN:ND2	1:A:223:ASN:H	1.78	0.81
1:C:220:ASN:ND2	1:C:223:ASN:H	1.80	0.80
1:D:220:ASN:ND2	1:D:223:ASN:H	1.80	0.79
1:D:225:LYS:HA	1:D:228:MET:HE3	1.64	0.79
1:C:222:GLU:HG3	3:C:553:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:CA	1:A:3:LYS:CE	2.52	0.76
1:C:385:ALA:HA	1:C:388:ASN:HD22	1.50	0.76
1:A:225:LYS:HA	1:A:228:MET:HE3	1.69	0.74
1:B:385:ALA:HA	1:B:388:ASN:HD22	1.51	0.73
1:B:122:LYS:HE2	1:B:314:ARG:HH22	1.53	0.73
1:C:429:ILE:HD11	1:C:450:LEU:HD12	1.69	0.73
1:C:369:LYS:HD3	1:C:370:TYR:N	2.04	0.72
1:B:225:LYS:HA	1:B:228:MET:HE3	1.72	0.72
1:B:429:ILE:HD11	1:B:450:LEU:HD12	1.71	0.71
1:D:1:MET:HE1	1:D:11:ARG:H	1.54	0.71
1:C:225:LYS:HA	1:C:228:MET:HE3	1.71	0.71
1:B:369:LYS:HD3	1:B:370:TYR:N	2.05	0.71
1:A:416:VAL:CG2	1:A:442:TYR:HB3	2.20	0.71
1:D:392:GLU:O	1:D:396:GLU:HG2	1.90	0.70
1:C:369:LYS:HD3	1:C:370:TYR:H	1.56	0.70
1:A:108:ASN:HD22	1:A:109:GLY:H	1.39	0.70
1:B:369:LYS:HD3	1:B:370:TYR:H	1.55	0.70
1:A:369:LYS:HD3	1:A:370:TYR:N	2.07	0.70
1:B:373:ILE:HB	1:B:443:LEU:HD12	1.75	0.69
1:A:220:ASN:C	1:A:220:ASN:HD22	1.94	0.69
1:B:108:ASN:HD22	1:B:109:GLY:H	1.38	0.69
1:D:220:ASN:C	1:D:220:ASN:HD22	1.94	0.69
1:D:416:VAL:CG2	1:D:442:TYR:HB3	2.21	0.69
1:B:220:ASN:C	1:B:220:ASN:HD22	1.96	0.68
1:B:3:LYS:HE3	1:B:3:LYS:HA	1.75	0.68
1:D:369:LYS:HD3	1:D:370:TYR:N	2.09	0.68
1:D:220:ASN:HD21	1:D:223:ASN:H	1.42	0.68
1:C:108:ASN:HD22	1:C:109:GLY:H	1.40	0.67
1:C:220:ASN:HD22	1:C:220:ASN:C	1.95	0.67
1:B:220:ASN:HD21	1:B:223:ASN:H	1.41	0.67
1:B:306:LYS:HG3	3:B:532:HOH:O	1.95	0.67
1:D:316:LEU:HD11	1:D:324:GLY:HA3	1.77	0.66
1:A:369:LYS:HD3	1:A:370:TYR:H	1.60	0.66
1:A:220:ASN:HD21	1:A:223:ASN:H	1.42	0.66
1:C:122:LYS:HG2	1:C:314:ARG:HH12	1.60	0.66
1:D:369:LYS:HD3	1:D:370:TYR:H	1.61	0.66
1:B:222:GLU:HG3	3:B:644:HOH:O	1.95	0.65
1:D:108:ASN:HD22	1:D:109:GLY:H	1.44	0.65
1:D:377:ARG:HH12	1:D:447:ILE:HG23	1.62	0.65
1:A:392:GLU:O	1:A:396:GLU:HG2	1.96	0.64
1:D:326:GLU:HB2	1:D:327:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:HE21	1:A:207:GLN:N	1.95	0.63
1:A:374:LYS:HE3	1:A:430:PHE:CE2	2.34	0.62
1:C:220:ASN:HD21	1:C:223:ASN:H	1.45	0.62
1:C:292:ASP:O	1:C:296:LYS:HG2	2.00	0.62
1:D:207:GLN:N	1:D:207:GLN:HE21	1.96	0.62
1:A:326:GLU:HB2	1:A:327:GLU:OE1	2.00	0.62
1:B:449:LEU:HD23	1:B:452:LYS:HD3	1.83	0.61
1:C:179:VAL:HG21	1:C:194:LEU:CD1	2.31	0.61
1:C:28:MET:HE3	3:C:459:HOH:O	2.00	0.61
1:D:383:ARG:HH11	1:D:425:PRO:HA	1.65	0.61
1:A:179:VAL:HG21	1:A:194:LEU:CD1	2.31	0.61
1:B:179:VAL:HG21	1:B:194:LEU:CD1	2.31	0.61
1:A:3:LYS:HG3	1:A:133:PHE:CZ	2.36	0.60
1:C:416:VAL:CG2	1:C:442:TYR:HB3	2.30	0.60
1:B:390:VAL:HG13	1:B:449:LEU:HB3	1.83	0.60
1:C:445:LEU:O	1:C:445:LEU:HD13	2.02	0.60
1:C:207:GLN:HE21	1:C:207:GLN:N	1.98	0.59
1:C:116:ASN:OD1	1:C:118:MET:HG2	2.02	0.59
1:B:326:GLU:HB2	1:B:327:GLU:OE1	2.01	0.59
1:A:3:LYS:CA	1:A:3:LYS:HE3	2.26	0.59
1:B:392:GLU:O	1:B:396:GLU:HG2	2.03	0.59
1:C:390:VAL:HG13	1:C:449:LEU:HB3	1.85	0.59
1:B:445:LEU:HD13	1:B:445:LEU:O	2.01	0.59
1:C:449:LEU:HD23	1:C:452:LYS:HD3	1.85	0.59
1:A:383:ARG:NH1	1:A:424:GLU:O	2.35	0.58
1:B:374:LYS:HE3	1:B:430:PHE:CZ	2.38	0.58
1:D:179:VAL:HG21	1:D:194:LEU:CD1	2.34	0.58
1:C:326:GLU:HB2	1:C:327:GLU:OE1	2.03	0.58
1:C:130:GLU:CG	1:C:134:LYS:HE2	2.34	0.58
1:A:3:LYS:HE2	1:A:3:LYS:CA	2.27	0.58
1:B:20:PRO:HG3	1:B:56:MET:SD	2.44	0.58
1:B:292:ASP:O	1:B:296:LYS:HG2	2.03	0.58
1:D:28:MET:HE3	3:D:460:HOH:O	2.05	0.57
1:D:1:MET:HE1	1:D:11:ARG:N	2.19	0.57
1:C:392:GLU:O	1:C:396:GLU:HG2	2.04	0.57
1:B:122:LYS:HE2	1:B:314:ARG:NH2	2.19	0.57
1:B:330:GLY:HA3	1:B:340:ARG:HD3	1.87	0.57
1:B:374:LYS:HE3	1:B:430:PHE:CE2	2.40	0.57
1:B:416:VAL:CG2	1:B:442:TYR:HB3	2.31	0.57
1:D:426:ILE:HG22	1:D:427:ILE:N	2.20	0.56
1:A:28:MET:HE3	3:A:463:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ALA:O	1:B:395:ARG:HG3	2.05	0.56
1:A:314:ARG:NH1	3:A:521:HOH:O	2.38	0.56
1:B:130:GLU:CG	1:B:134:LYS:HE2	2.35	0.56
1:D:1:MET:HE1	1:D:11:ARG:HD2	1.87	0.56
1:C:391:ALA:O	1:C:395:ARG:HG3	2.06	0.56
1:D:330:GLY:HA3	1:D:340:ARG:HD3	1.88	0.56
1:A:377:ARG:HH12	1:A:447:ILE:HG23	1.71	0.56
1:A:130:GLU:CG	1:A:134:LYS:HE2	2.36	0.55
1:C:122:LYS:HE2	1:C:314:ARG:HH22	1.72	0.55
1:B:1:MET:O	1:B:5:PHE:O	2.25	0.55
1:A:330:GLY:HA3	1:A:340:ARG:HD3	1.88	0.54
1:C:427:ILE:O	1:C:427:ILE:HG23	2.07	0.54
1:D:130:GLU:CG	1:D:134:LYS:HE2	2.37	0.54
1:D:394:ALA:O	1:D:399:TYR:HB2	2.07	0.54
1:B:155:LYS:HB3	1:B:156:PRO:HD3	1.88	0.54
1:C:175:PRO:HG2	1:C:199:CYS:SG	2.48	0.54
1:C:11:ARG:HH22	1:C:111:LYS:NZ	2.06	0.53
1:D:387:VAL:HG22	1:D:427:ILE:HD11	1.89	0.53
1:D:391:ALA:O	1:D:395:ARG:HG3	2.08	0.53
1:A:385:ALA:O	1:A:389:LYS:HG3	2.08	0.53
1:B:149:ARG:NH2	3:B:546:HOH:O	2.33	0.53
1:B:41:LYS:NZ	1:B:41:LYS:HB2	2.23	0.53
1:A:316:LEU:HD11	1:A:324:GLY:HA3	1.90	0.53
1:D:25:LYS:HE3	1:D:135:GLU:HG2	1.91	0.53
1:B:207:GLN:HE21	1:B:207:GLN:N	2.02	0.53
1:D:3:LYS:HG2	1:D:133:PHE:CE2	2.44	0.53
1:A:412:GLU:HG3	1:A:413:ASP:N	2.24	0.53
1:D:427:ILE:HG23	1:D:427:ILE:O	2.09	0.52
1:A:292:ASP:O	1:A:296:LYS:HG2	2.09	0.52
1:D:383:ARG:NH1	1:D:425:PRO:HA	2.25	0.52
1:D:359:LYS:HB2	1:D:362:GLU:HG3	1.92	0.52
1:B:423:THR:HB	1:B:424:GLU:OE1	2.09	0.52
1:A:20:PRO:HG3	1:A:56:MET:SD	2.50	0.52
1:B:377:ARG:HH12	1:B:447:ILE:HG23	1.75	0.52
1:D:123:GLU:CD	1:D:123:GLU:H	2.13	0.52
1:C:41:LYS:NZ	1:C:41:LYS:HB2	2.24	0.52
1:D:20:PRO:HG3	1:D:56:MET:SD	2.49	0.52
1:B:373:ILE:CB	1:B:443:LEU:HD12	2.40	0.51
1:C:253:ASP:HB2	1:C:254:GLU:OE1	2.10	0.51
1:D:383:ARG:HD2	1:D:426:ILE:O	2.10	0.51
1:C:130:GLU:HG2	1:C:134:LYS:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ASN:OD1	1:D:118:MET:HG2	2.11	0.51
1:D:207:GLN:H	1:D:207:GLN:NE2	1.99	0.51
1:D:214:ALA:O	1:D:215:ARG:HB3	2.10	0.51
1:B:130:GLU:HG2	1:B:134:LYS:HE2	1.92	0.51
1:B:427:ILE:HG23	1:B:427:ILE:O	2.09	0.51
1:C:330:GLY:HA3	1:C:340:ARG:HD3	1.92	0.51
1:D:108:ASN:HD22	1:D:109:GLY:N	2.09	0.51
1:B:4:LEU:HD12	1:B:5:PHE:CE1	2.45	0.51
1:A:108:ASN:HD22	1:A:109:GLY:N	2.07	0.51
1:A:387:VAL:HG22	1:A:427:ILE:HD11	1.93	0.51
1:B:403:THR:HA	1:B:406:GLY:O	2.11	0.51
1:A:260:GLN:HB3	1:A:262:ASP:OD1	2.12	0.50
1:B:426:ILE:HG22	1:B:427:ILE:N	2.27	0.50
1:A:25:LYS:HE3	1:A:135:GLU:HG2	1.93	0.50
1:A:428:ARG:HB3	1:A:430:PHE:HE1	1.76	0.50
1:B:413:ASP:HB3	1:B:442:TYR:OH	2.12	0.50
1:C:1:MET:O	1:C:3:LYS:O	2.29	0.50
1:D:281:LEU:C	1:D:281:LEU:HD23	2.31	0.50
1:A:254:GLU:CG	3:A:512:HOH:O	2.59	0.50
1:C:276:LYS:NZ	3:C:614:HOH:O	2.44	0.50
1:C:423:THR:HB	1:C:424:GLU:OE1	2.12	0.50
1:D:108:ASN:ND2	1:D:109:GLY:H	2.09	0.50
1:D:383:ARG:NH1	1:D:424:GLU:O	2.43	0.50
1:B:359:LYS:HB2	1:B:362:GLU:HG3	1.94	0.49
1:A:130:GLU:HG2	1:A:134:LYS:HE2	1.93	0.49
1:A:429:ILE:HD11	1:A:450:LEU:HD12	1.93	0.49
1:B:100:ALA:HB2	1:B:108:ASN:HA	1.94	0.49
1:A:123:GLU:CD	1:A:123:GLU:H	2.14	0.49
1:B:108:ASN:HD22	1:B:109:GLY:N	2.08	0.49
1:B:11:ARG:HH22	1:B:111:LYS:NZ	2.10	0.49
1:B:377:ARG:O	1:B:427:ILE:HG22	2.13	0.49
1:B:387:VAL:HG22	1:B:427:ILE:HD11	1.93	0.49
1:D:220:ASN:C	1:D:220:ASN:ND2	2.65	0.49
1:D:374:LYS:HE3	1:D:430:PHE:CE2	2.47	0.49
1:A:116:ASN:OD1	1:A:118:MET:HG2	2.12	0.49
1:A:427:ILE:HG23	1:A:427:ILE:O	2.11	0.49
1:C:426:ILE:HG22	1:C:427:ILE:N	2.27	0.49
1:D:1:MET:CE	1:D:11:ARG:HD2	2.41	0.49
1:B:116:ASN:OD1	1:B:118:MET:HG2	2.12	0.49
1:B:122:LYS:CE	1:B:314:ARG:HH22	2.24	0.49
1:C:260:GLN:HB3	1:C:262:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLN:HB3	1:D:262:ASP:OD1	2.11	0.49
1:D:91:ASN:HB3	3:D:619:HOH:O	2.12	0.49
1:C:377:ARG:O	1:C:427:ILE:HG22	2.13	0.49
1:C:450:LEU:O	1:C:453:ALA:HB3	2.13	0.48
1:C:20:PRO:HG3	1:C:56:MET:SD	2.52	0.48
1:B:123:GLU:H	1:B:123:GLU:CD	2.16	0.48
1:B:399:TYR:HE1	1:B:445:LEU:HD21	1.78	0.48
1:A:281:LEU:HD23	1:A:281:LEU:C	2.33	0.48
1:A:450:LEU:HD23	1:A:454:LEU:HD13	1.95	0.48
1:D:11:ARG:HH22	1:D:111:LYS:NZ	2.10	0.48
1:D:386:ILE:O	1:D:390:VAL:HG23	2.13	0.48
1:B:224:LEU:O	1:B:228:MET:HG3	2.13	0.48
1:A:383:ARG:HH11	1:A:425:PRO:HA	1.78	0.48
1:B:399:TYR:CE1	1:B:445:LEU:HD21	2.48	0.48
1:B:393:MET:HE1	1:B:453:ALA:HA	1.93	0.48
1:D:155:LYS:HB3	1:D:156:PRO:HD3	1.96	0.48
1:A:108:ASN:ND2	1:A:109:GLY:H	2.08	0.48
1:A:443:LEU:HD22	1:A:447:ILE:HD11	1.96	0.48
1:B:254:GLU:OE1	1:B:254:GLU:N	2.47	0.48
1:B:253:ASP:HB2	1:B:254:GLU:OE1	2.14	0.48
1:C:413:ASP:HB3	1:C:442:TYR:OH	2.14	0.48
1:C:399:TYR:CE1	1:C:445:LEU:HD21	2.49	0.48
1:D:417:LEU:HB3	1:D:430:PHE:HB2	1.95	0.48
1:B:175:PRO:HG2	1:B:199:CYS:SG	2.54	0.47
1:A:80:THR:HB	1:A:81:PRO:HD3	1.95	0.47
1:C:377:ARG:HH12	1:C:447:ILE:HG23	1.80	0.47
1:C:399:TYR:HE1	1:C:445:LEU:HD21	1.79	0.47
1:A:285:VAL:HG21	1:A:405:ASP:HB3	1.97	0.47
1:D:251:PHE:CD2	1:D:264:THR:HG21	2.50	0.47
1:B:394:ALA:O	1:B:399:TYR:HB2	2.14	0.47
1:A:426:ILE:HG22	1:A:427:ILE:N	2.28	0.47
1:B:393:MET:HE3	1:B:453:ALA:HB2	1.96	0.47
1:C:394:ALA:O	1:C:399:TYR:HB2	2.14	0.47
1:D:100:ALA:HB2	1:D:108:ASN:HA	1.97	0.47
1:C:214:ALA:O	1:C:215:ARG:HB3	2.14	0.47
1:C:220:ASN:ND2	1:C:220:ASN:C	2.65	0.47
1:C:429:ILE:HD11	1:C:450:LEU:CD1	2.42	0.47
1:A:155:LYS:HB3	1:A:156:PRO:HD3	1.97	0.47
1:A:253:ASP:HB2	1:A:254:GLU:OE1	2.15	0.47
1:B:447:ILE:O	1:B:451:GLU:HG3	2.14	0.47
1:B:389:LYS:C	1:B:393:MET:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HH22	1:A:111:LYS:NZ	2.12	0.46
1:A:237:ASP:O	1:A:238:PHE:HB3	2.15	0.46
1:B:254:GLU:CG	3:B:476:HOH:O	2.63	0.46
1:D:292:ASP:O	1:D:296:LYS:HG2	2.14	0.46
1:B:108:ASN:ND2	1:B:109:GLY:H	2.10	0.46
1:D:428:ARG:HB3	1:D:430:PHE:HE1	1.79	0.46
1:A:220:ASN:C	1:A:220:ASN:ND2	2.64	0.46
1:A:383:ARG:NH1	1:A:425:PRO:HA	2.29	0.46
1:B:1:MET:O	1:B:2:GLY:C	2.54	0.46
1:B:443:LEU:HD23	1:B:443:LEU:O	2.15	0.46
1:C:155:LYS:HB3	1:C:156:PRO:HD3	1.97	0.46
1:B:220:ASN:C	1:B:220:ASN:ND2	2.67	0.46
1:C:108:ASN:HD22	1:C:109:GLY:N	2.09	0.46
1:A:11:ARG:NH2	3:A:625:HOH:O	2.48	0.46
1:D:356:SER:CB	1:D:363:LEU:HD21	2.46	0.46
1:A:320:ASN:HB2	3:A:594:HOH:O	2.15	0.46
1:C:445:LEU:HD13	1:C:445:LEU:C	2.36	0.46
1:D:336:HIS:CD2	1:D:337:VAL:HG22	2.51	0.46
1:D:429:ILE:HD11	1:D:450:LEU:HD12	1.98	0.46
1:B:85:TRP:HB2	1:B:337:VAL:HG11	1.98	0.46
1:B:167:VAL:CG1	1:B:171:LYS:HE3	2.46	0.45
1:C:254:GLU:CG	3:C:568:HOH:O	2.63	0.45
1:B:100:ALA:HB2	1:B:108:ASN:CA	2.47	0.45
1:D:449:LEU:HA	1:D:452:LYS:HG2	1.98	0.45
1:D:88:LYS:HE3	3:D:485:HOH:O	2.15	0.45
1:B:445:LEU:HD13	1:B:445:LEU:C	2.37	0.45
1:C:100:ALA:HB2	1:C:108:ASN:CA	2.46	0.45
1:D:215:ARG:HG2	1:D:216:ASN:O	2.15	0.45
1:D:237:ASP:O	1:D:238:PHE:HB3	2.16	0.45
1:D:377:ARG:HH22	1:D:447:ILE:HD13	1.81	0.45
1:A:254:GLU:OE1	1:A:254:GLU:N	2.50	0.45
1:A:336:HIS:CD2	1:A:337:VAL:HG22	2.51	0.45
1:C:1:MET:C	1:C:3:LYS:O	2.55	0.45
1:D:100:ALA:HB2	1:D:108:ASN:CA	2.46	0.45
1:A:330:GLY:CA	1:A:340:ARG:HD3	2.47	0.45
1:B:11:ARG:NH2	3:B:570:HOH:O	2.33	0.45
1:A:175:PRO:HG2	1:A:199:CYS:SG	2.57	0.45
1:A:254:GLU:HG2	3:A:512:HOH:O	2.17	0.45
1:D:40:LYS:HD2	3:D:598:HOH:O	2.16	0.45
1:A:254:GLU:HG3	3:A:512:HOH:O	2.17	0.45
1:A:359:LYS:HB2	1:A:362:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:O	1:B:393:MET:HE2	2.17	0.45
1:D:80:THR:HB	1:D:81:PRO:HD3	1.98	0.45
1:A:445:LEU:HD13	1:A:445:LEU:O	2.16	0.45
1:C:25:LYS:HE3	1:C:135:GLU:HG2	1.99	0.45
1:C:403:THR:HA	1:C:406:GLY:O	2.17	0.45
1:D:1:MET:HE1	1:D:10:VAL:HA	1.98	0.45
1:D:259:ILE:N	1:D:259:ILE:HD12	2.32	0.45
1:D:330:GLY:CA	1:D:340:ARG:HD3	2.46	0.45
1:A:371:TYR:O	1:A:432:GLU:HA	2.17	0.44
1:C:85:TRP:HB2	1:C:337:VAL:HG11	1.99	0.44
1:D:377:ARG:HH12	1:D:447:ILE:CG2	2.28	0.44
1:A:41:LYS:HB2	1:A:41:LYS:NZ	2.32	0.44
1:B:122:LYS:HG2	1:B:314:ARG:HH12	1.83	0.44
1:B:429:ILE:HD11	1:B:450:LEU:CD1	2.43	0.44
1:D:253:ASP:HB2	1:D:254:GLU:OE1	2.17	0.44
1:C:1:MET:HE3	1:C:6:GLY:HA3	2.00	0.44
1:D:403:THR:HA	1:D:406:GLY:O	2.17	0.44
1:B:183:ASN:OD1	1:B:213:PRO:HD2	2.17	0.44
1:C:254:GLU:N	1:C:254:GLU:OE1	2.50	0.44
1:C:387:VAL:HG22	1:C:427:ILE:HD11	2.00	0.44
1:A:149:ARG:NH2	3:A:602:HOH:O	2.45	0.44
1:A:7:THR:HB	1:A:309:ASP:HB2	2.00	0.44
1:B:214:ALA:O	1:B:215:ARG:HB3	2.18	0.44
1:B:260:GLN:HB3	1:B:262:ASP:OD1	2.17	0.44
1:C:336:HIS:CD2	1:C:337:VAL:HG22	2.53	0.44
1:A:100:ALA:HB2	1:A:108:ASN:CA	2.48	0.44
1:A:173:ARG:HG3	1:A:354:ALA:HA	2.00	0.44
1:B:281:LEU:C	1:B:281:LEU:HD23	2.38	0.43
1:B:377:ARG:HH12	1:B:447:ILE:CG2	2.31	0.43
1:C:108:ASN:ND2	1:C:109:GLY:H	2.12	0.43
1:C:377:ARG:HH22	1:C:447:ILE:HD13	1.83	0.43
1:D:421:SER:HB3	1:D:424:GLU:O	2.18	0.43
1:B:237:ASP:O	1:B:238:PHE:HB3	2.18	0.43
1:C:316:LEU:HD11	1:C:324:GLY:HA3	1.99	0.43
1:A:11:ARG:NH1	3:A:614:HOH:O	2.51	0.43
1:D:1:MET:CE	1:D:10:VAL:HA	2.48	0.43
1:A:100:ALA:HB2	1:A:108:ASN:HA	1.99	0.43
1:A:19:THR:HB	1:A:20:PRO:CD	2.49	0.43
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.83	0.43
1:A:391:ALA:O	1:A:395:ARG:HG3	2.19	0.43
1:B:371:TYR:O	1:B:432:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LYS:HG2	1:C:314:ARG:NH1	2.31	0.43
1:C:237:ASP:O	1:C:238:PHE:HB3	2.19	0.43
1:D:130:GLU:HG2	1:D:134:LYS:HE2	1.99	0.43
1:A:4:LEU:HD21	1:A:22:PHE:CE1	2.53	0.43
1:C:183:ASN:OD1	1:C:213:PRO:HD2	2.18	0.43
1:C:447:ILE:O	1:C:451:GLU:HG3	2.18	0.43
1:B:411:PHE:HE1	1:B:416:VAL:HG23	1.84	0.43
1:C:373:ILE:HB	1:C:443:LEU:HD12	2.00	0.43
1:B:374:LYS:HG2	1:B:430:PHE:CD2	2.54	0.43
1:D:445:LEU:HD13	1:D:445:LEU:O	2.17	0.43
1:D:58:LYS:HB3	1:D:58:LYS:HE2	1.79	0.43
1:B:7:THR:HB	1:B:309:ASP:HB2	2.01	0.43
1:C:411:PHE:HE1	1:C:416:VAL:HG23	1.84	0.43
1:D:175:PRO:HG2	1:D:199:CYS:SG	2.59	0.42
1:D:1:MET:O	1:D:5:PHE:O	2.36	0.42
1:D:395:ARG:HH21	1:D:403:THR:HG23	1.84	0.42
1:A:413:ASP:OD1	1:A:433:ALA:HB1	2.20	0.42
1:C:281:LEU:HD23	1:C:281:LEU:C	2.40	0.42
1:B:377:ARG:HH22	1:B:447:ILE:HD13	1.83	0.42
1:C:443:LEU:O	1:C:443:LEU:HD23	2.18	0.42
1:D:385:ALA:O	1:D:389:LYS:HG3	2.19	0.42
1:A:58:LYS:HB3	1:A:58:LYS:HE2	1.80	0.42
1:B:122:LYS:HE2	1:B:314:ARG:HH12	1.84	0.42
1:C:100:ALA:HB2	1:C:108:ASN:HA	2.01	0.42
1:A:374:LYS:HG2	1:A:430:PHE:CD2	2.54	0.42
1:A:390:VAL:HG13	1:A:449:LEU:HB3	2.02	0.42
1:A:85:TRP:HB2	1:A:337:VAL:HG11	2.02	0.42
1:B:310:LEU:O	1:B:314:ARG:HG3	2.19	0.42
1:C:389:LYS:C	1:C:393:MET:HE2	2.40	0.42
1:D:408:LYS:HA	1:D:416:VAL:O	2.19	0.42
1:C:1:MET:CE	1:C:6:GLY:HA3	2.49	0.42
1:D:224:LEU:O	1:D:228:MET:HG3	2.20	0.42
1:B:178:VAL:HG23	1:B:236:ALA:CB	2.49	0.42
1:B:80:THR:HB	1:B:81:PRO:HD3	2.01	0.42
1:C:7:THR:HB	1:C:309:ASP:HB2	2.02	0.42
1:A:167:VAL:CG1	1:A:171:LYS:HE3	2.50	0.42
1:A:79:PRO:HB3	1:A:246:ALA:HB3	2.02	0.41
1:A:327:GLU:H	1:A:327:GLU:CD	2.19	0.41
1:C:173:ARG:HD2	1:C:173:ARG:O	2.19	0.41
1:A:383:ARG:HG2	1:A:420:ALA:HB1	2.02	0.41
1:B:178:VAL:HG23	1:B:236:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLU:CD	1:C:123:GLU:H	2.22	0.41
1:D:179:VAL:HG21	1:D:194:LEU:HD12	2.01	0.41
1:D:183:ASN:OD1	1:D:213:PRO:HD2	2.20	0.41
1:A:259:ILE:N	1:A:259:ILE:HD12	2.35	0.41
1:A:449:LEU:HA	1:A:452:LYS:HG2	2.03	0.41
1:B:25:LYS:HE3	1:B:135:GLU:HG2	2.02	0.41
1:B:316:LEU:HD11	1:B:324:GLY:HA3	2.02	0.41
1:D:212:PHE:N	1:D:213:PRO:HD3	2.36	0.41
1:B:449:LEU:O	1:B:453:ALA:HB2	2.20	0.41
1:C:179:VAL:HG21	1:C:194:LEU:HD11	2.01	0.41
1:D:41:LYS:HB2	1:D:41:LYS:NZ	2.35	0.41
1:B:254:GLU:HG3	3:B:476:HOH:O	2.21	0.41
1:B:449:LEU:HA	1:B:452:LYS:HG2	2.02	0.41
1:C:385:ALA:O	1:C:389:LYS:HG3	2.21	0.41
1:C:449:LEU:HA	1:C:452:LYS:HG2	2.02	0.41
1:A:1:MET:SD	1:A:10:VAL:HG23	2.61	0.41
1:C:405:ASP:OD1	1:C:419:ARG:NH1	2.54	0.41
1:D:250:VAL:HG11	1:D:258:PHE:CE1	2.55	0.41
1:A:403:THR:HA	1:A:406:GLY:O	2.20	0.41
1:C:167:VAL:CG1	1:C:171:LYS:HE3	2.51	0.41
1:C:330:GLY:CA	1:C:340:ARG:HD3	2.51	0.41
1:D:7:THR:HB	1:D:309:ASP:HB2	2.02	0.41
1:A:240:VAL:HG11	1:A:346:VAL:HG21	2.03	0.41
1:C:359:LYS:HB2	1:C:362:GLU:HG3	2.02	0.41
1:A:356:SER:CB	1:A:363:LEU:HD21	2.51	0.41
1:A:80:THR:N	1:A:81:PRO:CD	2.83	0.41
1:B:4:LEU:HB3	1:B:129:GLU:HG2	2.02	0.41
1:C:224:LEU:O	1:C:228:MET:HG3	2.21	0.41
1:C:356:SER:CB	1:C:363:LEU:HD21	2.51	0.41
1:A:19:THR:HB	1:A:20:PRO:HD2	2.03	0.41
1:B:318:GLU:OE1	1:B:318:GLU:HA	2.21	0.41
1:B:424:GLU:HA	1:B:425:PRO:HD3	1.89	0.41
1:C:207:GLN:NE2	1:C:207:GLN:H	2.01	0.41
1:B:385:ALA:O	1:B:389:LYS:HG3	2.22	0.40
1:C:386:ILE:O	1:C:390:VAL:HG23	2.21	0.40
1:A:214:ALA:O	1:A:215:ARG:HB3	2.20	0.40
1:B:386:ILE:O	1:B:390:VAL:HG23	2.21	0.40
1:A:3:LYS:HG3	1:A:133:PHE:CE2	2.56	0.40
1:A:383:ARG:HD2	1:A:426:ILE:O	2.22	0.40
1:A:379:VAL:HG21	1:A:427:ILE:HG21	2.03	0.40
1:B:11:ARG:HH22	1:B:111:LYS:HZ1	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLU:HG2	3:B:476:HOH:O	2.21	0.40
1:D:175:PRO:HB3	1:D:353:PHE:CE2	2.56	0.40
1:D:426:ILE:CG2	1:D:427:ILE:N	2.83	0.40
1:A:394:ALA:O	1:A:399:TYR:HB2	2.20	0.40
1:D:440:GLN:HG3	1:D:444:ASN:HD21	1.87	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	453/455 (100%)	431 (95%)	20 (4%)	2 (0%)	34	30
1	B	453/455 (100%)	425 (94%)	26 (6%)	2 (0%)	34	30
1	C	453/455 (100%)	428 (94%)	22 (5%)	3 (1%)	22	16
1	D	453/455 (100%)	429 (95%)	21 (5%)	3 (1%)	22	16
All	All	1812/1820 (100%)	1713 (94%)	89 (5%)	10 (1%)	25	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	LEU
1	D	428	ARG
1	B	4	LEU
1	D	3	LYS
1	A	428	ARG
1	B	428	ARG
1	C	428	ARG
1	A	4	LEU
1	D	4	LEU
1	C	215	ARG

### 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	368/368 (100%)	354 (96%)	14 (4%)	33	31
1	B	368/368 (100%)	356 (97%)	12 (3%)	38	37
1	C	368/368 (100%)	357 (97%)	11 (3%)	41	41
1	D	368/368 (100%)	357 (97%)	11 (3%)	41	41
All	All	1472/1472 (100%)	1424 (97%)	48 (3%)	38	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LEU
1	A	11	ARG
1	A	108	ASN
1	A	173	ARG
1	A	176	PHE
1	A	207	GLN
1	A	215	ARG
1	A	220	ASN
1	A	254	GLU
1	A	260	GLN
1	A	309	ASP
1	A	413	ASP
1	A	443	LEU
1	B	3	LYS
1	B	4	LEU
1	B	11	ARG
1	B	108	ASN
1	B	173	ARG
1	B	176	PHE
1	B	207	GLN
1	B	215	ARG
1	B	220	ASN
1	B	254	GLU

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Mol	Chain	Res	Type
1	B	264	THR
1	B	309	ASP
1	C	3	LYS
1	C	4	LEU
1	C	11	ARG
1	C	15	ASN
1	C	108	ASN
1	C	173	ARG
1	C	207	GLN
1	C	215	ARG
1	C	220	ASN
1	C	254	GLU
1	C	309	ASP
1	D	4	LEU
1	D	11	ARG
1	D	108	ASN
1	D	173	ARG
1	D	207	GLN
1	D	215	ARG
1	D	220	ASN
1	D	254	GLU
1	D	309	ASP
1	D	314	ARG
1	D	443	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	103	ASN
1	A	108	ASN
1	A	207	GLN
1	A	220	ASN
1	A	223	ASN
1	A	289	ASN
1	A	388	ASN
1	A	444	ASN
1	B	15	ASN
1	B	103	ASN
1	B	108	ASN
1	B	207	GLN
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	223	ASN
1	B	289	ASN
1	B	388	ASN
1	B	444	ASN
1	C	15	ASN
1	C	103	ASN
1	C	108	ASN
1	C	207	GLN
1	C	220	ASN
1	C	223	ASN
1	C	289	ASN
1	C	388	ASN
1	C	444	ASN
1	D	15	ASN
1	D	103	ASN
1	D	108	ASN
1	D	207	GLN
1	D	220	ASN
1	D	223	ASN
1	D	289	ASN
1	D	388	ASN
1	D	444	ASN

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	455/455 (100%)	0.16	34 (7%)	14 13	13, 29, 73, 89	0
1	B	455/455 (100%)	0.85	68 (14%)	2 2	11, 27, 88, 100	0
1	C	455/455 (100%)	0.37	39 (8%)	10 9	12, 28, 87, 99	0
1	D	455/455 (100%)	0.25	47 (10%)	6 6	13, 30, 82, 100	0
All	All	1820/1820 (100%)	0.41	188 (10%)	6 6	11, 28, 84, 100	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	VAL	13.3
1	B	453	ALA	10.9
1	B	427	ILE	9.9
1	B	450	LEU	9.2
1	B	425	PRO	9.2
1	B	422	GLY	8.7
1	B	454	LEU	8.7
1	B	1	MET	8.3
1	D	1	MET	8.1
1	D	455	SER	7.9
1	B	376	LYS	7.8
1	B	455	SER	7.7
1	B	446	GLY	7.3
1	B	382	ASP	7.2
1	B	377	ARG	7.2
1	B	388	ASN	7.0
1	B	380	GLU	7.0
1	C	427	ILE	6.4
1	B	385	ALA	6.4
1	B	375	THR	6.3
1	B	426	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	379	VAL	6.2
1	B	449	LEU	6.1
1	B	398	GLY	6.0
1	B	448	GLU	6.0
1	B	420	ALA	5.9
1	C	1	MET	5.9
1	B	378	HIS	5.8
1	B	381	GLY	5.7
1	C	379	VAL	5.7
1	C	378	HIS	5.5
1	B	409	ILE	5.4
1	B	386	ILE	5.3
1	B	430	PHE	5.3
1	D	389	LYS	5.3
1	B	394	ALA	5.2
1	B	2	GLY	5.0
1	B	429	ILE	5.0
1	D	454	LEU	4.9
1	B	406	GLY	4.9
1	B	396	GLU	4.8
1	C	450	LEU	4.8
1	B	442	TYR	4.8
1	D	449	LEU	4.7
1	A	449	LEU	4.7
1	D	452	LYS	4.7
1	A	455	SER	4.7
1	B	399	TYR	4.6
1	B	389	LYS	4.6
1	B	445	LEU	4.5
1	D	427	ILE	4.5
1	B	451	GLU	4.5
1	B	392	GLU	4.5
1	C	455	SER	4.5
1	D	379	VAL	4.4
1	D	375	THR	4.4
1	B	3	LYS	4.3
1	B	395	ARG	4.3
1	B	401	VAL	4.2
1	B	391	ALA	4.2
1	B	411	PHE	4.1
1	A	1	MET	4.1
1	D	374	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	399	TYR	4.1
1	D	424	GLU	4.0
1	A	427	ILE	4.0
1	D	450	LEU	4.0
1	A	426	ILE	3.9
1	D	396	GLU	3.9
1	C	425	PRO	3.9
1	B	416	VAL	3.9
1	B	371	TYR	3.9
1	C	454	LEU	3.8
1	B	452	LYS	3.8
1	C	426	ILE	3.7
1	C	412	GLU	3.7
1	D	451	GLU	3.7
1	D	395	ARG	3.7
1	B	384	HIS	3.6
1	D	453	ALA	3.6
1	B	374	LYS	3.6
1	D	3	LYS	3.6
1	A	413	ASP	3.6
1	B	418	VAL	3.6
1	B	421	SER	3.6
1	D	425	PRO	3.6
1	B	428	ARG	3.6
1	C	380	GLU	3.5
1	D	399	TYR	3.4
1	B	373	ILE	3.3
1	C	371	TYR	3.3
1	A	378	HIS	3.3
1	A	396	GLU	3.3
1	C	7	THR	3.3
1	A	452	LYS	3.2
1	A	437	GLU	3.2
1	C	430	PHE	3.2
1	D	430	PHE	3.2
1	D	448	GLU	3.2
1	A	430	PHE	3.2
1	C	222	GLU	3.2
1	A	424	GLU	3.2
1	B	437	GLU	3.2
1	A	381	GLY	3.1
1	B	407	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	410	ILE	3.1
1	C	3	LYS	3.1
1	C	424	GLU	3.1
1	B	419	ARG	3.0
1	C	2	GLY	3.0
1	B	387	VAL	3.0
1	B	423	THR	3.0
1	C	381	GLY	3.0
1	A	377	ARG	2.9
1	A	425	PRO	2.9
1	D	378	HIS	2.9
1	C	386	ILE	2.9
1	A	454	LEU	2.9
1	D	327	GLU	2.8
1	A	429	ILE	2.8
1	D	387	VAL	2.8
1	B	397	ARG	2.8
1	D	2	GLY	2.8
1	B	410	ILE	2.8
1	C	382	ASP	2.8
1	C	453	ALA	2.7
1	B	412	GLU	2.7
1	B	424	GLU	2.7
1	C	449	LEU	2.7
1	A	412	GLU	2.7
1	D	40	LYS	2.7
1	C	376	LYS	2.6
1	B	307	VAL	2.6
1	A	2	GLY	2.6
1	D	443	LEU	2.6
1	B	436	LYS	2.6
1	C	389	LYS	2.6
1	D	7	THR	2.6
1	B	441	GLU	2.5
1	D	446	GLY	2.5
1	D	426	ILE	2.5
1	A	418	VAL	2.5
1	C	377	ARG	2.5
1	A	386	ILE	2.5
1	A	389	LYS	2.5
1	A	399	TYR	2.5
1	D	410	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	411	PHE	2.4
1	B	222	GLU	2.4
1	C	394	ALA	2.4
1	C	451	GLU	2.4
1	C	452	LYS	2.4
1	B	402	ASP	2.4
1	C	384	HIS	2.4
1	D	447	ILE	2.4
1	D	371	TYR	2.4
1	C	276	LYS	2.3
1	D	416	VAL	2.3
1	A	375	THR	2.3
1	A	394	ALA	2.3
1	D	442	TYR	2.3
1	C	441	GLU	2.3
1	D	380	GLU	2.3
1	D	382	ASP	2.2
1	D	429	ILE	2.2
1	B	309	ASP	2.2
1	A	453	ALA	2.2
1	C	385	ALA	2.2
1	C	428	ARG	2.2
1	D	377	ARG	2.2
1	D	393	MET	2.2
1	C	422	GLY	2.2
1	D	413	ASP	2.2
1	A	4	LEU	2.2
1	C	442	TYR	2.2
1	A	446	GLY	2.2
1	B	417	LEU	2.1
1	A	388	ASN	2.1
1	A	445	LEU	2.1
1	A	222	GLU	2.1
1	D	445	LEU	2.1
1	D	418	VAL	2.1
1	D	444	ASN	2.0
1	C	383	ARG	2.0
1	D	388	ASN	2.0
1	A	441	GLU	2.0
1	C	413	ASP	2.0
1	D	436	LYS	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( $\text{\AA}^2$ )	Q<0.9
2	MG	C	456	1/1	0.89	0.10	29,29,29,29	0
2	MG	D	456	1/1	0.92	0.07	34,34,34,34	0
2	MG	A	456	1/1	0.95	0.07	32,32,32,32	0
2	MG	B	456	1/1	0.96	0.09	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.