



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 12:53 am GMT

PDB ID : 1UU2  
Title : Histidinol-phosphate aminotransferase (HisC) from *Thermotoga maritima* (apo-form)  
Authors : Vega, M.C.; Fernandez, F.J.; Lehmann, F.; Wilmanns, M.  
Deposited on : 2003-12-13  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

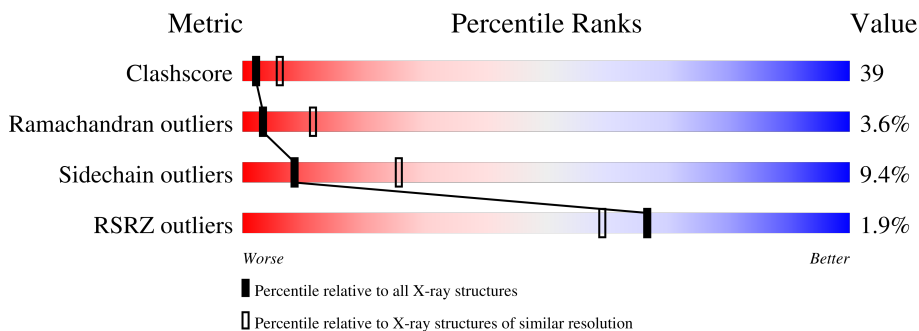
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of 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	335	 43% 46% 6% 5%
1	B	335	 2% 33% 53% 8% 5%

## 2 Entry composition [i](#)

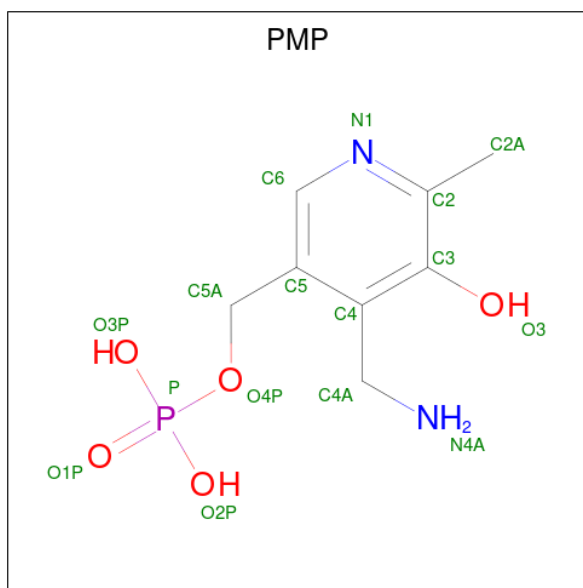
There are 4 unique types of molecules in this entry. The entry contains 5385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HISTIDINOL-PHOSPHATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	Total	C	N	O	S	48	0	1
			2655	1704	448	494	9			
1	B	319	Total	C	N	O	S	40	0	1
			2630	1689	444	488	9			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

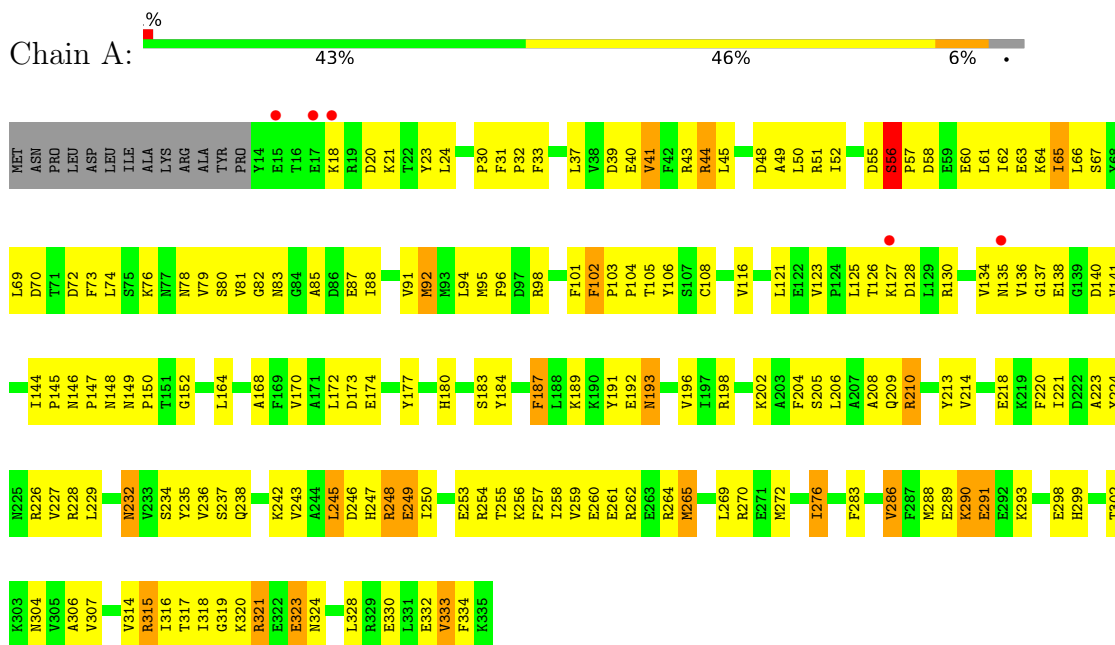
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	31	Total O 31 31	0	0

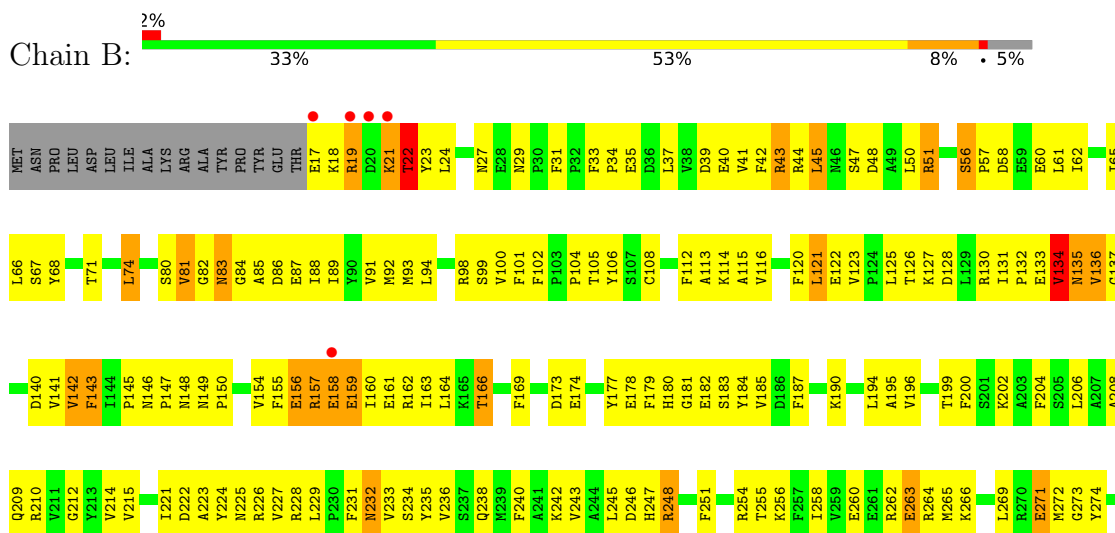
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HISTIDINOL-PHOSPHATE AMINOTRANSFERASE



#### • Molecule 1: HISTIDINOL-PHOSPHATE AMINOTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.65Å 98.56Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.80 19.91 – 2.79	Depositor EDS
% Data completeness (in resolution range)	89.5 (19.91-2.80) 89.7 (19.91-2.79)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.288 0.232 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.1	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: PMP, EDO

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	0.34	0/2711	0.58	0/3655
1	B	0.37	0/2686	0.77	6/3622 (0.2%)
All	All	0.35	0/5397	0.68	6/7277 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	MET	N-CA-C	8.13	132.94	111.00
1	B	288	MET	CB-CA-C	-6.06	98.28	110.40
1	B	288	MET	CB-CG-SD	-5.48	95.96	112.40
1	B	287	PHE	N-CA-C	5.39	125.56	111.00
1	B	288	MET	C-N-CA	-5.27	108.53	121.70
1	B	22	THR	N-CA-C	-5.23	96.87	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	2655	0	2621	183	0
1	B	2630	0	2595	244	0
2	A	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	1	0
3	A	4	0	6	3	0
4	A	35	0	0	0	0
4	B	31	0	0	3	0
All	All	5385	0	5234	407	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 39.

All (407) 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:56:SER:HB2	1:A:57:PRO:HD3	1.26	1.13
1:B:290:LYS:HG2	1:B:291:GLU:H	0.95	1.07
1:A:56:SER:HB2	1:A:57:PRO:CD	1.89	1.02
1:B:290:LYS:HG2	1:B:291:GLU:N	1.72	1.00
1:B:91:VAL:HG21	1:B:224:TYR:HE1	1.29	0.98
1:A:193:ASN:HD22	1:A:193:ASN:H	1.13	0.97
1:B:289:GLU:O	1:B:290:LYS:HB3	1.61	0.97
1:B:17:GLU:HG2	1:B:18:LYS:N	1.80	0.94
1:A:226:ARG:HH21	1:A:226:ARG:HG3	1.37	0.90
1:B:289:GLU:HB2	1:B:293:LYS:HG2	1.56	0.88
1:B:289:GLU:HG3	1:B:293:LYS:CE	2.05	0.86
1:A:58:ASP:HB2	1:A:238:GLN:NE2	1.90	0.86
1:B:232:ASN:HD22	1:B:232:ASN:H	1.24	0.84
1:A:32:PRO:HB3	1:B:48:ASP:HA	1.59	0.84
1:B:17:GLU:HG2	1:B:18:LYS:H	1.42	0.84
1:A:209:GLN:HE22	1:B:236:VAL:H	1.23	0.83
1:B:262:ARG:HB2	1:B:318:ILE:HD13	1.60	0.82
1:B:289:GLU:CG	1:B:293:LYS:HE2	2.10	0.81
1:B:290:LYS:CG	1:B:291:GLU:H	1.88	0.81
1:B:293:LYS:HD3	1:B:296:LEU:HD21	1.61	0.80
1:B:91:VAL:HG21	1:B:224:TYR:CE1	2.17	0.80
1:B:61:LEU:HD13	1:B:238:GLN:HE21	1.46	0.79
1:B:136:VAL:HB	1:B:166:THR:HB	1.62	0.79
1:B:262:ARG:HB2	1:B:318:ILE:CD1	2.12	0.79
1:B:56:SER:HB3	1:B:57:PRO:HD3	1.62	0.78
1:A:236:VAL:H	1:B:209:GLN:HE22	1.28	0.78
1:B:289:GLU:HB2	1:B:293:LYS:CG	2.13	0.78
1:B:289:GLU:HG3	1:B:293:LYS:HE2	1.64	0.78
1:B:19:ARG:O	1:B:19:ARG:HG2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:N	1:A:290:LYS:HD2	1.99	0.77
1:B:300:LEU:HB3	1:B:305:VAL:HB	1.65	0.77
1:B:61:LEU:O	1:B:65:ILE:HG12	1.85	0.77
1:B:163:ILE:O	1:B:166:THR:HG23	1.85	0.76
1:A:232:ASN:H	1:A:232:ASN:HD22	1.34	0.75
1:A:18:LYS:HE3	1:A:306:ALA:HB2	1.69	0.74
1:A:232:ASN:H	1:A:232:ASN:ND2	1.86	0.74
1:A:250:ILE:HD12	1:A:250:ILE:H	1.52	0.74
1:B:104:PRO:HD2	1:B:125:LEU:HD12	1.68	0.74
1:A:91:VAL:HG21	1:A:224:TYR:HE1	1.52	0.74
3:A:1637:EDO:H22	1:B:184:TYR:HD1	1.52	0.73
1:B:232:ASN:H	1:B:232:ASN:ND2	1.83	0.73
1:A:126:THR:HG22	1:A:128:ASP:H	1.54	0.73
1:A:265:MET:HG3	1:A:328:LEU:HD21	1.68	0.73
1:A:226:ARG:HG3	1:A:226:ARG:NH2	2.02	0.72
1:A:41:VAL:HG12	1:A:243:VAL:HG21	1.71	0.72
1:B:19:ARG:O	1:B:19:ARG:CG	2.37	0.72
1:B:293:LYS:HA	1:B:296:LEU:HG	1.71	0.72
1:A:193:ASN:HD22	1:A:193:ASN:N	1.80	0.71
1:B:56:SER:HB3	1:B:57:PRO:CD	2.20	0.71
1:B:93:MET:HE1	1:B:112:PHE:HB3	1.72	0.71
1:B:136:VAL:HB	1:B:166:THR:CB	2.21	0.70
1:B:289:GLU:HG3	1:B:293:LYS:NZ	2.07	0.70
1:A:193:ASN:H	1:A:193:ASN:ND2	1.88	0.70
1:B:88:ILE:HD12	1:B:88:ILE:H	1.56	0.70
1:B:177:TYR:CD2	1:B:183:SER:HB3	2.27	0.70
1:B:323:GLU:O	1:B:326:MET:HB3	1.92	0.70
1:B:39:ASP:O	1:B:43:ARG:HG3	1.90	0.70
1:A:150:PRO:HB2	1:A:315:ARG:HG3	1.73	0.69
1:A:91:VAL:HG21	1:A:224:TYR:CE1	2.28	0.69
1:A:254:ARG:O	1:A:258:ILE:HG13	1.93	0.69
1:A:49:ALA:O	1:A:52:ILE:HG12	1.92	0.69
1:B:174:GLU:OE1	1:B:183:SER:HB2	1.93	0.68
1:B:56:SER:CB	1:B:57:PRO:HD3	2.23	0.68
1:A:236:VAL:HG11	1:B:236:VAL:HG11	1.74	0.68
1:A:64:LYS:O	1:A:67:SER:HB3	1.94	0.68
1:B:22:THR:HG23	1:B:22:THR:O	1.94	0.68
1:B:293:LYS:HD3	1:B:296:LEU:CD2	2.24	0.67
1:A:134:VAL:HG23	1:A:136:VAL:HG23	1.77	0.67
1:A:126:THR:HG22	1:A:127:LYS:N	2.11	0.66
1:A:232:ASN:HD22	1:A:232:ASN:N	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PRO:HA	1:A:173:ASP:HB3	1.78	0.66
1:B:161:GLU:HA	1:B:164:LEU:HD12	1.77	0.66
1:A:276:ILE:HD13	1:A:276:ILE:H	1.62	0.65
1:B:102:PHE:O	1:B:105:THR:HG23	1.97	0.65
1:B:145:PRO:HA	1:B:173:ASP:HB3	1.78	0.65
1:B:98:ARG:HB3	1:B:140:ASP:OD1	1.96	0.65
1:B:271:GLU:HA	1:B:271:GLU:OE1	1.96	0.65
1:B:93:MET:HE1	1:B:112:PHE:C	2.17	0.65
1:B:21:LYS:HD2	1:B:21:LYS:N	2.13	0.64
1:B:290:LYS:O	1:B:292:GLU:N	2.30	0.64
1:B:303:LYS:HE3	4:B:2028:HOH:O	1.98	0.64
1:B:289:GLU:HG2	1:B:293:LYS:HE2	1.80	0.63
1:A:57:PRO:HD3	1:A:228:ARG:NH2	2.13	0.63
1:B:45:LEU:HD12	1:B:45:LEU:C	2.19	0.63
1:B:224:TYR:CE2	1:B:228:ARG:HD3	2.34	0.63
1:A:62:ILE:O	1:A:66:LEU:HD23	1.99	0.62
1:A:58:ASP:HB2	1:A:238:GLN:HE21	1.62	0.62
1:B:308:ARG:HE	1:B:308:ARG:HA	1.64	0.62
1:A:286:VAL:HG13	1:A:314:VAL:HG23	1.82	0.62
1:B:42:PHE:C	1:B:44:ARG:H	2.01	0.62
1:B:81:VAL:HG13	1:B:233:VAL:HG11	1.81	0.61
1:B:160:ILE:HD12	1:B:184:TYR:CD2	2.35	0.61
1:B:21:LYS:HD2	1:B:21:LYS:H	1.65	0.61
1:B:87:GLU:O	1:B:91:VAL:HG22	1.99	0.61
1:B:232:ASN:HD22	1:B:232:ASN:N	1.89	0.61
1:A:257:PHE:HZ	1:A:321:ARG:HG3	1.65	0.61
1:B:133:GLU:O	1:B:134:VAL:HG13	2.01	0.61
1:B:327:ILE:O	1:B:331:LEU:HB2	2.01	0.61
1:A:247:HIS:HB3	1:A:250:ILE:HD13	1.81	0.61
1:B:27:ASN:HD21	1:B:315:ARG:HD3	1.64	0.60
1:B:254:ARG:O	1:B:258:ILE:HG13	2.00	0.60
1:A:65:ILE:HG22	1:A:69:LEU:HD13	1.82	0.60
1:B:299:HIS:O	1:B:302:THR:HG22	2.00	0.60
1:A:257:PHE:CZ	1:A:321:ARG:HG3	2.36	0.60
1:A:330:GLU:O	1:A:333:VAL:HG12	2.00	0.60
1:A:286:VAL:HG13	1:A:314:VAL:CG2	2.32	0.60
1:A:232:ASN:HA	1:B:83:ASN:HD21	1.67	0.59
1:B:68:TYR:HA	1:B:248:ARG:NH2	2.17	0.59
1:A:106:TYR:CE2	1:A:108:CYS:HB2	2.38	0.59
1:B:58:ASP:H	1:B:238:GLN:HE22	1.51	0.59
1:B:290:LYS:O	1:B:293:LYS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:HD3	1:A:228:ARG:HH22	1.67	0.58
1:A:299:HIS:O	1:A:302:THR:HB	2.03	0.58
1:A:321:ARG:N	1:A:321:ARG:HD2	2.17	0.58
1:B:91:VAL:HA	1:B:94:LEU:HD12	1.85	0.58
1:A:69:LEU:HD23	1:A:74:LEU:HD13	1.85	0.58
1:A:87:GLU:O	1:A:91:VAL:HG22	2.03	0.58
1:A:164:LEU:HD13	1:A:170:VAL:CG2	2.34	0.58
1:A:291:GLU:HA	1:A:291:GLU:OE1	2.04	0.58
1:B:290:LYS:CG	1:B:291:GLU:N	2.56	0.58
1:B:296:LEU:HD12	1:B:296:LEU:C	2.24	0.58
1:A:255:THR:O	1:A:259:VAL:HG13	2.04	0.57
1:B:99:SER:O	1:B:120:PHE:HA	2.03	0.57
1:B:256:LYS:O	1:B:260:GLU:HG3	2.03	0.57
1:B:292:GLU:OE2	1:B:292:GLU:HA	2.04	0.57
1:A:24:LEU:HD22	1:A:317:THR:O	2.04	0.57
1:B:289:GLU:HB3	1:B:292:GLU:HB3	1.86	0.57
1:B:311:ARG:O	1:B:312:GLU:HB2	2.05	0.57
1:B:260:GLU:O	1:B:264:ARG:HB2	2.05	0.56
1:A:32:PRO:CB	1:B:48:ASP:HA	2.34	0.56
1:A:224:TYR:CE2	1:A:228:ARG:HD3	2.41	0.56
1:A:60:GLU:OE1	1:A:60:GLU:N	2.31	0.55
1:A:83:ASN:HD21	1:B:232:ASN:HA	1.71	0.55
1:A:205:SER:HB3	1:B:51:ARG:HB3	1.88	0.55
1:B:56:SER:CB	1:B:57:PRO:CD	2.83	0.55
1:B:289:GLU:CB	1:B:292:GLU:HB3	2.36	0.55
1:B:263:GLU:OE2	1:B:266:LYS:HE2	2.05	0.55
1:A:130:ARG:HH11	1:A:130:ARG:HB3	1.72	0.55
1:B:81:VAL:HG22	1:B:212:GLY:O	2.07	0.55
1:B:93:MET:HE1	1:B:112:PHE:CB	2.35	0.55
1:B:58:ASP:N	1:B:238:GLN:HE22	2.05	0.55
1:A:136:VAL:HG12	1:A:168:ALA:HB2	1.88	0.55
1:A:184:TYR:O	1:A:187:PHE:HB2	2.07	0.54
1:A:78:ASN:ND2	1:A:218:GLU:HG2	2.21	0.54
1:B:22:THR:O	1:B:22:THR:CG2	2.55	0.54
1:B:293:LYS:C	1:B:295:ARG:N	2.58	0.54
1:A:276:ILE:H	1:A:276:ILE:CD1	2.21	0.54
1:A:50:LEU:HD12	1:B:33:PHE:HB3	1.90	0.54
1:A:69:LEU:HD23	1:A:74:LEU:CD1	2.38	0.54
1:B:50:LEU:HD23	1:B:235:TYR:HD2	1.72	0.54
1:B:233:VAL:HG23	1:B:233:VAL:O	2.08	0.53
1:A:40:GLU:CD	1:A:44:ARG:HD3	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:O	1:B:142:VAL:HA	2.08	0.53
1:A:146:ASN:HA	1:A:147:PRO:C	2.28	0.53
1:B:42:PHE:C	1:B:44:ARG:N	2.60	0.53
1:B:41:VAL:HG21	1:B:240:PHE:CE1	2.43	0.53
1:B:80:SER:HB2	1:B:221:ILE:HG23	1.90	0.53
1:B:160:ILE:O	1:B:164:LEU:HG	2.09	0.53
1:A:283:PHE:CD2	1:A:315:ARG:HD3	2.44	0.53
1:B:85:ALA:O	1:B:89:ILE:HD13	2.09	0.53
1:A:73:PHE:H	1:A:73:PHE:HD1	1.55	0.53
1:A:164:LEU:HD13	1:A:170:VAL:HG21	1.90	0.52
1:A:261:GLU:OE2	1:A:264:ARG:NH1	2.42	0.52
1:A:289:GLU:C	1:A:290:LYS:HD2	2.29	0.52
1:B:85:ALA:HB2	1:B:199:THR:HB	1.91	0.52
1:B:160:ILE:HD12	1:B:184:TYR:CE2	2.44	0.52
1:B:183:SER:OG	1:B:185:VAL:HG23	2.09	0.52
1:A:62:ILE:O	1:A:66:LEU:CD2	2.57	0.52
1:B:156:GLU:HA	1:B:156:GLU:OE1	2.09	0.52
1:A:58:ASP:HB3	1:A:61:LEU:H	1.75	0.52
1:A:56:SER:CB	1:A:57:PRO:HD3	2.18	0.51
1:A:62:ILE:HA	1:A:65:ILE:HG13	1.91	0.51
1:A:172:LEU:CD2	1:A:184:TYR:HB2	2.40	0.51
1:A:234:SER:HG	1:A:237:SER:HG	1.59	0.51
1:B:37:LEU:O	1:B:41:VAL:HG23	2.10	0.51
1:B:58:ASP:HB3	1:B:61:LEU:HB2	1.91	0.51
1:B:262:ARG:HB2	1:B:318:ILE:HD11	1.92	0.51
1:A:50:LEU:HA	1:B:208:ALA:HB3	1.92	0.51
1:A:55:ASP:O	1:A:56:SER:O	2.29	0.51
1:A:58:ASP:HB2	1:A:238:GLN:HE22	1.72	0.51
1:B:58:ASP:HB2	1:B:238:GLN:NE2	2.26	0.51
1:A:105:THR:HA	1:A:149:ASN:O	2.10	0.51
1:A:262:ARG:HB2	1:A:318:ILE:CD1	2.40	0.51
1:B:23:TYR:C	1:B:24:LEU:HD22	2.31	0.51
1:B:126:THR:HG23	1:B:130:ARG:O	2.11	0.51
1:B:154:VAL:HG21	1:B:180:HIS:CD2	2.45	0.51
1:B:121:LEU:HD13	1:B:123:VAL:HG23	1.91	0.51
1:B:321:ARG:HA	1:B:324:ASN:HD22	1.75	0.51
1:A:238:GLN:O	1:A:242:LYS:HG3	2.11	0.51
1:B:136:VAL:CB	1:B:166:THR:HB	2.37	0.50
1:B:94:LEU:CD2	1:B:116:VAL:HG13	2.42	0.50
1:B:223:ALA:O	1:B:227:VAL:HG23	2.11	0.50
1:B:24:LEU:HD22	1:B:24:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HB3	1:A:123:VAL:O	2.10	0.50
1:B:88:ILE:HD12	1:B:88:ILE:N	2.23	0.50
1:A:262:ARG:HB2	1:A:318:ILE:HD13	1.93	0.50
1:B:37:LEU:HD21	1:B:247:HIS:CD2	2.46	0.50
1:B:150:PRO:HB3	1:B:310:PHE:CE2	2.46	0.50
1:A:226:ARG:HH21	1:A:226:ARG:CG	2.15	0.50
1:A:126:THR:CG2	1:A:127:LYS:N	2.75	0.49
1:A:174:GLU:HB2	1:A:198:ARG:HD3	1.93	0.49
1:B:93:MET:HE1	1:B:113:ALA:N	2.27	0.49
1:B:37:LEU:HB3	1:B:243:VAL:CG1	2.41	0.49
1:B:262:ARG:HG3	1:B:318:ILE:HD11	1.93	0.49
1:A:96:PHE:CG	1:A:141:VAL:HB	2.47	0.49
1:A:102:PHE:HB2	1:A:125:LEU:HD21	1.93	0.49
1:B:29:ASN:HB2	1:B:202:LYS:O	2.12	0.49
1:A:72:ASP:OD2	1:A:73:PHE:HD1	1.95	0.49
1:A:121:LEU:HD22	1:A:123:VAL:CG2	2.43	0.49
1:A:174:GLU:HG3	1:A:196:VAL:HG13	1.95	0.49
1:A:144:ILE:HD12	1:A:170:VAL:HG13	1.94	0.49
1:A:208:ALA:HB3	1:B:50:LEU:HA	1.94	0.49
1:A:20:ASP:OD2	1:A:304:ASN:HA	2.12	0.49
1:A:269:LEU:HD23	1:A:272:MET:HE2	1.95	0.49
1:B:143:PHE:N	1:B:143:PHE:CD2	2.81	0.49
1:B:289:GLU:HB2	1:B:293:LYS:HG3	1.92	0.49
1:A:30:PRO:HG2	1:A:31:PHE:CE1	2.48	0.49
1:A:177:TYR:O	1:A:180:HIS:O	2.29	0.49
1:B:177:TYR:HD2	1:B:183:SER:HB3	1.74	0.49
1:B:178:GLU:H	1:B:178:GLU:CD	2.17	0.49
1:A:172:LEU:HD21	1:A:184:TYR:CD2	2.48	0.48
1:A:307:VAL:HG11	1:A:316:ILE:HD12	1.95	0.48
1:A:80:SER:HB2	1:A:221:ILE:HG23	1.95	0.48
1:A:288:MET:HB3	1:A:293:LYS:HB2	1.94	0.48
1:B:21:LYS:H	1:B:21:LYS:CD	2.17	0.48
1:B:234:SER:O	1:B:238:GLN:HG3	2.13	0.48
1:A:98:ARG:HH21	1:A:140:ASP:CG	2.17	0.48
1:A:141:VAL:O	1:A:141:VAL:HG13	2.14	0.48
1:B:141:VAL:O	1:B:141:VAL:HG13	2.14	0.48
1:A:204:PHE:O	1:A:205:SER:C	2.52	0.48
1:B:86:ASP:OD2	2:B:1335:PMP:H5A2	2.13	0.48
1:A:321:ARG:HD2	1:A:321:ARG:H	1.76	0.48
1:B:57:PRO:HB3	1:B:62:ILE:HD11	1.95	0.48
1:B:81:VAL:CG1	1:B:233:VAL:HG11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG22	1:B:225:ASN:ND2	2.28	0.48
1:B:91:VAL:CG2	1:B:224:TYR:HE1	2.15	0.48
1:A:235:TYR:HB3	1:B:209:GLN:NE2	2.28	0.48
1:A:198:ARG:HB2	1:A:213:TYR:CZ	2.49	0.48
1:A:82:GLY:HA3	1:A:88:ILE:HD11	1.95	0.47
1:B:136:VAL:HG23	1:B:137:GLY:N	2.29	0.47
1:B:157:ARG:HD2	1:B:158:GLU:HB3	1.94	0.47
1:B:282:ASN:C	1:B:318:ILE:HD12	2.35	0.47
1:A:73:PHE:CE1	1:A:189:LYS:HE3	2.49	0.47
1:B:321:ARG:HB3	1:B:321:ARG:HH11	1.80	0.47
1:A:56:SER:HB2	1:A:228:ARG:HH22	1.78	0.47
1:B:157:ARG:HD2	1:B:158:GLU:N	2.29	0.47
1:B:125:LEU:HD23	1:B:132:PRO:HD3	1.97	0.47
1:A:85:ALA:HB3	2:A:1335:PMP:H5A2	1.97	0.47
1:A:224:TYR:CZ	1:A:228:ARG:HD3	2.50	0.47
1:A:229:LEU:HD22	1:B:86:ASP:HB3	1.97	0.47
1:B:277:THR:OG1	1:B:285:PHE:HB3	2.15	0.47
1:A:48:ASP:O	1:A:51:ARG:HG2	2.15	0.47
1:A:134:VAL:HG23	1:A:134:VAL:O	2.15	0.47
1:B:33:PHE:CD1	1:B:34:PRO:HD2	2.50	0.47
1:B:156:GLU:O	1:B:157:ARG:C	2.53	0.47
1:A:250:ILE:H	1:A:250:ILE:CD1	2.25	0.47
3:A:1637:EDO:C2	1:B:184:TYR:HD1	2.25	0.47
1:B:199:THR:OG1	1:B:200:PHE:N	2.48	0.47
1:B:238:GLN:O	1:B:242:LYS:HE2	2.13	0.47
1:B:289:GLU:HG3	1:B:293:LYS:HZ3	1.79	0.47
1:A:265:MET:SD	1:A:324:ASN:HB3	2.54	0.46
1:B:27:ASN:O	1:B:202:LYS:HD2	2.15	0.46
1:A:126:THR:HG22	1:A:127:LYS:H	1.79	0.46
1:B:141:VAL:HA	1:B:169:PHE:O	2.15	0.46
1:A:91:VAL:O	1:A:94:LEU:HB2	2.15	0.46
1:A:248:ARG:HG3	1:A:249:GLU:OE1	2.16	0.46
1:A:270:ARG:HE	1:A:276:ILE:HD11	1.79	0.46
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.80	0.46
1:A:40:GLU:OE2	1:A:43:ARG:HB3	2.16	0.46
1:B:292:GLU:O	1:B:295:ARG:HB3	2.16	0.46
1:A:31:PHE:O	1:B:51:ARG:HD2	2.15	0.46
1:B:17:GLU:CG	1:B:18:LYS:N	2.64	0.46
1:B:60:GLU:OE1	1:B:242:LYS:HD2	2.15	0.46
1:A:103:PRO:HA	1:A:104:PRO:C	2.36	0.46
1:A:126:THR:HB	1:A:130:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD21	1:B:194:LEU:HD13	1.97	0.46
1:A:91:VAL:HA	1:A:94:LEU:HD12	1.98	0.46
1:A:18:LYS:CE	1:A:306:ALA:HB2	2.43	0.45
1:A:64:LYS:HE2	1:A:246:ASP:OD1	2.16	0.45
1:A:37:LEU:O	1:A:41:VAL:HG13	2.15	0.45
1:A:223:ALA:O	1:A:226:ARG:HB2	2.16	0.45
1:A:333:VAL:O	1:A:333:VAL:HG13	2.16	0.45
1:B:154:VAL:HG21	1:B:180:HIS:NE2	2.31	0.45
1:A:177:TYR:CD2	1:A:183:SER:HB3	2.51	0.45
1:B:62:ILE:O	1:B:66:LEU:HD13	2.16	0.45
1:B:293:LYS:C	1:B:295:ARG:H	2.20	0.45
1:B:296:LEU:O	1:B:300:LEU:HG	2.16	0.45
1:A:136:VAL:HG12	1:A:137:GLY:N	2.32	0.45
1:B:125:LEU:HA	1:B:132:PRO:HG3	1.98	0.45
1:A:323:GLU:OE1	1:A:323:GLU:HA	2.16	0.45
1:B:174:GLU:CD	1:B:183:SER:HB2	2.36	0.45
1:B:332:GLU:C	1:B:334:PHE:H	2.20	0.45
1:A:56:SER:CB	1:A:228:ARG:HH22	2.30	0.45
1:A:94:LEU:CD2	1:A:116:VAL:HG13	2.47	0.45
1:B:82:GLY:O	1:B:84:GLY:N	2.49	0.45
1:B:91:VAL:O	1:B:94:LEU:HB2	2.17	0.45
1:B:221:ILE:O	1:B:224:TYR:HB3	2.17	0.45
1:A:30:PRO:HG2	1:A:31:PHE:CD1	2.52	0.45
1:A:209:GLN:NE2	1:B:236:VAL:H	2.03	0.45
1:A:320:LYS:O	1:A:323:GLU:N	2.49	0.45
1:B:93:MET:CE	1:B:112:PHE:HB3	2.44	0.44
1:B:131:ILE:HD12	1:B:159:GLU:HB3	1.98	0.44
1:B:299:HIS:C	1:B:299:HIS:CD2	2.90	0.44
1:A:88:ILE:O	1:A:92:MET:HB2	2.17	0.44
1:B:271:GLU:C	1:B:273:GLY:H	2.20	0.44
1:A:227:VAL:HA	1:B:115:ALA:HB1	1.99	0.44
1:A:234:SER:O	1:A:238:GLN:HG3	2.18	0.44
1:B:94:LEU:HD23	1:B:116:VAL:HG13	1.98	0.44
1:B:136:VAL:HB	1:B:166:THR:OG1	2.17	0.44
1:A:73:PHE:CD1	1:A:73:PHE:N	2.81	0.44
1:A:123:VAL:HG21	1:A:134:VAL:HG11	1.99	0.44
1:A:32:PRO:HB2	1:B:47:SER:O	2.18	0.44
1:A:57:PRO:HG3	1:A:81:VAL:HG22	1.99	0.44
1:B:134:VAL:HB	1:B:135:ASN:H	1.68	0.44
1:B:289:GLU:CB	1:B:293:LYS:CG	2.91	0.44
1:A:95:MET:HE1	1:A:220:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:HB2	1:A:150:PRO:HD2	1.99	0.44
1:A:250:ILE:HD12	1:A:250:ILE:N	2.28	0.44
1:B:194:LEU:HG	1:B:195:ALA:N	2.33	0.44
1:A:33:PHE:O	1:B:47:SER:OG	2.35	0.43
1:A:191:TYR:HB3	1:A:193:ASN:ND2	2.33	0.43
1:B:157:ARG:HD2	1:B:158:GLU:H	1.82	0.43
1:B:88:ILE:H	1:B:88:ILE:CD1	2.27	0.43
1:B:127:LYS:HG3	1:B:128:ASP:OD1	2.18	0.43
1:A:148:ASN:O	1:A:152:GLY:HA2	2.18	0.43
1:B:272:MET:HB3	1:B:274:TYR:CE1	2.53	0.43
1:B:65:ILE:HD13	1:B:245:LEU:HD11	2.01	0.43
1:B:91:VAL:HG23	1:B:92:MET:N	2.34	0.43
1:B:148:ASN:HB2	1:B:155:PHE:CE1	2.53	0.43
1:B:214:VAL:HG22	1:B:215:VAL:N	2.33	0.43
1:B:272:MET:SD	1:B:332:GLU:HB2	2.58	0.43
1:A:333:VAL:O	1:A:333:VAL:HG22	2.19	0.43
1:B:105:THR:HA	1:B:149:ASN:O	2.19	0.43
1:B:305:VAL:HG12	1:B:306:ALA:N	2.33	0.43
1:B:311:ARG:O	1:B:312:GLU:CB	2.66	0.43
1:A:45:LEU:C	1:A:45:LEU:HD23	2.38	0.43
1:A:134:VAL:CG2	1:A:136:VAL:HG23	2.46	0.43
1:A:276:ILE:CD1	1:A:276:ILE:N	2.81	0.43
1:A:102:PHE:HB2	1:A:125:LEU:CD2	2.49	0.43
1:A:234:SER:OG	1:A:237:SER:OG	2.29	0.43
1:A:256:LYS:O	1:A:259:VAL:HG22	2.18	0.43
1:B:146:ASN:HA	1:B:147:PRO:C	2.38	0.43
1:B:222:ASP:O	1:B:226:ARG:HG3	2.19	0.43
1:B:265:MET:HB2	1:B:328:LEU:HD11	2.00	0.43
1:B:19:ARG:HG3	1:B:21:LYS:HD3	2.01	0.43
1:B:71:THR:HG21	1:B:74:LEU:HD11	2.00	0.43
1:B:163:ILE:C	1:B:166:THR:HG23	2.39	0.43
1:A:262:ARG:HG3	1:A:318:ILE:HD11	2.00	0.43
1:B:45:LEU:HD12	1:B:45:LEU:O	2.17	0.43
1:A:39:ASP:O	1:A:43:ARG:HB2	2.19	0.42
1:A:304:ASN:N	1:A:304:ASN:ND2	2.67	0.42
1:A:307:VAL:HB	1:A:316:ILE:HD13	2.01	0.42
1:B:297:LEU:HD11	1:B:314:VAL:HG11	2.00	0.42
1:A:137:GLY:O	1:A:138:GLU:C	2.58	0.42
1:A:210:ARG:HE	1:B:231:PHE:HB2	1.83	0.42
1:B:226:ARG:HG2	1:B:226:ARG:NH1	2.35	0.42
1:B:269:LEU:HD22	1:B:331:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:HE1	1:B:333:VAL:HG23	1.84	0.42
1:B:177:TYR:CE2	1:B:183:SER:HB3	2.54	0.42
1:A:30:PRO:HB3	1:A:319:GLY:HA2	2.02	0.42
1:A:130:ARG:HB3	1:A:130:ARG:NH1	2.34	0.42
1:B:121:LEU:HD22	1:B:122:GLU:N	2.33	0.42
1:B:58:ASP:H	1:B:238:GLN:NE2	2.15	0.42
1:B:85:ALA:HA	1:B:88:ILE:HD13	2.01	0.42
1:B:204:PHE:HA	1:B:251:PHE:CD2	2.54	0.42
1:B:255:THR:O	1:B:256:LYS:C	2.57	0.42
1:A:172:LEU:HD21	1:A:184:TYR:HD2	1.83	0.42
1:B:278:ASP:OD1	1:B:280:ARG:NH2	2.53	0.42
1:A:79:VAL:HG12	1:A:80:SER:N	2.35	0.42
1:B:158:GLU:O	1:B:158:GLU:HG3	2.18	0.42
1:A:60:GLU:O	1:A:63:GLU:HB2	2.19	0.42
1:B:289:GLU:CB	1:B:293:LYS:HG2	2.39	0.42
1:A:209:GLN:NE2	1:B:236:VAL:HG23	2.35	0.42
1:A:332:GLU:C	1:A:334:PHE:H	2.23	0.42
1:B:226:ARG:HB3	4:B:2026:HOH:O	2.20	0.42
1:B:106:TYR:CE2	1:B:108:CYS:HB2	2.55	0.41
1:B:222:ASP:HA	1:B:225:ASN:HB2	2.02	0.41
1:B:246:ASP:C	1:B:247:HIS:ND1	2.73	0.41
1:B:299:HIS:HE1	1:B:333:VAL:CG2	2.32	0.41
1:A:193:ASN:N	1:A:193:ASN:ND2	2.53	0.41
1:A:18:LYS:O	1:A:23:TYR:CE1	2.72	0.41
1:A:82:GLY:HA3	1:A:88:ILE:CD1	2.50	0.41
1:B:40:GLU:O	1:B:40:GLU:HG2	2.20	0.41
1:B:131:ILE:HA	1:B:132:PRO:HD3	1.92	0.41
1:B:37:LEU:HB3	1:B:243:VAL:HG11	2.03	0.41
1:B:221:ILE:HG22	1:B:225:ASN:HD21	1.86	0.41
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.80	0.41
3:A:1637:EDO:H21	1:B:182:GLU:OE2	2.20	0.41
1:B:145:PRO:O	1:B:148:ASN:HA	2.21	0.41
1:B:179:PHE:CE1	1:B:282:ASN:HB3	2.55	0.41
1:A:48:ASP:OD1	1:A:51:ARG:HD3	2.21	0.41
1:B:31:PHE:HD2	1:B:254:ARG:HD3	1.85	0.41
1:A:187:PHE:HD2	1:A:187:PHE:HA	1.71	0.41
1:B:271:GLU:C	1:B:273:GLY:N	2.74	0.41
1:B:143:PHE:N	1:B:143:PHE:HD2	2.19	0.41
1:B:157:ARG:CD	1:B:158:GLU:H	2.34	0.41
1:A:106:TYR:CZ	1:A:108:CYS:HB2	2.56	0.40
1:A:259:VAL:HG23	1:A:260:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HG11	1:B:233:VAL:HG21	2.02	0.40
1:B:114:LYS:HE3	1:B:114:LYS:HB2	1.88	0.40
1:B:145:PRO:HG2	1:B:148:ASN:OD1	2.21	0.40
1:B:162:ARG:NH2	4:B:2020:HOH:O	2.54	0.40
1:A:58:ASP:HB3	1:A:61:LEU:HB3	2.01	0.40
1:B:185:VAL:HG22	1:B:196:VAL:HG11	2.01	0.40
1:B:187:PHE:HD1	1:B:187:PHE:HA	1.81	0.40
1:B:185:VAL:O	1:B:185:VAL:HG12	2.20	0.40
1:B:322:GLU:H	1:B:322:GLU:HG3	1.59	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	320/335 (96%)	284 (89%)	27 (8%)	9 (3%)	5	17
1	B	317/335 (95%)	263 (83%)	40 (13%)	14 (4%)	2	8
All	All	637/670 (95%)	547 (86%)	67 (10%)	23 (4%)	3	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	290	LYS
1	B	21	LYS
1	B	22	THR
1	B	56	SER
1	B	134	VAL
1	B	288	MET
1	B	290	LYS
1	A	333	VAL

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Mol	Chain	Res	Type
1	B	83	ASN
1	B	135	ASN
1	B	159	GLU
1	B	181	GLY
1	B	210	ARG
1	B	292	GLU
1	A	21	LYS
1	A	76	LYS
1	A	210	ARG
1	A	291	GLU
1	B	289	GLU
1	B	136	VAL
1	A	70	ASP
1	A	248	ARG

### 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	288/301 (96%)	263 (91%)	25 (9%)	10	30
1	B	285/301 (95%)	256 (90%)	29 (10%)	7	22
All	All	573/602 (95%)	519 (91%)	54 (9%)	8	26

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

Mol	Chain	Res	Type
1	A	41	VAL
1	A	44	ARG
1	A	56	SER
1	A	65	ILE
1	A	92	MET
1	A	101	PHE
1	A	102	PHE
1	A	135	ASN
1	A	187	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	192	GLU
1	A	193	ASN
1	A	202	LYS
1	A	206	LEU
1	A	214	VAL
1	A	232	ASN
1	A	245	LEU
1	A	249	GLU
1	A	253	GLU
1	A	265	MET
1	A	276	ILE
1	A	286	VAL
1	A	298	GLU
1	A	315	ARG
1	A	321	ARG
1	A	323	GLU
1	B	19	ARG
1	B	35	GLU
1	B	43	ARG
1	B	45	LEU
1	B	51	ARG
1	B	67	SER
1	B	74	LEU
1	B	81	VAL
1	B	101	PHE
1	B	121	LEU
1	B	134	VAL
1	B	142	VAL
1	B	143	PHE
1	B	156	GLU
1	B	157	ARG
1	B	158	GLU
1	B	166	THR
1	B	190	LYS
1	B	206	LEU
1	B	229	LEU
1	B	232	ASN
1	B	248	ARG
1	B	263	GLU
1	B	271	GLU
1	B	289	GLU
1	B	290	LYS

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Mol	Chain	Res	Type
1	B	292	GLU
1	B	321	ARG
1	B	322	GLU

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	83	ASN
1	A	135	ASN
1	A	193	ASN
1	A	209	GLN
1	A	232	ASN
1	A	238	GLN
1	B	27	ASN
1	B	83	ASN
1	B	209	GLN
1	B	232	ASN
1	B	238	GLN
1	B	299	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PMP	A	1335	-	15,15,16	1.28	1 (6%)	20,22,23	1.03	0
3	EDO	A	1637	-	3,3,3	0.49	0	2,2,2	0.28	0
2	PMP	B	1335	-	15,15,16	1.39	2 (13%)	20,22,23	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMP	A	1335	-	-	3/6/6/8	0/1/1/1
3	EDO	A	1637	-	-	0/1/1/1	-
2	PMP	B	1335	-	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1335	PMP	P-O1P	3.35	1.61	1.50
2	A	1335	PMP	P-O1P	3.33	1.61	1.50
2	B	1335	PMP	C2A-C2	2.05	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1335	PMP	O2P-P-O4P	2.14	112.42	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1335	PMP	C5A-O4P-P-O1P
2	A	1335	PMP	C5A-O4P-P-O2P
2	A	1335	PMP	C5A-O4P-P-O3P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1335	PMP	1	0
3	A	1637	EDO	3	0
2	B	1335	PMP	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	322/335 (96%)	-0.41	5 (1%) 72 66	40, 62, 85, 99	17 (5%)
1	B	319/335 (95%)	-0.23	7 (2%) 62 52	43, 69, 96, 99	13 (4%)
All	All	641/670 (95%)	-0.32	12 (1%) 66 59	40, 65, 93, 99	30 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLU	3.1
1	B	20	ASP	2.9
1	B	158	GLU	2.5
1	B	333	VAL	2.5
1	B	21	LYS	2.4
1	B	17	GLU	2.4
1	A	18	LYS	2.3
1	B	288	MET	2.3
1	B	19	ARG	2.2
1	A	127	LYS	2.0
1	A	17	GLU	2.0
1	A	135	ASN	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 monosaccharides 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	EDO	A	1637	4/4	0.89	0.33	50,50,51,51	0
2	PMP	B	1335	15/16	0.97	0.14	47,58,66,66	0
2	PMP	A	1335	15/16	0.97	0.10	39,55,65,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.