



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID : 2ZC0  
Title : Crystal structure of an archaeal alanine:glyoxylate aminotransferase  
Authors : Sakuraba, H.; Yoneda, K.; Tsuge, H.; Ohshima, T.  
Deposited on : 2007-10-31  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

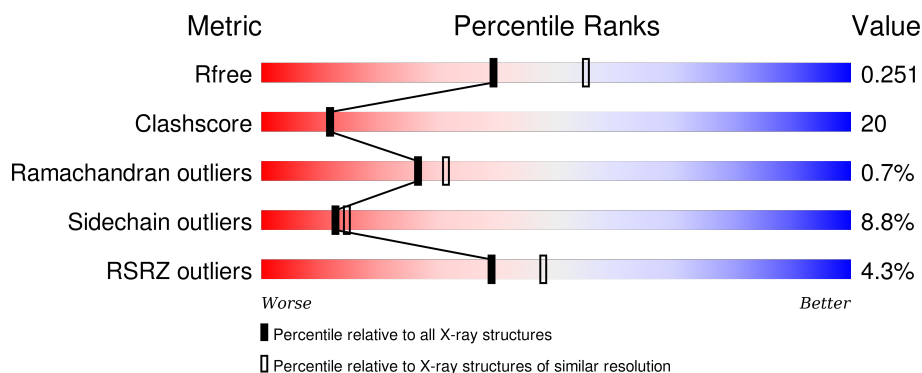
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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	407	<div> <div>3%</div> <div>64%</div> <div>32%</div> <div>.</div> </div>
1	B	407	<div> <div>%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>
1	C	407	<div> <div>6%</div> <div>57%</div> <div>37%</div> <div>5%</div> </div>
1	D	407	<div> <div>6%</div> <div>63%</div> <div>32%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PMP	A	409	-	-	-	X
3	PMP	B	409	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12914 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.

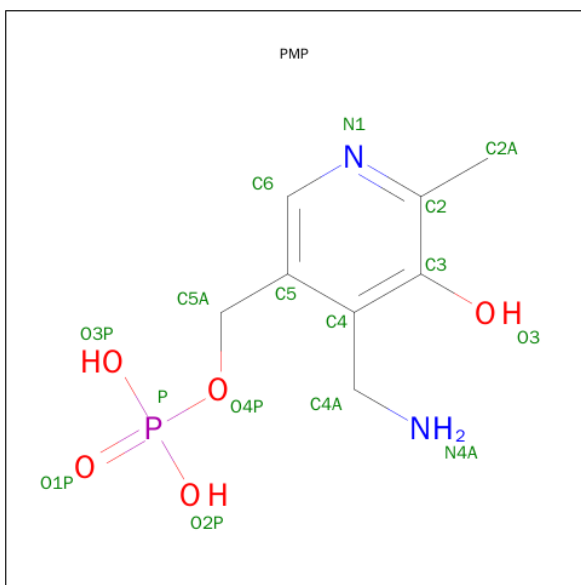
- Molecule 1 is a protein called Alanine glyoxylate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	B	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	C	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			
1	D	405	Total	C	N	O	S	0	0	0
			3111	2007	513	578	13			

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

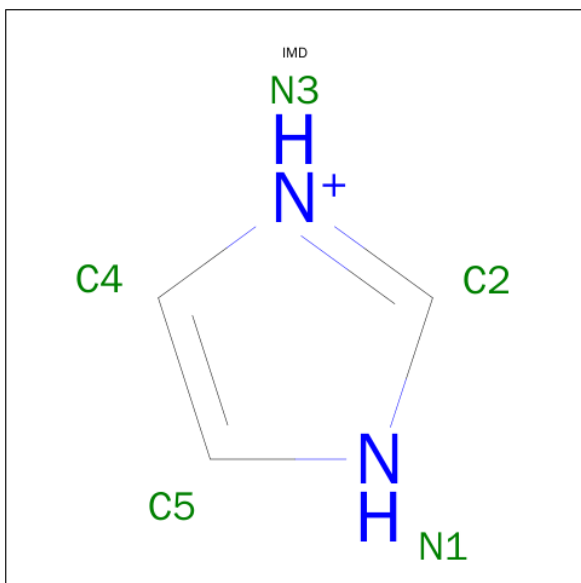
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	C	1	Total C N 5 3 2	0	0
4	D	1	Total C N 5 3 2	0	0

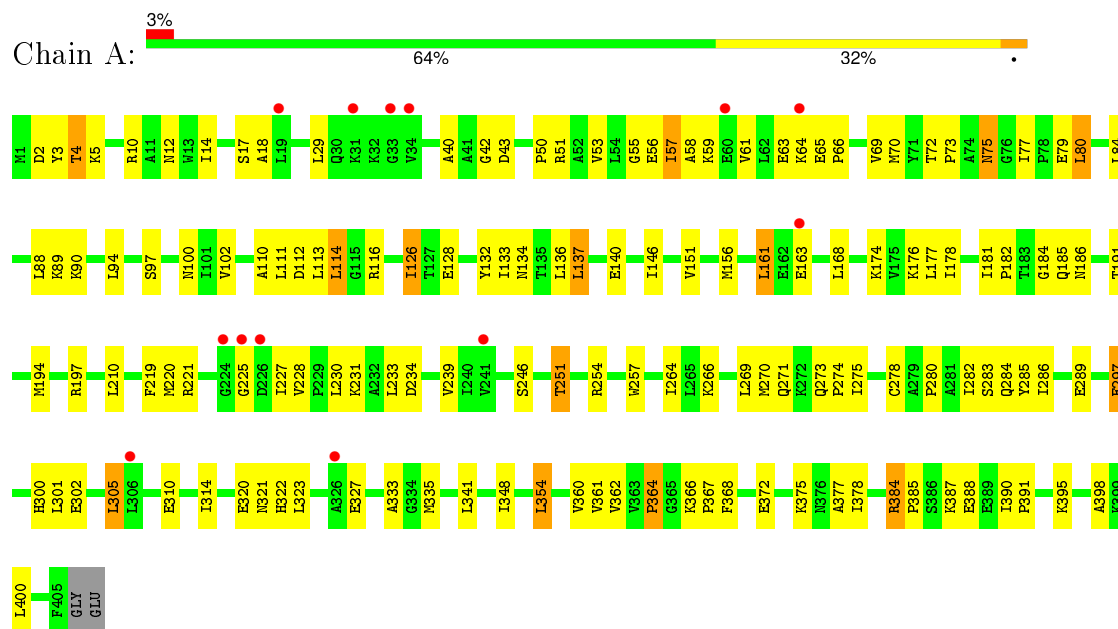
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	120	Total O 120 120	0	0
5	C	85	Total O 85 85	0	0
5	D	84	Total O 84 84	0	0

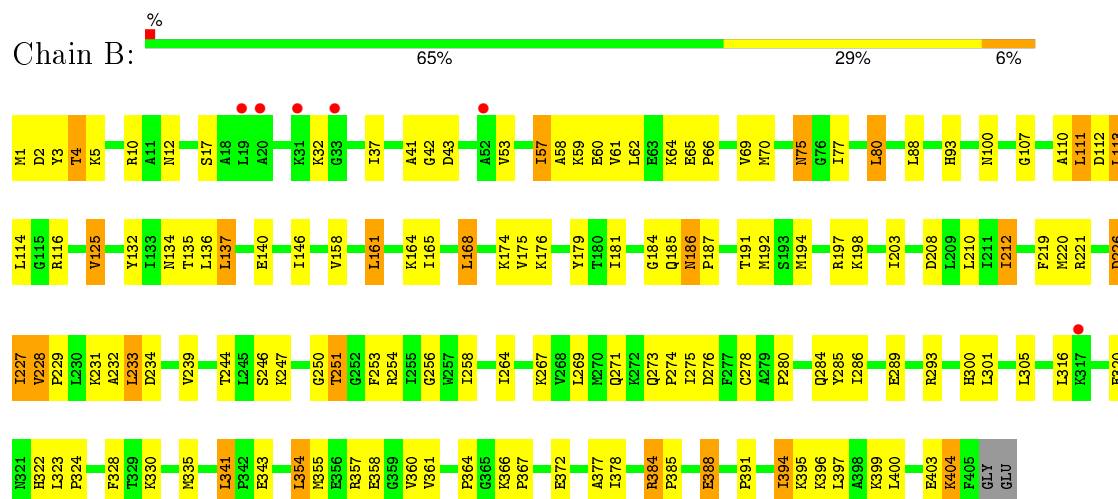
### 3 Residue-property plots

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

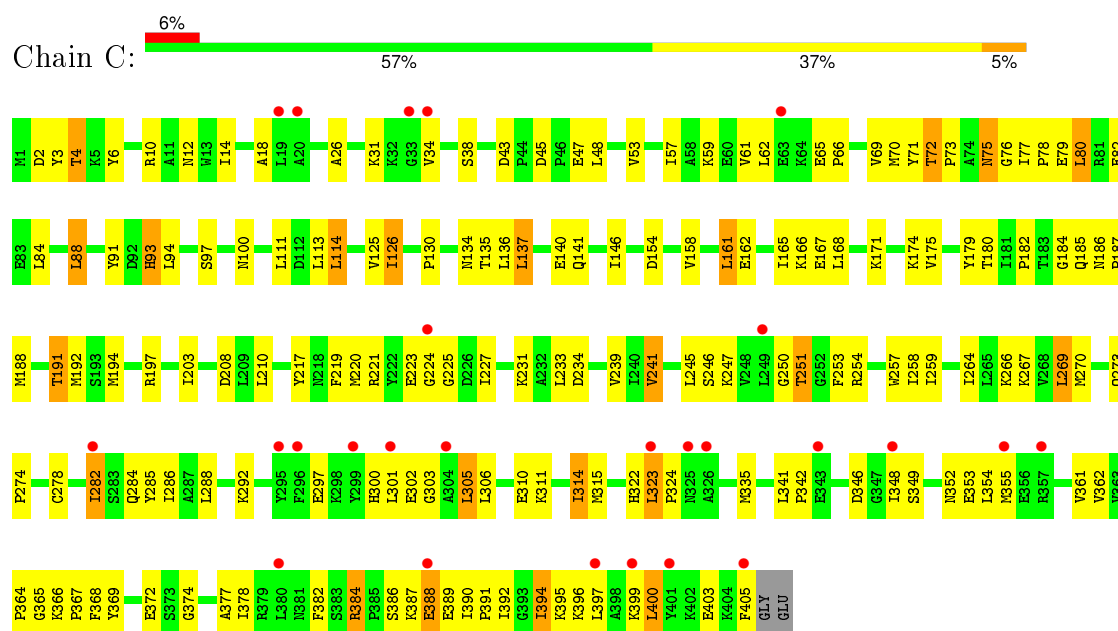
- Molecule 1: Alanine glyoxylate transaminase



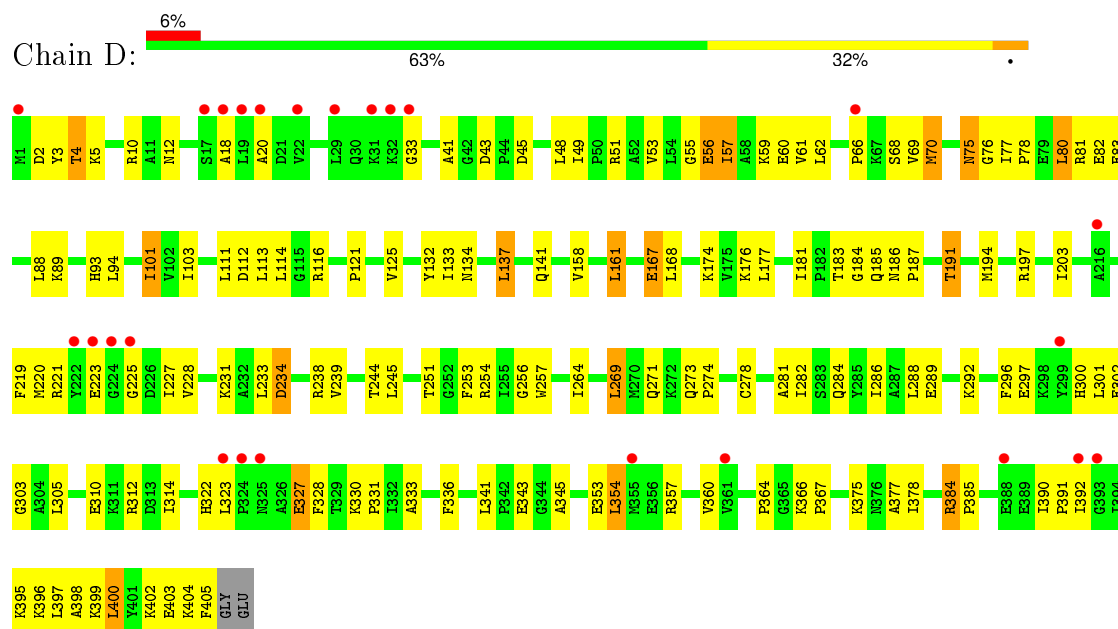
- Molecule 1: Alanine glyoxylate transaminase



- Molecule 1: Alanine glyoxylate transaminase



• Molecule 1: Alanine glyoxylate transaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.69Å 112.52Å 207.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.30 25.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.40-2.30) 98.0 (25.82-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	58.13 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.261 0.238 , 0.251	Depositor DCC
$R_{free}$ test set	4011 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 79851 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.41	0/3169	0.67	1/4279 (0.0%)
1	B	0.41	0/3169	0.71	3/4279 (0.1%)
1	C	0.38	0/3169	0.65	0/4279
1	D	0.44	2/3169 (0.1%)	0.68	0/4279
All	All	0.41	2/12676 (0.0%)	0.68	4/17116 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	225	GLY	C-N	10.18	1.57	1.34
1	D	220	MET	C-N	6.40	1.48	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	186	ASN	N-CA-C	-5.42	96.35	111.00
1	B	186	ASN	N-CA-C	-5.28	96.75	111.00
1	B	226	ASP	CB-CG-OD1	-5.03	113.77	118.30

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	3111	0	3162	147	0
1	B	3111	0	3162	129	0
1	C	3111	0	3162	152	0
1	D	3111	0	3162	136	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	16	0	11	2	0
3	B	16	0	11	3	0
3	C	16	0	11	1	0
3	D	16	0	11	1	0
4	A	5	0	4	0	0
4	B	5	0	4	0	0
4	C	5	0	4	0	0
4	D	5	0	4	0	0
5	A	93	0	0	12	0
5	B	120	0	0	9	0
5	C	85	0	0	10	0
5	D	84	0	0	9	0
All	All	12914	0	12708	511	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 20.

All (511) 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:C:354:LEU:HD11	1:C:397:LEU:HD23	1.35	1.08
1:C:221:ARG:HD3	1:C:227:ILE:HD11	1.38	1.04
1:B:184:GLY:H	1:B:191:THR:HG22	1.25	1.01
1:B:57:ILE:HD11	1:B:286:ILE:HA	1.40	0.99
1:A:57:ILE:HD11	1:A:286:ILE:HA	1.41	0.99
1:B:221:ARG:HD2	1:B:227:ILE:HD11	1.40	0.99
1:A:12:ASN:HD21	1:C:174:LYS:H	1.11	0.99
1:A:184:GLY:H	1:A:191:THR:HG22	1.21	0.98
1:B:174:LYS:H	1:D:12:ASN:HD21	1.07	0.96
1:D:57:ILE:HD11	1:D:286:ILE:HA	1.48	0.96
1:C:241:VAL:HG13	1:C:259:ILE:HB	1.45	0.95
1:A:134:ASN:HD21	1:B:273:GLN:HG2	1.35	0.91
1:D:223:GLU:HG3	1:D:312:ARG:HH22	1.33	0.91
1:A:174:LYS:H	1:C:12:ASN:HD21	1.15	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LEU:HD13	1:D:378:ILE:HD13	1.56	0.88
1:B:12:ASN:HD21	1:D:174:LYS:H	1.21	0.87
1:B:191:THR:HG23	5:B:421:HOH:O	1.75	0.85
1:C:72:THR:HG22	1:C:278:CYS:HB2	1.55	0.85
1:B:111:LEU:HD12	1:B:212:ILE:HD11	1.58	0.84
1:C:134:ASN:HD21	1:D:273:GLN:HG2	1.44	0.83
1:A:231:LYS:HD3	1:A:239:VAL:HG22	1.61	0.81
1:C:97:SER:HB3	1:C:100:ASN:HD22	1.47	0.78
1:B:404:LYS:HE2	1:B:404:LYS:HA	1.65	0.77
1:D:404:LYS:HE2	1:D:404:LYS:HA	1.67	0.77
1:A:251:THR:HG22	1:B:70:MET:HA	1.66	0.77
1:C:251:THR:HG22	1:D:70:MET:HA	1.66	0.77
1:C:341:LEU:HD13	1:C:378:ILE:HD13	1.68	0.76
1:C:70:MET:HA	1:D:251:THR:HG22	1.66	0.76
1:D:384:ARG:HH11	1:D:384:ARG:HB3	1.51	0.76
1:A:75:ASN:H	1:A:75:ASN:HD22	1.30	0.76
1:D:57:ILE:HD13	1:D:289:GLU:HB2	1.68	0.75
1:A:75:ASN:N	1:A:75:ASN:HD22	1.83	0.75
1:D:2:ASP:OD2	1:D:4:THR:HB	1.87	0.75
1:B:111:LEU:CD1	1:B:212:ILE:HD11	2.17	0.75
1:D:184:GLY:H	1:D:191:THR:HG22	1.50	0.75
1:B:364:PRO:O	1:B:377:ALA:O	2.05	0.75
1:D:75:ASN:HB3	1:D:269:LEU:HD11	1.69	0.74
1:B:125:VAL:HG13	1:B:146:ILE:HD13	1.69	0.74
1:A:246:SER:HB2	1:A:251:THR:HA	1.69	0.74
1:D:133:ILE:HD12	1:D:134:ASN:H	1.53	0.74
1:C:353:GLU:HB3	1:C:400:LEU:HD11	1.68	0.74
1:C:61:VAL:HG21	1:C:285:TYR:HB3	1.67	0.74
1:D:390:ILE:HB	1:D:391:PRO:HD3	1.68	0.74
1:D:101:ILE:HD11	1:D:103:ILE:HD13	1.69	0.74
1:A:70:MET:HA	1:B:251:THR:HG22	1.70	0.73
1:D:399:LYS:O	1:D:403:GLU:HB2	1.89	0.73
1:B:246:SER:HB2	1:B:251:THR:HA	1.68	0.72
5:C:413:HOH:O	1:D:10:ARG:HD2	1.88	0.72
1:B:42:GLY:O	1:B:335:MET:HE1	1.89	0.72
1:A:57:ILE:HD13	1:A:289:GLU:HB2	1.70	0.72
1:A:321:ASN:HB2	5:A:486:HOH:O	1.90	0.72
1:C:136:LEU:O	1:C:140:GLU:HG3	1.89	0.71
1:A:136:LEU:HD22	1:A:146:ILE:HD13	1.72	0.71
1:B:322:HIS:HB2	5:B:506:HOH:O	1.91	0.71
1:A:75:ASN:ND2	1:A:75:ASN:H	1.89	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HE2	1:B:59:LYS:HD3	1.72	0.70
1:A:126:ILE:HG23	1:A:178:ILE:HG12	1.73	0.70
1:D:176:LYS:HG3	1:D:177:LEU:HG	1.73	0.70
1:A:133:ILE:HD12	1:A:134:ASN:H	1.57	0.70
1:A:75:ASN:HB3	1:A:269:LEU:HD11	1.74	0.70
1:C:297:GLU:O	1:C:302:GLU:HG2	1.91	0.70
1:A:136:LEU:O	1:A:140:GLU:HG3	1.92	0.69
1:A:377:ALA:O	1:A:378:ILE:HD12	1.92	0.69
1:B:221:ARG:CD	1:B:227:ILE:HD11	2.21	0.68
1:B:355:MET:HE2	1:B:361:VAL:HG13	1.75	0.68
1:A:133:ILE:HG21	5:A:495:HOH:O	1.93	0.68
1:D:18:ALA:C	1:D:20:ALA:H	1.97	0.68
1:B:220:MET:HE1	1:B:335:MET:HB3	1.76	0.68
1:A:191:THR:HG23	5:A:490:HOH:O	1.92	0.68
1:D:391:PRO:O	1:D:395:LYS:HB2	1.94	0.67
1:C:114:LEU:HD13	1:C:258:ILE:HD13	1.77	0.67
1:A:133:ILE:HD12	1:A:134:ASN:N	2.09	0.67
1:C:273:GLN:HG2	1:D:134:ASN:HD21	1.60	0.67
1:B:107:GLY:O	1:B:111:LEU:HD22	1.95	0.66
1:B:231:LYS:HD3	1:B:239:VAL:HG22	1.78	0.66
1:C:184:GLY:H	1:C:191:THR:HG22	1.59	0.66
1:C:390:ILE:HB	1:C:391:PRO:HD3	1.77	0.66
1:A:174:LYS:H	1:C:12:ASN:ND2	1.92	0.66
1:A:10:ARG:HD2	5:B:419:HOH:O	1.94	0.66
1:C:365:GLY:HA2	1:C:368:PHE:CD1	2.31	0.65
1:C:384:ARG:HB3	1:C:384:ARG:HH11	1.62	0.65
1:D:133:ILE:HD12	1:D:134:ASN:N	2.12	0.65
1:C:43:ASP:OD1	1:C:251:THR:HG21	1.97	0.65
1:C:314:ILE:HD11	1:C:391:PRO:HD3	1.78	0.65
1:C:264:ILE:HG13	1:D:3:TYR:HB3	1.78	0.65
1:A:341:LEU:HD13	1:A:378:ILE:HD13	1.79	0.65
1:B:228:VAL:HG23	1:B:232:ALA:HB3	1.80	0.63
1:C:234:ASP:CG	1:C:239:VAL:HG13	2.18	0.63
1:D:223:GLU:HG3	1:D:312:ARG:NH2	2.10	0.62
1:C:62:LEU:O	1:D:51:ARG:HB3	1.97	0.62
1:D:343:GLU:H	1:D:343:GLU:CD	2.03	0.62
1:D:322:HIS:CE1	1:D:395:LYS:NZ	2.67	0.62
1:A:194:MET:HA	1:A:197:ARG:HD3	1.82	0.62
1:A:50:PRO:HB2	1:A:53:VAL:HB	1.81	0.62
1:B:234:ASP:CG	1:B:239:VAL:HG13	2.20	0.61
1:A:221:ARG:HG2	1:A:333:ALA:HB2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LYS:HD3	1:D:239:VAL:HG22	1.81	0.61
1:C:191:THR:HG23	5:C:418:HOH:O	2.01	0.61
1:C:390:ILE:O	1:C:394:ILE:HG23	2.01	0.61
1:B:43:ASP:OD1	1:B:251:THR:HG21	1.99	0.61
1:A:51:ARG:HB3	1:B:62:LEU:O	2.01	0.61
1:A:348:ILE:HG22	1:A:364:PRO:HB3	1.82	0.61
1:D:366:LYS:HD3	1:D:375:LYS:HA	1.82	0.61
1:C:77:ILE:HG13	1:C:80:LEU:HB2	1.83	0.61
1:C:377:ALA:O	1:C:378:ILE:HD12	2.00	0.61
1:B:17:SER:HB2	1:B:137:LEU:HD21	1.82	0.61
1:C:253:PHE:HE2	1:D:69:VAL:HG23	1.65	0.61
1:C:349:SER:HA	1:C:352:ASN:HD22	1.65	0.60
1:B:174:LYS:H	1:D:12:ASN:ND2	1.90	0.60
1:A:377:ALA:C	1:A:378:ILE:HD12	2.21	0.60
1:B:93:HIS:HE1	1:B:226:ASP:OD1	1.84	0.60
1:A:43:ASP:OD1	1:A:251:THR:HG21	1.99	0.60
1:D:384:ARG:N	1:D:385:PRO:HD2	2.17	0.60
1:D:384:ARG:HB3	1:D:384:ARG:NH1	2.16	0.60
1:B:75:ASN:HB3	1:B:269:LEU:HD11	1.84	0.60
1:C:10:ARG:HD3	5:D:436:HOH:O	2.02	0.60
1:A:390:ILE:HB	1:A:391:PRO:HD3	1.83	0.60
1:D:43:ASP:OD1	1:D:251:THR:HG21	2.02	0.60
1:D:18:ALA:CB	1:D:367:PRO:HG2	2.32	0.60
1:A:227:ILE:O	1:A:227:ILE:HG13	2.01	0.60
1:C:2:ASP:OD2	1:C:4:THR:HB	2.02	0.60
1:A:72:THR:HG22	1:A:278:CYS:SG	2.42	0.59
1:D:392:ILE:HG22	1:D:396:LYS:HE3	1.83	0.59
1:A:126:ILE:C	1:A:126:ILE:HD13	2.21	0.59
1:A:5:LYS:HE2	5:C:437:HOH:O	2.02	0.59
1:B:77:ILE:H	1:B:284:GLN:HE22	1.51	0.59
1:A:72:THR:HG22	1:A:278:CYS:HB2	1.84	0.59
1:A:5:LYS:HE3	1:C:208:ASP:HB3	1.85	0.58
1:B:247:LYS:NZ	3:B:409:PMP:H4A1	2.17	0.58
1:A:133:ILE:HG23	1:A:368:PHE:HA	1.85	0.58
1:C:254:ARG:NE	1:C:254:ARG:HA	2.18	0.58
1:A:72:THR:OG1	1:A:77:ILE:HG23	2.04	0.58
1:A:234:ASP:CG	1:A:239:VAL:HG13	2.24	0.57
1:A:79:GLU:H	1:A:79:GLU:CD	2.08	0.57
1:C:323:LEU:N	1:C:324:PRO:HD3	2.18	0.57
1:D:221:ARG:HG2	1:D:333:ALA:HB2	1.86	0.57
1:D:81:ARG:HG2	1:D:101:ILE:HG13	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG2	5:A:474:HOH:O	2.03	0.57
1:D:53:VAL:HG23	5:D:428:HOH:O	2.05	0.57
1:D:101:ILE:HD11	1:D:103:ILE:CD1	2.34	0.57
1:D:297:GLU:O	1:D:302:GLU:HG2	2.05	0.56
1:A:53:VAL:O	1:A:57:ILE:HG23	2.05	0.56
1:A:12:ASN:HD21	1:C:174:LYS:N	1.93	0.56
1:C:72:THR:OG1	1:C:77:ILE:HG23	2.05	0.56
1:C:278:CYS:O	1:D:254:ARG:HD2	2.05	0.56
1:D:384:ARG:H	1:D:385:PRO:HD2	1.71	0.56
1:C:18:ALA:HB3	1:C:367:PRO:HG3	1.87	0.56
1:D:353:GLU:HG2	1:D:357:ARG:HD3	1.87	0.56
1:D:185:GLN:HG2	1:D:186:ASN:N	2.20	0.56
1:C:372:GLU:HG2	5:C:488:HOH:O	2.04	0.56
1:D:167:GLU:HG2	5:D:425:HOH:O	2.05	0.56
1:B:366:LYS:HB3	1:B:367:PRO:HD3	1.88	0.56
1:D:364:PRO:O	1:D:377:ALA:O	2.23	0.56
1:C:246:SER:HB2	1:C:251:THR:HA	1.86	0.56
1:D:322:HIS:CE1	1:D:395:LYS:HZ2	2.24	0.56
1:D:76:GLY:HA2	1:D:284:GLN:HE22	1.70	0.56
1:C:65:GLU:OE1	1:C:66:PRO:HD2	2.06	0.56
1:D:366:LYS:HB3	1:D:367:PRO:HD3	1.88	0.55
1:C:3:TYR:HB3	1:D:264:ILE:HG13	1.88	0.55
1:D:322:HIS:NE2	1:D:395:LYS:HD2	2.21	0.55
1:C:266:LYS:HE3	1:C:270:MET:HE1	1.89	0.55
1:C:77:ILE:HB	1:C:79:GLU:OE1	2.07	0.55
1:C:388:GLU:O	1:C:391:PRO:HD2	2.06	0.55
1:D:244:THR:HA	1:D:256:GLY:HA2	1.88	0.55
1:C:391:PRO:O	1:C:395:LYS:HB2	2.06	0.55
1:A:354:LEU:HD22	1:A:360:VAL:HB	1.89	0.55
1:D:75:ASN:N	1:D:75:ASN:HD22	2.04	0.55
1:D:322:HIS:HE1	5:D:494:HOH:O	1.89	0.55
1:D:66:PRO:O	1:D:69:VAL:HG12	2.07	0.55
1:C:66:PRO:O	1:C:69:VAL:HG12	2.06	0.55
1:A:42:GLY:CA	1:A:335:MET:CE	2.84	0.55
1:B:316:LEU:O	1:B:320:GLU:HG3	2.06	0.55
1:A:254:ARG:HD2	1:B:278:CYS:O	2.07	0.54
1:A:72:THR:HG22	1:A:278:CYS:CB	2.38	0.54
1:C:59:LYS:HB2	1:D:59:LYS:HB2	1.89	0.54
1:C:254:ARG:HH12	3:C:409:PMP:P	2.30	0.54
1:C:399:LYS:O	1:C:403:GLU:HB2	2.08	0.54
1:A:184:GLY:N	1:A:191:THR:HG22	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASP:HB3	1:D:48:LEU:HG	1.90	0.54
1:A:388:GLU:O	1:A:391:PRO:HD2	2.08	0.54
1:A:322:HIS:CE1	1:A:395:LYS:HG2	2.42	0.54
1:C:253:PHE:CE2	1:D:69:VAL:HG23	2.43	0.54
1:B:280:PRO:O	1:B:284:GLN:HG3	2.08	0.54
1:C:288:LEU:O	1:C:292:LYS:HG3	2.08	0.54
1:C:346:ASP:OD2	1:C:348:ILE:HG13	2.08	0.54
1:D:158:VAL:O	1:D:161:LEU:HB3	2.08	0.54
1:D:234:ASP:CG	1:D:239:VAL:HG13	2.28	0.53
5:A:475:HOH:O	1:B:10:ARG:HD2	2.08	0.53
1:C:322:HIS:C	1:C:324:PRO:HD3	2.28	0.53
1:A:4:THR:HG23	5:C:484:HOH:O	2.08	0.53
1:C:297:GLU:HA	1:C:301:LEU:HB2	1.91	0.53
1:D:328:PHE:CE1	1:D:330:LYS:HE3	2.43	0.53
1:C:245:LEU:HG	1:C:257:TRP:HZ3	1.74	0.53
1:C:70:MET:HA	1:D:251:THR:CG2	2.37	0.53
1:C:366:LYS:N	1:C:367:PRO:HD2	2.23	0.53
1:C:137:LEU:O	1:C:141:GLN:HG2	2.09	0.53
1:B:354:LEU:HD22	1:B:360:VAL:HB	1.90	0.53
1:B:174:LYS:N	1:D:12:ASN:HD21	1.91	0.53
1:A:282:ILE:HG13	1:A:283:SER:N	2.24	0.53
1:A:42:GLY:HA2	1:A:335:MET:CE	2.38	0.53
1:A:384:ARG:HB3	1:A:384:ARG:HH11	1.73	0.53
1:D:89:LYS:C	1:D:89:LYS:HD3	2.29	0.53
1:A:72:THR:HG21	1:A:284:GLN:OE1	2.09	0.53
1:A:72:THR:CG2	1:A:278:CYS:HB2	2.39	0.52
1:B:2:ASP:OD2	1:B:4:THR:HB	2.09	0.52
1:B:208:ASP:HB3	1:D:5:LYS:HZ1	1.75	0.52
1:D:75:ASN:HD22	1:D:75:ASN:H	1.57	0.52
1:D:227:ILE:HG13	1:D:227:ILE:O	2.08	0.52
1:C:78:PRO:O	1:C:82:GLU:HG3	2.09	0.52
1:C:246:SER:HA	1:C:250:GLY:O	2.09	0.52
1:D:77:ILE:HG13	1:D:80:LEU:HB2	1.91	0.52
1:B:247:LYS:HZ1	3:B:409:PMP:H4A1	1.74	0.52
1:D:328:PHE:HE1	1:D:330:LYS:HE3	1.75	0.52
1:C:61:VAL:HG21	1:C:285:TYR:CB	2.37	0.52
1:A:273:GLN:HB3	1:A:274:PRO:HD3	1.91	0.52
1:D:297:GLU:HA	1:D:301:LEU:HB2	1.92	0.52
1:D:219:PHE:O	1:D:300:HIS:HE1	1.93	0.52
1:A:12:ASN:ND2	1:C:174:LYS:H	1.94	0.52
1:B:179:TYR:HA	1:B:212:ILE:HG23	1.92	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:TYR:N	1:D:251:THR:HG23	2.25	0.52
1:C:217:TYR:CE2	1:C:247:LYS:HE3	2.44	0.52
1:D:288:LEU:HD11	1:D:292:LYS:HE3	1.90	0.52
1:B:61:VAL:HG11	1:B:285:TYR:HB3	1.91	0.51
1:C:38:SER:HB2	1:C:361:VAL:HB	1.92	0.51
1:C:306:LEU:H	1:C:306:LEU:HD22	1.74	0.51
1:C:88:LEU:HB3	1:C:94:LEU:HB3	1.91	0.51
5:A:482:HOH:O	1:B:59:LYS:HD2	2.11	0.51
1:C:310:GLU:OE1	1:C:387:LYS:HE2	2.10	0.51
1:A:254:ARG:HH12	3:A:409:PMP:P	2.33	0.51
1:C:185:GLN:HG2	1:C:186:ASN:N	2.25	0.51
1:C:62:LEU:HD12	1:D:55:GLY:HA2	1.93	0.51
1:A:181:ILE:HB	1:A:185:GLN:HG3	1.92	0.51
1:D:341:LEU:CD1	1:D:378:ILE:HD13	2.37	0.51
1:C:75:ASN:HD22	1:C:75:ASN:N	2.07	0.51
1:A:282:ILE:HG23	5:A:417:HOH:O	2.11	0.51
1:D:273:GLN:HB3	1:D:274:PRO:HD3	1.92	0.51
1:D:181:ILE:HB	1:D:185:GLN:HG3	1.93	0.51
1:B:37:ILE:CB	5:B:515:HOH:O	2.57	0.51
1:A:57:ILE:HG13	1:A:58:ALA:N	2.25	0.51
1:A:366:LYS:HD3	1:A:375:LYS:HA	1.93	0.51
1:C:267:LYS:HE3	5:D:412:HOH:O	2.10	0.51
1:B:57:ILE:HD13	1:B:289:GLU:HB2	1.92	0.51
1:D:322:HIS:CE1	5:D:494:HOH:O	2.63	0.51
1:C:75:ASN:HB3	1:C:269:LEU:HD11	1.93	0.50
1:B:391:PRO:O	1:B:395:LYS:HB2	2.10	0.50
1:A:310:GLU:OE1	1:A:387:LYS:HD2	2.10	0.50
1:B:136:LEU:O	1:B:140:GLU:HG3	2.11	0.50
1:A:388:GLU:HB2	5:A:422:HOH:O	2.11	0.50
1:A:3:TYR:HB3	1:B:264:ILE:HG13	1.92	0.50
1:A:174:LYS:N	1:C:12:ASN:HD21	1.98	0.50
1:B:358:GLU:HB3	1:B:396:LYS:HD3	1.92	0.50
1:A:14:ILE:HD13	1:B:271:GLN:HB3	1.93	0.50
1:A:10:ARG:HD3	5:B:447:HOH:O	2.11	0.50
1:C:75:ASN:ND2	1:C:75:ASN:H	2.10	0.50
1:D:183:THR:HA	1:D:191:THR:HB	1.94	0.50
1:A:69:VAL:HG22	1:B:250:GLY:HA3	1.94	0.50
1:C:231:LYS:HD3	1:C:239:VAL:HG22	1.93	0.49
1:A:297:GLU:HG2	1:A:301:LEU:HD12	1.92	0.49
1:D:57:ILE:HD12	1:D:61:VAL:HG23	1.95	0.49
1:C:94:LEU:HD11	1:C:231:LYS:HG3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:VAL:HG13	1:D:203:ILE:HD12	1.94	0.49
1:A:61:VAL:HG11	1:A:285:TYR:HB3	1.94	0.49
1:B:194:MET:HA	1:B:197:ARG:HD3	1.95	0.49
1:D:364:PRO:O	1:D:378:ILE:HA	2.12	0.49
1:A:126:ILE:HD12	1:A:178:ILE:HG12	1.95	0.49
1:C:266:LYS:HE3	1:C:270:MET:CE	2.41	0.49
1:C:282:ILE:O	1:C:286:ILE:HG13	2.13	0.49
1:D:89:LYS:HA	1:D:94:LEU:O	2.12	0.49
1:B:60:GLU:HG3	1:B:64:LYS:HE2	1.94	0.49
1:C:194:MET:HG2	1:C:227:ILE:HG22	1.93	0.49
1:B:271:GLN:O	1:B:274:PRO:HD2	2.12	0.49
1:B:208:ASP:HB3	1:D:5:LYS:NZ	2.27	0.49
1:A:176:LYS:HG3	1:A:177:LEU:HG	1.94	0.49
1:D:191:THR:HG23	5:D:473:HOH:O	2.13	0.49
1:A:59:LYS:CE	1:B:59:LYS:HD3	2.42	0.49
1:C:91:TYR:CE2	1:C:301:LEU:HD11	2.48	0.49
1:C:300:HIS:O	1:C:305:LEU:HB2	2.13	0.49
1:D:56:GLU:O	1:D:60:GLU:HG3	2.13	0.49
1:B:366:LYS:N	1:B:367:PRO:CD	2.75	0.49
1:A:53:VAL:O	1:A:57:ILE:CG2	2.61	0.48
1:D:75:ASN:H	1:D:75:ASN:ND2	2.11	0.48
1:C:130:PRO:HD3	1:C:369:TYR:CE1	2.47	0.48
1:B:301:LEU:HA	1:B:305:LEU:HD12	1.95	0.48
1:A:273:GLN:HG2	1:B:134:ASN:HD21	1.77	0.48
1:A:297:GLU:O	1:A:302:GLU:HG2	2.12	0.48
1:C:364:PRO:O	1:C:377:ALA:O	2.31	0.48
1:C:69:VAL:HG23	1:D:253:PHE:CE2	2.48	0.48
1:A:322:HIS:HE1	1:A:395:LYS:HE2	1.79	0.48
1:B:289:GLU:HG2	5:B:433:HOH:O	2.12	0.48
1:D:395:LYS:NZ	5:D:494:HOH:O	2.18	0.48
1:C:93:HIS:NE2	5:C:494:HOH:O	2.33	0.48
1:C:45:ASP:OD2	1:C:47:GLU:HB2	2.14	0.48
1:A:63:GLU:HG3	1:A:64:LYS:HG3	1.95	0.48
1:D:327:GLU:OE1	1:D:327:GLU:HA	2.13	0.48
1:A:89:LYS:HD3	1:A:90:LYS:N	2.29	0.48
1:A:151:VAL:HG12	1:A:156:MET:HA	1.96	0.48
1:D:245:LEU:HG	1:D:257:TRP:HZ3	1.78	0.48
1:A:84:LEU:O	1:A:88:LEU:HD13	2.14	0.48
1:A:55:GLY:HA2	1:B:62:LEU:HD12	1.96	0.48
1:C:69:VAL:HG23	1:D:253:PHE:HE2	1.78	0.48
1:B:208:ASP:HB3	1:D:5:LYS:HE3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HG13	1:B:3:TYR:HB3	1.95	0.48
1:B:244:THR:HA	1:B:256:GLY:HA2	1.95	0.48
1:C:219:PHE:O	1:C:300:HIS:HE1	1.97	0.47
1:D:18:ALA:C	1:D:20:ALA:N	2.66	0.47
1:A:77:ILE:H	1:A:284:GLN:HE22	1.61	0.47
1:B:181:ILE:HB	1:B:185:GLN:HG3	1.97	0.47
1:C:72:THR:HG23	1:C:73:PRO:O	2.14	0.47
1:C:310:GLU:O	1:C:314:ILE:CG2	2.63	0.47
1:C:311:LYS:HA	1:C:314:ILE:HG23	1.97	0.47
1:B:388:GLU:HB2	5:B:445:HOH:O	2.15	0.47
1:A:323:LEU:HD21	1:A:398:ALA:HB2	1.96	0.47
1:B:377:ALA:C	1:B:378:ILE:HD12	2.35	0.47
1:A:77:ILE:HB	1:A:79:GLU:OE1	2.14	0.47
1:A:42:GLY:HA2	1:A:335:MET:HE3	1.96	0.47
1:B:384:ARG:N	1:B:385:PRO:HD2	2.30	0.47
1:C:79:GLU:H	1:C:79:GLU:CD	2.18	0.47
1:C:254:ARG:HD2	1:D:278:CYS:O	2.14	0.47
1:C:175:VAL:HG12	5:C:484:HOH:O	2.15	0.47
1:D:77:ILE:H	1:D:284:GLN:NE2	2.13	0.47
1:B:341:LEU:HD13	1:B:378:ILE:HD13	1.95	0.47
1:A:126:ILE:CG2	1:A:178:ILE:HG12	2.42	0.47
1:C:175:VAL:CG2	5:C:485:HOH:O	2.63	0.47
1:C:269:LEU:HA	1:C:269:LEU:HD13	1.74	0.47
1:D:323:LEU:HD21	1:D:398:ALA:HB2	1.96	0.47
1:D:94:LEU:HD11	1:D:231:LYS:HG3	1.96	0.46
1:B:208:ASP:HB3	1:D:5:LYS:CE	2.45	0.46
1:C:377:ALA:C	1:C:378:ILE:HD12	2.36	0.46
1:C:140:GLU:HG2	1:C:146:ILE:HD13	1.97	0.46
1:C:297:GLU:HA	1:C:301:LEU:HD12	1.97	0.46
1:B:75:ASN:HB3	1:B:269:LEU:CD1	2.45	0.46
1:A:132:TYR:CZ	1:A:134:ASN:HB2	2.50	0.46
1:B:231:LYS:CD	1:B:239:VAL:HG22	2.45	0.46
1:A:176:LYS:CG	1:A:177:LEU:HG	2.46	0.46
1:C:354:LEU:HD21	1:C:397:LEU:HA	1.96	0.46
1:B:175:VAL:HG22	1:B:176:LYS:N	2.30	0.46
1:A:110:ALA:O	1:A:114:LEU:HD22	2.16	0.46
1:C:273:GLN:HB3	1:C:274:PRO:HD3	1.97	0.46
1:B:228:VAL:CG2	1:B:233:LEU:HD13	2.46	0.46
1:A:156:MET:SD	1:A:161:LEU:HG	2.56	0.46
1:C:75:ASN:HD22	1:C:75:ASN:H	1.62	0.46
5:A:418:HOH:O	1:B:267:LYS:HE3	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:VAL:HG21	1:B:233:LEU:HD13	1.97	0.46
1:B:60:GLU:CD	1:B:293:ARG:HH22	2.19	0.46
1:C:57:ILE:O	1:C:61:VAL:HG12	2.16	0.46
1:D:231:LYS:CD	1:D:239:VAL:HG22	2.46	0.46
1:A:42:GLY:CA	1:A:335:MET:HE3	2.45	0.46
1:C:354:LEU:HD12	1:C:362:VAL:HG21	1.98	0.45
1:D:322:HIS:HE1	1:D:395:LYS:NZ	2.12	0.45
1:D:161:LEU:HD13	1:D:203:ILE:HG21	1.97	0.45
1:A:42:GLY:C	1:A:335:MET:HE3	2.37	0.45
1:C:310:GLU:O	1:C:314:ILE:HG22	2.17	0.45
1:B:93:HIS:NE2	1:B:226:ASP:OD2	2.49	0.45
1:B:185:GLN:HG2	1:B:186:ASN:N	2.32	0.45
1:B:254:ARG:HH12	3:B:409:PMP:P	2.39	0.45
1:B:42:GLY:C	1:B:335:MET:HE1	2.36	0.45
1:A:384:ARG:N	1:A:385:PRO:HD2	2.32	0.45
1:C:245:LEU:HG	1:C:257:TRP:CZ3	2.52	0.45
1:A:182:PRO:O	1:A:191:THR:HA	2.16	0.45
1:D:341:LEU:HB3	1:D:345:ALA:HB3	1.98	0.45
1:D:366:LYS:N	1:D:367:PRO:CD	2.79	0.45
1:C:231:LYS:CD	1:C:239:VAL:HG22	2.46	0.45
1:A:278:CYS:O	1:B:254:ARG:HD2	2.16	0.45
1:D:221:ARG:HD3	1:D:227:ILE:CD1	2.46	0.45
1:D:305:LEU:HD23	1:D:305:LEU:O	2.17	0.45
1:C:221:ARG:NH2	1:C:225:GLY:O	2.48	0.45
1:B:57:ILE:HD12	1:B:61:VAL:HG23	1.99	0.45
1:A:2:ASP:OD2	1:A:4:THR:HG22	2.17	0.45
1:A:322:HIS:CE1	1:A:395:LYS:HE2	2.52	0.45
1:C:386:SER:OG	1:C:389:GLU:HG3	2.17	0.45
1:A:57:ILE:HD12	1:A:61:VAL:HG23	1.98	0.45
1:B:42:GLY:CA	1:B:335:MET:HE3	2.47	0.45
1:C:282:ILE:HG13	5:C:438:HOH:O	2.17	0.45
1:C:167:GLU:O	1:C:171:LYS:HG3	2.17	0.45
1:A:220:MET:HE3	1:A:335:MET:HB3	1.99	0.44
1:B:60:GLU:OE1	1:B:293:ARG:NH2	2.46	0.44
1:D:281:ALA:HB3	5:D:447:HOH:O	2.16	0.44
1:B:273:GLN:HB3	1:B:274:PRO:HD3	1.98	0.44
1:C:394:ILE:O	1:C:394:ILE:HD12	2.17	0.44
1:B:75:ASN:C	1:B:75:ASN:HD22	2.20	0.44
1:B:219:PHE:O	1:B:300:HIS:HE1	2.00	0.44
1:A:219:PHE:O	1:A:300:HIS:HE1	2.00	0.44
1:A:72:THR:HG23	1:A:73:PRO:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:THR:HG21	1:C:179:TYR:CZ	2.52	0.44
1:C:135:THR:HG21	1:C:179:TYR:CE1	2.52	0.44
1:C:315:MET:HE3	1:C:382:PHE:HB3	1.98	0.44
1:D:137:LEU:O	1:D:141:GLN:HG2	2.17	0.44
1:A:65:GLU:OE1	1:A:66:PRO:HD2	2.18	0.44
1:B:57:ILE:HG13	1:B:58:ALA:N	2.33	0.44
1:A:231:LYS:CD	1:A:239:VAL:HG22	2.42	0.44
1:A:29:LEU:HA	5:A:481:HOH:O	2.18	0.44
1:A:362:VAL:HG22	5:A:429:HOH:O	2.17	0.44
1:A:112:ASP:O	1:A:116:ARG:HG3	2.18	0.44
1:B:323:LEU:N	1:B:324:PRO:CD	2.81	0.44
1:A:133:ILE:HG13	1:A:368:PHE:CE2	2.52	0.44
1:A:194:MET:HE1	1:A:228:VAL:HG22	2.00	0.44
1:B:77:ILE:CG1	1:B:80:LEU:HB2	2.48	0.44
1:D:296:PHE:O	1:D:300:HIS:HB3	2.18	0.44
1:C:154:ASP:O	1:C:192:MET:HA	2.18	0.44
1:A:136:LEU:CD2	1:A:146:ILE:HD13	2.45	0.44
5:A:496:HOH:O	1:C:4:THR:CG2	2.66	0.44
1:D:310:GLU:O	1:D:314:ILE:HG13	2.18	0.44
1:D:194:MET:HE1	1:D:228:VAL:HG22	2.00	0.44
1:A:102:VAL:O	1:A:257:TRP:HA	2.18	0.44
1:D:354:LEU:HA	1:D:400:LEU:HD12	2.00	0.44
1:B:112:ASP:O	1:B:116:ARG:HG3	2.18	0.44
1:A:384:ARG:HB3	1:A:384:ARG:NH1	2.32	0.43
1:A:266:LYS:HE3	1:A:270:MET:CE	2.48	0.43
1:B:93:HIS:CE1	1:B:226:ASP:OD1	2.69	0.43
1:B:328:PHE:CE1	1:B:330:LYS:HE3	2.53	0.43
1:C:14:ILE:HD13	1:D:271:GLN:HB3	1.99	0.43
1:B:192:MET:HG2	1:B:197:ARG:HG3	1.99	0.43
1:B:228:VAL:HA	1:B:229:PRO:HD3	1.91	0.43
1:A:80:LEU:HD12	1:A:284:GLN:HB3	2.00	0.43
1:D:238:ARG:NH2	1:D:238:ARG:HG2	2.34	0.43
1:A:300:HIS:O	1:A:305:LEU:HB2	2.18	0.43
1:D:77:ILE:H	1:D:284:GLN:HE22	1.67	0.43
1:C:84:LEU:HA	1:C:84:LEU:HD23	1.92	0.43
1:A:271:GLN:O	1:A:274:PRO:HD2	2.19	0.43
1:C:220:MET:CE	1:C:335:MET:HB3	2.49	0.43
1:B:42:GLY:HA2	1:B:335:MET:HE3	2.00	0.43
1:C:335:MET:HA	1:C:382:PHE:CZ	2.53	0.43
1:C:162:GLU:HG2	1:C:166:LYS:HD2	2.01	0.42
1:C:158:VAL:CG1	1:C:203:ILE:HD12	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:NE	1:B:254:ARG:HA	2.34	0.42
1:C:75:ASN:ND2	1:C:75:ASN:N	2.66	0.42
1:A:128:GLU:HG3	1:A:156:MET:CE	2.50	0.42
1:B:158:VAL:HG13	1:B:203:ILE:HD12	2.01	0.42
1:C:161:LEU:HD22	1:C:165:ILE:HD11	2.01	0.42
1:A:97:SER:HB3	1:A:100:ASN:HD22	1.83	0.42
1:A:282:ILE:O	1:A:286:ILE:HG13	2.19	0.42
1:C:175:VAL:HG23	5:C:485:HOH:O	2.19	0.42
1:D:53:VAL:O	1:D:57:ILE:HG23	2.20	0.42
1:C:53:VAL:O	1:C:57:ILE:HG13	2.19	0.42
1:B:1:MET:N	5:B:524:HOH:O	2.53	0.42
1:B:194:MET:HG2	1:B:227:ILE:HG22	2.01	0.42
1:B:111:LEU:HD12	1:B:212:ILE:CD1	2.38	0.42
1:D:238:ARG:HG2	1:D:238:ARG:HH21	1.84	0.42
1:C:180:THR:C	1:C:182:PRO:HD3	2.40	0.42
1:B:100:ASN:HD22	1:B:100:ASN:N	2.17	0.42
1:B:164:LYS:O	1:B:168:LEU:HD22	2.19	0.42
1:B:399:LYS:O	1:B:403:GLU:HG2	2.19	0.42
1:D:57:ILE:HD13	1:D:289:GLU:CB	2.44	0.42
1:A:77:ILE:HG13	1:A:80:LEU:HB2	2.02	0.42
1:B:65:GLU:HA	1:B:66:PRO:HD2	1.90	0.42
1:C:392:ILE:HG22	1:C:396:LYS:HE3	2.02	0.42
1:A:57:ILE:HD13	1:A:289:GLU:CB	2.45	0.42
1:C:72:THR:HG21	1:C:284:GLN:OE1	2.19	0.42
1:C:59:LYS:C	1:C:59:LYS:HD2	2.40	0.42
1:D:62:LEU:HD23	1:D:68:SER:OG	2.19	0.42
1:A:17:SER:HB2	1:A:137:LEU:HD21	2.01	0.42
1:A:282:ILE:HG21	1:B:253:PHE:CE1	2.55	0.42
1:D:254:ARG:HH12	3:D:409:PMP:P	2.43	0.42
1:D:184:GLY:H	1:D:191:THR:CG2	2.25	0.42
1:B:276:ASP:C	1:B:276:ASP:OD1	2.59	0.42
1:C:192:MET:HG2	1:C:197:ARG:HG3	2.02	0.41
1:B:42:GLY:CA	1:B:335:MET:CE	2.98	0.41
1:A:18:ALA:HB3	1:A:367:PRO:HG2	2.01	0.41
1:A:89:LYS:C	1:A:89:LYS:HD3	2.41	0.41
1:C:342:PRO:HG2	1:C:405:PHE:CD2	2.55	0.41
1:D:112:ASP:O	1:D:116:ARG:HG3	2.20	0.41
1:B:61:VAL:HG11	1:B:285:TYR:CB	2.51	0.41
1:B:113:LEU:HA	1:B:113:LEU:HD12	1.74	0.41
1:A:134:ASN:ND2	1:B:273:GLN:HG2	2.17	0.41
1:C:97:SER:HB3	1:C:100:ASN:ND2	2.24	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD11	1:A:231:LYS:HG3	2.01	0.41
1:A:197:ARG:HB3	1:A:230:LEU:HD23	2.02	0.41
1:A:221:ARG:HA	1:A:333:ALA:CB	2.50	0.41
1:D:77:ILE:HA	1:D:78:PRO:HD3	1.94	0.41
1:D:194:MET:HA	1:D:197:ARG:HD3	2.01	0.41
1:D:354:LEU:HD22	1:D:354:LEU:O	2.21	0.41
1:B:357:ARG:NH1	1:B:403:GLU:OE2	2.53	0.41
1:C:194:MET:HA	1:C:197:ARG:HD3	2.02	0.41
1:C:45:ASP:OD2	1:C:48:LEU:HG	2.21	0.41
1:C:126:ILE:HG13	1:C:126:ILE:O	2.21	0.41
1:B:53:VAL:O	1:B:57:ILE:HG23	2.21	0.41
1:C:76:GLY:HA2	1:C:284:GLN:HE22	1.86	0.41
1:A:366:LYS:N	1:A:367:PRO:CD	2.83	0.41
1:B:394:ILE:HA	1:B:397:LEU:HB3	2.02	0.41
1:B:110:ALA:HB1	1:B:258:ILE:HG13	2.03	0.41
1:D:392:ILE:O	1:D:396:LYS:HG3	2.21	0.41
1:C:3:TYR:HA	1:C:6:TYR:HD1	1.86	0.41
1:C:185:GLN:OE1	1:C:188:MET:HB2	2.20	0.41
1:A:314:ILE:HD11	1:A:387:LYS:HZ2	1.86	0.41
1:C:26:ALA:HB2	1:C:355:MET:SD	2.61	0.41
1:B:343:GLU:H	1:B:343:GLU:CD	2.22	0.41
1:D:402:LYS:HA	1:D:402:LYS:HD3	1.90	0.41
1:B:221:ARG:HD2	1:B:227:ILE:CD1	2.30	0.41
1:D:360:VAL:CG2	1:D:396:LYS:HD2	2.51	0.41
1:D:78:PRO:O	1:D:82:GLU:HG3	2.21	0.41
1:C:38:SER:CB	1:C:361:VAL:HB	2.51	0.41
1:B:161:LEU:O	1:B:165:ILE:HG13	2.21	0.41
1:B:198:LYS:HE3	5:B:518:HOH:O	2.20	0.41
1:C:227:ILE:HG12	1:C:227:ILE:H	1.69	0.41
1:A:69:VAL:HG23	1:B:253:PHE:CE2	2.56	0.41
1:B:135:THR:HG21	1:B:179:TYR:CE1	2.56	0.41
1:D:132:TYR:CZ	1:D:134:ASN:HB2	2.56	0.41
1:B:132:TYR:CZ	1:B:134:ASN:HB2	2.56	0.40
1:C:267:LYS:HA	1:C:267:LYS:HD3	1.88	0.40
1:A:42:GLY:CA	1:A:335:MET:HE1	2.51	0.40
1:D:83:GLU:HG3	1:D:288:LEU:HD12	2.04	0.40
1:A:40:ALA:HB2	1:A:361:VAL:HG12	2.03	0.40
1:A:282:ILE:HD13	1:B:253:PHE:CD1	2.56	0.40
1:A:126:ILE:O	1:A:126:ILE:HD13	2.22	0.40
1:A:280:PRO:HG3	1:B:280:PRO:HG2	2.03	0.40
1:B:77:ILE:HG13	1:B:80:LEU:H	1.85	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:HG21	1:D:49:ILE:HG21	2.03	0.40
1:A:254:ARG:NH1	3:A:409:PMP:O2P	2.54	0.40
1:D:331:PRO:HG2	1:D:336:PHE:O	2.22	0.40
1:C:369:TYR:CD2	1:C:374:GLY:HA3	2.57	0.40
1:A:128:GLU:HG3	1:A:156:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/407 (99%)	387 (96%)	14 (4%)	2 (0%)	34	41
1	B	403/407 (99%)	377 (94%)	24 (6%)	2 (0%)	34	41
1	C	403/407 (99%)	380 (94%)	19 (5%)	4 (1%)	19	21
1	D	403/407 (99%)	374 (93%)	25 (6%)	4 (1%)	19	21
All	All	1612/1628 (99%)	1518 (94%)	82 (5%)	12 (1%)	26	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	VAL
1	D	33	GLY
1	D	41	ALA
1	B	32	LYS
1	B	41	ALA
1	C	31	LYS
1	C	224	GLY
1	A	364	PRO
1	A	225	GLY
1	D	234	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	303	GLY
1	C	303	GLY

### 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	321/338 (95%)	297 (92%)	24 (8%)	17	21
1	B	321/338 (95%)	291 (91%)	30 (9%)	11	13
1	C	321/338 (95%)	291 (91%)	30 (9%)	11	13
1	D	321/338 (95%)	292 (91%)	29 (9%)	12	14
All	All	1284/1352 (95%)	1171 (91%)	113 (9%)	12	14

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	56	GLU
1	A	57	ILE
1	A	75	ASN
1	A	80	LEU
1	A	111	LEU
1	A	113	LEU
1	A	114	LEU
1	A	126	ILE
1	A	137	LEU
1	A	161	LEU
1	A	168	LEU
1	A	210	LEU
1	A	233	LEU
1	A	251	THR
1	A	275	ILE
1	A	297	GLU
1	A	305	LEU
1	A	320	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	327	GLU
1	A	354	LEU
1	A	372	GLU
1	A	384	ARG
1	A	400	LEU
1	B	4	THR
1	B	5	LYS
1	B	57	ILE
1	B	69	VAL
1	B	75	ASN
1	B	80	LEU
1	B	88	LEU
1	B	111	LEU
1	B	113	LEU
1	B	114	LEU
1	B	125	VAL
1	B	137	LEU
1	B	161	LEU
1	B	168	LEU
1	B	187	PRO
1	B	210	LEU
1	B	212	ILE
1	B	227	ILE
1	B	228	VAL
1	B	233	LEU
1	B	251	THR
1	B	275	ILE
1	B	341	LEU
1	B	354	LEU
1	B	372	GLU
1	B	384	ARG
1	B	388	GLU
1	B	394	ILE
1	B	400	LEU
1	B	404	LYS
1	C	4	THR
1	C	72	THR
1	C	75	ASN
1	C	80	LEU
1	C	88	LEU
1	C	93	HIS
1	C	111	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	113	LEU
1	C	114	LEU
1	C	125	VAL
1	C	126	ILE
1	C	137	LEU
1	C	161	LEU
1	C	168	LEU
1	C	187	PRO
1	C	191	THR
1	C	210	LEU
1	C	223	GLU
1	C	233	LEU
1	C	241	VAL
1	C	251	THR
1	C	269	LEU
1	C	282	ILE
1	C	305	LEU
1	C	314	ILE
1	C	323	LEU
1	C	384	ARG
1	C	388	GLU
1	C	394	ILE
1	C	400	LEU
1	D	4	THR
1	D	56	GLU
1	D	57	ILE
1	D	70	MET
1	D	75	ASN
1	D	80	LEU
1	D	88	LEU
1	D	93	HIS
1	D	101	ILE
1	D	111	LEU
1	D	113	LEU
1	D	114	LEU
1	D	121	PRO
1	D	125	VAL
1	D	137	LEU
1	D	161	LEU
1	D	167	GLU
1	D	168	LEU
1	D	187	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	191	THR
1	D	233	LEU
1	D	269	LEU
1	D	282	ILE
1	D	327	GLU
1	D	354	LEU
1	D	384	ARG
1	D	397	LEU
1	D	400	LEU
1	D	405	PHE

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
1	A	100	ASN
1	A	134	ASN
1	A	300	HIS
1	A	321	ASN
1	A	322	HIS
1	B	12	ASN
1	B	75	ASN
1	B	93	HIS
1	B	100	ASN
1	B	273	GLN
1	B	284	GLN
1	B	300	HIS
1	C	12	ASN
1	C	75	ASN
1	C	100	ASN
1	C	134	ASN
1	C	273	GLN
1	C	300	HIS
1	C	321	ASN
1	C	352	ASN
1	D	12	ASN
1	D	75	ASN
1	D	100	ASN
1	D	134	ASN
1	D	273	GLN
1	D	284	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	300	HIS
1	D	322	HIS

### 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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
3	PMP	A	409	-	16,16,16	5.61	9 (56%)	20,23,23	1.64	4 (20%)
4	IMD	A	410	2	3,5,5	0.29	0	4,5,5	0.62	0
3	PMP	B	409	-	16,16,16	5.61	9 (56%)	20,23,23	1.65	4 (20%)
4	IMD	B	410	2	3,5,5	0.43	0	4,5,5	0.58	0
3	PMP	C	409	-	16,16,16	5.51	7 (43%)	20,23,23	1.63	3 (15%)
4	IMD	C	410	2	3,5,5	0.37	0	4,5,5	0.62	0
3	PMP	D	409	-	16,16,16	5.68	9 (56%)	20,23,23	1.87	4 (20%)
4	IMD	D	410	2	3,5,5	0.44	0	4,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	A	409	-	-	0/8/8/8	0/1/1/1
4	IMD	A	410	2	-	0/0/0/0	0/1/1/1
3	PMP	B	409	-	-	0/8/8/8	0/1/1/1
4	IMD	B	410	2	-	0/0/0/0	0/1/1/1
3	PMP	C	409	-	-	0/8/8/8	0/1/1/1
4	IMD	C	410	2	-	0/0/0/0	0/1/1/1
3	PMP	D	409	-	-	0/8/8/8	0/1/1/1
4	IMD	D	410	2	-	0/0/0/0	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	409	PMP	O4P-C5A	-8.39	1.09	1.44
3	C	409	PMP	O4P-C5A	-8.21	1.10	1.44
3	B	409	PMP	O4P-C5A	-8.11	1.10	1.44
3	A	409	PMP	O4P-C5A	-7.99	1.11	1.44
3	C	409	PMP	C6-N1	2.09	1.38	1.34
3	D	409	PMP	P-O4P	2.12	1.67	1.60
3	B	409	PMP	P-O4P	2.16	1.67	1.60
3	D	409	PMP	C6-N1	2.17	1.39	1.34
3	A	409	PMP	P-O4P	2.19	1.67	1.60
3	B	409	PMP	C6-N1	2.29	1.39	1.34
3	B	409	PMP	C3-C2	2.33	1.42	1.40
3	A	409	PMP	C6-N1	2.35	1.39	1.34
3	D	409	PMP	C3-C2	2.47	1.42	1.40
3	A	409	PMP	C3-C2	2.51	1.42	1.40
3	C	409	PMP	C3-C4	2.96	1.44	1.40
3	A	409	PMP	C3-C4	3.16	1.45	1.40
3	B	409	PMP	C3-C4	3.44	1.45	1.40
3	D	409	PMP	C3-C4	3.45	1.45	1.40
3	B	409	PMP	P-O3P	7.56	1.81	1.54
3	A	409	PMP	P-O3P	7.57	1.81	1.54
3	C	409	PMP	P-O3P	7.62	1.82	1.54
3	D	409	PMP	P-O3P	7.66	1.82	1.54
3	C	409	PMP	C5-C4	9.49	1.54	1.40
3	A	409	PMP	C5-C4	10.00	1.54	1.40
3	D	409	PMP	P-O2P	10.16	1.91	1.54
3	B	409	PMP	P-O2P	10.23	1.91	1.54
3	C	409	PMP	P-O2P	10.24	1.91	1.54
3	A	409	PMP	P-O2P	10.25	1.91	1.54
3	B	409	PMP	C5-C4	10.37	1.55	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	409	PMP	C5-C4	10.53	1.55	1.40
3	B	409	PMP	P-O1P	11.51	1.89	1.51
3	C	409	PMP	P-O1P	11.75	1.89	1.51
3	D	409	PMP	P-O1P	11.75	1.89	1.51
3	A	409	PMP	P-O1P	11.81	1.90	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	409	PMP	C5-C6-N1	-3.25	118.22	123.86
3	A	409	PMP	C5-C6-N1	-3.07	118.53	123.86
3	D	409	PMP	C5-C6-N1	-3.05	118.57	123.86
3	B	409	PMP	C5-C6-N1	-3.04	118.58	123.86
3	A	409	PMP	O3P-P-O4P	2.32	113.24	106.56
3	B	409	PMP	O3P-P-O4P	2.53	113.86	106.56
3	D	409	PMP	O4P-C5A-C5	2.80	113.63	108.99
3	C	409	PMP	C6-N1-C2	2.82	125.03	119.28
3	A	409	PMP	C6-N1-C2	2.83	125.05	119.28
3	B	409	PMP	C6-N1-C2	2.92	125.23	119.28
3	D	409	PMP	C6-N1-C2	2.93	125.25	119.28
3	B	409	PMP	O4P-P-O1P	4.06	117.47	107.14
3	A	409	PMP	O4P-P-O1P	4.30	118.09	107.14
3	C	409	PMP	O4P-P-O1P	4.34	118.19	107.14
3	D	409	PMP	O4P-P-O1P	5.15	120.25	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	PMP	2	0
3	B	409	PMP	3	0
3	C	409	PMP	1	0
3	D	409	PMP	1	0

## 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	405/407 (99%)	0.15	13 (3%) 51 60	24, 46, 75, 102	0
1	B	405/407 (99%)	0.09	6 (1%) 76 81	23, 42, 69, 100	0
1	C	405/407 (99%)	0.33	26 (6%) 23 31	26, 48, 98, 109	0
1	D	405/407 (99%)	0.34	25 (6%) 24 32	24, 49, 83, 102	0
All	All	1620/1628 (99%)	0.23	70 (4%) 39 48	23, 46, 85, 109	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	ALA	6.0
1	D	19	LEU	6.0
1	B	19	LEU	5.9
1	D	31	LYS	5.0
1	B	33	GLY	4.6
1	D	20	ALA	4.5
1	D	29	LEU	4.0
1	C	325	ASN	3.7
1	C	399	LYS	3.7
1	A	225	GLY	3.6
1	C	19	LEU	3.6
1	C	348	ILE	3.6
1	D	33	GLY	3.6
1	D	66	PRO	3.5
1	D	223	GLU	3.4
1	C	299	TYR	3.4
1	B	31	LYS	3.4
1	D	32	LYS	3.4
1	D	388	GLU	3.1
1	C	20	ALA	3.1
1	D	225	GLY	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	392	ILE	3.0
1	D	323	LEU	2.9
1	A	241	VAL	2.9
1	D	355	MET	2.9
1	D	18	ALA	2.9
1	C	34	VAL	2.9
1	C	355	MET	2.8
1	D	17	SER	2.8
1	C	323	LEU	2.7
1	C	304	ALA	2.7
1	C	343	GLU	2.7
1	C	63	GLU	2.6
1	D	299	TYR	2.6
1	C	405	PHE	2.6
1	C	224	GLY	2.5
1	C	33	GLY	2.5
1	C	296	PHE	2.5
1	A	60	GLU	2.5
1	C	357	ARG	2.4
1	D	224	GLY	2.4
1	C	326	ALA	2.3
1	C	282	ILE	2.3
1	A	19	LEU	2.3
1	C	388	GLU	2.3
1	C	249	LEU	2.3
1	A	33	GLY	2.3
1	A	31	LYS	2.3
1	A	306	LEU	2.3
1	D	393	GLY	2.2
1	B	52	ALA	2.2
1	A	163	GLU	2.2
1	A	326	ALA	2.2
1	C	380	LEU	2.2
1	D	325	ASN	2.2
1	A	224	GLY	2.2
1	B	317	LYS	2.1
1	D	361	VAL	2.1
1	C	397	LEU	2.1
1	A	226	ASP	2.1
1	C	295	TYR	2.1
1	D	222	TYR	2.1
1	C	301	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	324	PRO	2.1
1	D	22	VAL	2.1
1	C	401	TYR	2.1
1	D	1	MET	2.1
1	A	64	LYS	2.1
1	A	34	VAL	2.1
1	D	216	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PMP	A	409	16/16	0.93	0.24	3.84	48,59,61,66	0
3	PMP	B	409	16/16	0.94	0.23	2.05	41,54,57,61	0
4	IMD	D	410	5/5	0.99	0.17	1.93	51,51,52,53	0
3	PMP	C	409	16/16	0.92	0.24	1.85	57,62,63,63	0
3	PMP	D	409	16/16	0.90	0.23	1.59	56,61,62,63	0
4	IMD	A	410	5/5	0.94	0.14	0.59	44,44,44,45	0
4	IMD	C	410	5/5	0.96	0.11	0.30	52,52,52,53	0
4	IMD	B	410	5/5	0.99	0.10	0.05	44,45,46,46	0
2	ZN	C	408	1/1	0.98	0.07	-	42,42,42,42	0
2	ZN	B	408	1/1	0.99	0.09	-	38,38,38,38	0
2	ZN	D	408	1/1	0.99	0.08	-	45,45,45,45	0
2	ZN	A	408	1/1	0.96	0.11	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.