



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:05 AM GMT

PDB ID : 3KRP  
Title : Mint heterotetrameric geranyl pyrophosphate synthase in complex with magnesium and GPP  
Authors : Chang, T.-H.; Hsieh, F.-L.; Ko, T.-P.; Wang, A.H.-J.  
Deposited on : 2009-11-19  
Resolution : 2.42 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

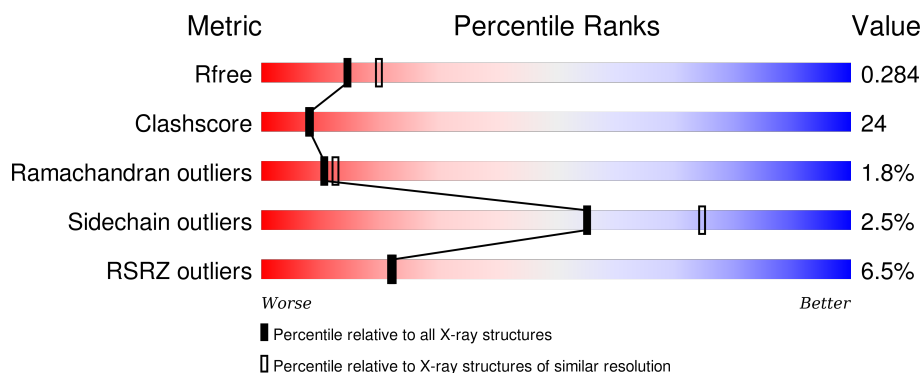
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	295	<div> <div>2%</div> <div>61% 32% 5%</div> </div>
1	D	295	<div> <div>8%</div> <div>53% 42% . .</div> </div>
2	B	274	<div> <div>9%</div> <div>53% 40% . 7%</div> </div>
2	C	274	<div> <div>6%</div> <div>55% 35% . 5%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9010 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 Geranyl diphosphate synthase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2120	1338	372	392	18			
1	D	284	Total	C	N	O	S	0	0	0
			2155	1359	378	400	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9SBR3
D	1	MET	-	EXPRESSION TAG	UNP Q9SBR3

- Molecule 2 is a protein called Geranyl diphosphate synthase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1929	1216	334	365	14			
2	C	259	Total	C	N	O	S	0	0	0
			1954	1233	339	368	14			

There are 18 discrepancies between the modelled and reference sequences:

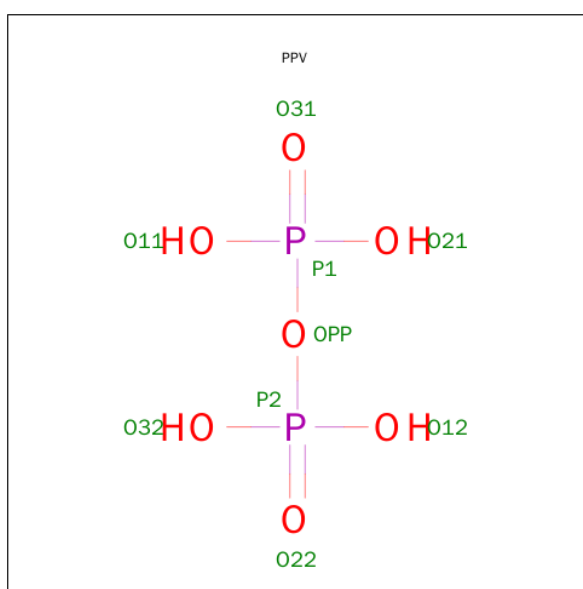
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP Q9SBR4
B	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	1	MET	-	EXPRESSION TAG	UNP Q9SBR4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4

- Molecule 3 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $\text{H}_4\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

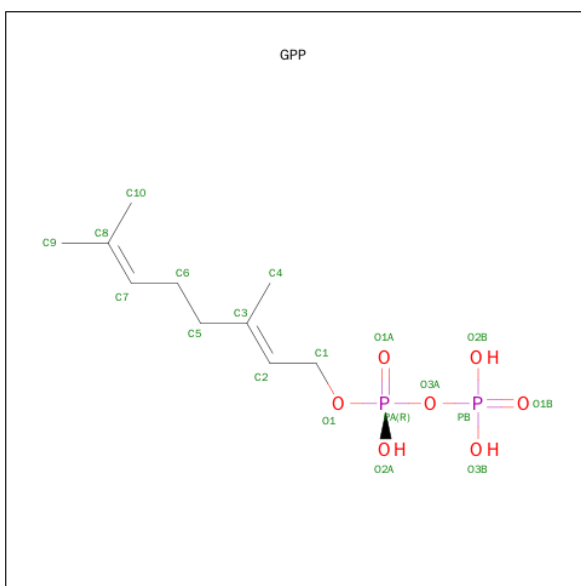
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

- Molecule 6 is GERANYL DIPHOSPHATE (three-letter code: GPP) (formula:  $C_{10}H_{20}O_7P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	O	P	0	0
			19	10	7	2		

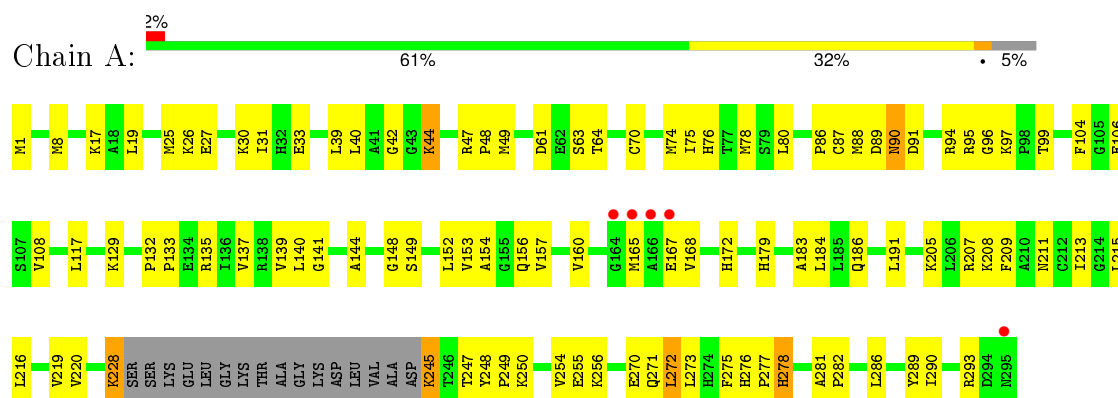
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	224	Total 224	O 224	0	0
7	B	177	Total 177	O 177	0	0
7	C	221	Total 221	O 221	0	0
7	D	194	Total 194	O 194	0	0

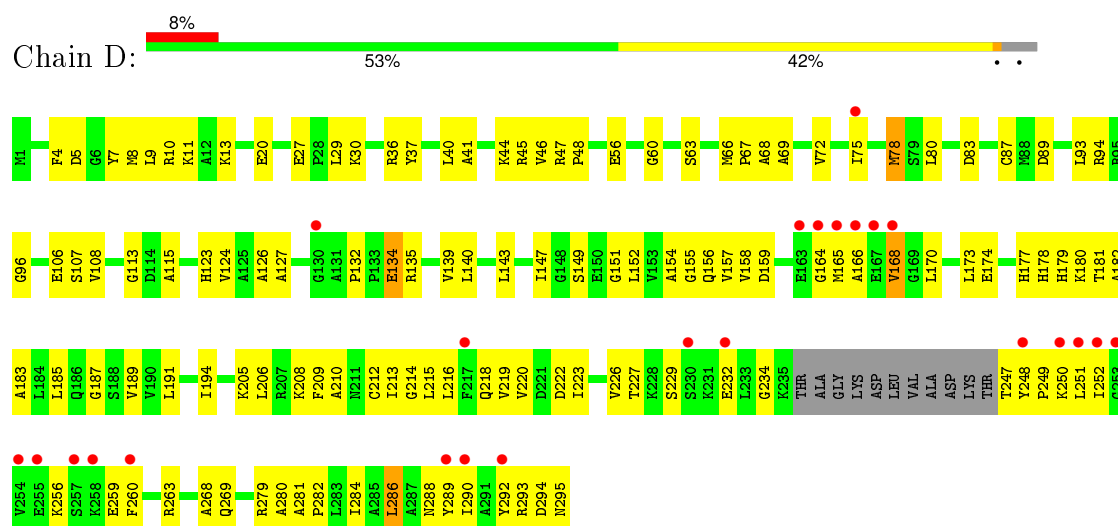
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

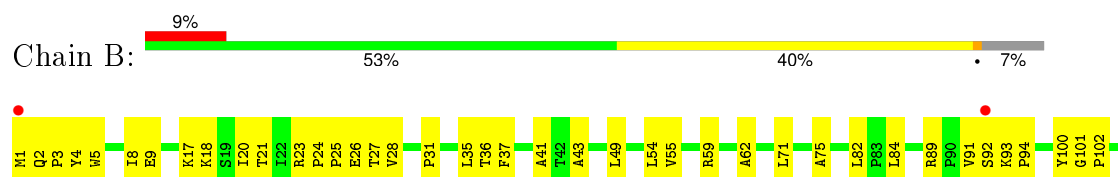
#### • Molecule 1: Geranyl diphosphate synthase large subunit

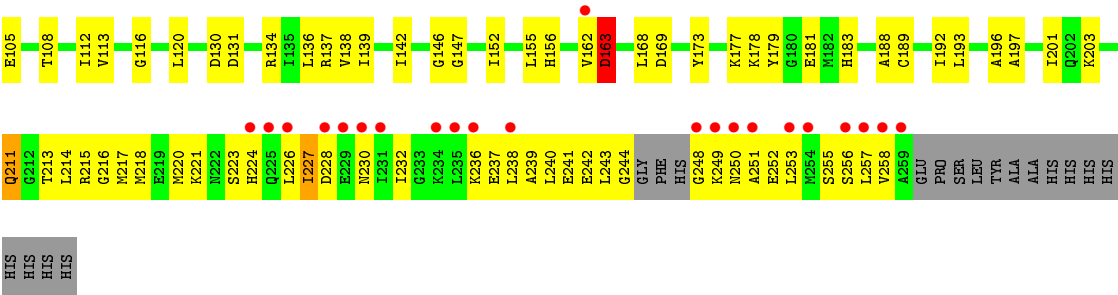


#### • Molecule 1: Geranyl diphosphate synthase large subunit

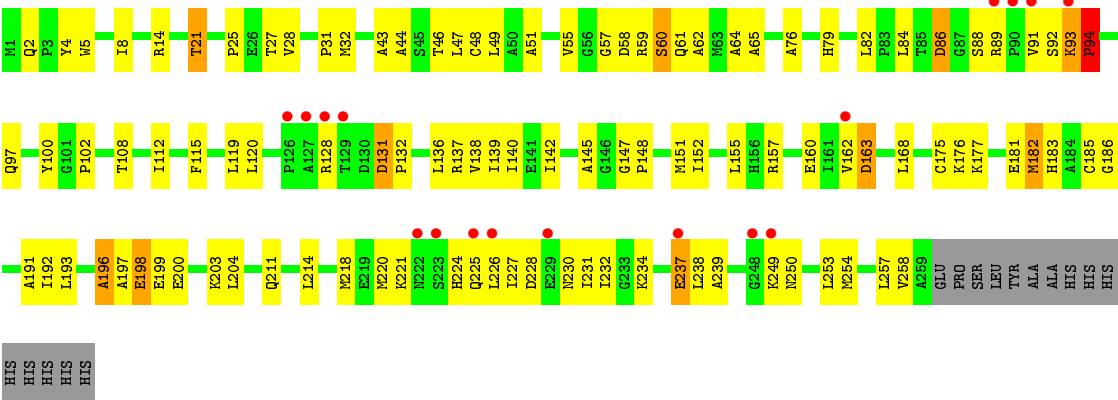


#### • Molecule 2: Geranyl diphosphate synthase small subunit





● Molecule 2: Geranyl diphosphate synthase small subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.26Å 109.02Å 182.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.42 29.62 – 2.24	Depositor EDS
% Data completeness (in resolution range)	85.9 (30.00-2.42) 83.1 (29.62-2.24)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.284 0.224 , 0.284	Depositor DCC
$R_{free}$ test set	1790 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	1.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.7	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 43365 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: MG, GPP, EDO, PPV

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	0.40	0/2155	0.59	0/2903
1	D	0.37	0/2190	0.59	0/2948
2	B	0.35	0/1965	0.57	0/2656
2	C	0.37	0/1993	0.57	0/2695
All	All	0.38	0/8303	0.58	0/11202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2120	0	2146	81	0
1	D	2155	0	2182	130	0
2	B	1929	0	1928	117	0
2	C	1954	0	1948	93	0
3	A	9	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	C	4	0	6	1	0
6	D	19	0	17	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	224	0	0	13	0
7	B	177	0	0	16	0
7	C	221	0	0	11	0
7	D	194	0	0	13	0
All	All	9010	0	8227	401	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 24.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ARG:HB2	2:B:24:PRO:HD2	1.37	1.06
2:B:249:LYS:HE2	2:B:253:LEU:HD13	1.46	0.98
2:B:8:ILE:HG12	2:B:59:ARG:HH12	1.28	0.97
2:C:163:ASP:HA	7:C:702:HOH:O	1.65	0.95
1:A:168:VAL:HG13	1:A:172:HIS:HB3	1.48	0.94
2:B:249:LYS:HD3	2:B:253:LEU:HB2	1.49	0.93
2:C:221:LYS:HD3	2:C:227:ILE:HG22	1.50	0.90
2:C:43:ALA:O	2:C:47:LEU:HB2	1.70	0.90
2:C:14:ARG:HG2	7:C:535:HOH:O	1.73	0.88
1:A:139:VAL:HG13	1:A:191:LEU:HD22	1.57	0.85
2:B:248:GLY:N	2:B:251:ALA:HB3	1.91	0.84
1:D:260:PHE:HD1	1:D:263:ARG:HH21	1.25	0.84
2:B:55:VAL:HG11	2:B:196:ALA:HB2	1.60	0.82
2:C:8:ILE:HG23	2:C:49:LEU:HD12	1.63	0.81
2:C:28:VAL:HG22	1:D:157:VAL:CG2	2.11	0.81
2:B:2:GLN:HB2	2:B:3:PRO:HD3	1.63	0.80
1:A:289:TYR:O	1:A:293:ARG:HG2	1.82	0.79
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.46	0.79
1:A:277:PRO:HD2	1:A:278:HIS:CE1	2.17	0.78
1:D:10:ARG:HD2	7:D:394:HOH:O	1.84	0.78
1:D:139:VAL:HG13	1:D:191:LEU:HD22	1.64	0.77
1:A:76:HIS:CE1	1:A:80:LEU:HD11	2.20	0.77
2:C:214:LEU:O	2:C:218:MET:HG2	1.86	0.76
1:D:9:LEU:O	1:D:13:LYS:HD3	1.86	0.75
2:C:199:GLU:O	2:C:203:LYS:HG2	1.87	0.74
1:A:256:LYS:HE2	7:A:378:HOH:O	1.87	0.73
1:D:216:LEU:O	1:D:220:VAL:HG23	1.88	0.73
2:B:2:GLN:HB2	2:B:3:PRO:CD	2.19	0.72
1:A:183:ALA:HB3	7:A:341:HOH:O	1.89	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:GLN:NE2	7:C:773:HOH:O	2.22	0.71
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.73	0.71
1:A:1:MET:N	7:A:352:HOH:O	2.23	0.71
2:B:138:VAL:O	2:B:142:ILE:HG13	1.91	0.71
2:B:249:LYS:O	2:B:253:LEU:N	2.24	0.70
2:C:137:ARG:HD3	2:C:192:ILE:HD13	1.72	0.70
2:B:28:VAL:O	2:B:31:PRO:HD2	1.91	0.70
2:C:230:ASN:O	2:C:234:LYS:HG3	1.92	0.70
1:A:165:MET:HE1	7:A:757:HOH:O	1.91	0.70
2:C:182:MET:HE3	2:C:182:MET:HA	1.73	0.70
2:B:221:LYS:HG3	2:B:227:ILE:HG21	1.72	0.70
2:C:221:LYS:HD3	2:C:227:ILE:CG2	2.20	0.69
1:A:256:LYS:HE3	7:A:379:HOH:O	1.91	0.69
2:B:248:GLY:O	2:B:252:GLU:HB2	1.91	0.69
1:A:286:LEU:O	1:A:290:ILE:HG13	1.93	0.69
2:B:23:ARG:HB2	2:B:24:PRO:CD	2.19	0.69
2:B:137:ARG:HD3	2:B:192:ILE:HD13	1.75	0.69
2:B:253:LEU:HD12	2:B:256:SER:OG	1.93	0.68
1:D:20:GLU:HA	1:D:40:LEU:HD11	1.75	0.68
2:B:1:MET:HG3	2:B:2:GLN:H	1.57	0.68
1:D:135:ARG:NH1	7:D:368:HOH:O	2.27	0.68
2:B:25:PRO:HB2	2:B:27:THR:HG22	1.76	0.68
2:C:62:ALA:HA	2:C:193:LEU:HD13	1.74	0.67
1:A:19:LEU:HD22	1:A:39:LEU:HD21	1.75	0.67
1:D:168:VAL:HG23	1:D:251:LEU:HD21	1.75	0.67
1:A:64:THR:HG23	1:A:129:LYS:O	1.94	0.67
1:A:149:SER:HB2	7:A:493:HOH:O	1.92	0.67
1:D:252:ILE:O	1:D:256:LYS:HB2	1.94	0.67
2:B:227:ILE:O	2:B:227:ILE:HG13	1.93	0.67
2:B:220:MET:HB3	2:B:224:HIS:HE1	1.59	0.67
2:B:8:ILE:HG12	2:B:59:ARG:NH1	2.06	0.67
2:C:58:ASP:OD1	2:C:61:GLN:HG3	1.95	0.66
2:B:168:LEU:HD21	2:B:226:LEU:HB2	1.77	0.66
2:C:86:ASP:OD2	1:D:106:GLU:HG3	1.96	0.66
1:D:260:PHE:HD1	1:D:263:ARG:NH2	1.93	0.66
2:B:177:LYS:O	7:B:508:HOH:O	2.13	0.66
1:D:208:LYS:HD2	7:D:694:HOH:O	1.95	0.66
2:B:249:LYS:CD	2:B:253:LEU:HB2	2.23	0.65
1:D:170:LEU:O	1:D:174:GLU:HB2	1.96	0.65
1:A:96:GLY:C	1:A:97:LYS:HD2	2.15	0.65
1:D:80:LEU:HD23	6:D:900:GPP:H92	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HG2	7:A:546:HOH:O	1.96	0.65
1:A:90:ASN:O	7:A:412:HOH:O	2.13	0.65
2:B:43:ALA:HB3	2:B:183:HIS:HE1	1.62	0.65
2:B:43:ALA:HB3	2:B:183:HIS:CE1	2.32	0.64
1:D:151:GLY:O	1:D:179:HIS:HB3	1.97	0.64
2:B:188:ALA:O	2:B:192:ILE:HG13	1.97	0.64
2:B:92:SER:C	2:B:94:PRO:HD2	2.18	0.64
1:A:245:LYS:O	1:A:245:LYS:HD2	1.97	0.64
1:D:208:LYS:HE2	7:D:529:HOH:O	1.96	0.64
1:A:276:HIS:HB3	1:A:278:HIS:ND1	2.12	0.64
1:D:251:LEU:HG	7:D:665:HOH:O	1.96	0.64
2:B:177:LYS:NZ	2:B:181:GLU:OE2	2.32	0.63
1:A:153:VAL:O	1:A:157:VAL:HG23	1.97	0.63
2:B:214:LEU:O	2:B:218:MET:HG2	1.98	0.63
2:C:214:LEU:HD21	2:C:232:ILE:HG23	1.81	0.63
2:B:236:LYS:O	2:B:240:LEU:HG	1.97	0.63
1:A:149:SER:CB	7:A:493:HOH:O	2.47	0.63
2:C:175:CYS:SG	2:C:220:MET:HG3	2.38	0.63
2:C:191:ALA:HB2	2:C:204:LEU:HD12	1.80	0.63
2:C:64:ALA:HB3	7:C:350:HOH:O	1.98	0.62
2:B:136:LEU:O	2:B:136:LEU:HD12	1.99	0.62
2:B:71:LEU:HD22	2:B:112:ILE:HG23	1.82	0.62
2:C:136:LEU:O	2:C:140:ILE:HG13	2.00	0.62
2:B:1:MET:HG3	2:B:2:GLN:N	2.14	0.62
2:C:28:VAL:HG22	1:D:157:VAL:HG21	1.82	0.62
1:D:187:GLY:O	1:D:191:LEU:HG	1.99	0.62
1:A:30:LYS:HE2	1:A:108:VAL:HG21	1.81	0.62
2:C:51:ALA:HA	2:C:254:MET:HE3	1.82	0.62
1:D:132:PRO:HB2	1:D:134:GLU:OE2	2.00	0.61
1:D:220:VAL:HG22	7:D:576:HOH:O	2.01	0.61
1:A:86:PRO:HG2	1:A:106:GLU:OE2	2.01	0.61
1:D:139:VAL:CG1	1:D:191:LEU:HD22	2.31	0.61
1:D:93:LEU:HG	1:D:234:GLY:O	2.00	0.61
2:C:65:ALA:HA	2:C:120:LEU:HD21	1.83	0.60
2:C:25:PRO:HB2	2:C:27:THR:HG22	1.83	0.60
2:C:227:ILE:O	2:C:227:ILE:HG23	2.01	0.60
1:D:93:LEU:HD11	1:D:96:GLY:HA2	1.83	0.60
1:A:270:GLU:HA	1:A:273:LEU:HG	1.84	0.60
1:A:76:HIS:NE2	1:A:80:LEU:HD11	2.17	0.60
1:A:61:ASP:OD2	1:A:63:SER:HB3	2.03	0.59
2:B:179:TYR:OH	7:B:306:HOH:O	2.16	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LYS:HE2	1:D:108:VAL:HG21	1.84	0.59
1:D:7:TYR:HA	1:D:10:ARG:HH11	1.67	0.59
2:B:221:LYS:HG3	2:B:227:ILE:CG2	2.32	0.59
2:C:237:GLU:O	2:C:239:ALA:N	2.36	0.59
2:B:31:PRO:HA	2:B:100:TYR:CE2	2.38	0.58
2:C:162:VAL:HG12	2:C:163:ASP:OD1	2.04	0.58
1:D:20:GLU:HA	1:D:40:LEU:CD1	2.33	0.58
1:D:256:LYS:HA	1:D:259:GLU:CD	2.24	0.58
2:C:181:GLU:HA	2:C:181:GLU:OE2	2.04	0.58
2:B:240:LEU:HD21	2:B:258:VAL:HG21	1.86	0.58
2:B:257:LEU:HD21	7:B:505:HOH:O	2.03	0.58
1:D:177:HIS:ND1	1:D:218:GLN:HG2	2.19	0.57
1:A:228:LYS:NZ	1:A:228:LYS:HB2	2.19	0.57
2:C:92:SER:C	2:C:94:PRO:HD2	2.25	0.57
2:C:93:LYS:N	2:C:94:PRO:HD2	2.20	0.57
2:B:147:GLY:HA3	7:B:296:HOH:O	2.04	0.57
2:C:79:HIS:HA	2:C:82:LEU:HG	1.87	0.57
1:D:83:ASP:O	1:D:89:ASP:HB2	2.05	0.57
2:B:137:ARG:NH1	7:B:499:HOH:O	2.37	0.57
2:B:23:ARG:CB	2:B:24:PRO:HD2	2.24	0.56
2:B:213:THR:O	2:B:217:MET:HB2	2.05	0.56
1:D:222:ASP:HB3	1:D:249:PRO:HD2	1.87	0.56
1:D:208:LYS:HG2	7:D:529:HOH:O	2.05	0.56
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.87	0.56
2:B:120:LEU:HD11	2:B:142:ILE:HD12	1.87	0.56
1:A:88:MET:HE3	1:A:160:VAL:HG21	1.87	0.56
2:C:58:ASP:HB2	7:C:634:HOH:O	2.05	0.56
2:B:54:LEU:HB2	2:B:250:ASN:OD1	2.05	0.56
1:A:133:PRO:O	1:A:137:VAL:HG23	2.05	0.56
1:D:180:LYS:HG2	6:D:900:GPP:H62	1.86	0.56
2:C:102:PRO:HB2	1:D:87:CYS:HB2	1.87	0.56
2:B:55:VAL:CG1	2:B:196:ALA:HB2	2.33	0.56
1:D:252:ILE:O	1:D:256:LYS:HE3	2.06	0.56
1:D:7:TYR:HA	1:D:10:ARG:NH1	2.21	0.55
1:D:263:ARG:HB2	1:D:263:ARG:NH1	2.21	0.55
2:B:214:LEU:HD23	2:B:258:VAL:HG12	1.88	0.55
2:B:9:GLU:OE1	7:B:503:HOH:O	2.18	0.55
2:C:43:ALA:HB3	2:C:183:HIS:HE1	1.72	0.55
2:B:220:MET:HB3	2:B:224:HIS:CE1	2.40	0.55
2:B:168:LEU:HD21	2:B:226:LEU:CB	2.37	0.55
1:A:205:LYS:HD3	1:A:271:GLN:O	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:221:LYS:HD2	2:C:225:GLN:HA	1.89	0.55
2:C:4:TYR:CE2	2:C:8:ILE:HD11	2.42	0.55
1:A:75:ILE:O	1:A:78:MET:HG3	2.07	0.55
1:D:289:TYR:O	1:D:293:ARG:HB3	2.07	0.55
2:C:44:ALA:CB	2:C:183:HIS:HA	2.37	0.55
1:A:95:ARG:HG2	1:A:95:ARG:NH1	2.22	0.54
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.89	0.54
1:A:87:CYS:HB2	2:B:102:PRO:HB2	1.89	0.54
2:B:137:ARG:HD2	7:B:499:HOH:O	2.07	0.54
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.73	0.54
1:D:294:ASP:O	1:D:295:ASN:HB3	2.07	0.54
1:D:229:SER:OG	1:D:232:GLU:HG3	2.08	0.53
1:D:280:ALA:O	1:D:284:ILE:HG13	2.08	0.53
1:D:37:TYR:O	1:D:41:ALA:HB2	2.08	0.53
1:A:140:LEU:HD13	2:B:139:ILE:HD13	1.91	0.53
2:B:93:LYS:N	2:B:94:PRO:HD2	2.22	0.53
2:C:92:SER:CB	2:C:94:PRO:HD2	2.38	0.53
1:A:31:ILE:HD11	2:B:156:HIS:CD2	2.43	0.53
2:C:108:THR:O	2:C:112:ILE:HG12	2.08	0.53
1:D:177:HIS:ND1	1:D:218:GLN:CG	2.72	0.53
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.91	0.53
1:D:149:SER:O	1:D:154:ALA:HB2	2.08	0.53
2:B:91:VAL:O	2:B:91:VAL:HG23	2.09	0.53
1:D:123:HIS:O	1:D:127:ALA:HB3	2.09	0.53
2:B:155:LEU:HD23	2:B:178:LYS:HE3	1.91	0.53
1:D:223:ILE:O	1:D:227:THR:HG23	2.10	0.52
1:D:66:MET:HB3	1:D:67:PRO:HD3	1.92	0.52
2:C:84:LEU:HD12	2:C:89:ARG:HG2	1.92	0.52
1:D:135:ARG:HG3	1:D:135:ARG:NH1	2.21	0.52
1:A:186:GLN:NE2	1:A:211:ASN:OD1	2.42	0.52
1:D:75:ILE:HD13	1:D:147:ILE:HD13	1.90	0.52
2:B:41:ALA:HB1	7:B:300:HOH:O	2.10	0.52
2:C:214:LEU:HD13	2:C:214:LEU:C	2.30	0.52
2:B:62:ALA:HA	2:B:193:LEU:HD13	1.91	0.52
2:B:258:VAL:HG22	7:B:616:HOH:O	2.11	0.51
1:A:94:ARG:HG2	1:A:95:ARG:HG3	1.93	0.51
2:C:157:ARG:O	2:C:160:GLU:HB2	2.10	0.51
1:D:178:HIS:O	1:D:182:ALA:HB3	2.11	0.51
2:C:43:ALA:HB3	2:C:183:HIS:CE1	2.46	0.51
1:A:89:ASP:OD1	7:A:733:HOH:O	2.18	0.51
2:C:8:ILE:CG2	2:C:49:LEU:HD12	2.37	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:GLU:HA	1:D:60:GLY:O	2.11	0.50
1:D:215:LEU:O	1:D:219:VAL:HG23	2.10	0.50
1:D:222:ASP:CG	1:D:247:THR:HB	2.30	0.50
1:D:279:ARG:O	1:D:282:PRO:HD2	2.10	0.50
2:B:17:LYS:HG3	2:B:37:PHE:CE2	2.46	0.50
2:B:4:TYR:O	2:B:8:ILE:HG13	2.11	0.50
2:B:249:LYS:HD2	2:B:253:LEU:HD22	1.93	0.50
2:C:51:ALA:HA	2:C:254:MET:CE	2.41	0.50
1:D:93:LEU:HD11	1:D:96:GLY:CA	2.41	0.50
2:B:5:TRP:HZ2	2:B:253:LEU:HG	1.77	0.50
2:B:146:GLY:O	2:B:152:ILE:HG12	2.11	0.50
2:C:177:LYS:HA	2:C:181:GLU:HG2	1.93	0.50
2:C:88:SER:OG	1:D:107:SER:HB3	2.12	0.50
1:D:250:LYS:HD3	7:D:665:HOH:O	2.10	0.49
1:D:183:ALA:HB3	7:D:313:HOH:O	2.12	0.49
2:B:242:GLU:O	2:B:243:LEU:HD23	2.12	0.49
1:A:148:GLY:O	1:A:153:VAL:HB	2.12	0.49
2:B:75:ALA:CB	2:B:113:VAL:HG23	2.42	0.49
2:C:211:GLN:HG2	2:C:258:VAL:HG12	1.95	0.49
1:D:248:TYR:HB2	1:D:249:PRO:HD3	1.95	0.49
2:B:162:VAL:O	2:B:162:VAL:HG12	2.13	0.49
1:A:209:PHE:CE1	1:A:272:LEU:HD11	2.48	0.49
2:C:221:LYS:CD	2:C:227:ILE:HG22	2.33	0.49
1:D:212:CYS:C	1:D:214:GLY:H	2.14	0.49
1:D:288:ASN:O	1:D:292:TYR:HD1	1.96	0.49
2:B:221:LYS:HD3	2:B:227:ILE:HB	1.95	0.49
2:B:239:ALA:O	2:B:242:GLU:HB2	2.13	0.49
1:D:69:ALA:O	1:D:72:VAL:HG22	2.12	0.49
2:B:101:GLY:O	2:B:105:GLU:HG3	2.13	0.48
2:B:179:TYR:CD1	2:B:216:GLY:HA3	2.48	0.48
1:A:8:MET:SD	1:A:49:MET:HG3	2.53	0.48
2:C:59:ARG:HG3	2:C:60:SER:N	2.28	0.48
2:C:8:ILE:HG22	2:C:46:THR:HG22	1.95	0.48
2:C:93:LYS:N	2:C:94:PRO:CD	2.76	0.48
1:A:148:GLY:HA3	7:B:335:HOH:O	2.11	0.48
2:B:230:ASN:HB3	7:B:279:HOH:O	2.13	0.48
1:A:208:LYS:HE3	1:A:271:GLN:CD	2.34	0.48
2:B:21:THR:HG22	2:B:21:THR:O	2.13	0.48
2:B:71:LEU:HD12	2:B:116:GLY:HA2	1.95	0.48
1:D:288:ASN:ND2	7:D:310:HOH:O	2.47	0.48
1:A:152:LEU:HA	1:A:179:HIS:O	2.12	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:LYS:HE3	7:C:286:HOH:O	2.12	0.48
2:C:55:VAL:HG21	2:C:196:ALA:HB2	1.95	0.48
1:A:247:THR:HG21	7:A:736:HOH:O	2.13	0.48
1:D:47:ARG:HG2	1:D:185:LEU:HD23	1.95	0.48
7:C:291:HOH:O	1:D:149:SER:HB2	2.12	0.48
1:A:70:CYS:O	1:A:74:MET:HG3	2.13	0.48
2:B:253:LEU:C	2:B:255:SER:N	2.67	0.47
2:C:197:ALA:O	2:C:198:GLU:C	2.52	0.47
1:A:168:VAL:CG1	1:A:172:HIS:HB3	2.33	0.47
2:C:168:LEU:HD13	2:C:231:ILE:HG13	1.95	0.47
2:B:20:ILE:HD12	2:B:36:THR:HG21	1.95	0.47
1:D:78:MET:HE3	1:D:113:GLY:O	2.14	0.47
1:D:4:PHE:HB2	1:D:8:MET:HE1	1.96	0.47
1:A:19:LEU:HB3	1:A:40:LEU:HD21	1.96	0.47
2:C:249:LYS:O	2:C:253:LEU:HG	2.15	0.47
2:B:173:TYR:CE2	1:D:29:LEU:HD21	2.49	0.47
2:C:228:ASP:OD1	2:C:230:ASN:HB2	2.15	0.47
2:B:228:ASP:OD2	2:B:230:ASN:HB2	2.15	0.47
2:B:258:VAL:HG13	7:B:616:HOH:O	2.14	0.47
2:B:203:LYS:HD2	2:B:244:GLY:H	1.79	0.47
2:C:139:ILE:HG21	1:D:140:LEU:HD13	1.96	0.47
1:D:164:GLY:O	1:D:166:ALA:N	2.48	0.47
1:A:89:ASP:HB3	1:A:91:ASP:OD1	2.14	0.47
2:B:248:GLY:N	7:B:714:HOH:O	2.48	0.47
2:C:48:CYS:HA	2:C:186:GLY:O	2.15	0.47
2:C:131:ASP:N	2:C:132:PRO:HD2	2.30	0.47
2:B:1:MET:CG	2:B:2:GLN:N	2.77	0.47
2:C:128:ARG:HB3	2:C:128:ARG:NH1	2.30	0.47
1:D:4:PHE:HB2	1:D:8:MET:CE	2.45	0.46
1:D:222:ASP:OD2	1:D:247:THR:HB	2.15	0.46
1:D:27:GLU:HB2	7:D:578:HOH:O	2.14	0.46
2:B:197:ALA:O	2:B:201:ILE:HG13	2.14	0.46
2:B:216:GLY:O	2:B:220:MET:HG2	2.15	0.46
2:B:226:LEU:O	2:B:228:ASP:N	2.47	0.46
1:D:181:THR:HG21	1:D:218:GLN:HB2	1.97	0.46
2:B:1:MET:O	2:B:5:TRP:CD1	2.68	0.46
2:C:46:THR:HG23	5:C:902:EDO:O2	2.16	0.46
1:D:93:LEU:HD12	1:D:94:ARG:H	1.81	0.46
1:D:214:GLY:C	1:D:216:LEU:N	2.68	0.46
1:A:19:LEU:HD22	1:A:39:LEU:CD2	2.45	0.46
2:C:93:LYS:O	2:C:94:PRO:C	2.54	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ILE:HA	1:D:226:VAL:HG12	1.97	0.46
2:C:32:MET:HA	2:C:108:THR:CG2	2.46	0.46
1:D:286:LEU:O	1:D:290:ILE:HG13	2.15	0.46
1:D:157:VAL:HG23	1:D:158:VAL:N	2.31	0.46
1:A:25:MET:O	1:A:26:LYS:HB3	2.16	0.46
2:C:151:MET:O	2:C:155:LEU:HG	2.16	0.46
2:C:28:VAL:HG22	1:D:157:VAL:HG23	1.93	0.46
1:A:186:GLN:HG3	1:A:207:ARG:HG3	1.96	0.46
2:C:115:PHE:CE1	2:C:119:LEU:HD11	2.51	0.45
2:C:199:GLU:HG3	2:C:200:GLU:N	2.31	0.45
1:D:134:GLU:CD	1:D:134:GLU:H	2.19	0.45
1:D:5:ASP:O	1:D:9:LEU:HB2	2.15	0.45
2:B:257:LEU:HD11	7:B:505:HOH:O	2.16	0.45
1:A:97:LYS:N	1:A:97:LYS:HD2	2.31	0.45
1:A:167:GLU:CG	7:A:546:HOH:O	2.60	0.45
1:A:27:GLU:OE1	2:C:157:ARG:NH2	2.50	0.45
2:B:20:ILE:CD1	2:B:36:THR:HG21	2.47	0.45
2:B:253:LEU:HD12	2:B:256:SER:HG	1.81	0.45
2:B:1:MET:HG3	2:B:2:GLN:HG2	1.98	0.45
1:D:212:CYS:C	1:D:214:GLY:N	2.70	0.45
2:B:162:VAL:O	2:B:163:ASP:HB2	2.17	0.45
2:B:130:ASP:O	2:B:134:ARG:HG3	2.17	0.45
1:D:178:HIS:HE1	7:D:362:HOH:O	1.99	0.45
2:C:21:THR:HG22	7:C:766:HOH:O	2.17	0.45
1:D:135:ARG:O	1:D:139:VAL:HG23	2.17	0.44
2:B:137:ARG:HD3	2:B:192:ILE:HG21	1.98	0.44
1:D:222:ASP:HB3	1:D:249:PRO:CD	2.47	0.44
1:A:132:PRO:O	1:A:135:ARG:N	2.46	0.44
2:B:4:TYR:CE2	2:B:8:ILE:HD11	2.52	0.44
1:D:263:ARG:HH11	1:D:263:ARG:HB2	1.82	0.44
1:D:7:TYR:O	1:D:11:LYS:HG2	2.18	0.44
2:B:237:GLU:HG2	2:B:241:GLU:OE2	2.16	0.44
1:A:149:SER:C	1:A:154:ALA:HB2	2.37	0.44
1:A:132:PRO:HG2	1:A:135:ARG:HB2	1.99	0.44
2:C:25:PRO:HG2	2:C:28:VAL:CG2	2.48	0.44
1:D:135:ARG:CG	1:D:135:ARG:HH11	2.20	0.44
2:C:44:ALA:HB2	2:C:183:HIS:CD2	2.52	0.44
1:D:135:ARG:NH1	1:D:135:ARG:CG	2.81	0.44
2:C:86:ASP:OD2	1:D:106:GLU:CG	2.63	0.44
2:C:31:PRO:HG3	2:C:100:TYR:CE1	2.53	0.43
1:D:212:CYS:HB3	1:D:268:ALA:HB2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:GLN:HE22	1:D:288:ASN:HD21	1.64	0.43
2:C:5:TRP:CZ2	2:C:257:LEU:HB2	2.53	0.43
1:D:205:LYS:NZ	7:D:365:HOH:O	2.50	0.43
2:B:211:GLN:CD	2:B:257:LEU:HD23	2.39	0.43
2:B:203:LYS:HE3	2:B:243:LEU:HA	2.00	0.43
1:A:33:GLU:HG2	1:A:104:PHE:CE2	2.53	0.43
1:A:44:LYS:NZ	1:A:44:LYS:HB2	2.33	0.43
1:A:213:ILE:HA	1:A:216:LEU:HB3	2.00	0.43
1:A:245:LYS:HD3	1:A:250:LYS:NZ	2.33	0.43
2:B:8:ILE:HG23	2:B:49:LEU:HD12	1.99	0.43
1:A:88:MET:CE	1:A:160:VAL:HG21	2.48	0.43
1:A:78:MET:HE3	1:A:117:LEU:HB2	1.99	0.43
2:B:93:LYS:N	2:B:94:PRO:CD	2.82	0.43
2:C:59:ARG:HG2	7:C:635:HOH:O	2.19	0.43
1:A:27:GLU:HG3	1:D:27:GLU:HB3	2.01	0.43
1:A:219:VAL:HG22	1:A:248:TYR:CE2	2.53	0.43
1:A:276:HIS:HA	1:A:277:PRO:HD3	1.91	0.43
1:D:222:ASP:O	1:D:226:VAL:HG12	2.18	0.43
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.93	0.43
1:D:209:PHE:CZ	1:D:213:ILE:HD13	2.54	0.43
1:D:168:VAL:O	1:D:168:VAL:HG23	2.19	0.42
1:A:247:THR:HB	1:A:249:PRO:HD2	2.00	0.42
2:B:18:LYS:O	2:B:18:LYS:HG2	2.19	0.42
1:D:189:VAL:HG21	1:D:210:ALA:HB2	2.00	0.42
1:A:96:GLY:N	7:A:730:HOH:O	2.38	0.42
2:B:82:LEU:HD21	2:B:105:GLU:HB2	2.01	0.42
1:D:256:LYS:HA	1:D:259:GLU:OE1	2.20	0.42
1:A:272:LEU:HA	1:A:275:PHE:CE1	2.54	0.42
1:A:216:LEU:O	1:A:220:VAL:HG23	2.20	0.42
1:D:179:HIS:HA	1:D:183:ALA:HB2	2.02	0.42
1:D:214:GLY:C	1:D:216:LEU:H	2.21	0.42
2:B:137:ARG:CD	2:B:192:ILE:HD13	2.47	0.42
1:D:248:TYR:C	1:D:250:LYS:H	2.23	0.42
1:A:47:ARG:HE	1:A:184:LEU:HD23	1.85	0.42
2:C:88:SER:CB	1:D:107:SER:H	2.33	0.42
1:D:152:LEU:C	1:D:152:LEU:HD23	2.40	0.42
2:B:35:LEU:HD12	2:B:108:THR:HG21	2.02	0.42
2:C:148:PRO:HA	2:C:152:ILE:HB	2.01	0.42
2:C:28:VAL:O	2:C:31:PRO:HD2	2.20	0.42
1:A:156:GLN:O	1:A:156:GLN:HG3	2.20	0.42
1:A:254:VAL:O	1:A:255:GLU:C	2.58	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:VAL:HG13	1:D:226:VAL:O	2.18	0.41
1:D:45:ARG:HB3	1:D:48:PRO:HG2	2.01	0.41
2:B:2:GLN:H	2:B:2:GLN:HG2	1.67	0.41
2:C:182:MET:O	2:C:185:CYS:HB3	2.20	0.41
2:B:25:PRO:C	2:B:27:THR:H	2.24	0.41
1:A:141:GLY:O	1:A:144:ALA:HB3	2.20	0.41
2:B:169:ASP:CG	1:D:36:ARG:HE	2.23	0.41
1:D:135:ARG:HD3	1:D:194:ILE:O	2.21	0.41
1:D:168:VAL:CG2	1:D:251:LEU:HD21	2.45	0.41
1:A:140:LEU:HD13	2:B:139:ILE:HG21	2.01	0.41
1:D:189:VAL:CG1	1:D:206:LEU:HB3	2.51	0.41
1:D:20:GLU:HG2	1:D:40:LEU:HD13	2.01	0.41
2:B:238:LEU:O	2:B:242:GLU:HG2	2.21	0.41
2:B:84:LEU:HD12	2:B:89:ARG:HB3	2.03	0.41
1:D:293:ARG:HG3	1:D:293:ARG:HH21	1.86	0.41
1:D:47:ARG:N	1:D:48:PRO:HD2	2.36	0.41
1:D:156:GLN:O	1:D:159:ASP:HB3	2.21	0.41
2:B:5:TRP:CZ2	2:B:253:LEU:HG	2.56	0.41
2:B:138:VAL:HG22	2:B:189:CYS:SG	2.61	0.41
2:B:181:GLU:HB2	7:B:508:HOH:O	2.21	0.41
1:D:155:GLY:O	1:D:159:ASP:HB2	2.20	0.41
2:C:138:VAL:O	2:C:142:ILE:HG13	2.21	0.41
2:C:92:SER:HB2	2:C:94:PRO:HD2	2.02	0.41
2:C:2:GLN:HG2	7:C:476:HOH:O	2.21	0.41
1:D:44:LYS:HB2	1:D:46:VAL:HG23	2.03	0.41
1:A:248:TYR:N	1:A:249:PRO:CD	2.84	0.40
2:C:139:ILE:HD13	1:D:140:LEU:HD13	2.03	0.40
2:C:148:PRO:HB3	1:D:115:ALA:HB1	2.04	0.40
2:C:76:ALA:HB2	2:C:151:MET:CE	2.52	0.40
1:D:4:PHE:CE1	1:D:5:ASP:OD1	2.75	0.40
2:C:140:ILE:HD13	1:D:126:ALA:HB2	2.03	0.40
1:D:75:ILE:O	1:D:78:MET:HG3	2.21	0.40
1:D:269:GLN:HE22	1:D:288:ASN:ND2	2.19	0.40
2:C:2:GLN:HB2	2:C:5:TRP:HD1	1.86	0.40
2:C:147:GLY:HA3	7:C:341:HOH:O	2.21	0.40
1:D:143:LEU:HD13	1:D:191:LEU:HD11	2.03	0.40
1:D:214:GLY:O	1:D:216:LEU:N	2.55	0.40
2:C:145:ALA:HB1	2:C:182:MET:HE3	2.03	0.40
2:C:93:LYS:HA	2:C:93:LYS:HE2	2.03	0.40
2:B:54:LEU:HD13	2:B:250:ASN:OD1	2.22	0.40
2:B:49:LEU:HD22	2:B:59:ARG:HG3	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LEU:HD11	2:B:232:ILE:HG23	2.03	0.40
1:D:173:LEU:HD11	1:D:177:HIS:HE2	1.87	0.40
2:B:215:ARG:NH2	7:B:325:HOH:O	2.50	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	275/295 (93%)	252 (92%)	22 (8%)	1 (0%)	39	54
1	D	280/295 (95%)	252 (90%)	25 (9%)	3 (1%)	17	24
2	B	252/274 (92%)	218 (86%)	30 (12%)	4 (2%)	12	15
2	C	257/274 (94%)	224 (87%)	22 (9%)	11 (4%)	3	2
All	All	1064/1138 (94%)	946 (89%)	99 (9%)	19 (2%)	11	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	SER
2	B	227	ILE
2	C	94	PRO
2	C	196	ALA
2	C	198	GLU
2	C	238	LEU
1	D	165	MET
1	D	168	VAL
1	A	42	GLY
2	C	57	GLY
2	C	224	HIS
2	C	226	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	237	GLU
2	B	26	GLU
2	C	91	VAL
2	B	163	ASP
2	C	60	SER
2	C	163	ASP
1	D	286	LEU

### 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	222/234 (95%)	214 (96%)	8 (4%)	42	62
1	D	226/234 (97%)	223 (99%)	3 (1%)	76	89
2	B	199/214 (93%)	196 (98%)	3 (2%)	72	86
2	C	201/214 (94%)	194 (96%)	7 (4%)	43	63
All	All	848/896 (95%)	827 (98%)	21 (2%)	55	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	44	LYS
1	A	90	ASN
1	A	99	THR
1	A	228	LYS
1	A	245	LYS
1	A	272	LEU
1	A	278	HIS
2	B	131	ASP
2	B	163	ASP
2	B	211	GLN
2	C	21	THR
2	C	86	ASP
2	C	93	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	94	PRO
2	C	131	ASP
2	C	182	MET
2	C	250	ASN
1	D	63	SER
1	D	78	MET
1	D	134	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	179	HIS
1	A	186	GLN
1	A	211	ASN
2	B	34	HIS
2	B	81	HIS
2	B	156	HIS
2	B	183	HIS
2	B	202	GLN
2	B	206	ASN
2	B	224	HIS
2	C	33	HIS
1	D	265	ASN
1	D	288	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	PPV	A	901	4	6,8,8	1.32	0	11,13,13	2.06	1 (9%)
5	EDO	C	902	-	3,3,3	0.47	0	2,2,2	0.45	0
6	GPP	D	900	-	16,18,18	2.12	6 (37%)	21,25,25	1.40	3 (14%)

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	PPV	A	901	4	-	0/6/6/6	0/0/0/0
5	EDO	C	902	-	-	0/1/1/1	0/0/0/0
6	GPP	D	900	-	-	0/19/19/19	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	900	GPP	C6-C7	-3.96	1.39	1.50
6	D	900	GPP	C1-C2	-2.86	1.39	1.49
6	D	900	GPP	C7-C8	2.40	1.39	1.32
6	D	900	GPP	PA-O1A	2.83	1.61	1.51
6	D	900	GPP	PB-O1B	3.15	1.61	1.51
6	D	900	GPP	C2-C3	3.26	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	PPV	P2-OPP-P1	-6.45	111.03	132.67
6	D	900	GPP	PA-O3A-PB	-3.55	120.76	132.67
6	D	900	GPP	C10-C8-C9	2.11	119.81	114.64
6	D	900	GPP	C4-C3-C5	2.78	119.66	115.41



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	902	EDO	1	0
6	D	900	GPP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	279/295 (94%)	-0.28	5 (1%) 71 70	28, 42, 65, 95	0
1	D	284/295 (96%)	0.24	24 (8%) 13 13	30, 47, 109, 125	0
2	B	256/274 (93%)	0.25	24 (9%) 11 10	32, 50, 128, 145	0
2	C	259/274 (94%)	0.15	17 (6%) 22 21	30, 50, 97, 106	0
All	All	1078/1138 (94%)	0.09	70 (6%) 22 22	28, 46, 104, 145	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	LEU	8.7
2	B	250	ASN	8.6
2	C	127	ALA	8.2
2	B	226	LEU	7.3
1	D	258	LYS	7.2
2	B	248	GLY	7.2
2	B	259	ALA	6.9
2	B	249	LYS	6.0
1	D	257	SER	6.0
2	C	249	LYS	5.5
1	D	255	GLU	5.1
1	D	165	MET	5.0
1	A	166	ALA	4.8
2	C	126	PRO	4.7
2	B	251	ALA	4.1
2	B	235	LEU	4.1
2	C	89	ARG	4.1
2	B	231	ILE	4.0
1	D	168	VAL	3.9
2	B	234	LYS	3.9
1	D	260	PHE	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	164	GLY	3.8
2	B	1	MET	3.8
2	B	224	HIS	3.6
2	C	226	LEU	3.6
1	D	292	TYR	3.6
1	D	289	TYR	3.5
2	B	254	MET	3.4
2	C	128	ARG	3.4
1	D	254	VAL	3.3
1	A	165	MET	3.3
1	D	290	ILE	3.2
1	D	250	LYS	3.1
2	B	258	VAL	3.1
1	D	167	GLU	3.1
1	D	163	GLU	3.0
2	C	222	ASN	3.0
1	D	253	GLY	2.9
1	D	248	TYR	2.9
1	D	230	SER	2.9
1	D	252	ILE	2.8
2	C	93	LYS	2.8
1	D	217	PHE	2.7
2	B	92	SER	2.7
1	D	130	GLY	2.6
2	C	225	GLN	2.6
2	B	225	GLN	2.6
2	C	223	SER	2.5
2	B	253	LEU	2.4
2	C	162	VAL	2.4
2	B	257	LEU	2.4
1	A	164	GLY	2.4
2	B	238	LEU	2.4
1	A	167	GLU	2.3
2	B	230	ASN	2.3
2	B	229	GLU	2.3
2	B	236	LYS	2.3
2	C	129	THR	2.2
2	C	237	GLU	2.2
1	D	232	GLU	2.1
2	B	256	SER	2.1
2	C	248	GLY	2.1
2	C	91	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	295	ASN	2.1
2	B	162	VAL	2.1
1	D	75	ILE	2.0
2	C	90	PRO	2.0
2	B	228	ASP	2.0
1	D	166	ALA	2.0
2	C	229	GLU	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
5	EDO	C	902	4/4	0.96	0.17	1.41	35,37,38,38	0
3	PPV	A	901	9/9	0.90	0.12	0.01	83,84,86,87	0
6	GPP	D	900	19/19	0.94	0.19	-0.05	53,61,68,69	0
4	MG	D	904	1/1	0.80	0.10	-1.33	57,57,57,57	0
4	MG	A	906	1/1	0.72	0.09	-	96,96,96,96	0
4	MG	D	903	1/1	0.91	0.09	-	48,48,48,48	0
4	MG	A	905	1/1	0.85	0.09	-	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.