



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 03:43 AM EDT

PDB ID : 3HGK  
Title : crystal structure of effect protein AvrptoB complexed with kinase Pto  
Authors : Dong, J.; Fan, F.; Gu, L.; Chai, J.  
Deposited on : 2009-05-14  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

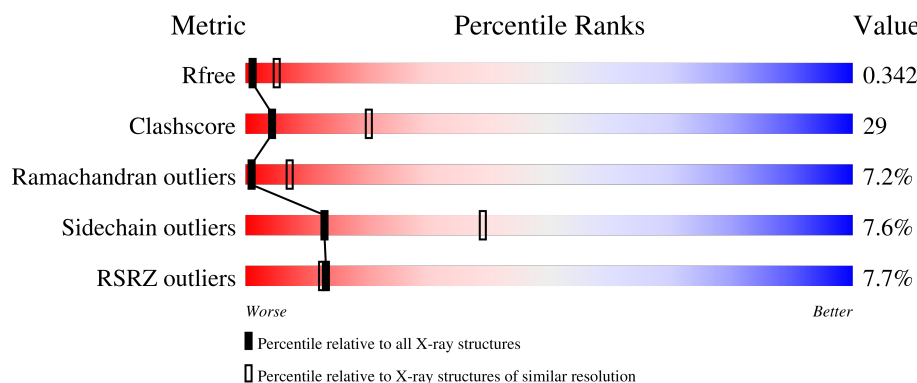
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	327	<div> <div>9%</div> <div>35%</div> <div>45%</div> <div>8%</div> <div>12%</div> </div>
1	B	327	<div> <div>6%</div> <div>39%</div> <div>39%</div> <div>9%</div> <div>12%</div> </div>
1	C	327	<div> <div>5%</div> <div>40%</div> <div>38%</div> <div>9%</div> <div>13%</div> </div>
1	D	327	<div> <div>8%</div> <div>40%</div> <div>41%</div> <div>7%</div> <div>12%</div> </div>
2	E	85	<div> <div>5%</div> <div>64%</div> <div>25%</div> <div>9%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	85	
2	G	85	
2	H	85	

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
1	SEP	B	198	-	-	-	X
1	SEP	C	198	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11599 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 Protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2308	1462	398	435	2	11			
1	B	288	Total	C	N	O	P	S	0	0	0
			2306	1459	398	436	2	11			
1	C	286	Total	C	N	O	P	S	0	0	0
			2293	1451	396	433	2	11			
1	D	288	Total	C	N	O	P	S	0	0	0
			2308	1462	398	435	2	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	GLY	ASP	engineered mutation	UNP Q40234
A	322	HIS	-	expression tag	UNP Q40234
A	323	HIS	-	expression tag	UNP Q40234
A	324	HIS	-	expression tag	UNP Q40234
A	325	HIS	-	expression tag	UNP Q40234
A	326	HIS	-	expression tag	UNP Q40234
A	327	HIS	-	expression tag	UNP Q40234
B	193	GLY	ASP	engineered mutation	UNP Q40234
B	322	HIS	-	expression tag	UNP Q40234
B	323	HIS	-	expression tag	UNP Q40234
B	324	HIS	-	expression tag	UNP Q40234
B	325	HIS	-	expression tag	UNP Q40234
B	326	HIS	-	expression tag	UNP Q40234
B	327	HIS	-	expression tag	UNP Q40234
C	193	GLY	ASP	engineered mutation	UNP Q40234
C	322	HIS	-	expression tag	UNP Q40234
C	323	HIS	-	expression tag	UNP Q40234
C	324	HIS	-	expression tag	UNP Q40234
C	325	HIS	-	expression tag	UNP Q40234
C	326	HIS	-	expression tag	UNP Q40234
C	327	HIS	-	expression tag	UNP Q40234

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	193	GLY	ASP	engineered mutation	UNP Q40234
D	322	HIS	-	expression tag	UNP Q40234
D	323	HIS	-	expression tag	UNP Q40234
D	324	HIS	-	expression tag	UNP Q40234
D	325	HIS	-	expression tag	UNP Q40234
D	326	HIS	-	expression tag	UNP Q40234
D	327	HIS	-	expression tag	UNP Q40234

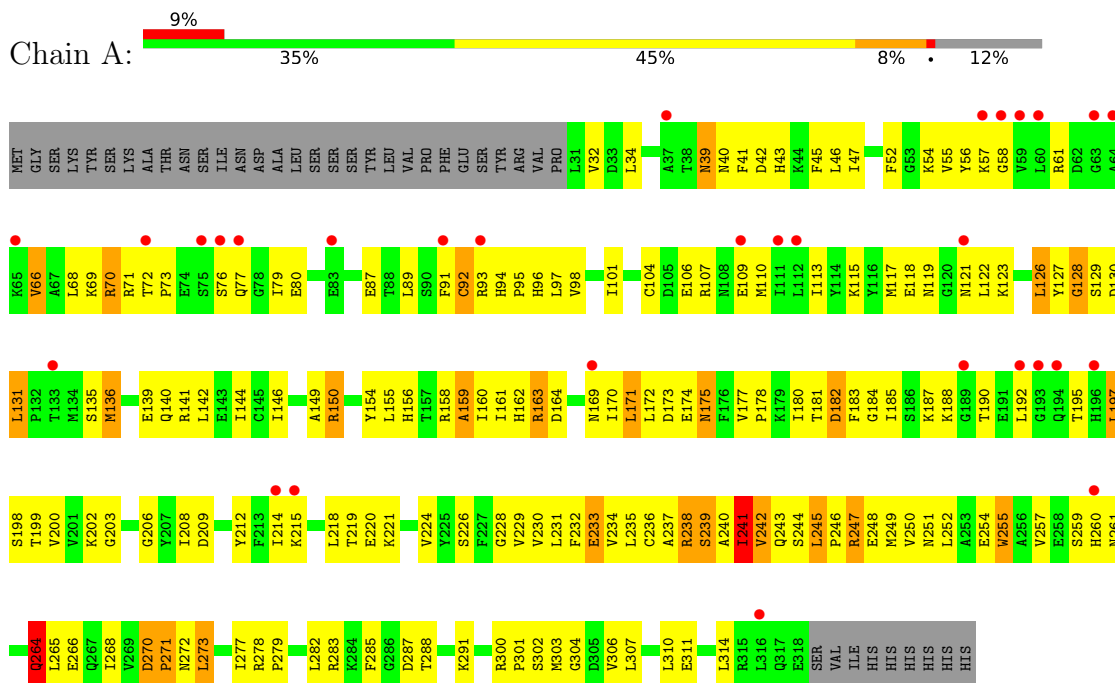
- Molecule 2 is a protein called Effector protein hopAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	F	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	G	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	H	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			

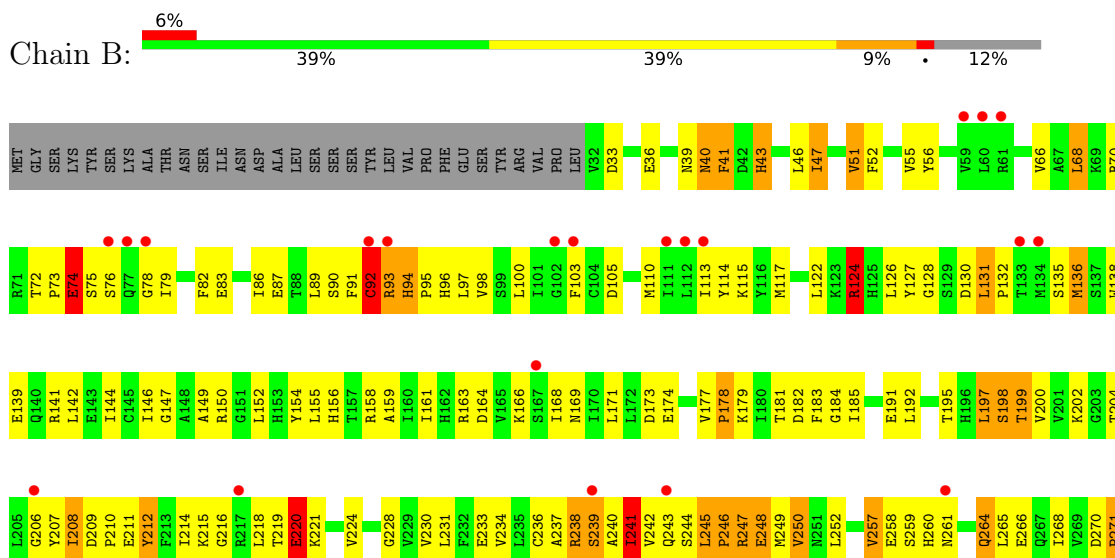
### 3 Residue-property plots [i](#)

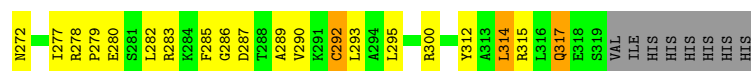
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein kinase

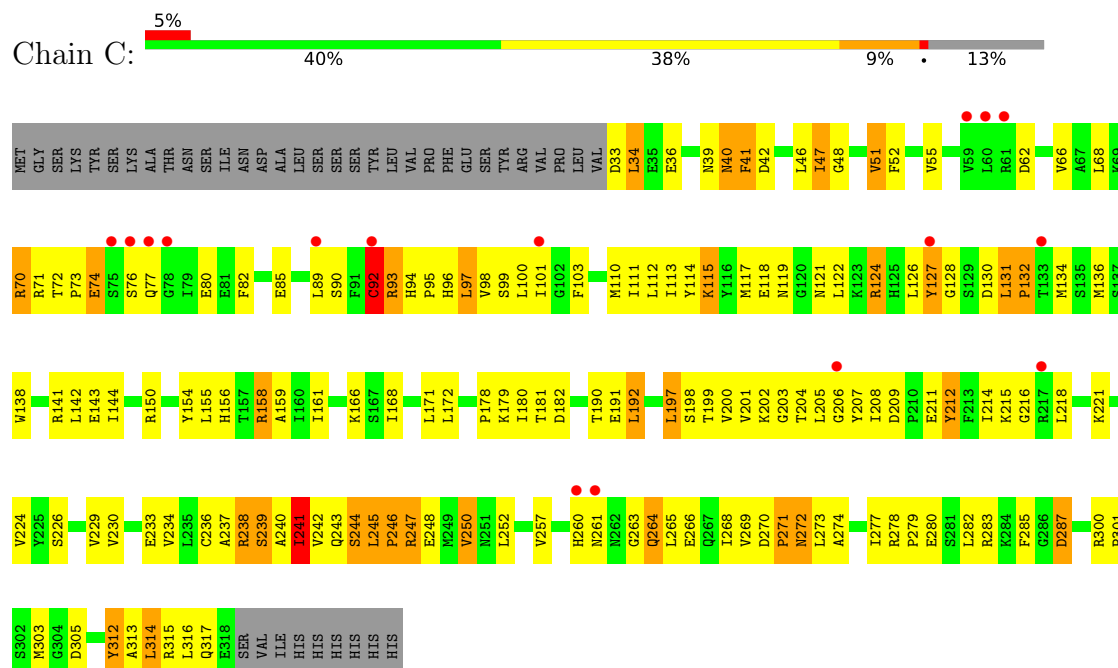


#### • Molecule 1: Protein kinase

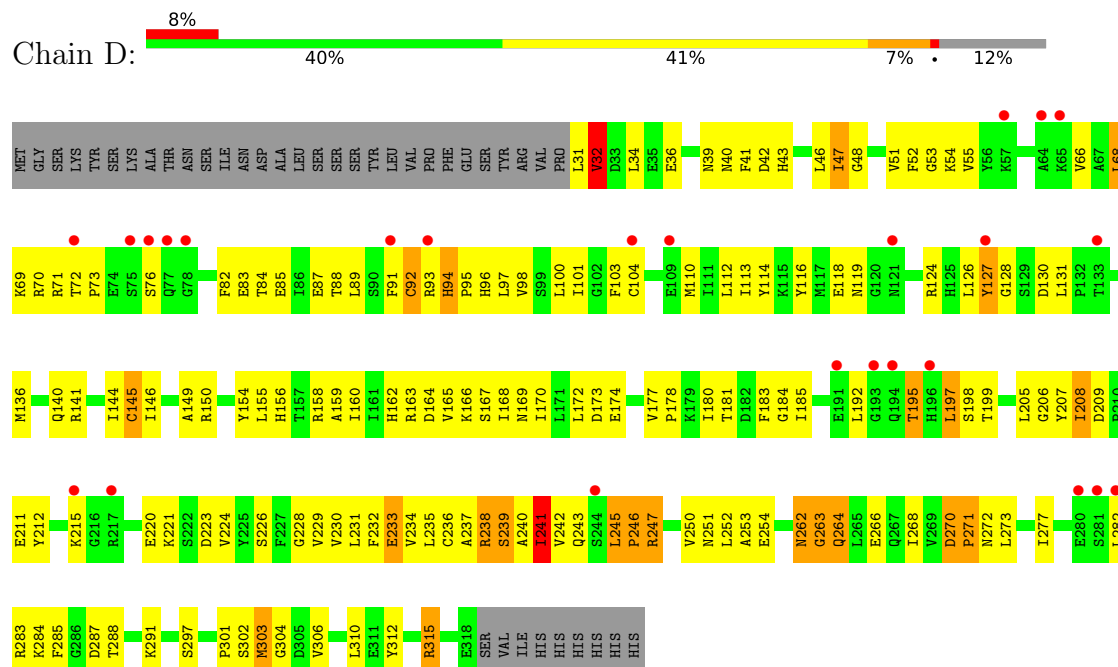




- Molecule 1: Protein kinase



- Molecule 1: Protein kinase



- Molecule 2: Effector protein hopAB2

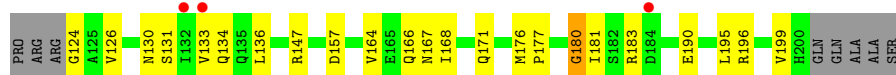




- Molecule 2: Effector protein hopAB2



- Molecule 2: Effector protein hopAB2



- Molecule 2: Effector protein hopAB2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.07Å 104.47Å 298.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 44.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.30) 99.6 (44.96-3.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.317 , 0.331 0.329 , 0.342	Depositor DCC
$R_{free}$ test set	1508 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.1	Xtriage
Anisotropy	0.895	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 20.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7970e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO

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	0.51	1/2331 (0.0%)	0.66	0/3143
1	B	0.51	0/2329	0.68	1/3140 (0.0%)
1	C	0.49	0/2316	0.67	0/3122
1	D	0.50	0/2331	0.65	0/3143
2	E	0.38	0/605	0.50	0/814
2	F	0.41	0/605	0.51	0/814
2	G	0.59	2/605 (0.3%)	0.58	1/814 (0.1%)
2	H	0.40	0/605	0.51	0/814
All	All	0.49	3/11727 (0.0%)	0.64	2/15804 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	124	GLY	C-O	-7.03	1.12	1.23
2	G	124	GLY	CA-C	-5.72	1.42	1.51
1	A	126	LEU	C-N	-5.23	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	124	GLY	N-CA-C	-7.49	94.38	113.10
1	B	47	ILE	N-CA-C	6.44	128.40	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2308	0	2301	172	0
1	B	2306	0	2295	156	0
1	C	2293	0	2281	175	0
1	D	2308	0	2301	141	0
2	E	596	0	585	18	0
2	F	596	0	585	17	0
2	G	596	0	585	18	0
2	H	596	0	585	17	0
All	All	11599	0	11518	671	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 29.

All (671) 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:B:245:LEU:HB3	1:D:240:ALA:HB2	1.38	1.06
1:B:240:ALA:HB2	1:D:245:LEU:HB3	1.40	1.03
1:C:238:ARG:HD2	1:C:252:LEU:HD13	1.43	0.98
1:A:203:GLY:HA3	1:A:208:ILE:HD11	1.43	0.97
1:C:77:GLN:HE21	1:C:80:GLU:HB2	1.26	0.97
1:A:268:ILE:HD13	1:C:268:ILE:HD13	1.45	0.96
1:A:240:ALA:HB2	1:C:245:LEU:HB3	1.47	0.95
1:B:247:ARG:HG3	1:B:248:GLU:H	1.29	0.95
1:D:127:TYR:HB3	1:D:239:SER:HB3	1.47	0.94
1:D:89:LEU:O	1:D:92:CYS:SG	2.28	0.92
1:B:159:ALA:HB2	1:B:192:LEU:HA	1.49	0.92
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.35	0.91
1:C:278:ARG:H	1:C:317:GLN:HE21	1.12	0.90
1:C:278:ARG:H	1:C:317:GLN:NE2	1.67	0.90
1:B:268:ILE:HD13	1:D:268:ILE:HD13	1.54	0.90
1:A:245:LEU:HB3	1:C:240:ALA:HB2	1.51	0.90
1:A:89:LEU:O	1:A:92:CYS:SG	2.31	0.88
1:B:247:ARG:HG3	1:B:248:GLU:N	1.87	0.87
1:C:159:ALA:HB2	1:C:192:LEU:HA	1.57	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:O	1:C:234:VAL:HG23	1.74	0.87
2:E:183:ARG:NH1	2:H:183:ARG:HB2	1.91	0.85
1:A:118:GLU:HG3	1:A:174:GLU:HG2	1.58	0.85
1:A:203:GLY:CA	1:A:208:ILE:HD11	2.06	0.85
2:E:183:ARG:HB2	2:H:183:ARG:NH1	1.91	0.83
1:B:97:LEU:HD21	1:B:155:LEU:HD11	1.60	0.83
1:B:277:ILE:HG21	1:B:282:LEU:HB2	1.59	0.82
1:B:259:SER:HB3	1:B:266:GLU:HB2	1.60	0.82
1:A:123:LYS:HG3	1:A:239:SER:OG	1.79	0.82
1:B:240:ALA:HB1	1:B:243:GLN:HB2	1.59	0.82
1:D:52:PHE:CE2	1:D:76:SER:HB2	2.14	0.82
1:B:224:VAL:HG12	1:B:292:CYS:HB3	1.62	0.81
1:D:126:LEU:HD13	1:D:233:GLU:O	1.80	0.81
1:B:66:VAL:HG21	1:B:113:ILE:CG2	2.10	0.81
1:B:209:ASP:HB3	1:B:212:TYR:HB2	1.62	0.81
1:C:144:ILE:HG23	1:C:178:PRO:HG3	1.61	0.80
2:E:183:ARG:HD3	2:H:183:ARG:HD3	1.64	0.80
1:D:94:HIS:ND1	1:D:95:PRO:HD2	1.97	0.79
1:A:91:PHE:HB3	1:A:158:ARG:HH12	1.45	0.79
1:C:209:ASP:HB3	1:C:212:TYR:CB	2.13	0.79
1:C:266:GLU:HB3	1:C:269:VAL:HG23	1.63	0.79
1:B:244:SER:O	1:D:127:TYR:HE2	1.65	0.79
1:B:277:ILE:CG2	1:B:282:LEU:HB2	2.12	0.79
1:B:243:GLN:HG3	1:B:246:PRO:HD3	1.65	0.78
1:B:247:ARG:CG	1:B:248:GLU:H	1.93	0.78
2:F:183:ARG:NH1	2:G:183:ARG:HB2	1.98	0.78
1:B:94:HIS:ND1	1:B:95:PRO:HD2	1.99	0.78
1:B:127:TYR:HB3	1:B:239:SER:HB3	1.67	0.76
1:B:244:SER:O	1:D:127:TYR:CE2	2.39	0.76
1:B:245:LEU:HD12	1:D:243:GLN:OE1	1.85	0.76
1:B:52:PHE:CE2	1:B:76:SER:HB2	2.20	0.76
1:C:77:GLN:NE2	1:C:80:GLU:HB2	2.00	0.75
1:A:136:MET:CG	1:A:140:GLN:HG2	2.16	0.75
1:B:241:ILE:HG12	1:B:242:VAL:N	2.02	0.75
1:A:271:PRO:HB3	1:C:247:ARG:HG3	1.69	0.74
1:C:238:ARG:O	1:C:238:ARG:HD3	1.86	0.74
1:A:146:ILE:HG12	1:A:310:LEU:HB3	1.69	0.74
1:A:161:ILE:HG22	1:A:163:ARG:HG3	1.69	0.74
1:A:238:ARG:C	1:A:240:ALA:H	1.86	0.74
1:C:94:HIS:HB3	1:C:97:LEU:HB2	1.69	0.74
1:B:178:PRO:O	1:B:179:LYS:HG2	1.86	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASP:HB3	1:C:212:TYR:HB2	1.69	0.73
1:C:264:GLN:HB3	1:C:266:GLU:HG3	1.70	0.73
1:D:240:ALA:O	1:D:242:VAL:N	2.21	0.72
1:B:260:HIS:HA	1:B:265:LEU:HA	1.70	0.72
1:D:136:MET:HG3	1:D:140:GLN:HG2	1.71	0.72
1:D:270:ASP:HB2	1:D:271:PRO:HD2	1.72	0.71
1:B:278:ARG:H	1:B:317:GLN:HE21	1.39	0.71
1:D:127:TYR:HB3	1:D:239:SER:CB	2.21	0.71
2:E:183:ARG:CZ	2:H:183:ARG:HB2	2.20	0.71
1:D:91:PHE:HB3	1:D:158:ARG:HH12	1.56	0.71
1:A:91:PHE:CB	1:A:158:ARG:HH12	2.03	0.71
1:B:238:ARG:NH2	1:B:250:VAL:O	2.24	0.71
1:C:117:MET:HG3	1:C:171:LEU:HD23	1.72	0.71
1:B:230:VAL:O	1:B:234:VAL:HG23	1.91	0.70
1:B:271:PRO:HB3	1:D:247:ARG:HG3	1.74	0.70
1:A:271:PRO:CB	1:C:247:ARG:HG3	2.22	0.70
1:A:170:ILE:HG22	1:A:170:ILE:O	1.90	0.70
1:A:197:LEU:HD23	1:A:197:LEU:H	1.56	0.70
1:A:271:PRO:HB3	1:C:247:ARG:CG	2.22	0.69
1:B:243:GLN:OE1	1:D:245:LEU:HD12	1.92	0.69
1:A:270:ASP:HB2	1:A:271:PRO:HD2	1.74	0.69
1:B:66:VAL:HG23	1:B:114:TYR:O	1.92	0.69
1:C:205:LEU:HD21	2:G:180:GLY:HA3	1.73	0.69
1:C:236:CYS:HA	1:C:270:ASP:HA	1.73	0.69
1:A:155:LEU:HD21	1:A:183:PHE:HE2	1.57	0.69
1:A:136:MET:HG3	1:A:140:GLN:HG2	1.74	0.69
1:C:154:TYR:O	1:C:158:ARG:HG3	1.93	0.69
1:B:283:ARG:O	1:B:287:ASP:HB2	1.92	0.68
1:A:247:ARG:HG3	1:A:248:GLU:H	1.58	0.68
1:B:127:TYR:HB3	1:B:239:SER:CB	2.24	0.68
1:A:52:PHE:CE2	1:A:76:SER:HB2	2.29	0.68
1:B:238:ARG:HD2	1:B:252:LEU:HD13	1.75	0.68
1:A:117:MET:HG3	1:A:171:LEU:HD23	1.75	0.68
1:B:214:ILE:HG13	1:B:215:LYS:HG3	1.76	0.68
1:C:94:HIS:ND1	1:C:95:PRO:HD2	2.09	0.68
1:C:197:LEU:HD23	1:C:197:LEU:H	1.59	0.68
1:A:127:TYR:HB3	1:A:239:SER:HB3	1.77	0.67
1:A:240:ALA:HB1	1:A:243:GLN:HB2	1.76	0.67
1:D:228:GLY:HA2	1:D:231:LEU:HD12	1.76	0.67
1:B:209:ASP:HB3	1:B:212:TYR:CB	2.23	0.67
1:B:135:SER:HB3	1:D:247:ARG:HH22	1.60	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:O	1:A:242:VAL:N	2.28	0.67
1:A:135:SER:HB3	1:C:247:ARG:HH22	1.60	0.67
1:D:277:ILE:CG2	1:D:282:LEU:HB2	2.24	0.66
1:D:209:ASP:HB3	1:D:212:TYR:HB3	1.78	0.66
1:B:141:ARG:HD3	1:B:234:VAL:HG12	1.78	0.66
1:D:83:GLU:O	1:D:87:GLU:HG2	1.96	0.66
1:B:156:HIS:CD2	1:B:220:GLU:HB2	2.31	0.66
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.06	0.66
1:C:238:ARG:C	1:C:240:ALA:H	1.98	0.66
1:D:226:SER:O	1:D:230:VAL:HG23	1.96	0.66
1:A:195:THR:HB	1:A:197:LEU:HD22	1.78	0.65
1:C:243:GLN:HG3	1:C:246:PRO:HD3	1.78	0.65
1:D:277:ILE:HG21	1:D:282:LEU:HB2	1.77	0.65
1:B:277:ILE:HD13	1:B:282:LEU:HD13	1.77	0.65
1:D:238:ARG:C	1:D:240:ALA:H	1.99	0.65
2:H:186:GLU:HA	2:H:189:ILE:HD12	1.78	0.65
1:A:206:GLY:C	1:A:241:ILE:HD11	2.16	0.65
1:C:130:ASP:O	1:C:131:LEU:HB3	1.95	0.65
1:D:243:GLN:HE21	1:D:245:LEU:N	1.94	0.65
1:D:238:ARG:HB3	1:D:252:LEU:HD12	1.79	0.65
1:B:166:LYS:HB2	1:B:207:TYR:CZ	2.32	0.65
1:C:126:LEU:HD13	1:C:233:GLU:O	1.95	0.65
1:C:283:ARG:O	1:C:287:ASP:HB2	1.96	0.65
1:D:52:PHE:HE2	1:D:76:SER:HB2	1.57	0.64
1:B:236:CYS:SG	1:B:252:LEU:HD11	2.37	0.64
1:C:171:LEU:HD11	1:C:181:THR:HG21	1.78	0.64
1:D:206:GLY:C	1:D:241:ILE:HD11	2.17	0.64
1:A:54:LYS:HG3	1:A:73:PRO:HG2	1.79	0.64
1:B:66:VAL:CG2	1:B:113:ILE:CG2	2.75	0.64
1:B:314:LEU:O	1:B:314:LEU:HD12	1.98	0.64
1:C:66:VAL:CG2	1:C:113:ILE:HG22	2.28	0.64
2:G:176:MET:HA	2:G:180:GLY:HA2	1.79	0.64
1:B:210:PRO:O	1:B:214:ILE:HG23	1.98	0.64
1:C:209:ASP:HB3	1:C:212:TYR:HB3	1.79	0.64
1:D:238:ARG:HD2	1:D:252:LEU:HD12	1.80	0.64
1:A:230:VAL:O	1:A:234:VAL:HG23	1.97	0.64
1:C:313:ALA:HA	1:C:316:LEU:HD12	1.80	0.64
1:A:161:ILE:HG21	1:A:218:LEU:HD11	1.80	0.63
1:B:66:VAL:HG21	1:B:113:ILE:HG22	1.79	0.63
1:C:166:LYS:HE3	1:C:168:ILE:HD12	1.81	0.63
2:G:133:VAL:HG22	2:G:195:LEU:HD12	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LYS:HG3	1:D:73:PRO:HG2	1.79	0.63
1:C:221:LYS:NZ	1:C:300:ARG:O	2.32	0.63
1:A:209:ASP:HB3	1:A:212:TYR:HB3	1.80	0.63
1:D:43:HIS:CE1	1:D:70:ARG:HH21	2.17	0.63
1:A:43:HIS:CE1	1:A:70:ARG:HH21	2.16	0.62
1:A:68:LEU:HD12	1:A:113:ILE:HG12	1.81	0.62
1:A:158:ARG:O	1:A:160:ILE:HG13	1.99	0.62
1:D:230:VAL:O	1:D:234:VAL:HG23	1.99	0.62
1:A:135:SER:CB	1:C:247:ARG:HH22	2.13	0.62
1:D:236:CYS:HA	1:D:270:ASP:HA	1.82	0.62
1:D:263:GLY:O	1:D:264:GLN:HB2	1.99	0.62
1:B:241:ILE:HG12	1:B:242:VAL:H	1.64	0.61
1:A:301:PRO:HG2	1:A:306:VAL:CG2	2.30	0.61
1:B:166:LYS:HE3	1:B:168:ILE:HD12	1.82	0.61
1:A:58:GLY:O	1:A:66:VAL:HG12	2.00	0.61
2:E:176:MET:HA	2:E:180:GLY:HA2	1.81	0.61
1:B:66:VAL:CG2	1:B:113:ILE:HG22	2.30	0.61
2:H:176:MET:HA	2:H:180:GLY:HA2	1.82	0.61
1:B:243:GLN:HE21	1:B:245:LEU:N	1.98	0.61
1:C:278:ARG:N	1:C:317:GLN:NE2	2.46	0.61
1:D:243:GLN:HG3	1:D:246:PRO:HD2	1.82	0.61
1:A:243:GLN:O	1:A:250:VAL:HG23	2.01	0.61
1:C:90:SER:C	1:C:92:CYS:H	2.03	0.61
1:D:270:ASP:HB2	1:D:271:PRO:CD	2.30	0.61
1:B:43:HIS:CE1	1:B:70:ARG:HH21	2.19	0.60
1:B:183:PHE:O	1:B:185:ILE:N	2.34	0.60
1:A:238:ARG:NH2	1:A:250:VAL:O	2.35	0.60
1:D:96:HIS:O	1:D:97:LEU:HD12	2.01	0.60
1:B:197:LEU:H	1:B:197:LEU:CD2	2.15	0.60
1:C:171:LEU:HD12	1:C:171:LEU:N	2.15	0.60
1:C:89:LEU:CD2	1:C:100:LEU:HB2	2.32	0.60
1:C:89:LEU:HD23	1:C:100:LEU:HB2	1.84	0.60
1:C:229:VAL:HG11	1:C:241:ILE:HD12	1.83	0.60
1:A:243:GLN:OE1	1:C:245:LEU:HD12	2.01	0.60
1:A:126:LEU:HD13	1:A:233:GLU:O	2.02	0.60
1:C:156:HIS:CE1	1:C:303:MET:HG2	2.37	0.60
1:B:96:HIS:O	1:B:97:LEU:HD12	2.01	0.59
1:D:69:LYS:HD3	1:D:71:ARG:HH21	1.68	0.59
1:A:238:ARG:O	1:A:240:ALA:N	2.34	0.59
1:C:240:ALA:HB1	1:C:243:GLN:HB2	1.85	0.59
1:C:238:ARG:O	1:C:240:ALA:N	2.35	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:O	1:B:90:SER:N	2.28	0.59
1:C:178:PRO:O	1:C:179:LYS:HG2	2.03	0.59
1:A:203:GLY:HA3	1:A:208:ILE:CD1	2.25	0.58
1:A:214:ILE:HG13	1:A:215:LYS:HG3	1.83	0.58
1:B:171:LEU:N	1:B:171:LEU:HD12	2.17	0.58
1:C:312:TYR:O	1:C:315:ARG:HB3	2.02	0.58
1:D:127:TYR:CB	1:D:239:SER:HB3	2.26	0.58
1:A:175:ASN:OD1	1:A:175:ASN:N	2.37	0.58
1:B:241:ILE:CG1	1:B:242:VAL:N	2.67	0.58
1:C:93:ARG:O	1:C:94:HIS:HB2	2.01	0.58
1:D:284:LYS:HE2	1:D:312:TYR:HD2	1.68	0.58
1:A:245:LEU:HD12	1:C:243:GLN:OE1	2.03	0.58
1:B:292:CYS:O	1:B:300:ARG:HD3	2.03	0.58
1:C:260:HIS:HA	1:C:265:LEU:HA	1.86	0.58
1:A:236:CYS:O	1:A:237:ALA:HB3	2.03	0.58
1:D:236:CYS:O	1:D:237:ALA:HB3	2.03	0.58
1:A:301:PRO:HG2	1:A:306:VAL:HG23	1.86	0.58
1:C:197:LEU:H	1:C:197:LEU:CD2	2.17	0.57
1:C:278:ARG:N	1:C:317:GLN:HE21	1.93	0.57
1:B:72:THR:N	1:B:73:PRO:CD	2.67	0.57
1:B:245:LEU:HB3	1:D:240:ALA:CB	2.24	0.57
1:B:154:TYR:O	1:B:158:ARG:HG3	2.04	0.57
1:B:130:ASP:O	1:B:131:LEU:HB3	2.02	0.57
1:B:238:ARG:O	1:B:238:ARG:HD3	2.04	0.57
1:A:91:PHE:O	1:A:93:ARG:N	2.37	0.57
1:A:122:LEU:HD13	1:A:144:ILE:HG21	1.86	0.57
1:B:238:ARG:C	1:B:240:ALA:H	2.06	0.57
1:D:264:GLN:OE1	1:D:266:GLU:HA	2.05	0.57
1:C:214:ILE:HG13	1:C:215:LYS:HG3	1.86	0.57
1:C:214:ILE:HG13	1:C:215:LYS:N	2.19	0.57
1:A:159:ALA:HB2	1:A:192:LEU:HA	1.86	0.57
1:A:283:ARG:O	1:A:287:ASP:HB2	2.04	0.57
1:C:270:ASP:HB2	1:C:271:PRO:HD2	1.86	0.57
1:B:271:PRO:CB	1:D:247:ARG:HG3	2.35	0.56
1:C:314:LEU:HD12	1:C:314:LEU:O	2.05	0.56
1:A:264:GLN:OE1	1:A:266:GLU:HG2	2.05	0.56
1:B:124:ARG:O	1:B:124:ARG:HD3	2.04	0.56
1:A:162:HIS:HE1	1:A:182:ASP:O	1.88	0.56
1:C:212:TYR:O	1:C:216:GLY:N	2.33	0.56
1:D:166:LYS:HE3	1:D:168:ILE:HD12	1.88	0.56
1:A:155:LEU:HD21	1:A:183:PHE:CE2	2.40	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	1:A:155:LEU:HD11	1.88	0.56
1:C:52:PHE:CE2	1:C:76:SER:HB2	2.41	0.56
1:C:241:ILE:HG12	1:C:242:VAL:N	2.20	0.56
1:D:312:TYR:O	1:D:315:ARG:HB3	2.05	0.56
2:F:133:VAL:HG22	2:F:195:LEU:HD12	1.87	0.56
1:A:119:ASN:ND2	1:A:173:ASP:O	2.38	0.55
1:A:155:LEU:HD23	1:A:160:ILE:HG21	1.88	0.55
1:A:161:ILE:CG2	1:A:163:ARG:HG3	2.34	0.55
1:D:238:ARG:HD2	1:D:252:LEU:HB2	1.88	0.55
1:C:97:LEU:HD11	1:C:155:LEU:HD13	1.88	0.55
1:B:221:LYS:NZ	1:B:300:ARG:O	2.37	0.55
1:C:94:HIS:HD2	1:C:154:TYR:CD2	2.25	0.55
1:C:98:VAL:HG21	1:C:181:THR:HB	1.87	0.55
1:B:135:SER:CB	1:D:247:ARG:HH22	2.19	0.55
1:A:45:PHE:HA	1:A:56:TYR:HE2	1.72	0.55
1:A:162:HIS:O	1:A:162:HIS:ND1	2.34	0.55
1:B:94:HIS:ND1	1:B:95:PRO:CD	2.68	0.55
1:D:232:PHE:C	1:D:234:VAL:H	2.09	0.55
1:B:163:ARG:NH2	1:B:199:TPO:O1P	2.37	0.55
1:D:149:ALA:HA	1:D:303:MET:CE	2.37	0.55
1:C:161:ILE:CD1	1:C:197:LEU:HD21	2.37	0.55
1:C:257:VAL:O	1:C:261:ASN:HB3	2.07	0.55
1:D:232:PHE:HB2	1:D:252:LEU:HD21	1.88	0.55
1:A:136:MET:HG2	1:A:140:GLN:HG2	1.89	0.54
1:B:155:LEU:HD21	1:B:183:PHE:HE2	1.73	0.54
1:C:171:LEU:H	1:C:171:LEU:CD1	2.20	0.54
1:A:66:VAL:HG23	1:A:101:ILE:HD12	1.88	0.54
1:A:104:CYS:O	1:A:110:MET:HA	2.08	0.54
1:B:126:LEU:HD13	1:B:233:GLU:O	2.07	0.54
1:C:72:THR:N	1:C:73:PRO:CD	2.71	0.54
1:D:197:LEU:HD23	1:D:197:LEU:H	1.73	0.54
1:B:197:LEU:H	1:B:197:LEU:HD23	1.72	0.54
1:D:162:HIS:O	1:D:162:HIS:ND1	2.38	0.54
1:A:130:ASP:O	1:A:131:LEU:HB3	2.06	0.54
1:A:229:VAL:HG11	1:A:241:ILE:HD12	1.89	0.54
1:C:277:ILE:HG21	1:C:282:LEU:HD13	1.88	0.54
1:D:96:HIS:HD2	1:D:150:ARG:HB3	1.71	0.54
1:D:209:ASP:HB3	1:D:212:TYR:CB	2.37	0.54
1:C:51:VAL:HG22	2:G:157:ASP:HB3	1.90	0.54
1:D:48:GLY:HA3	1:D:55:VAL:HB	1.88	0.54
1:D:232:PHE:CB	1:D:252:LEU:HD21	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HD2	1:A:252:LEU:HB2	1.90	0.53
1:B:161:ILE:HG21	1:B:218:LEU:HD11	1.90	0.53
2:G:130:ASN:O	2:G:134:GLN:HG2	2.08	0.53
1:B:236:CYS:O	1:B:271:PRO:HD3	2.08	0.53
2:E:183:ARG:HB2	2:H:183:ARG:CZ	2.37	0.53
2:F:183:ARG:HD3	2:G:183:ARG:HD3	1.89	0.53
1:C:238:ARG:C	1:C:240:ALA:N	2.61	0.53
2:F:176:MET:HA	2:F:180:GLY:HA2	1.89	0.53
1:A:238:ARG:C	1:A:240:ALA:N	2.57	0.53
1:B:169:ASN:O	1:B:181:THR:HG22	2.08	0.53
2:H:133:VAL:HG22	2:H:195:LEU:HD12	1.91	0.53
1:C:277:ILE:CG2	1:C:282:LEU:HB2	2.38	0.53
1:A:127:TYR:CD2	1:A:128:GLY:N	2.77	0.53
1:C:89:LEU:HD23	1:C:100:LEU:HD12	1.92	0.52
1:D:72:THR:N	1:D:73:PRO:CD	2.72	0.52
1:A:66:VAL:HG21	1:A:113:ILE:CG2	2.39	0.52
1:A:136:MET:O	1:A:141:ARG:NH1	2.43	0.52
1:C:209:ASP:O	1:C:212:TYR:HB3	2.09	0.52
1:D:238:ARG:O	1:D:240:ALA:N	2.28	0.52
1:A:232:PHE:HB2	1:A:252:LEU:HD21	1.92	0.52
1:D:119:ASN:HB2	1:D:172:LEU:HB2	1.91	0.52
1:C:66:VAL:HG21	1:C:113:ILE:CG2	2.39	0.52
1:B:211:GLU:O	1:B:215:LYS:HB2	2.09	0.52
1:A:180:ILE:HD13	1:A:180:ILE:N	2.24	0.52
1:A:238:ARG:HD2	1:A:252:LEU:CD1	2.39	0.52
1:C:117:MET:CG	1:C:171:LEU:HD23	2.38	0.52
2:E:167:ASN:O	2:E:171:GLN:HG3	2.10	0.52
1:B:238:ARG:C	1:B:240:ALA:N	2.64	0.52
1:C:94:HIS:ND1	1:C:95:PRO:CD	2.73	0.52
1:D:271:PRO:HD2	1:D:273:LEU:HD12	1.91	0.52
1:B:289:ALA:O	1:B:293:LEU:HG	2.10	0.52
1:C:171:LEU:CD1	1:C:181:THR:HG21	2.39	0.52
1:C:221:LYS:O	1:C:224:VAL:HB	2.09	0.52
1:D:159:ALA:HB2	1:D:192:LEU:HA	1.92	0.52
1:B:259:SER:O	1:B:264:GLN:N	2.41	0.52
1:C:94:HIS:HD2	1:C:154:TYR:CG	2.28	0.52
1:D:170:ILE:O	1:D:170:ILE:HG22	2.10	0.52
2:H:151:ARG:HG2	2:H:155:ASN:ND2	2.25	0.52
1:C:94:HIS:CD2	1:C:154:TYR:CG	2.98	0.51
1:D:166:LYS:HB2	1:D:207:TYR:CZ	2.44	0.51
1:A:163:ARG:NH2	1:A:202:LYS:HD2	2.26	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:CB	1:A:271:PRO:HD2	2.40	0.51
1:B:240:ALA:CB	1:D:245:LEU:HB3	2.26	0.51
2:E:195:LEU:O	2:E:199:VAL:HG23	2.10	0.51
1:C:117:MET:HG3	1:C:171:LEU:CD2	2.41	0.51
1:D:94:HIS:CD2	1:D:154:TYR:CG	2.98	0.51
2:F:148:ASN:HA	2:F:151:ARG:NH1	2.25	0.51
1:A:232:PHE:CB	1:A:252:LEU:HD21	2.40	0.51
1:A:72:THR:N	1:A:73:PRO:CD	2.74	0.51
1:A:139:GLU:O	1:A:142:LEU:N	2.43	0.51
1:B:240:ALA:O	1:B:241:ILE:HG23	2.11	0.51
1:C:243:GLN:HG3	1:C:246:PRO:CD	2.40	0.51
2:F:151:ARG:HG2	2:F:155:ASN:HD21	1.75	0.51
1:A:277:ILE:CG2	1:A:282:LEU:HB2	2.41	0.51
1:D:91:PHE:CB	1:D:158:ARG:HH12	2.22	0.51
1:A:150:ARG:HD3	1:A:307:LEU:HD21	1.94	0.50
1:A:180:ILE:HG22	1:A:181:THR:N	2.26	0.50
2:H:151:ARG:HG2	2:H:155:ASN:HD21	1.77	0.50
1:C:82:PHE:CE2	1:C:112:LEU:HG	2.46	0.50
1:B:72:THR:H	1:B:73:PRO:HD3	1.77	0.50
1:B:94:HIS:HB3	1:B:97:LEU:HB2	1.93	0.50
1:C:90:SER:C	1:C:92:CYS:N	2.65	0.50
1:C:171:LEU:HD12	1:C:171:LEU:H	1.76	0.50
2:G:147:ARG:NH1	2:G:196:ARG:HG3	2.27	0.50
1:B:66:VAL:CG2	1:B:114:TYR:O	2.60	0.50
1:B:236:CYS:O	1:B:237:ALA:HB3	2.12	0.50
1:B:89:LEU:HD23	1:B:100:LEU:HB2	1.93	0.50
1:B:164:ASP:O	1:B:169:ASN:ND2	2.45	0.50
1:C:221:LYS:CE	1:C:300:ARG:O	2.60	0.50
1:D:146:ILE:HG12	1:D:310:LEU:HB3	1.92	0.50
1:B:43:HIS:HD2	1:B:56:TYR:CE1	2.30	0.49
1:B:135:SER:HB3	1:D:247:ARG:NH2	2.25	0.49
1:C:66:VAL:HG21	1:C:113:ILE:HG22	1.94	0.49
1:C:127:TYR:O	1:C:239:SER:CB	2.61	0.49
1:A:55:VAL:HA	1:A:68:LEU:O	2.12	0.49
1:A:66:VAL:CG2	1:A:113:ILE:CG2	2.90	0.49
1:C:166:LYS:HB2	1:C:207:TYR:CZ	2.47	0.49
1:A:155:LEU:HD23	1:A:160:ILE:CG2	2.42	0.49
1:A:270:ASP:HB2	1:A:271:PRO:CD	2.42	0.49
1:B:79:ILE:HG13	1:B:110:MET:CE	2.42	0.49
1:B:238:ARG:O	1:B:240:ALA:N	2.45	0.49
1:C:66:VAL:CG2	1:C:113:ILE:CG2	2.90	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:HIS:CD2	1:D:220:GLU:HB2	2.47	0.49
1:D:238:ARG:C	1:D:240:ALA:N	2.63	0.49
1:D:85:GLU:O	1:D:89:LEU:HB3	2.12	0.49
1:B:228:GLY:O	1:B:231:LEU:HB2	2.12	0.49
1:C:171:LEU:N	1:C:171:LEU:CD1	2.75	0.49
1:C:236:CYS:SG	1:C:269:VAL:HG12	2.51	0.49
1:C:240:ALA:O	1:C:241:ILE:HG23	2.13	0.49
1:C:240:ALA:O	1:C:242:VAL:N	2.44	0.49
1:D:97:LEU:HD11	1:D:155:LEU:CD1	2.43	0.49
1:D:224:VAL:HG21	1:D:301:PRO:O	2.12	0.49
1:D:89:LEU:HD23	1:D:100:LEU:HD12	1.95	0.49
1:B:171:LEU:HD11	1:B:181:THR:HG21	1.94	0.49
1:A:251:ASN:HB3	1:A:254:GLU:HB2	1.95	0.49
1:A:162:HIS:HD2	1:A:180:ILE:HG21	1.76	0.48
1:B:51:VAL:HG22	2:E:157:ASP:HB3	1.95	0.48
1:C:89:LEU:HD11	1:C:98:VAL:O	2.12	0.48
1:A:195:THR:HB	1:A:197:LEU:CD2	2.43	0.48
1:A:264:GLN:HB3	1:A:266:GLU:CG	2.43	0.48
1:D:264:GLN:CD	1:D:266:GLU:HG2	2.34	0.48
1:A:94:HIS:CD2	1:A:154:TYR:CD1	3.01	0.48
1:B:257:VAL:HG12	1:B:258:GLU:N	2.29	0.48
1:B:270:ASP:HB2	1:B:271:PRO:HD2	1.95	0.48
1:A:98:VAL:HG23	1:A:180:ILE:O	2.13	0.48
1:A:221:LYS:HD2	1:A:300:ARG:HB2	1.95	0.48
1:B:240:ALA:O	1:B:242:VAL:N	2.46	0.48
1:B:286:GLY:O	1:B:290:VAL:HG23	2.12	0.48
1:D:238:ARG:HD2	1:D:252:LEU:CD1	2.42	0.48
1:A:127:TYR:CD1	1:C:246:PRO:O	2.67	0.48
1:D:98:VAL:HG23	1:D:180:ILE:O	2.13	0.48
1:B:247:ARG:HG3	1:B:249:MET:H	1.79	0.48
1:D:232:PHE:O	1:D:234:VAL:N	2.47	0.48
1:B:206:GLY:C	1:B:241:ILE:HD11	2.33	0.48
1:B:265:LEU:HD11	1:B:283:ARG:HG3	1.96	0.48
2:H:189:ILE:HG23	2:H:192:ARG:HH12	1.78	0.48
1:D:306:VAL:O	1:D:310:LEU:HG	2.14	0.48
1:B:219:THR:O	1:B:221:LYS:N	2.47	0.47
1:D:232:PHE:C	1:D:234:VAL:N	2.66	0.47
1:B:90:SER:C	1:B:92:CYS:H	2.16	0.47
1:C:36:GLU:HB2	1:C:103:PHE:CE1	2.48	0.47
1:D:211:GLU:HG3	1:D:215:LYS:HD2	1.96	0.47
1:D:262:ASN:O	1:D:264:GLN:N	2.41	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:VAL:O	2:F:137:VAL:HG23	2.14	0.47
1:B:74:GLU:CD	1:B:74:GLU:N	2.68	0.47
1:B:171:LEU:N	1:B:171:LEU:CD1	2.77	0.47
1:C:55:VAL:HA	1:C:68:LEU:O	2.13	0.47
2:F:148:ASN:HA	2:F:151:ARG:HH12	1.77	0.47
1:A:247:ARG:C	1:A:249:MET:H	2.17	0.47
1:B:136:MET:O	1:B:141:ARG:NH1	2.46	0.47
1:C:98:VAL:HG23	1:C:180:ILE:O	2.13	0.47
1:B:72:THR:N	1:B:73:PRO:HD3	2.28	0.47
1:D:302:SER:O	1:D:304:GLY:N	2.48	0.47
1:A:238:ARG:O	1:A:238:ARG:HD3	2.14	0.47
1:D:238:ARG:HB3	1:D:252:LEU:CD1	2.43	0.47
1:A:156:HIS:CD2	1:A:220:GLU:HB2	2.50	0.47
1:B:144:ILE:HA	1:B:178:PRO:CG	2.45	0.47
2:F:133:VAL:HA	2:F:136:LEU:HD12	1.95	0.47
1:C:203:GLY:HA3	1:C:208:ILE:HD11	1.97	0.47
1:D:55:VAL:HA	1:D:68:LEU:O	2.15	0.47
1:C:122:LEU:HD21	1:C:234:VAL:HG22	1.96	0.47
1:C:161:ILE:HD11	1:C:197:LEU:HD21	1.96	0.47
1:A:45:PHE:HA	1:A:56:TYR:CE2	2.49	0.47
1:A:260:HIS:HA	1:A:265:LEU:HA	1.96	0.47
1:B:83:GLU:O	1:B:87:GLU:HG2	2.15	0.47
1:B:144:ILE:HA	1:B:178:PRO:HG3	1.96	0.47
1:C:171:LEU:O	1:C:172:LEU:HD23	2.15	0.47
1:C:161:ILE:HG21	1:C:218:LEU:HD11	1.97	0.46
1:D:104:CYS:O	1:D:110:MET:HA	2.15	0.46
1:D:277:ILE:HG22	1:D:282:LEU:HB2	1.96	0.46
2:E:134:GLN:HA	2:E:134:GLN:NE2	2.30	0.46
1:C:48:GLY:HA3	1:C:55:VAL:HB	1.97	0.46
1:C:68:LEU:HD13	1:C:113:ILE:HG23	1.98	0.46
1:D:273:LEU:HD13	1:D:277:ILE:HD11	1.97	0.46
1:A:149:ALA:HB3	1:A:307:LEU:HD13	1.97	0.46
1:D:164:ASP:OD2	1:D:169:ASN:ND2	2.46	0.46
1:A:228:GLY:HA2	1:A:231:LEU:HD12	1.97	0.46
1:C:93:ARG:HG3	1:C:93:ARG:HH11	1.80	0.46
1:C:199:TPO:OG1	1:C:200:VAL:N	2.48	0.46
1:C:247:ARG:HB3	1:C:248:GLU:H	1.39	0.46
2:G:131:SER:O	2:G:134:GLN:HB2	2.16	0.46
1:A:221:LYS:O	1:A:224:VAL:N	2.48	0.46
1:C:142:LEU:HD21	1:C:285:PHE:CD1	2.49	0.46
1:C:266:GLU:CB	1:C:269:VAL:HG23	2.42	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HG23	1:D:178:PRO:HB3	1.97	0.46
1:A:146:ILE:CD1	1:A:311:GLU:HA	2.46	0.46
1:A:162:HIS:CE1	1:A:182:ASP:O	2.69	0.46
1:B:55:VAL:HA	1:B:68:LEU:O	2.15	0.46
1:D:145:CYS:SG	1:D:231:LEU:HD23	2.55	0.46
1:B:199:TPO:OG1	1:B:200:VAL:N	2.49	0.46
1:A:251:ASN:HD22	2:F:178:MET:HB3	1.79	0.46
1:D:288:THR:O	1:D:291:LYS:N	2.49	0.46
1:A:240:ALA:O	1:A:241:ILE:HG23	2.15	0.46
1:C:277:ILE:HG21	1:C:282:LEU:HB2	1.97	0.46
1:D:31:LEU:O	1:D:32:VAL:HG23	2.16	0.46
1:D:180:ILE:HG22	1:D:181:THR:N	2.30	0.46
1:C:144:ILE:HA	1:C:178:PRO:CG	2.46	0.46
1:B:211:GLU:CG	1:B:215:LYS:HD2	2.46	0.45
1:A:77:GLN:C	1:A:79:ILE:H	2.20	0.45
1:A:77:GLN:HE21	1:A:80:GLU:H	1.65	0.45
1:A:208:ILE:HG22	1:A:209:ASP:O	2.16	0.45
1:A:249:MET:HB2	1:A:255:TRP:NE1	2.30	0.45
2:H:147:ARG:NH1	2:H:196:ARG:HG3	2.31	0.45
1:A:96:HIS:O	1:A:97:LEU:HD12	2.17	0.45
1:A:209:ASP:HB3	1:A:212:TYR:CB	2.47	0.45
1:A:242:VAL:CG2	2:F:179:HIS:HA	2.47	0.45
1:A:277:ILE:HG21	1:A:282:LEU:HB2	1.98	0.45
1:B:122:LEU:HD21	1:B:234:VAL:HG22	1.99	0.45
1:B:135:SER:CB	1:D:247:ARG:NH2	2.79	0.45
1:C:47:ILE:HG13	1:C:48:GLY:H	1.82	0.45
2:F:147:ARG:NH1	2:F:196:ARG:HG3	2.31	0.45
1:A:162:HIS:CD2	1:A:180:ILE:HG21	2.52	0.45
1:A:270:ASP:CB	1:A:271:PRO:CD	2.94	0.45
1:D:243:GLN:O	1:D:250:VAL:HG23	2.17	0.45
1:A:177:VAL:HA	1:A:178:PRO:HD2	1.83	0.45
1:C:40:ASN:CG	1:C:41:PHE:N	2.71	0.45
1:B:66:VAL:HG13	1:B:68:LEU:HD21	1.99	0.45
1:B:166:LYS:NZ	1:B:204:THR:OG1	2.35	0.45
1:C:301:PRO:HB2	1:C:305:ASP:HB2	1.99	0.45
1:A:69:LYS:HD3	1:A:71:ARG:HH21	1.82	0.44
1:A:264:GLN:HB3	1:A:266:GLU:HG2	1.99	0.44
1:B:36:GLU:HB2	1:B:103:PHE:CE1	2.52	0.44
1:C:77:GLN:HE21	1:C:80:GLU:CB	2.13	0.44
1:C:101:ILE:HD11	1:C:115:LYS:HG3	1.99	0.44
1:D:118:GLU:HG3	1:D:174:GLU:HG2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:CYS:O	1:D:237:ALA:CB	2.64	0.44
2:E:133:VAL:HG22	2:E:195:LEU:HD12	1.99	0.44
1:A:119:ASN:HB2	1:A:172:LEU:HB2	1.99	0.44
1:A:121:ASN:HA	1:A:171:LEU:HA	1.97	0.44
1:B:247:ARG:HG2	1:B:249:MET:HG2	1.99	0.44
1:D:221:LYS:CB	1:D:297:SER:HB2	2.47	0.44
2:E:166:GLN:HE21	2:E:170:ARG:HH21	1.65	0.44
1:B:117:MET:HG3	1:B:171:LEU:HB3	2.00	0.44
1:B:211:GLU:HG3	1:B:215:LYS:HD2	1.98	0.44
1:C:82:PHE:HE2	1:C:112:LEU:HG	1.80	0.44
1:A:232:PHE:C	1:A:234:VAL:N	2.71	0.44
1:A:302:SER:C	1:A:304:GLY:H	2.21	0.44
1:B:117:MET:HG3	1:B:171:LEU:HD23	2.00	0.44
1:C:72:THR:N	1:C:73:PRO:HD3	2.32	0.44
1:C:190:THR:C	1:C:192:LEU:H	2.20	0.44
1:D:94:HIS:HD2	1:D:154:TYR:CD2	2.35	0.44
2:G:195:LEU:O	2:G:199:VAL:HG23	2.17	0.44
1:A:170:ILE:O	1:A:170:ILE:CG2	2.62	0.44
1:A:190:THR:N	1:A:195:THR:HG21	2.33	0.44
1:C:144:ILE:HA	1:C:178:PRO:HG3	1.99	0.44
1:D:68:LEU:N	1:D:68:LEU:HD22	2.32	0.44
2:G:126:VAL:HG22	2:G:190:GLU:CD	2.38	0.44
1:C:270:ASP:HB2	1:C:271:PRO:CD	2.47	0.44
1:D:232:PHE:O	1:D:235:LEU:N	2.50	0.44
1:B:138:TRP:CH2	1:B:285:PHE:CD1	3.06	0.44
1:C:96:HIS:O	1:C:97:LEU:HD12	2.18	0.44
1:C:206:GLY:C	1:C:241:ILE:HD11	2.38	0.44
1:C:211:GLU:HG2	1:C:215:LYS:HD2	2.00	0.44
1:D:270:ASP:CB	1:D:271:PRO:CD	2.95	0.44
2:G:133:VAL:HA	2:G:136:LEU:HD12	2.00	0.44
2:G:176:MET:N	2:G:177:PRO:CD	2.81	0.44
1:D:251:ASN:O	1:D:254:GLU:N	2.43	0.43
2:H:193:GLY:HA2	2:H:196:ARG:NH1	2.33	0.43
1:A:142:LEU:HD13	1:A:314:LEU:HA	2.00	0.43
1:A:278:ARG:HG2	1:A:279:PRO:HD2	2.00	0.43
1:C:92:CYS:SG	1:C:99:SER:HA	2.58	0.43
1:C:156:HIS:HE1	1:C:303:MET:HG2	1.78	0.43
1:C:171:LEU:CD1	1:C:181:THR:CG2	2.96	0.43
1:C:236:CYS:O	1:C:271:PRO:HD3	2.18	0.43
1:C:271:PRO:C	1:C:273:LEU:H	2.22	0.43
1:D:158:ARG:O	1:D:160:ILE:HG13	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:GLU:HA	2:F:189:ILE:HD12	2.00	0.43
1:C:204:THR:O	1:C:208:ILE:HG12	2.18	0.43
1:C:212:TYR:C	1:C:212:TYR:CD1	2.90	0.43
1:D:47:ILE:HG13	1:D:48:GLY:H	1.83	0.43
1:B:173:ASP:OD1	1:B:177:VAL:HG23	2.18	0.43
1:A:243:GLN:HE21	1:A:245:LEU:N	2.17	0.43
1:C:203:GLY:CA	1:C:208:ILE:HD11	2.49	0.43
1:D:66:VAL:HG23	1:D:101:ILE:HD12	2.00	0.43
1:B:93:ARG:HD2	1:B:93:ARG:HA	1.22	0.43
1:B:98:VAL:HG21	1:B:181:THR:HB	2.00	0.43
1:C:41:PHE:C	1:C:41:PHE:CD1	2.92	0.43
1:C:136:MET:O	1:C:141:ARG:NH1	2.50	0.43
1:D:165:VAL:HB	1:D:226:SER:HB3	2.01	0.43
1:D:284:LYS:HE2	1:D:312:TYR:CD2	2.50	0.43
1:A:150:ARG:HD3	1:A:307:LEU:HD11	2.00	0.43
1:A:302:SER:O	1:A:304:GLY:N	2.51	0.43
1:B:139:GLU:O	1:B:142:LEU:N	2.51	0.43
1:C:74:GLU:C	1:C:76:SER:H	2.22	0.43
1:D:94:HIS:HD2	1:D:154:TYR:CG	2.36	0.43
1:A:164:ASP:OD2	1:A:169:ASN:ND2	2.48	0.43
1:A:245:LEU:HD13	1:C:240:ALA:HA	2.00	0.43
1:C:156:HIS:CE1	1:C:303:MET:CG	3.01	0.43
1:C:201:VAL:HB	2:G:166:GLN:OE1	2.18	0.43
1:C:238:ARG:NH2	1:C:250:VAL:O	2.52	0.43
1:D:231:LEU:O	1:D:234:VAL:HB	2.19	0.43
2:H:136:LEU:O	2:H:141:ALA:N	2.52	0.43
1:A:70:ARG:HD2	1:A:109:GLU:OE1	2.18	0.43
1:A:265:LEU:HD21	1:A:283:ARG:HG3	2.01	0.43
1:B:146:ILE:O	1:B:149:ALA:HB3	2.18	0.43
1:C:41:PHE:C	1:C:41:PHE:HD1	2.21	0.43
1:A:46:LEU:HD13	1:A:57:LYS:HB3	2.01	0.43
1:B:94:HIS:CD2	1:B:154:TYR:CG	3.07	0.43
1:D:136:MET:CG	1:D:140:GLN:HG2	2.45	0.43
1:D:242:VAL:O	1:D:242:VAL:HG13	2.18	0.43
1:D:263:GLY:O	1:D:264:GLN:CB	2.66	0.43
1:A:190:THR:H	1:A:195:THR:HG21	1.85	0.42
1:C:127:TYR:C	1:C:127:TYR:CD2	2.92	0.42
1:C:158:ARG:HE	1:C:158:ARG:HB3	1.63	0.42
1:D:47:ILE:HD13	1:D:116:TYR:HE1	1.84	0.42
1:D:84:THR:O	1:D:88:THR:HB	2.18	0.42
2:E:154:MET:HG2	2:E:181:ILE:HG22	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:C	1:B:91:PHE:N	2.71	0.42
1:B:96:HIS:HD2	1:B:150:ARG:HB3	1.82	0.42
1:D:36:GLU:HB2	1:D:103:PHE:CE1	2.54	0.42
1:D:53:GLY:HA2	1:D:73:PRO:HD2	2.01	0.42
1:D:85:GLU:HG3	1:D:183:PHE:HB2	2.00	0.42
2:E:147:ARG:NH1	2:E:196:ARG:HG3	2.34	0.42
2:F:135:GLN:O	2:F:139:GLU:N	2.44	0.42
2:H:126:VAL:HG22	2:H:190:GLU:CD	2.40	0.42
1:A:243:GLN:NE2	1:A:244:SER:N	2.67	0.42
1:B:89:LEU:CD2	1:B:100:LEU:HB2	2.49	0.42
1:D:240:ALA:O	1:D:241:ILE:HG23	2.19	0.42
2:G:164:VAL:O	2:G:168:ILE:HG13	2.19	0.42
1:A:117:MET:CG	1:A:171:LEU:HD23	2.46	0.42
1:A:226:SER:O	1:A:230:VAL:HG23	2.19	0.42
1:A:235:LEU:HB2	1:A:285:PHE:HE2	1.84	0.42
1:C:33:ASP:OD1	1:C:34:LEU:N	2.52	0.42
1:C:96:HIS:HD2	1:C:150:ARG:HB3	1.83	0.42
1:C:221:LYS:HE2	1:C:300:ARG:O	2.19	0.42
1:C:245:LEU:H	1:C:246:PRO:CD	2.31	0.42
1:A:158:ARG:HE	1:A:158:ARG:HB3	1.49	0.42
1:A:187:LYS:HG2	1:A:197:LEU:HD11	2.01	0.42
1:A:232:PHE:O	1:A:234:VAL:N	2.52	0.42
1:A:241:ILE:HG12	1:A:242:VAL:N	2.33	0.42
1:B:96:HIS:NE2	1:B:147:GLY:HA2	2.34	0.42
1:B:198:SEP:HB3	1:B:216:GLY:O	2.19	0.42
1:A:238:ARG:HD2	1:A:252:LEU:HD13	2.01	0.42
1:A:273:LEU:HD13	1:A:277:ILE:HD11	2.00	0.42
2:E:136:LEU:O	2:E:141:ALA:N	2.51	0.42
1:A:183:PHE:O	1:A:185:ILE:N	2.52	0.42
1:A:236:CYS:O	1:A:237:ALA:CB	2.66	0.42
1:D:283:ARG:O	1:D:287:ASP:HB2	2.20	0.42
1:B:74:GLU:O	1:B:76:SER:N	2.46	0.42
1:B:202:LYS:O	1:B:208:ILE:CD1	2.67	0.42
1:B:278:ARG:O	1:B:280:GLU:N	2.53	0.42
1:C:236:CYS:O	1:C:237:ALA:HB3	2.18	0.42
1:D:252:LEU:C	1:D:252:LEU:HD23	2.40	0.42
1:B:94:HIS:HD2	1:B:154:TYR:CD2	2.38	0.42
1:D:238:ARG:O	1:D:238:ARG:HD3	2.19	0.42
1:A:187:LYS:HG3	1:A:188:LYS:N	2.35	0.42
1:C:74:GLU:N	1:C:74:GLU:CD	2.73	0.42
1:C:117:MET:HG3	1:C:171:LEU:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ARG:HA	1:C:279:PRO:HD2	1.72	0.42
1:D:97:LEU:HD11	1:D:155:LEU:HD11	2.02	0.42
1:A:288:THR:O	1:A:291:LYS:N	2.53	0.41
1:C:93:ARG:HA	1:C:93:ARG:HD3	1.27	0.41
1:C:126:LEU:HD21	1:C:234:VAL:HG13	2.02	0.41
1:D:68:LEU:HD12	1:D:113:ILE:HG12	2.01	0.41
1:D:85:GLU:OE2	1:D:114:TYR:OH	2.31	0.41
1:D:285:PHE:CD2	1:D:285:PHE:C	2.94	0.41
2:F:151:ARG:HG2	2:F:155:ASN:ND2	2.35	0.41
1:A:68:LEU:CD1	1:A:113:ILE:HG12	2.49	0.41
1:B:142:LEU:HD21	1:B:285:PHE:CD1	2.56	0.41
1:A:146:ILE:HD13	1:A:311:GLU:HA	2.00	0.41
1:A:238:ARG:HB3	1:A:252:LEU:CD1	2.51	0.41
1:A:302:SER:C	1:A:304:GLY:N	2.73	0.41
1:B:200:VAL:O	1:B:202:LYS:HG3	2.20	0.41
1:B:219:THR:C	1:B:221:LYS:N	2.74	0.41
1:C:238:ARG:HG3	1:C:238:ARG:HH11	1.85	0.41
2:G:167:ASN:O	2:G:171:GLN:HG3	2.19	0.41
1:A:98:VAL:HG21	1:A:181:THR:HB	2.03	0.41
1:B:78:GLY:O	1:B:82:PHE:HB2	2.20	0.41
2:F:147:ARG:CG	2:F:195:LEU:HB3	2.50	0.41
1:A:163:ARG:NH1	1:A:185:ILE:O	2.53	0.41
1:B:89:LEU:C	1:B:91:PHE:H	2.23	0.41
1:B:197:LEU:HD23	1:B:218:LEU:O	2.20	0.41
1:B:245:LEU:H	1:B:246:PRO:CD	2.33	0.41
1:C:36:GLU:HB2	1:C:103:PHE:CZ	2.56	0.41
1:C:205:LEU:HD21	2:G:180:GLY:CA	2.45	0.41
2:E:133:VAL:O	2:E:137:VAL:HG23	2.21	0.41
1:A:257:VAL:O	1:A:261:ASN:HB3	2.20	0.41
1:A:278:ARG:CG	1:A:279:PRO:HD2	2.50	0.41
1:B:40:ASN:CG	1:B:41:PHE:N	2.73	0.41
1:B:259:SER:O	1:B:265:LEU:N	2.46	0.41
1:C:85:GLU:O	1:C:89:LEU:HB3	2.20	0.41
1:D:195:THR:HB	1:D:197:LEU:CD2	2.51	0.41
1:D:220:GLU:O	1:D:223:ASP:HB2	2.21	0.41
1:A:287:ASP:O	1:A:291:LYS:HG3	2.21	0.41
1:C:226:SER:O	1:C:230:VAL:HG23	2.21	0.41
1:D:141:ARG:O	1:D:145:CYS:HB2	2.21	0.41
1:A:94:HIS:ND1	1:A:95:PRO:HD2	2.36	0.41
1:C:71:ARG:HB2	1:C:110:MET:HG3	2.02	0.41
1:D:91:PHE:O	1:D:93:ARG:N	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG12	1:A:32:VAL:O	2.21	0.41
1:A:39:ASN:ND2	1:A:106:GLU:OE2	2.54	0.41
1:A:106:GLU:HG2	1:A:107:ARG:HG3	2.03	0.41
1:A:127:TYR:CE2	1:C:244:SER:O	2.73	0.41
1:A:259:SER:HB3	1:A:266:GLU:HB2	2.03	0.41
1:B:142:LEU:HD21	1:B:285:PHE:HD1	1.86	0.41
1:B:161:ILE:HD13	1:B:218:LEU:HG	2.03	0.41
1:C:138:TRP:CD1	1:C:277:ILE:HG12	2.56	0.41
1:D:82:PHE:CE2	1:D:112:LEU:HG	2.55	0.41
1:D:229:VAL:HG22	1:D:253:ALA:HB2	2.01	0.41
2:H:133:VAL:HG21	2:H:194:ALA:HB1	2.02	0.41
1:B:122:LEU:HD13	1:B:144:ILE:HG21	2.03	0.41
1:C:70:ARG:HG2	1:C:111:ILE:HG12	2.03	0.41
1:D:207:TYR:O	1:D:208:ILE:C	2.59	0.41
1:A:199:TPO:OG1	1:A:200:VAL:N	2.54	0.40
1:C:98:VAL:HG12	1:C:114:TYR:HD2	1.86	0.40
1:C:271:PRO:HB2	1:C:272:ASN:H	1.71	0.40
1:C:117:MET:O	1:C:119:ASN:N	2.55	0.40
1:C:132:PRO:C	1:C:134:MET:N	2.74	0.40
1:C:240:ALA:CB	1:C:243:GLN:HB2	2.50	0.40
1:D:173:ASP:OD2	1:D:177:VAL:HB	2.21	0.40
1:D:205:LEU:HD12	1:D:205:LEU:HA	1.96	0.40
1:A:39:ASN:ND2	1:A:106:GLU:CD	2.75	0.40
1:B:98:VAL:HG22	1:B:179:LYS:HB3	2.03	0.40
1:B:245:LEU:H	1:B:246:PRO:HD3	1.85	0.40
1:C:200:VAL:O	1:C:202:LYS:HG3	2.22	0.40
2:E:164:VAL:O	2:E:168:ILE:HG13	2.21	0.40
2:E:182:SER:HB3	2:E:185:SER:HB2	2.02	0.40
2:F:183:ARG:HB2	2:G:183:ARG:NH1	2.36	0.40
2:H:176:MET:HA	2:H:180:GLY:CA	2.49	0.40
1:A:197:LEU:H	1:A:197:LEU:CD2	2.30	0.40
1:C:132:PRO:C	1:C:134:MET:H	2.24	0.40
1:D:238:ARG:HD3	1:D:240:ALA:HB3	2.03	0.40
1:D:251:ASN:HB3	1:D:254:GLU:HB2	2.04	0.40
1:B:161:ILE:CD1	1:B:197:LEU:HD21	2.51	0.40
1:C:121:ASN:HA	1:C:171:LEU:HA	2.03	0.40
1:C:238:ARG:O	1:C:238:ARG:CD	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	284/327 (87%)	209 (74%)	54 (19%)	21 (7%)	1	7
1	B	284/327 (87%)	194 (68%)	63 (22%)	27 (10%)	0	4
1	C	282/327 (86%)	201 (71%)	60 (21%)	21 (7%)	1	7
1	D	284/327 (87%)	209 (74%)	49 (17%)	26 (9%)	1	4
2	E	75/85 (88%)	62 (83%)	11 (15%)	2 (3%)	5	26
2	F	75/85 (88%)	62 (83%)	11 (15%)	2 (3%)	5	26
2	G	75/85 (88%)	61 (81%)	12 (16%)	2 (3%)	5	26
2	H	75/85 (88%)	67 (89%)	6 (8%)	2 (3%)	5	26
All	All	1434/1648 (87%)	1065 (74%)	266 (18%)	103 (7%)	1	7

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	47	ILE
1	A	92	CYS
1	B	39	ASN
1	B	47	ILE
1	B	51	VAL
1	B	184	GLY
1	C	39	ASN
1	C	47	ILE
1	C	51	VAL
1	C	127	TYR
1	C	263	GLY
1	D	39	ASN
1	D	47	ILE
1	D	92	CYS
1	D	239	SER
1	D	264	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	181	ILE
2	F	181	ILE
2	G	181	ILE
2	H	181	ILE
1	A	128	GLY
1	A	129	SER
1	A	159	ALA
1	A	171	LEU
1	A	184	GLY
1	A	239	SER
1	A	241	ILE
1	A	247	ARG
1	A	264	GLN
1	B	40	ASN
1	B	74	GLU
1	B	92	CYS
1	B	124	ARG
1	B	128	GLY
1	B	220	GLU
1	B	239	SER
1	B	241	ILE
1	B	246	PRO
1	B	261	ASN
1	C	40	ASN
1	C	92	CYS
1	C	118	GLU
1	C	192	LEU
1	C	239	SER
1	C	241	ILE
1	C	245	LEU
1	C	246	PRO
1	D	51	VAL
1	D	128	GLY
1	D	163	ARG
1	D	241	ILE
1	D	247	ARG
1	D	263	GLY
1	D	303	MET
2	E	180	GLY
2	F	180	GLY
2	H	180	GLY
1	A	163	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	245	LEU
1	B	43	HIS
1	B	182	ASP
1	B	271	PRO
1	B	295	LEU
1	C	124	ARG
1	C	128	GLY
1	C	132	PRO
1	C	182	ASP
1	C	191	GLU
1	D	34	LEU
1	D	184	GLY
1	D	233	GLU
1	D	245	LEU
2	G	180	GLY
1	A	40	ASN
1	A	182	ASP
1	A	233	GLU
1	A	271	PRO
1	A	303	MET
1	B	245	LEU
1	C	131	LEU
1	C	271	PRO
1	C	274	ALA
1	D	40	ASN
1	D	130	ASP
1	D	131	LEU
1	D	167	SER
1	D	262	ASN
1	A	246	PRO
1	B	131	LEU
1	B	174	GLU
1	B	191	GLU
1	D	271	PRO
1	A	131	LEU
1	B	75	SER
1	D	32	VAL
1	D	127	TYR
1	B	178	PRO
1	D	208	ILE
1	D	246	PRO
1	B	132	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	208	ILE
1	B	279	PRO

### 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	251/287 (88%)	230 (92%)	21 (8%)	11	35
1	B	251/287 (88%)	221 (88%)	30 (12%)	5	20
1	C	249/287 (87%)	222 (89%)	27 (11%)	6	24
1	D	251/287 (88%)	235 (94%)	16 (6%)	17	46
2	E	62/68 (91%)	62 (100%)	0	100	100
2	F	62/68 (91%)	62 (100%)	0	100	100
2	G	62/68 (91%)	62 (100%)	0	100	100
2	H	62/68 (91%)	61 (98%)	1 (2%)	62	79
All	All	1250/1420 (88%)	1155 (92%)	95 (8%)	13	39

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	PHE
1	A	42	ASP
1	A	61	ARG
1	A	66	VAL
1	A	70	ARG
1	A	87	GLU
1	A	115	LYS
1	A	136	MET
1	A	150	ARG
1	A	175	ASN
1	A	197	LEU
1	A	219	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	238	ARG
1	A	241	ILE
1	A	242	VAL
1	A	255	TRP
1	A	264	GLN
1	A	270	ASP
1	A	272	ASN
1	A	273	LEU
1	B	33	ASP
1	B	41	PHE
1	B	46	LEU
1	B	68	LEU
1	B	74	GLU
1	B	92	CYS
1	B	93	ARG
1	B	94	HIS
1	B	105	ASP
1	B	115	LYS
1	B	124	ARG
1	B	136	MET
1	B	152	LEU
1	B	195	THR
1	B	197	LEU
1	B	212	TYR
1	B	220	GLU
1	B	238	ARG
1	B	241	ILE
1	B	247	ARG
1	B	248	GLU
1	B	250	VAL
1	B	257	VAL
1	B	264	GLN
1	B	272	ASN
1	B	292	CYS
1	B	312	TYR
1	B	314	LEU
1	B	315	ARG
1	B	317	GLN
1	C	34	LEU
1	C	41	PHE
1	C	42	ASP
1	C	46	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	62	ASP
1	C	70	ARG
1	C	74	GLU
1	C	92	CYS
1	C	93	ARG
1	C	97	LEU
1	C	115	LYS
1	C	124	ARG
1	C	143	GLU
1	C	158	ARG
1	C	197	LEU
1	C	212	TYR
1	C	238	ARG
1	C	241	ILE
1	C	244	SER
1	C	247	ARG
1	C	250	VAL
1	C	264	GLN
1	C	272	ASN
1	C	280	GLU
1	C	287	ASP
1	C	312	TYR
1	C	314	LEU
1	D	32	VAL
1	D	41	PHE
1	D	42	ASP
1	D	46	LEU
1	D	68	LEU
1	D	94	HIS
1	D	124	ARG
1	D	145	CYS
1	D	185	ILE
1	D	195	THR
1	D	197	LEU
1	D	238	ARG
1	D	241	ILE
1	D	270	ASP
1	D	272	ASN
1	D	315	ARG
2	H	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	77	GLN
1	A	262	ASN
1	B	39	ASN
1	B	77	GLN
1	B	243	GLN
1	B	272	ASN
1	B	317	GLN
1	C	39	ASN
1	C	77	GLN
1	C	96	HIS
1	C	156	HIS
1	C	272	ASN
1	C	317	GLN
1	D	77	GLN
1	D	94	HIS
1	D	96	HIS
1	D	119	ASN
1	D	243	GLN
1	D	262	ASN
1	D	272	ASN
2	E	130	ASN
2	E	134	GLN
2	E	155	ASN
2	E	175	ASN
2	F	130	ASN
2	F	134	GLN
2	F	155	ASN
2	G	130	ASN
2	G	134	GLN
2	G	155	ASN
2	H	134	GLN
2	H	155	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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$
1	TPO	B	199	1	8,10,11	1.19	1 (12%)	10,14,16	0.95	0
1	TPO	D	199	1	8,10,11	1.11	1 (12%)	10,14,16	0.99	0
1	SEP	C	198	1	8,9,10	2.18	3 (37%)	8,12,14	1.34	1 (12%)
1	SEP	B	198	1	8,9,10	1.98	3 (37%)	8,12,14	1.73	2 (25%)
1	TPO	A	199	1	8,10,11	0.98	0	10,14,16	1.01	0
1	SEP	D	198	1	8,9,10	1.77	3 (37%)	8,12,14	1.50	2 (25%)
1	SEP	A	198	1	8,9,10	1.87	3 (37%)	8,12,14	1.50	2 (25%)
1	TPO	C	199	1	8,10,11	0.91	0	10,14,16	0.98	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
1	TPO	B	199	1	-	2/9/11/13	-
1	TPO	D	199	1	-	2/9/11/13	-
1	SEP	C	198	1	-	4/5/8/10	-
1	SEP	B	198	1	-	4/5/8/10	-
1	TPO	A	199	1	-	1/9/11/13	-
1	SEP	D	198	1	-	4/5/8/10	-
1	SEP	A	198	1	-	4/5/8/10	-
1	TPO	C	199	1	-	1/9/11/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	SEP	P-O1P	4.65	1.65	1.50
1	B	198	SEP	P-O1P	4.18	1.64	1.50
1	A	198	SEP	P-O1P	3.82	1.62	1.50
1	D	198	SEP	P-O1P	3.69	1.62	1.50
1	C	198	SEP	P-O2P	2.72	1.65	1.54
1	B	199	TPO	P-OG1	2.71	1.64	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	SEP	P-O3P	2.33	1.63	1.54
1	D	199	TPO	P-OG1	2.33	1.63	1.59
1	B	198	SEP	P-O3P	2.32	1.63	1.54
1	B	198	SEP	P-O2P	2.26	1.63	1.54
1	A	198	SEP	P-O3P	2.17	1.63	1.54
1	A	198	SEP	P-O2P	2.17	1.63	1.54
1	D	198	SEP	P-O2P	2.08	1.62	1.54
1	D	198	SEP	P-O3P	2.06	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	SEP	P-OG-CB	-3.72	108.03	118.30
1	C	198	SEP	P-OG-CB	-3.37	109.03	118.30
1	A	198	SEP	OG-CB-CA	2.80	110.87	108.14
1	D	198	SEP	OG-CB-CA	2.56	110.64	108.14
1	D	198	SEP	P-OG-CB	-2.52	111.36	118.30
1	A	198	SEP	P-OG-CB	-2.12	112.46	118.30
1	B	198	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	199	TPO	N-CA-CB-OG1
1	B	198	SEP	N-CA-CB-OG
1	B	198	SEP	CB-OG-P-O1P
1	B	199	TPO	N-CA-CB-OG1
1	C	198	SEP	N-CA-CB-OG
1	C	198	SEP	CB-OG-P-O2P
1	C	198	SEP	CB-OG-P-O3P
1	C	199	TPO	N-CA-CB-OG1
1	D	198	SEP	N-CA-CB-OG
1	D	198	SEP	CB-OG-P-O1P
1	D	198	SEP	CB-OG-P-O2P
1	D	198	SEP	CB-OG-P-O3P
1	D	199	TPO	N-CA-CB-OG1
1	A	198	SEP	CB-OG-P-O1P
1	C	198	SEP	CB-OG-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	198	SEP	CB-OG-P-O3P
1	B	198	SEP	CB-OG-P-O2P
1	B	199	TPO	O-C-CA-CB
1	D	199	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	199	TPO	2	0
1	B	198	SEP	1	0
1	A	199	TPO	1	0
1	C	199	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	286/327 (87%)	0.64	30 (10%) 6 6	48, 81, 109, 115	0
1	B	286/327 (87%)	0.43	21 (7%) 15 15	50, 74, 98, 107	0
1	C	284/327 (86%)	0.47	16 (5%) 24 23	47, 75, 99, 110	0
1	D	286/327 (87%)	0.62	25 (8%) 10 10	50, 82, 103, 109	0
2	E	77/85 (90%)	0.48	4 (5%) 27 25	74, 90, 105, 107	0
2	F	77/85 (90%)	0.62	5 (6%) 18 18	72, 85, 109, 113	0
2	G	77/85 (90%)	0.46	3 (3%) 39 37	83, 102, 113, 115	0
2	H	77/85 (90%)	0.50	7 (9%) 9 9	76, 85, 95, 101	0
All	All	1450/1648 (87%)	0.53	111 (7%) 13 12	47, 81, 105, 115	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	194	ALA	6.7
1	B	92	CYS	5.3
1	D	75	SER	5.2
1	D	133	THR	4.9
1	B	77	GLN	4.9
1	A	63	GLY	4.8
1	A	75	SER	4.7
1	D	194	GLN	4.4
1	C	92	CYS	4.4
1	C	60	LEU	4.2
1	B	133	THR	4.1
1	D	77	GLN	4.1
1	A	194	GLN	4.1
1	D	193	GLY	4.0
1	A	77	GLN	4.0
1	A	189	GLY	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	77	GLN	3.8
1	A	57	LYS	3.8
1	C	59	VAL	3.7
2	G	132	ILE	3.5
1	A	133	THR	3.5
1	B	60	LEU	3.5
1	C	261	ASN	3.4
2	H	197	ARG	3.4
1	A	193	GLY	3.4
1	A	109	GLU	3.3
2	F	191	LEU	3.2
2	F	195	LEU	3.2
1	B	261	ASN	3.2
1	D	280	GLU	3.1
1	C	133	THR	3.1
1	B	111	ILE	3.1
1	D	65	LYS	3.0
2	H	195	LEU	3.0
1	B	102	GLY	3.0
1	D	78	GLY	3.0
1	D	72	THR	3.0
1	C	217	ARG	2.9
1	A	60	LEU	2.9
1	D	215	LYS	2.9
1	A	72	THR	2.8
2	H	194	ALA	2.8
2	G	133	VAL	2.8
2	E	172	HIS	2.7
1	C	260	HIS	2.7
1	D	191	GLU	2.7
1	C	61	ARG	2.7
1	D	109	GLU	2.7
1	D	76	SER	2.7
2	F	150	LEU	2.6
1	A	192	LEU	2.6
2	E	175	ASN	2.6
1	C	78	GLY	2.6
1	D	244	SER	2.6
1	D	282	LEU	2.6
1	A	196	HIS	2.6
1	D	91	PHE	2.6
1	D	127	TYR	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	93	ARG	2.5
1	A	65	LYS	2.5
1	C	206	GLY	2.5
1	C	101	ILE	2.5
2	G	184	ASP	2.5
1	A	316	LEU	2.5
1	B	239	SER	2.5
1	D	281	SER	2.5
1	A	91	PHE	2.4
1	B	113	ILE	2.4
2	H	133	VAL	2.4
1	B	217	ARG	2.3
1	A	64	ALA	2.3
1	B	103	PHE	2.3
1	C	127	TYR	2.3
1	D	196	HIS	2.3
1	C	75	SER	2.3
2	H	161	PHE	2.3
1	A	58	GLY	2.3
1	A	215	LYS	2.3
1	D	93	ARG	2.3
1	A	76	SER	2.3
1	A	169	ASN	2.3
1	B	59	VAL	2.3
1	B	134	MET	2.2
1	C	89	LEU	2.2
1	B	167	SER	2.2
1	A	121	ASN	2.2
1	A	93	ARG	2.2
1	D	217	ARG	2.2
2	H	143	ILE	2.2
1	A	37	ALA	2.2
1	B	112	LEU	2.2
1	D	121	ASN	2.2
1	D	64	ALA	2.1
1	A	112	LEU	2.1
1	B	243	GLN	2.1
1	A	214	ILE	2.1
1	D	104	CYS	2.1
1	B	76	SER	2.1
1	A	83	GLU	2.1
1	B	206	GLY	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	111	ILE	2.1
1	A	59	VAL	2.1
1	B	78	GLY	2.1
1	C	76	SER	2.1
2	H	193	GLY	2.1
2	E	171	GLN	2.0
2	E	136	LEU	2.0
2	F	143	ILE	2.0
1	D	57	LYS	2.0
1	B	61	ARG	2.0
1	A	260	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	B	198	10/11	0.48	0.46	78,82,83,88	0
1	SEP	C	198	10/11	0.53	0.48	82,85,86,89	0
1	SEP	A	198	10/11	0.70	0.22	84,85,86,90	0
1	SEP	D	198	10/11	0.79	0.23	78,79,81,85	0
1	TPO	C	199	11/12	0.84	0.25	82,83,85,88	0
1	TPO	B	199	11/12	0.85	0.18	79,79,80,80	0
1	TPO	A	199	11/12	0.85	0.20	83,83,85,87	0
1	TPO	D	199	11/12	0.86	0.17	79,80,81,82	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.