



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:14 PM GMT

PDB ID : 1SMK  
Title : Mature and translocatable forms of glyoxysomal malate dehydrogenase have different activities and stabilities but similar crystal structures  
Authors : Cox, B.; Chit, M.M.; Weaver, T.; Bailey, J.; Gietl, C.; Bell, E.; Banaszak, L.  
Deposited on : 2004-03-09  
Resolution : 2.50 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

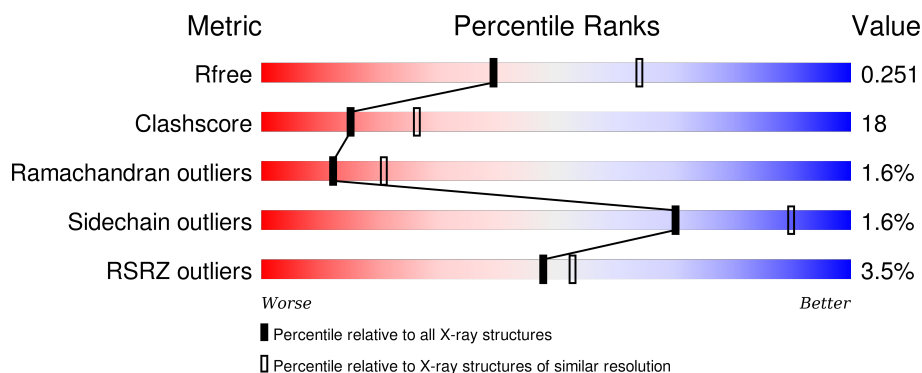
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	326	<div> <div>2%</div> <div>72%</div> <div>21%</div> <div>• •</div> </div>
1	B	326	<div> <div>3%</div> <div>69%</div> <div>26%</div> <div>•</div> </div>
1	C	326	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	D	326	<div> <div>5%</div> <div>67%</div> <div>29%</div> <div>• •</div> </div>
1	E	326	<div> <div>5%</div> <div>52%</div> <div>43%</div> <div>• •</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	F	326	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%68%25%<div>..</div></div>	
1	G	326	<div><div></div><div></div><div></div><div></div><div></div></div> <div>5%59%35%<div>..</div></div>	
1	H	326	<div><div></div><div></div><div></div><div></div><div></div></div> <div>5%58%36%<div>..</div></div>	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18870 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 Malate dehydrogenase, glyoxysomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	B	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	C	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	D	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	E	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	F	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	G	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			
1	H	313	Total	C	N	O	S	0	0	0
			2309	1469	396	431	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	HIS	-	EXPRESSION TAG	UNP P19446
A	358	HIS	-	EXPRESSION TAG	UNP P19446
A	359	HIS	-	EXPRESSION TAG	UNP P19446
A	360	HIS	-	EXPRESSION TAG	UNP P19446
A	361	HIS	-	EXPRESSION TAG	UNP P19446
A	362	HIS	-	EXPRESSION TAG	UNP P19446
B	357	HIS	-	EXPRESSION TAG	UNP P19446
B	358	HIS	-	EXPRESSION TAG	UNP P19446
B	359	HIS	-	EXPRESSION TAG	UNP P19446
B	360	HIS	-	EXPRESSION TAG	UNP P19446
B	361	HIS	-	EXPRESSION TAG	UNP P19446
B	362	HIS	-	EXPRESSION TAG	UNP P19446
C	357	HIS	-	EXPRESSION TAG	UNP P19446

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	358	HIS	-	EXPRESSION TAG	UNP P19446
C	359	HIS	-	EXPRESSION TAG	UNP P19446
C	360	HIS	-	EXPRESSION TAG	UNP P19446
C	361	HIS	-	EXPRESSION TAG	UNP P19446
C	362	HIS	-	EXPRESSION TAG	UNP P19446
D	357	HIS	-	EXPRESSION TAG	UNP P19446
D	358	HIS	-	EXPRESSION TAG	UNP P19446
D	359	HIS	-	EXPRESSION TAG	UNP P19446
D	360	HIS	-	EXPRESSION TAG	UNP P19446
D	361	HIS	-	EXPRESSION TAG	UNP P19446
D	362	HIS	-	EXPRESSION TAG	UNP P19446
E	357	HIS	-	EXPRESSION TAG	UNP P19446
E	358	HIS	-	EXPRESSION TAG	UNP P19446
E	359	HIS	-	EXPRESSION TAG	UNP P19446
E	360	HIS	-	EXPRESSION TAG	UNP P19446
E	361	HIS	-	EXPRESSION TAG	UNP P19446
E	362	HIS	-	EXPRESSION TAG	UNP P19446
F	357	HIS	-	EXPRESSION TAG	UNP P19446
F	358	HIS	-	EXPRESSION TAG	UNP P19446
F	359	HIS	-	EXPRESSION TAG	UNP P19446
F	360	HIS	-	EXPRESSION TAG	UNP P19446
F	361	HIS	-	EXPRESSION TAG	UNP P19446
F	362	HIS	-	EXPRESSION TAG	UNP P19446
G	357	HIS	-	EXPRESSION TAG	UNP P19446
G	358	HIS	-	EXPRESSION TAG	UNP P19446
G	359	HIS	-	EXPRESSION TAG	UNP P19446
G	360	HIS	-	EXPRESSION TAG	UNP P19446
G	361	HIS	-	EXPRESSION TAG	UNP P19446
G	362	HIS	-	EXPRESSION TAG	UNP P19446
H	357	HIS	-	EXPRESSION TAG	UNP P19446
H	358	HIS	-	EXPRESSION TAG	UNP P19446
H	359	HIS	-	EXPRESSION TAG	UNP P19446
H	360	HIS	-	EXPRESSION TAG	UNP P19446
H	361	HIS	-	EXPRESSION TAG	UNP P19446
H	362	HIS	-	EXPRESSION TAG	UNP P19446

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			13	6	7		

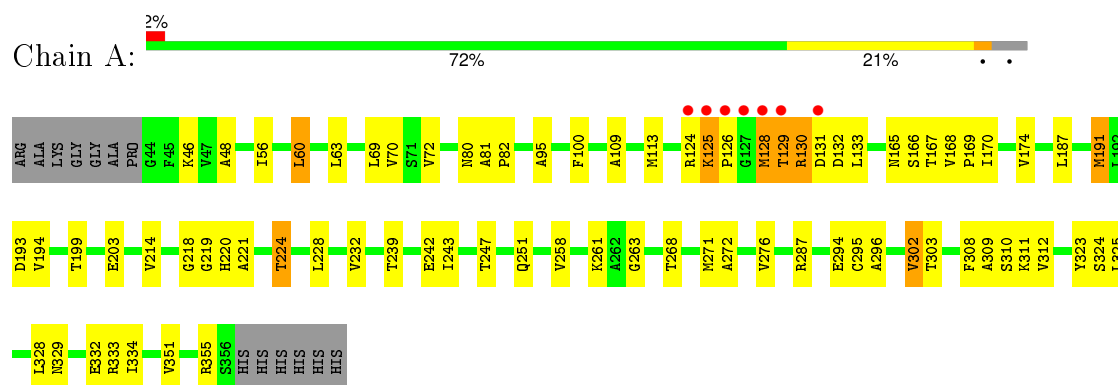
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	48	Total	O	0	0
			48	48		
3	C	114	Total	O	0	0
			114	114		
3	D	45	Total	O	0	0
			45	45		
3	E	17	Total	O	0	0
			17	17		
3	F	46	Total	O	0	0
			46	46		
3	G	18	Total	O	0	0
			18	18		
3	H	18	Total	O	0	0
			18	18		

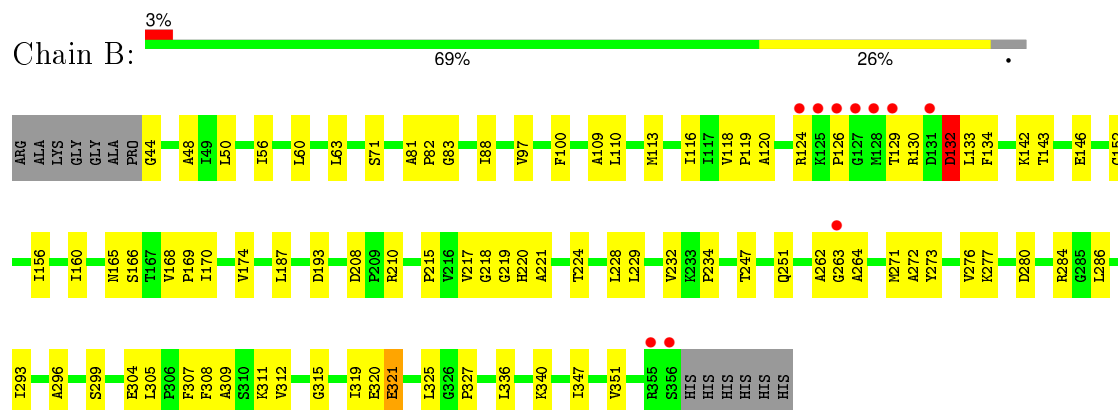
### 3 Residue-property plots [i](#)

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

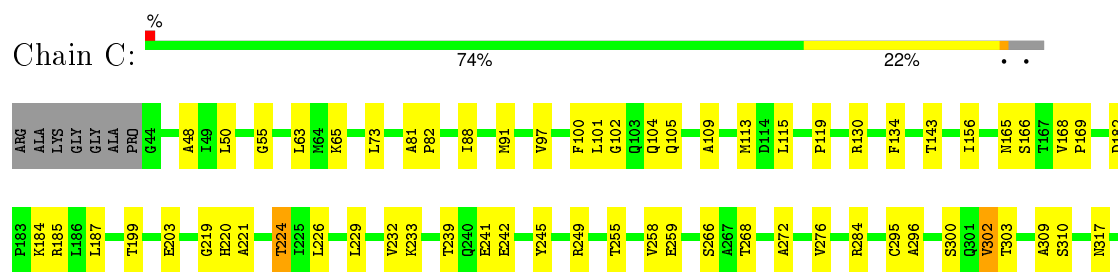
- Molecule 1: Malate dehydrogenase, glyoxysomal

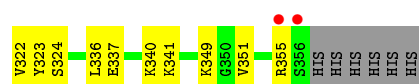


- Molecule 1: Malate dehydrogenase, glyoxysomal

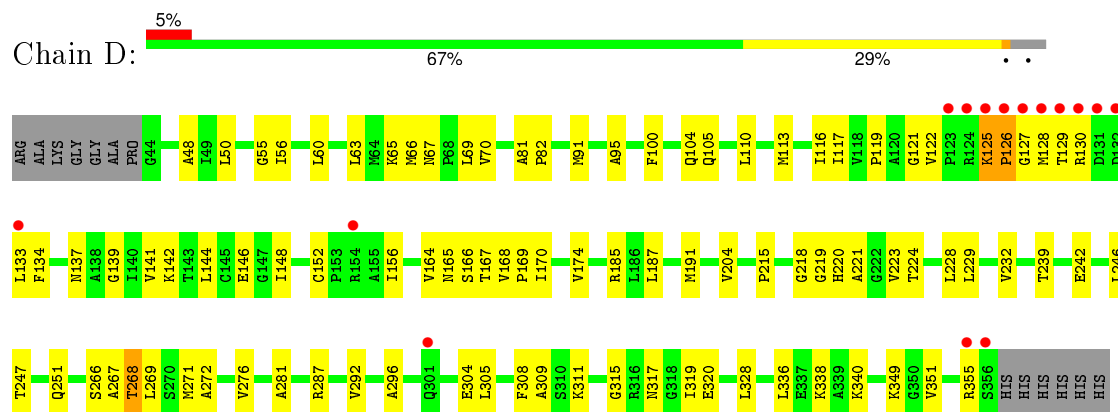


- Molecule 1: Malate dehydrogenase, glyoxysomal

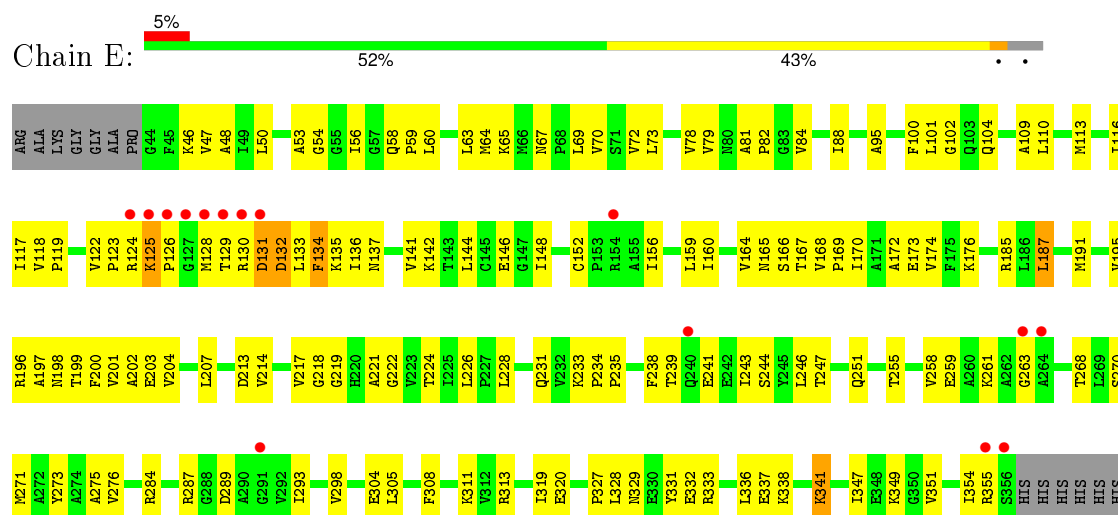




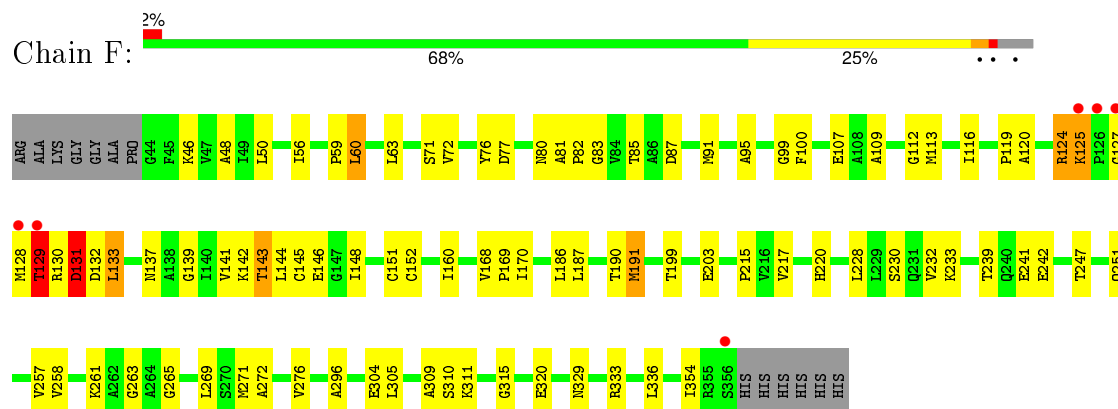
- Molecule 1: Malate dehydrogenase, glyoxysomal



- Molecule 1: Malate dehydrogenase, glyoxysomal



- Molecule 1: Malate dehydrogenase, glyoxysomal



- Molecule 1: Malate dehydrogenase, glyoxysomal



Frequency	Percentage
5%	5%
59%	59%
35%	35%



Frequency	Percentage
Very often	5%
Often	58%
Sometimes	36%
Rarely	• •
Never	• •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.43Å 88.05Å 138.82Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	13.00 – 2.50 19.80 – 2.48	Depositor EDS
% Data completeness (in resolution range)	85.3 (13.00-2.50) 85.2 (19.80-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.47Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.254 0.204 , 0.251	Depositor DCC
$R_{free}$ test set	4931 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.8	EDS
Estimated twinning fraction	0.022 for l,k,-h 0.019 for h,-k,-l 0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 100388 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CIT

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	0.38	0/2345	0.62	0/3179
1	B	0.35	0/2345	0.62	0/3179
1	C	0.38	0/2345	0.63	0/3179
1	D	0.35	0/2345	0.60	0/3179
1	E	0.32	0/2345	0.57	0/3179
1	F	0.34	0/2345	0.61	0/3179
1	G	0.31	0/2345	0.57	0/3179
1	H	0.32	0/2345	0.59	0/3179
All	All	0.34	0/18760	0.60	0/25432

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	2309	0	2393	67	0
1	B	2309	0	2393	76	0
1	C	2309	0	2393	59	0
1	D	2309	0	2393	83	0
1	E	2309	0	2393	125	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2309	0	2393	65	0
1	G	2309	0	2393	102	0
1	H	2309	0	2393	103	0
2	C	13	0	5	0	0
3	A	79	0	0	1	0
3	B	48	0	0	0	0
3	C	114	0	0	2	0
3	D	45	0	0	8	0
3	E	17	0	0	3	0
3	F	46	0	0	0	0
3	G	18	0	0	0	0
3	H	18	0	0	0	0
All	All	18870	0	19149	659	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 18.

All (659) 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:H:125:LYS:HB3	1:H:126:PRO:HD2	1.40	1.01
1:C:165:ASN:HD21	1:C:224:THR:HG21	1.24	1.01
1:B:165:ASN:HD21	1:B:224:THR:HG21	1.31	0.95
1:B:221:ALA:O	1:B:224:THR:HG22	1.66	0.94
1:A:124:ARG:HA	1:A:128:MET:HG3	1.49	0.93
1:B:116:ILE:HD11	1:B:152:CYS:SG	2.12	0.90
1:C:101:LEU:H	1:C:105:GLN:NE2	1.70	0.89
1:B:293:ILE:HD11	1:H:262:ALA:HA	1.55	0.88
1:E:48:ALA:HB2	1:E:113:MET:HG3	1.56	0.87
1:H:165:ASN:HD21	1:H:224:THR:HG21	1.38	0.87
1:A:125:LYS:HB2	1:A:126:PRO:HD3	1.55	0.87
1:D:116:ILE:HD11	1:D:152:CYS:SG	2.15	0.86
1:E:60:LEU:HD12	1:E:276:VAL:HG23	1.56	0.86
1:E:201:VAL:HG21	1:E:214:VAL:HG21	1.59	0.84
1:G:125:LYS:HB2	1:G:126:PRO:HD2	1.62	0.81
1:E:116:ILE:HD11	1:E:152:CYS:SG	2.20	0.81
1:G:116:ILE:HD11	1:G:152:CYS:SG	2.22	0.80
1:C:185:ARG:HH22	1:C:317:ASN:HD22	1.27	0.80
1:D:221:ALA:H	1:D:224:THR:CG2	1.94	0.80
1:E:221:ALA:H	1:E:224:THR:HG22	1.47	0.79
1:G:199:THR:O	1:G:203:GLU:HG3	1.81	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:THR:HG23	1:B:130:ARG:H	1.47	0.79
1:E:187:LEU:HA	1:E:298:VAL:HG12	1.63	0.79
1:E:125:LYS:HB3	1:E:126:PRO:HD2	1.66	0.78
1:H:221:ALA:O	1:H:224:THR:HG22	1.83	0.78
1:G:303:THR:HG22	1:G:305:LEU:H	1.49	0.77
1:A:333:ARG:HD3	1:C:245:TYR:CD2	2.19	0.77
1:F:116:ILE:HD11	1:F:152:CYS:SG	2.24	0.77
1:D:304:GLU:HG2	1:D:305:LEU:HD12	1.66	0.77
1:A:199:THR:O	1:A:203:GLU:HG3	1.85	0.77
1:H:221:ALA:H	1:H:224:THR:CG2	1.97	0.76
1:D:221:ALA:H	1:D:224:THR:HG22	1.50	0.76
1:D:215:PRO:HB3	1:D:311:LYS:HE2	1.67	0.76
1:E:199:THR:O	1:E:203:GLU:HG3	1.85	0.76
1:E:168:VAL:HB	1:E:169:PRO:HD3	1.66	0.76
1:F:124:ARG:HE	1:F:265:GLY:H	1.34	0.76
1:F:247:THR:O	1:F:251:GLN:HG3	1.86	0.76
1:B:247:THR:O	1:B:251:GLN:HG3	1.86	0.75
1:C:65:LYS:HG2	1:C:91:MET:HE3	1.69	0.75
1:E:221:ALA:O	1:E:224:THR:HG22	1.86	0.75
1:A:302:VAL:HG22	1:A:324:SER:HA	1.69	0.74
1:A:165:ASN:HD21	1:A:224:THR:HG21	1.51	0.74
1:D:165:ASN:HD21	1:D:224:THR:HG21	1.50	0.74
1:E:124:ARG:HA	1:E:128:MET:HE2	1.68	0.74
1:G:304:GLU:HG2	1:G:305:LEU:HD12	1.70	0.73
1:B:130:ARG:HE	1:B:132:ASP:HA	1.53	0.73
1:F:50:LEU:HD13	1:F:144:LEU:HD22	1.71	0.73
1:G:56:ILE:HD13	1:G:271:MET:HG2	1.69	0.72
1:A:130:ARG:C	1:A:132:ASP:H	1.93	0.72
1:D:221:ALA:O	1:D:224:THR:HG22	1.89	0.72
1:H:199:THR:O	1:H:203:GLU:HG3	1.89	0.72
1:A:302:VAL:HG12	1:A:303:THR:HG23	1.70	0.72
1:E:298:VAL:HG11	1:E:319:ILE:HD11	1.69	0.72
1:G:168:VAL:HB	1:G:169:PRO:HD3	1.70	0.72
1:H:336:LEU:HG	1:H:340:LYS:HE3	1.71	0.71
1:H:125:LYS:HB3	1:H:126:PRO:CD	2.19	0.71
1:E:221:ALA:H	1:E:224:THR:CG2	2.02	0.71
1:B:304:GLU:HG2	1:B:305:LEU:HD12	1.72	0.70
1:D:185:ARG:HH22	1:D:317:ASN:HD22	1.40	0.70
1:H:193:ASP:OD2	1:H:220:HIS:HD2	1.73	0.70
1:D:110:LEU:HD22	1:D:116:ILE:HD13	1.72	0.70
1:F:239:THR:OG1	1:F:242:GLU:HG3	1.92	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:GLY:HA3	1:F:320:GLU:HG2	1.73	0.70
1:D:133:LEU:HD13	1:D:137:ASN:HD22	1.56	0.70
1:E:102:GLY:HA3	1:E:104:GLN:HE22	1.57	0.69
1:H:125:LYS:HZ3	1:H:126:PRO:HD2	1.58	0.69
1:E:124:ARG:HH12	1:E:258:VAL:HG21	1.58	0.69
1:C:102:GLY:HA3	1:C:104:GLN:NE2	2.08	0.69
1:F:56:ILE:HD13	1:F:271:MET:HG2	1.75	0.68
1:H:217:VAL:HG12	1:H:310:SER:HA	1.73	0.68
1:D:133:LEU:HD13	1:D:137:ASN:ND2	2.08	0.68
1:B:130:ARG:C	1:B:132:ASP:H	1.96	0.68
1:H:239:THR:OG1	1:H:242:GLU:HG3	1.94	0.68
1:B:305:LEU:HD12	1:B:305:LEU:H	1.58	0.68
1:A:247:THR:O	1:A:251:GLN:HG3	1.94	0.67
1:E:58:GLN:HB2	1:E:59:PRO:HD3	1.75	0.67
1:H:125:LYS:HB3	1:H:125:LYS:HZ2	1.58	0.67
1:F:142:LYS:O	1:F:146:GLU:HG3	1.94	0.67
1:B:166:SER:O	1:B:169:PRO:HD2	1.95	0.67
1:G:81:ALA:HB3	1:G:82:PRO:HD3	1.75	0.67
1:B:221:ALA:H	1:B:224:THR:CG2	2.08	0.67
1:C:101:LEU:H	1:C:105:GLN:HE21	1.43	0.67
1:E:122:VAL:HG22	1:E:137:ASN:OD1	1.95	0.67
1:E:79:VAL:HA	1:E:101:LEU:HD11	1.77	0.67
1:H:300:SER:HB2	1:H:302:VAL:HG23	1.77	0.66
1:A:56:ILE:HD13	1:A:271:MET:HG2	1.77	0.66
1:H:116:ILE:HD11	1:H:152:CYS:SG	2.35	0.66
1:C:221:ALA:H	1:C:224:THR:HG22	1.58	0.66
1:H:156:ILE:HD13	1:H:185:ARG:HG2	1.76	0.66
1:H:47:VAL:HG22	1:H:115:LEU:HB3	1.78	0.66
1:G:142:LYS:O	1:G:146:GLU:HG3	1.94	0.66
1:A:46:LYS:HG2	1:A:72:VAL:HB	1.77	0.66
1:C:88:ILE:HG23	1:C:91:MET:CE	2.26	0.65
1:G:167:THR:HA	1:G:170:ILE:HD12	1.78	0.65
1:H:125:LYS:NZ	1:H:126:PRO:HD2	2.12	0.65
1:A:329:ASN:OD1	1:A:332:GLU:HG3	1.95	0.65
1:B:272:ALA:O	1:B:276:VAL:HG23	1.97	0.65
1:D:168:VAL:HB	1:D:169:PRO:HD3	1.77	0.65
1:D:125:LYS:HB3	1:D:126:PRO:CD	2.26	0.65
1:E:333:ARG:HD3	1:G:245:TYR:CD2	2.32	0.65
1:G:46:LYS:HB3	1:G:113:MET:HE1	1.77	0.65
1:D:266:SER:HB2	3:D:390:HOH:O	1.96	0.65
1:A:124:ARG:CA	1:A:128:MET:HG3	2.24	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:LEU:HD21	1:G:117:ILE:HG21	1.79	0.65
1:F:139:GLY:O	1:F:143:THR:HG23	1.97	0.64
1:B:142:LYS:O	1:B:146:GLU:HG3	1.97	0.64
1:A:128:MET:O	1:A:129:THR:HG22	1.98	0.64
1:H:63:LEU:CB	1:H:276:VAL:HG21	2.28	0.64
1:C:272:ALA:O	1:C:276:VAL:HG23	1.97	0.64
1:A:219:GLY:CA	1:A:224:THR:HG23	2.28	0.63
1:D:247:THR:O	1:D:251:GLN:HG3	1.98	0.63
1:E:165:ASN:HD21	1:E:224:THR:HG21	1.63	0.63
1:B:305:LEU:HD12	1:B:305:LEU:N	2.14	0.63
1:D:336:LEU:HD11	1:D:340:LYS:HE3	1.81	0.63
1:H:125:LYS:HB3	1:H:125:LYS:NZ	2.14	0.63
1:E:247:THR:O	1:E:251:GLN:HG3	1.99	0.63
1:B:56:ILE:HD13	1:B:271:MET:HG2	1.79	0.63
1:A:219:GLY:HA3	1:A:224:THR:HG23	1.81	0.63
1:E:64:MET:HE2	1:E:117:ILE:HD11	1.80	0.63
1:E:196:ARG:HB3	1:E:200:PHE:CE2	2.34	0.63
1:B:193:ASP:OD2	1:B:220:HIS:HD2	1.82	0.63
1:G:170:ILE:O	1:G:174:VAL:HG23	1.99	0.62
1:E:222:GLY:O	1:E:251:GLN:HB3	1.99	0.62
1:B:273:TYR:CZ	1:B:277:LYS:HD2	2.33	0.62
1:E:56:ILE:HD13	1:E:271:MET:HG2	1.81	0.62
1:F:199:THR:O	1:F:203:GLU:HG3	1.98	0.62
1:D:268:THR:HG22	1:D:269:LEU:N	2.14	0.62
1:E:197:ALA:O	1:E:201:VAL:HG23	2.00	0.62
1:A:334:ILE:HA	1:C:241:GLU:HG3	1.80	0.62
1:H:130:ARG:C	1:H:132:ASP:H	2.03	0.62
1:D:133:LEU:HD12	1:D:134:PHE:N	2.15	0.62
1:H:166:SER:C	1:H:169:PRO:HD2	2.20	0.62
1:E:123:PRO:CG	1:E:125:LYS:HE3	2.30	0.61
1:C:102:GLY:HA3	1:C:104:GLN:HE22	1.64	0.61
1:D:60:LEU:HD21	1:D:117:ILE:HG21	1.82	0.61
1:E:129:THR:O	1:E:130:ARG:HB2	2.01	0.61
1:E:166:SER:O	1:E:170:ILE:HG13	2.00	0.61
1:A:193:ASP:OD2	1:A:220:HIS:HD2	1.84	0.61
1:G:154:ARG:HH21	1:G:185:ARG:HH21	1.48	0.61
1:G:125:LYS:C	1:G:125:LYS:HD2	2.22	0.60
1:D:56:ILE:HD13	1:D:271:MET:HG2	1.82	0.60
1:A:60:LEU:HD12	1:A:60:LEU:O	2.00	0.60
1:E:351:VAL:O	1:E:355:ARG:HG3	2.01	0.60
1:E:63:LEU:CB	1:E:276:VAL:HG21	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ALA:O	1:C:309:ALA:HA	2.01	0.60
1:D:228:LEU:HD22	1:D:328:LEU:HD22	1.83	0.60
1:E:60:LEU:CD1	1:E:276:VAL:HG23	2.30	0.60
1:E:142:LYS:O	1:E:146:GLU:HG3	2.02	0.60
1:C:268:THR:HG21	3:D:388:HOH:O	2.01	0.60
1:H:63:LEU:HB2	1:H:276:VAL:HG21	1.82	0.60
1:H:170:ILE:O	1:H:174:VAL:HG23	2.02	0.60
1:E:219:GLY:C	1:E:224:THR:HG23	2.23	0.59
1:G:129:THR:HG22	1:G:130:ARG:N	2.17	0.59
1:G:154:ARG:HH21	1:G:185:ARG:NH2	2.00	0.59
1:H:144:LEU:O	1:H:148:ILE:HG13	2.02	0.59
1:B:315:GLY:HA3	1:B:320:GLU:HG3	1.83	0.59
1:E:63:LEU:HB2	1:E:276:VAL:HG21	1.84	0.59
1:G:218:GLY:HA2	1:G:308:PHE:CZ	2.38	0.59
1:E:239:THR:O	1:E:243:ILE:HG13	2.03	0.59
1:C:55:GLY:O	1:C:268:THR:HG23	2.03	0.59
1:A:48:ALA:HB2	1:A:113:MET:HG3	1.84	0.59
1:H:247:THR:O	1:H:251:GLN:HG3	2.03	0.59
1:F:100:PHE:CG	1:F:109:ALA:HB2	2.38	0.59
1:F:133:LEU:C	1:F:133:LEU:HD12	2.23	0.59
1:F:124:ARG:HH22	1:F:258:VAL:HG22	1.67	0.59
1:G:173:GLU:OE1	1:G:355:ARG:HD2	2.02	0.59
1:F:129:THR:O	1:F:131:ASP:N	2.36	0.59
1:B:124:ARG:HH12	1:B:126:PRO:HA	1.68	0.58
1:H:326:GLY:O	1:H:328:LEU:HD13	2.04	0.58
1:A:69:LEU:HD21	1:A:287:ARG:NH1	2.18	0.58
1:D:125:LYS:O	1:D:127:GLY:N	2.35	0.58
1:H:163:PRO:HG2	1:H:166:SER:HB2	1.86	0.58
1:B:48:ALA:HB2	1:B:113:MET:HG3	1.86	0.58
1:A:221:ALA:H	1:A:224:THR:CG2	2.15	0.58
1:G:166:SER:O	1:G:169:PRO:HD2	2.03	0.58
1:D:127:GLY:C	1:D:129:THR:H	2.06	0.58
1:G:202:ALA:HB1	1:G:207:LEU:O	2.04	0.58
1:H:60:LEU:HD21	1:H:117:ILE:HG21	1.85	0.58
1:F:124:ARG:NH2	1:F:258:VAL:HG22	2.18	0.58
1:G:195:VAL:HG13	1:H:92:ASP:H	1.69	0.58
1:E:347:ILE:O	1:E:351:VAL:HG23	2.04	0.58
1:D:219:GLY:C	1:D:224:THR:HG23	2.24	0.57
1:F:127:GLY:C	1:F:129:THR:H	2.06	0.57
1:H:221:ALA:H	1:H:224:THR:HG22	1.68	0.57
1:A:130:ARG:O	1:A:132:ASP:N	2.37	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:MET:HE2	1:H:191:MET:HA	1.85	0.57
1:G:329:ASN:OD1	1:G:332:GLU:HG3	2.04	0.57
1:D:229:LEU:O	1:D:232:VAL:HG12	2.04	0.57
1:E:110:LEU:HD22	1:E:116:ILE:HD13	1.87	0.57
1:G:166:SER:C	1:G:169:PRO:HD2	2.25	0.57
1:E:123:PRO:HG2	1:E:125:LYS:HE3	1.84	0.57
1:H:107:GLU:HG3	1:H:151:CYS:SG	2.45	0.57
1:B:133:LEU:HD23	1:B:134:PHE:H	1.69	0.57
1:D:315:GLY:HA3	1:D:320:GLU:HG2	1.87	0.57
1:D:156:ILE:HD13	1:D:185:ARG:HG2	1.86	0.57
1:E:329:ASN:O	1:E:333:ARG:HG3	2.04	0.57
1:G:172:ALA:O	1:G:176:LYS:HG3	2.05	0.57
1:C:219:GLY:CA	1:C:224:THR:HG23	2.35	0.56
1:D:125:LYS:HB3	1:D:126:PRO:HD2	1.86	0.56
1:H:165:ASN:ND2	1:H:224:THR:HG21	2.17	0.56
1:G:129:THR:O	1:G:130:ARG:HB2	2.06	0.56
1:E:202:ALA:HB1	1:E:207:LEU:O	2.06	0.56
1:C:88:ILE:HA	1:C:91:MET:HE2	1.86	0.56
1:F:187:LEU:HD12	1:F:187:LEU:N	2.21	0.56
1:H:125:LYS:O	1:H:127:GLY:N	2.35	0.56
1:F:124:ARG:HE	1:F:265:GLY:N	2.02	0.56
1:G:47:VAL:HG22	1:G:115:LEU:HB3	1.87	0.56
1:A:166:SER:C	1:A:169:PRO:HD2	2.27	0.56
1:E:217:VAL:HG23	1:E:226:LEU:HB3	1.88	0.56
1:A:302:VAL:CG2	1:A:324:SER:HA	2.36	0.56
1:E:124:ARG:HA	1:E:128:MET:CE	2.34	0.56
1:F:215:PRO:HG2	1:F:228:LEU:HB2	1.88	0.55
1:F:215:PRO:HB3	1:F:311:LYS:HE3	1.87	0.55
1:E:69:LEU:HD21	1:E:287:ARG:NH1	2.22	0.55
1:G:223:VAL:HA	1:G:251:GLN:NE2	2.21	0.55
1:D:142:LYS:O	1:D:146:GLU:HG3	2.06	0.55
1:B:215:PRO:HG2	1:B:228:LEU:HB2	1.89	0.55
1:H:347:ILE:O	1:H:351:VAL:HG23	2.06	0.55
1:A:166:SER:O	1:A:170:ILE:HG13	2.06	0.55
1:E:130:ARG:HD3	1:E:133:LEU:HD13	1.88	0.55
1:H:337:GLU:O	1:H:341:LYS:HG3	2.07	0.55
1:C:65:LYS:HG2	1:C:91:MET:CE	2.36	0.55
1:A:170:ILE:O	1:A:174:VAL:HG23	2.07	0.55
1:C:302:VAL:HG21	1:C:323:TYR:O	2.07	0.55
1:E:50:LEU:O	1:E:119:PRO:HD2	2.07	0.55
1:F:125:LYS:HB2	1:F:128:MET:CB	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:LEU:CD1	1:H:276:VAL:HG21	2.37	0.54
1:B:215:PRO:HB3	1:B:311:LYS:HE2	1.89	0.54
1:A:70:VAL:O	1:A:95:ALA:HB2	2.07	0.54
1:G:124:ARG:HD3	1:G:136:ILE:CD1	2.37	0.54
1:B:63:LEU:CB	1:B:276:VAL:HG21	2.37	0.54
1:E:234:PRO:HB3	1:H:105:GLN:HG2	1.89	0.54
1:B:156:ILE:HD11	1:B:286:LEU:HD21	1.89	0.54
1:D:65:LYS:HD2	1:D:95:ALA:HB3	1.88	0.54
1:C:63:LEU:HB2	1:C:276:VAL:HG21	1.88	0.54
1:E:284:ARG:HD2	3:E:375:HOH:O	2.07	0.54
1:E:191:MET:O	1:E:195:VAL:HG23	2.07	0.54
1:B:221:ALA:H	1:B:224:THR:HG22	1.73	0.54
1:C:185:ARG:NH2	1:C:317:ASN:HD22	2.03	0.54
1:B:166:SER:C	1:B:169:PRO:HD2	2.28	0.54
1:B:169:PRO:HG3	1:B:307:PHE:CD2	2.41	0.54
1:F:125:LYS:HB2	1:F:128:MET:HB2	1.90	0.54
1:H:122:VAL:HG22	1:H:137:ASN:OD1	2.08	0.54
1:G:46:LYS:HG2	1:G:72:VAL:HB	1.89	0.54
1:D:272:ALA:O	1:D:276:VAL:HG23	2.08	0.54
1:D:305:LEU:N	1:D:305:LEU:HD12	2.23	0.54
1:F:124:ARG:HH21	1:F:265:GLY:C	2.10	0.54
1:B:63:LEU:HB2	1:B:276:VAL:HG21	1.90	0.54
1:A:130:ARG:C	1:A:132:ASP:N	2.61	0.54
1:B:129:THR:HG23	1:B:130:ARG:N	2.21	0.54
1:A:221:ALA:H	1:A:224:THR:HG22	1.73	0.54
1:D:130:ARG:HE	1:D:130:ARG:HA	1.72	0.54
1:C:302:VAL:HG12	1:C:303:THR:HG23	1.90	0.54
1:G:104:GLN:HG2	1:G:105:GLN:N	2.22	0.54
1:D:100:PHE:HA	1:D:105:GLN:NE2	2.23	0.53
1:E:100:PHE:CG	1:E:109:ALA:HB2	2.43	0.53
1:A:302:VAL:HG13	1:A:325:LEU:HG	1.90	0.53
1:D:63:LEU:CB	1:D:276:VAL:HG21	2.39	0.53
1:H:125:LYS:CB	1:H:126:PRO:HD2	2.27	0.53
1:E:221:ALA:N	1:E:224:THR:CG2	2.72	0.53
1:E:124:ARG:HH12	1:E:258:VAL:CG2	2.22	0.53
1:G:48:ALA:HB2	1:G:113:MET:HG2	1.90	0.53
1:A:168:VAL:HB	1:A:169:PRO:HD3	1.91	0.53
1:E:270:SER:HB3	1:F:87:ASP:O	2.09	0.53
1:F:85:THR:HG21	1:F:99:GLY:N	2.23	0.53
1:F:71:SER:O	1:F:95:ALA:HA	2.08	0.53
1:C:168:VAL:HB	1:C:169:PRO:HD3	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:ILE:CD1	1:H:185:ARG:HG2	2.39	0.53
1:E:133:LEU:C	1:E:133:LEU:HD23	2.29	0.53
1:D:50:LEU:O	1:D:119:PRO:HD2	2.09	0.53
1:E:313:ARG:HH21	1:E:320:GLU:CG	2.21	0.53
1:A:167:THR:HA	1:A:170:ILE:HD12	1.90	0.53
1:E:137:ASN:O	1:E:141:VAL:HG23	2.09	0.53
1:G:46:LYS:C	1:G:113:MET:HE3	2.28	0.53
1:E:338:LYS:HA	1:E:341:LYS:HD2	1.91	0.53
1:E:156:ILE:HD13	1:E:185:ARG:HG2	1.91	0.53
1:H:71:SER:O	1:H:95:ALA:HA	2.09	0.53
1:H:308:PHE:HE2	1:H:325:LEU:HD21	1.73	0.52
1:H:70:VAL:O	1:H:95:ALA:HB2	2.08	0.52
1:D:296:ALA:O	1:D:309:ALA:HA	2.09	0.52
1:E:327:PRO:HB3	1:G:249:ARG:CZ	2.39	0.52
1:G:170:ILE:HG23	1:G:354:ILE:HD11	1.91	0.52
1:B:234:PRO:HB3	1:G:105:GLN:HG2	1.91	0.52
1:G:304:GLU:HG2	1:G:305:LEU:N	2.24	0.52
1:E:60:LEU:HD12	1:E:276:VAL:CG2	2.33	0.52
1:D:137:ASN:O	1:D:141:VAL:HG23	2.10	0.52
1:A:311:LYS:HB2	1:A:323:TYR:HB2	1.92	0.52
1:D:317:ASN:HA	3:D:369:HOH:O	2.10	0.52
1:G:191:MET:O	1:G:195:VAL:HG23	2.10	0.52
1:F:304:GLU:HG2	1:F:305:LEU:HD13	1.92	0.51
1:A:294:GLU:O	1:A:312:VAL:HG22	2.11	0.51
1:D:219:GLY:CA	1:D:224:THR:HG23	2.41	0.51
1:B:229:LEU:O	1:B:232:VAL:HG23	2.10	0.51
1:G:205:LEU:HD21	1:G:238:PHE:CE1	2.46	0.51
1:B:229:LEU:HA	1:B:232:VAL:HG23	1.92	0.51
1:B:44:GLY:HA3	1:B:71:SER:HB3	1.91	0.51
1:H:221:ALA:H	1:H:224:THR:HG21	1.74	0.51
1:F:124:ARG:HG2	1:F:124:ARG:HH11	1.76	0.51
1:D:218:GLY:HA2	1:D:308:PHE:CZ	2.46	0.51
1:E:134:PHE:CD2	1:E:349:LYS:HE2	2.45	0.51
1:F:145:CYS:HA	1:F:148:ILE:HD12	1.93	0.51
1:E:131:ASP:C	1:E:133:LEU:H	2.13	0.51
1:G:273:TYR:CZ	1:G:277:LYS:HD2	2.45	0.51
1:G:201:VAL:HG21	1:G:214:VAL:HG21	1.93	0.51
1:H:48:ALA:HB2	1:H:113:MET:HG3	1.92	0.51
1:G:46:LYS:HB3	1:G:113:MET:CE	2.40	0.51
1:B:320:GLU:O	1:B:321:GLU:HB2	2.11	0.51
1:F:63:LEU:HB2	1:F:276:VAL:HG21	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:VAL:HG13	1:H:263:GLY:HA2	1.91	0.51
1:B:217:VAL:HG11	1:B:325:LEU:HD22	1.93	0.51
1:B:187:LEU:HG	1:B:319:ILE:HD11	1.91	0.51
1:B:130:ARG:C	1:B:132:ASP:N	2.63	0.50
1:D:63:LEU:HB2	1:D:276:VAL:HG21	1.92	0.50
1:A:243:ILE:HD13	3:A:434:HOH:O	2.11	0.50
1:B:262:ALA:O	1:B:264:ALA:N	2.39	0.50
1:B:50:LEU:HD12	1:B:118:VAL:HG22	1.91	0.50
1:E:273:TYR:CD2	1:F:91:MET:HG2	2.46	0.50
1:D:239:THR:OG1	1:D:242:GLU:HG3	2.11	0.50
1:E:124:ARG:O	1:E:125:LYS:HB2	2.12	0.50
1:C:239:THR:OG1	1:C:242:GLU:HG3	2.10	0.50
1:E:198:ASN:OD1	1:E:213:ASP:HA	2.11	0.50
1:C:134:PHE:CG	1:C:349:LYS:HE2	2.47	0.50
1:H:214:VAL:HG22	1:H:232:VAL:HG22	1.93	0.50
1:F:46:LYS:HD2	1:F:112:GLY:O	2.10	0.50
1:B:156:ILE:CD1	1:B:286:LEU:HD21	2.42	0.50
1:A:239:THR:OG1	1:A:242:GLU:HG3	2.11	0.50
1:G:337:GLU:O	1:G:341:LYS:HG3	2.11	0.50
1:E:304:GLU:H	1:E:304:GLU:CD	2.15	0.50
1:G:240:GLN:HA	1:G:243:ILE:HD12	1.92	0.50
1:E:329:ASN:OD1	1:E:332:GLU:HG3	2.12	0.50
1:F:272:ALA:O	1:F:276:VAL:HG23	2.12	0.49
1:E:187:LEU:HD12	1:E:187:LEU:N	2.27	0.49
1:F:296:ALA:O	1:F:309:ALA:HA	2.12	0.49
1:A:125:LYS:CB	1:A:126:PRO:HD3	2.34	0.49
1:E:125:LYS:HB3	1:E:126:PRO:CD	2.40	0.49
1:G:303:THR:CG2	1:G:305:LEU:HD13	2.42	0.49
1:B:299:SER:HA	1:B:307:PHE:CD1	2.48	0.49
1:B:336:LEU:HG	1:B:340:LYS:HE3	1.94	0.49
1:B:193:ASP:OD2	1:B:220:HIS:CD2	2.65	0.49
1:G:338:LYS:HA	1:G:341:LYS:HD2	1.94	0.49
1:E:204:VAL:HG21	1:E:246:LEU:HD21	1.95	0.49
1:G:122:VAL:HG21	1:G:136:ILE:HG21	1.94	0.49
1:E:221:ALA:N	1:E:224:THR:HG22	2.21	0.49
1:E:337:GLU:O	1:E:341:LYS:HG3	2.13	0.49
1:A:81:ALA:HB3	1:A:82:PRO:HD3	1.94	0.49
1:H:125:LYS:C	1:H:127:GLY:H	2.16	0.49
1:C:130:ARG:NH2	3:C:1314:HOH:O	2.45	0.49
1:B:347:ILE:O	1:B:351:VAL:HG23	2.12	0.49
1:G:100:PHE:CG	1:G:109:ALA:HB2	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:N	1:C:105:GLN:HE21	2.09	0.49
1:H:351:VAL:HG12	1:H:351:VAL:O	2.12	0.49
1:C:229:LEU:O	1:C:232:VAL:HG12	2.13	0.49
1:A:166:SER:O	1:A:169:PRO:HD2	2.12	0.49
1:E:164:VAL:HA	1:E:167:THR:OG1	2.13	0.49
1:A:125:LYS:N	1:A:128:MET:HG3	2.28	0.49
1:G:154:ARG:NH2	1:G:185:ARG:NH2	2.61	0.49
1:E:218:GLY:HA2	1:E:308:PHE:CZ	2.48	0.49
1:H:258:VAL:CG1	1:H:263:GLY:HA2	2.42	0.48
1:E:47:VAL:HG11	1:E:64:MET:HE3	1.94	0.48
1:E:166:SER:C	1:E:169:PRO:HD2	2.34	0.48
1:F:170:ILE:HG23	1:F:354:ILE:CG1	2.43	0.48
1:E:81:ALA:HB3	1:E:82:PRO:HD3	1.95	0.48
1:F:144:LEU:O	1:F:148:ILE:HG13	2.14	0.48
1:H:308:PHE:CE2	1:H:325:LEU:HD21	2.48	0.48
1:H:296:ALA:O	1:H:309:ALA:HA	2.13	0.48
1:D:156:ILE:CD1	1:D:185:ARG:HG2	2.44	0.48
1:B:124:ARG:HH11	1:B:124:ARG:HG3	1.78	0.48
1:H:85:THR:HG23	1:H:97:VAL:HG22	1.94	0.48
1:B:293:ILE:HA	1:B:312:VAL:O	2.13	0.48
1:C:48:ALA:HB2	1:C:113:MET:HG3	1.94	0.48
1:E:67:ASN:HB3	1:E:70:VAL:HG23	1.96	0.48
1:E:261:LYS:HG2	1:F:83:GLY:HA3	1.94	0.48
1:D:134:PHE:CD2	1:D:349:LYS:HE2	2.49	0.48
1:D:166:SER:C	1:D:169:PRO:HD2	2.33	0.48
1:H:337:GLU:HG3	1:H:341:LYS:HE3	1.96	0.48
1:E:53:ALA:HA	1:E:84:VAL:HG21	1.96	0.48
1:C:73:LEU:O	1:C:97:VAL:HA	2.14	0.48
1:C:351:VAL:O	1:C:355:ARG:HG3	2.12	0.48
1:B:81:ALA:HB3	1:B:82:PRO:HD3	1.96	0.48
1:A:129:THR:C	1:A:131:ASP:H	2.16	0.48
1:D:110:LEU:HD22	1:D:116:ILE:CD1	2.43	0.48
1:A:228:LEU:HD22	1:A:328:LEU:HD22	1.96	0.48
1:B:116:ILE:CD1	1:B:152:CYS:SG	2.96	0.47
1:C:182:ASP:OD1	1:C:184:LYS:HG2	2.14	0.47
1:H:168:VAL:HB	1:H:169:PRO:HD3	1.94	0.47
1:D:174:VAL:HG13	3:D:384:HOH:O	2.14	0.47
1:D:116:ILE:CD1	1:D:152:CYS:SG	2.97	0.47
1:A:63:LEU:HB2	1:A:276:VAL:HG21	1.96	0.47
1:E:63:LEU:HB3	1:E:276:VAL:HG21	1.97	0.47
1:B:143:THR:HA	1:B:146:GLU:OE1	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ASN:HD21	1:G:221:ALA:H	1.61	0.47
1:A:351:VAL:O	1:A:355:ARG:HG3	2.14	0.47
1:G:63:LEU:HB2	1:G:276:VAL:HG21	1.95	0.47
1:G:286:LEU:HA	1:G:316:ARG:HA	1.96	0.47
1:H:50:LEU:O	1:H:119:PRO:HD2	2.13	0.47
1:D:48:ALA:HB2	1:D:113:MET:HG3	1.95	0.47
1:B:219:GLY:C	1:B:224:THR:HG23	2.35	0.47
1:C:184:LYS:NZ	1:C:185:ARG:NH1	2.62	0.47
1:G:165:ASN:HD21	1:G:221:ALA:N	2.13	0.47
1:H:46:LYS:HG2	1:H:72:VAL:HB	1.96	0.47
1:D:104:GLN:OE1	1:D:104:GLN:N	2.38	0.47
1:E:46:LYS:HB3	1:E:113:MET:SD	2.55	0.47
1:H:185:ARG:HG3	1:H:185:ARG:HH11	1.79	0.47
1:E:293:ILE:HG21	1:E:311:LYS:HE2	1.96	0.47
1:F:128:MET:O	1:F:128:MET:HG3	2.15	0.47
1:E:204:VAL:CG2	1:E:246:LEU:HD21	2.44	0.47
1:B:327:PRO:HB3	1:H:249:ARG:CZ	2.45	0.47
1:H:56:ILE:HD13	1:H:271:MET:HG2	1.97	0.47
1:C:221:ALA:O	1:C:224:THR:HB	2.15	0.47
1:B:130:ARG:HG2	1:B:132:ASP:H	1.79	0.47
1:E:320:GLU:OE1	1:E:320:GLU:HA	2.15	0.47
1:E:60:LEU:HD13	1:E:275:ALA:HB3	1.97	0.46
1:B:168:VAL:HB	1:B:169:PRO:HD3	1.96	0.46
1:E:235:PRO:HG2	1:H:100:PHE:CE2	2.50	0.46
1:G:56:ILE:CD1	1:G:271:MET:HG2	2.41	0.46
1:F:336:LEU:HD12	1:F:336:LEU:O	2.16	0.46
1:E:104:GLN:CD	1:E:104:GLN:H	2.19	0.46
1:C:336:LEU:HG	1:C:340:LYS:HE3	1.97	0.46
1:H:79:VAL:HA	1:H:101:LEU:HD11	1.96	0.46
1:C:300:SER:HB2	1:C:322:VAL:HG11	1.97	0.46
1:C:81:ALA:HB3	1:C:82:PRO:HD3	1.97	0.46
1:G:298:VAL:HG11	1:G:319:ILE:HD11	1.96	0.46
1:F:257:VAL:O	1:F:261:LYS:HG3	2.15	0.46
1:A:125:LYS:H	1:A:128:MET:HG3	1.81	0.46
1:H:217:VAL:HB	1:H:309:ALA:O	2.15	0.46
1:H:232:VAL:CG1	1:H:233:LYS:N	2.78	0.46
1:D:187:LEU:HG	1:D:319:ILE:HD11	1.96	0.46
1:B:130:ARG:HG2	1:B:130:ARG:O	2.16	0.46
1:H:129:THR:O	1:H:130:ARG:C	2.54	0.46
1:A:272:ALA:O	1:A:276:VAL:HG23	2.15	0.46
1:H:78:VAL:HG23	1:H:79:VAL:HG13	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:LEU:O	1:G:119:PRO:HD2	2.16	0.46
1:A:296:ALA:O	1:A:309:ALA:HA	2.16	0.46
1:C:88:ILE:HD13	1:C:91:MET:HE2	1.98	0.46
1:C:104:GLN:H	1:C:104:GLN:CD	2.18	0.46
1:E:144:LEU:O	1:E:148:ILE:HG13	2.16	0.46
1:H:215:PRO:HG2	1:H:228:LEU:HB2	1.98	0.46
1:F:168:VAL:HB	1:F:169:PRO:HD3	1.97	0.46
1:B:56:ILE:CD1	1:B:271:MET:HG2	2.46	0.46
1:B:280:ASP:OD2	1:B:284:ARG:NH1	2.49	0.46
1:E:122:VAL:HG11	1:E:136:ILE:HG21	1.97	0.46
1:G:47:VAL:N	1:G:113:MET:HE3	2.31	0.46
1:H:130:ARG:C	1:H:132:ASP:N	2.69	0.46
1:E:244:SER:HA	1:E:331:TYR:OH	2.16	0.46
1:H:55:GLY:O	1:H:268:THR:HG23	2.15	0.46
1:F:56:ILE:O	1:F:59:PRO:HD2	2.17	0.45
1:E:47:VAL:O	1:E:73:LEU:HA	2.16	0.45
1:B:133:LEU:HD23	1:B:134:PHE:N	2.31	0.45
1:G:104:GLN:HG2	1:G:105:GLN:HG3	1.97	0.45
1:F:170:ILE:HG23	1:F:354:ILE:HG12	1.97	0.45
1:D:220:HIS:HD2	3:D:395:HOH:O	1.98	0.45
1:C:255:THR:HG22	1:C:259:GLU:OE2	2.16	0.45
1:F:217:VAL:HG12	1:F:310:SER:HA	1.97	0.45
1:G:200:PHE:HA	1:G:203:GLU:OE1	2.16	0.45
1:G:163:PRO:O	1:G:167:THR:HG23	2.16	0.45
1:H:147:GLY:HA2	1:H:150:LYS:HB3	1.99	0.45
1:H:204:VAL:HG21	1:H:246:LEU:HD21	1.98	0.45
1:E:133:LEU:O	1:E:135:LYS:N	2.49	0.45
1:D:305:LEU:HD12	1:D:305:LEU:H	1.82	0.45
1:H:153:PRO:HB2	1:H:180:THR:HB	1.99	0.45
1:G:270:SER:HB3	1:H:87:ASP:O	2.17	0.45
1:A:214:VAL:HG22	1:A:232:VAL:HG23	1.99	0.45
1:B:305:LEU:CD1	1:B:305:LEU:H	2.28	0.45
1:A:60:LEU:C	1:A:60:LEU:HD12	2.36	0.45
1:E:132:ASP:OD1	1:E:132:ASP:N	2.47	0.45
1:G:125:LYS:HB2	1:G:126:PRO:CD	2.42	0.45
1:E:313:ARG:HH21	1:E:320:GLU:HG3	1.82	0.45
1:G:187:LEU:HD22	1:G:278:PHE:HZ	1.80	0.45
1:D:164:VAL:HA	1:D:167:THR:OG1	2.16	0.45
1:E:333:ARG:NH2	1:G:204:VAL:HG13	2.32	0.45
1:G:195:VAL:HG12	1:H:90:HIS:O	2.16	0.45
1:H:137:ASN:O	1:H:141:VAL:HG23	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ILE:O	1:E:160:ILE:HG22	2.17	0.45
1:E:172:ALA:O	1:E:176:LYS:HG3	2.17	0.45
1:E:46:LYS:HG2	1:E:72:VAL:CG2	2.46	0.45
1:E:221:ALA:O	1:E:224:THR:CG2	2.61	0.45
1:A:221:ALA:O	1:A:224:THR:HB	2.17	0.45
1:H:166:SER:O	1:H:169:PRO:HD2	2.16	0.45
1:D:351:VAL:HG12	1:D:355:ARG:HG3	1.99	0.45
1:G:241:GLU:OE1	1:G:242:GLU:HG3	2.17	0.45
1:D:204:VAL:CG2	1:D:246:LEU:HD21	2.47	0.45
1:G:125:LYS:NZ	1:G:127:GLY:HA3	2.32	0.44
1:H:132:ASP:C	1:H:134:PHE:H	2.19	0.44
1:G:129:THR:CG2	1:G:130:ARG:N	2.80	0.44
1:H:85:THR:OG1	1:H:99:GLY:HA3	2.17	0.44
1:H:81:ALA:HB3	1:H:82:PRO:HD3	2.00	0.44
1:D:127:GLY:C	1:D:129:THR:N	2.71	0.44
1:G:60:LEU:HD21	1:G:117:ILE:CG2	2.44	0.44
1:F:190:THR:HG22	1:F:220:HIS:HB2	1.97	0.44
1:G:134:PHE:O	1:G:138:ALA:HB2	2.17	0.44
1:G:173:GLU:HB3	1:G:354:ILE:HG21	2.00	0.44
1:C:284:ARG:HD2	3:C:1380:HOH:O	2.18	0.44
1:F:137:ASN:O	1:F:141:VAL:HG23	2.17	0.44
1:D:164:VAL:HG13	1:D:168:VAL:HG23	2.00	0.44
1:E:56:ILE:HG12	1:E:268:THR:HA	1.98	0.44
1:B:296:ALA:O	1:B:309:ALA:HA	2.18	0.44
1:C:199:THR:O	1:C:203:GLU:HG3	2.17	0.44
1:E:226:LEU:HD22	1:E:336:LEU:HA	2.00	0.44
1:E:233:LYS:HA	1:E:234:PRO:C	2.38	0.44
1:G:63:LEU:CB	1:G:276:VAL:HG21	2.47	0.44
1:G:149:ALA:HB2	1:G:175:PHE:CD1	2.52	0.44
1:F:329:ASN:O	1:F:333:ARG:HG2	2.17	0.44
1:G:98:ARG:HH11	1:G:98:ARG:HG2	1.83	0.44
1:D:221:ALA:N	1:D:224:THR:HG22	2.26	0.44
1:E:243:ILE:HG22	1:E:331:TYR:CE2	2.53	0.44
1:A:56:ILE:HG12	1:A:268:THR:HA	2.00	0.44
1:B:119:PRO:HA	1:B:160:ILE:HB	2.00	0.44
1:A:191:MET:HE2	1:A:194:VAL:HB	2.00	0.44
1:H:218:GLY:HA2	1:H:308:PHE:CZ	2.53	0.43
1:E:67:ASN:HB3	1:E:70:VAL:CG2	2.48	0.43
1:G:262:ALA:C	1:G:264:ALA:H	2.21	0.43
1:D:100:PHE:HA	1:D:105:GLN:HE21	1.83	0.43
1:C:258:VAL:HG22	1:C:266:SER:HB3	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD12	1:C:187:LEU:N	2.33	0.43
1:G:300:SER:HB2	1:G:302:VAL:HG23	1.99	0.43
1:G:143:THR:HA	1:G:146:GLU:OE1	2.18	0.43
1:E:228:LEU:HD22	1:E:328:LEU:HD22	2.00	0.43
1:C:300:SER:CB	1:C:322:VAL:HG11	2.48	0.43
1:G:197:ALA:O	1:G:201:VAL:HG23	2.19	0.43
1:G:198:ASN:OD1	1:G:214:VAL:N	2.49	0.43
1:C:337:GLU:OE2	1:C:341:LYS:HE3	2.19	0.43
1:F:191:MET:CE	1:F:191:MET:HA	2.48	0.43
1:H:50:LEU:HD13	1:H:144:LEU:HD22	2.01	0.43
1:F:186:LEU:C	1:F:187:LEU:HD12	2.39	0.43
1:C:134:PHE:CD2	1:C:349:LYS:HE2	2.54	0.43
1:B:327:PRO:HB3	1:H:249:ARG:NH1	2.33	0.43
1:F:119:PRO:HA	1:F:160:ILE:HB	2.01	0.43
1:F:76:TYR:CD1	1:F:77:ASP:N	2.86	0.43
1:H:187:LEU:N	1:H:187:LEU:HD12	2.33	0.43
1:C:50:LEU:O	1:C:119:PRO:HD2	2.19	0.43
1:B:110:LEU:O	1:B:113:MET:HG2	2.19	0.43
1:F:63:LEU:CB	1:F:276:VAL:HG21	2.48	0.43
1:E:293:ILE:CG2	1:E:311:LYS:HE2	2.49	0.43
1:G:239:THR:C	1:G:241:GLU:N	2.71	0.43
1:G:138:ALA:HB1	1:G:353:PHE:CE2	2.54	0.43
1:H:230:SER:HB3	1:H:329:ASN:ND2	2.34	0.43
1:C:115:LEU:HD12	1:C:156:ILE:O	2.18	0.43
1:A:333:ARG:HB3	1:C:241:GLU:OE2	2.18	0.43
1:E:228:LEU:HA	1:E:332:GLU:OE2	2.19	0.43
1:G:48:ALA:CB	1:G:113:MET:HG2	2.48	0.43
1:F:107:GLU:HG3	1:F:151:CYS:SG	2.58	0.43
1:A:295:CYS:HA	1:A:310:SER:O	2.18	0.43
1:E:46:LYS:HB3	1:E:113:MET:CE	2.49	0.43
1:F:124:ARG:HG2	1:F:124:ARG:NH1	2.33	0.43
1:G:115:LEU:HD12	1:G:156:ILE:O	2.18	0.43
1:G:76:TYR:CG	1:G:77:ASP:N	2.86	0.43
1:A:128:MET:C	1:A:130:ARG:H	2.20	0.43
1:H:217:VAL:HG21	1:H:325:LEU:HD22	1.99	0.43
1:C:295:CYS:HA	1:C:310:SER:O	2.19	0.43
1:E:65:LYS:HG2	1:E:88:ILE:HG23	2.01	0.43
1:E:46:LYS:HG2	1:E:72:VAL:HB	1.99	0.43
1:G:303:THR:HG22	1:G:304:GLU:N	2.33	0.43
1:D:130:ARG:HA	1:D:130:ARG:NE	2.32	0.43
1:D:67:ASN:HB3	1:D:70:VAL:HG23	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:350:GLY:C	1:H:352:SER:H	2.23	0.43
1:E:58:GLN:HB3	1:F:269:LEU:HD11	2.01	0.42
1:E:54:GLY:HA3	3:E:368:HOH:O	2.18	0.42
1:C:220:HIS:O	1:C:220:HIS:CG	2.72	0.42
1:C:100:PHE:CG	1:C:109:ALA:HB2	2.53	0.42
1:D:215:PRO:HG2	1:D:228:LEU:HB2	2.01	0.42
1:D:315:GLY:HA3	1:D:320:GLU:CG	2.48	0.42
1:A:124:ARG:HB3	1:A:128:MET:HB2	2.00	0.42
1:F:258:VAL:CG1	1:F:263:GLY:HA2	2.49	0.42
1:D:166:SER:O	1:D:169:PRO:HD2	2.19	0.42
1:H:60:LEU:HD12	1:H:276:VAL:CG2	2.49	0.42
1:F:46:LYS:HG2	1:F:72:VAL:HG22	2.02	0.42
1:D:204:VAL:HG21	1:D:246:LEU:HD21	2.01	0.42
1:G:49:ILE:CD1	1:G:61:ALA:HA	2.49	0.42
1:F:60:LEU:O	1:F:60:LEU:HD12	2.19	0.42
1:A:128:MET:HE3	1:A:133:LEU:HD13	2.01	0.42
1:G:303:THR:HG21	1:G:305:LEU:HD13	2.01	0.42
1:F:127:GLY:C	1:F:129:THR:N	2.71	0.42
1:H:171:ALA:O	1:H:174:VAL:HB	2.20	0.42
1:G:244:SER:HA	1:G:331:TYR:OH	2.20	0.42
1:B:130:ARG:HG3	1:B:132:ASP:HA	2.02	0.42
1:H:336:LEU:CG	1:H:340:LYS:HE3	2.44	0.42
1:H:193:ASP:OD2	1:H:220:HIS:CD2	2.64	0.42
1:C:63:LEU:CB	1:C:276:VAL:HG21	2.50	0.42
1:H:119:PRO:HA	1:H:160:ILE:HB	2.01	0.42
1:B:88:ILE:HG22	1:B:97:VAL:HG11	2.02	0.42
1:E:118:VAL:HB	1:E:159:LEU:HD12	2.01	0.42
1:A:100:PHE:CG	1:A:109:ALA:HB2	2.54	0.42
1:B:170:ILE:O	1:B:174:VAL:HG23	2.20	0.42
1:D:139:GLY:O	1:D:142:LYS:HB3	2.20	0.42
1:G:303:THR:HG23	1:G:304:GLU:OE1	2.20	0.42
1:B:166:SER:O	1:B:170:ILE:HG13	2.20	0.42
1:F:81:ALA:HB3	1:F:82:PRO:HD3	2.02	0.42
1:D:185:ARG:NH2	3:D:369:HOH:O	2.53	0.42
1:E:123:PRO:HG3	1:E:125:LYS:HE3	2.01	0.41
1:G:166:SER:O	1:G:170:ILE:HG13	2.20	0.41
1:F:56:ILE:CD1	1:F:271:MET:HG2	2.47	0.41
1:E:129:THR:O	1:E:130:ARG:CB	2.64	0.41
1:B:81:ALA:N	1:B:82:PRO:CD	2.83	0.41
1:G:76:TYR:HE1	1:G:102:GLY:O	2.03	0.41
1:E:104:GLN:N	1:E:104:GLN:CD	2.74	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ALA:N	1:E:82:PRO:CD	2.83	0.41
1:F:230:SER:HB3	1:F:329:ASN:ND2	2.35	0.41
1:F:48:ALA:HB2	1:F:113:MET:HG3	2.01	0.41
1:D:315:GLY:HA2	3:D:374:HOH:O	2.20	0.41
1:H:229:LEU:HA	1:H:232:VAL:HG23	2.02	0.41
1:D:121:GLY:O	1:D:122:VAL:HG13	2.19	0.41
1:E:255:THR:O	1:E:259:GLU:HB2	2.20	0.41
1:D:69:LEU:HD21	1:D:287:ARG:NH1	2.36	0.41
1:B:218:GLY:HA2	1:B:308:PHE:CZ	2.56	0.41
1:B:60:LEU:HD12	1:B:276:VAL:HG22	2.02	0.41
1:C:166:SER:C	1:C:169:PRO:HD2	2.41	0.41
1:G:306:PRO:HG2	1:G:347:ILE:HD13	2.02	0.41
1:G:315:GLY:HA3	1:G:320:GLU:CD	2.41	0.41
1:E:174:VAL:HG13	3:E:370:HOH:O	2.20	0.41
1:C:302:VAL:HG22	1:C:324:SER:HA	2.02	0.41
1:C:226:LEU:HD22	1:C:336:LEU:HA	2.02	0.41
1:D:223:VAL:HG21	1:D:338:LYS:HE2	2.01	0.41
1:H:104:GLN:O	1:H:104:GLN:HG2	2.19	0.41
1:A:218:GLY:HA2	1:A:308:PHE:CZ	2.56	0.41
1:H:67:ASN:HA	1:H:68:PRO:HD2	1.91	0.41
1:C:249:ARG:HG2	1:C:249:ARG:HH11	1.86	0.41
1:G:124:ARG:HH21	1:G:128:MET:CB	2.34	0.41
1:A:219:GLY:HA3	1:A:224:THR:CG2	2.50	0.41
1:E:78:VAL:O	1:E:79:VAL:HG13	2.20	0.41
1:B:142:LYS:HE2	1:B:146:GLU:OE2	2.21	0.41
1:B:234:PRO:HB3	1:G:105:GLN:CD	2.41	0.41
1:H:253:GLY:O	1:H:256:GLU:HB2	2.20	0.41
1:D:133:LEU:HD12	1:D:133:LEU:C	2.41	0.41
1:A:81:ALA:N	1:A:82:PRO:CD	2.84	0.41
1:A:258:VAL:CG1	1:A:263:GLY:HA2	2.51	0.41
1:G:284:ARG:O	1:G:289:ASP:HB2	2.20	0.41
1:D:144:LEU:O	1:D:148:ILE:HG13	2.21	0.41
1:B:208:ASP:OD1	1:B:210:ARG:HB2	2.21	0.41
1:G:330:GLU:HA	1:G:333:ARG:CZ	2.51	0.41
1:H:221:ALA:N	1:H:224:THR:HG22	2.35	0.41
1:H:132:ASP:C	1:H:134:PHE:N	2.73	0.41
1:E:238:PHE:HB2	1:E:243:ILE:HG12	2.02	0.41
1:G:198:ASN:OD1	1:G:213:ASP:HA	2.21	0.41
1:H:85:THR:HG21	1:H:99:GLY:N	2.36	0.41
1:A:125:LYS:N	1:A:128:MET:CG	2.84	0.40
1:D:166:SER:O	1:D:170:ILE:HG13	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:SER:O	1:D:267:ALA:C	2.59	0.40
1:A:60:LEU:HD13	1:A:276:VAL:HG22	2.03	0.40
1:G:129:THR:HG22	1:G:130:ARG:H	1.84	0.40
1:D:66:MET:HG3	1:D:91:MET:HE1	2.03	0.40
1:A:261:LYS:HG2	1:B:83:GLY:HA3	2.04	0.40
1:D:81:ALA:N	1:D:82:PRO:CD	2.85	0.40
1:F:232:VAL:CG1	1:F:233:LYS:N	2.83	0.40
1:D:281:ALA:O	1:D:292:VAL:HG11	2.21	0.40
1:D:55:GLY:O	1:D:268:THR:HG23	2.21	0.40
1:F:63:LEU:CD1	1:F:276:VAL:HG21	2.51	0.40
1:E:173:GLU:HB3	1:E:354:ILE:HG21	2.01	0.40
1:E:228:LEU:HD13	1:E:231:GLN:NE2	2.37	0.40
1:C:232:VAL:HG22	1:C:233:LYS:N	2.35	0.40
1:E:70:VAL:O	1:E:95:ALA:HB2	2.21	0.40
1:G:262:ALA:O	1:G:264:ALA:N	2.54	0.40
1:B:100:PHE:CG	1:B:109:ALA:HB2	2.56	0.40
1:H:169:PRO:HB3	1:H:351:VAL:CG2	2.51	0.40
1:H:329:ASN:OD1	1:H:332:GLU:HG3	2.22	0.40
1:G:127:GLY:O	1:G:128:MET:HG3	2.21	0.40
1:D:127:GLY:O	1:D:129:THR:N	2.54	0.40
1:D:220:HIS:CE1	3:D:379:HOH:O	2.75	0.40
1:H:182:ASP:C	1:H:184:LYS:H	2.25	0.40
1:A:187:LEU:N	1:A:187:LEU:HD12	2.35	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	311/326 (95%)	296 (95%)	11 (4%)	4 (1%)	15 26
1	B	311/326 (95%)	294 (94%)	13 (4%)	4 (1%)	15 26

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	311/326 (95%)	300 (96%)	11 (4%)	0	100	100
1	D	311/326 (95%)	292 (94%)	16 (5%)	3 (1%)	19	34
1	E	311/326 (95%)	285 (92%)	20 (6%)	6 (2%)	10	16
1	F	311/326 (95%)	295 (95%)	9 (3%)	7 (2%)	8	12
1	G	311/326 (95%)	281 (90%)	24 (8%)	6 (2%)	10	16
1	H	311/326 (95%)	283 (91%)	19 (6%)	9 (3%)	6	8
All	All	2488/2608 (95%)	2326 (94%)	123 (5%)	39 (2%)	12	21

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	ASP
1	F	130	ARG
1	H	80	ASN
1	A	80	ASN
1	A	128	MET
1	A	130	ARG
1	B	263	GLY
1	E	134	PHE
1	F	129	THR
1	F	131	ASP
1	G	130	ARG
1	H	94	GLY
1	H	125	LYS
1	A	125	LYS
1	E	263	GLY
1	E	341	LYS
1	H	95	ALA
1	B	321	GLU
1	E	132	ASP
1	F	120	ALA
1	F	125	LYS
1	G	80	ASN
1	G	136	ILE
1	G	263	GLY
1	H	130	ARG
1	H	131	ASP
1	D	128	MET
1	E	125	LYS
1	F	80	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	124	ARG
1	G	127	GLY
1	B	120	ALA
1	E	131	ASP
1	G	125	LYS
1	H	126	PRO
1	H	183	PRO
1	D	125	LYS
1	D	126	PRO
1	H	152	CYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/256 (96%)	242 (98%)	5 (2%)	63	86
1	B	247/256 (96%)	246 (100%)	1 (0%)	93	98
1	C	247/256 (96%)	244 (99%)	3 (1%)	78	93
1	D	247/256 (96%)	245 (99%)	2 (1%)	86	96
1	E	247/256 (96%)	243 (98%)	4 (2%)	70	90
1	F	247/256 (96%)	239 (97%)	8 (3%)	46	74
1	G	247/256 (96%)	243 (98%)	4 (2%)	70	90
1	H	247/256 (96%)	243 (98%)	4 (2%)	70	90
All	All	1976/2048 (96%)	1945 (98%)	31 (2%)	70	90

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	129	THR
1	A	191	MET
1	A	224	THR
1	A	302	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	132	ASP
1	C	143	THR
1	C	224	THR
1	C	302	VAL
1	D	191	MET
1	D	268	THR
1	E	187	LEU
1	E	241	GLU
1	E	289	ASP
1	E	305	LEU
1	F	60	LEU
1	F	129	THR
1	F	131	ASP
1	F	132	ASP
1	F	133	LEU
1	F	143	THR
1	F	191	MET
1	F	241	GLU
1	G	113	MET
1	G	125	LYS
1	G	191	MET
1	G	241	GLU
1	H	191	MET
1	H	248	ASP
1	H	289	ASP
1	H	301	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	220	HIS
1	B	158	ASN
1	B	220	HIS
1	C	103	GLN
1	C	104	GLN
1	C	105	GLN
1	C	317	ASN
1	D	105	GLN
1	D	317	ASN
1	E	104	GLN
1	E	158	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	158	ASN
1	H	103	GLN
1	H	158	ASN
1	H	162	ASN
1	H	220	HIS
1	H	301	GLN

### 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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	C	1313	-	3,12,12	1.78	1 (33%)	3,17,17	1.76	1 (33%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	C	1313	-	-	0/6/16/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1313	CIT	C4-C3	2.38	1.58	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1313	CIT	C3-C4-C5	-2.86	110.39	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	313/326 (96%)	-0.38	7 (2%) 65 69	14, 27, 48, 126	0
1	B	313/326 (96%)	-0.18	10 (3%) 51 56	18, 34, 65, 131	0
1	C	313/326 (96%)	-0.54	2 (0%) 90 91	15, 26, 38, 62	0
1	D	313/326 (96%)	-0.06	15 (4%) 34 39	18, 37, 65, 130	0
1	E	313/326 (96%)	0.24	15 (4%) 34 39	24, 52, 76, 130	0
1	F	313/326 (96%)	-0.25	6 (1%) 70 73	19, 35, 57, 112	0
1	G	313/326 (96%)	0.15	17 (5%) 29 33	25, 50, 80, 122	0
1	H	313/326 (96%)	0.09	15 (4%) 34 39	28, 46, 80, 140	0
All	All	2504/2608 (96%)	-0.12	87 (3%) 48 53	14, 38, 73, 140	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	MET	11.1
1	A	129	THR	9.3
1	D	128	MET	8.2
1	D	129	THR	8.2
1	F	128	MET	7.8
1	H	126	PRO	7.5
1	B	129	THR	6.7
1	H	127	GLY	6.3
1	B	128	MET	5.7
1	B	127	GLY	5.7
1	D	126	PRO	5.6
1	B	126	PRO	5.6
1	E	124	ARG	5.5
1	E	130	ARG	5.4
1	A	124	ARG	5.4
1	H	124	ARG	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	129	THR	4.8
1	E	126	PRO	4.7
1	E	129	THR	4.6
1	G	127	GLY	4.6
1	D	356	SER	4.5
1	E	131	ASP	4.4
1	E	355	ARG	4.3
1	H	129	THR	4.3
1	G	130	ARG	4.3
1	G	124	ARG	4.2
1	F	126	PRO	4.1
1	G	356	SER	4.1
1	H	125	LYS	4.1
1	A	128	MET	4.0
1	D	124	ARG	3.9
1	A	125	LYS	3.8
1	H	356	SER	3.8
1	F	127	GLY	3.8
1	D	125	LYS	3.7
1	D	127	GLY	3.7
1	E	356	SER	3.7
1	A	126	PRO	3.6
1	A	127	GLY	3.6
1	G	355	ARG	3.6
1	B	131	ASP	3.5
1	D	132	ASP	3.4
1	H	130	ARG	3.4
1	D	355	ARG	3.3
1	E	125	LYS	3.2
1	E	127	GLY	3.1
1	H	355	ARG	3.1
1	F	125	LYS	3.0
1	D	133	LEU	2.9
1	B	125	LYS	2.9
1	B	356	SER	2.9
1	D	131	ASP	2.8
1	E	128	MET	2.8
1	H	177	LYS	2.7
1	F	356	SER	2.6
1	H	44	GLY	2.6
1	G	128	MET	2.6
1	H	304	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	129	THR	2.6
1	A	131	ASP	2.6
1	G	331	TYR	2.5
1	G	341	LYS	2.5
1	D	130	ARG	2.5
1	G	178	ALA	2.5
1	B	355	ARG	2.4
1	H	133	LEU	2.4
1	D	123	PRO	2.4
1	E	291	GLY	2.4
1	G	133	LEU	2.4
1	G	123	PRO	2.4
1	E	240	GLN	2.3
1	E	154	ARG	2.3
1	B	124	ARG	2.3
1	G	154	ARG	2.3
1	D	154	ARG	2.2
1	D	301	GLN	2.2
1	E	263	GLY	2.2
1	G	263	GLY	2.1
1	E	264	ALA	2.1
1	H	291	GLY	2.1
1	C	356	SER	2.1
1	H	179	GLY	2.1
1	G	240	GLN	2.1
1	B	263	GLY	2.1
1	G	348	GLU	2.1
1	C	355	ARG	2.0
1	G	116	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
2	CIT	C	1313	13/13	0.94	0.15	1.28	28,36,46,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.