



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:21 pm BST

PDB ID : 2CFQ  
Title : Sugar Free Lactose Permease at neutral pH  
Authors : Mirza, O.; Guan, L.; Verner, G.; Iwata, S.; Kaback, H.R.  
Deposited on : 2006-02-22  
Resolution : 2.95 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

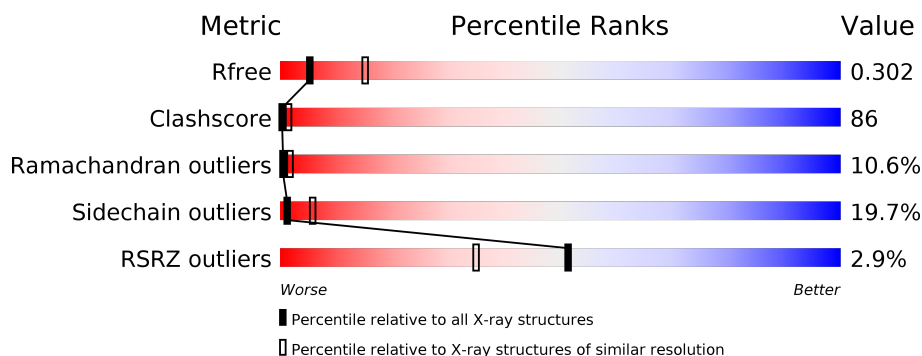
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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	417	<div> <div>3%</div> <div>18%</div> <div>62%</div> <div>18%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3295 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 LACTOSE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	53	0	0
			3290	2222	506	541	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	engineered mutation	UNP P02920

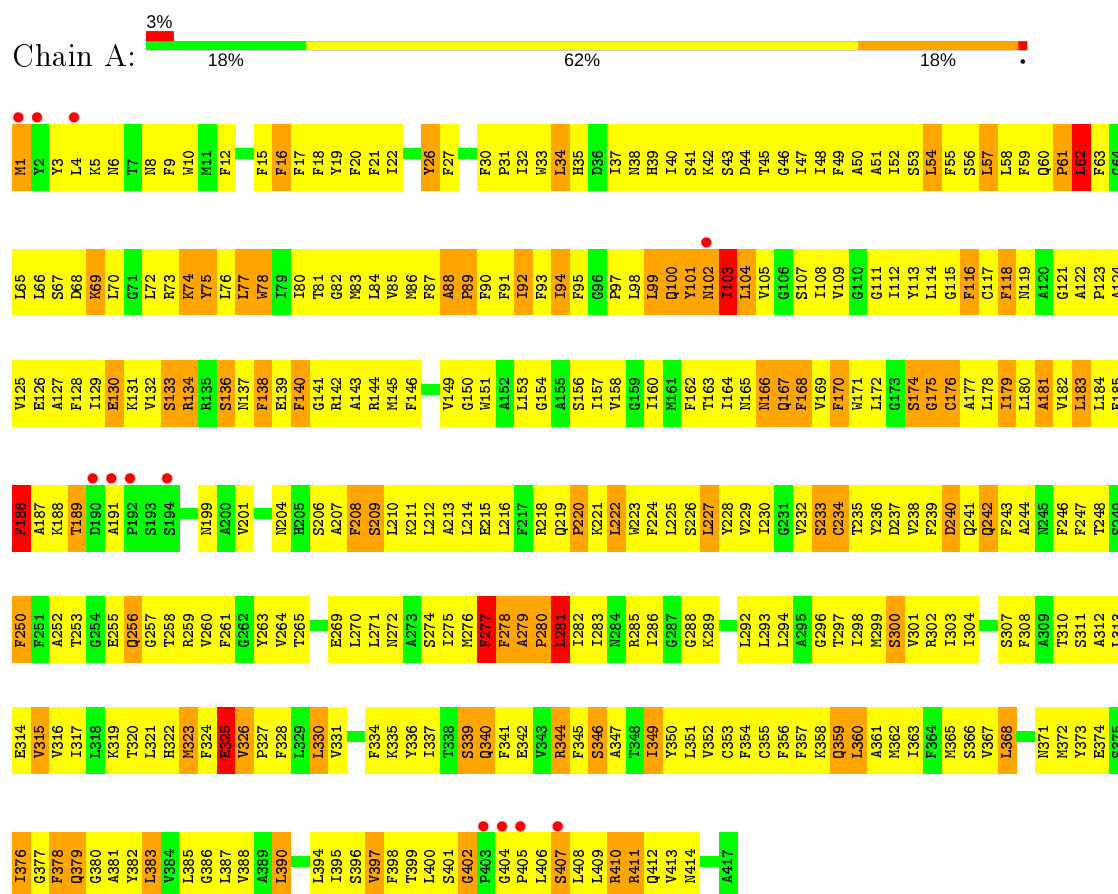
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Hg	0	0
			5	5		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: LACTOSE PERMEASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.47Å 122.47Å 187.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 2.95 11.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	82.6 (9.99-2.95) 81.2 (11.99-2.81)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.262 , 0.298 0.264 , 0.302	Depositor DCC
$R_{free}$ test set	909 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 121.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.66	0/3387	0.91	1/4588 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ILE	N-CA-C	-10.31	83.15	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3332	561	0
2	A	5	0	0	0	0
All	All	3295	0	3332	561	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 86.

All (561) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:VAL:HA	1:A:178:LEU:HG	1.26	1.13
1:A:330:LEU:HD23	1:A:331:VAL:HG23	1.42	1.02
1:A:358:LYS:O	1:A:362:MET:HG3	1.60	1.00
1:A:330:LEU:H	1:A:330:LEU:HD13	1.22	0.99
1:A:334:PHE:HD2	1:A:335:LYS:HD2	1.25	0.98
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.46	0.97
1:A:411:ARG:HA	1:A:411:ARG:HE	1.30	0.96
1:A:101:TYR:O	1:A:103:ILE:HG12	1.66	0.96
1:A:22:ILE:HG13	1:A:177:ALA:CB	1.96	0.96
1:A:85:VAL:HG22	1:A:178:LEU:HD11	1.47	0.96
1:A:330:LEU:HD22	1:A:331:VAL:H	1.29	0.95
1:A:180:LEU:N	1:A:180:LEU:HD12	1.80	0.94
1:A:234:CYS:SG	1:A:362:MET:HG2	2.08	0.93
1:A:98:LEU:HB3	1:A:107:SER:HB2	1.51	0.93
1:A:209:SER:H	1:A:212:LEU:HD12	1.31	0.92
1:A:90:PHE:HA	1:A:94:ILE:HD12	1.52	0.92
1:A:100:GLN:C	1:A:102:ASN:H	1.70	0.91
1:A:1:MET:H2	1:A:4:LEU:HG	1.36	0.90
1:A:337:ILE:HD12	1:A:349:ILE:HG21	1.51	0.90
1:A:54:LEU:O	1:A:54:LEU:HG	1.72	0.90
1:A:297:THR:O	1:A:301:VAL:HG23	1.72	0.89
1:A:92:ILE:HD12	1:A:92:ILE:H	1.36	0.89
1:A:51:ALA:HB3	1:A:112:ILE:HD12	1.55	0.89
1:A:85:VAL:CA	1:A:178:LEU:HG	2.01	0.89
1:A:51:ALA:HB3	1:A:112:ILE:CD1	2.03	0.89
1:A:407:SER:HB3	1:A:411:ARG:HB3	1.51	0.88
1:A:22:ILE:HG13	1:A:177:ALA:HB3	1.54	0.87
1:A:296:GLY:O	1:A:300:SER:HB2	1.75	0.87
1:A:74:LYS:H	1:A:74:LYS:HE3	1.40	0.87
1:A:394:LEU:O	1:A:397:VAL:HG23	1.74	0.86
1:A:330:LEU:CD2	1:A:331:VAL:HG23	2.05	0.86
1:A:409:LEU:HA	1:A:413:VAL:HB	1.57	0.85
1:A:12:PHE:HD2	1:A:129:ILE:HG12	1.41	0.85
1:A:342:GLU:HB2	1:A:345:PHE:CD1	2.10	0.85
1:A:334:PHE:CD2	1:A:335:LYS:HD2	2.12	0.84
1:A:279:ALA:O	1:A:283:ILE:HG12	1.77	0.84
1:A:178:LEU:HD13	1:A:179:ILE:N	1.94	0.82
1:A:54:LEU:O	1:A:57:LEU:HD22	1.79	0.82
1:A:74:LYS:HD3	1:A:188:LYS:HD2	1.59	0.82
1:A:238:VAL:O	1:A:241:GLN:HG2	1.80	0.82
1:A:116:PHE:HD2	1:A:117:CYS:N	1.78	0.81
1:A:246:PHE:HB2	1:A:378:PHE:CD2	2.16	0.81

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CD2	1:A:399:THR:HB	2.15	0.81
1:A:92:ILE:N	1:A:92:ILE:HD12	1.95	0.81
1:A:77:LEU:HD21	1:A:185:PHE:CZ	2.15	0.81
1:A:282:ILE:HG23	1:A:285:ARG:HH21	1.46	0.80
1:A:172:LEU:O	1:A:176:CYS:HB3	1.82	0.79
1:A:154:GLY:O	1:A:158:VAL:HG23	1.82	0.79
1:A:311:SER:OG	1:A:314:GLU:HG3	1.82	0.79
1:A:92:ILE:H	1:A:92:ILE:CD1	1.95	0.79
1:A:210:LEU:O	1:A:214:LEU:HG	1.82	0.79
1:A:8:ASN:ND2	1:A:189:THR:OG1	2.16	0.78
1:A:139:GLU:O	1:A:142:ARG:N	2.16	0.78
1:A:88:ALA:HB3	1:A:89:PRO:CD	2.13	0.78
1:A:278:PHE:HB3	1:A:282:ILE:HD11	1.65	0.77
1:A:62:LEU:O	1:A:66:LEU:HD12	1.84	0.77
1:A:85:VAL:HG13	1:A:178:LEU:HD12	1.67	0.77
1:A:396:SER:C	1:A:398:PHE:H	1.86	0.77
1:A:22:ILE:CG1	1:A:177:ALA:HB3	2.15	0.76
1:A:91:PHE:HA	1:A:95:PHE:HB3	1.67	0.76
1:A:99:LEU:HD23	1:A:107:SER:OG	1.84	0.76
1:A:330:LEU:CD2	1:A:331:VAL:H	1.98	0.76
1:A:326:VAL:HG13	1:A:330:LEU:HD11	1.66	0.75
1:A:88:ALA:O	1:A:92:ILE:HD13	1.85	0.75
1:A:108:ILE:O	1:A:112:ILE:HG13	1.87	0.75
1:A:312:ALA:O	1:A:315:VAL:HG12	1.85	0.75
1:A:46:GLY:O	1:A:50:ALA:HB2	1.87	0.75
1:A:264:VAL:HB	1:A:319:LYS:HD2	1.68	0.74
1:A:180:LEU:C	1:A:182:VAL:H	1.89	0.74
1:A:85:VAL:HG22	1:A:178:LEU:CD1	2.18	0.74
1:A:210:LEU:HG	1:A:214:LEU:HD11	1.68	0.74
1:A:70:LEU:CD2	1:A:73:ARG:HB2	2.18	0.74
1:A:74:LYS:CD	1:A:188:LYS:HD2	2.18	0.74
1:A:221:LYS:NZ	1:A:340:GLN:O	2.20	0.73
1:A:178:LEU:HD13	1:A:178:LEU:C	2.08	0.73
1:A:178:LEU:O	1:A:182:VAL:HG12	1.89	0.73
1:A:316:VAL:HG12	1:A:316:VAL:O	1.89	0.72
1:A:302:ARG:HH21	1:A:319:LYS:HA	1.55	0.72
1:A:408:LEU:O	1:A:413:VAL:HG23	1.90	0.72
1:A:100:GLN:C	1:A:102:ASN:N	2.41	0.71
1:A:368:LEU:O	1:A:372:MET:HB2	1.89	0.71
1:A:410:ARG:HA	1:A:410:ARG:HH11	1.55	0.71
1:A:411:ARG:HH21	1:A:414:ASN:HD21	1.39	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:O	1:A:81:THR:HG23	1.91	0.71
1:A:35:HIS:O	1:A:39:HIS:HA	1.90	0.70
1:A:1:MET:N	1:A:4:LEU:HG	2.06	0.70
1:A:136:SER:HB3	1:A:138:PHE:CE1	2.27	0.70
1:A:294:LEU:O	1:A:298:ILE:HG12	1.91	0.70
1:A:351:LEU:HD23	1:A:351:LEU:C	2.11	0.70
1:A:368:LEU:O	1:A:368:LEU:HD12	1.91	0.70
1:A:410:ARG:HA	1:A:410:ARG:NH1	2.06	0.70
1:A:241:GLN:HE21	1:A:366:SER:HB2	1.57	0.69
1:A:271:LEU:HD21	1:A:324:PHE:CE1	2.26	0.69
1:A:225:LEU:HD12	1:A:336:TYR:CE2	2.27	0.69
1:A:121:GLY:O	1:A:125:VAL:HG23	1.93	0.69
1:A:185:PHE:O	1:A:188:LYS:HD3	1.92	0.69
1:A:293:LEU:HD13	1:A:397:VAL:HG13	1.74	0.68
1:A:74:LYS:H	1:A:74:LYS:CE	2.05	0.68
1:A:41:SER:HB3	1:A:44:ASP:HB2	1.76	0.68
1:A:83:MET:SD	1:A:117:CYS:SG	2.91	0.68
1:A:90:PHE:HA	1:A:94:ILE:CD1	2.24	0.68
1:A:330:LEU:HD22	1:A:331:VAL:N	2.08	0.68
1:A:396:SER:C	1:A:398:PHE:N	2.45	0.68
1:A:93:PHE:C	1:A:94:ILE:HG13	2.13	0.67
1:A:84:LEU:HD21	1:A:117:CYS:SG	2.34	0.67
1:A:185:PHE:O	1:A:187:ALA:N	2.28	0.67
1:A:180:LEU:HD12	1:A:180:LEU:H	1.54	0.67
1:A:47:ILE:HD13	1:A:367:VAL:HG22	1.76	0.67
1:A:54:LEU:N	1:A:363:ILE:CD1	2.57	0.67
1:A:172:LEU:HG	1:A:176:CYS:HB3	1.77	0.66
1:A:208:PHE:N	1:A:208:PHE:HD1	1.93	0.66
1:A:233:SER:O	1:A:236:TYR:N	2.28	0.66
1:A:57:LEU:C	1:A:57:LEU:HD23	2.15	0.66
1:A:170:PHE:HD1	1:A:170:PHE:H	1.44	0.66
1:A:238:VAL:HA	1:A:241:GLN:HG2	1.78	0.66
1:A:62:LEU:HD23	1:A:62:LEU:C	2.16	0.66
1:A:282:ILE:HA	1:A:285:ARG:HE	1.61	0.66
1:A:335:LYS:O	1:A:339:SER:OG	2.12	0.65
1:A:307:SER:C	1:A:379:GLN:HE21	1.98	0.65
1:A:260:VAL:O	1:A:264:VAL:HG23	1.97	0.65
1:A:278:PHE:H	1:A:278:PHE:HD1	1.43	0.65
1:A:325:GLU:OE2	1:A:326:VAL:N	2.29	0.65
1:A:52:ILE:HD13	1:A:112:ILE:HG23	1.78	0.65
1:A:230:ILE:HD11	1:A:357:PHE:HB3	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:OD1	1:A:167:GLN:N	2.30	0.65
1:A:208:PHE:CD1	1:A:208:PHE:N	2.62	0.65
1:A:32:ILE:CG2	1:A:162:PHE:HE2	2.09	0.65
1:A:51:ALA:CB	1:A:112:ILE:HD12	2.27	0.65
1:A:68:ASP:C	1:A:70:LEU:H	2.01	0.65
1:A:90:PHE:CE2	1:A:95:PHE:HB2	2.32	0.64
1:A:282:ILE:O	1:A:286:ILE:HG22	1.98	0.64
1:A:12:PHE:CD2	1:A:129:ILE:HG12	2.30	0.64
1:A:38:ASN:HB2	1:A:40:ILE:HD11	1.79	0.64
1:A:206:SER:OG	1:A:207:ALA:N	2.28	0.64
1:A:38:ASN:HA	1:A:100:GLN:HE22	1.63	0.63
1:A:409:LEU:C	1:A:410:ARG:HD2	2.18	0.63
1:A:342:GLU:OE1	1:A:344:ARG:HD3	1.97	0.63
1:A:280:PRO:O	1:A:281:LEU:C	2.36	0.63
1:A:330:LEU:CD2	1:A:331:VAL:N	2.61	0.63
1:A:174:SER:O	1:A:178:LEU:HB3	1.99	0.63
1:A:30:PHE:HB3	1:A:31:PRO:HD3	1.79	0.63
1:A:278:PHE:O	1:A:281:LEU:HB3	1.99	0.62
1:A:85:VAL:HG13	1:A:178:LEU:CD1	2.29	0.62
1:A:180:LEU:N	1:A:180:LEU:CD1	2.55	0.62
1:A:92:ILE:HD11	1:A:170:PHE:CB	2.29	0.62
1:A:232:VAL:HG12	1:A:299:MET:SD	2.40	0.62
1:A:116:PHE:CD2	1:A:116:PHE:C	2.73	0.62
1:A:122:ALA:N	1:A:123:PRO:HD2	2.15	0.61
1:A:73:ARG:HB3	1:A:75:TYR:CD1	2.35	0.61
1:A:180:LEU:O	1:A:182:VAL:N	2.33	0.61
1:A:246:PHE:HB2	1:A:378:PHE:CE2	2.34	0.61
1:A:34:LEU:O	1:A:38:ASN:HB2	2.00	0.61
1:A:88:ALA:C	1:A:92:ILE:HD13	2.20	0.61
1:A:100:GLN:O	1:A:102:ASN:N	2.31	0.61
1:A:298:ILE:N	1:A:298:ILE:HD13	2.14	0.61
1:A:298:ILE:O	1:A:299:MET:C	2.39	0.61
1:A:313:LEU:O	1:A:317:ILE:HG12	1.99	0.61
1:A:407:SER:HB3	1:A:411:ARG:CB	2.30	0.61
1:A:233:SER:O	1:A:234:CYS:C	2.38	0.61
1:A:170:PHE:O	1:A:174:SER:HB2	2.01	0.61
1:A:210:LEU:HG	1:A:214:LEU:CD1	2.31	0.60
1:A:89:PRO:O	1:A:93:PHE:HB2	2.00	0.60
1:A:238:VAL:O	1:A:241:GLN:CG	2.49	0.60
1:A:182:VAL:HG13	1:A:183:LEU:N	2.17	0.60
1:A:225:LEU:O	1:A:229:VAL:HG23	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:O	1:A:69:LYS:HB3	2.00	0.60
1:A:282:ILE:HA	1:A:285:ARG:NE	2.16	0.60
1:A:356:PHE:O	1:A:360:LEU:HB2	2.01	0.60
1:A:323:MET:O	1:A:327:PRO:HD2	2.01	0.60
1:A:376:ILE:HD12	1:A:380:GLY:HA3	1.83	0.60
1:A:337:ILE:HD12	1:A:349:ILE:CG2	2.28	0.59
1:A:178:LEU:CD1	1:A:179:ILE:N	2.65	0.59
1:A:280:PRO:HG2	1:A:281:LEU:H	1.67	0.59
1:A:146:PHE:O	1:A:149:VAL:HG12	2.01	0.59
1:A:278:PHE:CB	1:A:282:ILE:HD11	2.31	0.59
1:A:108:ILE:HB	1:A:112:ILE:HD11	1.84	0.59
1:A:236:TYR:CG	1:A:299:MET:HG2	2.37	0.59
1:A:112:ILE:O	1:A:112:ILE:HG22	2.02	0.59
1:A:59:PHE:CD2	1:A:116:PHE:HB2	2.38	0.59
1:A:38:ASN:CA	1:A:100:GLN:HE22	2.16	0.59
1:A:105:VAL:O	1:A:108:ILE:HG13	2.02	0.59
1:A:359:GLN:O	1:A:363:ILE:HG12	2.02	0.59
1:A:279:ALA:C	1:A:283:ILE:HG12	2.23	0.59
1:A:185:PHE:O	1:A:186:PHE:C	2.40	0.59
1:A:279:ALA:O	1:A:280:PRO:C	2.40	0.59
1:A:88:ALA:HA	1:A:92:ILE:HD13	1.84	0.59
1:A:88:ALA:O	1:A:89:PRO:C	2.42	0.58
1:A:211:LYS:O	1:A:215:GLU:N	2.36	0.58
1:A:241:GLN:NE2	1:A:366:SER:HB2	2.16	0.58
1:A:82:GLY:HA2	1:A:85:VAL:HG23	1.85	0.58
1:A:89:PRO:O	1:A:94:ILE:HD12	2.03	0.58
1:A:233:SER:O	1:A:235:THR:N	2.36	0.58
1:A:258:THR:O	1:A:261:PHE:N	2.35	0.58
1:A:178:LEU:HD13	1:A:179:ILE:CA	2.33	0.58
1:A:41:SER:HB3	1:A:44:ASP:CB	2.33	0.58
1:A:54:LEU:HA	1:A:363:ILE:HD11	1.86	0.58
1:A:236:TYR:O	1:A:239:PHE:HB3	2.04	0.58
1:A:45:THR:HA	1:A:48:ILE:HD12	1.86	0.57
1:A:68:ASP:C	1:A:70:LEU:N	2.56	0.57
1:A:93:PHE:O	1:A:94:ILE:HG13	2.04	0.57
1:A:48:ILE:HG12	1:A:108:ILE:CG2	2.34	0.57
1:A:160:ILE:HD11	1:A:263:TYR:CZ	2.39	0.57
1:A:15:PHE:HA	1:A:184:LEU:HD12	1.85	0.57
1:A:21:PHE:CE1	1:A:154:GLY:HA2	2.40	0.57
1:A:326:VAL:HG12	1:A:327:PRO:N	2.19	0.57
1:A:88:ALA:CB	1:A:89:PRO:HD3	2.28	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD23	1:A:323:MET:CB	2.34	0.57
1:A:383:LEU:HD23	1:A:387:LEU:HD11	1.86	0.57
1:A:280:PRO:O	1:A:283:ILE:N	2.38	0.57
1:A:180:LEU:C	1:A:182:VAL:N	2.59	0.57
1:A:186:PHE:HD1	1:A:187:ALA:N	2.03	0.57
1:A:260:VAL:HA	1:A:263:TYR:CD1	2.40	0.56
1:A:33:TRP:HA	1:A:37:ILE:HD13	1.86	0.56
1:A:32:ILE:HG22	1:A:162:PHE:HE2	1.68	0.56
1:A:271:LEU:HD21	1:A:324:PHE:HE1	1.69	0.56
1:A:186:PHE:CD1	1:A:187:ALA:N	2.73	0.56
1:A:253:THR:HG22	1:A:255:GLU:H	1.70	0.56
1:A:26:TYR:CE1	1:A:27:PHE:HD1	2.22	0.56
1:A:282:ILE:HA	1:A:285:ARG:HH21	1.70	0.56
1:A:54:LEU:N	1:A:363:ILE:HD12	2.20	0.56
1:A:85:VAL:HA	1:A:178:LEU:CG	2.18	0.56
1:A:126:GLU:OE2	1:A:144:ARG:NE	2.36	0.56
1:A:307:SER:C	1:A:308:PHE:HD1	2.08	0.56
1:A:65:LEU:HD23	1:A:65:LEU:N	2.20	0.56
1:A:74:LYS:N	1:A:74:LYS:HE3	2.15	0.56
1:A:88:ALA:CB	1:A:89:PRO:CD	2.83	0.56
1:A:12:PHE:CE2	1:A:128:PHE:HE1	2.24	0.56
1:A:376:ILE:O	1:A:376:ILE:HG23	2.06	0.56
1:A:48:ILE:HG12	1:A:108:ILE:HG21	1.87	0.56
1:A:282:ILE:HA	1:A:285:ARG:NH2	2.21	0.56
1:A:172:LEU:HG	1:A:176:CYS:CB	2.35	0.56
1:A:238:VAL:CA	1:A:241:GLN:HG2	2.35	0.56
1:A:409:LEU:HA	1:A:413:VAL:CB	2.32	0.55
1:A:339:SER:O	1:A:340:GLN:NE2	2.39	0.55
1:A:51:ALA:HB3	1:A:112:ILE:HD13	1.86	0.55
1:A:216:LEU:O	1:A:219:GLN:N	2.40	0.55
1:A:170:PHE:CD1	1:A:170:PHE:N	2.74	0.55
1:A:327:PRO:O	1:A:330:LEU:HD22	2.06	0.55
1:A:12:PHE:HE2	1:A:128:PHE:CE1	2.24	0.55
1:A:60:GLN:N	1:A:61:PRO:CD	2.70	0.55
1:A:225:LEU:HD21	1:A:354:PHE:HE1	1.71	0.55
1:A:15:PHE:HE2	1:A:125:VAL:HG13	1.72	0.55
1:A:324:PHE:CD1	1:A:324:PHE:N	2.75	0.55
1:A:34:LEU:HA	1:A:38:ASN:HD22	1.72	0.55
1:A:26:TYR:HB2	1:A:87:PHE:CZ	2.41	0.55
1:A:307:SER:C	1:A:379:GLN:NE2	2.60	0.55
1:A:410:ARG:HA	1:A:414:ASN:HB3	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:185:PHE:HZ	1.71	0.54
1:A:70:LEU:HD21	1:A:73:ARG:HB2	1.89	0.54
1:A:179:ILE:C	1:A:182:VAL:HG12	2.27	0.54
1:A:98:LEU:HB3	1:A:107:SER:CB	2.32	0.54
1:A:209:SER:N	1:A:212:LEU:HD12	2.13	0.54
1:A:279:ALA:HA	1:A:282:ILE:HD12	1.88	0.54
1:A:282:ILE:CG2	1:A:285:ARG:HH21	2.19	0.54
1:A:108:ILE:HB	1:A:112:ILE:CD1	2.38	0.54
1:A:269:GLU:C	1:A:271:LEU:H	2.11	0.54
1:A:238:VAL:C	1:A:241:GLN:HG2	2.28	0.54
1:A:47:ILE:CD1	1:A:367:VAL:HG22	2.37	0.54
1:A:381:ALA:O	1:A:385:LEU:HG	2.07	0.54
1:A:91:PHE:N	1:A:91:PHE:CD1	2.76	0.54
1:A:153:LEU:N	1:A:153:LEU:HD12	2.23	0.53
1:A:278:PHE:N	1:A:278:PHE:CD1	2.76	0.53
1:A:279:ALA:HB3	1:A:280:PRO:CD	2.38	0.53
1:A:35:HIS:HA	1:A:40:ILE:H	1.74	0.53
1:A:153:LEU:O	1:A:157:ILE:HD13	2.08	0.53
1:A:157:ILE:HG22	1:A:158:VAL:N	2.23	0.53
1:A:247:PHE:CE1	1:A:315:VAL:HG13	2.43	0.53
1:A:57:LEU:CD2	1:A:58:LEU:HG	2.38	0.53
1:A:253:THR:H	1:A:256:GLN:HG2	1.74	0.53
1:A:22:ILE:HG13	1:A:177:ALA:HB1	1.87	0.53
1:A:282:ILE:HG23	1:A:285:ARG:NH2	2.20	0.53
1:A:272:ASN:OD1	1:A:327:PRO:HG3	2.09	0.53
1:A:300:SER:OG	1:A:390:LEU:HB2	2.09	0.53
1:A:66:LEU:O	1:A:70:LEU:HB2	2.07	0.53
1:A:178:LEU:HD13	1:A:179:ILE:HA	1.90	0.53
1:A:326:VAL:HG12	1:A:327:PRO:CD	2.38	0.53
1:A:289:LYS:HD2	1:A:402:GLY:HA2	1.91	0.53
1:A:83:MET:C	1:A:84:LEU:HD23	2.28	0.53
1:A:410:ARG:HD2	1:A:410:ARG:N	2.24	0.53
1:A:116:PHE:CD2	1:A:117:CYS:N	2.66	0.53
1:A:282:ILE:HG12	1:A:285:ARG:NH2	2.25	0.53
1:A:41:SER:HB3	1:A:44:ASP:CG	2.30	0.53
1:A:289:LYS:HE2	1:A:400:LEU:O	2.09	0.52
1:A:139:GLU:O	1:A:140:PHE:C	2.45	0.52
1:A:324:PHE:N	1:A:324:PHE:HD1	2.05	0.52
1:A:57:LEU:HD23	1:A:58:LEU:HG	1.91	0.52
1:A:271:LEU:HD23	1:A:323:MET:HB2	1.92	0.52
1:A:46:GLY:O	1:A:50:ALA:CB	2.57	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:O	1:A:130:GLU:N	2.41	0.52
1:A:186:PHE:CD1	1:A:186:PHE:C	2.81	0.52
1:A:26:TYR:HE1	1:A:27:PHE:HD1	1.57	0.52
1:A:55:PHE:C	1:A:57:LEU:H	2.11	0.52
1:A:177:ALA:O	1:A:181:ALA:HB3	2.10	0.52
1:A:326:VAL:HG12	1:A:327:PRO:HD3	1.92	0.52
1:A:54:LEU:CA	1:A:363:ILE:CD1	2.88	0.52
1:A:88:ALA:CA	1:A:92:ILE:HD13	2.39	0.52
1:A:16:PHE:CE1	1:A:129:ILE:HG21	2.45	0.52
1:A:279:ALA:O	1:A:280:PRO:O	2.27	0.52
1:A:323:MET:O	1:A:327:PRO:CD	2.57	0.52
1:A:90:PHE:CA	1:A:94:ILE:HD12	2.33	0.52
1:A:238:VAL:HA	1:A:241:GLN:CG	2.39	0.52
1:A:325:GLU:O	1:A:326:VAL:C	2.47	0.52
1:A:54:LEU:N	1:A:363:ILE:HD11	2.25	0.52
1:A:122:ALA:N	1:A:123:PRO:CD	2.73	0.52
1:A:85:VAL:HG22	1:A:178:LEU:CG	2.40	0.52
1:A:123:PRO:HG2	1:A:124:ALA:H	1.74	0.52
1:A:153:LEU:CD1	1:A:153:LEU:N	2.73	0.52
1:A:77:LEU:HD21	1:A:185:PHE:CE2	2.45	0.51
1:A:38:ASN:CB	1:A:40:ILE:HD11	2.39	0.51
1:A:26:TYR:C	1:A:26:TYR:CD1	2.83	0.51
1:A:80:ILE:O	1:A:84:LEU:HG	2.10	0.51
1:A:56:SER:CB	1:A:119:ASN:HB3	2.40	0.51
1:A:225:LEU:HD12	1:A:336:TYR:HE2	1.75	0.51
1:A:55:PHE:C	1:A:57:LEU:N	2.64	0.51
1:A:66:LEU:HB3	1:A:76:LEU:HD13	1.92	0.51
1:A:160:ILE:HD11	1:A:263:TYR:OH	2.10	0.51
1:A:57:LEU:HD23	1:A:58:LEU:N	2.25	0.51
1:A:136:SER:O	1:A:137:ASN:CG	2.49	0.51
1:A:228:TYR:CD1	1:A:228:TYR:C	2.84	0.51
1:A:127:ALA:O	1:A:128:PHE:C	2.50	0.51
1:A:26:TYR:HB2	1:A:87:PHE:HZ	1.76	0.51
1:A:283:ILE:HA	1:A:286:ILE:CG2	2.41	0.51
1:A:411:ARG:NH2	1:A:414:ASN:HD21	2.08	0.51
1:A:133:SER:HA	1:A:138:PHE:CD2	2.46	0.51
1:A:160:ILE:HD11	1:A:263:TYR:CE2	2.45	0.51
1:A:324:PHE:H	1:A:324:PHE:HD1	1.59	0.51
1:A:330:LEU:N	1:A:330:LEU:HD13	2.06	0.51
1:A:178:LEU:CD1	1:A:178:LEU:C	2.78	0.50
1:A:77:LEU:HG	1:A:77:LEU:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:O	1:A:70:LEU:HD23	2.11	0.50
1:A:246:PHE:HD2	1:A:378:PHE:HD2	1.58	0.50
1:A:258:THR:O	1:A:259:ARG:C	2.49	0.50
1:A:85:VAL:CG2	1:A:178:LEU:HD11	2.32	0.50
1:A:210:LEU:O	1:A:213:ALA:HB3	2.11	0.50
1:A:293:LEU:HD13	1:A:397:VAL:CG1	2.41	0.50
1:A:394:LEU:O	1:A:397:VAL:CG2	2.54	0.50
1:A:77:LEU:HA	1:A:80:ILE:HD12	1.93	0.50
1:A:9:PHE:CZ	1:A:142:ARG:HG2	2.47	0.50
1:A:316:VAL:O	1:A:317:ILE:HD13	2.12	0.50
1:A:183:LEU:C	1:A:183:LEU:HD23	2.32	0.49
1:A:378:PHE:O	1:A:380:GLY:N	2.45	0.49
1:A:112:ILE:O	1:A:113:TYR:CD2	2.66	0.49
1:A:278:PHE:N	1:A:278:PHE:HD1	2.10	0.49
1:A:408:LEU:O	1:A:409:LEU:HD23	2.12	0.49
1:A:410:ARG:CA	1:A:410:ARG:HH11	2.22	0.49
1:A:32:ILE:N	1:A:32:ILE:HD12	2.27	0.49
1:A:91:PHE:HD1	1:A:91:PHE:H	1.60	0.49
1:A:242:GLN:HE21	1:A:373:TYR:HD2	1.58	0.49
1:A:88:ALA:O	1:A:90:PHE:N	2.45	0.49
1:A:108:ILE:HD12	1:A:109:VAL:N	2.28	0.49
1:A:22:ILE:CG1	1:A:177:ALA:CB	2.77	0.49
1:A:224:PHE:CD2	1:A:399:THR:CB	2.92	0.49
1:A:175:GLY:O	1:A:176:CYS:C	2.50	0.49
1:A:253:THR:HB	1:A:256:GLN:HB3	1.94	0.49
1:A:373:TYR:O	1:A:377:GLY:HA2	2.13	0.49
1:A:92:ILE:HG22	1:A:93:PHE:CD1	2.47	0.49
1:A:409:LEU:CA	1:A:413:VAL:HB	2.37	0.49
1:A:69:LYS:CG	1:A:69:LYS:O	2.60	0.49
1:A:93:PHE:HD1	1:A:93:PHE:N	2.11	0.49
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.30	0.49
1:A:303:ILE:HG21	1:A:386:GLY:N	2.28	0.49
1:A:236:TYR:CD1	1:A:299:MET:HG2	2.48	0.48
1:A:75:TYR:O	1:A:78:TRP:HB2	2.13	0.48
1:A:141:GLY:O	1:A:145:MET:HG3	2.12	0.48
1:A:66:LEU:O	1:A:68:ASP:N	2.47	0.48
1:A:56:SER:HB2	1:A:119:ASN:HB3	1.95	0.48
1:A:62:LEU:HD23	1:A:63:PHE:N	2.28	0.48
1:A:10:TRP:HA	1:A:10:TRP:CE3	2.48	0.48
1:A:352:VAL:HG12	1:A:353:CYS:N	2.27	0.48
1:A:60:GLN:HB2	1:A:61:PRO:HD3	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:CB	1:A:76:LEU:HD13	2.44	0.48
1:A:143:ALA:O	1:A:146:PHE:CB	2.61	0.48
1:A:220:PRO:O	1:A:223:TRP:N	2.47	0.48
1:A:240:ASP:OD1	1:A:302:ARG:NH1	2.47	0.48
1:A:349:ILE:HG22	1:A:350:TYR:N	2.29	0.48
1:A:61:PRO:O	1:A:63:PHE:N	2.47	0.48
1:A:54:LEU:CA	1:A:363:ILE:HD11	2.44	0.48
1:A:43:SER:HB2	1:A:371:ASN:HD22	1.79	0.48
1:A:143:ALA:O	1:A:146:PHE:HB3	2.14	0.47
1:A:246:PHE:HE2	1:A:379:GLN:HG2	1.79	0.47
1:A:74:LYS:O	1:A:75:TYR:C	2.51	0.47
1:A:166:ASN:ND2	1:A:167:GLN:N	2.61	0.47
1:A:91:PHE:CD2	1:A:170:PHE:HE2	2.32	0.47
1:A:175:GLY:O	1:A:178:LEU:N	2.47	0.47
1:A:233:SER:OG	1:A:358:LYS:HE3	2.15	0.47
1:A:242:GLN:O	1:A:244:ALA:N	2.48	0.47
1:A:32:ILE:CD1	1:A:32:ILE:H	2.27	0.47
1:A:404:GLY:N	1:A:405:PRO:HD3	2.28	0.47
1:A:47:ILE:CG2	1:A:47:ILE:O	2.62	0.47
1:A:66:LEU:O	1:A:70:LEU:CB	2.62	0.47
1:A:179:ILE:HA	1:A:182:VAL:CG1	2.43	0.47
1:A:260:VAL:O	1:A:263:TYR:HB2	2.14	0.47
1:A:73:ARG:HD2	1:A:73:ARG:N	2.29	0.47
1:A:132:VAL:HG12	1:A:138:PHE:CZ	2.50	0.47
1:A:269:GLU:O	1:A:271:LEU:N	2.48	0.47
1:A:361:ALA:O	1:A:365:MET:HG3	2.14	0.47
1:A:93:PHE:CD1	1:A:93:PHE:N	2.80	0.47
1:A:10:TRP:HA	1:A:10:TRP:HE3	1.79	0.47
1:A:19:TYR:HD2	1:A:20:PHE:CD1	2.32	0.47
1:A:282:ILE:HA	1:A:285:ARG:CZ	2.44	0.47
1:A:69:LYS:O	1:A:69:LYS:HG3	2.15	0.47
1:A:130:GLU:OE2	1:A:131:LYS:HG2	2.15	0.47
1:A:408:LEU:O	1:A:412:GLN:HB3	2.15	0.47
1:A:73:ARG:HB3	1:A:75:TYR:HD1	1.78	0.47
1:A:97:PRO:O	1:A:98:LEU:C	2.51	0.46
1:A:272:ASN:O	1:A:276:MET:HB2	2.14	0.46
1:A:326:VAL:O	1:A:327:PRO:C	2.51	0.46
1:A:260:VAL:HA	1:A:263:TYR:HD1	1.79	0.46
1:A:66:LEU:HD13	1:A:76:LEU:CD1	2.45	0.46
1:A:368:LEU:HA	1:A:371:ASN:HB2	1.98	0.46
1:A:395:ILE:HD13	1:A:395:ILE:HA	1.82	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:HG22	1:A:382:TYR:O	2.16	0.46
1:A:340:GLN:HB3	1:A:341:PHE:CE1	2.51	0.46
1:A:47:ILE:HG22	1:A:47:ILE:O	2.15	0.46
1:A:49:PHE:HB3	1:A:241:GLN:NE2	2.31	0.46
1:A:250:PHE:CD2	1:A:311:SER:O	2.69	0.46
1:A:91:PHE:HD1	1:A:91:PHE:N	2.13	0.46
1:A:12:PHE:CE2	1:A:128:PHE:CE1	3.02	0.45
1:A:127:ALA:O	1:A:130:GLU:OE1	2.33	0.45
1:A:378:PHE:O	1:A:381:ALA:N	2.49	0.45
1:A:139:GLU:O	1:A:141:GLY:N	2.49	0.45
1:A:227:LEU:HD22	1:A:227:LEU:HA	1.47	0.45
1:A:274:SER:O	1:A:277:PHE:HB2	2.15	0.45
1:A:16:PHE:CE1	1:A:144:ARG:HG2	2.52	0.45
1:A:17:PHE:O	1:A:17:PHE:CG	2.70	0.45
1:A:17:PHE:CE1	1:A:150:GLY:HA2	2.51	0.45
1:A:38:ASN:O	1:A:100:GLN:NE2	2.50	0.45
1:A:54:LEU:CA	1:A:363:ILE:HD12	2.46	0.45
1:A:59:PHE:O	1:A:60:GLN:C	2.55	0.45
1:A:32:ILE:HG21	1:A:162:PHE:HE2	1.78	0.45
1:A:342:GLU:O	1:A:345:PHE:HB2	2.16	0.45
1:A:182:VAL:CG1	1:A:183:LEU:N	2.79	0.45
1:A:283:ILE:HA	1:A:286:ILE:HG22	1.99	0.45
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.87	0.45
1:A:383:LEU:HD23	1:A:387:LEU:CD1	2.46	0.45
1:A:47:ILE:HD13	1:A:367:VAL:CG2	2.44	0.45
1:A:157:ILE:N	1:A:157:ILE:HD12	2.32	0.45
1:A:3:TYR:HA	1:A:6:ASN:HB3	1.97	0.45
1:A:169:VAL:C	1:A:171:TRP:N	2.70	0.45
1:A:74:LYS:HG2	1:A:185:PHE:CE2	2.51	0.45
1:A:355:CYS:O	1:A:359:GLN:HB2	2.16	0.45
1:A:185:PHE:C	1:A:187:ALA:N	2.71	0.45
1:A:304:ILE:HD11	1:A:386:GLY:C	2.38	0.45
1:A:75:TYR:O	1:A:78:TRP:N	2.37	0.45
1:A:9:PHE:CE1	1:A:143:ALA:HB2	2.51	0.45
1:A:88:ALA:HB2	1:A:170:PHE:O	2.17	0.44
1:A:283:ILE:CA	1:A:286:ILE:HG22	2.47	0.44
1:A:321:LEU:C	1:A:323:MET:N	2.71	0.44
1:A:289:LYS:CE	1:A:402:GLY:HA2	2.47	0.44
1:A:54:LEU:HA	1:A:363:ILE:CD1	2.47	0.44
1:A:330:LEU:H	1:A:330:LEU:CD1	2.02	0.44
1:A:42:LYS:HB3	1:A:374:GLU:OE1	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:SER:O	1:A:402:GLY:O	2.36	0.44
1:A:3:TYR:HA	1:A:6:ASN:CB	2.46	0.44
1:A:100:GLN:HB2	1:A:100:GLN:HE21	1.51	0.44
1:A:48:ILE:C	1:A:50:ALA:N	2.70	0.44
1:A:56:SER:O	1:A:60:GLN:HG3	2.18	0.44
1:A:86:MET:O	1:A:87:PHE:C	2.55	0.44
1:A:113:TYR:O	1:A:116:PHE:HB3	2.18	0.44
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.84	0.44
1:A:256:GLN:HB2	1:A:256:GLN:HE21	1.47	0.44
1:A:38:ASN:HB2	1:A:40:ILE:CD1	2.47	0.44
1:A:167:GLN:O	1:A:169:VAL:N	2.41	0.43
1:A:183:LEU:C	1:A:185:PHE:H	2.22	0.43
1:A:282:ILE:HG13	1:A:282:ILE:H	1.42	0.43
1:A:89:PRO:C	1:A:94:ILE:HD12	2.38	0.43
1:A:30:PHE:N	1:A:31:PRO:CD	2.81	0.43
1:A:334:PHE:C	1:A:334:PHE:CD2	2.91	0.43
1:A:269:GLU:C	1:A:271:LEU:N	2.72	0.43
1:A:83:MET:O	1:A:84:LEU:HD23	2.18	0.43
1:A:172:LEU:O	1:A:176:CYS:N	2.51	0.43
1:A:183:LEU:HD23	1:A:184:LEU:HD23	2.01	0.43
1:A:316:VAL:CG1	1:A:316:VAL:O	2.60	0.43
1:A:73:ARG:N	1:A:73:ARG:CD	2.81	0.43
1:A:345:PHE:O	1:A:346:SER:C	2.57	0.43
1:A:297:THR:C	1:A:298:ILE:HD13	2.38	0.43
1:A:6:ASN:ND2	1:A:137:ASN:OD1	2.51	0.43
1:A:149:VAL:O	1:A:153:LEU:HD13	2.19	0.43
1:A:178:LEU:O	1:A:180:LEU:N	2.52	0.43
1:A:15:PHE:CA	1:A:184:LEU:HD12	2.48	0.43
1:A:108:ILE:O	1:A:109:VAL:C	2.57	0.42
1:A:413:VAL:O	1:A:413:VAL:HG12	2.19	0.42
1:A:248:THR:HG22	1:A:257:GLY:O	2.19	0.42
1:A:411:ARG:HE	1:A:411:ARG:CA	2.12	0.42
1:A:77:LEU:HD23	1:A:77:LEU:C	2.39	0.42
1:A:264:VAL:HG11	1:A:319:LYS:HB3	2.01	0.42
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.81	0.42
1:A:346:SER:OG	1:A:347:ALA:N	2.52	0.42
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.88	0.42
1:A:5:LYS:O	1:A:5:LYS:HD3	2.20	0.42
1:A:256:GLN:HG3	1:A:257:GLY:N	2.33	0.42
1:A:302:ARG:CZ	1:A:322:HIS:HB2	2.50	0.42
1:A:49:PHE:HB3	1:A:241:GLN:HE22	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.82	0.42
1:A:98:LEU:O	1:A:99:LEU:C	2.54	0.42
1:A:101:TYR:O	1:A:103:ILE:CG1	2.52	0.42
1:A:108:ILE:O	1:A:112:ILE:N	2.52	0.42
1:A:209:SER:OG	1:A:210:LEU:N	2.50	0.42
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.74	0.42
1:A:53:SER:C	1:A:363:ILE:HD11	2.40	0.42
1:A:32:ILE:N	1:A:32:ILE:CD1	2.83	0.42
1:A:82:GLY:HA2	1:A:85:VAL:CG2	2.49	0.42
1:A:271:LEU:O	1:A:275:ILE:HG12	2.19	0.42
1:A:220:PRO:C	1:A:222:LEU:N	2.73	0.42
1:A:281:LEU:O	1:A:285:ARG:HG3	2.19	0.42
1:A:351:LEU:CD2	1:A:351:LEU:C	2.81	0.42
1:A:340:GLN:HB3	1:A:341:PHE:CD1	2.55	0.41
1:A:224:PHE:CG	1:A:399:THR:HB	2.53	0.41
1:A:410:ARG:CA	1:A:414:ASN:HB3	2.49	0.41
1:A:91:PHE:HB2	1:A:92:ILE:HD12	2.01	0.41
1:A:219:GLN:O	1:A:222:LEU:HB3	2.20	0.41
1:A:77:LEU:CG	1:A:77:LEU:O	2.68	0.41
1:A:157:ILE:CD1	1:A:157:ILE:H	2.33	0.41
1:A:307:SER:O	1:A:379:GLN:NE2	2.53	0.41
1:A:32:ILE:HG22	1:A:162:PHE:CE2	2.51	0.41
1:A:390:LEU:O	1:A:390:LEU:HG	2.19	0.41
1:A:88:ALA:HA	1:A:170:PHE:HB3	2.02	0.41
1:A:163:THR:OG1	1:A:164:ILE:N	2.52	0.41
1:A:180:LEU:CD1	1:A:180:LEU:H	2.25	0.41
1:A:47:ILE:HA	1:A:47:ILE:HD13	1.76	0.41
1:A:88:ALA:HA	1:A:92:ILE:CD1	2.48	0.41
1:A:185:PHE:O	1:A:188:LYS:CD	2.67	0.41
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.50	0.41
1:A:90:PHE:HD2	1:A:91:PHE:CE1	2.39	0.41
1:A:117:CYS:O	1:A:118:PHE:CG	2.74	0.41
1:A:166:ASN:C	1:A:166:ASN:ND2	2.74	0.41
1:A:241:GLN:HB2	1:A:242:GLN:H	1.59	0.41
1:A:224:PHE:N	1:A:224:PHE:CD1	2.88	0.41
1:A:341:PHE:CD1	1:A:341:PHE:N	2.89	0.41
1:A:90:PHE:HD2	1:A:91:PHE:CD1	2.39	0.41
1:A:3:TYR:HE2	1:A:138:PHE:HA	1.86	0.41
1:A:297:THR:O	1:A:301:VAL:CG2	2.56	0.41
1:A:314:GLU:O	1:A:317:ILE:HB	2.20	0.41
1:A:342:GLU:O	1:A:345:PHE:N	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HD11	1:A:170:PHE:HB2	2.02	0.41
1:A:108:ILE:HG13	1:A:108:ILE:H	1.58	0.41
1:A:113:TYR:C	1:A:115:GLY:H	2.22	0.41
1:A:17:PHE:CD2	1:A:18:PHE:CE1	3.08	0.41
1:A:326:VAL:O	1:A:330:LEU:HD13	2.21	0.41
1:A:340:GLN:C	1:A:341:PHE:CD1	2.95	0.41
1:A:82:GLY:CA	1:A:85:VAL:HG23	2.50	0.41
1:A:143:ALA:O	1:A:146:PHE:HB2	2.21	0.41
1:A:35:HIS:O	1:A:39:HIS:CA	2.66	0.41
1:A:304:ILE:HD11	1:A:386:GLY:O	2.20	0.41
1:A:105:VAL:C	1:A:107:SER:H	2.24	0.40
1:A:108:ILE:HG13	1:A:109:VAL:H	1.85	0.40
1:A:123:PRO:HG2	1:A:124:ALA:N	2.36	0.40
1:A:240:ASP:O	1:A:241:GLN:C	2.58	0.40
1:A:246:PHE:HD2	1:A:378:PHE:CD2	2.38	0.40
1:A:32:ILE:HD12	1:A:32:ILE:H	1.85	0.40
1:A:342:GLU:HB3	1:A:344:ARG:HG2	2.02	0.40
1:A:219:GLN:HA	1:A:220:PRO:HD3	1.75	0.40
1:A:104:LEU:HA	1:A:107:SER:OG	2.22	0.40
1:A:327:PRO:O	1:A:331:VAL:HB	2.21	0.40
1:A:349:ILE:HG22	1:A:350:TYR:CD1	2.57	0.40
1:A:19:TYR:HD2	1:A:20:PHE:CE1	2.39	0.40
1:A:241:GLN:NE2	1:A:366:SER:CB	2.84	0.40
1:A:92:ILE:HG22	1:A:93:PHE:HD1	1.85	0.40
1:A:56:SER:HB3	1:A:119:ASN:HB3	2.03	0.40
1:A:121:GLY:N	1:A:123:PRO:HD2	2.37	0.40
1:A:351:LEU:HD23	1:A:351:LEU:O	2.21	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	415/417 (100%)	276 (66%)	95 (23%)	44 (11%)	<b>0</b> <b>2</b>

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	75	TYR
1	A	243	PHE
1	A	252	ALA
1	A	279	ALA
1	A	288	GLY
1	A	325	GLU
1	A	346	SER
1	A	379	GLN
1	A	61	PRO
1	A	62	LEU
1	A	67	SER
1	A	88	ALA
1	A	181	ALA
1	A	186	PHE
1	A	201	VAL
1	A	234	CYS
1	A	270	LEU
1	A	281	LEU
1	A	378	PHE
1	A	402	GLY
1	A	99	LEU
1	A	102	ASN
1	A	134	ARG
1	A	140	PHE
1	A	175	GLY
1	A	204	ASN
1	A	233	SER
1	A	250	PHE
1	A	280	PRO
1	A	326	VAL
1	A	407	SER
1	A	26	TYR
1	A	111	GLY
1	A	118	PHE
1	A	168	PHE
1	A	191	ALA
1	A	277	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	156	SER
1	A	328	PHE
1	A	89	PRO
1	A	179	ILE
1	A	220	PRO
1	A	94	ILE

### 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	345/345 (100%)	277 (80%)	68 (20%)	<b>1</b> <b>6</b>

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	PHE
1	A	54	LEU
1	A	57	LEU
1	A	62	LEU
1	A	69	LYS
1	A	74	LYS
1	A	77	LEU
1	A	78	TRP
1	A	92	ILE
1	A	100	GLN
1	A	101	TYR
1	A	103	ILE
1	A	104	LEU
1	A	114	LEU
1	A	116	PHE
1	A	130	GLU
1	A	133	SER
1	A	134	ARG
1	A	136	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	138	PHE
1	A	151	TRP
1	A	166	ASN
1	A	167	GLN
1	A	168	PHE
1	A	170	PHE
1	A	174	SER
1	A	176	CYS
1	A	183	LEU
1	A	186	PHE
1	A	189	THR
1	A	199	ASN
1	A	208	PHE
1	A	209	SER
1	A	218	ARG
1	A	222	LEU
1	A	226	SER
1	A	227	LEU
1	A	237	ASP
1	A	240	ASP
1	A	242	GLN
1	A	256	GLN
1	A	265	THR
1	A	277	PHE
1	A	278	PHE
1	A	281	LEU
1	A	300	SER
1	A	310	THR
1	A	315	VAL
1	A	320	THR
1	A	323	MET
1	A	325	GLU
1	A	330	LEU
1	A	339	SER
1	A	340	GLN
1	A	344	ARG
1	A	349	ILE
1	A	359	GLN
1	A	360	LEU
1	A	368	LEU
1	A	376	ILE
1	A	383	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	388	VAL
1	A	390	LEU
1	A	397	VAL
1	A	406	LEU
1	A	410	ARG
1	A	411	ARG

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	ASN
1	A	60	GLN
1	A	100	GLN
1	A	102	ASN
1	A	166	ASN
1	A	241	GLN
1	A	256	GLN
1	A	340	GLN
1	A	359	GLN
1	A	371	ASN
1	A	379	GLN
1	A	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.



There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	408/417 (97%)	-0.40	12 (2%)	51 35	44, 77, 138, 186	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	GLY	10.6
1	A	405	PRO	7.5
1	A	194	SER	5.4
1	A	192	PRO	5.0
1	A	2	TYR	3.1
1	A	407	SER	2.8
1	A	403	PRO	2.7
1	A	4	LEU	2.6
1	A	102	ASN	2.6
1	A	191	ALA	2.5
1	A	1	MET	2.2
1	A	190	ASP	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	HG	A	501	1/1	0.90	0.10	200,200,200,200	1
2	HG	A	504	1/1	0.95	0.12	127,127,127,127	1
2	HG	A	502	1/1	0.98	0.04	73,73,73,73	1
2	HG	A	505	1/1	0.99	0.03	44,44,44,44	1
2	HG	A	503	1/1	0.99	0.05	67,67,67,67	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.