



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:08 am GMT

PDB ID : 2CFP  
Title : SUGAR FREE LACTOSE PERMEASE AT ACIDIC PH  
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Deposited on : 2006-02-22  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

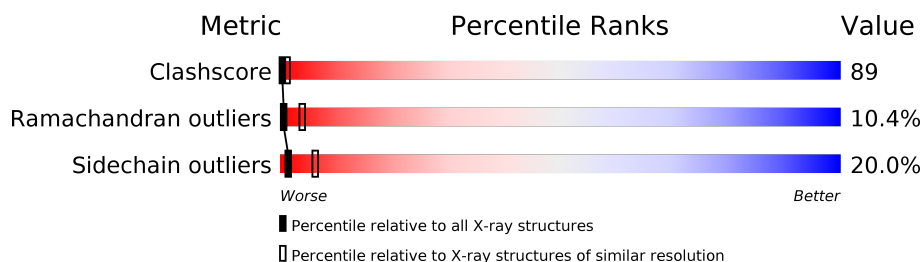
# 1 Overall quality at a glance

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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	417	

## 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	76	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).

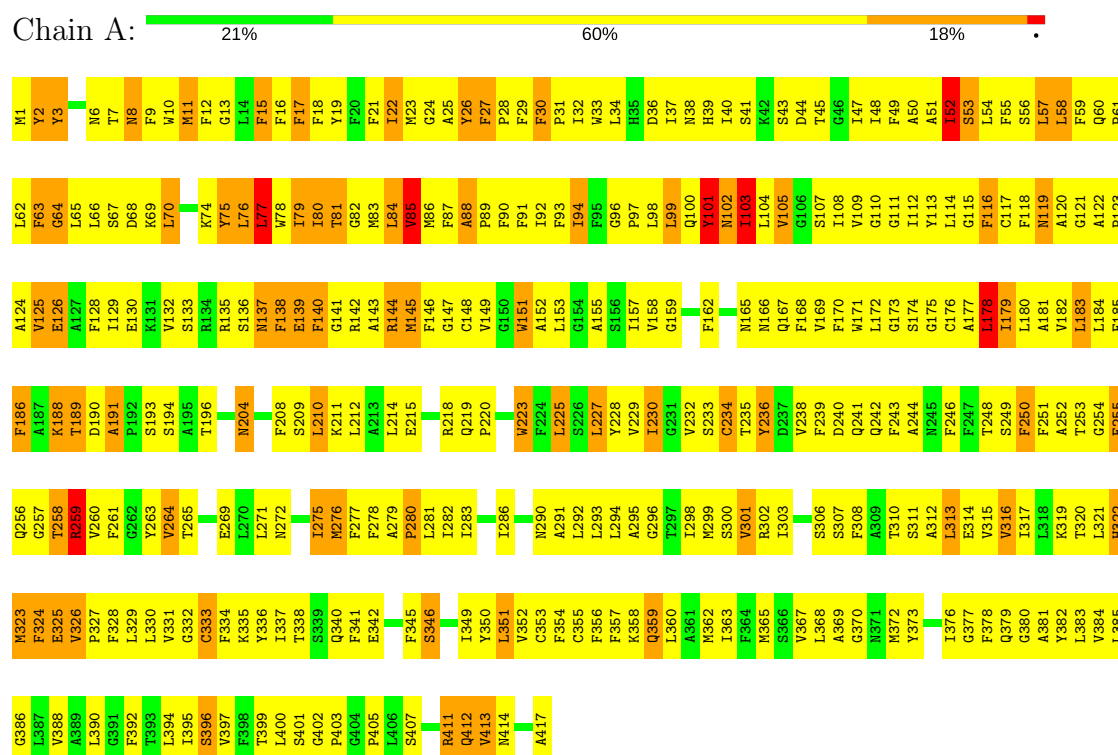
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Hg	0	0
			5	5		

### 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.

Note EDS was not executed.

#### • Molecule 1: LACTOSE PERMEASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.92Å 123.92Å 190.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.30	Depositor
% Data completeness (in resolution range)	80.7 (14.98-3.30)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.286 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

## 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	0.63	1/3387 (0.0%)	0.92	6/4588 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	VAL	CB-CG2	-5.30	1.41	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	PHE	N-CA-C	-7.21	91.52	111.00
1	A	193	SER	N-CA-C	6.95	129.75	111.00
1	A	103	ILE	CB-CA-C	-5.73	100.15	111.60
1	A	102	ASN	C-N-CA	5.67	135.88	121.70
1	A	102	ASN	CA-C-N	-5.64	104.80	117.20
1	A	103	ILE	N-CA-C	-5.14	97.13	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	3330	576	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
All	All	3295	0	3330	576	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 89.

All (576) 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:172:LEU:O	1:A:176:CYS:HB3	1.39	1.22
1:A:337:ILE:HD12	1:A:338:THR:H	1.16	1.11
1:A:51:ALA:HB1	1:A:112:ILE:HD13	1.25	1.10
1:A:109:VAL:HA	1:A:112:ILE:HD12	1.35	1.08
1:A:81:THR:O	1:A:85:VAL:HG22	1.54	1.08
1:A:337:ILE:HD12	1:A:338:THR:N	1.71	1.04
1:A:178:LEU:HG	1:A:179:ILE:H	1.17	1.04
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.40	1.03
1:A:85:VAL:HG13	1:A:178:LEU:HD13	1.41	1.02
1:A:94:ILE:O	1:A:98:LEU:HD12	1.60	1.01
1:A:137:ASN:ND2	1:A:137:ASN:H	1.51	1.00
1:A:2:TYR:H	1:A:2:TYR:HD2	1.02	1.00
1:A:307:SER:HB2	1:A:383:LEU:HG	1.41	0.99
1:A:108:ILE:HG22	1:A:112:ILE:HD11	1.44	0.99
1:A:104:LEU:HG	1:A:108:ILE:HD11	1.42	0.98
1:A:108:ILE:O	1:A:112:ILE:HG13	1.64	0.98
1:A:22:ILE:CG1	1:A:177:ALA:HB2	1.95	0.96
1:A:54:LEU:O	1:A:58:LEU:HB2	1.63	0.96
1:A:116:PHE:HD1	1:A:117:CYS:N	1.66	0.94
1:A:312:ALA:O	1:A:315:VAL:HG22	1.68	0.94
1:A:236:TYR:HD1	1:A:303:ILE:HD11	1.35	0.91
1:A:238:VAL:O	1:A:241:GLN:HG2	1.70	0.91
1:A:137:ASN:N	1:A:137:ASN:HD22	1.68	0.91
1:A:116:PHE:C	1:A:116:PHE:HD1	1.74	0.90
1:A:178:LEU:HG	1:A:179:ILE:N	1.87	0.90
1:A:17:PHE:C	1:A:17:PHE:HD2	1.75	0.90
1:A:51:ALA:CB	1:A:112:ILE:HD13	2.01	0.90
1:A:138:PHE:HD2	1:A:139:GLU:H	1.20	0.90
1:A:209:SER:H	1:A:212:LEU:HD13	1.37	0.89
1:A:30:PHE:HB3	1:A:31:PRO:HD3	1.54	0.89
1:A:137:ASN:H	1:A:137:ASN:HD22	0.93	0.88
1:A:1:MET:HA	1:A:3:TYR:HE2	1.34	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG13	1:A:177:ALA:HB2	1.52	0.88
1:A:373:TYR:HE1	1:A:382:TYR:HE1	1.22	0.87
1:A:116:PHE:C	1:A:116:PHE:CD1	2.48	0.87
1:A:85:VAL:HB	1:A:86:MET:HE3	1.55	0.86
1:A:1:MET:HA	1:A:3:TYR:CE2	2.10	0.85
1:A:396:SER:HA	1:A:399:THR:OG1	1.76	0.84
1:A:85:VAL:HA	1:A:178:LEU:HD22	1.59	0.84
1:A:359:GLN:O	1:A:363:ILE:HG13	1.77	0.84
1:A:165:ASN:HD21	1:A:167:GLN:HB2	1.41	0.83
1:A:299:MET:O	1:A:303:ILE:HG12	1.78	0.83
1:A:190:ASP:CG	1:A:191:ALA:H	1.83	0.83
1:A:230:ILE:HD12	1:A:357:PHE:HB3	1.61	0.83
1:A:8:ASN:HD21	1:A:189:THR:HB	1.44	0.83
1:A:17:PHE:CD2	1:A:17:PHE:C	2.51	0.82
1:A:229:VAL:O	1:A:233:SER:HB3	1.78	0.82
1:A:300:SER:HB3	1:A:390:LEU:HB2	1.60	0.81
1:A:84:LEU:HD21	1:A:117:CYS:HB3	1.64	0.80
1:A:109:VAL:CA	1:A:112:ILE:HD12	2.10	0.80
1:A:256:GLN:O	1:A:260:VAL:HG12	1.82	0.80
1:A:407:SER:O	1:A:411:ARG:HB3	1.83	0.79
1:A:22:ILE:CD1	1:A:177:ALA:HB2	2.13	0.79
1:A:178:LEU:CG	1:A:179:ILE:N	2.45	0.78
1:A:74:LYS:HD2	1:A:74:LYS:N	1.98	0.78
1:A:61:PRO:HD3	1:A:355:CYS:SG	2.24	0.77
1:A:135:ARG:O	1:A:137:ASN:N	2.17	0.77
1:A:87:PHE:HD2	1:A:173:GLY:HA3	1.49	0.77
1:A:98:LEU:HB3	1:A:107:SER:HB2	1.67	0.76
1:A:173:GLY:O	1:A:177:ALA:HB3	1.86	0.76
1:A:411:ARG:HH11	1:A:411:ARG:HG3	1.51	0.76
1:A:22:ILE:CG1	1:A:177:ALA:CB	2.63	0.76
1:A:84:LEU:HD21	1:A:117:CYS:CB	2.17	0.75
1:A:113:TYR:C	1:A:115:GLY:H	1.87	0.75
1:A:180:LEU:HD22	1:A:180:LEU:N	2.02	0.74
1:A:8:ASN:O	1:A:12:PHE:N	2.19	0.74
1:A:144:ARG:C	1:A:146:PHE:H	1.89	0.74
1:A:165:ASN:ND2	1:A:167:GLN:H	1.84	0.74
1:A:264:VAL:HG11	1:A:319:LYS:HD2	1.68	0.74
1:A:78:TRP:HD1	1:A:185:PHE:HD1	1.37	0.73
1:A:47:ILE:CG2	1:A:108:ILE:HD13	2.18	0.73
1:A:276:MET:C	1:A:278:PHE:H	1.90	0.73
1:A:85:VAL:CA	1:A:178:LEU:HD22	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB3	1:A:89:PRO:CD	2.18	0.73
1:A:22:ILE:HD11	1:A:177:ALA:HB2	1.70	0.72
1:A:22:ILE:CD1	1:A:22:ILE:N	2.53	0.72
1:A:37:ILE:HG22	1:A:38:ASN:ND2	2.04	0.71
1:A:116:PHE:CD1	1:A:117:CYS:N	2.56	0.71
1:A:281:LEU:HG	1:A:282:ILE:N	2.04	0.71
1:A:66:LEU:C	1:A:66:LEU:HD23	2.11	0.71
1:A:77:LEU:HD21	1:A:185:PHE:CZ	2.25	0.70
1:A:278:PHE:C	1:A:280:PRO:HD2	2.12	0.70
1:A:165:ASN:HD22	1:A:168:PHE:H	1.39	0.70
1:A:256:GLN:O	1:A:257:GLY:C	2.29	0.70
1:A:411:ARG:NH1	1:A:411:ARG:HG3	2.04	0.70
1:A:412:GLN:C	1:A:412:GLN:CD	2.49	0.70
1:A:75:TYR:O	1:A:79:ILE:HG22	1.91	0.70
1:A:30:PHE:H	1:A:31:PRO:CD	2.05	0.70
1:A:180:LEU:CD2	1:A:180:LEU:H	2.05	0.70
1:A:83:MET:C	1:A:85:VAL:H	1.94	0.70
1:A:112:ILE:O	1:A:112:ILE:HG22	1.90	0.69
1:A:22:ILE:HG13	1:A:177:ALA:CB	2.22	0.69
1:A:251:PHE:CB	1:A:256:GLN:HB3	2.22	0.69
1:A:98:LEU:HB3	1:A:107:SER:CB	2.22	0.69
1:A:313:LEU:HD22	1:A:317:ILE:HD11	1.75	0.69
1:A:307:SER:HB2	1:A:383:LEU:CG	2.21	0.69
1:A:120:ALA:O	1:A:123:PRO:HG2	1.93	0.69
1:A:80:ILE:HD11	1:A:121:GLY:HA3	1.75	0.69
1:A:22:ILE:HD12	1:A:22:ILE:N	2.08	0.69
1:A:87:PHE:CD2	1:A:173:GLY:HA3	2.28	0.69
1:A:12:PHE:O	1:A:16:PHE:HB2	1.93	0.68
1:A:308:PHE:O	1:A:310:THR:HG23	1.94	0.68
1:A:330:LEU:HD23	1:A:331:VAL:N	2.08	0.68
1:A:326:VAL:N	1:A:327:PRO:HD2	2.09	0.68
1:A:65:LEU:HD11	1:A:208:PHE:HZ	1.58	0.68
1:A:34:LEU:HB3	1:A:40:ILE:HG21	1.75	0.68
1:A:70:LEU:HD11	1:A:76:LEU:HB2	1.74	0.68
1:A:271:LEU:HD23	1:A:271:LEU:O	1.92	0.68
1:A:303:ILE:HG21	1:A:386:GLY:CA	2.24	0.68
1:A:179:ILE:HG22	1:A:180:LEU:HD22	1.75	0.68
1:A:209:SER:N	1:A:212:LEU:HD13	2.07	0.68
1:A:78:TRP:HD1	1:A:185:PHE:CD1	2.11	0.68
1:A:313:LEU:CD2	1:A:317:ILE:HD11	2.24	0.67
1:A:82:GLY:C	1:A:85:VAL:CG2	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:CG	1:A:108:ILE:HD11	2.21	0.67
1:A:29:PHE:CE1	1:A:158:VAL:HG13	2.29	0.67
1:A:376:ILE:HG13	1:A:381:ALA:N	2.09	0.67
1:A:301:VAL:HG12	1:A:302:ARG:N	2.10	0.67
1:A:16:PHE:HD2	1:A:144:ARG:HA	1.60	0.67
1:A:334:PHE:O	1:A:336:TYR:N	2.29	0.66
1:A:17:PHE:HA	1:A:147:GLY:HA2	1.78	0.66
1:A:257:GLY:O	1:A:261:PHE:CB	2.43	0.66
1:A:337:ILE:CD1	1:A:338:THR:H	2.03	0.66
1:A:78:TRP:CD1	1:A:185:PHE:HD1	2.13	0.66
1:A:94:ILE:HG22	1:A:98:LEU:CD1	2.25	0.65
1:A:119:ASN:O	1:A:123:PRO:HD2	1.96	0.65
1:A:271:LEU:HD21	1:A:324:PHE:CE1	2.31	0.65
1:A:77:LEU:O	1:A:77:LEU:HG	1.95	0.65
1:A:7:THR:HG22	1:A:8:ASN:N	2.09	0.65
1:A:94:ILE:HG22	1:A:98:LEU:HD11	1.77	0.65
1:A:80:ILE:HD11	1:A:121:GLY:CA	2.26	0.65
1:A:85:VAL:HG12	1:A:178:LEU:HD22	1.78	0.65
1:A:326:VAL:HG23	1:A:327:PRO:HD3	1.78	0.65
1:A:211:LYS:HA	1:A:214:LEU:HD12	1.78	0.65
1:A:60:GLN:N	1:A:61:PRO:HD2	2.12	0.64
1:A:298:ILE:HG22	1:A:299:MET:N	2.13	0.64
1:A:376:ILE:HD11	1:A:381:ALA:HA	1.78	0.64
1:A:379:GLN:O	1:A:382:TYR:HB2	1.97	0.64
1:A:12:PHE:HD2	1:A:129:ILE:HG13	1.62	0.64
1:A:278:PHE:CD2	1:A:282:ILE:HD11	2.32	0.64
1:A:257:GLY:O	1:A:261:PHE:N	2.29	0.63
1:A:81:THR:HB	1:A:182:VAL:CG1	2.27	0.63
1:A:85:VAL:HA	1:A:178:LEU:CB	2.28	0.63
1:A:302:ARG:NH1	1:A:322:HIS:HB2	2.14	0.63
1:A:55:PHE:O	1:A:59:PHE:HD1	1.80	0.63
1:A:82:GLY:HA2	1:A:85:VAL:HG21	1.79	0.63
1:A:180:LEU:N	1:A:180:LEU:CD2	2.61	0.63
1:A:254:GLY:C	1:A:256:GLN:H	2.02	0.63
1:A:373:TYR:CE1	1:A:382:TYR:HE1	2.09	0.63
1:A:137:ASN:ND2	1:A:137:ASN:N	2.30	0.63
1:A:238:VAL:HA	1:A:241:GLN:OE1	1.98	0.63
1:A:255:GLU:O	1:A:255:GLU:HG2	1.99	0.63
1:A:53:SER:HB2	1:A:363:ILE:CG1	2.29	0.62
1:A:85:VAL:CB	1:A:86:MET:HE3	2.28	0.62
1:A:8:ASN:HD21	1:A:189:THR:CB	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:O	1:A:218:ARG:HB3	1.99	0.62
1:A:264:VAL:CG1	1:A:319:LYS:HD2	2.29	0.62
1:A:334:PHE:HD1	1:A:337:ILE:HD11	1.64	0.62
1:A:16:PHE:CD2	1:A:144:ARG:HA	2.34	0.62
1:A:313:LEU:O	1:A:316:VAL:HB	1.99	0.62
1:A:413:VAL:O	1:A:413:VAL:CG1	2.46	0.62
1:A:23:MET:O	1:A:25:ALA:N	2.33	0.62
1:A:276:MET:C	1:A:278:PHE:N	2.51	0.62
1:A:51:ALA:HB1	1:A:112:ILE:CD1	2.16	0.62
1:A:85:VAL:HA	1:A:178:LEU:CD2	2.28	0.62
1:A:26:TYR:CD1	1:A:27:PHE:N	2.68	0.62
1:A:3:TYR:HB3	1:A:138:PHE:CE1	2.35	0.61
1:A:74:LYS:CD	1:A:74:LYS:N	2.63	0.61
1:A:17:PHE:HD2	1:A:18:PHE:N	1.98	0.61
1:A:47:ILE:HG22	1:A:108:ILE:HD13	1.80	0.61
1:A:125:VAL:C	1:A:129:ILE:HD13	2.20	0.61
1:A:307:SER:CB	1:A:383:LEU:HG	2.24	0.61
1:A:23:MET:C	1:A:25:ALA:H	2.04	0.61
1:A:342:GLU:HB2	1:A:345:PHE:CD2	2.36	0.61
1:A:394:LEU:O	1:A:397:VAL:HB	2.00	0.61
1:A:327:PRO:HG2	1:A:328:PHE:HD1	1.66	0.61
1:A:48:ILE:CD1	1:A:108:ILE:HG23	2.29	0.61
1:A:155:ALA:O	1:A:158:VAL:HG12	2.00	0.61
1:A:85:VAL:HA	1:A:178:LEU:HB2	1.83	0.61
1:A:123:PRO:HA	1:A:126:GLU:OE1	2.01	0.61
1:A:34:LEU:C	1:A:40:ILE:HG22	2.21	0.61
1:A:311:SER:O	1:A:314:GLU:HB2	2.01	0.60
1:A:49:PHE:HA	1:A:52:ILE:HG13	1.83	0.60
1:A:57:LEU:C	1:A:57:LEU:HD23	2.20	0.60
1:A:18:PHE:O	1:A:22:ILE:CD1	2.49	0.60
1:A:334:PHE:O	1:A:338:THR:HG22	2.01	0.60
1:A:65:LEU:HD11	1:A:208:PHE:CZ	2.37	0.60
1:A:2:TYR:N	1:A:2:TYR:CD2	2.58	0.60
1:A:313:LEU:HD13	1:A:314:GLU:N	2.15	0.60
1:A:380:GLY:HA2	1:A:383:LEU:HD12	1.84	0.60
1:A:204:ASN:HD22	1:A:204:ASN:N	2.00	0.60
1:A:238:VAL:HA	1:A:241:GLN:CD	2.21	0.60
1:A:223:TRP:CE3	1:A:223:TRP:HA	2.37	0.60
1:A:360:LEU:O	1:A:363:ILE:HB	2.02	0.60
1:A:15:PHE:C	1:A:15:PHE:CD2	2.75	0.60
1:A:261:PHE:O	1:A:264:VAL:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:O	1:A:85:VAL:CG2	2.42	0.59
1:A:113:TYR:C	1:A:115:GLY:N	2.56	0.59
1:A:3:TYR:H	1:A:3:TYR:HD2	1.50	0.59
1:A:209:SER:OG	1:A:210:LEU:N	2.34	0.59
1:A:52:ILE:HA	1:A:112:ILE:CG2	2.33	0.59
1:A:9:PHE:C	1:A:11:MET:H	2.06	0.59
1:A:77:LEU:HD21	1:A:185:PHE:HZ	1.66	0.59
1:A:306:SER:O	1:A:379:GLN:OE1	2.20	0.59
1:A:395:ILE:HG22	1:A:399:THR:CG2	2.33	0.59
1:A:313:LEU:HD22	1:A:317:ILE:CD1	2.32	0.58
1:A:74:LYS:HD2	1:A:74:LYS:H	1.64	0.58
1:A:334:PHE:O	1:A:337:ILE:HG13	2.03	0.58
1:A:84:LEU:N	1:A:84:LEU:CD2	2.66	0.58
1:A:17:PHE:CD2	1:A:18:PHE:N	2.72	0.58
1:A:33:TRP:O	1:A:37:ILE:HB	2.03	0.58
1:A:48:ILE:HD13	1:A:108:ILE:HG23	1.85	0.58
1:A:7:THR:O	1:A:10:TRP:N	2.36	0.58
1:A:107:SER:O	1:A:108:ILE:C	2.39	0.58
1:A:411:ARG:HH11	1:A:411:ARG:CG	2.17	0.58
1:A:180:LEU:HD22	1:A:180:LEU:H	1.65	0.57
1:A:18:PHE:O	1:A:22:ILE:HD13	2.04	0.57
1:A:30:PHE:N	1:A:31:PRO:CD	2.67	0.57
1:A:108:ILE:CG2	1:A:112:ILE:HD11	2.26	0.57
1:A:151:TRP:CD1	1:A:152:ALA:N	2.72	0.57
1:A:165:ASN:HD22	1:A:167:GLN:H	1.52	0.57
1:A:172:LEU:C	1:A:176:CYS:HB3	2.21	0.57
1:A:337:ILE:CD1	1:A:338:THR:N	2.58	0.57
1:A:230:ILE:CD1	1:A:357:PHE:HB3	2.32	0.57
1:A:53:SER:HB2	1:A:363:ILE:HG12	1.86	0.57
1:A:84:LEU:HD23	1:A:84:LEU:N	2.19	0.57
1:A:276:MET:CE	1:A:330:LEU:HD22	2.35	0.57
1:A:372:MET:HE1	1:A:384:VAL:HG11	1.86	0.57
1:A:74:LYS:HE2	1:A:188:LYS:HB2	1.87	0.57
1:A:286:ILE:HG22	1:A:286:ILE:O	2.03	0.57
1:A:31:PRO:HA	1:A:34:LEU:HD12	1.87	0.57
1:A:299:MET:CG	1:A:325:GLU:HG3	2.34	0.57
1:A:49:PHE:CE1	1:A:241:GLN:HB2	2.38	0.57
1:A:70:LEU:HD11	1:A:76:LEU:CB	2.35	0.57
1:A:210:LEU:C	1:A:214:LEU:HD12	2.24	0.57
1:A:48:ILE:HD13	1:A:108:ILE:CG2	2.34	0.57
1:A:8:ASN:O	1:A:11:MET:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:VAL:CG1	1:A:178:LEU:HD22	2.34	0.56
1:A:251:PHE:HB3	1:A:256:GLN:HB3	1.86	0.56
1:A:313:LEU:O	1:A:317:ILE:HD12	2.05	0.56
1:A:89:PRO:O	1:A:93:PHE:HB2	2.05	0.56
1:A:190:ASP:CG	1:A:191:ALA:N	2.55	0.56
1:A:232:VAL:HG12	1:A:232:VAL:O	2.04	0.56
1:A:257:GLY:O	1:A:261:PHE:HB2	2.05	0.56
1:A:275:ILE:O	1:A:278:PHE:HB3	2.04	0.56
1:A:326:VAL:HG23	1:A:327:PRO:CD	2.35	0.56
1:A:140:PHE:C	1:A:142:ARG:H	2.08	0.56
1:A:412:GLN:OE1	1:A:413:VAL:HA	2.05	0.56
1:A:264:VAL:CG1	1:A:265:THR:N	2.69	0.56
1:A:327:PRO:HG2	1:A:328:PHE:CD1	2.41	0.56
1:A:9:PHE:CD2	1:A:10:TRP:N	2.74	0.56
1:A:2:TYR:N	1:A:2:TYR:HD2	1.86	0.56
1:A:271:LEU:HD21	1:A:324:PHE:HE1	1.70	0.56
1:A:178:LEU:CD1	1:A:179:ILE:N	2.69	0.56
1:A:295:ALA:O	1:A:299:MET:HG3	2.06	0.56
1:A:413:VAL:O	1:A:413:VAL:HG13	2.05	0.56
1:A:243:PHE:CD2	1:A:243:PHE:O	2.60	0.55
1:A:395:ILE:O	1:A:397:VAL:N	2.39	0.55
1:A:85:VAL:CG1	1:A:178:LEU:HD13	2.26	0.55
1:A:334:PHE:C	1:A:336:TYR:H	2.09	0.55
1:A:233:SER:OG	1:A:358:LYS:HE2	2.05	0.55
1:A:22:ILE:CD1	1:A:22:ILE:H	2.18	0.55
1:A:92:ILE:O	1:A:97:PRO:HG2	2.06	0.55
1:A:108:ILE:HG22	1:A:112:ILE:CD1	2.27	0.55
1:A:12:PHE:CD2	1:A:129:ILE:HG13	2.41	0.55
1:A:143:ALA:O	1:A:146:PHE:HB3	2.07	0.55
1:A:165:ASN:ND2	1:A:167:GLN:HB2	2.17	0.55
1:A:32:ILE:N	1:A:32:ILE:HD12	2.21	0.55
1:A:34:LEU:HB3	1:A:40:ILE:CG2	2.36	0.55
1:A:350:TYR:O	1:A:351:LEU:HD12	2.05	0.55
1:A:83:MET:N	1:A:85:VAL:HG23	2.22	0.55
1:A:23:MET:C	1:A:25:ALA:N	2.60	0.54
1:A:330:LEU:C	1:A:330:LEU:HD23	2.26	0.54
1:A:412:GLN:OE1	1:A:412:GLN:O	2.24	0.54
1:A:13:GLY:O	1:A:146:PHE:HD2	1.90	0.54
1:A:141:GLY:O	1:A:145:MET:HG3	2.07	0.54
1:A:178:LEU:HD12	1:A:179:ILE:N	2.22	0.54
1:A:57:LEU:O	1:A:61:PRO:CD	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:C	1:A:83:MET:H	2.11	0.54
1:A:99:LEU:O	1:A:102:ASN:ND2	2.40	0.54
1:A:183:LEU:C	1:A:185:PHE:H	2.11	0.54
1:A:125:VAL:O	1:A:129:ILE:HD13	2.07	0.54
1:A:81:THR:CB	1:A:182:VAL:HG12	2.37	0.54
1:A:54:LEU:HD23	1:A:55:PHE:CZ	2.43	0.54
1:A:242:GLN:HB2	1:A:373:TYR:OH	2.07	0.54
1:A:281:LEU:O	1:A:282:ILE:C	2.46	0.54
1:A:184:LEU:C	1:A:185:PHE:HD2	2.10	0.53
1:A:225:LEU:C	1:A:227:LEU:N	2.61	0.53
1:A:76:LEU:C	1:A:76:LEU:CD1	2.77	0.53
1:A:30:PHE:H	1:A:31:PRO:HD2	1.72	0.53
1:A:144:ARG:C	1:A:146:PHE:N	2.60	0.53
1:A:246:PHE:HD2	1:A:378:PHE:CB	2.21	0.53
1:A:372:MET:CE	1:A:384:VAL:HG11	2.38	0.53
1:A:74:LYS:CD	1:A:74:LYS:H	2.19	0.53
1:A:260:VAL:HA	1:A:263:TYR:HB2	1.89	0.53
1:A:82:GLY:HA2	1:A:85:VAL:CG2	2.38	0.53
1:A:279:ALA:HA	1:A:282:ILE:HD12	1.89	0.53
1:A:22:ILE:HD11	1:A:177:ALA:CB	2.38	0.53
1:A:212:LEU:HD12	1:A:212:LEU:H	1.73	0.53
1:A:232:VAL:HG22	1:A:392:PHE:HB2	1.90	0.53
1:A:76:LEU:C	1:A:78:TRP:H	2.12	0.53
1:A:394:LEU:C	1:A:394:LEU:HD23	2.29	0.53
1:A:49:PHE:O	1:A:50:ALA:C	2.46	0.53
1:A:223:TRP:HE3	1:A:223:TRP:HA	1.74	0.53
1:A:258:THR:O	1:A:260:VAL:N	2.42	0.53
1:A:175:GLY:O	1:A:176:CYS:C	2.48	0.52
1:A:3:TYR:N	1:A:3:TYR:CD2	2.77	0.52
1:A:3:TYR:N	1:A:3:TYR:HD2	2.07	0.52
1:A:82:GLY:CA	1:A:85:VAL:CG2	2.87	0.52
1:A:248:THR:HA	1:A:257:GLY:HA3	1.90	0.52
1:A:334:PHE:CD1	1:A:337:ILE:HD11	2.44	0.52
1:A:113:TYR:N	1:A:113:TYR:CD1	2.78	0.52
1:A:22:ILE:HG21	1:A:84:LEU:CD1	2.40	0.52
1:A:29:PHE:CE1	1:A:159:GLY:HA2	2.45	0.52
1:A:286:ILE:CG2	1:A:286:ILE:O	2.57	0.52
1:A:294:LEU:HD23	1:A:328:PHE:CD2	2.45	0.52
1:A:380:GLY:O	1:A:384:VAL:HG23	2.08	0.52
1:A:3:TYR:CG	1:A:138:PHE:CE1	2.98	0.52
1:A:34:LEU:O	1:A:40:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG21	1:A:108:ILE:HD13	1.91	0.52
1:A:109:VAL:C	1:A:111:GLY:H	2.13	0.52
1:A:303:ILE:CG2	1:A:386:GLY:CA	2.88	0.52
1:A:57:LEU:HD23	1:A:58:LEU:N	2.24	0.52
1:A:82:GLY:C	1:A:85:VAL:HG23	2.29	0.52
1:A:115:GLY:O	1:A:119:ASN:OD1	2.29	0.51
1:A:165:ASN:ND2	1:A:167:GLN:N	2.56	0.51
1:A:184:LEU:O	1:A:185:PHE:HD2	1.92	0.51
1:A:66:LEU:CD2	1:A:66:LEU:C	2.77	0.51
1:A:340:GLN:HG2	1:A:401:SER:CB	2.41	0.51
1:A:21:PHE:CD2	1:A:176:CYS:SG	3.04	0.51
1:A:334:PHE:C	1:A:336:TYR:N	2.64	0.51
1:A:96:GLY:C	1:A:98:LEU:H	2.14	0.51
1:A:378:PHE:O	1:A:382:TYR:CD1	2.64	0.51
1:A:172:LEU:O	1:A:176:CYS:CB	2.33	0.51
1:A:17:PHE:CA	1:A:147:GLY:HA2	2.41	0.51
1:A:108:ILE:O	1:A:112:ILE:CG1	2.50	0.51
1:A:26:TYR:HD1	1:A:27:PHE:N	2.07	0.51
1:A:301:VAL:CG1	1:A:302:ARG:N	2.73	0.51
1:A:325:GLU:C	1:A:327:PRO:HD2	2.30	0.51
1:A:32:ILE:HD11	1:A:244:ALA:HB1	1.91	0.51
1:A:41:SER:OG	1:A:44:ASP:OD2	2.26	0.51
1:A:60:GLN:N	1:A:61:PRO:CD	2.74	0.51
1:A:377:GLY:O	1:A:378:PHE:C	2.47	0.51
1:A:36:ASP:O	1:A:37:ILE:HD12	2.11	0.51
1:A:79:ILE:HG12	1:A:79:ILE:O	2.10	0.51
1:A:81:THR:HG21	1:A:182:VAL:HG12	1.93	0.51
1:A:360:LEU:HA	1:A:363:ILE:HD12	1.93	0.51
1:A:62:LEU:HD23	1:A:62:LEU:C	2.32	0.51
1:A:83:MET:C	1:A:85:VAL:N	2.64	0.50
1:A:82:GLY:CA	1:A:85:VAL:HG21	2.41	0.50
1:A:100:GLN:O	1:A:102:ASN:N	2.44	0.50
1:A:323:MET:HA	1:A:326:VAL:HG22	1.93	0.50
1:A:17:PHE:HB2	1:A:147:GLY:HA2	1.92	0.50
1:A:303:ILE:O	1:A:306:SER:HB2	2.11	0.50
1:A:84:LEU:CD2	1:A:117:CYS:HB3	2.38	0.50
1:A:251:PHE:HB2	1:A:256:GLN:HB3	1.93	0.50
1:A:264:VAL:HG13	1:A:265:THR:N	2.26	0.50
1:A:32:ILE:N	1:A:32:ILE:CD1	2.74	0.50
1:A:144:ARG:O	1:A:147:GLY:N	2.43	0.50
1:A:233:SER:O	1:A:234:CYS:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:N	1:A:327:PRO:CD	2.72	0.50
1:A:276:MET:HE1	1:A:330:LEU:HD22	1.93	0.50
1:A:48:ILE:HA	1:A:108:ILE:HG21	1.94	0.50
1:A:2:TYR:CD1	1:A:137:ASN:O	2.65	0.50
1:A:319:LYS:O	1:A:321:LEU:N	2.45	0.50
1:A:321:LEU:O	1:A:324:PHE:CB	2.60	0.50
1:A:392:PHE:HD1	1:A:395:ILE:HD12	1.77	0.50
1:A:276:MET:O	1:A:278:PHE:N	2.44	0.49
1:A:407:SER:OG	1:A:411:ARG:N	2.45	0.49
1:A:47:ILE:HG21	1:A:108:ILE:CD1	2.42	0.49
1:A:299:MET:HG2	1:A:325:GLU:HG3	1.94	0.49
1:A:116:PHE:C	1:A:118:PHE:H	2.15	0.49
1:A:359:GLN:O	1:A:363:ILE:CG1	2.54	0.49
1:A:44:ASP:HB3	1:A:104:LEU:HD21	1.94	0.49
1:A:9:PHE:C	1:A:11:MET:N	2.65	0.49
1:A:167:GLN:O	1:A:168:PHE:C	2.51	0.49
1:A:153:LEU:CD1	1:A:153:LEU:N	2.76	0.49
1:A:41:SER:O	1:A:45:THR:HG23	2.12	0.49
1:A:7:THR:O	1:A:8:ASN:C	2.51	0.49
1:A:16:PHE:HE2	1:A:144:ARG:CD	2.26	0.48
1:A:55:PHE:O	1:A:59:PHE:CD1	2.64	0.48
1:A:60:GLN:HG2	1:A:120:ALA:HA	1.95	0.48
1:A:88:ALA:CB	1:A:89:PRO:HD3	2.28	0.48
1:A:174:SER:O	1:A:178:LEU:N	2.47	0.48
1:A:119:ASN:O	1:A:123:PRO:CD	2.62	0.48
1:A:83:MET:HB2	1:A:84:LEU:HD23	1.95	0.48
1:A:140:PHE:C	1:A:142:ARG:N	2.66	0.48
1:A:19:TYR:O	1:A:22:ILE:HB	2.14	0.48
1:A:281:LEU:CG	1:A:282:ILE:N	2.74	0.48
1:A:290:ASN:HA	1:A:293:LEU:HB2	1.94	0.48
1:A:81:THR:HB	1:A:182:VAL:HG12	1.95	0.48
1:A:51:ALA:CB	1:A:112:ILE:CD1	2.83	0.48
1:A:264:VAL:O	1:A:265:THR:C	2.52	0.48
1:A:30:PHE:O	1:A:33:TRP:HB3	2.13	0.48
1:A:351:LEU:O	1:A:356:PHE:HB3	2.14	0.48
1:A:76:LEU:C	1:A:76:LEU:HD12	2.33	0.48
1:A:140:PHE:HB2	1:A:143:ALA:HB3	1.96	0.47
1:A:153:LEU:N	1:A:153:LEU:HD12	2.29	0.47
1:A:303:ILE:HG21	1:A:386:GLY:HA2	1.97	0.47
1:A:3:TYR:CD2	1:A:138:PHE:HE1	2.33	0.47
1:A:63:PHE:O	1:A:64:GLY:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:HD12	1:A:108:ILE:HG23	1.96	0.47
1:A:48:ILE:HA	1:A:108:ILE:CG2	2.44	0.47
1:A:251:PHE:HB3	1:A:256:GLN:CB	2.45	0.47
1:A:104:LEU:O	1:A:108:ILE:HG13	2.13	0.47
1:A:18:PHE:O	1:A:22:ILE:HD11	2.14	0.47
1:A:249:SER:OG	1:A:250:PHE:N	2.48	0.47
1:A:280:PRO:O	1:A:283:ILE:HB	2.15	0.47
1:A:373:TYR:HE1	1:A:382:TYR:CE1	2.14	0.47
1:A:84:LEU:O	1:A:178:LEU:HB3	2.15	0.47
1:A:29:PHE:CD1	1:A:158:VAL:HG13	2.49	0.47
1:A:151:TRP:HD1	1:A:152:ALA:N	2.13	0.47
1:A:22:ILE:HG12	1:A:177:ALA:CB	2.44	0.47
1:A:190:ASP:OD2	1:A:191:ALA:N	2.42	0.47
1:A:204:ASN:N	1:A:204:ASN:ND2	2.62	0.47
1:A:328:PHE:N	1:A:328:PHE:CD1	2.82	0.47
1:A:52:ILE:HA	1:A:112:ILE:HG23	1.97	0.47
1:A:303:ILE:HG21	1:A:386:GLY:N	2.29	0.47
1:A:319:LYS:O	1:A:320:THR:C	2.51	0.47
1:A:341:PHE:CD2	1:A:349:ILE:HD11	2.49	0.47
1:A:385:LEU:O	1:A:388:VAL:N	2.47	0.47
1:A:55:PHE:HB3	1:A:59:PHE:CD1	2.50	0.47
1:A:76:LEU:O	1:A:78:TRP:N	2.48	0.47
1:A:210:LEU:HD12	1:A:214:LEU:HD11	1.97	0.46
1:A:279:ALA:O	1:A:283:ILE:HG12	2.16	0.46
1:A:126:GLU:OE2	1:A:144:ARG:NH1	2.40	0.46
1:A:322:HIS:C	1:A:324:PHE:H	2.17	0.46
1:A:22:ILE:HD13	1:A:22:ILE:H	1.80	0.46
1:A:236:TYR:CD1	1:A:303:ILE:HD11	2.28	0.46
1:A:333:CYS:HG	1:A:354:PHE:HZ	1.64	0.46
1:A:94:ILE:HG22	1:A:98:LEU:HD12	1.96	0.46
1:A:328:PHE:HD1	1:A:328:PHE:H	1.64	0.46
1:A:165:ASN:HD22	1:A:168:PHE:N	2.10	0.46
1:A:276:MET:HE3	1:A:330:LEU:HD22	1.98	0.46
1:A:319:LYS:C	1:A:321:LEU:N	2.69	0.46
1:A:23:MET:HB3	1:A:151:TRP:HE3	1.80	0.45
1:A:333:CYS:O	1:A:337:ILE:HG13	2.16	0.45
1:A:79:ILE:O	1:A:79:ILE:CG1	2.63	0.45
1:A:74:LYS:NZ	1:A:189:THR:O	2.23	0.45
1:A:312:ALA:O	1:A:313:LEU:C	2.54	0.45
1:A:59:PHE:C	1:A:61:PRO:HD2	2.36	0.45
1:A:62:LEU:HD23	1:A:62:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:CD1	1:A:214:LEU:HD11	2.47	0.45
1:A:249:SER:O	1:A:251:PHE:N	2.49	0.45
1:A:271:LEU:HD21	1:A:324:PHE:CD1	2.51	0.45
1:A:349:ILE:HA	1:A:352:VAL:HG12	1.98	0.45
1:A:80:ILE:HD11	1:A:121:GLY:HA2	1.96	0.45
1:A:60:GLN:HB2	1:A:355:CYS:SG	2.57	0.45
1:A:412:GLN:CD	1:A:412:GLN:O	2.55	0.45
1:A:82:GLY:C	1:A:85:VAL:HG21	2.36	0.45
1:A:101:TYR:O	1:A:103:ILE:HG13	2.16	0.45
1:A:108:ILE:C	1:A:112:ILE:CD1	2.85	0.45
1:A:323:MET:HA	1:A:326:VAL:CG2	2.47	0.45
1:A:351:LEU:HG	1:A:355:CYS:HB3	1.98	0.45
1:A:395:ILE:HG22	1:A:399:THR:HG21	1.97	0.45
1:A:55:PHE:O	1:A:59:PHE:HB2	2.17	0.45
1:A:2:TYR:O	1:A:6:ASN:HB3	2.17	0.45
1:A:81:THR:CG2	1:A:182:VAL:HG12	2.47	0.45
1:A:275:ILE:HG22	1:A:276:MET:N	2.32	0.45
1:A:37:ILE:HG22	1:A:38:ASN:HD22	1.82	0.45
1:A:66:LEU:HD23	1:A:66:LEU:O	2.16	0.45
1:A:254:GLY:C	1:A:256:GLN:N	2.69	0.45
1:A:107:SER:O	1:A:110:GLY:N	2.50	0.44
1:A:11:MET:C	1:A:13:GLY:H	2.20	0.44
1:A:250:PHE:HB3	1:A:312:ALA:HA	1.99	0.44
1:A:88:ALA:CB	1:A:89:PRO:CD	2.89	0.44
1:A:76:LEU:O	1:A:79:ILE:HG23	2.17	0.44
1:A:92:ILE:O	1:A:97:PRO:CG	2.65	0.44
1:A:169:VAL:C	1:A:171:TRP:H	2.20	0.44
1:A:104:LEU:O	1:A:105:VAL:C	2.55	0.44
1:A:144:ARG:O	1:A:146:PHE:N	2.47	0.44
1:A:189:THR:HG23	1:A:190:ASP:N	2.31	0.44
1:A:232:VAL:CG2	1:A:392:PHE:HB2	2.47	0.44
1:A:340:GLN:HG2	1:A:401:SER:HB3	2.00	0.44
1:A:122:ALA:O	1:A:125:VAL:HB	2.17	0.44
1:A:236:TYR:CG	1:A:236:TYR:O	2.71	0.44
1:A:292:LEU:HD21	1:A:332:GLY:C	2.38	0.44
1:A:395:ILE:C	1:A:397:VAL:N	2.69	0.44
1:A:210:LEU:O	1:A:214:LEU:HD12	2.18	0.43
1:A:55:PHE:HB3	1:A:59:PHE:CE1	2.53	0.43
1:A:104:LEU:CD1	1:A:108:ILE:HD11	2.47	0.43
1:A:225:LEU:C	1:A:227:LEU:H	2.22	0.43
1:A:212:LEU:HD12	1:A:212:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:C	1:A:283:ILE:N	2.69	0.43
1:A:299:MET:SD	1:A:325:GLU:HG3	2.58	0.43
1:A:219:GLN:HG3	1:A:220:PRO:HD2	1.99	0.43
1:A:22:ILE:HG12	1:A:177:ALA:HB1	2.00	0.43
1:A:257:GLY:O	1:A:261:PHE:HB3	2.19	0.43
1:A:53:SER:HA	1:A:56:SER:HB3	2.01	0.43
1:A:125:VAL:O	1:A:126:GLU:C	2.56	0.43
1:A:158:VAL:O	1:A:162:PHE:HB2	2.18	0.43
1:A:17:PHE:HA	1:A:147:GLY:CA	2.48	0.43
1:A:239:PHE:O	1:A:243:PHE:HB2	2.18	0.43
1:A:236:TYR:OH	1:A:302:ARG:NH1	2.47	0.43
1:A:243:PHE:CG	1:A:243:PHE:O	2.71	0.43
1:A:279:ALA:N	1:A:280:PRO:CD	2.82	0.43
1:A:313:LEU:HD21	1:A:317:ILE:HD11	1.98	0.43
1:A:346:SER:O	1:A:349:ILE:HB	2.18	0.43
1:A:246:PHE:HB2	1:A:378:PHE:CD2	2.52	0.43
1:A:85:VAL:CG1	1:A:86:MET:HE3	2.49	0.43
1:A:282:ILE:HG22	1:A:286:ILE:HD12	2.01	0.43
1:A:317:ILE:C	1:A:319:LYS:N	2.72	0.43
1:A:349:ILE:O	1:A:353:CYS:HB2	2.19	0.43
1:A:394:LEU:HD23	1:A:394:LEU:O	2.19	0.42
1:A:3:TYR:CG	1:A:138:PHE:HE1	2.36	0.42
1:A:53:SER:O	1:A:56:SER:N	2.44	0.42
1:A:178:LEU:HD12	1:A:178:LEU:C	2.39	0.42
1:A:413:VAL:HG12	1:A:417:ALA:O	2.19	0.42
1:A:48:ILE:O	1:A:51:ALA:HB3	2.18	0.42
1:A:336:TYR:CD2	1:A:337:ILE:N	2.88	0.42
1:A:57:LEU:O	1:A:61:PRO:HG3	2.19	0.42
1:A:185:PHE:O	1:A:186:PHE:HD2	2.03	0.42
1:A:128:PHE:O	1:A:132:VAL:HG23	2.19	0.42
1:A:172:LEU:HD22	1:A:172:LEU:N	2.33	0.42
1:A:180:LEU:O	1:A:181:ALA:C	2.58	0.42
1:A:112:ILE:C	1:A:113:TYR:CD1	2.93	0.42
1:A:76:LEU:C	1:A:78:TRP:N	2.72	0.42
1:A:55:PHE:CD2	1:A:112:ILE:HG22	2.55	0.42
1:A:367:VAL:O	1:A:368:LEU:C	2.57	0.42
1:A:180:LEU:O	1:A:184:LEU:HG	2.19	0.42
1:A:283:ILE:HD12	1:A:291:ALA:HB1	2.01	0.42
1:A:350:TYR:N	1:A:350:TYR:CD1	2.88	0.42
1:A:373:TYR:CD1	1:A:378:PHE:HD1	2.38	0.42
1:A:66:LEU:O	1:A:68:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB2	1:A:170:PHE:O	2.20	0.41
1:A:302:ARG:CZ	1:A:322:HIS:HB2	2.49	0.41
1:A:329:LEU:O	1:A:333:CYS:HB2	2.20	0.41
1:A:333:CYS:SG	1:A:354:PHE:HZ	2.43	0.41
1:A:354:PHE:N	1:A:354:PHE:CD1	2.87	0.41
1:A:140:PHE:C	1:A:140:PHE:CD2	2.93	0.41
1:A:246:PHE:CD2	1:A:378:PHE:HB3	2.55	0.41
1:A:269:GLU:O	1:A:272:ASN:N	2.52	0.41
1:A:283:ILE:HD12	1:A:291:ALA:CB	2.50	0.41
1:A:258:THR:O	1:A:259:ARG:C	2.59	0.41
1:A:1:MET:SD	1:A:3:TYR:CE2	3.13	0.41
1:A:369:ALA:O	1:A:370:GLY:C	2.58	0.41
1:A:83:MET:N	1:A:85:VAL:CG2	2.83	0.41
1:A:276:MET:O	1:A:280:PRO:HD3	2.20	0.41
1:A:385:LEU:O	1:A:388:VAL:HB	2.20	0.41
1:A:81:THR:CB	1:A:182:VAL:CG1	2.94	0.41
1:A:109:VAL:O	1:A:111:GLY:N	2.54	0.41
1:A:109:VAL:N	1:A:112:ILE:HD12	2.33	0.41
1:A:228:TYR:CD1	1:A:228:TYR:C	2.94	0.41
1:A:359:GLN:OE1	1:A:359:GLN:HA	2.19	0.41
1:A:8:ASN:ND2	1:A:189:THR:HB	2.25	0.41
1:A:22:ILE:HG21	1:A:84:LEU:HD12	2.02	0.41
1:A:32:ILE:O	1:A:36:ASP:HB2	2.20	0.41
1:A:57:LEU:O	1:A:61:PRO:CG	2.69	0.41
1:A:121:GLY:O	1:A:124:ALA:N	2.53	0.41
1:A:223:TRP:CE3	1:A:223:TRP:CA	3.03	0.41
1:A:337:ILE:HD12	1:A:338:THR:CA	2.47	0.41
1:A:3:TYR:CB	1:A:138:PHE:CE1	3.03	0.41
1:A:16:PHE:HE2	1:A:144:ARG:HB2	1.86	0.41
1:A:279:ALA:O	1:A:280:PRO:C	2.59	0.41
1:A:239:PHE:CE2	1:A:303:ILE:HA	2.56	0.41
1:A:68:ASP:C	1:A:70:LEU:H	2.24	0.41
1:A:85:VAL:HG12	1:A:178:LEU:CD2	2.49	0.41
1:A:123:PRO:C	1:A:125:VAL:N	2.74	0.41
1:A:260:VAL:O	1:A:263:TYR:HB2	2.20	0.41
1:A:376:ILE:HD11	1:A:381:ALA:CA	2.49	0.41
1:A:121:GLY:O	1:A:122:ALA:C	2.60	0.40
1:A:251:PHE:CD1	1:A:251:PHE:N	2.90	0.40
1:A:43:SER:HA	1:A:370:GLY:C	2.41	0.40
1:A:43:SER:HA	1:A:370:GLY:O	2.21	0.40
1:A:7:THR:O	1:A:9:PHE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:MET:C	1:A:13:GLY:N	2.75	0.40
1:A:296:GLY:HA2	1:A:299:MET:HE2	2.02	0.40
1:A:303:ILE:CG2	1:A:386:GLY:HA3	2.51	0.40
1:A:337:ILE:HD12	1:A:338:THR:CB	2.52	0.40
1:A:3:TYR:HB3	1:A:138:PHE:CD1	2.56	0.40
1:A:19:TYR:O	1:A:22:ILE:HD13	2.22	0.40
1:A:30:PHE:HB3	1:A:31:PRO:CD	2.37	0.40
1:A:402:GLY:HA2	1:A:403:PRO:HD3	1.88	0.40
1:A:81:THR:HB	1:A:182:VAL:HG11	2.01	0.40
1:A:172:LEU:N	1:A:172:LEU:CD2	2.85	0.40
1:A:38:ASN:O	1:A:39:HIS:C	2.59	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	415/417 (100%)	238 (57%)	134 (32%)	43 (10%)	<b>0</b> <b>4</b>

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	103	ILE
1	A	105	VAL
1	A	136	SER
1	A	178	LEU
1	A	188	LYS
1	A	204	ASN
1	A	250	PHE
1	A	258	THR
1	A	280	PRO

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Mol	Chain	Res	Type
1	A	346	SER
1	A	405	PRO
1	A	414	ASN
1	A	24	GLY
1	A	26	TYR
1	A	52	ILE
1	A	63	PHE
1	A	67	SER
1	A	77	LEU
1	A	101	TYR
1	A	235	THR
1	A	259	ARG
1	A	335	LYS
1	A	396	SER
1	A	28	PRO
1	A	69	LYS
1	A	125	VAL
1	A	126	GLU
1	A	179	ILE
1	A	196	THR
1	A	210	LEU
1	A	322	HIS
1	A	145	MET
1	A	236	TYR
1	A	252	ALA
1	A	90	PHE
1	A	166	ASN
1	A	191	ALA
1	A	255	GLU
1	A	30	PHE
1	A	413	VAL
1	A	64	GLY
1	A	88	ALA

### 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%)	276 (80%)	69 (20%)	<b>1</b> <b>6</b>

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	3	TYR
1	A	11	MET
1	A	15	PHE
1	A	17	PHE
1	A	22	ILE
1	A	27	PHE
1	A	52	ILE
1	A	53	SER
1	A	57	LEU
1	A	58	LEU
1	A	70	LEU
1	A	75	TYR
1	A	76	LEU
1	A	77	LEU
1	A	79	ILE
1	A	80	ILE
1	A	81	THR
1	A	84	LEU
1	A	85	VAL
1	A	91	PHE
1	A	94	ILE
1	A	99	LEU
1	A	101	TYR
1	A	114	LEU
1	A	116	PHE
1	A	119	ASN
1	A	130	GLU
1	A	133	SER
1	A	137	ASN
1	A	139	GLU
1	A	140	PHE
1	A	144	ARG
1	A	148	CYS
1	A	149	VAL
1	A	151	TRP
1	A	157	ILE
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	183	LEU
1	A	186	PHE
1	A	189	THR
1	A	194	SER
1	A	223	TRP
1	A	225	LEU
1	A	227	LEU
1	A	230	ILE
1	A	234	CYS
1	A	240	ASP
1	A	253	THR
1	A	259	ARG
1	A	264	VAL
1	A	275	ILE
1	A	276	MET
1	A	277	PHE
1	A	301	VAL
1	A	313	LEU
1	A	316	VAL
1	A	323	MET
1	A	324	PHE
1	A	325	GLU
1	A	326	VAL
1	A	333	CYS
1	A	351	LEU
1	A	359	GLN
1	A	362	MET
1	A	365	MET
1	A	400	LEU
1	A	411	ARG
1	A	412	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	ASN
1	A	100	GLN
1	A	102	ASN
1	A	137	ASN
1	A	165	ASN
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	371	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.