



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

PDB ID : 3VLF
Title : Crystal structure of yeast proteasome interacting protein
Authors : Takagi, K.; Kim, S.; Kato, K.; Tanaka, K.; Saeki, Y.; Mizushima, T.
Deposited on : 2011-12-01
Resolution : 3.80 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
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

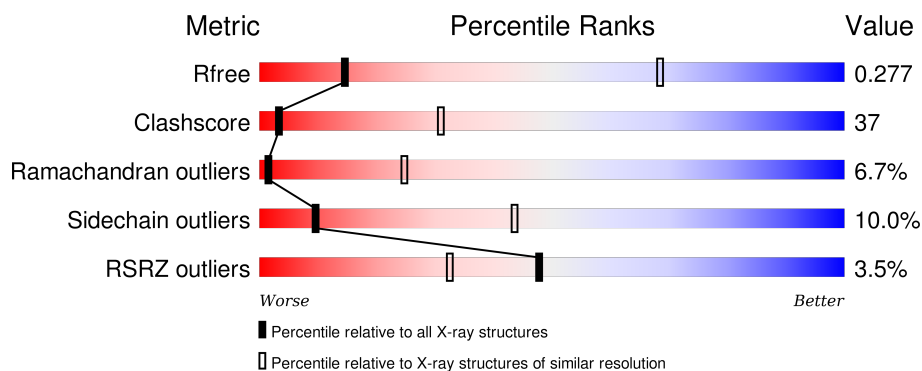
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 ≥ 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	500	<div> <div>5%</div> <div> <div>38%</div> <div>47%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	500	<div> <div>2%</div> <div> <div>31%</div> <div>49%</div> <div>9%</div> <div>9%</div> </div> </div>
2	B	88	<div> <div>32%</div> <div>41%</div> <div>10%</div> <div>17%</div> </div>
2	D	88	<div> <div>%</div> <div> <div>23%</div> <div>49%</div> <div>9%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8594 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 DNA mismatch repair protein HSM3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	Se	0	0	0
			3727	2403	596	715	5	8			
1	C	454	Total	C	N	O	S	Se	0	0	0
			3717	2396	594	714	5	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP P38348
A	-18	GLY	-	EXPRESSION TAG	UNP P38348
A	-17	SER	-	EXPRESSION TAG	UNP P38348
A	-16	SER	-	EXPRESSION TAG	UNP P38348
A	-15	HIS	-	EXPRESSION TAG	UNP P38348
A	-14	HIS	-	EXPRESSION TAG	UNP P38348
A	-13	HIS	-	EXPRESSION TAG	UNP P38348
A	-12	HIS	-	EXPRESSION TAG	UNP P38348
A	-11	HIS	-	EXPRESSION TAG	UNP P38348
A	-10	HIS	-	EXPRESSION TAG	UNP P38348
A	-9	SER	-	EXPRESSION TAG	UNP P38348
A	-8	SER	-	EXPRESSION TAG	UNP P38348
A	-7	GLY	-	EXPRESSION TAG	UNP P38348
A	-6	LEU	-	EXPRESSION TAG	UNP P38348
A	-5	VAL	-	EXPRESSION TAG	UNP P38348
A	-4	PRO	-	EXPRESSION TAG	UNP P38348
A	-3	ARG	-	EXPRESSION TAG	UNP P38348
A	-2	GLY	-	EXPRESSION TAG	UNP P38348
A	-1	SER	-	EXPRESSION TAG	UNP P38348
A	0	HIS	-	EXPRESSION TAG	UNP P38348
C	-19	MSE	-	EXPRESSION TAG	UNP P38348
C	-18	GLY	-	EXPRESSION TAG	UNP P38348
C	-17	SER	-	EXPRESSION TAG	UNP P38348
C	-16	SER	-	EXPRESSION TAG	UNP P38348
C	-15	HIS	-	EXPRESSION TAG	UNP P38348

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP P38348
C	-13	HIS	-	EXPRESSION TAG	UNP P38348
C	-12	HIS	-	EXPRESSION TAG	UNP P38348
C	-11	HIS	-	EXPRESSION TAG	UNP P38348
C	-10	HIS	-	EXPRESSION TAG	UNP P38348
C	-9	SER	-	EXPRESSION TAG	UNP P38348
C	-8	SER	-	EXPRESSION TAG	UNP P38348
C	-7	GLY	-	EXPRESSION TAG	UNP P38348
C	-6	LEU	-	EXPRESSION TAG	UNP P38348
C	-5	VAL	-	EXPRESSION TAG	UNP P38348
C	-4	PRO	-	EXPRESSION TAG	UNP P38348
C	-3	ARG	-	EXPRESSION TAG	UNP P38348
C	-2	GLY	-	EXPRESSION TAG	UNP P38348
C	-1	SER	-	EXPRESSION TAG	UNP P38348
C	0	HIS	-	EXPRESSION TAG	UNP P38348

- Molecule 2 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	Se	0	0	0
			575	357	110	103	2	3			
2	D	73	Total	C	N	O	S	Se	0	0	0
			575	357	110	103	2	3			

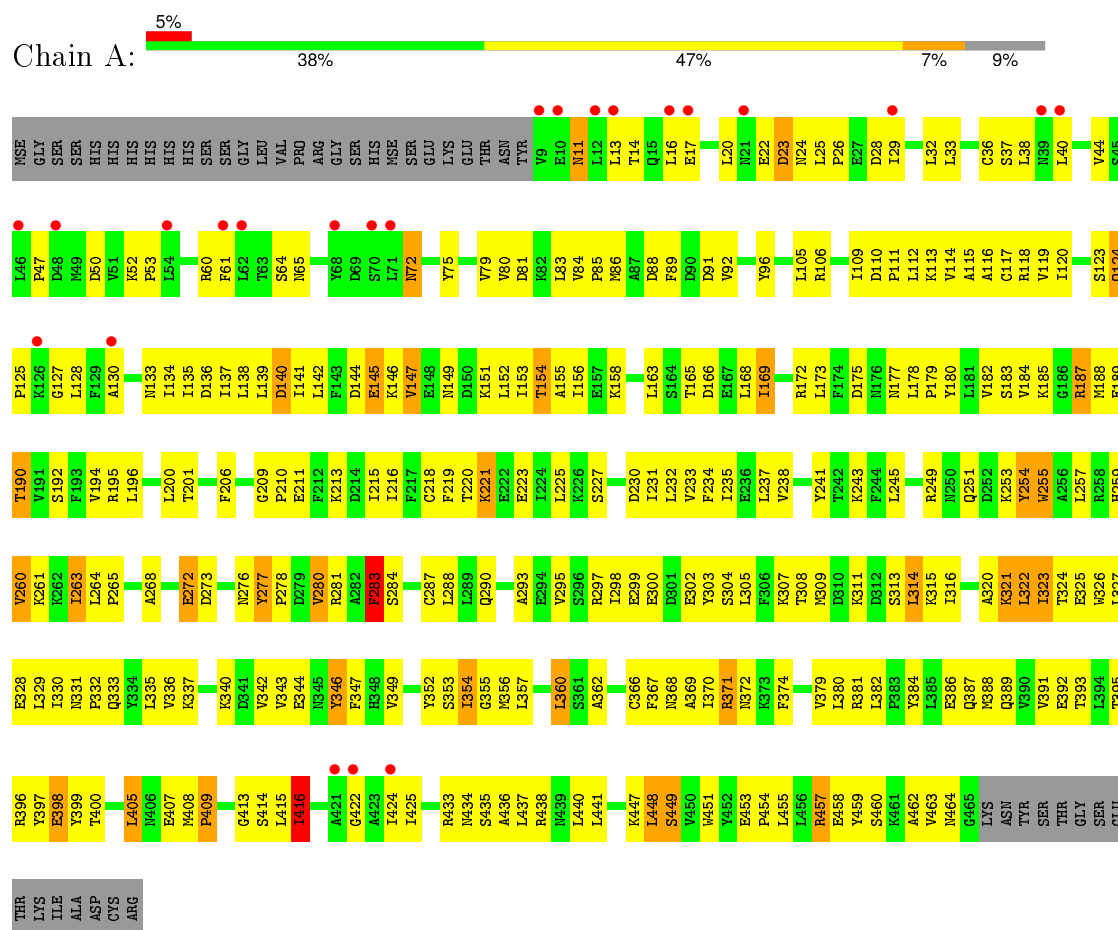
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	380	MSE	-	EXPRESSION TAG	UNP P33299
D	380	MSE	-	EXPRESSION TAG	UNP P33299

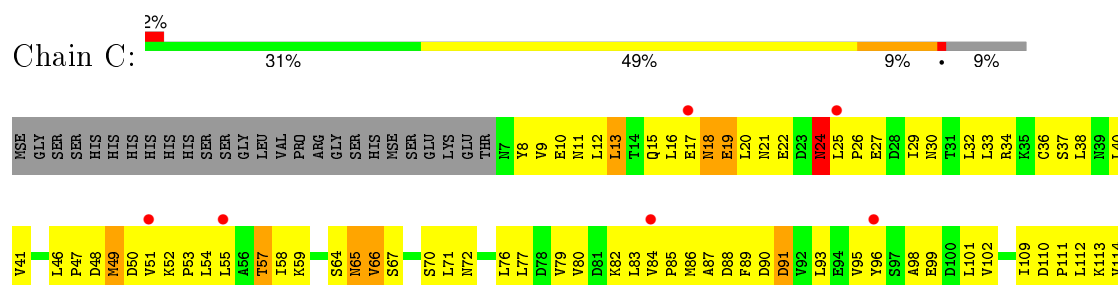
3 Residue-property plots

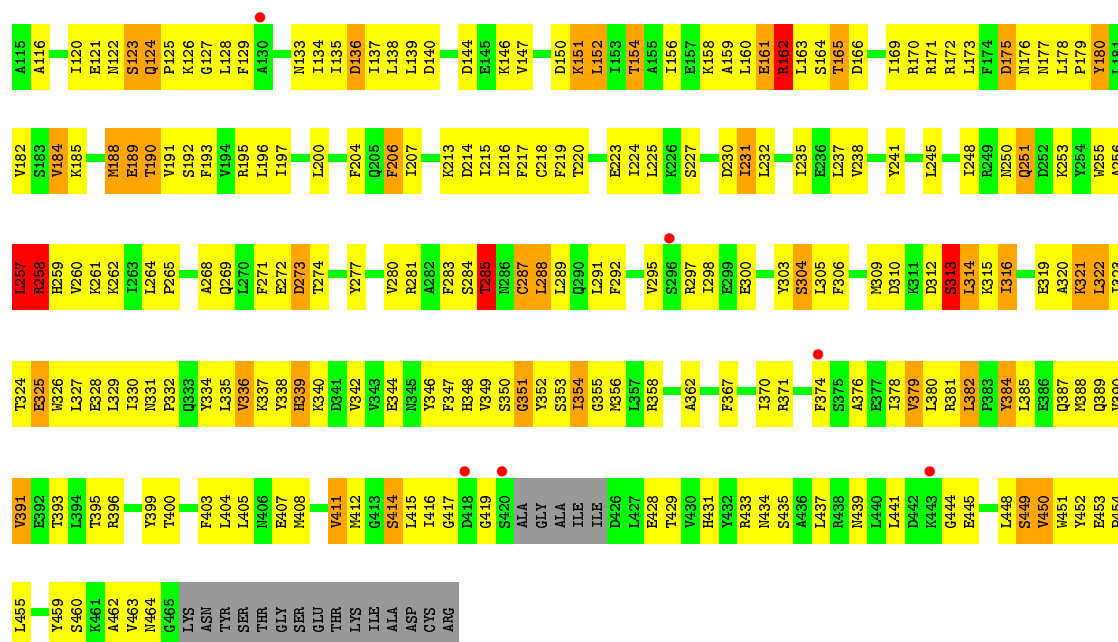
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: DNA mismatch repair protein HSM3

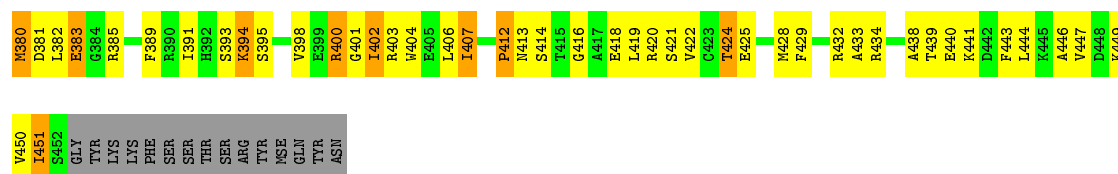


• Molecule 1: DNA mismatch repair protein HSM3

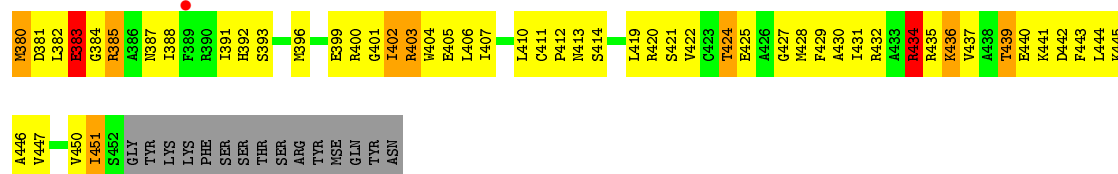




- Molecule 2: 26S protease regulatory subunit 7 homolog



- Molecule 2: 26S protease regulatory subunit 7 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	187.28 Å 187.28 Å 379.57 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.80 46.82 – 3.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.80) 99.1 (46.82-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.80 (at 3.77 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.278 0.251 , 0.277	Depositor DCC
R_{free} test set	1952 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	143.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 129.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39549 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0/3785	0.47	0/5114
1	C	0.36	0/3775	0.49	0/5099
2	B	0.34	0/579	0.47	0/769
2	D	0.36	0/579	0.47	0/769
All	All	0.37	0/8718	0.48	0/11751

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	3727	0	3763	236	0
1	C	3717	0	3742	309	0
2	B	575	0	598	50	0
2	D	575	0	598	65	0
All	All	8594	0	8701	642	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 37.

All (642) 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:464:ASN:OD1	1:C:82:LYS:NZ	1.93	1.01
1:C:88:ASP:HB3	1:C:91:ASP:HB2	1.42	1.01
1:C:124:GLN:HB2	1:C:125:PRO:HD3	1.43	0.98
1:A:320:ALA:HA	1:A:323:ILE:HG13	1.44	0.98
1:A:321:LYS:HD2	1:A:321:LYS:H	1.34	0.90
1:A:433:ARG:HH12	1:A:458:GLU:HG3	1.37	0.89
1:C:441:LEU:HD11	1:C:455:LEU:HB3	1.54	0.88
2:B:400:ARG:HG3	2:B:401:GLY:H	1.39	0.87
1:A:124:GLN:HB3	1:A:125:PRO:HD3	1.57	0.86
1:C:219:PHE:HE1	1:C:237:LEU:HD22	1.40	0.86
2:D:441:LYS:HA	2:D:444:LEU:HD13	1.58	0.85
1:A:393:THR:HA	1:A:396:ARG:HD3	1.59	0.84
1:A:263:ILE:HD13	1:A:263:ILE:H	1.42	0.84
2:B:391:ILE:HA	2:B:394:LYS:HE3	1.59	0.83
1:A:213:LYS:HB3	1:A:215:ILE:HG22	1.59	0.83
1:C:17:GLU:HG2	1:C:32:LEU:HD21	1.65	0.79
1:A:218:CYS:SG	1:A:259:HIS:HB3	2.24	0.77
1:C:16:LEU:O	1:C:20:LEU:HB2	1.83	0.77
2:D:422:VAL:HA	2:D:450:VAL:HG21	1.67	0.77
1:C:163:LEU:HD22	1:C:169:ILE:HD13	1.66	0.77
2:D:402:ILE:HA	2:D:440:GLU:HG3	1.67	0.77
1:A:453:GLU:HB2	1:A:454:PRO:HD3	1.66	0.77
1:C:285:THR:O	1:C:289:LEU:HB2	1.84	0.77
1:C:349:VAL:HG23	1:C:378:ILE:HG21	1.65	0.77
2:D:385:ARG:CZ	2:D:412:PRO:HA	2.16	0.75
1:C:265:PRO:HA	1:C:309:MSE:HE3	1.66	0.75
1:C:387:GLN:O	1:C:390:VAL:HG22	1.86	0.75
1:C:347:PHE:HD1	1:C:370:ILE:HG21	1.52	0.74
2:B:381:ASP:HA	2:B:385:ARG:HH12	1.53	0.74
1:C:40:LEU:HD11	1:C:46:LEU:HD21	1.69	0.74
1:A:238:VAL:HG11	1:A:288:LEU:HD23	1.70	0.73
1:C:382:LEU:HD12	1:C:382:LEU:H	1.53	0.73
1:A:330:ILE:HG22	1:A:335:LEU:HG	1.69	0.73
1:C:250:ASN:O	1:C:251:GLN:HG3	1.89	0.73
1:C:219:PHE:CE1	1:C:237:LEU:HD22	2.24	0.73
1:C:139:LEU:HD11	1:C:173:LEU:HD23	1.70	0.73
1:C:144:ASP:HB3	1:C:147:VAL:HG23	1.71	0.73
2:D:382:LEU:O	2:D:383:GLU:HG3	1.88	0.72
1:C:268:ALA:HB2	1:C:309:MSE:HE2	1.71	0.72
1:A:297:ARG:NH1	1:A:331:ASN:HA	2.03	0.72
1:C:166:ASP:HB3	1:C:169:ILE:HG22	1.71	0.72
1:C:178:LEU:O	1:C:182:VAL:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:O	1:A:327:LEU:HD12	1.89	0.71
1:C:459:TYR:O	1:C:463:VAL:HG22	1.89	0.71
1:A:37:SER:HA	1:A:40:LEU:HD12	1.72	0.71
2:B:419:LEU:HD22	2:B:419:LEU:H	1.56	0.70
1:C:324:THR:HG21	1:C:352:TYR:OH	1.92	0.70
1:C:25:LEU:HD11	1:C:66:VAL:HG12	1.73	0.70
1:C:367:PHE:CE1	1:C:400:THR:HA	2.27	0.69
1:C:389:GLN:O	1:C:393:THR:HG23	1.92	0.69
1:C:162:ARG:NH1	1:C:162:ARG:HB2	2.07	0.69
2:D:399:GLU:HB2	2:D:439:THR:HA	1.73	0.69
1:C:184:VAL:HB	1:C:196:LEU:HD22	1.75	0.69
1:A:257:LEU:HD22	1:A:298:ILE:HD11	1.74	0.69
1:C:80:VAL:O	1:C:84:VAL:HG23	1.94	0.68
1:C:238:VAL:HG11	1:C:288:LEU:HA	1.74	0.68
1:C:218:CYS:SG	1:C:259:HIS:HB3	2.33	0.68
2:D:385:ARG:NH1	2:D:412:PRO:HA	2.09	0.68
2:B:450:VAL:HG12	2:B:451:ILE:HD13	1.76	0.67
1:C:11:ASN:HB3	1:C:47:PRO:HG2	1.75	0.67
2:D:399:GLU:HG2	2:D:400:ARG:H	1.60	0.67
1:C:156:ILE:O	1:C:160:LEU:HD12	1.94	0.67
1:A:260:VAL:HA	1:A:263:ILE:HD11	1.77	0.67
1:C:135:ILE:HD12	1:C:172:ARG:HG2	1.76	0.67
1:C:388:MSE:HE3	1:C:433:ARG:HB2	1.75	0.67
1:C:367:PHE:HE1	1:C:400:THR:HA	1.60	0.67
1:C:245:LEU:O	1:C:248:ILE:HG22	1.96	0.66
1:A:325:GLU:O	1:A:329:LEU:HD12	1.96	0.66
1:C:109:ILE:HG23	1:C:111:PRO:HD2	1.77	0.66
1:C:416:ILE:HG12	1:C:454:PRO:HB2	1.77	0.66
1:C:33:LEU:HD13	1:C:76:LEU:HA	1.78	0.66
1:C:388:MSE:HE3	1:C:433:ARG:HG3	1.78	0.66
1:C:347:PHE:CD1	1:C:370:ILE:HG21	2.31	0.66
1:C:144:ASP:OD2	1:C:146:LYS:HB2	1.96	0.65
1:A:254:TYR:CE1	1:A:299:GLU:HG3	2.32	0.65
1:A:457:ARG:HG3	1:A:458:GLU:N	2.09	0.65
2:D:388:ILE:HD12	2:D:419:LEU:HD12	1.77	0.65
1:C:9:VAL:HG21	1:C:47:PRO:HG3	1.77	0.65
1:C:327:LEU:HB2	1:C:356:MSE:HG2	1.76	0.65
2:D:403:ARG:HG3	2:D:406:LEU:HD12	1.78	0.65
2:D:450:VAL:HG12	2:D:451:ILE:HD13	1.79	0.64
2:D:380:MSE:SE	2:D:388:ILE:HD11	2.47	0.64
1:C:220:THR:OG1	1:C:223:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:HG23	1:C:76:LEU:HD21	1.78	0.64
1:C:126:LYS:HG3	1:C:166:ASP:HB2	1.79	0.64
1:C:178:LEU:N	1:C:179:PRO:HD2	2.12	0.64
1:A:276:ASN:O	1:A:277:TYR:HB2	1.98	0.64
1:C:52:LYS:N	1:C:53:PRO:HD2	2.13	0.64
1:C:110:ASP:HA	1:C:113:LYS:HD3	1.78	0.63
1:C:358:ARG:HE	1:C:396:ARG:HH21	1.44	0.63
1:A:327:LEU:HD23	1:A:343:VAL:HG22	1.79	0.63
1:C:378:ILE:C	1:C:380:LEU:H	2.01	0.63
2:D:436:LYS:HD2	2:D:437:VAL:HG23	1.80	0.63
1:C:64:SER:O	1:C:65:ASN:HB2	1.97	0.63
1:C:441:LEU:CD1	1:C:455:LEU:HB3	2.28	0.63
1:C:29:ILE:HG22	1:C:71:LEU:HD23	1.81	0.62
1:C:384:TYR:CD2	1:C:388:MSE:HG2	2.34	0.62
1:C:391:VAL:O	1:C:395:THR:HG23	1.99	0.62
1:C:264:LEU:HD23	1:C:305:LEU:HD21	1.82	0.62
1:A:235:ILE:HD11	1:A:283:PHE:O	1.98	0.62
1:A:433:ARG:HH12	1:A:458:GLU:CG	2.11	0.62
1:C:391:VAL:HG12	1:C:404:LEU:HD11	1.81	0.62
1:C:358:ARG:HE	1:C:396:ARG:NH2	1.97	0.62
1:A:316:ILE:HD11	1:A:330:ILE:HG12	1.82	0.62
1:C:170:ARG:HH21	1:C:207:ILE:HA	1.65	0.62
1:A:436:ALA:O	1:A:440:LEU:HB2	2.00	0.62
1:A:324:THR:O	1:A:328:GLU:HG3	2.00	0.61
1:A:124:GLN:CB	1:A:125:PRO:HD3	2.28	0.61
1:C:297:ARG:HG2	1:C:331:ASN:HB2	1.82	0.61
1:C:332:PRO:HG3	1:C:362:ALA:HB3	1.81	0.61
1:C:193:PHE:HE1	1:C:237:LEU:HD21	1.64	0.61
1:C:109:ILE:CG2	1:C:111:PRO:HD2	2.30	0.61
1:A:158:LYS:HZ2	2:B:382:LEU:HG	1.65	0.61
2:B:400:ARG:HG3	2:B:401:GLY:N	2.15	0.61
2:D:422:VAL:HG22	2:D:450:VAL:HG11	1.82	0.61
1:A:13:LEU:HD23	1:A:16:LEU:HD23	1.81	0.61
1:C:351:GLY:O	1:C:354:ILE:HD13	2.00	0.61
2:D:444:LEU:HD12	2:D:444:LEU:H	1.65	0.61
1:A:264:LEU:HD13	1:A:295:VAL:HG22	1.81	0.61
1:C:172:ARG:HD3	1:C:176:ASN:HB2	1.83	0.61
1:A:149:ASN:ND2	1:A:152:LEU:HB2	2.16	0.61
1:A:321:LYS:HD2	1:A:321:LYS:N	2.10	0.60
1:A:268:ALA:HB2	1:A:309:MSE:HE3	1.83	0.60
1:A:434:ASN:ND2	1:A:462:ALA:HB1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD12	1:C:86:MSE:SE	2.51	0.60
1:C:289:LEU:HD22	1:C:329:LEU:HD22	1.83	0.60
2:D:382:LEU:O	2:D:384:GLY:N	2.34	0.60
2:D:434:ARG:HG2	2:D:434:ARG:HH11	1.66	0.60
1:C:388:MSE:HE3	1:C:433:ARG:CG	2.31	0.60
1:C:52:LYS:HB2	1:C:91:ASP:OD1	2.01	0.60
1:A:84:VAL:N	1:A:85:PRO:HD2	2.16	0.60
1:A:388:MSE:HG3	1:A:433:ARG:HB2	1.83	0.60
1:A:178:LEU:N	1:A:179:PRO:HD2	2.17	0.60
1:C:30:ASN:HA	1:C:71:LEU:HD22	1.84	0.60
2:B:412:PRO:HG2	2:B:413:ASN:H	1.66	0.60
1:C:204:PHE:O	1:C:207:ILE:HG22	2.02	0.60
1:A:354:ILE:O	1:A:354:ILE:HD13	2.01	0.60
1:A:434:ASN:HD21	1:A:462:ALA:HB1	1.67	0.60
1:A:264:LEU:N	1:A:265:PRO:HD2	2.17	0.59
2:D:425:GLU:O	2:D:428:MSE:HB2	2.02	0.59
1:C:303:TYR:HD1	1:C:334:TYR:HD1	1.50	0.59
1:A:321:LYS:CD	1:A:321:LYS:H	2.05	0.59
1:C:280:VAL:O	1:C:284:SER:HB2	2.03	0.59
1:A:440:LEU:O	1:A:448:LEU:HD11	2.03	0.59
1:C:30:ASN:HA	1:C:71:LEU:HD13	1.84	0.59
1:C:224:ILE:H	1:C:224:ILE:HD12	1.68	0.59
1:A:138:LEU:HD22	1:A:156:ILE:HG23	1.84	0.59
1:C:388:MSE:HE3	1:C:433:ARG:CB	2.33	0.59
1:C:388:MSE:O	1:C:391:VAL:HG23	2.03	0.58
1:C:151:LYS:HB2	1:C:151:LYS:NZ	2.18	0.58
1:A:180:TYR:O	1:A:183:SER:HB3	2.02	0.58
2:D:382:LEU:C	2:D:384:GLY:H	2.07	0.58
1:C:292:PHE:CD2	1:C:314:LEU:HD21	2.38	0.58
1:A:257:LEU:O	1:A:261:LYS:HB2	2.03	0.58
1:A:153:ILE:HD12	1:A:195:ARG:NH1	2.18	0.58
1:C:138:LEU:HD22	1:C:156:ILE:HG23	1.84	0.58
1:C:10:GLU:HB3	1:C:13:LEU:HG	1.84	0.58
1:C:29:ILE:HG22	1:C:71:LEU:CD2	2.34	0.58
1:A:144:ASP:OD1	1:A:146:LYS:HB2	2.04	0.58
1:C:162:ARG:HB2	1:C:162:ARG:HH11	1.67	0.58
1:A:52:LYS:H	1:A:53:PRO:HD2	1.69	0.58
1:A:178:LEU:O	1:A:182:VAL:HG23	2.03	0.57
1:C:367:PHE:HD1	1:C:399:TYR:HD1	1.52	0.57
1:A:52:LYS:N	1:A:53:PRO:HD2	2.18	0.57
1:A:460:SER:HA	1:C:38:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD21	1:A:342:VAL:HG12	1.86	0.57
1:C:156:ILE:O	1:C:159:ALA:HB3	2.04	0.57
1:A:221:LYS:O	1:A:225:LEU:HD12	2.04	0.57
1:C:84:VAL:N	1:C:85:PRO:HD2	2.20	0.57
1:A:249:ARG:HH11	1:A:297:ARG:HG2	1.68	0.57
1:C:309:MSE:O	1:C:314:LEU:HD12	2.04	0.57
2:B:402:ILE:HG12	2:B:440:GLU:HB2	1.85	0.57
1:A:245:LEU:HD11	1:A:264:LEU:HD11	1.87	0.57
1:A:297:ARG:HD3	1:A:331:ASN:HD22	1.70	0.57
2:B:420:ARG:HH11	2:B:420:ARG:HG2	1.69	0.57
1:A:249:ARG:NH1	1:A:297:ARG:HG2	2.20	0.56
1:A:50:ASP:OD2	1:A:52:LYS:HG2	2.03	0.56
1:A:435:SER:HA	1:A:438:ARG:NH1	2.19	0.56
1:C:54:LEU:O	1:C:58:ILE:HG13	2.06	0.56
1:A:249:ARG:HH11	1:A:297:ARG:HB3	1.70	0.56
2:D:436:LYS:H	2:D:436:LYS:CE	2.19	0.56
1:C:125:PRO:O	1:C:126:LYS:HG2	2.06	0.56
1:A:115:ALA:O	1:A:119:VAL:HG23	2.04	0.56
1:C:124:GLN:CB	1:C:125:PRO:HD3	2.29	0.56
2:B:429:PHE:HZ	2:B:449:LYS:HD2	1.70	0.56
2:D:403:ARG:HD3	2:D:440:GLU:OE2	2.05	0.56
1:A:145:GLU:HG2	1:A:189:GLU:OE1	2.05	0.56
1:A:354:ILE:HD11	1:A:389:GLN:HB3	1.88	0.56
2:D:430:ALA:HB1	2:D:435:ARG:HG3	1.87	0.56
2:D:428:MSE:HA	2:D:431:ILE:HD13	1.88	0.56
1:A:25:LEU:HD21	1:A:61:PHE:HE1	1.71	0.56
2:B:414:SER:HA	2:B:418:GLU:OE1	2.07	0.55
1:C:450:VAL:O	1:C:450:VAL:HG22	2.05	0.55
1:A:135:ILE:HD12	1:A:172:ARG:HG2	1.86	0.55
1:A:149:ASN:O	1:A:153:ILE:HG12	2.06	0.55
1:C:83:LEU:C	1:C:85:PRO:HD2	2.27	0.55
2:B:450:VAL:HG12	2:B:451:ILE:N	2.21	0.55
2:B:419:LEU:CD2	2:B:419:LEU:H	2.20	0.55
1:A:188:MSE:HE1	1:A:223:GLU:O	2.06	0.55
1:A:374:PHE:CD1	1:A:408:MSE:HE1	2.42	0.55
1:A:391:VAL:O	1:A:395:THR:HG23	2.07	0.55
1:C:79:VAL:O	1:C:83:LEU:HB2	2.06	0.55
1:A:333:GLN:HB3	1:A:337:LYS:NZ	2.21	0.55
1:A:340:LYS:HE2	1:A:344:GLU:OE2	2.06	0.55
1:C:336:VAL:C	1:C:338:TYR:H	2.10	0.55
1:C:47:PRO:C	1:C:49:MSE:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:ARG:O	2:D:424:THR:HG22	2.07	0.55
1:A:238:VAL:CG1	1:A:288:LEU:HD23	2.36	0.54
1:A:120:ILE:HG22	1:A:163:LEU:HD11	1.89	0.54
1:C:206:PHE:N	1:C:206:PHE:CD1	2.75	0.54
2:B:385:ARG:HG2	2:B:385:ARG:HH11	1.73	0.54
1:C:154:THR:CG2	2:D:383:GLU:HB3	2.37	0.54
1:A:81:ASP:HB2	1:A:118:ARG:HH11	1.71	0.54
1:A:154:THR:HG23	2:B:383:GLU:HG2	1.90	0.54
1:C:444:GLY:O	1:C:448:LEU:HD12	2.07	0.54
1:C:250:ASN:O	1:C:251:GLN:CG	2.55	0.54
2:D:427:GLY:O	2:D:431:ILE:HD12	2.08	0.54
1:A:380:LEU:HA	1:A:387:GLN:NE2	2.22	0.54
2:B:381:ASP:C	2:B:383:GLU:H	2.10	0.54
2:D:421:SER:HA	2:D:424:THR:CG2	2.38	0.54
1:A:219:PHE:HE1	1:A:237:LEU:HD22	1.73	0.54
1:A:303:TYR:O	1:A:307:LYS:HB2	2.08	0.54
1:A:89:PHE:CZ	1:A:123:SER:HA	2.43	0.54
1:A:125:PRO:C	1:A:127:GLY:H	2.11	0.53
1:A:33:LEU:HA	1:A:36:CYS:SG	2.49	0.53
1:C:272:GLU:O	1:C:274:THR:N	2.42	0.53
1:A:320:ALA:HA	1:A:323:ILE:CG1	2.27	0.53
1:A:343:VAL:HG13	1:A:360:LEU:HD21	1.91	0.53
1:C:71:LEU:HD12	1:C:72:ASN:H	1.72	0.53
1:A:332:PRO:HG3	1:A:362:ALA:HB3	1.89	0.53
2:D:439:THR:HG23	2:D:442:ASP:OD1	2.08	0.53
1:C:303:TYR:CD1	1:C:334:TYR:HD1	2.27	0.53
1:A:336:VAL:O	1:A:340:LYS:HB2	2.09	0.53
1:C:232:LEU:CD2	2:D:410:LEU:HD11	2.39	0.52
1:C:216:ILE:HD12	1:C:217:PHE:N	2.23	0.52
1:C:323:ILE:HG21	1:C:346:TYR:CG	2.44	0.52
1:C:163:LEU:HD22	1:C:169:ILE:CD1	2.37	0.52
1:C:163:LEU:C	1:C:165:THR:H	2.12	0.52
1:C:17:GLU:O	1:C:19:GLU:N	2.41	0.52
1:A:328:GLU:HG2	1:A:356:MSE:HG2	1.90	0.52
1:C:251:GLN:OE1	1:C:253:LYS:HE3	2.09	0.52
1:A:88:ASP:O	1:A:92:VAL:HG23	2.09	0.52
2:D:443:PHE:O	2:D:447:VAL:HG23	2.10	0.52
1:C:144:ASP:HB3	1:C:147:VAL:CG2	2.40	0.52
1:A:20:LEU:HD22	1:A:32:LEU:HD22	1.90	0.52
1:A:413:GLY:C	1:A:415:LEU:H	2.13	0.52
1:A:16:LEU:O	1:A:20:LEU:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD11	1:A:134:ILE:HG23	1.91	0.52
2:B:404:TRP:HZ3	2:B:443:PHE:CE1	2.28	0.52
1:C:124:GLN:H	1:C:124:GLN:CD	2.12	0.52
1:C:93:LEU:C	1:C:95:VAL:H	2.12	0.52
1:C:384:TYR:CE2	1:C:388:MSE:HE2	2.45	0.52
1:C:300:GLU:CD	1:C:305:LEU:H	2.12	0.52
2:B:429:PHE:CZ	2:B:449:LYS:HD2	2.45	0.52
1:A:166:ASP:OD2	1:A:168:LEU:HB2	2.10	0.51
1:C:379:VAL:HA	1:C:382:LEU:HD11	1.91	0.51
1:C:116:ALA:O	1:C:120:ILE:HG13	2.10	0.51
1:C:154:THR:HG21	2:D:383:GLU:HB3	1.90	0.51
1:A:145:GLU:HG3	1:A:192:SER:HB3	1.92	0.51
1:A:127:GLY:HA2	1:A:169:ILE:HD13	1.92	0.51
1:A:283:PHE:HE2	2:B:444:LEU:HB2	1.75	0.51
1:C:124:GLN:HB2	1:C:125:PRO:CD	2.27	0.51
1:A:300:GLU:OE1	1:A:305:LEU:N	2.44	0.51
1:A:441:LEU:HA	1:A:448:LEU:HD11	1.91	0.51
1:A:149:ASN:HD22	1:A:152:LEU:HB2	1.75	0.51
2:D:411:CYS:HB3	2:D:451:ILE:HG13	1.92	0.51
1:A:20:LEU:HG	1:A:26:PRO:HG2	1.92	0.51
1:C:284:SER:O	1:C:285:THR:C	2.49	0.51
1:C:196:LEU:O	1:C:200:LEU:HG	2.10	0.51
1:A:134:ILE:HA	1:A:137:ILE:HD12	1.91	0.51
1:C:403:PHE:CE2	1:C:408:MSE:HE2	2.46	0.51
1:A:116:ALA:O	1:A:120:ILE:HG13	2.11	0.51
1:C:358:ARG:NE	1:C:396:ARG:HH21	2.08	0.51
1:A:398:GLU:HG3	1:A:399:TYR:N	2.26	0.51
1:A:110:ASP:HB2	1:A:111:PRO:HD3	1.93	0.51
2:D:393:SER:HA	2:D:396:MSE:HG2	1.93	0.51
1:C:125:PRO:HD2	1:C:128:LEU:HB2	1.93	0.50
1:C:65:ASN:C	1:C:67:SER:H	2.15	0.50
1:C:180:TYR:HD1	1:C:180:TYR:C	2.14	0.50
2:B:419:LEU:HD22	2:B:419:LEU:N	2.26	0.50
1:C:109:ILE:HG22	1:C:112:LEU:H	1.77	0.50
1:C:37:SER:O	1:C:41:VAL:HG23	2.11	0.50
1:C:121:GLU:CB	1:C:159:ALA:HA	2.41	0.50
1:C:158:LYS:O	1:C:161:GLU:HB3	2.12	0.50
1:C:284:SER:HB3	1:C:288:LEU:CB	2.42	0.50
1:C:76:LEU:O	1:C:80:VAL:HG23	2.12	0.50
1:C:390:VAL:HG23	1:C:391:VAL:N	2.26	0.50
1:C:347:PHE:CD2	1:C:348:HIS:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:SER:C	1:C:451:TRP:H	2.15	0.50
1:C:445:GLU:HB2	1:C:452:TYR:CE2	2.47	0.50
1:A:263:ILE:N	1:A:263:ILE:HD13	2.19	0.50
2:D:385:ARG:HG3	2:D:385:ARG:HH11	1.76	0.50
1:A:333:GLN:HB3	1:A:337:LYS:HZ3	1.76	0.50
1:A:96:TYR:CD1	1:A:119:VAL:HG21	2.46	0.50
1:C:54:LEU:HG	1:C:58:ILE:HD11	1.93	0.50
1:C:230:ASP:O	1:C:232:LEU:N	2.45	0.50
1:C:371:ARG:NH1	1:C:403:PHE:HD1	2.08	0.50
1:C:10:GLU:O	1:C:13:LEU:HB2	2.11	0.49
1:C:136:ASP:OD1	1:C:172:ARG:HD2	2.12	0.49
1:C:385:LEU:HD23	1:C:429:THR:OG1	2.12	0.49
1:C:206:PHE:H	1:C:206:PHE:HD1	1.60	0.49
1:A:44:VAL:O	1:A:86:MSE:HE2	2.11	0.49
2:B:425:GLU:O	2:B:428:MSE:HB2	2.12	0.49
1:A:178:LEU:HD21	1:A:213:LYS:HG2	1.94	0.49
1:C:378:ILE:O	1:C:380:LEU:N	2.46	0.49
2:B:393:SER:C	2:B:395:SER:H	2.15	0.49
1:A:209:GLY:N	1:A:210:PRO:HD2	2.27	0.49
1:A:260:VAL:O	1:A:264:LEU:HG	2.13	0.49
1:C:268:ALA:O	1:C:271:PHE:HB3	2.13	0.49
1:C:310:ASP:O	1:C:315:LYS:HA	2.12	0.49
1:C:245:LEU:C	1:C:248:ILE:HG22	2.32	0.49
2:D:431:ILE:H	2:D:431:ILE:HD12	1.78	0.49
1:C:388:MSE:CE	1:C:433:ARG:HG3	2.43	0.49
1:A:249:ARG:HH11	1:A:297:ARG:CB	2.26	0.49
1:A:367:PHE:CE1	1:A:400:THR:HG22	2.48	0.49
1:C:283:PHE:HE1	2:D:445:LYS:HD2	1.78	0.49
1:A:124:GLN:HB3	1:A:125:PRO:CD	2.34	0.49
1:A:40:LEU:O	1:A:86:MSE:HE1	2.13	0.49
1:C:180:TYR:C	1:C:180:TYR:CD1	2.85	0.49
1:A:459:TYR:O	1:A:463:VAL:HG23	2.12	0.49
1:A:144:ASP:HB3	1:A:147:VAL:HG23	1.95	0.49
1:C:12:LEU:O	1:C:15:GLN:HB2	2.13	0.49
1:A:353:SER:HB2	1:A:356:MSE:HE3	1.95	0.48
1:C:322:LEU:HD13	1:C:325:GLU:HG3	1.95	0.48
2:B:389:PHE:CE2	2:B:419:LEU:HD12	2.47	0.48
1:C:405:LEU:HD23	1:C:412:MSE:SE	2.62	0.48
1:C:428:GLU:O	1:C:431:HIS:HB3	2.13	0.48
1:C:460:SER:O	1:C:464:ASN:HB2	2.12	0.48
1:C:50:ASP:OD2	1:C:53:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:446:ALA:O	2:D:450:VAL:N	2.43	0.48
1:C:295:VAL:O	1:C:298:ILE:HG13	2.12	0.48
2:D:404:TRP:HA	2:D:407:ILE:HG22	1.95	0.48
2:D:387:ASN:O	2:D:391:ILE:HD13	2.13	0.48
1:C:316:ILE:HG12	1:C:326:TRP:CG	2.49	0.48
1:A:194:VAL:HG11	2:B:406:LEU:HD22	1.95	0.48
1:A:111:PRO:O	1:A:114:VAL:HG12	2.12	0.48
1:C:51:VAL:C	1:C:53:PRO:HD2	2.34	0.48
1:C:121:GLU:HB3	1:C:159:ALA:HA	1.94	0.48
1:C:416:ILE:CG1	1:C:454:PRO:HB2	2.43	0.48
1:C:261:LYS:HB2	1:C:305:LEU:HD22	1.95	0.48
1:C:349:VAL:HG11	1:C:374:PHE:CD1	2.49	0.48
1:C:122:ASN:O	1:C:123:SER:C	2.51	0.48
1:C:133:ASN:HA	1:C:136:ASP:OD2	2.14	0.48
1:A:185:LYS:HE2	1:A:215:ILE:O	2.14	0.48
1:C:260:VAL:HG12	1:C:264:LEU:HD13	1.96	0.48
1:C:306:PHE:HZ	1:C:330:ILE:HD12	1.78	0.48
2:D:412:PRO:O	2:D:414:SER:N	2.47	0.48
1:A:272:GLU:HG3	1:A:273:ASP:N	2.28	0.48
1:A:457:ARG:HG3	1:A:458:GLU:H	1.77	0.48
1:C:281:ARG:O	1:C:285:THR:HG23	2.14	0.48
1:A:283:PHE:HZ	2:B:441:LYS:HB3	1.79	0.48
2:B:428:MSE:HB3	2:B:432:ARG:HH21	1.79	0.48
1:A:139:LEU:HD11	1:A:173:LEU:CD2	2.44	0.48
1:A:189:GLU:O	1:A:190:THR:C	2.51	0.47
1:A:130:ALA:HB2	1:A:169:ILE:HD12	1.96	0.47
1:A:189:GLU:HB3	1:A:192:SER:OG	2.14	0.47
1:C:269:GLN:O	1:C:272:GLU:HB3	2.14	0.47
2:D:385:ARG:HA	2:D:419:LEU:CD1	2.44	0.47
1:A:79:VAL:O	1:A:83:LEU:HG	2.13	0.47
1:C:93:LEU:HD21	1:C:124:GLN:HE22	1.80	0.47
1:C:232:LEU:HD22	2:D:410:LEU:HD11	1.95	0.47
2:D:382:LEU:O	2:D:382:LEU:HD23	2.14	0.47
1:A:276:ASN:O	1:A:277:TYR:CB	2.62	0.47
2:B:443:PHE:O	2:B:447:VAL:HG23	2.15	0.47
2:B:414:SER:HB2	2:B:418:GLU:HB2	1.96	0.47
1:C:135:ILE:CD1	1:C:169:ILE:HG13	2.43	0.47
1:C:185:LYS:HE3	1:C:219:PHE:CD2	2.50	0.47
1:C:19:GLU:HA	1:C:22:GLU:OE1	2.14	0.47
1:A:232:LEU:O	1:A:232:LEU:HD13	2.14	0.47
1:C:59:LYS:HB2	1:C:96:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD13	1:A:393:THR:HG21	1.96	0.47
1:A:392:GLU:OE2	1:A:396:ARG:HD2	2.13	0.47
1:C:19:GLU:C	1:C:21:ASN:H	2.18	0.47
1:C:189:GLU:O	1:C:190:THR:C	2.53	0.47
1:C:291:LEU:O	1:C:295:VAL:HG23	2.14	0.47
1:A:84:VAL:HG13	1:A:92:VAL:HG11	1.96	0.47
2:B:398:VAL:HG22	2:B:438:ALA:HB3	1.97	0.47
1:A:340:LYS:O	1:A:344:GLU:HB2	2.14	0.47
1:C:272:GLU:O	1:C:274:THR:HG23	2.14	0.47
1:A:447:LYS:O	1:A:449:SER:N	2.47	0.47
1:C:123:SER:HB3	1:C:126:LYS:HA	1.97	0.47
1:C:135:ILE:HD13	1:C:169:ILE:HG13	1.95	0.47
1:C:9:VAL:CG2	1:C:47:PRO:HG3	2.42	0.47
1:C:271:PHE:CE2	1:C:281:ARG:NE	2.82	0.47
1:C:289:LEU:HD22	1:C:329:LEU:CD2	2.43	0.47
1:C:327:LEU:CB	1:C:356:MSE:HG2	2.41	0.47
1:A:20:LEU:HB3	1:A:29:ILE:HD13	1.97	0.47
1:A:52:LYS:NZ	1:A:91:ASP:HB3	2.30	0.47
1:C:434:ASN:HD21	1:C:462:ALA:HB1	1.79	0.47
1:A:96:TYR:CE1	1:A:119:VAL:HG21	2.50	0.47
1:A:313:SER:O	1:A:315:LYS:N	2.48	0.47
1:A:422:GLY:C	1:A:424:ILE:H	2.17	0.47
1:C:125:PRO:C	1:C:127:GLY:H	2.18	0.46
2:D:407:ILE:HD11	2:D:443:PHE:HB3	1.97	0.46
1:A:72:ASN:HD22	1:A:72:ASN:C	2.16	0.46
1:A:293:ALA:HB2	1:A:329:LEU:HB3	1.96	0.46
1:C:110:ASP:O	1:C:114:VAL:HG23	2.15	0.46
1:C:152:LEU:HD22	1:C:156:ILE:HD11	1.97	0.46
1:A:125:PRO:C	1:A:127:GLY:N	2.69	0.46
1:C:171:ARG:CZ	1:C:171:ARG:HB3	2.46	0.46
1:A:367:PHE:C	1:A:369:ALA:H	2.19	0.46
2:B:389:PHE:O	2:B:393:SER:HB3	2.15	0.46
2:B:404:TRP:CZ3	2:B:443:PHE:CE1	3.04	0.46
2:B:422:VAL:HG11	2:B:447:VAL:HG22	1.98	0.46
1:A:17:GLU:HA	1:A:32:LEU:HD21	1.97	0.46
1:A:435:SER:HA	1:A:438:ARG:HH12	1.81	0.46
1:C:161:GLU:C	1:C:163:LEU:H	2.19	0.46
1:C:165:THR:HG22	1:C:206:PHE:CE2	2.50	0.46
1:A:213:LYS:C	1:A:215:ILE:H	2.20	0.46
1:A:219:PHE:O	1:A:263:ILE:HG21	2.15	0.46
2:B:400:ARG:NE	2:B:400:ARG:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:TRP:CE3	1:C:330:ILE:HD11	2.50	0.46
1:A:185:LYS:HD2	1:A:219:PHE:HE2	1.81	0.46
1:C:26:PRO:O	1:C:29:ILE:HG13	2.16	0.46
1:A:133:ASN:O	1:A:137:ILE:HG13	2.16	0.46
1:A:416:ILE:HD11	1:A:451:TRP:HE3	1.81	0.46
1:A:327:LEU:CD2	1:A:343:VAL:HA	2.46	0.45
1:C:25:LEU:HD11	1:C:66:VAL:CG1	2.41	0.45
1:A:142:LEU:O	1:A:195:ARG:HD2	2.17	0.45
1:C:10:GLU:HB3	1:C:13:LEU:CD2	2.47	0.45
1:A:163:LEU:C	1:A:165:THR:H	2.19	0.45
2:D:399:GLU:HG2	2:D:400:ARG:N	2.29	0.45
1:C:102:VAL:HG22	1:C:134:ILE:HG12	1.98	0.45
1:A:322:LEU:O	1:A:323:ILE:C	2.55	0.45
1:A:219:PHE:HE1	1:A:237:LEU:CD2	2.30	0.45
1:A:324:THR:HG23	1:A:325:GLU:H	1.81	0.45
1:C:399:TYR:CE1	1:C:400:THR:HG23	2.52	0.45
1:C:324:THR:O	1:C:328:GLU:HG2	2.17	0.45
1:C:384:TYR:CZ	1:C:388:MSE:HE2	2.52	0.45
1:C:232:LEU:HD23	2:D:444:LEU:HD21	1.99	0.45
1:C:367:PHE:O	1:C:370:ILE:HG13	2.17	0.45
1:C:34:ARG:O	1:C:38:LEU:HD12	2.17	0.45
1:A:201:THR:HG21	1:A:243:LYS:HD2	1.99	0.45
1:C:295:VAL:HA	1:C:298:ILE:HG13	1.99	0.45
1:C:10:GLU:HB3	1:C:13:LEU:CG	2.47	0.45
1:C:313:SER:HB2	1:C:314:LEU:H	1.57	0.45
1:A:249:ARG:HH11	1:A:297:ARG:CG	2.29	0.45
1:C:235:ILE:HG23	1:C:287:CYS:SG	2.57	0.45
1:C:185:LYS:HE3	1:C:219:PHE:HD2	1.80	0.45
1:A:185:LYS:HD3	1:A:216:ILE:HD12	1.99	0.45
1:C:325:GLU:O	1:C:329:LEU:HD13	2.17	0.45
1:C:453:GLU:N	1:C:454:PRO:HD2	2.32	0.45
2:B:398:VAL:CG1	2:B:402:ILE:HD12	2.47	0.45
1:A:23:ASP:HB3	1:A:24:ASN:H	1.54	0.45
1:C:12:LEU:HA	1:C:15:GLN:HE21	1.81	0.45
2:D:392:HIS:CE1	2:D:420:ARG:HH11	2.35	0.45
1:A:137:ILE:O	1:A:141:ILE:HG13	2.17	0.45
1:A:60:ARG:O	1:A:64:SER:HB3	2.16	0.45
1:C:125:PRO:C	1:C:127:GLY:N	2.71	0.44
2:D:400:ARG:HH11	2:D:400:ARG:HG3	1.82	0.44
1:A:425:ILE:HD12	1:A:425:ILE:N	2.31	0.44
1:C:321:LYS:N	1:C:321:LYS:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:ILE:HG21	2:D:404:TRP:CH2	2.52	0.44
1:C:411:VAL:HA	1:C:414:SER:OG	2.17	0.44
1:A:154:THR:CG2	2:B:383:GLU:HG2	2.47	0.44
1:A:140:ASP:O	1:A:144:ASP:HB2	2.18	0.44
2:B:383:GLU:HA	2:B:383:GLU:OE1	2.16	0.44
2:B:429:PHE:HE2	2:B:446:ALA:HA	1.82	0.44
1:C:52:LYS:N	1:C:53:PRO:CD	2.80	0.44
2:D:404:TRP:O	2:D:407:ILE:HG22	2.17	0.44
1:A:331:ASN:OD1	1:A:333:GLN:N	2.51	0.44
1:C:204:PHE:CD1	1:C:207:ILE:HG21	2.53	0.44
1:A:397:TYR:HB2	1:A:400:THR:OG1	2.17	0.44
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.82	0.44
1:C:322:LEU:HB3	1:C:326:TRP:NE1	2.33	0.44
1:A:347:PHE:CD2	1:A:370:ILE:HB	2.53	0.44
1:C:255:TRP:CZ3	1:C:256:ALA:HB2	2.53	0.44
1:C:195:ARG:HD3	2:D:405:GLU:OE1	2.18	0.44
1:C:264:LEU:HB3	1:C:265:PRO:HD3	2.00	0.44
1:C:250:ASN:C	1:C:251:GLN:HG3	2.37	0.44
1:C:11:ASN:HB3	1:C:47:PRO:CG	2.44	0.44
1:A:451:TRP:O	1:A:455:LEU:HG	2.18	0.44
1:C:339:HIS:HB3	1:C:342:VAL:CG2	2.48	0.44
1:A:407:GLU:C	1:A:409:PRO:HD3	2.38	0.44
1:A:368:ASN:HA	1:A:371:ARG:HG2	2.00	0.44
1:C:135:ILE:HA	1:C:138:LEU:HD12	1.99	0.44
1:C:30:ASN:OD1	1:C:71:LEU:HD13	2.16	0.44
1:C:272:GLU:HG3	1:C:273:ASP:N	2.33	0.44
1:C:412:MSE:HE2	1:C:451:TRP:CD2	2.53	0.44
1:A:11:ASN:HD22	1:A:14:THR:HB	1.82	0.44
1:C:124:GLN:OE1	1:C:124:GLN:N	2.51	0.43
1:C:241:TYR:CE1	1:C:260:VAL:HG13	2.53	0.43
1:C:245:LEU:CD2	1:C:295:VAL:HG22	2.48	0.43
1:C:412:MSE:HB3	1:C:412:MSE:HE3	1.90	0.43
1:C:437:LEU:O	1:C:441:LEU:HD13	2.17	0.43
1:C:10:GLU:OE1	1:C:13:LEU:HD21	2.18	0.43
1:A:139:LEU:HD11	1:A:173:LEU:HD23	2.00	0.43
1:C:20:LEU:HD23	1:C:26:PRO:HG2	2.00	0.43
1:A:316:ILE:HG12	1:A:326:TRP:CD2	2.53	0.43
1:A:425:ILE:HD12	1:A:425:ILE:H	1.84	0.43
1:A:379:VAL:O	1:A:382:LEU:HG	2.17	0.43
1:A:125:PRO:HD2	1:A:128:LEU:HB2	2.00	0.43
2:D:383:GLU:O	2:D:384:GLY:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TYR:O	1:A:184:VAL:HG23	2.17	0.43
1:C:188:MSE:HE2	1:C:188:MSE:HB3	1.71	0.43
1:C:380:LEU:HD21	1:C:411:VAL:HG23	2.00	0.43
2:D:385:ARG:HG3	2:D:385:ARG:NH1	2.34	0.43
1:A:24:ASN:O	1:A:25:LEU:HB2	2.19	0.43
1:A:109:ILE:O	1:A:113:LYS:HG3	2.18	0.43
1:A:11:ASN:HA	1:A:14:THR:OG1	2.18	0.43
1:C:159:ALA:O	1:C:163:LEU:HB2	2.19	0.43
1:C:77:LEU:O	1:C:80:VAL:HB	2.19	0.43
1:C:109:ILE:O	1:C:113:LYS:HG3	2.19	0.43
2:B:407:ILE:HD11	2:B:443:PHE:HB3	2.00	0.43
1:C:353:SER:O	1:C:354:ILE:C	2.56	0.43
1:C:336:VAL:C	1:C:338:TYR:N	2.71	0.43
1:A:105:LEU:O	1:A:113:LYS:HE2	2.19	0.43
1:A:178:LEU:N	1:A:179:PRO:CD	2.82	0.43
2:D:382:LEU:C	2:D:384:GLY:N	2.72	0.43
1:A:210:PRO:HG2	1:A:211:GLU:H	1.83	0.43
1:C:316:ILE:HD11	1:C:330:ILE:HG13	2.01	0.43
1:C:24:ASN:HA	1:C:24:ASN:HD22	1.62	0.43
2:D:422:VAL:CG2	2:D:450:VAL:HG11	2.47	0.43
2:D:402:ILE:HG21	2:D:404:TRP:CZ2	2.53	0.43
1:C:268:ALA:HB2	1:C:309:MSE:CE	2.42	0.43
1:C:314:LEU:N	1:C:314:LEU:HD12	2.33	0.43
2:D:436:LYS:NZ	2:D:437:VAL:HG23	2.33	0.43
1:A:109:ILE:HB	1:A:112:LEU:HB3	1.99	0.43
1:C:166:ASP:HB3	1:C:169:ILE:CG2	2.46	0.43
2:B:385:ARG:NH1	2:B:385:ARG:HG2	2.33	0.43
1:C:47:PRO:O	1:C:49:MSE:N	2.52	0.43
1:C:245:LEU:HD21	1:C:295:VAL:HG22	2.01	0.43
1:C:327:LEU:HD23	1:C:335:LEU:HD13	2.01	0.43
2:D:392:HIS:NE2	2:D:420:ARG:HG2	2.33	0.43
1:C:320:ALA:HA	1:C:323:ILE:HG12	2.00	0.43
1:C:225:LEU:HD23	1:C:277:TYR:OH	2.19	0.43
1:A:253:LYS:C	1:A:255:TRP:H	2.22	0.43
1:C:121:GLU:HA	1:C:163:LEU:CD1	2.49	0.42
1:C:163:LEU:O	1:C:169:ILE:HG21	2.18	0.42
1:C:193:PHE:O	1:C:197:ILE:HG13	2.19	0.42
1:A:336:VAL:O	1:A:336:VAL:HG22	2.19	0.42
1:C:403:PHE:HE2	1:C:408:MSE:HE2	1.84	0.42
1:A:196:LEU:O	1:A:200:LEU:HG	2.18	0.42
1:C:85:PRO:HA	1:C:122:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD21	1:C:124:GLN:NE2	2.34	0.42
2:D:385:ARG:HA	2:D:419:LEU:HD13	2.01	0.42
1:C:178:LEU:N	1:C:179:PRO:CD	2.81	0.42
2:D:436:LYS:H	2:D:436:LYS:HE3	1.83	0.42
1:C:428:GLU:H	1:C:428:GLU:CD	2.23	0.42
1:A:72:ASN:HB3	1:A:75:TYR:HD2	1.84	0.42
1:A:302:GLU:O	1:A:302:GLU:HG3	2.20	0.42
1:A:227:SER:HB2	1:A:233:VAL:HG12	1.99	0.42
1:C:110:ASP:N	1:C:111:PRO:CD	2.82	0.42
1:A:353:SER:CB	1:A:356:MSE:HE3	2.49	0.42
1:A:234:PHE:CE2	1:A:280:VAL:HG13	2.55	0.42
1:A:277:TYR:N	1:A:278:PRO:CD	2.82	0.42
1:A:146:LYS:HD2	1:A:146:LYS:H	1.84	0.42
1:A:187:ARG:HD2	1:A:192:SER:OG	2.20	0.42
1:A:133:ASN:ND2	1:A:137:ILE:HD11	2.35	0.42
2:B:424:THR:HG21	1:C:459:TYR:HE2	1.85	0.42
1:A:232:LEU:HD23	2:B:444:LEU:HD21	2.00	0.42
1:C:85:PRO:HG2	1:C:86:MSE:H	1.84	0.42
1:A:322:LEU:HA	1:A:325:GLU:OE1	2.19	0.42
1:C:231:ILE:HG23	1:C:232:LEU:N	2.35	0.42
1:C:310:ASP:O	1:C:314:LEU:O	2.37	0.42
1:C:340:LYS:HE2	1:C:344:GLU:OE1	2.19	0.42
1:C:152:LEU:O	1:C:156:ILE:HG13	2.20	0.42
1:A:241:TYR:HE1	1:A:260:VAL:HG12	1.85	0.42
1:C:271:PHE:HE2	1:C:281:ARG:NE	2.17	0.42
1:C:295:VAL:C	1:C:297:ARG:H	2.22	0.42
1:A:52:LYS:N	1:A:53:PRO:CD	2.83	0.42
1:C:46:LEU:CD1	1:C:86:MSE:HB2	2.49	0.42
1:C:433:ARG:HG2	1:C:437:LEU:HD13	2.02	0.42
1:C:347:PHE:HE1	1:C:370:ILE:HD13	1.84	0.42
1:A:261:LYS:HG2	1:A:305:LEU:HD22	2.00	0.42
1:A:80:VAL:O	1:A:84:VAL:HG23	2.20	0.42
1:A:413:GLY:C	1:A:415:LEU:N	2.73	0.42
1:C:257:LEU:O	1:C:258:ARG:C	2.58	0.42
1:A:124:GLN:CB	1:A:125:PRO:CD	2.95	0.42
2:D:382:LEU:C	2:D:383:GLU:HG3	2.41	0.41
1:A:230:ASP:O	1:A:232:LEU:N	2.53	0.41
1:A:84:VAL:N	1:A:85:PRO:CD	2.81	0.41
1:A:81:ASP:OD1	1:A:118:ARG:HD3	2.20	0.41
1:C:319:GLU:HB3	1:C:321:LYS:HD2	2.02	0.41
1:A:177:ASN:C	1:A:179:PRO:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PHE:CZ	1:C:330:ILE:HD12	2.55	0.41
2:B:381:ASP:C	2:B:383:GLU:N	2.73	0.41
1:A:220:THR:HG23	1:A:223:GLU:OE1	2.19	0.41
2:B:380:MSE:HB2	2:B:380:MSE:HE2	1.99	0.41
1:A:241:TYR:CZ	1:A:263:ILE:HG13	2.56	0.41
1:C:101:LEU:HD21	1:C:120:ILE:HG12	2.02	0.41
1:A:114:VAL:HG23	1:A:155:ALA:CB	2.50	0.41
2:B:433:ALA:O	2:B:434:ARG:HG2	2.20	0.41
1:C:54:LEU:HA	1:C:57:THR:OG1	2.20	0.41
2:D:436:LYS:H	2:D:436:LYS:CD	2.33	0.41
1:C:40:LEU:CD1	1:C:46:LEU:HD21	2.45	0.41
1:A:324:THR:HG23	1:A:325:GLU:N	2.36	0.41
1:A:388:MSE:N	1:A:388:MSE:HE2	2.35	0.41
2:B:416:GLY:O	2:B:419:LEU:HD23	2.20	0.41
2:B:407:ILE:HD11	2:B:444:LEU:HD23	2.02	0.41
1:A:220:THR:OG1	1:A:223:GLU:HG3	2.20	0.41
1:A:109:ILE:HG22	1:A:112:LEU:H	1.86	0.41
1:A:255:TRP:CD1	1:A:255:TRP:C	2.92	0.41
1:C:33:LEU:HA	1:C:36:CYS:SG	2.60	0.41
1:C:190:THR:HG21	2:D:403:ARG:NH1	2.35	0.41
1:C:300:GLU:OE1	1:C:305:LEU:N	2.54	0.41
1:A:234:PHE:O	1:A:238:VAL:HG23	2.21	0.41
1:C:354:ILE:HG22	1:C:355:GLY:N	2.35	0.41
1:A:187:ARG:HG3	1:A:188:MSE:N	2.34	0.41
1:C:435:SER:O	1:C:439:ASN:ND2	2.54	0.41
2:D:429:PHE:HA	2:D:432:ARG:HH11	1.85	0.41
1:C:128:LEU:HD22	1:C:129:PHE:CD1	2.56	0.41
1:A:353:SER:C	1:A:355:GLY:N	2.74	0.41
1:A:433:ARG:O	1:A:437:LEU:HG	2.19	0.41
1:C:193:PHE:CE1	1:C:197:ILE:HD11	2.56	0.41
1:A:13:LEU:HD13	1:A:36:CYS:HA	2.01	0.41
1:C:30:ASN:CA	1:C:71:LEU:HD22	2.51	0.41
1:C:260:VAL:C	1:C:262:LYS:H	2.23	0.41
1:C:331:ASN:ND2	1:C:334:TYR:H	2.18	0.41
2:B:420:ARG:NH1	2:B:420:ARG:HG2	2.33	0.41
1:A:374:PHE:HD1	1:A:408:MSE:HE1	1.83	0.41
1:A:405:LEU:HD13	1:A:405:LEU:HA	1.83	0.41
1:C:378:ILE:HA	1:C:381:ARG:HG2	2.02	0.41
1:C:417:GLY:C	1:C:419:GLY:H	2.24	0.41
2:D:412:PRO:C	2:D:414:SER:N	2.75	0.41
1:C:353:SER:O	1:C:355:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ILE:O	2:B:402:ILE:HG22	2.21	0.41
1:A:38:LEU:O	1:A:38:LEU:HD13	2.21	0.41
1:C:300:GLU:OE2	1:C:304:SER:HB2	2.21	0.40
1:C:66:VAL:O	1:C:66:VAL:HG12	2.21	0.40
1:C:213:LYS:C	1:C:215:ILE:H	2.24	0.40
1:C:102:VAL:HG13	1:C:137:ILE:CD1	2.51	0.40
1:C:133:ASN:O	1:C:137:ILE:HG13	2.21	0.40
1:A:327:LEU:HD21	1:A:343:VAL:HA	2.03	0.40
1:C:340:LYS:HE2	1:C:344:GLU:CD	2.41	0.40
1:A:454:PRO:O	1:A:458:GLU:HB2	2.22	0.40
1:A:264:LEU:N	1:A:265:PRO:CD	2.83	0.40
1:C:284:SER:HB3	1:C:288:LEU:HB3	2.04	0.40
1:C:349:VAL:O	1:C:350:SER:HB3	2.22	0.40
1:C:47:PRO:C	1:C:49:MSE:N	2.74	0.40
1:A:366:CYS:O	1:A:369:ALA:HB3	2.21	0.40
1:C:156:ILE:HG22	1:C:160:LEU:HD11	2.02	0.40
1:C:55:LEU:C	1:C:95:VAL:HG11	2.41	0.40
1:A:295:VAL:HG11	1:A:309:MSE:SE	2.71	0.40
2:B:407:ILE:CD1	2:B:443:PHE:HB3	2.51	0.40
1:C:224:ILE:O	1:C:227:SER:OG	2.34	0.40
1:A:117:CYS:SG	1:A:156:ILE:HG12	2.61	0.40
1:C:171:ARG:O	1:C:175:ASP:HB3	2.21	0.40
1:A:384:TYR:HE1	1:A:414:SER:O	2.05	0.40
1:A:333:GLN:O	1:A:337:LYS:HG3	2.21	0.40
1:C:177:ASN:C	1:C:179:PRO:HD2	2.41	0.40
1:C:269:GLN:O	1:C:272:GLU:N	2.52	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	455/500 (91%)	366 (80%)	67 (15%)	22 (5%)	3	32
1	C	450/500 (90%)	330 (73%)	83 (18%)	37 (8%)	1	18
2	B	71/88 (81%)	55 (78%)	11 (16%)	5 (7%)	1	23
2	D	71/88 (81%)	50 (70%)	15 (21%)	6 (8%)	1	17
All	All	1047/1176 (89%)	801 (76%)	176 (17%)	70 (7%)	1	25

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	190	THR
1	A	231	ILE
1	A	281	ARG
1	A	449	SER
1	C	18	ASN
1	C	65	ASN
1	C	70	SER
1	C	161	GLU
1	C	190	THR
1	C	231	ILE
1	C	258	ARG
1	C	273	ASP
1	C	285	THR
1	C	313	SER
1	C	354	ILE
2	D	383	GLU
1	A	260	VAL
1	A	284	SER
1	A	314	LEU
2	B	400	ARG
2	B	402	ILE
1	C	48	ASP
1	C	66	VAL
1	C	191	VAL
1	C	214	ASP
1	C	304	SER
1	C	351	GLY
1	C	376	ALA
1	C	379	VAL
1	C	449	SER
1	C	450	VAL
2	D	381	ASP

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Mol	Chain	Res	Type
2	D	401	GLY
2	D	413	ASN
1	A	47	PRO
1	A	254	TYR
1	A	283	PHE
1	A	346	TYR
1	A	448	LEU
1	C	27	GLU
1	C	49	MSE
1	C	87	ALA
1	C	162	ARG
1	C	164	SER
1	C	257	LEU
1	C	312	ASP
1	C	407	GLU
1	A	280	VAL
2	B	394	LYS
2	B	412	PRO
1	C	175	ASP
1	C	251	GLN
1	C	337	LYS
2	D	434	ARG
1	A	23	ASP
1	A	277	TYR
1	A	304	SER
1	A	409	PRO
1	C	24	ASN
1	C	98	ALA
1	C	339	HIS
2	B	403	ARG
1	C	123	SER
1	A	416	ILE
1	A	349	VAL
1	A	323	ILE
2	D	402	ILE
1	A	147	VAL
1	C	316	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	424/452 (94%)	385 (91%)	39 (9%)	11	48
1	C	424/452 (94%)	382 (90%)	42 (10%)	10	44
2	B	62/72 (86%)	55 (89%)	7 (11%)	7	38
2	D	62/72 (86%)	53 (86%)	9 (14%)	4	27
All	All	972/1048 (93%)	875 (90%)	97 (10%)	9	43

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	22	GLU
1	A	28	ASP
1	A	65	ASN
1	A	72	ASN
1	A	136	ASP
1	A	140	ASP
1	A	145	GLU
1	A	151	LYS
1	A	154	THR
1	A	169	ILE
1	A	175	ASP
1	A	187	ARG
1	A	206	PHE
1	A	221	LYS
1	A	251	GLN
1	A	255	TRP
1	A	263	ILE
1	A	272	GLU
1	A	283	PHE
1	A	287	CYS
1	A	290	GLN
1	A	308	THR
1	A	311	LYS
1	A	314	LEU
1	A	321	LYS
1	A	322	LEU
1	A	346	TYR

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Mol	Chain	Res	Type
1	A	352	TYR
1	A	354	ILE
1	A	360	LEU
1	A	371	ARG
1	A	372	ASN
1	A	381	ARG
1	A	386	GLU
1	A	398	GLU
1	A	405	LEU
1	A	416	ILE
1	A	457	ARG
2	B	380	MSE
2	B	383	GLU
2	B	407	ILE
2	B	421	SER
2	B	424	THR
2	B	439	THR
2	B	451	ILE
1	C	8	TYR
1	C	13	LEU
1	C	18	ASN
1	C	19	GLU
1	C	24	ASN
1	C	57	THR
1	C	89	PHE
1	C	90	ASP
1	C	91	ASP
1	C	99	GLU
1	C	124	GLN
1	C	136	ASP
1	C	140	ASP
1	C	150	ASP
1	C	151	LYS
1	C	152	LEU
1	C	154	THR
1	C	162	ARG
1	C	165	THR
1	C	180	TYR
1	C	184	VAL
1	C	188	MSE
1	C	189	GLU
1	C	192	SER

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Mol	Chain	Res	Type
1	C	206	PHE
1	C	257	LEU
1	C	258	ARG
1	C	285	THR
1	C	287	CYS
1	C	288	LEU
1	C	313	SER
1	C	314	LEU
1	C	321	LYS
1	C	322	LEU
1	C	325	GLU
1	C	336	VAL
1	C	382	LEU
1	C	384	TYR
1	C	391	VAL
1	C	411	VAL
1	C	414	SER
1	C	415	LEU
2	D	380	MSE
2	D	383	GLU
2	D	385	ARG
2	D	403	ARG
2	D	424	THR
2	D	434	ARG
2	D	436	LYS
2	D	439	THR
2	D	451	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	15	GLN
1	A	21	ASN
1	A	24	ASN
1	A	65	ASN
1	A	72	ASN
1	A	149	ASN
1	A	177	ASN
1	A	333	GLN
1	A	348	HIS
1	A	434	ASN

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Mol	Chain	Res	Type
1	C	24	ASN
1	C	122	ASN
1	C	124	GLN
1	C	177	ASN
1	C	239	ASN
1	C	276	ASN
1	C	290	GLN
1	C	331	ASN
1	C	333	GLN
1	C	387	GLN
1	C	389	GLN
1	C	439	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	449/500 (89%)	0.35	23 (5%) 32 21	87, 158, 255, 289	0
1	C	446/500 (89%)	0.24	12 (2%) 58 42	102, 156, 216, 274	0
2	B	70/88 (79%)	0.12	0 100 100	106, 154, 195, 221	0
2	D	70/88 (79%)	0.15	1 (1%) 78 63	98, 144, 178, 202	0
All	All	1035/1176 (88%)	0.27	36 (3%) 48 32	87, 156, 236, 289	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	SER	6.7
1	A	13	LEU	4.6
1	A	421	ALA	4.5
1	A	29	ILE	4.5
1	A	39	ASN	4.2
1	A	422	GLY	4.1
1	A	17	GLU	3.5
1	A	21	ASN	3.5
1	A	10	GLU	3.3
1	A	62	LEU	3.3
1	C	17	GLU	3.0
1	A	68	TYR	3.0
1	A	9	VAL	3.0
1	A	46	LEU	2.8
1	C	96	TYR	2.6
1	C	25	LEU	2.5
1	A	12	LEU	2.5
1	C	84	VAL	2.4
1	C	51	VAL	2.4
1	A	71	LEU	2.4
1	C	130	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	55	LEU	2.4
1	A	48	ASP	2.4
1	C	374	PHE	2.3
1	C	418	ASP	2.3
1	A	61	PHE	2.3
1	C	420	SER	2.3
1	A	130	ALA	2.2
1	A	126	LYS	2.2
1	A	40	LEU	2.2
1	C	443	LYS	2.2
1	A	16	LEU	2.1
2	D	389	PHE	2.1
1	C	296	SER	2.1
1	A	424	ILE	2.1
1	A	54	LEU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.