



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 04:55 PM UTC

PDB ID : 3RTK / pdb_00003rtk
Title : Crystal structure of Cpn60.2 from Mycobacterium tuberculosis at 2.8Å
Authors : Shahar, A.; Melamed-Frank, M.; Kashi, Y.; Adir, N.
Deposited on : 2011-05-03
Resolution : 2.80 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

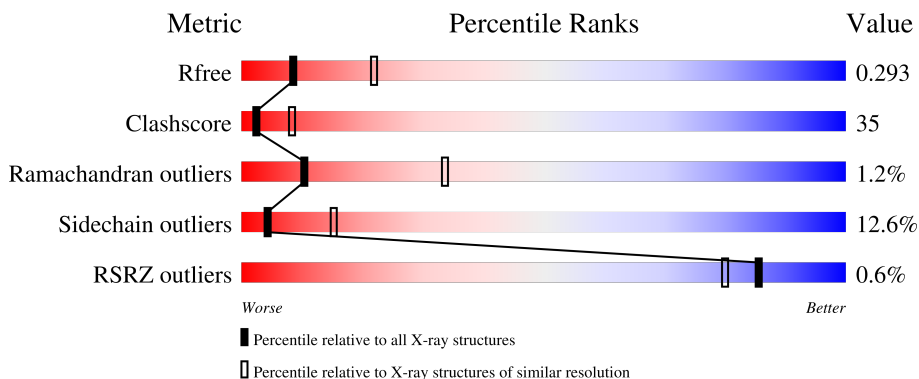
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	546	 38% 38% 5% 18%
1	B	546	 41% 33% 8% 18%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6629 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 60 kDa chaperonin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	Total	C	N	O	S	0	0	0
			3315	2076	567	668	4			
1	B	447	Total	C	N	O	S	0	0	0
			3305	2071	566	664	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	HIS	-	expression tag	UNP P0A520
A	542	HIS	-	expression tag	UNP P0A520
A	543	HIS	-	expression tag	UNP P0A520
A	544	HIS	-	expression tag	UNP P0A520
A	545	HIS	-	expression tag	UNP P0A520
A	546	HIS	-	expression tag	UNP P0A520
B	541	HIS	-	expression tag	UNP P0A520
B	542	HIS	-	expression tag	UNP P0A520
B	543	HIS	-	expression tag	UNP P0A520
B	544	HIS	-	expression tag	UNP P0A520
B	545	HIS	-	expression tag	UNP P0A520
B	546	HIS	-	expression tag	UNP P0A520

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.19Å 111.98Å 77.28Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.0 (20.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.79Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.285 0.225 , 0.293	Depositor DCC
R_{free} test set	1192 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6629	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, 0.333 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: MG

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	0.58	0/3340	1.05	19/4514 (0.4%)
1	B	0.61	0/3330	1.02	15/4501 (0.3%)
All	All	0.60	0/6670	1.04	34/9015 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	VAL	N-CA-C	-10.21	92.30	107.51
1	A	153	ASP	CB-CA-C	8.80	124.16	109.99
1	A	139	THR	N-CA-C	8.77	122.28	110.35
1	B	406	GLU	CB-CA-C	-8.69	95.05	109.65
1	A	226	SER	CB-CA-C	8.09	126.52	110.42
1	A	276	ALA	CA-C-N	7.65	128.11	119.92
1	A	276	ALA	C-N-CA	7.65	128.11	119.92
1	A	340	ILE	N-CA-C	7.56	118.09	110.23
1	B	256	ALA	N-CA-C	-7.31	103.45	113.18
1	A	332	GLU	N-CA-C	7.24	121.66	111.52
1	B	492	ASP	CB-CA-C	7.13	124.22	110.17
1	A	340	ILE	CB-CA-C	-6.69	103.13	111.70
1	B	406	GLU	N-CA-C	6.65	121.80	113.43
1	A	138	GLU	CB-CA-C	6.21	122.78	110.42
1	B	491	ALA	N-CA-CB	6.02	121.48	110.76
1	B	496	VAL	N-CA-C	6.00	116.66	110.36
1	A	184	GLN	N-CA-C	5.88	118.82	109.24
1	A	178	SER	CB-CA-C	-5.84	99.91	111.60
1	B	205	ASP	CA-C-N	5.69	126.95	119.84
1	B	205	ASP	C-N-CA	5.69	126.95	119.84
1	B	203	VAL	N-CA-C	5.63	116.58	110.21
1	A	415	VAL	N-CA-C	5.62	121.03	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	N-CA-C	-5.56	100.07	108.52
1	A	166	LYS	N-CA-C	5.55	122.63	110.80
1	A	415	VAL	CB-CA-C	-5.55	102.19	111.29
1	A	70	ALA	N-CA-C	-5.50	104.67	111.33
1	B	458	GLU	CA-C-N	5.43	126.63	119.84
1	B	458	GLU	C-N-CA	5.43	126.63	119.84
1	A	227	THR	N-CA-C	5.43	118.34	110.42
1	B	382	ALA	CB-CA-C	-5.15	100.99	109.65
1	A	286	MET	N-CA-C	-5.15	105.74	112.23
1	B	324	THR	CB-CA-C	-5.15	102.60	112.43
1	A	250	GLU	N-CA-C	-5.11	105.71	111.28
1	B	361	GLU	CB-CA-C	-5.10	102.81	110.92

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	3315	0	3430	263	1
1	B	3305	0	3427	212	1
2	A	1	0	0	0	0
3	A	5	0	0	8	0
3	B	3	0	0	2	0
All	All	6629	0	6857	471	1

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 35.

All (471) 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:481:VAL:CG1	1:A:483:GLU:HG2	1.52	1.36
1:A:381:ALA:HB1	1:A:387:LEU:CD1	1.60	1.31
1:B:333:GLY:HA2	1:B:334:ALA:CB	1.57	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLY:CA	1:B:334:ALA:HB3	1.65	1.26
1:A:381:ALA:CB	1:A:387:LEU:HD21	1.65	1.25
1:A:381:ALA:HB2	1:A:387:LEU:CD2	1.67	1.24
1:A:381:ALA:CB	1:A:387:LEU:HD11	1.68	1.23
1:A:382:ALA:HA	1:A:383:THR:OG1	1.41	1.21
1:A:80:THR:O	1:A:81:ASP:CG	1.88	1.15
1:B:294:THR:HG23	1:B:316:GLY:HA3	1.19	1.15
1:A:294:THR:CG2	1:A:316:GLY:HA3	1.77	1.14
1:B:294:THR:CA	1:B:334:ALA:HB1	1.78	1.14
1:A:294:THR:HG23	1:A:316:GLY:HA3	1.29	1.13
1:A:481:VAL:HG12	1:A:483:GLU:HG2	1.28	1.11
1:A:191:MET:HE1	1:A:290:MET:HG3	1.34	1.09
1:B:294:THR:HA	1:B:334:ALA:CB	1.84	1.08
1:A:226:SER:O	1:A:256:ALA:HB2	1.52	1.07
1:A:481:VAL:HG11	1:A:483:GLU:HG2	1.32	1.07
1:A:481:VAL:HG12	1:A:483:GLU:CG	1.84	1.06
1:B:418:LEU:HD13	1:B:445:GLU:HB3	1.37	1.05
1:A:64:PRO:O	1:A:68:ILE:HG12	1.55	1.05
1:A:381:ALA:HB2	1:A:387:LEU:HD21	1.07	1.04
1:B:333:GLY:HA2	1:B:334:ALA:HB3	1.06	1.02
1:A:76:VAL:HG13	1:A:79:LYS:NZ	1.73	1.02
1:A:481:VAL:CG1	1:A:483:GLU:CG	2.40	1.00
1:A:476:ASN:HB3	1:A:479:THR:HB	1.46	0.96
1:A:382:ALA:HA	1:A:383:THR:HG1	1.21	0.96
1:A:172:VAL:HG13	1:A:192:ARG:CZ	1.95	0.95
1:B:254:GLY:O	1:B:255:GLU:HB2	1.63	0.94
1:A:232:LEU:O	1:A:236:GLU:HG3	1.68	0.93
1:B:312:LEU:H	1:B:312:LEU:HD12	1.30	0.93
1:B:140:LYS:H	1:B:140:LYS:HD2	1.33	0.93
1:A:381:ALA:CA	1:A:387:LEU:HD21	1.98	0.93
1:B:331:VAL:O	1:B:332:GLU:HB2	1.66	0.93
1:B:294:THR:HA	1:B:334:ALA:HB1	0.96	0.93
1:A:194:ASP:O	1:A:195:LYS:HG2	1.68	0.92
1:A:129:THR:OG1	1:A:423:THR:HG21	1.70	0.91
1:A:76:VAL:HA	1:A:79:LYS:HE3	1.52	0.91
1:B:293:LEU:HD22	1:B:293:LEU:O	1.70	0.91
1:B:332:GLU:OE2	1:B:332:GLU:HA	1.71	0.90
1:A:217:TYR:O	1:A:245:LEU:HD12	1.71	0.90
1:A:381:ALA:CB	1:A:387:LEU:CD1	2.39	0.90
1:A:448:LEU:HD23	1:A:466:VAL:HG11	1.54	0.90
1:A:125:LYS:HE2	1:A:423:THR:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:THR:CG2	1:B:316:GLY:HA3	2.02	0.88
1:A:226:SER:O	1:A:256:ALA:CB	2.21	0.88
1:A:183:LEU:H	1:A:183:LEU:HD12	1.38	0.88
1:B:418:LEU:HD22	1:B:448:LEU:HD23	1.56	0.87
1:A:294:THR:HG23	1:A:316:GLY:CA	2.04	0.87
1:A:381:ALA:CB	1:A:387:LEU:CD2	2.38	0.87
1:B:333:GLY:HA2	1:B:334:ALA:HB2	1.55	0.87
1:B:164:MET:HE1	1:B:405:VAL:HG21	1.55	0.86
1:B:331:VAL:O	1:B:331:VAL:CG2	2.23	0.86
1:B:410:VAL:CG1	1:B:416:THR:OG1	2.25	0.84
1:A:175:VAL:HG12	1:A:391:LYS:HG3	1.60	0.84
1:B:112:PRO:HB3	1:B:512:LEU:O	1.78	0.83
1:B:319:ARG:HB2	1:B:332:GLU:HG3	1.60	0.83
1:A:178:SER:HB2	1:A:378:LYS:HB3	1.61	0.81
1:A:475:LEU:O	1:A:485:LEU:HD11	1.81	0.81
1:B:271:SER:O	1:B:272:VAL:HG22	1.82	0.80
1:B:455:SER:HB3	1:B:457:LEU:HD12	1.61	0.80
1:B:237:LYS:HG3	1:B:312:LEU:HD11	1.63	0.80
1:B:410:VAL:HG11	1:B:416:THR:HG21	1.62	0.80
1:B:271:SER:O	1:B:272:VAL:CG2	2.30	0.80
1:A:80:THR:O	1:A:81:ASP:CB	2.29	0.80
1:A:76:VAL:HG13	1:A:79:LYS:CE	2.11	0.79
1:A:381:ALA:O	1:A:382:ALA:HB2	1.81	0.78
1:A:76:VAL:HG13	1:A:79:LYS:HZ1	1.45	0.78
1:B:333:GLY:HA3	1:B:334:ALA:HB3	1.65	0.78
1:B:294:THR:HG23	1:B:316:GLY:CA	2.08	0.77
1:A:382:ALA:CA	1:A:383:THR:OG1	2.30	0.77
1:B:331:VAL:O	1:B:332:GLU:CB	2.32	0.77
1:A:294:THR:HG22	1:A:296:GLY:H	1.50	0.76
1:B:331:VAL:O	1:B:331:VAL:HG23	1.84	0.76
1:A:396:ASP:O	1:A:400:ASN:HB2	1.86	0.75
1:A:381:ALA:O	1:A:382:ALA:CB	2.34	0.74
1:A:476:ASN:CB	1:A:479:THR:HB	2.17	0.74
1:B:418:LEU:CD2	1:B:448:LEU:HD23	2.16	0.74
1:A:227:THR:HG21	1:A:230:ASP:OD2	1.86	0.74
1:A:469:LEU:HD21	1:A:482:TYR:HB3	1.70	0.73
1:B:102:GLY:O	1:B:106:VAL:HG23	1.89	0.73
1:B:213:LEU:HD13	1:B:244:PRO:HB2	1.71	0.72
1:B:129:THR:O	1:B:132:LYS:HG2	1.89	0.72
1:A:451:ILE:HA	1:A:454:ASN:HD22	1.53	0.72
1:B:409:ILE:HG12	1:B:492:ASP:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:TYR:O	1:B:245:LEU:HD12	1.90	0.71
1:A:226:SER:C	1:A:256:ALA:HB2	2.15	0.71
1:A:447:PRO:HB2	3:A:550:HOH:O	1.89	0.71
1:A:383:THR:O	1:A:384:GLU:CB	2.39	0.70
1:A:231:LEU:HD13	1:A:235:LEU:HD21	1.73	0.70
1:A:294:THR:HG21	1:A:316:GLY:HA3	1.72	0.70
1:B:181:PHE:HA	1:B:380:GLY:HA3	1.73	0.69
1:B:101:GLU:HB3	1:B:439:ILE:HG12	1.73	0.69
1:A:234:LEU:O	1:A:238:VAL:HG23	1.92	0.69
1:A:383:THR:O	1:A:384:GLU:CG	2.41	0.68
1:A:212:VAL:O	1:A:213:LEU:HD23	1.93	0.68
1:A:394:ILE:O	1:A:398:VAL:HG23	1.94	0.67
1:B:410:VAL:HG13	1:B:416:THR:OG1	1.93	0.67
1:B:325:LYS:HZ3	1:B:325:LYS:HB3	1.58	0.67
1:B:64:PRO:O	1:B:68:ILE:HG22	1.95	0.66
1:B:389:GLU:HA	1:B:389:GLU:OE1	1.95	0.66
1:A:354:SER:O	1:A:360:ARG:NH2	2.29	0.66
1:B:358:TYR:O	1:B:361:GLU:HB2	1.96	0.66
1:B:407:GLU:OE1	1:B:495:LYS:HA	1.96	0.66
1:B:164:MET:HE2	1:B:169:ASN:OD1	1.95	0.65
1:B:288:GLN:OE1	1:B:288:GLN:HA	1.96	0.65
1:A:448:LEU:CD2	1:A:466:VAL:HG11	2.26	0.65
1:B:425:ASP:OD1	1:B:441:LYS:NZ	2.31	0.64
1:A:445:GLU:HG2	1:A:449:LYS:HE3	1.79	0.64
1:A:448:LEU:HD12	1:A:448:LEU:O	1.96	0.64
1:B:190:GLY:HA2	1:B:293:LEU:HD11	1.79	0.64
1:B:228:VAL:HG12	1:B:232:LEU:HG	1.78	0.64
1:B:458:GLU:HB3	1:B:461:VAL:HB	1.79	0.64
1:A:381:ALA:CB	1:A:387:LEU:CG	2.75	0.64
1:A:288:GLN:HE21	1:A:292:ILE:HD11	1.63	0.64
1:B:319:ARG:HB2	1:B:332:GLU:CG	2.27	0.64
1:A:212:VAL:C	1:A:213:LEU:HD23	2.22	0.64
1:A:383:THR:O	1:A:384:GLU:CD	2.41	0.64
1:A:159:LEU:HD11	1:A:185:LEU:HB2	1.79	0.63
1:A:216:PRO:HD2	1:A:318:ALA:O	1.98	0.63
1:B:72:LEU:O	1:B:76:VAL:HG23	1.98	0.63
1:B:128:GLU:HG3	1:B:129:THR:N	2.13	0.63
1:B:282:ARG:H	1:B:282:ARG:HD2	1.63	0.63
1:A:175:VAL:CG1	1:A:391:LYS:HG3	2.29	0.62
1:B:256:ALA:O	1:B:260:LEU:HG	1.98	0.62
1:A:119:ILE:HG23	1:A:440:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LYS:H	1:B:140:LYS:CD	2.08	0.62
1:B:132:LYS:HG3	1:B:133:GLY:N	2.15	0.62
1:B:228:VAL:HG23	1:B:255:GLU:OE1	2.00	0.62
1:A:115:LEU:O	1:A:119:ILE:HG13	1.99	0.62
1:B:164:MET:CE	1:B:405:VAL:HG21	2.28	0.62
1:A:208:ARG:O	1:A:210:GLU:HG3	1.99	0.62
1:A:381:ALA:HA	1:A:387:LEU:HD21	1.80	0.62
1:A:428:LYS:HB2	1:A:428:LYS:NZ	2.15	0.61
1:B:180:THR:HG22	1:B:181:PHE:H	1.65	0.61
1:B:482:TYR:HD1	1:B:482:TYR:H	1.46	0.61
1:A:226:SER:HA	1:A:253:GLU:O	2.00	0.61
1:A:475:LEU:HD13	1:A:482:TYR:CD1	2.36	0.61
1:A:511:PHE:H	1:A:511:PHE:HD2	1.49	0.61
1:B:325:LYS:HB3	1:B:325:LYS:NZ	2.16	0.61
1:A:191:MET:HE1	1:A:290:MET:CG	2.22	0.61
1:B:264:LYS:HA	1:B:269:PHE:O	2.00	0.61
1:A:342:GLY:O	1:A:345:ALA:HB3	2.01	0.61
1:A:390:ARG:O	1:A:394:ILE:HG13	2.01	0.61
1:B:125:LYS:HE2	1:B:423:THR:O	2.01	0.61
1:A:387:LEU:HG	3:A:548:HOH:O	2.01	0.60
1:B:239:ILE:HG12	1:B:269:PHE:CD1	2.36	0.60
1:A:119:ILE:O	1:A:123:VAL:HG23	2.01	0.60
1:A:117:ARG:HD2	1:A:433:GLU:OE2	2.01	0.60
1:B:213:LEU:HD11	1:B:271:SER:HA	1.83	0.60
1:A:428:LYS:NZ	1:A:430:GLU:HG2	2.15	0.60
1:B:271:SER:C	1:B:272:VAL:HG23	2.27	0.60
1:A:183:LEU:H	1:A:183:LEU:CD1	2.13	0.60
1:A:228:VAL:HG23	1:A:229:LYS:H	1.67	0.59
1:A:479:THR:HG22	1:A:481:VAL:HB	1.84	0.59
1:A:438:ASN:O	1:A:442:VAL:HG23	2.02	0.59
1:B:410:VAL:HG11	1:B:416:THR:CG2	2.31	0.59
1:B:202:PHE:HB3	1:B:272:VAL:HG13	1.83	0.59
1:A:451:ILE:HA	1:A:454:ASN:ND2	2.17	0.59
1:A:183:LEU:HD21	1:A:390:ARG:HH21	1.66	0.59
1:A:385:VAL:HG12	1:A:385:VAL:O	2.03	0.59
1:A:381:ALA:HB1	1:A:387:LEU:HD11	0.74	0.59
1:A:385:VAL:HA	3:A:551:HOH:O	2.03	0.59
1:B:204:THR:OG1	1:B:211:ALA:HA	2.03	0.59
1:B:312:LEU:HD12	1:B:312:LEU:N	2.12	0.59
1:B:271:SER:C	1:B:272:VAL:CG2	2.75	0.59
1:B:473:HIS:CD2	1:B:484:ASP:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD21	1:A:445:GLU:HG3	1.85	0.58
1:A:381:ALA:HB2	1:A:387:LEU:HD22	1.77	0.58
1:A:454:ASN:C	1:A:456:GLY:H	2.11	0.58
1:A:411:ALA:HB3	1:A:416:THR:HB	1.86	0.58
1:B:485:LEU:O	1:B:490:VAL:O	2.21	0.57
1:A:418:LEU:HD21	1:A:445:GLU:HA	1.86	0.57
1:B:331:VAL:O	1:B:331:VAL:HG22	2.03	0.57
1:B:405:VAL:HG12	1:B:405:VAL:O	2.04	0.57
1:A:383:THR:HA	3:A:548:HOH:O	2.02	0.57
1:B:125:LYS:O	1:B:128:GLU:HG2	2.05	0.57
1:A:119:ILE:HG23	1:A:440:VAL:HG23	1.85	0.57
1:B:159:LEU:HD11	1:B:185:LEU:HB2	1.86	0.57
1:A:287:LEU:HD23	1:A:290:MET:CE	2.35	0.56
1:A:183:LEU:HD11	1:A:390:ARG:HH21	1.69	0.56
1:B:226:SER:HB3	1:B:253:GLU:HB2	1.88	0.56
1:B:463:ALA:O	1:B:467:ARG:HB2	2.05	0.56
1:A:181:PHE:O	1:A:380:GLY:HA3	2.05	0.56
1:B:221:VAL:HG13	1:B:299:ILE:HG22	1.85	0.56
1:A:479:THR:HG22	1:A:481:VAL:CG2	2.35	0.56
1:A:237:LYS:NZ	1:A:311:ASP:OD1	2.39	0.56
1:B:180:THR:HG22	1:B:181:PHE:N	2.20	0.56
1:A:183:LEU:HD21	1:A:390:ARG:NH2	2.21	0.56
1:B:145:ALA:O	1:B:149:ILE:HG13	2.05	0.56
1:B:409:ILE:CG1	1:B:492:ASP:O	2.54	0.56
1:A:172:VAL:HG13	1:A:192:ARG:NE	2.21	0.55
1:A:144:ALA:HA	1:A:161:ALA:HB2	1.88	0.55
1:A:340:ILE:HG22	1:A:341:ALA:N	2.21	0.55
1:A:424:LEU:HD12	1:A:441:LYS:HB3	1.87	0.55
1:A:465:LYS:HB3	1:A:482:TYR:HE2	1.72	0.55
1:B:195:LYS:HD2	1:B:275:LYS:O	2.07	0.55
1:B:312:LEU:H	1:B:312:LEU:CD1	2.06	0.55
1:A:418:LEU:HD21	1:A:445:GLU:CG	2.37	0.55
1:A:287:LEU:HD23	1:A:290:MET:HE1	1.88	0.55
1:B:466:VAL:C	1:B:468:ASN:H	2.15	0.55
1:A:228:VAL:HG23	1:A:229:LYS:HE2	1.88	0.55
1:B:319:ARG:H	1:B:332:GLU:HB2	1.72	0.55
1:B:320:LYS:O	1:B:331:VAL:HG13	2.07	0.55
1:B:325:LYS:NZ	1:B:325:LYS:CB	2.70	0.55
1:A:200:GLY:O	1:A:203:VAL:HG23	2.07	0.55
1:A:125:LYS:HE2	1:A:423:THR:CG2	2.31	0.55
1:B:94:LEU:HD13	1:B:447:PRO:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HG3	1:A:284:LYS:N	2.21	0.54
1:B:167:VAL:HG12	1:B:167:VAL:O	2.08	0.54
1:B:301:GLU:HG2	1:B:306:THR:HA	1.89	0.54
1:A:80:THR:C	1:A:81:ASP:CG	2.73	0.54
1:A:188:THR:HB	1:B:282:ARG:HH22	1.73	0.54
1:A:226:SER:O	1:A:256:ALA:N	2.41	0.54
1:A:412:GLY:HA3	1:A:491:ALA:HA	1.89	0.54
1:B:425:ASP:C	1:B:427:LEU:H	2.15	0.54
1:B:205:ASP:OD1	1:B:208:ARG:HD3	2.08	0.54
1:B:359:ASP:OD1	1:B:359:ASP:N	2.33	0.54
1:A:445:GLU:O	1:A:449:LYS:HG2	2.07	0.54
1:B:421:ALA:HB3	1:B:422:PRO:HD3	1.90	0.54
1:B:145:ALA:O	1:B:148:ALA:HB3	2.09	0.53
1:A:80:THR:O	1:A:81:ASP:OD1	2.24	0.53
1:B:294:THR:O	1:B:334:ALA:HA	2.08	0.53
1:B:129:THR:HG23	1:B:132:LYS:HE2	1.91	0.53
1:B:164:MET:HE1	1:B:405:VAL:CG2	2.34	0.53
1:B:455:SER:CB	1:B:457:LEU:HD12	2.36	0.52
1:B:293:LEU:O	1:B:293:LEU:CD2	2.52	0.52
1:B:346:GLN:O	1:B:349:GLN:HB2	2.09	0.52
1:A:444:LEU:O	1:A:447:PRO:HD2	2.10	0.52
1:A:317:LYS:HE3	1:B:358:TYR:HB2	1.91	0.52
1:B:90:THR:O	1:B:94:LEU:HB2	2.09	0.52
1:B:123:VAL:HG13	1:B:501:LEU:HD13	1.91	0.52
1:A:237:LYS:CE	1:A:312:LEU:HG	2.40	0.52
1:B:265:ILE:C	1:B:267:GLY:N	2.65	0.52
1:A:101:GLU:O	1:A:105:ASN:ND2	2.41	0.51
1:A:487:ALA:C	1:A:489:GLY:N	2.67	0.51
1:B:482:TYR:CD1	1:B:482:TYR:N	2.78	0.51
1:A:306:THR:OG1	1:A:307:LEU:N	2.44	0.51
1:B:401:ALA:O	1:B:405:VAL:HG23	2.10	0.51
1:A:135:LYS:O	1:A:409:ILE:HG13	2.08	0.51
1:B:291:ALA:HB1	1:B:296:GLY:O	2.10	0.51
1:B:410:VAL:CG1	1:B:411:ALA:N	2.74	0.51
1:B:203:VAL:CG1	1:B:204:THR:N	2.73	0.51
1:A:92:THR:HG22	1:A:96:GLN:HE21	1.75	0.51
1:A:428:LYS:HB2	1:A:428:LYS:HZ2	1.76	0.51
1:A:487:ALA:O	1:A:489:GLY:N	2.44	0.51
1:B:498:ARG:HG3	1:B:499:SER:N	2.26	0.50
1:B:254:GLY:O	1:B:255:GLU:CB	2.44	0.50
1:A:90:THR:HG22	1:A:500:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:O	1:A:132:LYS:HG3	2.12	0.50
1:A:487:ALA:C	1:A:489:GLY:H	2.18	0.50
1:A:293:LEU:HD13	1:A:370:LEU:HD23	1.94	0.50
1:A:139:THR:OG1	1:A:141:GLU:HG2	2.10	0.50
1:B:264:LYS:HD2	1:B:264:LYS:C	2.37	0.50
1:A:203:VAL:O	1:A:264:LYS:NZ	2.41	0.50
1:A:410:VAL:HG13	1:A:494:VAL:HG22	1.94	0.50
1:A:124:GLU:O	1:A:125:LYS:C	2.53	0.50
1:A:122:ALA:O	1:A:126:VAL:HG23	2.12	0.49
1:A:410:VAL:HG13	1:A:494:VAL:CG2	2.42	0.49
1:A:231:LEU:HB3	1:A:235:LEU:HG	1.93	0.49
1:A:479:THR:HG22	1:A:481:VAL:HG23	1.93	0.49
1:B:290:MET:O	1:B:294:THR:HB	2.13	0.49
1:B:335:GLY:N	3:B:548:HOH:O	2.39	0.49
1:B:491:ALA:O	1:B:492:ASP:CG	2.55	0.49
1:A:93:VAL:HG21	1:A:450:GLN:HG2	1.94	0.49
1:A:178:SER:OG	1:A:179:ASN:N	2.42	0.49
1:A:77:ALA:C	1:A:79:LYS:H	2.21	0.49
1:A:507:ILE:O	1:A:508:ALA:C	2.55	0.49
1:B:67:LYS:O	1:B:71:GLU:HG3	2.12	0.49
1:B:88:THR:HB	3:B:549:HOH:O	2.13	0.49
1:A:64:PRO:O	1:A:68:ILE:CG1	2.45	0.49
1:A:382:ALA:H	1:A:383:THR:HA	1.77	0.49
1:A:421:ALA:HB3	1:A:422:PRO:HD3	1.95	0.49
1:B:310:ALA:HB1	1:B:314:LEU:HD12	1.95	0.49
1:B:418:LEU:CD1	1:B:445:GLU:HB3	2.25	0.49
1:A:358:TYR:C	1:A:360:ARG:N	2.70	0.49
1:B:219:LEU:HD13	1:B:234:LEU:HD21	1.94	0.49
1:B:226:SER:O	1:B:255:GLU:HB3	2.11	0.49
1:B:277:PRO:O	1:B:283:ARG:HG3	2.13	0.49
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.13	0.49
1:A:288:GLN:HE21	1:A:292:ILE:CD1	2.25	0.49
1:A:310:ALA:HB1	1:A:314:LEU:HD12	1.94	0.49
1:A:476:ASN:ND2	1:A:490:VAL:HG21	2.28	0.49
1:B:293:LEU:O	1:B:293:LEU:HD13	2.12	0.49
1:A:135:LYS:HD2	1:A:135:LYS:N	2.27	0.48
1:A:228:VAL:HG13	1:A:255:GLU:HB3	1.93	0.48
1:A:439:ILE:O	1:A:442:VAL:HB	2.13	0.48
1:A:93:VAL:HG22	1:A:446:ALA:HB1	1.95	0.48
1:A:123:VAL:HG13	1:A:501:LEU:HG	1.94	0.48
1:B:117:ARG:HH21	1:B:121:LYS:NZ	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:VAL:C	1:B:468:ASN:N	2.69	0.48
1:B:212:VAL:HG22	1:B:322:VAL:HG22	1.94	0.48
1:A:379:ALA:O	1:A:380:GLY:C	2.57	0.48
1:A:479:THR:HG22	1:A:481:VAL:CB	2.42	0.48
1:A:481:VAL:CB	1:A:483:GLU:HG2	2.36	0.48
1:A:205:ASP:C	1:A:205:ASP:OD1	2.56	0.48
1:B:169:ASN:CG	1:B:405:VAL:HG11	2.38	0.48
1:A:151:ALA:HB2	1:A:397:ALA:HB2	1.96	0.48
1:A:183:LEU:HD11	1:A:390:ARG:NH2	2.29	0.48
1:A:178:SER:CB	1:A:378:LYS:HB3	2.39	0.48
1:A:194:ASP:O	1:A:194:ASP:CG	2.57	0.48
1:A:160:ILE:O	1:A:164:MET:HG3	2.13	0.47
1:A:383:THR:O	1:A:384:GLU:HB2	2.15	0.47
1:A:156:ILE:O	1:A:157:GLY:C	2.57	0.47
1:A:184:GLN:O	1:A:377:ILE:HA	2.14	0.47
1:B:140:LYS:HD2	1:B:140:LYS:N	2.16	0.47
1:B:178:SER:HB2	1:B:378:LYS:HB3	1.97	0.47
1:A:479:THR:CG2	1:A:481:VAL:HB	2.45	0.47
1:A:454:ASN:C	1:A:456:GLY:N	2.70	0.47
1:B:370:LEU:HD23	1:B:370:LEU:HA	1.61	0.47
1:B:458:GLU:OE2	1:B:461:VAL:HG23	2.13	0.47
1:B:202:PHE:CB	1:B:272:VAL:HG13	2.44	0.47
1:B:237:LYS:HG3	1:B:312:LEU:CD1	2.40	0.47
1:A:458:GLU:O	1:A:459:PRO:C	2.58	0.46
1:B:132:LYS:CG	1:B:133:GLY:N	2.77	0.46
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.53	0.46
1:B:293:LEU:O	1:B:334:ALA:HB1	2.15	0.46
1:B:320:LYS:H	1:B:331:VAL:HG22	1.79	0.46
1:B:418:LEU:CD2	1:B:448:LEU:CD2	2.90	0.46
1:A:297:GLN:OE1	1:A:298:VAL:N	2.47	0.46
1:B:172:VAL:HB	1:B:374:VAL:HG22	1.97	0.46
1:B:465:LYS:O	1:B:465:LYS:HG2	2.14	0.46
1:A:299:ILE:O	1:A:299:ILE:HG22	2.16	0.46
1:A:421:ALA:C	1:A:423:THR:H	2.23	0.46
1:B:271:SER:O	1:B:272:VAL:HG23	2.08	0.46
1:A:89:THR:HG22	1:A:92:THR:H	1.81	0.46
1:A:176:GLU:O	1:A:378:LYS:HA	2.15	0.46
1:A:194:ASP:C	1:A:195:LYS:HG2	2.40	0.46
1:B:186:GLU:HG3	1:B:376:VAL:HB	1.97	0.46
1:B:239:ILE:HG12	1:B:269:PHE:HD1	1.79	0.46
1:A:382:ALA:N	1:A:383:THR:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:VAL:HG11	1:B:416:THR:CB	2.46	0.46
1:B:164:MET:O	1:B:168:GLY:CA	2.64	0.46
1:A:481:VAL:HG12	1:A:483:GLU:CB	2.43	0.46
1:B:265:ILE:C	1:B:267:GLY:H	2.23	0.46
1:B:249:ALA:O	1:B:250:GLU:C	2.59	0.46
1:B:294:THR:C	1:B:334:ALA:HA	2.41	0.46
1:A:166:LYS:HG3	1:A:187:LEU:HD11	1.97	0.45
1:A:383:THR:CA	3:A:548:HOH:O	2.62	0.45
1:A:384:GLU:N	3:A:548:HOH:O	2.32	0.45
1:A:473:HIS:CD2	1:A:484:ASP:CG	2.94	0.45
1:B:257:LEU:O	1:B:261:VAL:HG23	2.16	0.45
1:B:446:ALA:HB3	1:B:447:PRO:HD3	1.97	0.45
1:A:221:VAL:HG12	1:A:223:SER:H	1.80	0.45
1:B:310:ALA:CB	1:B:314:LEU:HD12	2.46	0.45
1:A:147:ALA:HB3	1:A:157:GLY:HA2	1.98	0.45
1:A:418:LEU:C	1:A:420:ALA:H	2.25	0.45
1:B:476:ASN:OD1	1:B:476:ASN:C	2.59	0.45
1:A:228:VAL:HG23	1:A:229:LYS:N	2.32	0.45
1:B:311:ASP:C	1:B:313:SER:N	2.74	0.45
1:A:63:ASP:O	1:A:67:LYS:HB2	2.17	0.45
1:A:100:ARG:HG2	1:A:101:GLU:N	2.32	0.45
1:A:213:LEU:HD13	1:A:244:PRO:HB2	1.98	0.45
1:B:465:LYS:O	1:B:465:LYS:CG	2.64	0.45
1:A:191:MET:HE2	1:A:191:MET:HB3	1.56	0.45
1:B:178:SER:HB2	1:B:378:LYS:HD2	1.99	0.45
1:A:430:GLU:N	1:A:434:ALA:HB2	2.32	0.45
1:B:149:ILE:HG21	1:B:489:GLY:O	2.17	0.45
1:A:166:LYS:CB	1:A:187:LEU:HD11	2.46	0.45
1:B:128:GLU:CG	1:B:129:THR:N	2.80	0.45
1:B:215:ASP:N	1:B:216:PRO:HD3	2.31	0.45
1:B:131:LEU:CD2	1:B:407:GLU:HB3	2.47	0.45
1:B:440:VAL:O	1:B:444:LEU:HG	2.17	0.45
1:B:462:VAL:O	1:B:466:VAL:HG23	2.17	0.45
1:B:193:PHE:CZ	1:B:328:THR:HB	2.52	0.44
1:A:332:GLU:O	1:A:332:GLU:CG	2.65	0.44
1:A:473:HIS:CD2	1:A:484:ASP:OD1	2.70	0.44
1:A:511:PHE:N	1:A:511:PHE:CD2	2.82	0.44
1:B:93:VAL:HG21	1:B:450:GLN:HG2	1.98	0.44
1:B:412:GLY:C	1:B:414:GLY:H	2.25	0.44
1:A:317:LYS:HG3	1:A:318:ALA:N	2.30	0.44
1:B:130:LEU:CD2	1:B:416:THR:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG13	1:A:142:GLN:HB3	2.00	0.44
1:A:184:GLN:HB2	1:A:378:LYS:HB2	1.98	0.44
1:A:203:VAL:HG13	1:A:210:GLU:O	2.17	0.44
1:B:198:ILE:HD12	1:B:273:ALA:CB	2.47	0.44
1:A:450:GLN:O	1:A:453:PHE:HB3	2.17	0.44
1:A:387:LEU:CD1	3:A:548:HOH:O	2.65	0.44
1:B:159:LEU:HD22	1:B:183:LEU:HD23	1.99	0.44
1:B:203:VAL:HG12	1:B:204:THR:N	2.33	0.44
1:B:212:VAL:C	1:B:213:LEU:HD23	2.42	0.44
1:A:175:VAL:O	1:A:391:LYS:HE3	2.18	0.43
1:A:188:THR:HB	1:B:282:ARG:NH2	2.31	0.43
1:A:418:LEU:C	1:A:420:ALA:N	2.73	0.43
1:B:404:ALA:O	1:B:408:GLY:HA2	2.17	0.43
1:A:332:GLU:O	1:A:333:GLY:C	2.61	0.43
1:A:435:THR:HA	1:A:438:ASN:HD22	1.83	0.43
1:A:479:THR:O	1:A:481:VAL:HG23	2.18	0.43
1:B:164:MET:O	1:B:168:GLY:N	2.52	0.43
1:A:172:VAL:HB	1:A:374:VAL:HG22	2.00	0.43
1:B:303:VAL:O	1:B:303:VAL:HG12	2.18	0.43
1:B:349:GLN:HA	1:B:349:GLN:OE1	2.18	0.43
1:A:475:LEU:HD12	1:A:476:ASN:H	1.83	0.43
1:B:380:GLY:O	1:B:381:ALA:HB2	2.19	0.43
1:B:129:THR:HA	1:B:132:LYS:HE2	2.00	0.43
1:A:446:ALA:O	1:A:449:LYS:HB2	2.19	0.43
1:B:139:THR:O	1:B:140:LYS:C	2.61	0.43
1:A:76:VAL:HG13	1:A:79:LYS:HZ2	1.72	0.42
1:A:237:LYS:HG2	1:A:312:LEU:HD11	1.99	0.42
1:A:167:VAL:O	1:A:167:VAL:HG13	2.18	0.42
1:A:448:LEU:HD12	1:A:448:LEU:C	2.44	0.42
1:A:458:GLU:HB3	1:A:461:VAL:HB	2.00	0.42
1:B:204:THR:C	1:B:206:PRO:HD3	2.44	0.42
1:A:166:LYS:HB3	1:A:187:LEU:HD11	2.00	0.42
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.74	0.42
1:A:226:SER:HB3	1:A:253:GLU:CG	2.49	0.42
1:A:457:LEU:O	1:A:459:PRO:HD3	2.19	0.42
1:A:476:ASN:OD1	1:A:477:ALA:N	2.53	0.42
1:B:166:LYS:HG3	1:B:187:LEU:HD11	2.02	0.42
1:B:228:VAL:HG22	1:B:255:GLU:O	2.20	0.42
1:B:474:GLY:O	1:B:485:LEU:HD21	2.19	0.42
1:B:262:VAL:C	1:B:264:LYS:N	2.78	0.42
1:B:311:ASP:HB3	1:B:313:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LYS:O	1:A:395:GLU:HG3	2.20	0.42
1:B:132:LYS:HG3	1:B:133:GLY:H	1.83	0.42
1:B:234:LEU:HD13	1:B:310:ALA:HB3	2.01	0.42
1:A:476:ASN:HD21	1:A:490:VAL:HG21	1.85	0.42
1:A:71:GLU:HA	1:A:71:GLU:OE1	2.18	0.42
1:A:237:LYS:CD	1:A:312:LEU:HG	2.49	0.42
1:A:320:LYS:HG2	1:A:321:VAL:N	2.35	0.42
1:A:384:GLU:C	1:A:386:GLU:N	2.77	0.42
1:A:423:THR:HG22	1:A:423:THR:O	2.20	0.42
1:A:435:THR:O	1:A:438:ASN:HB2	2.20	0.42
1:B:476:ASN:HB2	1:B:485:LEU:CD2	2.49	0.42
1:A:306:THR:HG23	1:A:308:GLU:O	2.19	0.42
1:A:348:ARG:O	1:A:352:GLU:HG2	2.20	0.42
1:B:481:VAL:O	1:B:483:GLU:HG2	2.20	0.42
1:A:137:VAL:HG13	1:A:142:GLN:CB	2.50	0.41
1:B:172:VAL:HG13	1:B:192:ARG:CZ	2.50	0.41
1:B:431:GLY:O	1:B:434:ALA:N	2.51	0.41
1:B:479:THR:HB	1:B:481:VAL:HG23	2.01	0.41
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.93	0.41
1:A:276:ALA:HA	1:A:277:PRO:HD3	1.69	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.87	0.41
1:B:115:LEU:HD11	1:B:435:THR:HB	2.02	0.41
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.87	0.41
1:B:293:LEU:HD22	1:B:293:LEU:C	2.30	0.41
1:B:418:LEU:HD23	1:B:448:LEU:CD2	2.50	0.41
1:B:425:ASP:C	1:B:427:LEU:N	2.78	0.41
1:B:469:LEU:HB3	1:B:470:PRO:HD2	2.02	0.41
1:A:210:GLU:HG2	1:A:324:THR:HG22	2.01	0.41
1:A:318:ALA:HB1	1:A:331:VAL:O	2.19	0.41
1:B:317:LYS:HB2	1:B:317:LYS:HE3	1.87	0.41
1:A:167:VAL:HG13	1:A:171:GLY:HA3	2.02	0.41
1:A:232:LEU:N	1:A:233:PRO:CD	2.83	0.41
1:B:65:TYR:CE2	1:B:103:LEU:HD13	2.54	0.41
1:B:72:LEU:HB3	1:B:511:PHE:HZ	1.85	0.41
1:A:225:VAL:O	1:A:252:VAL:HA	2.21	0.41
1:A:414:GLY:O	3:A:550:HOH:O	2.22	0.41
1:A:470:PRO:HG2	1:A:473:HIS:ND1	2.36	0.41
1:A:465:LYS:HB3	1:A:482:TYR:CE2	2.54	0.41
1:B:69:GLY:O	1:B:70:ALA:C	2.64	0.41
1:B:345:ALA:O	1:B:346:GLN:C	2.64	0.41
1:A:76:VAL:HG13	1:A:79:LYS:HE3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:HA	1:B:282:ARG:HH12	1.85	0.41
1:A:417:LEU:O	1:A:420:ALA:HB3	2.20	0.41
1:B:219:LEU:HD22	1:B:234:LEU:HD23	2.03	0.41
1:B:274:VAL:HG21	1:B:328:THR:OG1	2.21	0.41
1:A:428:LYS:HZ2	1:A:430:GLU:HG2	1.85	0.41
1:A:436:GLY:O	1:A:439:ILE:HB	2.20	0.41
1:A:194:ASP:O	1:A:194:ASP:OD1	2.39	0.40
1:A:326:ASP:C	1:A:327:GLU:HG3	2.46	0.40
1:A:384:GLU:C	1:A:386:GLU:H	2.28	0.40
1:A:412:GLY:CA	1:A:491:ALA:HA	2.51	0.40
1:A:362:LYS:O	1:A:365:GLU:HG2	2.22	0.40
1:A:462:VAL:HA	1:A:482:TYR:OH	2.20	0.40
1:A:475:LEU:HD11	1:A:480:GLY:C	2.47	0.40
1:A:162:GLU:O	1:A:165:ASP:N	2.49	0.40
1:A:347:ILE:HG21	1:A:367:LEU:HB2	2.03	0.40
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.79	0.40
1:B:299:ILE:HG22	1:B:299:ILE:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:TYR:OH	1:B:333:GLY:O[1_655]	1.66	0.54

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	444/546 (81%)	375 (84%)	62 (14%)	7 (2%)	7	27
1	B	443/546 (81%)	384 (87%)	55 (12%)	4 (1%)	14	41
All	All	887/1092 (81%)	759 (86%)	117 (13%)	11 (1%)	10	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	ALA
1	B	332	GLU
1	B	334	ALA
1	A	384	GLU
1	B	255	GLU
1	A	488	ALA
1	B	271	SER
1	A	359	ASP
1	A	112	PRO
1	A	422	PRO
1	A	459	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/419 (83%)	313 (90%)	33 (10%)	8	26
1	B	345/419 (82%)	291 (84%)	54 (16%)	2	9
All	All	691/838 (82%)	604 (87%)	87 (13%)	4	15

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	90	THR
1	A	100	ARG
1	A	127	THR
1	A	139	THR
1	A	141	GLU
1	A	166	LYS
1	A	167	VAL
1	A	169	ASN
1	A	170	GLU
1	A	179	ASN
1	A	183	LEU

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Mol	Chain	Res	Type
1	A	188	THR
1	A	227	THR
1	A	231	LEU
1	A	270	LYS
1	A	290	MET
1	A	294	THR
1	A	306	THR
1	A	317	LYS
1	A	320	LYS
1	A	329	THR
1	A	384	GLU
1	A	405	VAL
1	A	409	ILE
1	A	428	LYS
1	A	430	GLU
1	A	435	THR
1	A	445	GLU
1	A	448	LEU
1	A	466	VAL
1	A	483	GLU
1	A	514	THR
1	B	61	LEU
1	B	62	GLU
1	B	68	ILE
1	B	88	THR
1	B	93	VAL
1	B	115	LEU
1	B	126	VAL
1	B	129	THR
1	B	139	THR
1	B	140	LYS
1	B	149	ILE
1	B	164	MET
1	B	183	LEU
1	B	189	GLU
1	B	213	LEU
1	B	218	ILE
1	B	221	VAL
1	B	226	SER
1	B	231	LEU
1	B	247	ILE
1	B	255	GLU

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Mol	Chain	Res	Type
1	B	270	LYS
1	B	282	ARG
1	B	292	ILE
1	B	293	LEU
1	B	294	THR
1	B	306	THR
1	B	312	LEU
1	B	323	VAL
1	B	325	LYS
1	B	327	GLU
1	B	331	VAL
1	B	343	ARG
1	B	359	ASP
1	B	365	GLU
1	B	370	LEU
1	B	383	THR
1	B	384	GLU
1	B	393	ARG
1	B	399	ARG
1	B	409	ILE
1	B	410	VAL
1	B	423	THR
1	B	427	LEU
1	B	429	LEU
1	B	433	GLU
1	B	440	VAL
1	B	455	SER
1	B	458	GLU
1	B	486	LEU
1	B	498	ARG
1	B	501	LEU
1	B	510	LEU
1	B	511	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	111	ASN
1	A	169	ASN
1	A	288	GLN
1	A	392	HIS

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Mol	Chain	Res	Type
1	A	438	ASN
1	A	454	ASN
1	B	96	GLN
1	B	105	ASN
1	B	184	GLN
1	B	419	GLN
1	B	468	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

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, 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	448/546 (82%)	-0.14	3 (0%) 84 77	44, 83, 152, 167	0
1	B	447/546 (81%)	-0.34	2 (0%) 88 84	50, 74, 106, 122	0
All	All	895/1092 (81%)	-0.24	5 (0%) 85 80	44, 77, 137, 167	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	VAL	3.0
1	B	333	GLY	2.5
1	A	482	TYR	2.2
1	A	489	GLY	2.2
1	B	334	ALA	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 oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
2	MG	A	547	1/1	0.91	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.