



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 10:04 PM EDT

PDB ID : 3RTK
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

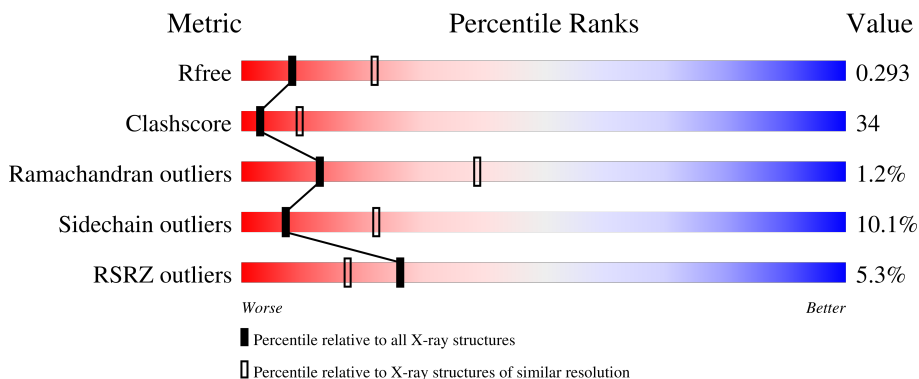
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	
1	B	546	

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	3315	2076	567	668	4	0	0	0
1	B	447	3305	2071	566	664	4	0	0	0

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 (three-letter code: 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 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.3 (19.98-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.79Å)	Xtriage
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	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.45	0/3340	0.72	5/4514 (0.1%)
1	B	0.47	0/3330	0.70	5/4501 (0.1%)
All	All	0.46	0/6670	0.71	10/9015 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	SER	CB-CA-C	8.64	126.52	110.10
1	B	491	ALA	N-CA-CB	8.13	121.48	110.10
1	B	406	GLU	CB-CA-C	-7.67	95.05	110.40
1	B	490	VAL	N-CA-C	-6.92	92.30	111.00
1	B	492	ASP	CB-CA-C	6.91	124.22	110.40
1	A	153	ASP	CB-CA-C	6.88	124.16	110.40
1	A	138	GLU	CB-CA-C	6.19	122.78	110.40
1	B	382	ALA	CB-CA-C	-6.07	100.99	110.10
1	A	178	SER	CB-CA-C	-5.36	99.91	110.10
1	A	81	ASP	CB-CG-OD2	5.23	123.01	118.30

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	256	1
1	B	3305	0	3427	205	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	457	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 34.

All (457) 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
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: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:80:THR:O	1:A:81:ASP:CG	1.88	1.11
1:A:481:VAL:HG12	1:A:483:GLU:HG2	1.28	1.11
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:333:GLY:CA	1:B:334:ALA:CB	2.30	0.92
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:MET:HE1	1:A:290:MET:HG3	1.69	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
1:B:217:TYR:O	1:B:245:LEU:HD12	1.90	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:164:MET:HE2	1:B:405:VAL:HG21	1.76	0.67
1:A:226:SER:C	1:A:256:ALA:HB2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:164:MET:CE	1:B:405:VAL:HG21	2.28	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
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: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:NZ	1:B:325:LYS:HB3	2.16	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:191:MET:CE	1:A:290:MET:HG3	2.30	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:212:VAL:C	1:A:213:LEU:HD23	2.22	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:383:THR:O	1:A:384:GLU:CD	2.41	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:473:HIS:CD2	1:B:484:ASP:HA	2.38	0.58
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: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:B:271:SER:C	1:B:272:VAL:HG23	2.27	0.55
1:A:287:LEU:HD23	1:A:290:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:B:271:SER:C	1:B:272:VAL:CG2	2.75	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:A:454:ASN:C	1:A:456:GLY:H	2.11	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:325:LYS:HB3	1:B:325:LYS:HZ3	1.73	0.53
1:B:129:THR:HG23	1:B:132:LYS:HE2	1.91	0.53
1:B:455:SER:CB	1:B:457:LEU:HD12	2.36	0.52
1:A:178:SER:OG	1:A:179:ASN:N	2.42	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:B:271:SER:O	1:B:272:VAL:HG23	2.08	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:A:101:GLU:O	1:A:105:ASN:ND2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ALA:O	1:B:405:VAL:HG23	2.10	0.51
1:B:164:MET:HE3	1:B:169:ASN:HA	1.93	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:B:466:VAL:C	1:B:468:ASN:H	2.15	0.50
1:A:90:THR:HG22	1:A:500:ALA:HB1	1.92	0.50
1:A:128:GLU:O	1:A:132:LYS:HG3	2.12	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:A:410:VAL:HG13	1:A:494:VAL:HG22	1.94	0.50
1:B:425:ASP:C	1:B:427:LEU:H	2.15	0.49
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:A:93:VAL:HG21	1:A:450:GLN:HG2	1.94	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:265:ILE:C	1:B:267:GLY:N	2.65	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: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:191:MET:HE1	1:A:290:MET:CG	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:212:VAL:HG22	1:B:322:VAL:HG22	1.94	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: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: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: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: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:A:487:ALA:C	1:A:489:GLY:N	2.67	0.47
1:B:202:PHE:CB	1:B:272:VAL:HG13	2.44	0.47
1:B:465:LYS:O	1:B:465:LYS:HG2	2.14	0.47
1:B:237:LYS:HG3	1:B:312:LEU:CD1	2.40	0.47
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:A:299:ILE:O	1:A:299:ILE:HG22	2.16	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: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
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:124:GLU:O	1:A:125:LYS:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:VAL:HG12	1:A:483:GLU:CB	2.43	0.46
1:A:487:ALA:C	1:A:489:GLY:H	2.18	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: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:B:264:LYS:HD2	1:B:264:LYS:C	2.37	0.45
1:A:228:VAL:HG23	1:A:229:LYS:N	2.32	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: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:A:77:ALA:C	1:A:79:LYS:H	2.21	0.44
1:A:203:VAL:O	1:A:264:LYS:NZ	2.41	0.44
1:B:193:PHE:CZ	1:B:328:THR:HB	2.52	0.44
1:B:491:ALA:O	1:B:492:ASP:CG	2.55	0.44
1:A:332:GLU:CG	1:A:332:GLU:O	2.65	0.44
1:A:473:HIS:CD2	1:A:484:ASP:OD1	2.70	0.44
1:A:507:ILE:O	1:A:508:ALA:C	2.55	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:A:191:MET:HB3	1:A:191:MET:HE3	1.40	0.44
1:A:317:LYS:HG3	1:A:318:ALA:N	2.30	0.44
1:A:358:TYR:C	1:A:360:ARG:N	2.70	0.44
1:B:130:LEU:CD2	1:B:416:THR:HG22	2.47	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:454:ASN:C	1:A:456:GLY:N	2.70	0.44
1:B:303:VAL:HG12	1:B:303:VAL:O	2.18	0.44
1:A:387:LEU:CD1	3:A:548:HOH:O	2.65	0.44
1:B:325:LYS:CB	1:B:325:LYS:HZ2	2.30	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:466:VAL:C	1:B:468:ASN:N	2.69	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:B:404:ALA:O	1:B:408:GLY:HA2	2.17	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:A:205:ASP:C	1:A:205:ASP:OD1	2.56	0.43
1:A:379:ALA:O	1:A:380:GLY:C	2.57	0.43
1:B:169:ASN:CG	1:B:405:VAL:HG11	2.38	0.43
1:B:349:GLN:HA	1:B:349:GLN:OE1	2.18	0.43
1:B:117:ARG:HH21	1:B:121:LYS:HZ2	1.67	0.43
1:A:194:ASP:O	1:A:194:ASP:CG	2.57	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:A:76:VAL:HG13	1:A:79:LYS:HZ2	1.72	0.42
1:A:156:ILE:O	1:A:157:GLY:C	2.57	0.42
1:A:237:LYS:HG2	1:A:312:LEU:HD11	1.99	0.42
1:B:265:ILE:C	1:B:267:GLY:H	2.23	0.42
1:A:167:VAL:O	1:A:167:VAL:HG13	2.18	0.42
1:A:458:GLU:HB3	1:A:461:VAL:HB	2.00	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: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:287:LEU:HA	1:A:290:MET:HE2	2.02	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: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:A:458:GLU:O	1:A:459:PRO:C	2.58	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:A:421:ALA:C	1:A:423:THR:H	2.23	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:418:LEU:HD23	1:B:448:LEU:CD2	2.50	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:B:476:ASN:OD1	1:B:476:ASN:C	2.59	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:249:ALA:O	1:B:250:GLU:C	2.59	0.41
1:B:294:THR:C	1:B:334:ALA:HA	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG13	1:A:79:LYS:HE3	1.99	0.41
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:473:HIS:CD2	1:A:484:ASP:CG	2.94	0.41
1:B:311:ASP:C	1:B:313:SER:N	2.74	0.40
1:A:194:ASP:O	1:A:194:ASP:OD1	2.39	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: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:A:418:LEU:C	1:A:420:ALA:H	2.25	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%)	9 31
1	B	443/546 (81%)	384 (87%)	55 (12%)	4 (1%)	17 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	887/1092 (81%)	759 (86%)	117 (13%)	11 (1%)	13 39

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%)	315 (91%)	31 (9%)	9 28
1	B	345/419 (82%)	306 (89%)	39 (11%)	6 18
All	All	691/838 (82%)	621 (90%)	70 (10%)	7 22

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	100	ARG
1	A	127	THR
1	A	135	LYS
1	A	139	THR
1	A	141	GLU
1	A	166	LYS

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Mol	Chain	Res	Type
1	A	167	VAL
1	A	169	ASN
1	A	170	GLU
1	A	179	ASN
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	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	74	LYS
1	B	88	THR
1	B	104	ARG
1	B	115	LEU
1	B	140	LYS
1	B	149	ILE
1	B	189	GLU
1	B	197	TYR
1	B	226	SER
1	B	247	ILE
1	B	255	GLU
1	B	264	LYS
1	B	282	ARG
1	B	293	LEU
1	B	294	THR

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Mol	Chain	Res	Type
1	B	306	THR
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	423	THR
1	B	429	LEU
1	B	433	GLU
1	B	455	SER
1	B	458	GLU
1	B	486	LEU
1	B	498	ARG
1	B	501	LEU
1	B	511	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	438	ASN
1	A	454	ASN
1	B	96	GLN
1	B	184	GLN
1	B	419	GLN
1	B	473	HIS

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 monosaccharides 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 [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	448/546 (82%)	0.20	34 (7%) 13 7	44, 83, 152, 167	0
1	B	447/546 (81%)	-0.04	13 (2%) 51 41	50, 74, 106, 122	0
All	All	895/1092 (81%)	0.08	47 (5%) 26 17	44, 77, 137, 167	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	5.4
1	A	309	ASN	5.1
1	A	382	ALA	4.1
1	A	381	ALA	3.8
1	A	61	LEU	3.7
1	A	455	SER	3.7
1	A	456	GLY	3.6
1	A	302	GLU	3.5
1	A	474	GLY	3.5
1	A	489	GLY	3.1
1	A	304	GLY	3.0
1	A	303	VAL	2.9
1	A	471	ALA	2.9
1	A	453	PHE	2.9
1	B	80	THR	2.8
1	B	88	THR	2.8
1	A	414	GLY	2.8
1	A	514	THR	2.8
1	B	179	ASN	2.7
1	A	181	PHE	2.7
1	A	79	LYS	2.7
1	A	487	ALA	2.6
1	B	266	ARG	2.6
1	A	80	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	482	TYR	2.5
1	B	303	VAL	2.4
1	A	78	LYS	2.4
1	B	302	GLU	2.4
1	A	478	GLN	2.4
1	B	229	LYS	2.4
1	A	393	ARG	2.3
1	B	194	ASP	2.3
1	A	460	GLY	2.3
1	A	413	GLY	2.2
1	B	426	GLU	2.2
1	A	458	GLU	2.2
1	B	381	ALA	2.2
1	A	479	THR	2.2
1	A	475	LEU	2.1
1	A	430	GLU	2.1
1	B	219	LEU	2.1
1	B	333	GLY	2.1
1	A	491	ALA	2.1
1	A	480	GLY	2.0
1	A	247	ILE	2.0
1	B	89	THR	2.0
1	A	306	THR	2.0

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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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2	MG	A	547	1/1	0.91	0.10	30,30,30,30	0
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6.5 Other polymers [i](#)

There are no such residues in this entry.