



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:54 PM GMT

PDB ID : 1WZM
Title : Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) mutatnt R469K
Authors : Mizuno, M.; Ichikawa, K.; Tonozyuka, T.; Ohtaki, A.; Shimura, Y.; Kamitori, S.; Nishikawa, A.; Sakano, Y.
Deposited on : 2005-03-06
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

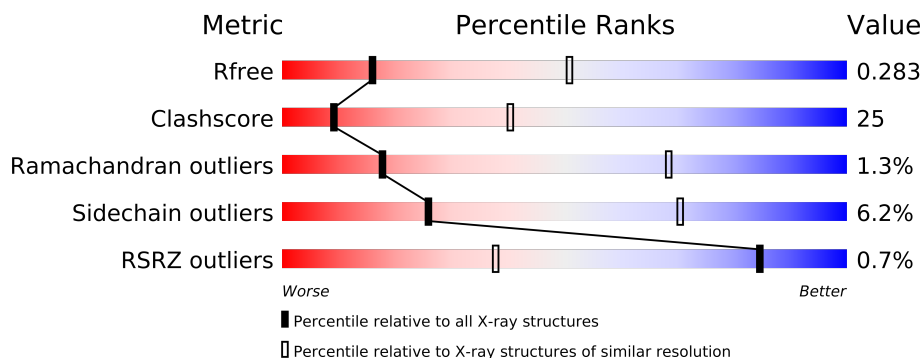
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9550 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alpha-amylase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4774	3056	829	874	15			
1	B	585	Total	C	N	O	S	0	0	0
			4774	3056	829	874	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	LYS	ARG	ENGINEERED	UNP Q08751
B	469	LYS	ARG	ENGINEERED	UNP Q08751

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

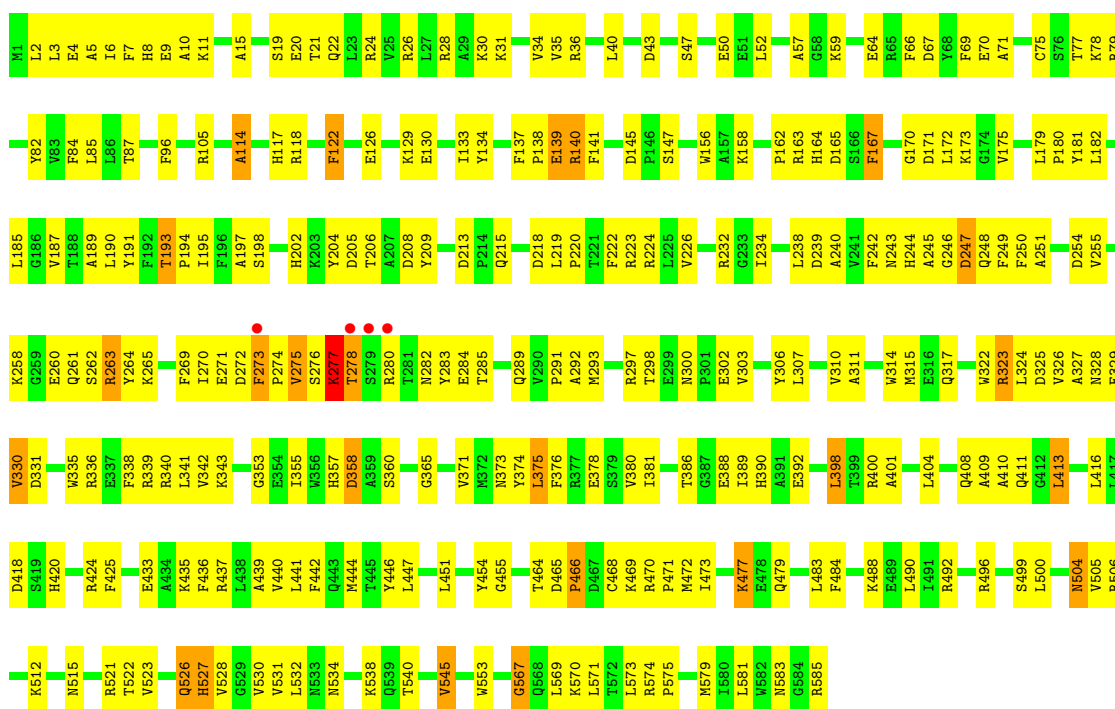
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

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.

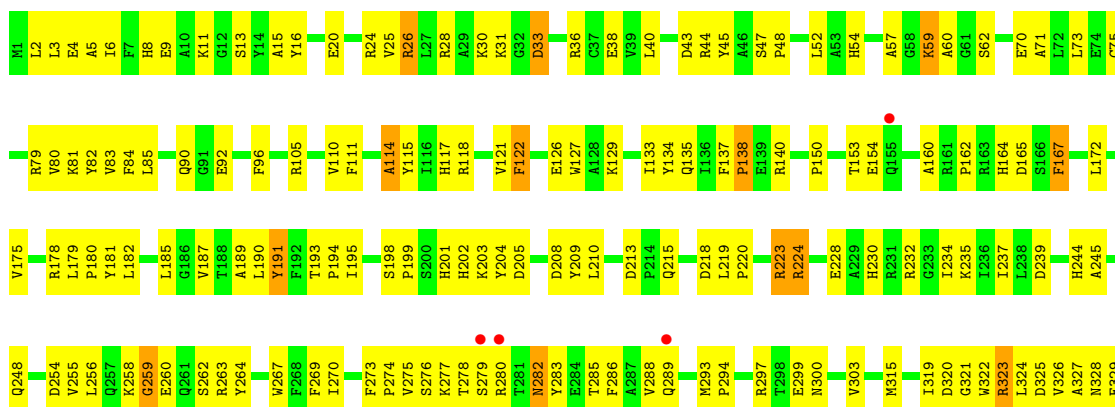
• Molecule 1: Alpha-amylase II

Chain A: 



• Molecule 1: Alpha-amylase II

Chain B: 



Y330	F425	D511
R336	L426	K512
E337	T427	Q513
F338	S428	A514
R339		
R340	G431	V520
L341	M432	R521
V342	E433	T522
K343	A434	V523
	K435	
A349	V440	Q526
L350	L441	R527
T351	F442	V528
V352	Q443	G529
E353	M444	
E354	L447	N533
T355		N534
M356	L451	R535
H357		
D358	Y454	Q539
D369		L542
	G459	L543
Y374	M460	Q544
L375	D465	V545
F376	P466	P546
	K469	E547
I381	R470	S548
R382	P471	
F383	M472	V553
	I473	C556
T386	W474	
E388	E475	K565
	E476	Q566
A391	K477	Q567
E392	E478	Q568
		L569
D395	L483	K570
		L571
L398	F486	R574
T399	Y487	R575
R400	K488	V576
A401	E489	Q577
	L490	G578
L404	I491	N579
E407	R492	T580
Q408	L493	L581
A409	R494	N582
A410	H495	N583
Q411	R496	G584
G412		R585
L413	S499	
V414	L500	
M415		
L416	N504	
L417	V505	
D418		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.66Å 115.90Å 112.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.53 – 3.20 51.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (51.53-3.20) 97.8 (51.53-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.80 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.293 0.209 , 0.283	Depositor DCC
R_{free} test set	2366 reflections (9.87%)	DCC
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 17.2	EDS
Estimated twinning fraction	0.024 for -h,l,k 0.025 for -k,-h,l 0.024 for l,-k,h 0.011 for l,h,k 0.011 for k,l,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23971 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9550	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/4904	0.66	0/6638
1	B	0.48	0/4904	0.64	0/6638
All	All	0.49	0/9808	0.65	0/13276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4607	248	0
1	B	4774	0	4607	229	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9550	0	9214	469	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (469) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.30	1.07
1:B:477:LYS:H	1:B:477:LYS:HD2	1.21	1.02
1:A:300:ASN:HD21	1:A:302:GLU:HB2	1.32	0.93
1:B:386:THR:OG1	1:B:388:GLU:HG3	1.68	0.93
1:A:300:ASN:HD22	1:A:303:VAL:HG23	1.33	0.93
1:B:410:ALA:HA	1:B:413:LEU:HD22	1.52	0.91
1:B:3:LEU:HA	1:B:6:ILE:HD12	1.56	0.84
1:A:330:VAL:HG22	1:A:335:TRP:NE1	1.93	0.84
1:B:542:LEU:HD11	1:B:568:GLN:NE2	1.92	0.83
1:B:409:ALA:O	1:B:413:LEU:HD13	1.78	0.82
1:A:540:THR:HG21	1:A:570:LYS:HE3	1.61	0.82
1:A:477:LYS:HD2	1:A:477:LYS:H	1.45	0.81
1:A:492:ARG:HD2	1:A:496:ARG:NH1	1.97	0.80
1:B:328:ASN:HB3	1:B:355:ILE:HD12	1.64	0.80
1:A:36:ARG:HB3	1:A:87:THR:HB	1.64	0.79
1:B:82:TYR:O	1:B:110:VAL:HG23	1.83	0.78
1:B:274:PRO:HD2	1:B:280:ARG:HH12	1.47	0.78
1:A:477:LYS:CD	1:A:477:LYS:H	1.94	0.77
1:B:542:LEU:HD11	1:B:568:GLN:HE22	1.49	0.76
1:A:338:PHE:O	1:A:342:VAL:HG23	1.86	0.76
1:A:374:TYR:CE1	1:A:375:LEU:HD13	2.21	0.75
1:A:416:LEU:HD23	1:A:416:LEU:H	1.51	0.74
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.70	0.72
1:B:288:VAL:HG12	1:B:289:GLN:HG2	1.71	0.72
1:A:141:PHE:HZ	1:A:182:LEU:HD21	1.52	0.72
1:B:392:GLU:HG3	1:B:512:LYS:HB3	1.71	0.72
1:A:381:ILE:HD13	1:A:425:PHE:HE1	1.53	0.71
1:A:328:ASN:CB	1:A:355:ILE:HD12	2.16	0.71
1:B:426:LEU:HD22	1:B:431:GLY:HA2	1.71	0.71
1:A:271:GLU:HG3	1:A:272:ASP:H	1.56	0.70
1:B:256:LEU:O	1:B:256:LEU:HD23	1.92	0.70
1:A:311:ALA:O	1:A:315:MET:HG2	1.91	0.70
1:B:62:SER:H	1:B:399:THR:HG21	1.56	0.70
1:A:141:PHE:CZ	1:A:182:LEU:HD21	2.26	0.69
1:A:444:MET:HG2	1:A:490:LEU:HB3	1.74	0.69
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.26	0.69
1:B:245:ALA:O	1:B:294:PRO:HD2	1.89	0.69
1:A:484:PHE:O	1:A:488:LYS:HG3	1.93	0.69
1:B:52:LEU:HD11	1:B:105:ARG:HH21	1.58	0.69
1:A:392:GLU:HG3	1:A:512:LYS:HB3	1.74	0.68
1:B:354:GLU:O	1:B:355:ILE:HD13	1.94	0.67
1:A:314:TRP:HA	1:A:317:GLN:HG2	1.76	0.67
1:A:8:HIS:HD2	1:A:26:ARG:O	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:LEU:HD21	1:A:528:VAL:HG11	1.76	0.66
1:B:569:LEU:HG	1:B:571:LEU:CD1	2.26	0.66
1:B:583:ASN:ND2	1:B:585:ARG:HB2	2.11	0.66
1:B:477:LYS:N	1:B:477:LYS:HD2	2.03	0.66
1:B:73:LEU:HD23	1:B:80:VAL:HG21	1.77	0.66
1:A:420:HIS:HB2	1:A:469:LYS:HE2	1.77	0.66
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.31	0.66
1:B:237:ILE:HD12	1:B:321:GLY:HA3	1.78	0.65
1:A:260:GLU:HB2	1:A:265:LYS:NZ	2.11	0.65
1:A:300:ASN:ND2	1:A:302:GLU:HB2	2.08	0.65
1:A:224:ARG:HE	1:A:224:ARG:HA	1.61	0.65
1:B:255:VAL:HA	1:B:262:SER:OG	1.96	0.65
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.77	0.65
1:A:400:ARG:O	1:A:404:LEU:HD13	1.96	0.65
1:A:133:ILE:HD13	1:A:189:ALA:HB3	1.77	0.65
1:B:160:ALA:O	1:B:162:PRO:HD3	1.97	0.65
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.32	0.64
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.79	0.64
1:A:275:VAL:HG12	1:A:282:ASN:HD21	1.63	0.64
1:B:392:GLU:CG	1:B:512:LYS:HB3	2.28	0.63
1:A:275:VAL:HA	1:A:282:ASN:HD21	1.62	0.63
1:B:583:ASN:HD21	1:B:585:ARG:HB2	1.62	0.63
1:A:260:GLU:HA	1:A:265:LYS:HE2	1.81	0.62
1:A:275:VAL:CG1	1:A:282:ASN:HD21	2.12	0.62
1:B:504:ASN:HD22	1:B:504:ASN:C	2.04	0.62
1:B:386:THR:HG1	1:B:388:GLU:HG3	1.65	0.61
1:B:543:LEU:HD12	1:B:571:LEU:HD13	1.82	0.61
1:A:273:PHE:CD1	1:A:274:PRO:HA	2.35	0.61
1:B:90:GLN:HB2	1:B:92:GLU:OE1	2.00	0.61
1:B:328:ASN:CB	1:B:355:ILE:HD12	2.30	0.61
1:A:441:LEU:O	1:A:441:LEU:HD23	2.00	0.61
1:A:162:PRO:HG2	1:A:470:ARG:HA	1.82	0.61
1:A:254:ASP:OD2	1:A:262:SER:HB2	2.00	0.61
1:A:401:ALA:O	1:A:404:LEU:HB2	2.01	0.61
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.83	0.60
1:B:417:LEU:HD11	1:B:443:GLN:NE2	2.16	0.60
1:B:213:ASP:OD1	1:B:215:GLN:HG2	2.02	0.60
1:B:60:ALA:HB2	1:B:70:GLU:HB2	1.82	0.60
1:B:319:ILE:HD11	1:B:322:TRP:CZ2	2.36	0.60
1:A:416:LEU:H	1:A:416:LEU:CD2	2.15	0.60
1:A:276:SER:O	1:A:277:LYS:HB2	2.02	0.60
1:A:8:HIS:HE1	1:A:82:TYR:OH	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:VAL:HG13	1:A:523:VAL:O	2.01	0.60
1:B:133:ILE:HB	1:B:451:LEU:HD12	1.83	0.60
1:B:179:LEU:HA	1:B:182:LEU:HD23	1.83	0.60
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.84	0.59
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.37	0.59
1:B:488:LYS:HB3	1:B:492:ARG:HH12	1.67	0.59
1:A:401:ALA:HA	1:A:404:LEU:HD22	1.83	0.59
1:A:328:ASN:O	1:B:114:ALA:HB1	2.02	0.59
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.02	0.59
1:B:110:VAL:HG22	1:B:111:PHE:O	2.03	0.59
1:B:338:PHE:O	1:B:342:VAL:HG23	2.02	0.59
1:B:545:VAL:HG21	1:B:569:LEU:HB2	1.83	0.59
1:B:244:HIS:CE1	1:B:293:MET:HG2	2.38	0.59
1:B:276:SER:HA	1:B:282:ASN:ND2	2.17	0.59
1:B:36:ARG:NH2	1:B:38:GLU:OE2	2.36	0.58
1:A:247:ASP:HB3	1:A:292:ALA:HA	1.85	0.58
1:A:224:ARG:NE	1:A:224:ARG:HA	2.19	0.58
1:B:285:THR:HB	1:B:293:MET:O	2.03	0.58
1:B:276:SER:OG	1:B:277:LYS:N	2.35	0.58
1:B:277:LYS:HG2	1:B:278:THR:N	2.17	0.58
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.17	0.58
1:A:336:ARG:NE	1:B:336:ARG:CZ	2.67	0.58
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.38	0.58
1:B:327:ALA:O	1:B:330:VAL:HG13	2.04	0.58
1:A:473:ILE:HG22	1:A:479:GLN:HG2	1.85	0.58
1:B:533:ASN:ND2	1:B:574:ARG:O	2.35	0.58
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.86	0.57
1:A:164:HIS:CD2	1:A:466:PRO:HD3	2.39	0.57
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.86	0.57
1:A:277:LYS:HE2	1:A:277:LYS:HA	1.87	0.57
1:A:300:ASN:ND2	1:A:303:VAL:H	2.01	0.57
1:B:133:ILE:HB	1:B:451:LEU:CD1	2.34	0.57
1:A:573:LEU:HD11	1:A:579:MET:HG3	1.87	0.57
1:B:504:ASN:HD21	1:B:522:THR:HB	1.68	0.57
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.52	0.57
1:B:526:GLN:HG3	1:B:585:ARG:OXT	2.04	0.57
1:B:278:THR:O	1:B:279:SER:HB2	2.04	0.57
1:B:357:HIS:O	1:B:358:ASP:C	2.43	0.57
1:A:540:THR:HA	1:A:571:LEU:O	2.04	0.56
1:A:269:PHE:HB2	1:A:284:GLU:HB3	1.87	0.56
1:A:206:THR:HG21	1:A:209:TYR:CE2	2.40	0.56
1:A:277:LYS:HE2	1:A:278:THR:H	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:38:GLU:OE1	1:B:54:HIS:HD2	1.89	0.56
1:A:477:LYS:HD2	1:A:477:LYS:N	2.18	0.56
1:A:114:ALA:HB1	1:B:328:ASN:O	2.05	0.56
1:A:532:LEU:HD12	1:A:532:LEU:N	2.21	0.56
1:A:376:PHE:O	1:A:380:VAL:HG23	2.06	0.56
1:B:274:PRO:HG2	1:B:280:ARG:NH2	2.20	0.56
1:A:8:HIS:CE1	1:A:82:TYR:OH	2.59	0.56
1:A:398:LEU:HD21	1:A:442:PHE:CZ	2.40	0.56
1:A:8:HIS:CD2	1:A:26:ARG:O	2.59	0.56
1:B:416:LEU:H	1:B:416:LEU:HD23	1.71	0.56
1:A:515:ASN:ND2	1:A:534:ASN:O	2.33	0.56
1:A:2:LEU:O	1:A:6:ILE:HD12	2.06	0.56
1:B:434:ALA:HB1	1:B:576:TYR:HD1	1.70	0.56
1:B:2:LEU:HD21	1:B:4:GLU:HB2	1.89	0.55
1:A:326:VAL:O	1:A:326:VAL:HG12	2.06	0.55
1:A:499:SER:HB3	1:A:526:GLN:OE1	2.07	0.55
1:B:178:ARG:O	1:B:181:TYR:HB3	2.06	0.55
1:A:247:ASP:CG	1:A:292:ALA:HA	2.27	0.55
1:B:218:ASP:OD1	1:B:220:PRO:HD2	2.06	0.55
1:B:444:MET:HG2	1:B:490:LEU:HB3	1.89	0.55
1:B:224:ARG:HA	1:B:224:ARG:HE	1.71	0.55
1:A:324:LEU:HB2	1:A:353:GLY:HA2	1.89	0.55
1:A:273:PHE:CG	1:A:274:PRO:HA	2.42	0.55
1:A:420:HIS:HB2	1:A:469:LYS:CE	2.35	0.55
1:A:269:PHE:O	1:A:283:TYR:HA	2.07	0.55
1:B:571:LEU:HD23	1:B:579:MET:SD	2.47	0.55
1:A:504:ASN:HD22	1:A:504:ASN:C	2.09	0.54
1:B:185:LEU:HD23	1:B:187:VAL:HG13	1.89	0.54
1:B:492:ARG:O	1:B:496:ARG:HG3	2.08	0.54
1:A:386:THR:OG1	1:A:388:GLU:HG3	2.07	0.54
1:A:31:LYS:HG3	1:A:67:ASP:OD2	2.07	0.54
1:A:416:LEU:HD12	1:A:418:ASP:O	2.08	0.54
1:B:569:LEU:HG	1:B:571:LEU:HD12	1.88	0.54
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.73	0.54
1:B:260:GLU:HB3	1:B:273:PHE:CZ	2.42	0.54
1:B:475:GLU:OE1	1:B:477:LYS:HD3	2.08	0.54
1:B:8:HIS:HD2	1:B:26:ARG:O	1.90	0.54
1:A:531:VAL:HG11	1:A:573:LEU:HD21	1.89	0.54
1:B:11:LYS:N	1:B:15:ALA:HB3	2.23	0.54
1:A:275:VAL:HG12	1:A:282:ASN:ND2	2.23	0.53
1:A:260:GLU:HB2	1:A:265:LYS:HZ1	1.73	0.53
1:B:383:PHE:CE1	1:B:391:ALA:HA	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:230:HIS:C	1:B:232:ARG:H	2.12	0.53
1:B:75:CYS:SG	1:B:80:VAL:HB	2.48	0.53
1:A:245:ALA:O	1:A:293:MET:HA	2.08	0.53
1:B:426:LEU:HD12	1:B:459:GLY:O	2.09	0.53
1:B:473:ILE:HG21	1:B:478:GLU:O	2.08	0.53
1:B:381:ILE:HA	1:B:425:PHE:HE1	1.73	0.53
1:A:19:SER:HB3	1:A:22:GLN:HE21	1.73	0.53
1:B:202:HIS:HB2	1:B:204:TYR:CD2	2.43	0.53
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.91	0.53
1:A:246:GLY:C	1:A:248:GLN:H	2.12	0.53
1:A:43:ASP:OD1	1:A:79:ARG:HG3	2.07	0.53
1:A:433:GLU:CD	1:A:437:ARG:HE	2.11	0.53
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.22	0.53
1:A:43:ASP:CG	1:A:77:THR:HG21	2.29	0.53
1:B:494:ARG:NH1	1:B:500:LEU:O	2.42	0.53
1:A:409:ALA:O	1:A:410:ALA:C	2.48	0.52
1:A:336:ARG:HE	1:B:336:ARG:CZ	2.22	0.52
1:B:440:VAL:O	1:B:444:MET:HB2	2.09	0.52
1:A:193:THR:HB	1:A:194:PRO:CD	2.39	0.52
1:B:198:SER:HB3	1:B:203:LYS:HD2	1.92	0.52
1:B:20:GLU:OE1	1:B:118:ARG:HB3	2.10	0.52
1:B:401:ALA:HA	1:B:404:LEU:HD13	1.91	0.52
1:A:258:LYS:O	1:A:261:GLN:HB2	2.09	0.52
1:A:270:ILE:HG22	1:A:271:GLU:N	2.24	0.52
1:A:19:SER:OG	1:A:22:GLN:HG3	2.09	0.52
1:B:488:LYS:HB3	1:B:492:ARG:NH1	2.24	0.52
1:B:500:LEU:HD21	1:B:528:VAL:HG11	1.91	0.52
1:A:505:VAL:HG22	1:A:521:ARG:CD	2.40	0.52
1:B:410:ALA:HA	1:B:413:LEU:CD2	2.34	0.52
1:A:242:PHE:HB3	1:A:307:LEU:HD13	1.91	0.52
1:A:28:ARG:HG2	1:A:66:PHE:CD2	2.45	0.52
1:B:44:ARG:HB2	1:B:79:ARG:HB3	1.92	0.52
1:A:277:LYS:HD3	1:A:280:ARG:HB3	1.92	0.52
1:B:315:MET:HA	1:B:319:ILE:HG12	1.91	0.52
1:A:31:LYS:HA	1:A:67:ASP:CG	2.30	0.52
1:B:165:ASP:HB2	1:B:201:HIS:HE1	1.75	0.52
1:A:358:ASP:OD1	1:A:360:SER:HB3	2.10	0.52
1:A:19:SER:CB	1:A:22:GLN:HE21	2.23	0.51
1:A:222:PHE:O	1:A:226:VAL:HG23	2.10	0.51
1:B:326:VAL:HG12	1:B:329:GLU:HG3	1.91	0.51
1:B:514:ALA:HB1	1:B:539:GLN:NE2	2.25	0.51
1:B:254:ASP:OD2	1:B:262:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:THR:HB	1:B:194:PRO:HD2	1.92	0.51
1:A:373:ASN:HD22	1:A:413:LEU:HB3	1.75	0.51
1:B:92:GLU:CD	1:B:92:GLU:H	2.14	0.51
1:B:416:LEU:CD2	1:B:416:LEU:H	2.23	0.51
1:A:505:VAL:HG22	1:A:521:ARG:HD2	1.91	0.51
1:A:59:LYS:HG3	1:A:69:PHE:CE1	2.46	0.51
1:A:137:PHE:CE1	1:A:139:GLU:HB3	2.46	0.51
1:A:250:PHE:CG	1:A:251:ALA:N	2.79	0.51
1:B:511:ASP:OD1	1:B:513:GLN:HB2	2.11	0.51
1:B:2:LEU:HD23	1:B:4:GLU:H	1.75	0.51
1:B:202:HIS:HE1	1:B:205:ASP:OD1	1.94	0.51
1:B:40:LEU:HB2	1:B:83:VAL:HG13	1.92	0.51
1:A:444:MET:HG2	1:A:490:LEU:CB	2.40	0.51
1:A:3:LEU:HA	1:A:6:ILE:HD13	1.91	0.51
1:A:454:TYR:CG	1:A:454:TYR:O	2.63	0.51
1:A:440:VAL:HG12	1:A:490:LEU:HD13	1.92	0.50
1:B:30:LYS:HB3	1:B:33:ASP:HB2	1.93	0.50
1:A:374:TYR:CE1	1:A:375:LEU:CD1	2.92	0.50
1:A:306:TYR:O	1:A:310:VAL:HG23	2.11	0.50
1:B:533:ASN:O	1:B:576:TYR:HA	2.11	0.50
1:A:574:ARG:HG2	1:A:575:PRO:HD2	1.94	0.50
1:A:271:GLU:HG3	1:A:272:ASP:N	2.25	0.50
1:A:545:VAL:O	1:A:567:GLY:HA2	2.11	0.50
1:A:171:ASP:OD1	1:A:173:LYS:HB3	2.12	0.50
1:A:328:ASN:HB3	1:A:355:ILE:CD1	2.22	0.50
1:B:395:ASP:O	1:B:399:THR:OG1	2.28	0.50
1:A:289:GLN:O	1:A:291:PRO:HD3	2.11	0.50
1:A:117:HIS:HB3	1:B:299:GLU:CD	2.32	0.50
1:B:351:ILE:N	1:B:369:ASP:OD2	2.34	0.50
1:A:52:LEU:HD11	1:A:105:ARG:NH2	2.26	0.50
1:A:374:TYR:CD1	1:A:375:LEU:HD13	2.47	0.50
1:B:160:ALA:HB3	1:B:471:PRO:HG3	1.92	0.50
1:B:165:ASP:HB2	1:B:201:HIS:CE1	2.47	0.50
1:B:193:THR:HB	1:B:194:PRO:CD	2.42	0.49
1:B:553:TRP:HB3	1:B:581:LEU:HB3	1.93	0.49
1:A:424:ARG:HH12	1:A:455:GLY:HA3	1.77	0.49
1:A:141:PHE:O	1:A:472:MET:HB3	2.13	0.49
1:A:273:PHE:CZ	1:A:275:VAL:HG22	2.46	0.49
1:B:504:ASN:C	1:B:504:ASN:ND2	2.64	0.49
1:A:446:TYR:CG	1:A:447:LEU:N	2.81	0.49
1:B:81:LYS:O	1:B:81:LYS:HG3	2.11	0.49
1:B:255:VAL:O	1:B:275:VAL:HG11	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:ASP:OD1	1:A:325:ASP:HB2	2.13	0.49
1:A:325:ASP:OD1	1:A:326:VAL:HG23	2.13	0.49
1:B:269:PHE:CE2	1:B:297:ARG:HG3	2.47	0.49
1:B:208:ASP:C	1:B:210:LEU:H	2.16	0.49
1:A:247:ASP:CB	1:A:292:ALA:HA	2.42	0.49
1:B:258:LYS:O	1:B:259:GLY:C	2.51	0.49
1:A:573:LEU:CD1	1:A:579:MET:HG3	2.42	0.48
1:B:121:VAL:O	1:B:122:PHE:C	2.52	0.48
1:A:272:ASP:OD1	1:A:282:ASN:HB3	2.13	0.48
1:A:273:PHE:CE2	1:A:275:VAL:HG13	2.48	0.48
1:A:181:TYR:HD2	1:A:182:LEU:HD22	1.78	0.48
1:A:271:GLU:CG	1:A:272:ASP:H	2.22	0.48
1:A:390:HIS:CD2	1:A:392:GLU:HB2	2.49	0.48
1:B:180:PRO:HG3	1:B:232:ARG:NH1	2.28	0.48
1:B:134:TYR:CZ	1:B:454:TYR:HA	2.49	0.48
1:A:5:ALA:HA	1:B:4:GLU:O	2.14	0.48
1:A:4:GLU:CD	1:B:30:LYS:HE3	2.34	0.48
1:B:339:ARG:O	1:B:343:LYS:HG2	2.14	0.48
1:A:269:PHE:HE2	1:A:297:ARG:HG3	1.78	0.48
1:A:583:ASN:HD21	1:A:585:ARG:HB2	1.79	0.48
1:B:320:ASP:O	1:B:349:ALA:HA	2.14	0.48
1:A:570:LYS:O	1:A:571:LEU:HD12	2.14	0.47
1:A:277:LYS:CE	1:A:278:THR:H	2.27	0.47
1:A:26:ARG:HD3	1:A:70:GLU:HG3	1.95	0.47
1:B:522:THR:HG23	1:B:526:GLN:O	2.14	0.47
1:A:262:SER:C	1:A:264:TYR:H	2.16	0.47
1:A:285:THR:HB	1:A:293:MET:O	2.14	0.47
1:B:504:ASN:HD22	1:B:504:ASN:N	2.13	0.47
1:A:77:THR:O	1:A:78:LYS:HB2	2.14	0.47
1:B:239:ASP:OD1	1:B:325:ASP:OD2	2.33	0.47
1:A:4:GLU:O	1:B:5:ALA:HA	2.15	0.47
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.95	0.47
1:A:330:VAL:HG22	1:A:335:TRP:CD1	2.49	0.47
1:B:8:HIS:ND1	1:B:9:GLU:N	2.62	0.47
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.50	0.47
1:A:505:VAL:O	1:A:506:ARG:HG2	2.15	0.47
1:A:137:PHE:HE1	1:A:139:GLU:HB3	1.79	0.47
1:A:470:ARG:HB3	1:A:471:PRO:HD2	1.96	0.47
1:B:202:HIS:HB2	1:B:204:TYR:HD2	1.80	0.47
1:B:494:ARG:HA	1:B:500:LEU:HD12	1.97	0.47
1:A:130:GLU:O	1:A:130:GLU:HG3	2.14	0.47
1:B:270:ILE:HG12	1:B:283:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:ASP:OD1	1:A:215:GLN:HG2	2.15	0.47
1:B:460:MET:SD	1:B:472:MET:HA	2.55	0.47
1:B:356:TRP:CZ3	1:B:374:TYR:HB3	2.50	0.47
1:B:47:SER:OG	1:B:48:PRO:HD2	2.15	0.47
1:B:499:SER:OG	1:B:523:VAL:HG12	2.14	0.47
1:A:339:ARG:O	1:A:343:LYS:HG2	2.15	0.47
1:A:545:VAL:N	1:A:567:GLY:O	2.42	0.46
1:A:410:ALA:CA	1:A:413:LEU:HD22	2.44	0.46
1:A:553:TRP:HB3	1:A:581:LEU:HB3	1.97	0.46
1:A:420:HIS:O	1:A:468:CYS:SG	2.73	0.46
1:A:219:LEU:HB2	1:A:220:PRO:HD3	1.97	0.46
1:B:52:LEU:CD1	1:B:105:ARG:HH21	2.26	0.46
1:B:276:SER:HA	1:B:282:ASN:HD21	1.78	0.46
1:A:324:LEU:HB3	1:A:327:ALA:HB2	1.98	0.46
1:A:251:ALA:O	1:A:255:VAL:HG23	2.14	0.46
1:B:520:VAL:HG22	1:B:529:GLY:HA2	1.96	0.46
1:B:321:GLY:HA2	1:B:350:LEU:O	2.16	0.46
1:A:193:THR:O	1:A:195:ILE:HG23	2.16	0.46
1:A:276:SER:O	1:A:277:LYS:CB	2.64	0.46
1:B:441:LEU:HD13	1:B:578:GLY:HA3	1.97	0.46
1:A:193:THR:HB	1:A:194:PRO:HD2	1.97	0.46
1:B:274:PRO:CG	1:B:280:ARG:HH22	2.29	0.46
1:B:228:GLU:O	1:B:232:ARG:HG3	2.16	0.46
1:B:300:ASN:HB3	1:B:303:VAL:HG23	1.98	0.46
1:B:278:THR:O	1:B:279:SER:CB	2.63	0.46
1:A:398:LEU:HD21	1:A:442:PHE:HZ	1.81	0.46
1:B:546:PRO:C	1:B:548:SER:H	2.19	0.45
1:B:443:GLN:O	1:B:443:GLN:HG3	2.09	0.45
1:A:269:PHE:O	1:A:284:GLU:N	2.45	0.45
1:B:2:LEU:HD23	1:B:4:GLU:OE2	2.16	0.45
1:B:487:TYR:O	1:B:490:LEU:HB2	2.17	0.45
1:A:499:SER:HA	1:A:523:VAL:CG1	2.47	0.45
1:A:353:GLY:O	1:A:371:VAL:HA	2.16	0.45
1:B:264:TYR:O	1:B:267:TRP:HB2	2.16	0.45
1:B:199:PRO:HG3	1:B:248:GLN:NE2	2.32	0.45
1:A:335:TRP:CE3	1:A:335:TRP:HA	2.52	0.45
1:A:158:LYS:HG3	1:A:473:ILE:HD11	1.98	0.45
1:A:11:LYS:N	1:A:15:ALA:HB3	2.32	0.45
1:B:24:ARG:HD2	1:B:70:GLU:HG2	1.99	0.45
1:B:43:ASP:OD1	1:B:79:ARG:HB2	2.17	0.45
1:A:202:HIS:HB2	1:A:204:TYR:HD2	1.81	0.45
1:B:127:TRP:CE3	1:B:235:LYS:HD2	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.98	0.45
1:A:528:VAL:HA	1:A:581:LEU:O	2.17	0.45
1:A:324:LEU:HD22	1:A:335:TRP:CH2	2.51	0.45
1:B:274:PRO:HG2	1:B:280:ARG:HH22	1.81	0.45
1:A:416:LEU:N	1:A:416:LEU:HD23	2.24	0.45
1:B:16:TYR:CE1	1:B:407:GLU:HG2	2.51	0.45
1:B:542:LEU:HD23	1:B:542:LEU:C	2.37	0.44
1:B:416:LEU:HB3	1:B:451:LEU:HD23	1.99	0.44
1:A:504:ASN:ND2	1:A:504:ASN:C	2.69	0.44
1:B:127:TRP:CD2	1:B:235:LYS:HD2	2.52	0.44
1:B:59:LYS:HB2	1:B:59:LYS:HE3	1.88	0.44
1:A:122:PHE:O	1:A:408:GLN:HG2	2.17	0.44
1:A:277:LYS:HB3	1:A:280:ARG:O	2.18	0.44
1:B:381:ILE:O	1:B:381:ILE:HG23	2.18	0.44
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.47	0.44
1:A:222:PHE:CZ	1:A:238:LEU:HD11	2.53	0.44
1:B:3:LEU:HA	1:B:6:ILE:CD1	2.40	0.44
1:A:30:LYS:HG3	1:A:31:LYS:N	2.33	0.44
1:B:381:ILE:HD11	1:B:428:SER:HB3	1.98	0.44
1:B:483:LEU:O	1:B:486:PHE:HB3	2.17	0.44
1:B:505:VAL:HG22	1:B:521:ARG:CD	2.48	0.44
1:A:179:LEU:N	1:A:180:PRO:CD	2.81	0.44
1:A:180:PRO:HG3	1:A:232:ARG:HH11	1.82	0.44
1:B:26:ARG:NH1	1:B:70:GLU:OE2	2.49	0.44
1:B:489:GLU:HG2	1:B:489:GLU:O	2.18	0.44
1:B:523:VAL:O	1:B:523:VAL:HG13	2.18	0.44
1:B:493:LEU:HD21	1:B:556:CYS:HB3	2.00	0.44
1:B:153:THR:HG22	1:B:154:GLU:N	2.33	0.44
1:A:410:ALA:HA	1:A:413:LEU:CD2	2.44	0.44
1:B:57:ALA:HA	1:B:70:GLU:O	2.17	0.44
1:B:219:LEU:HB2	1:B:220:PRO:HD3	1.98	0.44
1:A:527:HIS:HB2	1:A:583:ASN:CG	2.38	0.44
1:B:150:PRO:HG2	1:B:167:PHE:CE2	2.53	0.44
1:B:432:ASN:ND2	1:B:435:LYS:HE3	2.33	0.43
1:B:137:PHE:CZ	1:B:469:LYS:HD3	2.53	0.43
1:A:374:TYR:O	1:A:378:GLU:HG3	2.18	0.43
1:B:401:ALA:O	1:B:404:LEU:HB2	2.18	0.43
1:B:376:PHE:CZ	1:B:415:ASN:HB3	2.53	0.43
1:B:300:ASN:HB3	1:B:303:VAL:CG2	2.48	0.43
1:A:209:TYR:HB3	1:A:310:VAL:HG11	2.00	0.43
1:B:182:LEU:O	1:B:185:LEU:HB3	2.19	0.43
1:A:357:HIS:O	1:A:358:ASP:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:ALA:HA	1:B:235:LYS:H	1.83	0.43
1:A:185:LEU:HD23	1:A:187:VAL:HG13	2.00	0.43
1:A:263:ARG:O	1:A:263:ARG:HD2	2.18	0.43
1:A:40:LEU:HD12	1:A:40:LEU:N	2.33	0.43
1:A:138:PRO:O	1:A:170:GLY:HA3	2.19	0.43
1:B:126:GLU:O	1:B:129:LYS:HB2	2.19	0.43
1:A:163:ARG:NH1	1:A:165:ASP:OD1	2.50	0.43
1:A:9:GLU:O	1:A:11:LYS:N	2.45	0.43
1:A:167:PHE:HA	1:A:167:PHE:HD2	1.73	0.43
1:B:582:TRP:CZ2	1:B:584:GLY:HA2	2.54	0.43
1:A:43:ASP:OD2	1:A:79:ARG:NH1	2.51	0.43
1:A:275:VAL:O	1:A:276:SER:HB3	2.19	0.43
1:B:381:ILE:HA	1:B:425:PHE:CE1	2.53	0.43
1:A:190:LEU:HG	1:A:234:ILE:CG2	2.49	0.43
1:B:567:GLY:O	1:B:568:GLN:HG2	2.19	0.43
1:B:25:VAL:HG22	1:B:71:ALA:O	2.19	0.43
1:A:484:PHE:CD1	1:A:488:LYS:HD2	2.54	0.42
1:B:8:HIS:CG	1:B:9:GLU:N	2.86	0.42
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.54	0.42
1:B:465:ASP:OD1	1:B:466:PRO:HA	2.19	0.42
1:B:138:PRO:HG3	1:B:195:ILE:HG22	2.01	0.42
1:A:21:THR:HB	1:A:75:CYS:O	2.19	0.42
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.30	0.42
1:A:581:LEU:N	1:A:581:LEU:HD12	2.35	0.42
1:A:20:GLU:OE1	1:A:118:ARG:HB3	2.20	0.42
1:A:134:TYR:CD2	1:A:182:LEU:HD11	2.55	0.42
1:B:38:GLU:OE1	1:B:54:HIS:CD2	2.72	0.42
1:A:240:ALA:HB1	1:A:242:PHE:CE1	2.55	0.42
1:B:328:ASN:N	1:B:328:ASN:OD1	2.52	0.42
1:A:506:ARG:HH21	1:A:506:ARG:HG2	1.84	0.42
1:B:190:LEU:HG	1:B:234:ILE:HG21	2.00	0.42
1:A:24:ARG:HD2	1:A:70:GLU:OE2	2.19	0.42
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.55	0.42
1:B:356:TRP:HZ3	1:B:374:TYR:HB3	1.84	0.42
1:A:7:PHE:CG	1:A:8:HIS:N	2.87	0.42
1:B:504:ASN:N	1:B:504:ASN:ND2	2.66	0.42
1:B:381:ILE:HD13	1:B:381:ILE:O	2.19	0.42
1:A:145:ASP:OD1	1:A:147:SER:OG	2.28	0.42
1:B:323:ARG:HA	1:B:352:VAL:O	2.20	0.42
1:A:3:LEU:HA	1:A:6:ILE:CD1	2.49	0.42
1:A:180:PRO:HG3	1:A:232:ARG:NH1	2.35	0.42
1:B:6:ILE:HA	1:B:28:ARG:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:LEU:CD2	1:B:4:GLU:HB2	2.50	0.41
1:B:459:GLY:O	1:B:460:MET:C	2.58	0.41
1:A:530:VAL:HG12	1:A:532:LEU:HD11	2.02	0.41
1:A:249:PHE:O	1:A:250:PHE:C	2.57	0.41
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.55	0.41
1:A:271:GLU:HG2	1:A:282:ASN:O	2.20	0.41
1:A:401:ALA:HA	1:A:404:LEU:HD13	2.01	0.41
1:B:489:GLU:HA	1:B:492:ARG:CZ	2.50	0.41
1:B:440:VAL:HG12	1:B:490:LEU:CD1	2.50	0.41
1:B:81:LYS:CG	1:B:81:LYS:O	2.68	0.41
1:B:441:LEU:HD23	1:B:441:LEU:C	2.40	0.41
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.49	0.41
1:A:126:GLU:O	1:A:129:LYS:HB2	2.19	0.41
1:A:538:LYS:HB2	1:A:538:LYS:HE3	1.93	0.41
1:B:135:GLN:HG3	1:B:191:TYR:CE2	2.56	0.41
1:B:26:ARG:HD3	1:B:70:GLU:OE2	2.21	0.41
1:A:530:VAL:HA	1:A:579:MET:O	2.21	0.41
1:B:190:LEU:HG	1:B:234:ILE:CG2	2.51	0.41
1:A:172:LEU:O	1:A:175:VAL:N	2.53	0.41
1:A:464:THR:OG1	1:A:465:ASP:N	2.53	0.41
1:A:206:THR:HG21	1:A:209:TYR:CG	2.55	0.41
1:A:43:ASP:OD1	1:A:79:ARG:NH1	2.54	0.41
1:B:45:TYR:HD1	1:B:79:ARG:HH11	1.67	0.41
1:A:34:VAL:HG12	1:A:35:VAL:N	2.34	0.41
1:A:436:PHE:O	1:A:439:ALA:HB3	2.21	0.41
1:A:15:ALA:HA	1:A:24:ARG:O	2.21	0.41
1:A:198:SER:OG	1:A:205:ASP:OD1	2.31	0.41
1:A:140:ARG:HG2	1:A:469:LYS:O	2.20	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD13	1.95	0.41
1:B:400:ARG:O	1:B:401:ALA:C	2.59	0.41
1:B:447:LEU:HB2	1:B:505:VAL:HG21	2.03	0.41
1:A:389:ILE:HG13	1:A:389:ILE:O	2.20	0.41
1:B:31:LYS:HE2	1:B:62:SER:OG	2.20	0.41
1:B:326:VAL:CG1	1:B:329:GLU:HG3	2.51	0.41
1:B:267:TRP:CD2	1:B:303:VAL:HG22	2.56	0.41
1:B:115:TYR:HD1	1:B:117:HIS:CE1	2.39	0.40
1:A:8:HIS:ND1	1:A:9:GLU:N	2.69	0.40
1:A:435:LYS:O	1:A:436:PHE:C	2.60	0.40
1:A:376:PHE:CD1	1:A:376:PHE:C	2.95	0.40
1:A:205:ASP:O	1:A:246:GLY:HA3	2.22	0.40
1:A:504:ASN:HD21	1:A:522:THR:HB	1.85	0.40
1:B:127:TRP:CE2	1:B:235:LYS:HD2	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:172:LEU:O	1:B:175:VAL:N	2.54	0.40
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.56	0.40
1:B:182:LEU:H	1:B:182:LEU:HD22	1.87	0.40
1:A:219:LEU:N	1:A:220:PRO:CD	2.84	0.40
1:B:43:ASP:HA	1:B:79:ARG:O	2.21	0.40
1:B:398:LEU:HD21	1:B:442:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	520 (89%)	55 (9%)	8 (1%)	16	66
1	B	583/585 (100%)	512 (88%)	64 (11%)	7 (1%)	19	70
All	All	1166/1170 (100%)	1032 (88%)	119 (10%)	15 (1%)	18	68

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ALA
1	A	277	LYS
1	A	358	ASP
1	B	259	GLY
1	B	547	GLU
1	A	10	ALA
1	A	298	THR
1	B	460	MET
1	A	247	ASP
1	A	567	GLY
1	B	209	TYR
1	A	331	ASP
1	B	59	LYS
1	A	114	ALA

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Mol	Chain	Res	Type
1	B	138	PRO

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	493/493 (100%)	464 (94%)	29 (6%)	28	72
1	B	493/493 (100%)	461 (94%)	32 (6%)	24	68
All	All	986/986 (100%)	925 (94%)	61 (6%)	26	70

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	85	LEU
1	A	122	PHE
1	A	139	GLU
1	A	140	ARG
1	A	167	PHE
1	A	193	THR
1	A	223	ARG
1	A	263	ARG
1	A	273	PHE
1	A	275	VAL
1	A	277	LYS
1	A	278	THR
1	A	323	ARG
1	A	329	GLU
1	A	330	VAL
1	A	340	ARG
1	A	341	LEU
1	A	375	LEU
1	A	398	LEU
1	A	411	GLN
1	A	413	LEU
1	A	466	PRO
1	A	477	LYS

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Mol	Chain	Res	Type
1	A	483	LEU
1	A	504	ASN
1	A	526	GLN
1	A	527	HIS
1	A	545	VAL
1	B	13	SER
1	B	26	ARG
1	B	33	ASP
1	B	85	LEU
1	B	122	PHE
1	B	140	ARG
1	B	164	HIS
1	B	167	PHE
1	B	191	TYR
1	B	223	ARG
1	B	224	ARG
1	B	263	ARG
1	B	282	ASN
1	B	323	ARG
1	B	324	LEU
1	B	330	VAL
1	B	341	LEU
1	B	375	LEU
1	B	381	ILE
1	B	398	LEU
1	B	399	THR
1	B	411	GLN
1	B	413	LEU
1	B	416	LEU
1	B	418	ASP
1	B	426	LEU
1	B	443	GLN
1	B	483	LEU
1	B	504	ASN
1	B	535	ARG
1	B	565	LYS
1	B	568	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS

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Mol	Chain	Res	Type
1	A	22	GLN
1	A	112	GLN
1	A	135	GLN
1	A	155	GLN
1	A	244	HIS
1	A	282	ASN
1	A	300	ASN
1	A	346	ASN
1	A	504	ASN
1	A	527	HIS
1	A	539	GLN
1	A	544	GLN
1	B	8	HIS
1	B	54	HIS
1	B	90	GLN
1	B	117	HIS
1	B	135	GLN
1	B	155	GLN
1	B	215	GLN
1	B	244	HIS
1	B	248	GLN
1	B	346	ASN
1	B	367	GLN
1	B	504	ASN
1	B	539	GLN
1	B	544	GLN
1	B	568	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

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	585/585 (100%)	-0.18	4 (0%) 84 38	6, 27, 50, 52	0
1	B	585/585 (100%)	-0.05	4 (0%) 84 38	6, 33, 51, 52	0
All	All	1170/1170 (100%)	-0.11	8 (0%) 84 38	6, 30, 51, 52	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ARG	2.9
1	A	280	ARG	2.7
1	A	279	SER	2.4
1	A	278	THR	2.1
1	A	273	PHE	2.1
1	B	289	GLN	2.1
1	B	279	SER	2.0
1	B	155	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	B	602	1/1	0.06	-3.91	49,49,49,49	0
2	CA	A	601	1/1	0.07	-5.00	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.