Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2021 – 03:25 AM EDT

PDB ID	:	1WZM
Title	:	Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) mutatnt R469K
Authors	:	Mizuno, M.; Ichikawa, K.; Tonozuka, 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 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		25
Ramachandran outliers		1.3%
Sidechain outliers		6.2%
RSRZ outliers		3.2%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
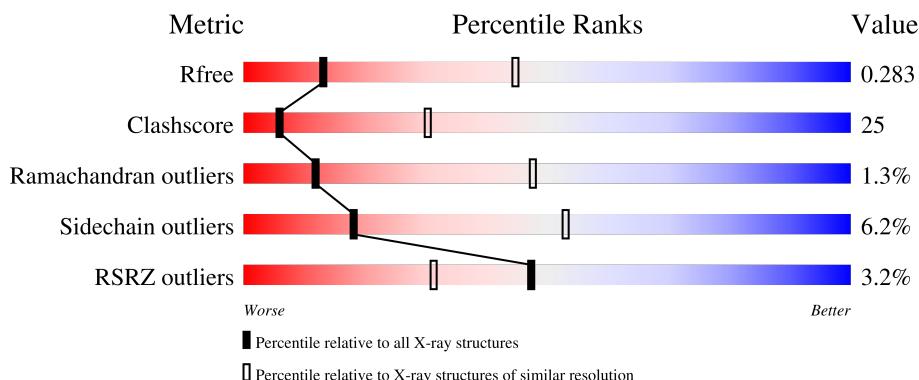
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	585	54% 42% •
1	B	585	53% 43% •
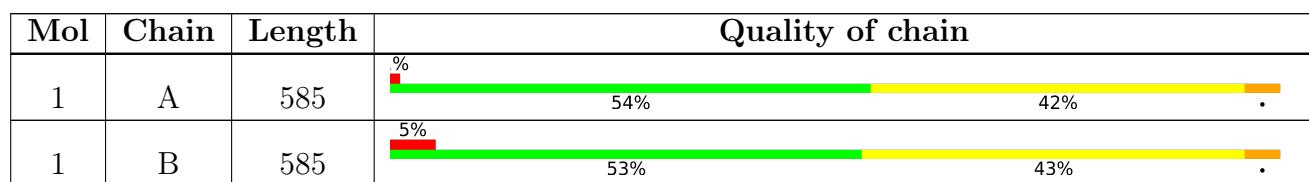
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9550 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 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 mutation	UNP Q08751
B	469	LYS	ARG	engineered mutation	UNP Q08751

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

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

3 Residue-property plots ⓘ

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

- Molecule 1: Alpha-amylase II
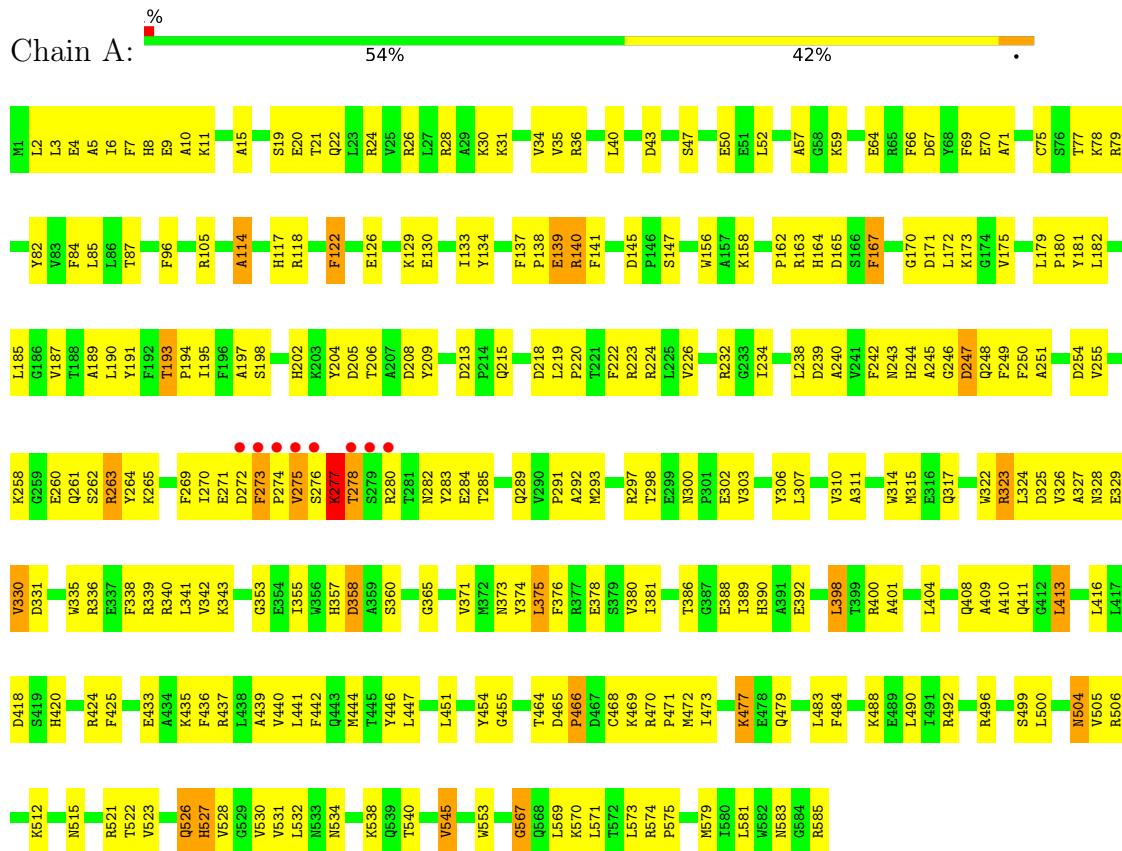
- Molecule 1: Alpha-amylase II
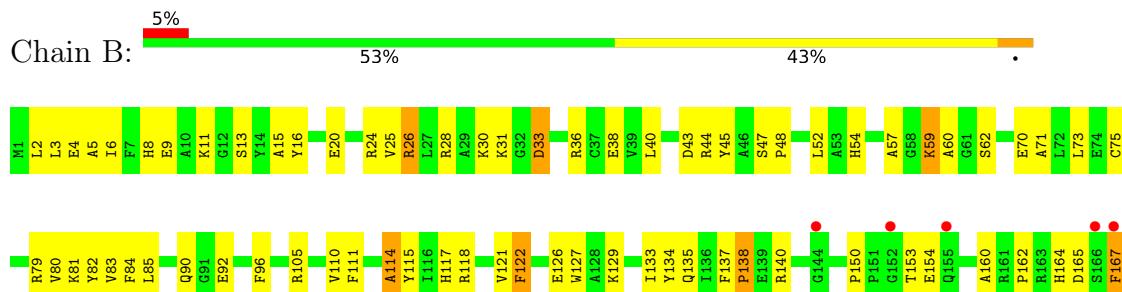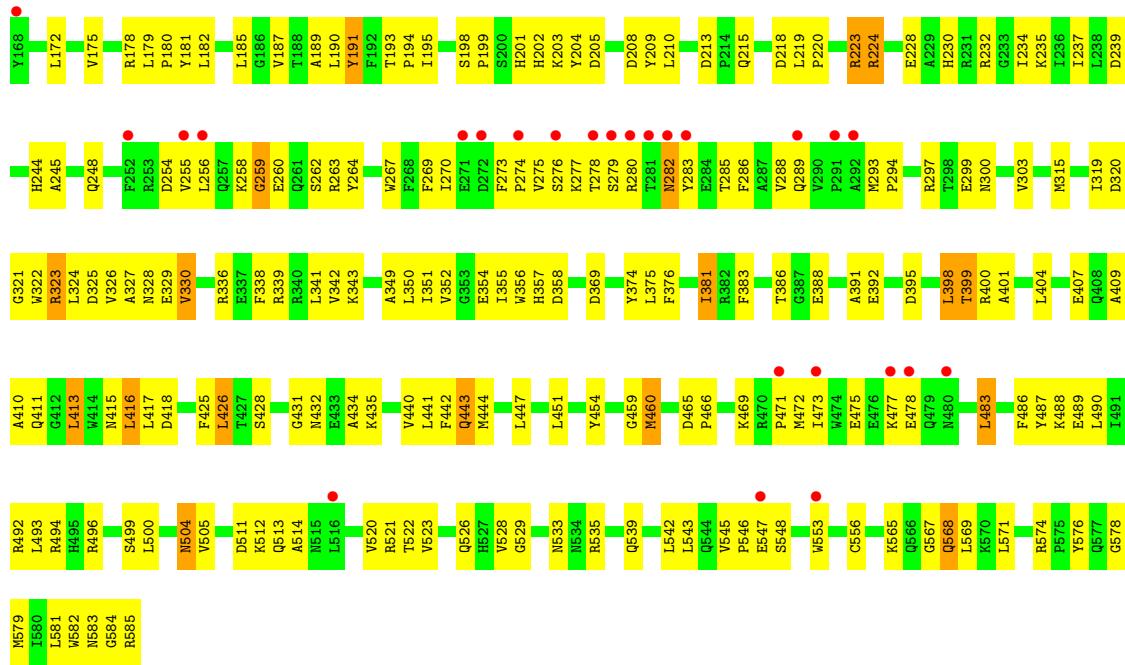
4   Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [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%)	wwPDB-VP
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 , 51.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47$, $< L^2 > = 0.30$	Xtriage
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
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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 Too-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 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	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

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 25.

All (469) 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: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:H	1:A:477:LYS:HD2	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:H	1:A:477:LYS:CD	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:H	1:A:416:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:HD2	1:A:26:ARG:O	1.76	0.67
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:73:LEU:HD23	1:B:80:VAL:HG21	1.77	0.66
1:B:477:LYS:HD2	1:B:477:LYS:N	2.03	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:A:260:GLU:HB2	1:A:265:LYS:NZ	2.11	0.65
1:B:237:ILE:HD12	1:B:321:GLY:HA3	1.78	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:400:ARG:O	1:A:404:LEU:HD13	1.96	0.65
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.77	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:C	1:B:504:ASN:HD22	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:8:HIS:HE1	1:A:82:TYR:OH	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:SER:O	1:A:277:LYS:HB2	2.02	0.60
1:A:416:LEU:H	1:A:416:LEU:CD2	2.15	0.60
1:A:523:VAL:O	1:A:523:VAL:HG13	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:A:247:ASP:HB3	1:A:292:ALA:HA	1.85	0.58
1:B:36:ARG:NH2	1:B:38:GLU:OE2	2.36	0.58
1:A:224:ARG:HA	1:A:224:ARG:NE	2.19	0.58
1:A:336:ARG:NE	1:B:336:ARG:CZ	2.67	0.58
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.17	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:285:THR:HB	1:B:293:MET:O	2.03	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:HA	1:A:277:LYS:HE2	1.87	0.57
1:A:300:ASN:ND2	1:A:303:VAL:H	2.01	0.57
1:A:573:LEU:HD11	1:A:579:MET:HG3	1.87	0.57
1:B:133:ILE:HB	1:B:451:LEU:CD1	2.34	0.57
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.52	0.57
1:B:504:ASN:HD21	1:B:522:THR:HB	1.68	0.57
1:B:278:THR:O	1:B:279:SER:HB2	2.04	0.57
1:B:526:GLN:HG3	1:B:585:ARG:OXT	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:38:GLU:OE1	1:B:54:HIS:HD2	1.89	0.56
1:A:114:ALA:HB1	1:B:328:ASN:O	2.05	0.56
1:A:376:PHE:O	1:A:380:VAL:HG23	2.06	0.56
1:A:477:LYS:HD2	1:A:477:LYS:N	2.18	0.56
1:A:532:LEU:N	1:A:532:LEU:HD12	2.21	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:B:274:PRO:HG2	1:B:280:ARG:NH2	2.20	0.56
1:A:8:HIS:CD2	1:A:26:ARG:O	2.59	0.56
1:A:515:ASN:ND2	1:A:534:ASN:O	2.33	0.56
1:B:416:LEU:HD23	1:B:416:LEU:H	1.71	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:A:326:VAL:HG12	1:A:326:VAL:O	2.06	0.55
1:B:2:LEU:HD21	1:B:4:GLU:HB2	1.89	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:224:ARG:HE	1:B:224:ARG:HA	1.71	0.55
1:B:444:MET:HG2	1:B:490:LEU:HB3	1.89	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:C	1:A:504:ASN:HD22	2.09	0.54
1:A:31:LYS:HG3	1:A:67:ASP:OD2	2.07	0.54
1:A:386:THR:OG1	1:A:388:GLU:HG3	2.07	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:416:LEU:HD12	1:A:418:ASP:O	2.08	0.54
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.73	0.54
1:B:569:LEU:HG	1:B:571:LEU:HD12	1.88	0.54
1:B:260:GLU:HB3	1:B:273:PHE:CZ	2.42	0.54
1:A:531:VAL:HG11	1:A:573:LEU:HD21	1.89	0.54
1:B:8:HIS:HD2	1:B:26:ARG:O	1.90	0.54
1:B:11:LYS:N	1:B:15:ALA:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLU:OE1	1:B:477:LYS:HD3	2.08	0.54
1:A:260:GLU:HB2	1:A:265:LYS:HZ1	1.73	0.53
1:A:275:VAL:HG12	1:A:282:ASN:ND2	2.23	0.53
1:B:230:HIS:C	1:B:232:ARG:H	2.12	0.53
1:B:383:PHE:CE1	1:B:391:ALA:HA	2.43	0.53
1:A:245:ALA:O	1:A:293:MET:HA	2.08	0.53
1:B:75:CYS:SG	1:B:80:VAL:HB	2.48	0.53
1:A:19:SER:HB3	1:A:22:GLN:HE21	1.73	0.53
1:B:381:ILE:HA	1:B:425:PHE:HE1	1.73	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: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:43:ASP:OD1	1:A:79:ARG:HG3	2.07	0.53
1:A:246:GLY:C	1:A:248:GLN:H	2.12	0.53
1:A:433:GLU:CD	1:A:437:ARG:HE	2.11	0.53
1:B:223:ARG:HH11	1:B:223:ARG:CG	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:336:ARG:HE	1:B:336:ARG:CZ	2.22	0.52
1:A:409:ALA:O	1:A:410:ALA:C	2.48	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:440:VAL:O	1:B:444:MET:HB2	2.09	0.52
1:A:258:LYS:O	1:A:261:GLN:HB2	2.09	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:19:SER:OG	1:A:22:GLN:HG3	2.09	0.52
1:A:270:ILE:HG22	1:A:271:GLU:N	2.24	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:A:28:ARG:HG2	1:A:66:PHE:CD2	2.45	0.52
1:A:242:PHE:HB3	1:A:307:LEU:HD13	1.91	0.52
1:B:44:ARG:HB2	1:B:79:ARG:HB3	1.92	0.52
1:B:410:ALA:HA	1:B:413:LEU:CD2	2.34	0.52
1:A:31:LYS:HA	1:A:67:ASP:CG	2.30	0.52
1:A:277:LYS:HD3	1:A:280:ARG:HB3	1.92	0.52
1:A:358:ASP:OD1	1:A:360:SER:HB3	2.10	0.52
1:B:165:ASP:HB2	1:B:201:HIS:HE1	1.75	0.52
1:B:315:MET:HA	1:B:319:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:THR:HB	1:B:194:PRO:HD2	1.92	0.51
1:B:254:ASP:OD2	1:B:262:SER:HB3	2.10	0.51
1:A:59:LYS:HG3	1:A:69:PHE:CE1	2.46	0.51
1:A:373:ASN:HD22	1:A:413:LEU:HB3	1.75	0.51
1:A:505:VAL:HG22	1:A:521:ARG:HD2	1.91	0.51
1:B:92:GLU:H	1:B:92:GLU:CD	2.14	0.51
1:B:416:LEU:H	1:B:416:LEU:CD2	2.23	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:40:LEU:HB2	1:B:83:VAL:HG13	1.92	0.51
1:B:202:HIS:HE1	1:B:205:ASP:OD1	1.94	0.51
1:A:3:LEU:HA	1:A:6:ILE:HD13	1.91	0.51
1:A:444:MET:HG2	1:A:490:LEU:CB	2.40	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:306:TYR:O	1:A:310:VAL:HG23	2.11	0.50
1:A:374:TYR:CE1	1:A:375:LEU:CD1	2.92	0.50
1:A:574:ARG:HG2	1:A:575:PRO:HD2	1.94	0.50
1:B:533:ASN:O	1:B:576:TYR:HA	2.11	0.50
1:A:271:GLU:HG3	1:A:272:ASP:N	2.25	0.50
1:A:171:ASP:OD1	1:A:173:LYS:HB3	2.12	0.50
1:A:545:VAL:O	1:A:567:GLY:HA2	2.11	0.50
1:A:117:HIS:HB3	1:B:299:GLU:CD	2.32	0.50
1:A:289:GLN:O	1:A:291:PRO:HD3	2.11	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:52:LEU:HD11	1:A:105:ARG:NH2	2.26	0.50
1:B:351:ILE:N	1:B:369:ASP:OD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:446:TYR:CG	1:A:447:LEU:N	2.81	0.49
1:B:504:ASN:C	1:B:504:ASN:ND2	2.64	0.49
1:B:81:LYS:O	1:B:81:LYS:HG3	2.11	0.49
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:255:VAL:O	1:B:275:VAL:HG11	2.12	0.49
1:B:208:ASP:C	1:B:210:LEU:H	2.16	0.49
1:B:269:PHE:CE2	1:B:297:ARG:HG3	2.47	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:134:TYR:CZ	1:B:454:TYR:HA	2.49	0.48
1:B:180:PRO:HG3	1:B:232:ARG:NH1	2.28	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:26:ARG:HD3	1:A:70:GLU:HG3	1.95	0.47
1:A:262:SER:C	1:A:264:TYR:H	2.16	0.47
1:A:277:LYS:CE	1:A:278:THR:H	2.27	0.47
1:A:570:LYS:O	1:A:571:LEU:HD12	2.14	0.47
1:B:522:THR:HG23	1:B:526:GLN:O	2.14	0.47
1:A:285:THR:HB	1:A:293:MET:O	2.14	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:B:504:ASN:HD22	1:B:504:ASN:N	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE1	1:A:139:GLU:HB3	1.79	0.47
1:A:505:VAL:O	1:A:506:ARG:HG2	2.15	0.47
1:A:130:GLU:HG3	1:A:130:GLU:O	2.14	0.47
1:A:213:ASP:OD1	1:A:215:GLN:HG2	2.15	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:270:ILE:HG12	1:B:283:TYR:HB3	1.97	0.47
1:B:494:ARG:HA	1:B:500:LEU:HD12	1.97	0.47
1:B:460:MET:SD	1:B:472:MET:HA	2.55	0.47
1:B:47:SER:OG	1:B:48:PRO:HD2	2.15	0.47
1:B:356:TRP:CZ3	1:B:374:TYR:HB3	2.50	0.47
1:A:339:ARG:O	1:A:343:LYS:HG2	2.15	0.47
1:B:499:SER:OG	1:B:523:VAL:HG12	2.14	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:219:LEU:HB2	1:A:220:PRO:HD3	1.97	0.46
1:A:420:HIS:O	1:A:468:CYS:SG	2.73	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:251:ALA:O	1:A:255:VAL:HG23	2.14	0.46
1:A:324:LEU:HB3	1:A:327:ALA:HB2	1.98	0.46
1:B:520:VAL:HG22	1:B:529:GLY:HA2	1.96	0.46
1:A:193:THR:O	1:A:195:ILE:HG23	2.16	0.46
1:B:321:GLY:HA2	1:B:350:LEU:O	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:228:GLU:O	1:B:232:ARG:HG3	2.16	0.46
1:B:274:PRO:CG	1:B:280:ARG:HH22	2.29	0.46
1:B:300:ASN:HB3	1:B:303:VAL:HG23	1.98	0.46
1:A:398:LEU:HD21	1:A:442:PHE:HZ	1.81	0.46
1:B:278:THR:O	1:B:279:SER:CB	2.63	0.46
1:B:546:PRO:C	1:B:548:SER:H	2.19	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:443:GLN:O	1:B:443:GLN:HG3	2.09	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:199:PRO:HG3	1:B:248:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:TYR:O	1:B:267:TRP:HB2	2.16	0.45
1:A:158:LYS:HG3	1:A:473:ILE:HD11	1.98	0.45
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.52	0.45
1:A:11:LYS:N	1:A:15:ALA:HB3	2.32	0.45
1:A:202:HIS:HB2	1:A:204:TYR:HD2	1.81	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:B:127:TRP:CE3	1:B:235:LYS:HD2	2.52	0.45
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:A:416:LEU:HD23	1:A:416:LEU:N	2.24	0.45
1:B:16:TYR:CE1	1:B:407:GLU:HG2	2.51	0.45
1:B:274:PRO:HG2	1:B:280:ARG:HH22	1.81	0.45
1:A:122:PHE:O	1:A:408:GLN:HG2	2.17	0.44
1:A:504:ASN:C	1:A:504:ASN:ND2	2.69	0.44
1:B:59:LYS:HB2	1:B:59:LYS:HE3	1.88	0.44
1:B:127:TRP:CD2	1:B:235:LYS:HD2	2.52	0.44
1:B:416:LEU:HB3	1:B:451:LEU:HD23	1.99	0.44
1:B:542:LEU:C	1:B:542:LEU:HD23	2.37	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:A:30:LYS:HG3	1:A:31:LYS:N	2.33	0.44
1:B:3:LEU:HA	1:B:6:ILE:CD1	2.40	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: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:505:VAL:HG22	1:B:521:ARG:CD	2.48	0.44
1:B:26:ARG:NH1	1:B:70:GLU:OE2	2.49	0.44
1:B:153:THR:HG22	1:B:154:GLU:N	2.33	0.44
1:B:489:GLU:O	1:B:489:GLU:HG2	2.18	0.44
1:B:493:LEU:HD21	1:B:556:CYS:HB3	2.00	0.44
1:B:523:VAL:O	1:B:523:VAL:HG13	2.18	0.44
1:A:410:ALA:HA	1:A:413:LEU:CD2	2.44	0.44
1:A:527:HIS:HB2	1:A:583:ASN:CG	2.38	0.44
1:B:57:ALA:HA	1:B:70:GLU:O	2.17	0.44
1:B:150:PRO:HG2	1:B:167:PHE:CE2	2.53	0.44
1:B:219:LEU:HB2	1:B:220:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PHE:CZ	1:B:469:LYS:HD3	2.53	0.43
1:B:432:ASN:ND2	1:B:435:LYS:HE3	2.33	0.43
1:A:374:TYR:O	1:A:378:GLU:HG3	2.18	0.43
1:B:376:PHE:CZ	1:B:415:ASN:HB3	2.53	0.43
1:B:401:ALA:O	1:B:404:LEU:HB2	2.18	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:A:357:HIS:O	1:A:358:ASP:C	2.56	0.43
1:B:182:LEU:O	1:B:185:LEU:HB3	2.19	0.43
1:A:40:LEU:N	1:A:40:LEU:HD12	2.33	0.43
1:A:138:PRO:O	1:A:170:GLY:HA3	2.19	0.43
1:A:163:ARG:NH1	1:A:165:ASP:OD1	2.50	0.43
1:A:185:LEU:HD23	1:A:187:VAL:HG13	2.00	0.43
1:A:263:ARG:HD2	1:A:263:ARG:O	2.18	0.43
1:B:126:GLU:O	1:B:129:LYS:HB2	2.19	0.43
1:B:189:ALA:HA	1:B:235:LYS:H	1.83	0.43
1:A:9:GLU:O	1:A:11:LYS:N	2.45	0.43
1:A:167:PHE:HD2	1:A:167:PHE:HA	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:190:LEU:HG	1:A:234:ILE:CG2	2.49	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:B:25:VAL:HG22	1:B:71:ALA:O	2.19	0.43
1:B:567:GLY:O	1:B:568:GLN:HG2	2.19	0.43
1:A:21:THR:HB	1:A:75:CYS:O	2.19	0.42
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:138:PRO:HG3	1:B:195:ILE:HG22	2.01	0.42
1:B:465:ASP:OD1	1:B:466:PRO:HA	2.19	0.42
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.54	0.42
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.30	0.42
1:A:581:LEU:HD12	1:A:581:LEU:N	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:A:240:ALA:HB1	1:A:242:PHE:CE1	2.55	0.42
1:B:38:GLU:OE1	1:B:54:HIS:CD2	2.72	0.42
1:A:506:ARG:HG2	1:A:506:ARG:HH21	1.84	0.42
1:B:190:LEU:HG	1:B:234:ILE:HG21	2.00	0.42
1:B:328:ASN:OD1	1:B:328:ASN:N	2.52	0.42
1:A:24:ARG:HD2	1:A:70:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:381:ILE:O	1:B:381:ILE:HD13	2.19	0.42
1:B:504:ASN:ND2	1:B:504:ASN:N	2.66	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:2:LEU:CD2	1:B:4:GLU:HB2	2.50	0.41
1:B:6:ILE:HA	1:B:28:ARG:O	2.20	0.41
1:A:122:PHE:CD2	1:A:365:GLY:HA2	2.55	0.41
1:A:249:PHE:O	1:A:250:PHE:C	2.57	0.41
1:A:530:VAL:HG12	1:A:532:LEU:HD11	2.02	0.41
1:B:459:GLY:O	1:B:460:MET:C	2.58	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:81:LYS:O	1:B:81:LYS:CG	2.68	0.41
1:B:440:VAL:HG12	1:B:490:LEU:CD1	2.50	0.41
1:B:441:LEU:HD23	1:B:441:LEU:C	2.40	0.41
1:B:489:GLU:HA	1:B:492:ARG:CZ	2.50	0.41
1:A:126:GLU:O	1:A:129:LYS:HB2	2.19	0.41
1:A:538:LYS:HE3	1:A:538:LYS:HB2	1.93	0.41
1:B:57:ALA:CB	1:B:71:ALA:HB2	2.49	0.41
1:B:135:GLN:HG3	1:B:191:TYR:CE2	2.56	0.41
1:A:172:LEU:O	1:A:175:VAL:N	2.53	0.41
1:A:530:VAL:HA	1:A:579:MET:O	2.21	0.41
1:B:26:ARG:HD3	1:B:70:GLU:OE2	2.21	0.41
1:B:190:LEU:HG	1:B:234:ILE:CG2	2.51	0.41
1:A:464:THR:OG1	1:A:465:ASP:N	2.53	0.41
1:A:34:VAL:HG12	1:A:35:VAL:N	2.34	0.41
1:A:43:ASP:OD1	1:A:79:ARG:NH1	2.54	0.41
1:A:206:THR:HG21	1:A:209:TYR:CG	2.55	0.41
1:A:436:PHE:O	1:A:439:ALA:HB3	2.21	0.41
1:B:45:TYR:HD1	1:B:79:ARG:HH11	1.67	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:HD13	1:A:219:LEU:HA	1.95	0.41
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.41
1:B:400:ARG:O	1:B:401:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LEU:HB2	1:B:505:VAL:HG21	2.03	0.41
1:B:31:LYS:HE2	1:B:62:SER:OG	2.20	0.41
1:B:267:TRP:CD2	1:B:303:VAL:HG22	2.56	0.41
1:B:326:VAL:CG1	1:B:329:GLU:HG3	2.51	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:205:ASP:O	1:A:246:GLY:HA3	2.22	0.40
1:A:376:PHE:CD1	1:A:376:PHE:C	2.95	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
1:B:172:LEU:O	1:B:175:VAL:N	2.54	0.40
1:A:219:LEU:N	1:A:220:PRO:CD	2.84	0.40
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.56	0.40
1:B:43:ASP:HA	1:B:79:ARG:O	2.21	0.40
1:B:182:LEU:HD22	1:B:182:LEU:H	1.87	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%)	11	46
1	B	583/585 (100%)	512 (88%)	64 (11%)	7 (1%)	13	49
All	All	1166/1170 (100%)	1032 (88%)	119 (10%)	15 (1%)	12	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ALA

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Mol	Chain	Res	Type
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
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%)	19	54
1	B	493/493 (100%)	461 (94%)	32 (6%)	17	51
All	All	986/986 (100%)	925 (94%)	61 (6%)	18	53

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
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 molecules 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 monosaccharides 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.

No monomer is involved in short contacts.

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%)	-0.21	8 (1%)	75	63	6, 27, 50, 52	0
1	B	585/585 (100%)	-0.02	30 (5%)	28	16	6, 33, 51, 52	0
All	All	1170/1170 (100%)	-0.11	38 (3%)	47	31	6, 30, 51, 52	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	SER	5.5
1	A	278	THR	4.7
1	B	276	SER	4.3
1	B	279	SER	4.3
1	B	278	THR	4.1
1	B	471	PRO	3.9
1	B	280	ARG	3.6
1	A	273	PHE	3.5
1	A	274	PRO	3.5
1	A	276	SER	3.2
1	B	256	LEU	3.1
1	A	280	ARG	3.1
1	B	272	ASP	3.1
1	B	274	PRO	3.0
1	A	272	ASP	3.0
1	B	547	GLU	2.8
1	B	281	THR	2.8
1	B	255	VAL	2.6
1	B	477	LYS	2.5
1	B	516	LEU	2.5
1	B	155	GLN	2.5
1	B	473	ILE	2.5
1	B	289	GLN	2.4
1	B	271	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	TYR	2.3
1	B	252	PHE	2.3
1	B	144	GLY	2.2
1	B	553	TRP	2.2
1	A	275	VAL	2.1
1	B	283	TYR	2.1
1	B	166	SER	2.1
1	B	292	ALA	2.1
1	B	478	GLU	2.1
1	B	282	ASN	2.1
1	B	480	ASN	2.0
1	B	152	GLY	2.0
1	B	167	PHE	2.0
1	B	291	PRO	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 monosaccharides 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. 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(Å^2)	Q<0.9
2	CA	B	602	1/1	0.95	0.06	49,49,49,49	0
2	CA	A	601	1/1	0.98	0.06	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.