



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:30 AM GMT

PDB ID : 1J38
Title : Crystal Structure of Drosophila AnCE
Authors : Kim, H.M.; Shin, D.R.; Lee, H.; Lee, J.-O.
Deposited on : 2003-01-20
Resolution : 2.60 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>

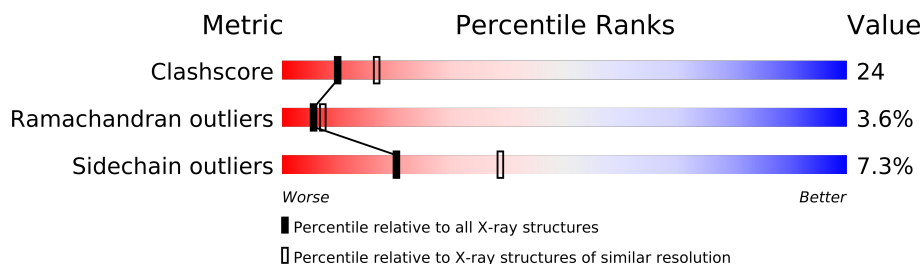
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	
1	B	607	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9806 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 angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	CONFLICT	UNP Q10714
A	53	ALA	ASN	CONFLICT	UNP Q10714
A	607	ILE	THR	CONFLICT	UNP Q10714
A	616	HIS	-	EXPRESSION TAG	UNP Q10714
A	617	HIS	-	EXPRESSION TAG	UNP Q10714
A	618	HIS	-	EXPRESSION TAG	UNP Q10714
A	619	HIS	-	EXPRESSION TAG	UNP Q10714
A	620	HIS	-	EXPRESSION TAG	UNP Q10714
B	51	ARG	GLY	CONFLICT	UNP Q10714
B	53	ALA	ASN	CONFLICT	UNP Q10714
B	607	ILE	THR	CONFLICT	UNP Q10714
B	616	HIS	-	EXPRESSION TAG	UNP Q10714
B	617	HIS	-	EXPRESSION TAG	UNP Q10714
B	618	HIS	-	EXPRESSION TAG	UNP Q10714
B	619	HIS	-	EXPRESSION TAG	UNP Q10714
B	620	HIS	-	EXPRESSION TAG	UNP Q10714

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	2	Total 2	O 2	0	0

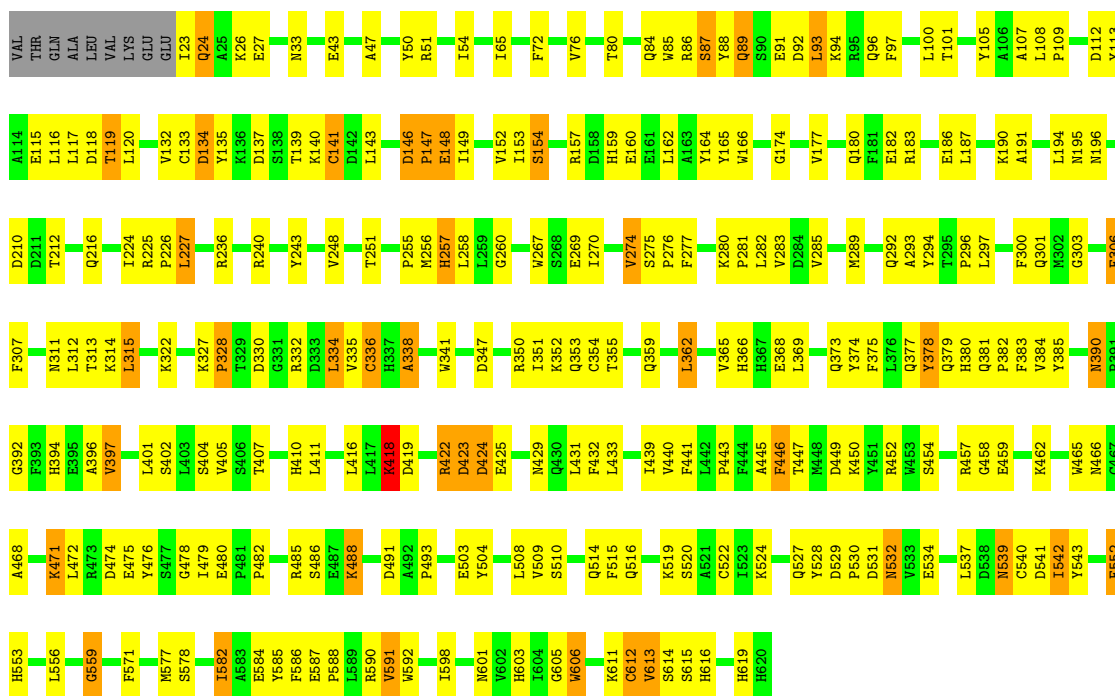
3 Residue-property plots

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.

Note EDS was not executed.

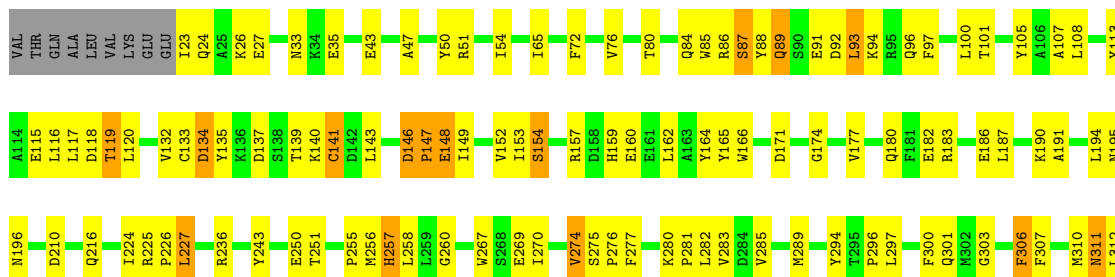
- Molecule 1: angiotensin converting enzyme

Chain A:



- Molecule 1: angiotensin converting enzyme

Chain B:



T313	V397	Y476	M577
K314	L401	S477	S578
L315	S402	G478	
		L479	
K322	V405	E480	I582
	S406	P481	A583
K327	T407	P482	E584
P328			Y585
T329		R485	F586
D330	H410	S486	E587
G331	L411	E487	P588
R332		K488	I589
D333	L416		R590
L334	L417	D491	V591
V335	K418	A492	W592
C336		P493	
H337	R422		N601
A338	D423	E503	V602
	D424	Y504	H603
W341	E425		I604
		L508	G605
D347	N429	V509	W606
	Q430	S510	
R350	L431	Q514	N610
I351	F432	F515	K611
K352	L433	Q516	G612
Q353			V613
C354	I439	K519	S614
T355	V440	S520	S615
	F441	A521	H616
Q359	L442	C522	H619
	P443	I523	H620
L362	F444	K524	
	A445		
V365	F446	Q527	
H366	T447	Y528	
H367	W448	D529	
E368	D449	P530	
L369	K450	D531	
	Y451	N532	
Q373	R452	W533	
Y374	W453	E534	
F375	S454		
L376		L537	
Q377	R457	D538	
Y378	G458	N539	
Q379	E459	C540	
H380		D541	
Q381		I542	
P382	K462	Y543	
F383	W465	F552	
V384	N466	H553	
Y385	C467		
	A468	L556	
N390	K471		
P391	L472	G559	
G392	R473		
F393	D474	F571	
H394	E475		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.43	0/5031	0.67	0/6814
1	B	0.45	0/5031	0.68	0/6814
All	All	0.44	0/10062	0.67	0/13628

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	4900	0	4696	221	2
1	B	4900	0	4696	230	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	9806	0	9392	450	2

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 24.

All (450) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.39	1.04
1:B:146:ASP:HB3	1:B:147:PRO:HD3	1.39	1.01
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.42	1.00
1:B:143:LEU:HD22	1:B:148:GLU:HG2	1.46	0.96
1:B:347:ASP:H	1:B:379:GLN:HE22	0.95	0.94
1:B:347:ASP:H	1:B:379:GLN:NE2	1.66	0.93
1:B:154:SER:HB2	1:B:269:GLU:HG2	1.51	0.92
1:A:347:ASP:H	1:A:379:GLN:HE22	0.96	0.92
1:A:154:SER:HB2	1:A:269:GLU:HG2	1.50	0.91
1:A:347:ASP:H	1:A:379:GLN:NE2	1.68	0.91
1:B:26:LYS:HB2	1:B:93:LEU:HD21	1.53	0.88
1:A:322:LYS:HB3	1:A:350:ARG:HD3	1.54	0.88
1:B:322:LYS:HB3	1:B:350:ARG:HD3	1.56	0.87
1:A:26:LYS:HB2	1:A:93:LEU:HD21	1.58	0.86
1:B:143:LEU:CD2	1:B:148:GLU:HG2	2.07	0.85
1:A:256:MET:O	1:A:257:HIS:ND1	2.08	0.85
1:B:115:GLU:O	1:B:119:THR:HG23	1.78	0.84
1:A:143:LEU:CD2	1:A:148:GLU:HG2	2.08	0.83
1:B:347:ASP:N	1:B:379:GLN:HE22	1.77	0.83
1:B:256:MET:O	1:B:257:HIS:ND1	2.12	0.83
1:A:115:GLU:O	1:A:119:THR:HG23	1.79	0.81
1:A:486:SER:HB2	1:A:614:SER:HA	1.66	0.77
1:B:285:VAL:HG11	1:B:416:LEU:HB3	1.67	0.77
1:A:146:ASP:HB3	1:A:147:PRO:CD	2.14	0.77
1:A:347:ASP:N	1:A:379:GLN:HE22	1.79	0.77
1:B:486:SER:HB2	1:B:614:SER:HA	1.65	0.77
1:B:488:LYS:HZ1	1:B:615:SER:HB2	1.51	0.76
1:B:146:ASP:HB3	1:B:147:PRO:CD	2.13	0.76
1:A:174:GLY:HA2	1:A:493:PRO:HB2	1.67	0.76
1:A:285:VAL:HG11	1:A:416:LEU:HB3	1.67	0.76
1:A:251:THR:HG22	1:A:603:HIS:CD2	2.21	0.75
1:B:251:THR:HG22	1:B:603:HIS:CD2	2.21	0.75
1:B:443:PRO:O	1:B:447:THR:HG23	1.87	0.75
1:A:143:LEU:HD22	1:A:148:GLU:CG	2.17	0.74
1:B:297:LEU:HG	1:B:301:GLN:HE21	1.53	0.74
1:B:143:LEU:HD22	1:B:148:GLU:CG	2.18	0.73
1:A:488:LYS:HZ1	1:A:615:SER:HB2	1.51	0.73
1:B:330:ASP:OD1	1:B:332:ARG:HB2	1.88	0.73
1:A:297:LEU:HG	1:A:301:GLN:HE21	1.54	0.72
1:B:516:GLN:NE2	1:B:578:SER:H	1.88	0.72
1:B:174:GLY:HA2	1:B:493:PRO:HB2	1.71	0.71
1:B:532:ASN:HD22	1:B:534:GLU:H	1.38	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:108:LEU:HD13	1:B:191:ALA:HB2	1.73	0.70
1:A:516:GLN:NE2	1:A:578:SER:H	1.89	0.70
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.27	0.69
1:A:89:GLN:H	1:A:89:GLN:NE2	1.91	0.69
1:A:330:ASP:OD1	1:A:332:ARG:HB2	1.93	0.69
1:A:532:ASN:HD22	1:A:534:GLU:H	1.39	0.69
1:B:89:GLN:H	1:B:89:GLN:NE2	1.91	0.68
1:B:315:LEU:HD21	1:B:369:LEU:HD11	1.74	0.68
1:A:97:PHE:O	1:A:101:THR:HG23	1.94	0.68
1:A:443:PRO:O	1:A:447:THR:HG23	1.94	0.68
1:A:108:LEU:HD13	1:A:191:ALA:HB2	1.75	0.68
1:A:509:VAL:HB	1:A:577:MET:CE	2.24	0.68
1:A:322:LYS:CB	1:A:350:ARG:HD3	2.23	0.67
1:A:315:LEU:HD21	1:A:369:LEU:HD11	1.75	0.67
1:B:590:ARG:NH1	1:B:591:VAL:HG12	2.10	0.67
1:B:97:PHE:O	1:B:101:THR:HG23	1.95	0.67
1:A:590:ARG:NH1	1:A:591:VAL:HG12	2.09	0.66
1:A:166:TRP:HH2	1:A:485:ARG:HD2	1.61	0.66
1:B:285:VAL:CG1	1:B:416:LEU:HB3	2.25	0.65
1:A:516:GLN:HE22	1:A:578:SER:H	1.42	0.65
1:B:276:PRO:HB3	1:B:592:TRP:CH2	2.31	0.65
1:A:285:VAL:CG1	1:A:416:LEU:HB3	2.26	0.65
1:A:89:GLN:H	1:A:89:GLN:CD	2.00	0.65
1:B:509:VAL:HB	1:B:577:MET:CE	2.26	0.65
1:A:177:VAL:HG22	1:A:180:GLN:HB2	1.79	0.65
1:B:516:GLN:HE22	1:B:578:SER:H	1.41	0.65
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.31	0.65
1:B:89:GLN:H	1:B:89:GLN:CD	1.99	0.64
1:A:166:TRP:CH2	1:A:485:ARG:HD2	2.33	0.64
1:A:43:GLU:HA	1:A:65:ILE:HG21	1.79	0.64
1:B:177:VAL:HG22	1:B:180:GLN:HB2	1.78	0.63
1:B:225:ARG:HB3	1:B:226:PRO:HD3	1.80	0.63
1:B:152:VAL:HG11	1:B:165:TYR:CD2	2.34	0.63
1:B:322:LYS:CB	1:B:350:ARG:HD3	2.27	0.63
1:A:471:LYS:O	1:A:475:GLU:HG3	1.99	0.63
1:A:285:VAL:H	1:A:359:GLN:NE2	1.96	0.63
1:B:297:LEU:HG	1:B:301:GLN:NE2	2.13	0.63
1:A:148:GLU:H	1:A:148:GLU:CD	2.00	0.62
1:B:532:ASN:ND2	1:B:534:GLU:H	1.98	0.62
1:A:509:VAL:HB	1:A:577:MET:HE1	1.81	0.61
1:B:285:VAL:H	1:B:359:GLN:NE2	1.98	0.61
1:A:297:LEU:HG	1:A:301:GLN:NE2	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:TRP:HH2	1:B:485:ARG:HD2	1.64	0.61
1:A:132:VAL:HG22	1:A:149:ILE:HD11	1.82	0.61
1:B:148:GLU:CD	1:B:148:GLU:H	2.04	0.61
1:B:296:PRO:HB3	1:B:355:THR:OG1	2.01	0.61
1:B:166:TRP:CH2	1:B:485:ARG:HD2	2.36	0.61
1:B:334:LEU:HD21	1:B:336:CYS:SG	2.41	0.60
1:A:296:PRO:HB3	1:A:355:THR:OG1	2.02	0.60
1:B:528:TYR:CE1	1:B:537:LEU:HB2	2.37	0.60
1:A:225:ARG:HB3	1:A:226:PRO:HD3	1.84	0.60
1:A:85:TRP:O	1:A:87:SER:N	2.35	0.60
1:A:532:ASN:ND2	1:A:534:GLU:H	1.99	0.59
1:A:598:ILE:CD1	1:B:35:GLU:HG2	2.33	0.59
1:A:365:VAL:O	1:A:369:LEU:HD23	2.03	0.59
1:B:96:GLN:O	1:B:100:LEU:HD23	2.03	0.59
1:A:613:VAL:HG23	1:A:614:SER:N	2.17	0.59
1:B:47:ALA:O	1:B:51:ARG:HG3	2.03	0.59
1:A:528:TYR:CE1	1:A:537:LEU:HB2	2.38	0.59
1:A:587:GLU:OE2	1:A:590:ARG:NH2	2.36	0.59
1:B:285:VAL:O	1:B:285:VAL:HG12	2.03	0.59
1:B:509:VAL:HB	1:B:577:MET:HE1	1.84	0.59
1:A:47:ALA:O	1:A:51:ARG:HG3	2.03	0.59
1:B:43:GLU:HA	1:B:65:ILE:HG21	1.84	0.59
1:B:552:PHE:O	1:B:556:LEU:HG	2.03	0.59
1:B:183:ARG:HH12	1:B:187:LEU:HD21	1.67	0.59
1:B:270:ILE:HD12	1:B:270:ILE:O	2.03	0.58
1:B:72:PHE:O	1:B:76:VAL:HG23	2.03	0.58
1:A:541:ASP:O	1:A:543:TYR:N	2.36	0.58
1:A:552:PHE:O	1:A:556:LEU:HG	2.02	0.58
1:B:520:SER:HB2	1:B:571:PHE:HE2	1.68	0.58
1:B:85:TRP:HA	1:B:88:TYR:CD1	2.38	0.58
1:A:162:LEU:HD13	1:A:257:HIS:O	2.02	0.58
1:B:537:LEU:O	1:B:537:LEU:HD13	2.03	0.58
1:A:183:ARG:HH12	1:A:187:LEU:HD21	1.69	0.58
1:A:270:ILE:HD12	1:A:270:ILE:O	2.03	0.58
1:A:251:THR:HG22	1:A:603:HIS:NE2	2.19	0.58
1:B:251:THR:HG22	1:B:603:HIS:NE2	2.19	0.58
1:A:72:PHE:O	1:A:76:VAL:HG23	2.04	0.58
1:A:520:SER:HB2	1:A:571:PHE:HE2	1.69	0.57
1:B:613:VAL:HG23	1:B:614:SER:N	2.19	0.57
1:A:96:GLN:O	1:A:100:LEU:HD23	2.04	0.57
1:B:91:GLU:HB3	1:B:94:LYS:NZ	2.20	0.57
1:B:446:PHE:O	1:B:450:LYS:HB2	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:VAL:O	1:B:369:LEU:HD23	2.04	0.57
1:A:277:PHE:H	1:A:429:ASN:HD21	1.52	0.57
1:A:488:LYS:HB2	1:A:488:LYS:HZ2	1.70	0.57
1:A:330:ASP:OD2	1:A:332:ARG:HD3	2.05	0.56
1:A:85:TRP:C	1:A:87:SER:H	2.08	0.56
1:B:257:HIS:ND1	1:B:482:PRO:HB3	2.21	0.56
1:A:537:LEU:HD13	1:A:537:LEU:O	2.05	0.56
1:B:385:TYR:HB3	1:B:559:GLY:O	2.04	0.56
1:A:256:MET:O	1:A:257:HIS:CB	2.53	0.56
1:A:257:HIS:ND1	1:A:482:PRO:HB3	2.20	0.56
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.40	0.56
1:A:85:TRP:HA	1:A:88:TYR:CD1	2.40	0.56
1:B:267:TRP:O	1:B:270:ILE:HG13	2.04	0.56
1:B:541:ASP:O	1:B:543:TYR:N	2.39	0.56
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.59	0.56
1:B:488:LYS:HZ2	1:B:488:LYS:HB2	1.70	0.56
1:A:251:THR:HG22	1:A:603:HIS:CE1	2.41	0.56
1:A:471:LYS:HD3	1:A:471:LYS:O	2.05	0.56
1:B:85:TRP:O	1:B:87:SER:N	2.38	0.56
1:B:162:LEU:HD13	1:B:257:HIS:O	2.04	0.56
1:A:105:TYR:O	1:A:108:LEU:HB2	2.05	0.56
1:B:587:GLU:OE2	1:B:590:ARG:NH2	2.38	0.56
1:B:280:LYS:HB3	1:B:281:PRO:HD2	1.88	0.56
1:B:105:TYR:O	1:B:108:LEU:HB2	2.05	0.56
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.41	0.56
1:A:91:GLU:HB3	1:A:94:LYS:NZ	2.20	0.56
1:A:116:LEU:O	1:A:120:LEU:HB2	2.05	0.56
1:B:277:PHE:H	1:B:429:ASN:HD21	1.53	0.56
1:A:446:PHE:O	1:A:450:LYS:HB2	2.06	0.56
1:B:85:TRP:C	1:B:87:SER:H	2.09	0.56
1:A:135:TYR:HB2	1:A:164:TYR:CD2	2.41	0.56
1:A:480:GLU:OE2	1:A:611:LYS:HE3	2.05	0.56
1:B:227:LEU:HD13	1:B:439:ILE:HD13	1.88	0.56
1:B:485:ARG:HD3	1:B:491:ASP:OD2	2.06	0.56
1:B:471:LYS:O	1:B:475:GLU:HG3	2.06	0.55
1:B:224:ILE:HG12	1:B:582:ILE:HD12	1.88	0.55
1:A:154:SER:HB2	1:A:269:GLU:CG	2.29	0.55
1:B:256:MET:O	1:B:257:HIS:CB	2.54	0.55
1:B:300:PHE:HE2	1:B:355:THR:HG21	1.71	0.55
1:A:485:ARG:HD3	1:A:491:ASP:OD2	2.06	0.55
1:B:51:ARG:HD2	1:B:341:TRP:CZ2	2.42	0.55
1:A:107:ALA:O	1:A:194:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:LYS:HB3	1:A:281:PRO:HD2	1.88	0.55
1:A:510:SER:O	1:A:514:GLN:HB3	2.07	0.55
1:B:116:LEU:O	1:B:120:LEU:HB2	2.06	0.55
1:A:267:TRP:O	1:A:270:ILE:HG13	2.05	0.55
1:A:377:GLN:HE22	1:A:553:HIS:CD2	2.25	0.55
1:B:251:THR:HG22	1:B:603:HIS:CE1	2.41	0.55
1:B:183:ARG:HH12	1:B:187:LEU:CD2	2.19	0.55
1:A:457:ARG:O	1:A:459:GLU:N	2.38	0.55
1:A:474:ASP:O	1:A:606:TRP:CZ3	2.60	0.54
1:A:515:PHE:CD2	1:A:582:ILE:HG23	2.42	0.54
1:B:135:TYR:HB2	1:B:164:TYR:CD2	2.42	0.54
1:A:285:VAL:HG12	1:A:285:VAL:O	2.06	0.54
1:A:183:ARG:HH12	1:A:187:LEU:CD2	2.21	0.54
1:A:454:SER:O	1:A:457:ARG:O	2.25	0.54
1:B:480:GLU:OE2	1:B:611:LYS:HE3	2.08	0.54
1:A:385:TYR:HB3	1:A:559:GLY:O	2.07	0.54
1:A:256:MET:O	1:A:257:HIS:CG	2.60	0.54
1:A:51:ARG:HD2	1:A:341:TRP:CZ2	2.43	0.54
1:B:515:PHE:CD2	1:B:582:ILE:HG23	2.43	0.54
1:B:377:GLN:HE22	1:B:553:HIS:CD2	2.25	0.54
1:B:159:HIS:CE1	1:B:160:GLU:HG3	2.43	0.54
1:B:405:VAL:O	1:B:411:LEU:HD21	2.08	0.54
1:A:159:HIS:CE1	1:A:160:GLU:HG3	2.43	0.54
1:A:76:VAL:O	1:A:80:THR:HG23	2.08	0.54
1:B:510:SER:O	1:B:514:GLN:HB3	2.07	0.54
1:B:330:ASP:OD2	1:B:332:ARG:HD3	2.08	0.53
1:B:471:LYS:HD3	1:B:471:LYS:O	2.07	0.53
1:B:422:ARG:HD2	1:B:422:ARG:O	2.07	0.53
1:A:143:LEU:HB3	1:A:148:GLU:HB2	1.89	0.53
1:A:478:GLY:O	1:A:479:ILE:HD12	2.07	0.53
1:A:422:ARG:O	1:A:422:ARG:HD2	2.08	0.53
1:B:527:GLN:HB3	1:B:540:CYS:HB2	1.90	0.53
1:B:76:VAL:O	1:B:80:THR:HG23	2.08	0.53
1:B:508:LEU:O	1:B:508:LEU:HD12	2.09	0.53
1:B:457:ARG:O	1:B:459:GLU:N	2.41	0.53
1:A:289:MET:HE1	1:A:362:LEU:HG	1.89	0.53
1:B:251:THR:HG22	1:B:603:HIS:CG	2.44	0.52
1:B:289:MET:HE1	1:B:362:LEU:HG	1.89	0.52
1:A:431:LEU:CD1	1:A:588:PRO:HG2	2.39	0.52
1:A:334:LEU:HD21	1:A:336:CYS:SG	2.50	0.52
1:A:152:VAL:HG11	1:A:165:TYR:CE2	2.44	0.52
1:A:300:PHE:HE2	1:A:355:THR:HG21	1.73	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:ARG:NH2	1:B:603:HIS:O	2.39	0.52
1:B:520:SER:HB2	1:B:571:PHE:CE2	2.44	0.52
1:B:478:GLY:O	1:B:479:ILE:HD12	2.10	0.52
1:B:327:LYS:HB2	1:B:354:CYS:SG	2.49	0.52
1:A:251:THR:HG22	1:A:603:HIS:CG	2.44	0.52
1:B:143:LEU:HB3	1:B:148:GLU:HB2	1.91	0.52
1:A:405:VAL:O	1:A:411:LEU:HD21	2.10	0.52
1:A:227:LEU:HD13	1:A:439:ILE:HD13	1.92	0.52
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.45	0.52
1:B:402:SER:HA	1:B:405:VAL:HG22	1.93	0.51
1:B:488:LYS:HB2	1:B:488:LYS:NZ	2.25	0.51
1:A:402:SER:HA	1:A:405:VAL:HG22	1.92	0.51
1:B:362:LEU:O	1:B:366:HIS:HD2	1.93	0.51
1:A:527:GLN:HB3	1:A:540:CYS:HB2	1.92	0.51
1:B:132:VAL:HG22	1:B:149:ILE:HD11	1.91	0.51
1:B:256:MET:O	1:B:257:HIS:CG	2.64	0.51
1:B:338:ALA:HB2	1:B:353:GLN:HG3	1.90	0.51
1:A:224:ILE:HG12	1:A:582:ILE:HD12	1.91	0.51
1:B:134:ASP:OD1	1:B:143:LEU:HD11	2.09	0.51
1:B:528:TYR:CG	1:B:537:LEU:HD23	2.46	0.51
1:B:96:GLN:O	1:B:100:LEU:CD2	2.58	0.51
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.31	0.51
1:B:537:LEU:HD13	1:B:585:TYR:HD1	1.76	0.51
1:A:541:ASP:OD2	1:A:541:ASP:O	2.29	0.51
1:A:133:CYS:HA	1:A:141:CYS:HA	1.91	0.51
1:A:338:ALA:HB2	1:A:353:GLN:HG3	1.92	0.51
1:B:154:SER:HB2	1:B:269:GLU:CG	2.33	0.51
1:B:152:VAL:HG11	1:B:165:TYR:CE2	2.45	0.51
1:B:454:SER:O	1:B:457:ARG:O	2.28	0.51
1:A:362:LEU:O	1:A:366:HIS:HD2	1.94	0.51
1:A:520:SER:HB2	1:A:571:PHE:CE2	2.46	0.51
1:A:33:ASN:HD22	1:A:383:PHE:HB3	1.75	0.50
1:B:190:LYS:O	1:B:194:LEU:HD13	2.11	0.50
1:A:134:ASP:OD1	1:A:143:LEU:HD11	2.10	0.50
1:B:113:TYR:CE2	1:B:117:LEU:HD11	2.46	0.50
1:A:541:ASP:C	1:A:543:TYR:H	2.15	0.50
1:A:157:ARG:HA	1:A:243:TYR:OH	2.11	0.50
1:A:255:PRO:HB2	1:A:258:LEU:HD12	1.94	0.50
1:B:183:ARG:NH1	1:B:187:LEU:HD21	2.26	0.50
1:A:327:LYS:HB2	1:A:354:CYS:SG	2.52	0.50
1:B:255:PRO:HB2	1:B:258:LEU:HD12	1.93	0.50
1:B:392:GLY:HA3	1:B:509:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:537:LEU:HD13	1:A:585:TYR:HD1	1.76	0.50
1:B:157:ARG:HA	1:B:243:TYR:OH	2.10	0.50
1:A:528:TYR:CG	1:A:537:LEU:HD23	2.46	0.50
1:A:392:GLY:HA3	1:A:509:VAL:CG2	2.41	0.50
1:B:33:ASN:ND2	1:B:384:VAL:H	2.10	0.50
1:A:96:GLN:O	1:A:100:LEU:CD2	2.59	0.50
1:B:431:LEU:CD1	1:B:588:PRO:HG2	2.41	0.50
1:B:33:ASN:HD22	1:B:383:PHE:HB3	1.75	0.49
1:B:381:GLN:HE21	1:B:382:PRO:HD2	1.77	0.49
1:B:143:LEU:HD22	1:B:148:GLU:CB	2.42	0.49
1:B:153:ILE:HG22	1:B:153:ILE:O	2.12	0.49
1:A:307:PHE:O	1:A:312:LEU:HB2	2.11	0.49
1:B:410:HIS:HB2	1:B:541:ASP:CG	2.33	0.49
1:A:439:ILE:HD11	1:A:586:PHE:CD2	2.47	0.49
1:A:381:GLN:HE21	1:A:382:PRO:HD2	1.77	0.49
1:A:450:LYS:HE2	1:A:476:TYR:OH	2.12	0.49
1:A:190:LYS:O	1:A:194:LEU:HD13	2.12	0.49
1:A:275:SER:CB	1:A:282:LEU:HD21	2.41	0.49
1:A:303:GLY:HA2	1:A:366:HIS:CE1	2.47	0.49
1:A:431:LEU:HD13	1:A:588:PRO:HG2	1.94	0.49
1:A:509:VAL:HB	1:A:577:MET:HE2	1.94	0.49
1:B:441:PHE:CE2	1:B:445:ALA:HB2	2.47	0.49
1:B:285:VAL:HG23	1:B:359:GLN:NE2	2.27	0.49
1:A:210:ASP:OD1	1:A:216:GLN:NE2	2.44	0.49
1:B:107:ALA:O	1:B:194:LEU:HD23	2.13	0.49
1:B:210:ASP:OD1	1:B:216:GLN:NE2	2.42	0.49
1:B:133:CYS:HA	1:B:141:CYS:HA	1.93	0.49
1:A:195:ASN:O	1:A:196:ASN:HB2	2.13	0.48
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.34	0.48
1:A:183:ARG:NH1	1:A:187:LEU:HD21	2.28	0.48
1:A:236:ARG:NH2	1:A:603:HIS:O	2.40	0.48
1:B:50:TYR:CZ	1:B:54:ILE:HG23	2.49	0.48
1:A:306:PHE:CE2	1:A:543:TYR:HA	2.48	0.48
1:B:541:ASP:O	1:B:541:ASP:OD2	2.31	0.48
1:B:195:ASN:O	1:B:196:ASN:HB2	2.14	0.48
1:A:485:ARG:O	1:A:612:CYS:HA	2.13	0.48
1:A:471:LYS:HD3	1:A:475:GLU:HG3	1.96	0.48
1:A:351:ILE:HD13	1:A:368:GLU:HB3	1.96	0.48
1:B:471:LYS:HD3	1:B:475:GLU:HG3	1.96	0.48
1:B:439:ILE:HD11	1:B:586:PHE:CD2	2.49	0.48
1:B:250:GLU:O	1:B:251:THR:OG1	2.27	0.47
1:B:289:MET:O	1:B:294:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:275:SER:CB	1:B:282:LEU:HD21	2.44	0.47
1:B:276:PRO:HD3	1:B:432:PHE:CD1	2.49	0.47
1:A:33:ASN:ND2	1:A:384:VAL:H	2.11	0.47
1:A:441:PHE:CE2	1:A:445:ALA:HB2	2.48	0.47
1:A:407:THR:HB	1:A:539:ASN:HD22	1.79	0.47
1:B:537:LEU:CD1	1:B:585:TYR:HD1	2.28	0.47
1:B:532:ASN:HD22	1:B:532:ASN:C	2.18	0.47
1:A:276:PRO:HD2	1:A:429:ASN:ND2	2.30	0.47
1:A:532:ASN:HD22	1:A:532:ASN:C	2.18	0.47
1:B:335:VAL:O	1:B:352:LYS:NZ	2.44	0.47
1:A:276:PRO:HD3	1:A:432:PHE:CD1	2.50	0.47
1:B:509:VAL:HB	1:B:577:MET:HE2	1.95	0.47
1:A:418:LYS:N	1:A:418:LYS:HD2	2.29	0.47
1:B:380:HIS:H	1:B:380:HIS:CD2	2.33	0.47
1:A:137:ASP:C	1:A:139:THR:H	2.18	0.47
1:A:289:MET:O	1:A:294:TYR:HB2	2.14	0.47
1:B:418:LYS:HD2	1:B:418:LYS:N	2.29	0.47
1:B:303:GLY:HA2	1:B:366:HIS:CE1	2.49	0.47
1:B:468:ALA:O	1:B:472:LEU:HB2	2.15	0.47
1:B:541:ASP:C	1:B:543:TYR:H	2.18	0.47
1:B:307:PHE:O	1:B:312:LEU:HB2	2.15	0.47
1:B:407:THR:HB	1:B:539:ASN:HD22	1.80	0.47
1:A:488:LYS:HB2	1:A:488:LYS:NZ	2.29	0.46
1:B:485:ARG:O	1:B:612:CYS:HA	2.16	0.46
1:B:306:PHE:CE2	1:B:543:TYR:HA	2.50	0.46
1:A:285:VAL:HG23	1:A:359:GLN:NE2	2.30	0.46
1:B:137:ASP:C	1:B:139:THR:H	2.18	0.46
1:B:439:ILE:HD11	1:B:586:PHE:CG	2.51	0.46
1:B:351:ILE:HD13	1:B:368:GLU:HB3	1.97	0.46
1:B:50:TYR:OH	1:B:54:ILE:HG23	2.15	0.46
1:B:431:LEU:HD13	1:B:588:PRO:HG2	1.97	0.46
1:A:146:ASP:CB	1:A:147:PRO:HD3	2.28	0.46
1:B:285:VAL:HG21	1:B:411:LEU:HD13	1.98	0.46
1:A:328:PRO:HG2	1:A:332:ARG:NH2	2.30	0.46
1:B:140:LYS:HE2	1:B:140:LYS:HB3	1.77	0.46
1:A:143:LEU:HD22	1:A:148:GLU:CB	2.45	0.45
1:B:277:PHE:CE2	1:B:425:GLU:HB3	2.52	0.45
1:B:100:LEU:HD21	1:B:384:VAL:HB	1.98	0.45
1:B:330:ASP:CG	1:B:332:ARG:HD3	2.37	0.45
1:B:276:PRO:HD2	1:B:429:ASN:ND2	2.30	0.45
1:B:171:ASP:OD1	1:B:485:ARG:NH2	2.36	0.45
1:B:328:PRO:HG2	1:B:332:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:PHE:CE2	1:A:425:GLU:HB3	2.51	0.45
1:B:153:ILE:O	1:B:260:GLY:HA2	2.16	0.45
1:A:519:LYS:HE3	1:A:584:GLU:OE2	2.16	0.45
1:B:614:SER:O	1:B:615:SER:HB3	2.17	0.45
1:B:450:LYS:HE2	1:B:476:TYR:OH	2.17	0.45
1:B:615:SER:OG	1:B:616:HIS:N	2.50	0.45
1:B:108:LEU:HD13	1:B:191:ALA:CB	2.42	0.45
1:B:275:SER:OG	1:B:282:LEU:HD11	2.17	0.45
1:B:54:ILE:HG13	1:B:334:LEU:HA	1.99	0.45
1:B:310:MET:HB2	1:B:312:LEU:HD12	1.99	0.45
1:B:274:VAL:O	1:B:274:VAL:HG13	2.16	0.45
1:A:275:SER:OG	1:A:282:LEU:HD11	2.17	0.44
1:A:108:LEU:HD13	1:A:191:ALA:CB	2.43	0.44
1:A:100:LEU:HD21	1:A:384:VAL:HB	1.99	0.44
1:A:375:PHE:HA	1:A:378:TYR:CE1	2.52	0.44
1:B:330:ASP:C	1:B:332:ARG:H	2.21	0.44
1:A:466:ASN:ND2	1:A:491:ASP:H	2.16	0.44
1:A:468:ALA:O	1:A:472:LEU:HB2	2.17	0.44
1:A:43:GLU:CA	1:A:65:ILE:HG21	2.46	0.44
1:B:256:MET:O	1:B:257:HIS:HB3	2.17	0.44
1:B:422:ARG:O	1:B:423:ASP:C	2.55	0.44
1:B:85:TRP:HA	1:B:88:TYR:CG	2.53	0.44
1:A:537:LEU:CD1	1:A:585:TYR:HD1	2.31	0.44
1:A:439:ILE:HD11	1:A:586:PHE:CG	2.53	0.44
1:A:380:HIS:H	1:A:380:HIS:CD2	2.35	0.44
1:A:274:VAL:O	1:A:274:VAL:HG13	2.17	0.44
1:A:452:ARG:NH2	1:A:504:TYR:HB2	2.32	0.44
1:A:256:MET:O	1:A:257:HIS:HB3	2.16	0.44
1:B:466:ASN:ND2	1:B:491:ASP:H	2.16	0.44
1:B:353:GLN:NE2	1:B:355:THR:HG22	2.33	0.44
1:A:524:LYS:HE3	1:A:571:PHE:O	2.18	0.44
1:A:422:ARG:O	1:A:423:ASP:C	2.56	0.44
1:A:522:CYS:SG	1:A:542:ILE:HG23	2.58	0.43
1:A:50:TYR:CZ	1:A:54:ILE:HG23	2.53	0.43
1:A:177:VAL:HG13	1:A:177:VAL:O	2.18	0.43
1:B:524:LYS:HE3	1:B:571:PHE:O	2.18	0.43
1:A:285:VAL:HG21	1:A:411:LEU:HD13	1.99	0.43
1:A:275:SER:HA	1:A:276:PRO:HD3	1.79	0.43
1:A:330:ASP:C	1:A:332:ARG:H	2.22	0.43
1:B:84:GLN:O	1:B:88:TYR:CE1	2.72	0.43
1:B:462:LYS:HA	1:B:465:TRP:CD1	2.53	0.43
1:A:23:ILE:O	1:A:23:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:475:GLU:O	1:B:606:TRP:HH2	2.01	0.43
1:B:183:ARG:NH1	1:B:187:LEU:CD2	2.82	0.43
1:A:615:SER:OG	1:A:616:HIS:N	2.51	0.43
1:A:475:GLU:O	1:A:606:TRP:HH2	2.01	0.43
1:B:519:LYS:HE3	1:B:584:GLU:OE2	2.18	0.43
1:B:522:CYS:SG	1:B:542:ILE:HG23	2.58	0.43
1:A:392:GLY:HA3	1:A:509:VAL:HG21	2.01	0.43
1:A:353:GLN:NE2	1:A:355:THR:HG22	2.34	0.43
1:B:605:GLY:C	1:B:606:TRP:CD1	2.92	0.43
1:A:508:LEU:O	1:A:508:LEU:HD12	2.18	0.43
1:B:23:ILE:HG12	1:B:23:ILE:O	2.19	0.43
1:A:153:ILE:HG22	1:A:153:ILE:O	2.18	0.43
1:B:327:LYS:CB	1:B:354:CYS:SG	3.07	0.43
1:B:177:VAL:O	1:B:177:VAL:HG13	2.17	0.43
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.54	0.43
1:A:313:THR:HB	1:A:373:GLN:HE22	1.84	0.42
1:A:335:VAL:O	1:A:352:LYS:NZ	2.44	0.42
1:B:611:LYS:HD3	1:B:611:LYS:HA	1.86	0.42
1:A:85:TRP:HA	1:A:88:TYR:CG	2.55	0.42
1:B:392:GLY:HA3	1:B:509:VAL:HG21	2.01	0.42
1:B:375:PHE:HA	1:B:378:TYR:CE1	2.55	0.42
1:B:51:ARG:HD2	1:B:341:TRP:CH2	2.54	0.42
1:B:313:THR:HB	1:B:373:GLN:HE22	1.85	0.42
1:B:267:TRP:CE2	1:B:440:VAL:HG11	2.55	0.42
1:B:327:LYS:HG3	1:B:354:CYS:SG	2.59	0.42
1:A:153:ILE:O	1:A:260:GLY:HA2	2.19	0.42
1:B:423:ASP:O	1:B:424:ASP:HB2	2.20	0.42
1:A:113:TYR:O	1:A:117:LEU:HG	2.19	0.42
1:B:113:TYR:O	1:B:117:LEU:HG	2.20	0.42
1:B:182:GLU:O	1:B:186:GLU:HG3	2.19	0.42
1:B:146:ASP:CB	1:B:147:PRO:HD3	2.28	0.42
1:B:143:LEU:HD22	1:B:148:GLU:HB3	2.02	0.42
1:A:423:ASP:O	1:A:424:ASP:HB2	2.20	0.42
1:A:527:GLN:HB3	1:A:540:CYS:CB	2.50	0.42
1:B:449:ASP:OD2	1:B:452:ARG:NH2	2.48	0.42
1:A:115:GLU:OE1	1:A:183:ARG:NH2	2.53	0.41
1:A:183:ARG:NH1	1:A:187:LEU:CD2	2.83	0.41
1:A:182:GLU:O	1:A:186:GLU:HG3	2.20	0.41
1:A:84:GLN:O	1:A:88:TYR:CE1	2.74	0.41
1:A:51:ARG:HD2	1:A:341:TRP:HZ2	1.84	0.41
1:A:23:ILE:O	1:A:24:GLN:O	2.38	0.41
1:A:529:ASP:O	1:A:531:ASP:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:ARG:HD2	1:A:341:TRP:CH2	2.55	0.41
1:A:240:ARG:HA	1:A:248:VAL:HB	2.02	0.41
1:B:143:LEU:HD23	1:B:148:GLU:HG2	1.96	0.41
1:B:452:ARG:NH2	1:B:504:TYR:HB2	2.35	0.41
1:B:528:TYR:OH	1:B:584:GLU:OE1	2.37	0.41
1:A:292:GLN:O	1:A:293:ALA:HB3	2.21	0.41
1:A:471:LYS:HA	1:A:471:LYS:HZ3	1.86	0.41
1:A:212:THR:O	1:A:216:GLN:HG3	2.20	0.41
1:A:605:GLY:C	1:A:606:TRP:CD1	2.94	0.41
1:A:449:ASP:OD2	1:A:452:ARG:NH2	2.47	0.41
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.79	0.41
1:B:610:ASN:HD22	1:B:610:ASN:HA	1.69	0.41
1:B:613:VAL:HG23	1:B:614:SER:H	1.86	0.41
1:B:85:TRP:C	1:B:87:SER:N	2.75	0.41
1:A:267:TRP:CE2	1:A:440:VAL:HG11	2.56	0.41
1:B:471:LYS:HZ3	1:B:471:LYS:HA	1.86	0.41
1:B:381:GLN:HE21	1:B:382:PRO:CD	2.34	0.41
1:B:311:ASN:HA	1:B:311:ASN:HD22	1.57	0.41
1:B:89:GLN:N	1:B:89:GLN:CD	2.72	0.40
1:A:381:GLN:HE21	1:A:382:PRO:CD	2.34	0.40
1:A:327:LYS:CB	1:A:354:CYS:SG	3.09	0.40
1:A:109:PRO:CG	1:A:112:ASP:OD2	2.69	0.40
1:A:382:PRO:O	1:A:383:PHE:C	2.60	0.40
1:A:396:ALA:O	1:A:397:VAL:C	2.60	0.40
1:B:410:HIS:HD2	1:B:541:ASP:OD1	2.05	0.40
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.49	0.40
1:B:380:HIS:N	1:B:380:HIS:CD2	2.89	0.40
1:B:529:ASP:O	1:B:531:ASP:N	2.54	0.40
1:B:275:SER:HA	1:B:276:PRO:HD3	1.80	0.40
1:B:270:ILE:H	1:B:270:ILE:HG13	1.81	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:A:619:HIS:NE2	1:B:134:ASP:OD2[1_554]	2.07	0.13
1:A:134:ASP:OD2	1:B:619:HIS:NE2[1_554]	2.17	0.03

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	596/607 (98%)	517 (87%)	58 (10%)	21 (4%)	6	8
1	B	596/607 (98%)	518 (87%)	56 (9%)	22 (4%)	5	7
All	All	1192/1214 (98%)	1035 (87%)	114 (10%)	43 (4%)	5	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	147	PRO
1	A	418	LYS
1	A	542	ILE
1	B	24	GLN
1	B	147	PRO
1	B	418	LYS
1	B	542	ILE
1	A	86	ARG
1	A	87	SER
1	A	338	ALA
1	A	423	ASP
1	A	424	ASP
1	A	613	VAL
1	B	86	ARG
1	B	87	SER
1	B	338	ALA
1	B	423	ASP
1	B	424	ASP
1	B	613	VAL
1	A	559	GLY
1	B	141	CYS
1	B	283	VAL
1	B	559	GLY
1	A	141	CYS
1	A	257	HIS
1	A	283	VAL

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Mol	Chain	Res	Type
1	A	390	ASN
1	B	257	HIS
1	B	390	ASN
1	A	148	GLU
1	A	397	VAL
1	A	458	GLY
1	B	148	GLU
1	B	397	VAL
1	B	616	HIS
1	B	146	ASP
1	A	530	PRO
1	A	591	VAL
1	B	458	GLY
1	B	530	PRO
1	B	591	VAL
1	A	146	ASP

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	522/530 (98%)	483 (92%)	39 (8%)	19	36
1	B	522/530 (98%)	485 (93%)	37 (7%)	21	40
All	All	1044/1060 (98%)	968 (93%)	76 (7%)	20	38

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	89	GLN
1	A	92	ASP
1	A	93	LEU
1	A	118	ASP
1	A	119	THR
1	A	134	ASP
1	A	154	SER
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	274	VAL
1	A	306	PHE
1	A	311	ASN
1	A	314	LYS
1	A	315	LEU
1	A	328	PRO
1	A	334	LEU
1	A	336	CYS
1	A	362	LEU
1	A	374	TYR
1	A	378	TYR
1	A	390	ASN
1	A	394	HIS
1	A	401	LEU
1	A	404	SER
1	A	418	LYS
1	A	419	ASP
1	A	422	ARG
1	A	433	LEU
1	A	446	PHE
1	A	471	LYS
1	A	488	LYS
1	A	503	GLU
1	A	532	ASN
1	A	539	ASN
1	A	552	PHE
1	A	582	ILE
1	A	601	ASN
1	A	606	TRP
1	A	612	CYS
1	B	27	GLU
1	B	89	GLN
1	B	92	ASP
1	B	93	LEU
1	B	118	ASP
1	B	119	THR
1	B	134	ASP
1	B	154	SER
1	B	227	LEU
1	B	274	VAL
1	B	306	PHE
1	B	311	ASN

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Mol	Chain	Res	Type
1	B	314	LYS
1	B	315	LEU
1	B	328	PRO
1	B	334	LEU
1	B	336	CYS
1	B	362	LEU
1	B	374	TYR
1	B	378	TYR
1	B	390	ASN
1	B	394	HIS
1	B	401	LEU
1	B	418	LYS
1	B	422	ARG
1	B	433	LEU
1	B	446	PHE
1	B	471	LYS
1	B	488	LYS
1	B	503	GLU
1	B	532	ASN
1	B	539	ASN
1	B	552	PHE
1	B	582	ILE
1	B	601	ASN
1	B	606	TRP
1	B	612	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	ASN
1	A	41	ASN
1	A	89	GLN
1	A	159	HIS
1	A	301	GLN
1	A	311	ASN
1	A	317	GLN
1	A	337	HIS
1	A	359	GLN
1	A	366	HIS
1	A	373	GLN
1	A	377	GLN

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Mol	Chain	Res	Type
1	A	379	GLN
1	A	380	HIS
1	A	381	GLN
1	A	410	HIS
1	A	429	ASN
1	A	464	ASN
1	A	466	ASN
1	A	514	GLN
1	A	516	GLN
1	A	527	GLN
1	A	532	ASN
1	A	539	ASN
1	A	554	ASN
1	A	610	ASN
1	B	31	ASN
1	B	33	ASN
1	B	41	ASN
1	B	89	GLN
1	B	159	HIS
1	B	301	GLN
1	B	311	ASN
1	B	337	HIS
1	B	359	GLN
1	B	366	HIS
1	B	373	GLN
1	B	377	GLN
1	B	379	GLN
1	B	380	HIS
1	B	381	GLN
1	B	410	HIS
1	B	429	ASN
1	B	464	ASN
1	B	466	ASN
1	B	514	GLN
1	B	516	GLN
1	B	527	GLN
1	B	532	ASN
1	B	539	ASN
1	B	554	ASN
1	B	601	ASN
1	B	610	ASN

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.