



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:29 PM UTC

PDB ID : 1J38 / pdb_00001j38
Title : Crystal Structure of Drosophila AnCE
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Deposited on : 2003-01-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

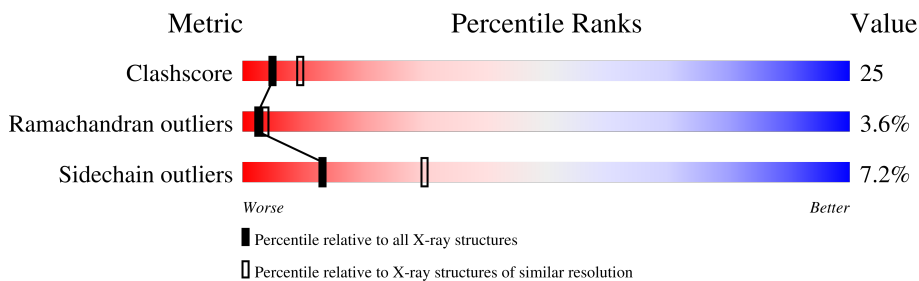
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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 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 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 (CCD ID: ZN) (formula: Zn).

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

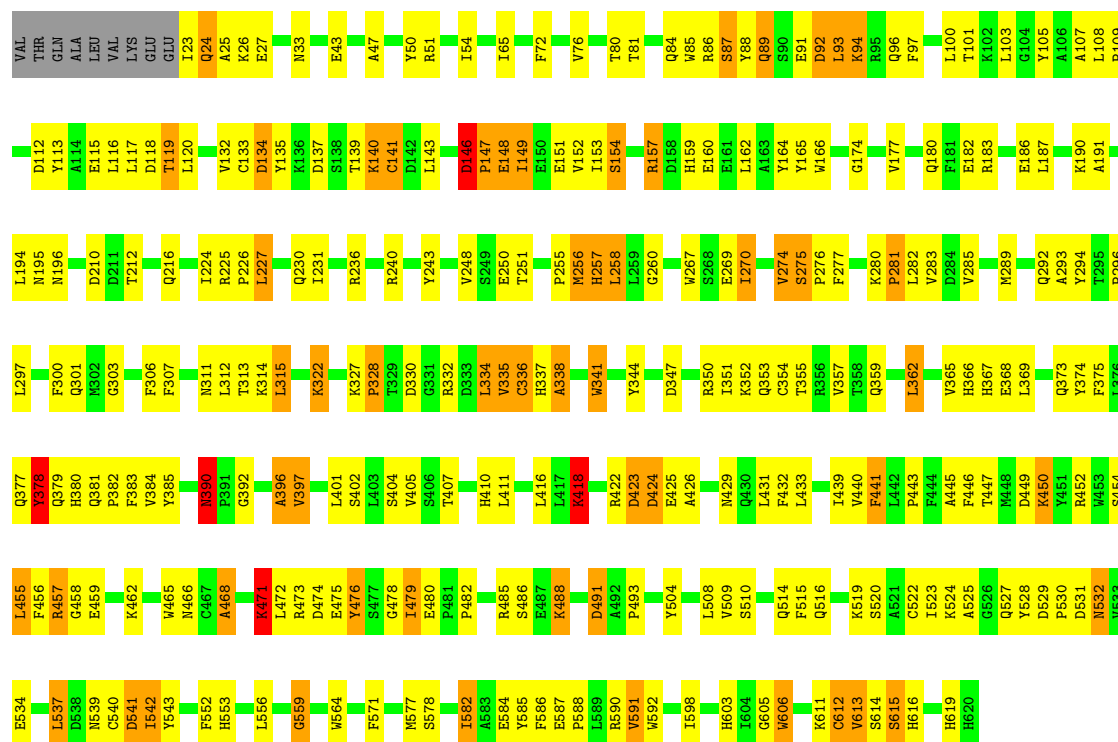
3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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.

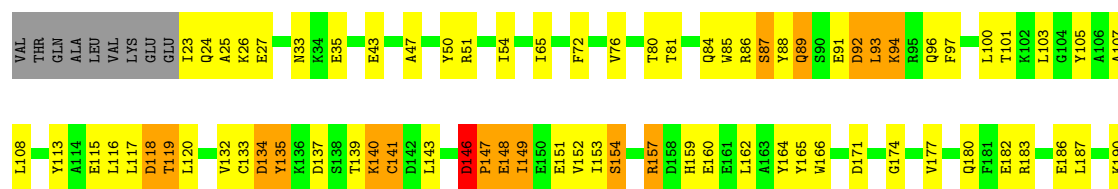
- Molecule 1: angiotensin converting enzyme

Chain A: 



- Molecule 1: angiotensin converting enzyme

Chain B: 



N539	C540	D541	I542	Y543	F552	H553	L556	G559	W564	F571	M577	S578	I582	A583	E584	Y585	F586	E587	P588	L589	R590	V591	W592	H603	T604	G605	W606	M610	K611	C612	V613	S614	S615	H616	H619	H620																
W465	N466	C467	A468	F469	W470	K471	L472	R473	D474	E475	Y476	S477	G478	L479	E480	P481	P482	R485	S486	E487	K488	D491	A492	P493	A494	K495	Y496	Y504	L508	V509	S510	Q514	F515	Q516	K519	S520	A521	C522	I523	K524	A525	G526	Q527	Y528	D529	P530	D531	N532	W533	E534	L537	D538
V384	Y385	K390	F391	G392	A396	V397	L401	S402	W405	S406	T407	H410	L411	L416	L417	K418	R422	D423	D424	E425	A426	N429	Q430	L431	F432	L433	T439	V440	F441	L442	P443	F444	A445	F446	T447	P448	D449	K450	Y451	R452	W453	S454	L455	F456	R457	G458	E459	K462				
A191	F306	F307	M310	N311	L312	T313	K314	L315	K322	K327	P328	T329	D330	G331	R332	D333	L334	V335	C336	H337	A338	W341	Y344	D347	R350	I351	K352	Q353	C354	T355	Q359	L362	V365	H366	H367	E368	L369	Q373	Y374	F375	L376	Q377	Y378	Q379	H380	Q381	P382	F383				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.51	0/5031	1.05	34/6814 (0.5%)
1	B	0.53	0/5031	1.05	35/6814 (0.5%)
All	All	0.52	0/10062	1.05	69/13628 (0.5%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	N-CA-C	-8.97	101.65	114.12
1	B	426	ALA	N-CA-C	-8.78	102.34	113.23
1	B	491	ASP	N-CA-C	8.74	123.24	112.23
1	A	491	ASP	N-CA-C	8.72	123.22	112.23
1	A	426	ALA	N-CA-C	-8.66	102.72	113.28
1	A	258	LEU	N-CA-C	-8.57	102.21	114.12
1	B	92	ASP	N-CA-C	-8.32	102.16	111.14
1	A	146	ASP	CA-C-N	-8.23	109.55	119.84
1	A	146	ASP	C-N-CA	-8.23	109.55	119.84
1	B	146	ASP	CA-C-N	-7.85	110.02	119.84
1	B	146	ASP	C-N-CA	-7.85	110.02	119.84
1	B	275	SER	CA-C-N	7.82	129.61	119.84
1	B	275	SER	C-N-CA	7.82	129.61	119.84
1	A	275	SER	CA-C-N	7.75	129.53	119.84
1	A	275	SER	C-N-CA	7.75	129.53	119.84
1	A	476	TYR	N-CA-C	7.66	121.11	111.69
1	A	92	ASP	N-CA-C	-7.63	102.89	111.14
1	B	396	ALA	N-CA-C	7.42	119.37	111.28
1	B	25	ALA	N-CA-C	-7.18	103.53	114.16
1	A	25	ALA	N-CA-C	-7.03	103.76	114.16
1	A	396	ALA	N-CA-C	6.93	118.83	111.28
1	A	357	VAL	N-CA-C	6.67	113.35	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LYS	N-CA-C	6.56	118.23	111.14
1	B	457	ARG	N-CA-C	-6.49	98.69	109.46
1	A	140	LYS	N-CA-C	6.45	118.11	111.14
1	B	390	ASN	CA-C-N	6.41	127.85	119.84
1	B	390	ASN	C-N-CA	6.41	127.85	119.84
1	A	149	ILE	N-CA-C	6.33	117.00	110.36
1	A	457	ARG	N-CA-C	-6.33	98.90	108.96
1	B	256	MET	N-CA-C	-6.23	102.27	110.43
1	A	81	THR	N-CA-C	-6.14	104.65	111.71
1	B	81	THR	N-CA-C	-6.06	104.74	111.71
1	A	390	ASN	CA-C-N	6.02	127.37	119.84
1	A	390	ASN	C-N-CA	6.02	127.37	119.84
1	B	341	TRP	N-CA-C	5.99	118.72	109.07
1	B	441	PHE	N-CA-C	5.96	117.45	111.07
1	A	468	ALA	N-CA-C	-5.91	104.92	111.71
1	B	149	ILE	N-CA-C	5.89	116.55	110.36
1	A	341	TRP	N-CA-C	5.88	118.54	109.07
1	B	231	ILE	N-CA-C	-5.88	106.08	111.67
1	A	231	ILE	N-CA-C	-5.87	106.09	111.67
1	A	441	PHE	N-CA-C	5.86	117.34	111.07
1	B	254	ILE	N-CA-C	5.84	114.68	108.95
1	B	471	LYS	N-CA-C	-5.84	105.04	111.82
1	B	476	TYR	N-CA-C	5.82	120.54	112.45
1	A	378	TYR	N-CA-C	5.78	119.93	112.41
1	B	378	TYR	N-CA-C	5.75	119.89	112.41
1	A	256	MET	N-CA-C	-5.72	102.94	110.43
1	A	344	TYR	N-CA-C	5.63	119.45	112.24
1	B	344	TYR	N-CA-C	5.55	119.34	112.24
1	B	468	ALA	N-CA-C	-5.55	105.23	111.28
1	B	230	GLN	N-CA-C	-5.30	106.77	113.18
1	A	230	GLN	N-CA-C	-5.27	106.80	113.18
1	B	450	LYS	N-CA-C	-5.27	105.65	111.71
1	A	541	ASP	N-CA-C	5.25	119.75	113.23
1	B	455	LEU	N-CA-C	-5.22	103.57	111.56
1	B	473	ARG	N-CA-C	-5.20	105.68	112.23
1	A	471	LYS	N-CA-C	-5.18	105.81	111.82
1	A	322	LYS	N-CA-C	5.18	119.23	113.02
1	B	281	PRO	N-CA-C	5.18	119.21	111.14
1	B	470	TRP	N-CA-C	5.17	117.00	111.36
1	A	615	SER	N-CA-C	5.17	121.80	110.80
1	B	525	ALA	N-CA-C	-5.13	101.96	109.81
1	A	450	LYS	N-CA-C	-5.12	105.83	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	ASP	N-CA-C	5.09	119.54	113.23
1	A	473	ARG	N-CA-C	-5.08	105.83	112.23
1	A	281	PRO	N-CA-C	5.06	119.03	111.14
1	A	455	LEU	N-CA-C	-5.03	103.87	111.56
1	B	135	TYR	N-CA-C	-5.03	106.25	112.38

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	4900	0	4696	233	2
1	B	4900	0	4696	238	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	470	2

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 (470) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:256:MET:O	1:A:257:HIS:ND1	2.08	0.85
1:B:143:LEU:CD2	1:B:148:GLU:HG2	2.07	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:509:VAL:HB	1:A:577:MET:HE1	1.60	0.82
1:A:488:LYS:HZ2	1:A:488:LYS:HB2	1.42	0.82
1:A:115:GLU:O	1:A:119:THR:HG23	1.79	0.81
1:B:509:VAL:HB	1:B:577:MET:HE1	1.63	0.81
1:B:488:LYS:HZ1	1:B:615:SER:HB2	1.46	0.79
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: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: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
1:A:516:GLN:NE2	1:A:578:SER:H	1.89	0.70
1:B:108:LEU:HD13	1:B:191:ALA:HB2	1.73	0.70
1:A:89:GLN:H	1:A:89:GLN:CD	2.00	0.70
1:A:89:GLN:H	1:A:89:GLN:NE2	1.91	0.69
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.27	0.69
1:A:330:ASP:OD1	1:A:332:ARG:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:HD22	1:A:534:GLU:H	1.39	0.69
1:B:89:GLN:CD	1:B:89:GLN:H	1.99	0.68
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:322:LYS:CB	1:A:350:ARG:HD3	2.23	0.67
1:A:148:GLU:CD	1:A:148:GLU:H	2.00	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:A:509:VAL:HB	1:A:577:MET:CE	2.24	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:148:GLU:CD	1:B:148:GLU:H	2.04	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:177:VAL:HG22	1:A:180:GLN:HB2	1.79	0.65
1:A:285:VAL:CG1	1:A:416:LEU:HB3	2.26	0.65
1:B:509:VAL:HB	1:B:577:MET:CE	2.26	0.65
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.31	0.65
1:B:516:GLN:HE22	1:B:578:SER:H	1.41	0.65
1:A:43:GLU:HA	1:A:65:ILE:HG21	1.79	0.64
1:A:166:TRP:CH2	1:A:485:ARG:HD2	2.33	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:B:532:ASN:ND2	1:B:534:GLU:H	1.98	0.62
1:A:85:TRP:C	1:A:87:SER:H	2.08	0.61
1:A:297:LEU:HG	1:A:301:GLN:NE2	2.15	0.61
1:B:166:TRP:HH2	1:B:485:ARG:HD2	1.64	0.61
1:B:285:VAL:H	1:B:359:GLN:NE2	1.98	0.61
1:A:132:VAL:HG22	1:A:149:ILE:HD11	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TRP:C	1:B:87:SER:H	2.09	0.60
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:528:TYR:CE1	1:A:537:LEU:HB2	2.38	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:587:GLU:OE2	1:A:590:ARG:NH2	2.36	0.59
1:B:285:VAL:HG12	1:B:285:VAL:O	2.03	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:72:PHE:O	1:B:76:VAL:HG23	2.03	0.58
1:B:270:ILE:HD12	1:B:270:ILE:O	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:85:TRP:HA	1:B:88:TYR:CD1	2.38	0.58
1:B:520:SER:HB2	1:B:571:PHE:HE2	1.68	0.58
1:A:162:LEU:HD13	1:A:257:HIS:O	2.02	0.58
1:B:537:LEU:HD13	1:B:537:LEU:O	2.03	0.58
1:A:390:ASN:HD22	1:A:564:TRP:CG	2.21	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:A:72:PHE:O	1:A:76:VAL:HG23	2.04	0.58
1:B:251:THR:HG22	1:B:603:HIS:NE2	2.19	0.58
1:B:390:ASN:HD22	1:B:564:TRP:CG	2.22	0.58
1:A:520:SER:HB2	1:A:571:PHE:HE2	1.69	0.57
1:A:96:GLN:O	1:A:100:LEU:HD23	2.04	0.57
1:B:613:VAL:HG23	1:B:614:SER:N	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASP:OD2	1:A:332:ARG:HD3	2.05	0.56
1:A:537:LEU:HD13	1:A:537:LEU:O	2.05	0.56
1:B:257:HIS:ND1	1:B:482:PRO:HB3	2.21	0.56
1:B:385:TYR:HB3	1:B:559:GLY:O	2.04	0.56
1:A:85:TRP:HA	1:A:88:TYR:CD1	2.40	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:B:267:TRP:O	1:B:270:ILE:HG13	2.04	0.56
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.59	0.56
1:B:541:ASP:O	1:B:543:TYR:N	2.39	0.56
1:A:251:THR:HG22	1:A:603:HIS:CE1	2.41	0.56
1:A:471:LYS:O	1:A:471:LYS:HD3	2.05	0.56
1:B:85:TRP:O	1:B:87:SER:N	2.38	0.56
1:A:105:TYR:O	1:A:108:LEU:HB2	2.05	0.56
1:B:162:LEU:HD13	1:B:257:HIS:O	2.04	0.56
1:B:280:LYS:HB3	1:B:281:PRO:HD2	1.88	0.56
1:B:587:GLU:OE2	1:B:590:ARG:NH2	2.38	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:105:TYR:O	1:B:108:LEU:HB2	2.05	0.56
1:A:446:PHE:O	1:A:450:LYS:HB2	2.06	0.56
1:B:277:PHE:H	1:B:429:ASN:HD21	1.53	0.56
1:A:135:TYR:HB2	1:A:164:TYR:CD2	2.41	0.56
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.31	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:224:ILE:HG12	1:B:582:ILE:HD12	1.88	0.55
1:B:471:LYS:O	1:B:475:GLU:HG3	2.06	0.55
1:A:154:SER:HB2	1:A:269:GLU:CG	2.29	0.55
1:A:256:MET:O	1:A:257:HIS:CB	2.53	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
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:A:541:ASP:C	1:A:543:TYR:H	2.15	0.55
1:B:116:LEU:O	1:B:120:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:183:ARG:HH12	1:B:187:LEU:CD2	2.19	0.55
1:B:251:THR:HG22	1:B:603:HIS:CE1	2.41	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:410:HIS:HB2	1:B:541:ASP:CG	2.33	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:51:ARG:HD2	1:A:341:TRP:CZ2	2.43	0.54
1:A:256:MET:O	1:A:257:HIS:CG	2.60	0.54
1:B:377:GLN:HE22	1:B:553:HIS:CD2	2.25	0.54
1:B:515:PHE:CD2	1:B:582:ILE:HG23	2.43	0.54
1:B:159:HIS:CE1	1:B:160:GLU:HG3	2.43	0.54
1:A:159:HIS:CE1	1:A:160:GLU:HG3	2.43	0.54
1:B:405:VAL:O	1:B:411:LEU:HD21	2.08	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:422:ARG:HD2	1:B:422:ARG:O	2.07	0.53
1:B:471:LYS:O	1:B:471:LYS:HD3	2.07	0.53
1:A:143:LEU:HB3	1:A:148:GLU:HB2	1.89	0.53
1:A:422:ARG:HD2	1:A:422:ARG:O	2.08	0.53
1:A:478:GLY:O	1:A:479:ILE:HD12	2.07	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:HD12	1:B:508:LEU:O	2.09	0.53
1:B:457:ARG:O	1:B:459:GLU:N	2.41	0.53
1:B:251:THR:HG22	1:B:603:HIS:CG	2.44	0.52
1:A:334:LEU:HD21	1:A:336:CYS:SG	2.50	0.52
1:A:431:LEU:CD1	1:A:588:PRO:HG2	2.39	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
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.34	0.52
1:B:236:ARG:NH2	1:B:603:HIS:O	2.39	0.52
1:B:327:LYS:HB2	1:B:354:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLY:O	1:B:479:ILE:HD12	2.10	0.52
1:B:520:SER:HB2	1:B:571:PHE:CE2	2.44	0.52
1:A:251:THR:HG22	1:A:603:HIS:CG	2.44	0.52
1:B:532:ASN:HD22	1:B:532:ASN:C	2.18	0.52
1:A:405:VAL:O	1:A:411:LEU:HD21	2.10	0.52
1:B:143:LEU:HB3	1:B:148:GLU:HB2	1.91	0.52
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.45	0.52
1:A:227:LEU:HD13	1:A:439:ILE:HD13	1.92	0.52
1:A:137:ASP:C	1:A:139:THR:H	2.18	0.52
1:A:402:SER:HA	1:A:405:VAL:HG22	1.92	0.51
1:A:527:GLN:HB3	1:A:540:CYS:HB2	1.92	0.51
1:B:362:LEU:O	1:B:366:HIS:HD2	1.93	0.51
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:532:ASN:HD22	1:A:532:ASN:C	2.18	0.51
1:B:132:VAL:HG22	1:B:149:ILE:HD11	1.91	0.51
1:A:224:ILE:HG12	1:A:582:ILE:HD12	1.91	0.51
1:B:137:ASP:C	1:B:139:THR:H	2.18	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:B:541:ASP:C	1:B:543:TYR:H	2.18	0.51
1:B:96:GLN:O	1:B:100:LEU:CD2	2.58	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:A:133:CYS:HA	1:A:141:CYS:HA	1.91	0.51
1:A:541:ASP:O	1:A:541:ASP:OD2	2.29	0.51
1:B:537:LEU:HD13	1:B:585:TYR:HD1	1.76	0.51
1:A:338:ALA:HB2	1:A:353:GLN:HG3	1.92	0.51
1:A:362:LEU:O	1:A:366:HIS:HD2	1.94	0.51
1:B:152:VAL:HG11	1:B:165:TYR:CE2	2.45	0.51
1:B:154:SER:HB2	1:B:269:GLU:CG	2.33	0.51
1:B:454:SER:O	1:B:457:ARG:O	2.28	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:A:335:VAL:O	1:A:352:LYS:NZ	2.44	0.50
1:B:113:TYR:CE2	1:B:117:LEU:HD11	2.46	0.50
1:B:335:VAL:O	1:B:352:LYS:NZ	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:NH1	1:B:187:LEU:HD21	2.26	0.50
1:B:330:ASP:CG	1:B:332:ARG:HD3	2.37	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: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:B:392:GLY:HA3	1:B:509:VAL:CG2	2.41	0.50
1:A:528:TYR:CG	1:A:537:LEU:HD23	2.46	0.50
1:A:96:GLN:O	1:A:100:LEU:CD2	2.59	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: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:A:307:PHE:O	1:A:312:LEU:HB2	2.11	0.49
1:B:143:LEU:HD22	1:B:148:GLU:CB	2.42	0.49
1:A:439:ILE:HD11	1:A:586:PHE:CD2	2.47	0.49
1:B:153:ILE:O	1:B:153:ILE:HG22	2.12	0.49
1:A:190:LYS:O	1:A:194:LEU:HD13	2.12	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: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:B:441:PHE:CE2	1:B:445:ALA:HB2	2.47	0.49
1:A:210:ASP:OD1	1:A:216:GLN:NE2	2.44	0.49
1:B:285:VAL:HG23	1:B:359:GLN:NE2	2.27	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:422:ARG:O	1:B:423:ASP:C	2.55	0.49
1:B:133:CYS:HA	1:B:141:CYS:HA	1.93	0.49
1:A:422:ARG:O	1:A:423:ASP:C	2.56	0.48
1:A:195:ASN:O	1:A:196:ASN:HB2	2.13	0.48
1:B:330:ASP:C	1:B:332:ARG:H	2.21	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:A:306:PHE:CE2	1:A:543:TYR:HA	2.48	0.48
1:A:330:ASP:C	1:A:332:ARG:H	2.22	0.48
1:B:50:TYR:CZ	1:B:54:ILE:HG23	2.49	0.48
1:B:195:ASN:O	1:B:196:ASN:HB2	2.14	0.48
1:B:541:ASP:O	1:B:541:ASP:OD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LYS:HD3	1:A:475:GLU:HG3	1.96	0.48
1:A:485:ARG:O	1:A:612:CYS:HA	2.13	0.48
1:A:351:ILE:HD13	1:A:368:GLU:HB3	1.96	0.48
1:B:439:ILE:HD11	1:B:586:PHE:CD2	2.49	0.48
1:B:471:LYS:HD3	1:B:475:GLU:HG3	1.96	0.48
1:B:605:GLY:C	1:B:606:TRP:CD1	2.92	0.47
1:B:289:MET:O	1:B:294:TYR:HB2	2.14	0.47
1:A:33:ASN:ND2	1:A:384:VAL:H	2.11	0.47
1:A:407:THR:HB	1:A:539:ASN:HD22	1.79	0.47
1:A:441:PHE:CE2	1:A:445:ALA:HB2	2.48	0.47
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:B:537:LEU:CD1	1:B:585:TYR:HD1	2.28	0.47
1:A:276:PRO:HD2	1:A:429:ASN:ND2	2.30	0.47
1:A:276:PRO:HD3	1:A:432:PHE:CD1	2.50	0.47
1:A:418:LYS:HD2	1:A:418:LYS:N	2.29	0.47
1:B:380:HIS:CD2	1:B:380:HIS:H	2.33	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:A:85:TRP:C	1:A:87:SER:N	2.73	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: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:B:306:PHE:CE2	1:B:543:TYR:HA	2.50	0.46
1:B:485:ARG:O	1:B:612:CYS:HA	2.16	0.46
1:A:285:VAL:HG23	1:A:359:GLN:NE2	2.30	0.46
1:A:605:GLY:C	1:A:606:TRP:CD1	2.94	0.46
1:B:351:ILE:HD13	1:B:368:GLU:HB3	1.97	0.46
1:B:439:ILE:HD11	1:B:586:PHE:CG	2.51	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:A:328:PRO:HG2	1:A:332:ARG:NH2	2.30	0.46
1:B:85:TRP:C	1:B:87:SER:N	2.75	0.46
1:B:140:LYS:HB3	1:B:140:LYS:HE2	1.77	0.46
1:B:285:VAL:HG21	1:B:411:LEU:HD13	1.98	0.46
1:A:143:LEU:HD22	1:A:148:GLU:CB	2.45	0.45
1:A:289:MET:HE1	1:A:362:LEU:HG	1.97	0.45
1:B:100:LEU:HD21	1:B:384:VAL:HB	1.98	0.45
1:B:277:PHE:CE2	1:B:425:GLU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:OD1	1:B:485:ARG:NH2	2.36	0.45
1:B:276:PRO:HD2	1:B:429:ASN:ND2	2.30	0.45
1:A:277:PHE:CE2	1:A:425:GLU:HB3	2.51	0.45
1:A:519:LYS:HE3	1:A:584:GLU:OE2	2.16	0.45
1:B:153:ILE:O	1:B:260:GLY:HA2	2.16	0.45
1:B:328:PRO:HG2	1:B:332:ARG:NH2	2.31	0.45
1:A:488:LYS:NZ	1:A:615:SER:HB2	2.31	0.45
1:B:614:SER:O	1:B:615:SER:HB3	2.17	0.45
1:A:488:LYS:HZ2	1:A:488:LYS:CB	2.19	0.45
1:B:450:LYS:HE2	1:B:476:TYR:OH	2.17	0.45
1:A:382:PRO:O	1:A:383:PHE:C	2.60	0.45
1:A:396:ALA:O	1:A:397:VAL:C	2.60	0.45
1:B:289:MET:HE1	1:B:362:LEU:HG	1.99	0.45
1:A:353:GLN:CD	1:A:355:THR:HG22	2.42	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:274:VAL:O	1:B:274:VAL:HG13	2.16	0.45
1:B:310:MET:HB2	1:B:312:LEU:HD12	1.99	0.45
1:A:100:LEU:HD21	1:A:384:VAL:HB	1.99	0.44
1:A:108:LEU:HD13	1:A:191:ALA:CB	2.43	0.44
1:A:275:SER:OG	1:A:282:LEU:HD11	2.17	0.44
1:A:375:PHE:HA	1:A:378:TYR:CE1	2.52	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:B:353:GLN:CD	1:B:355:THR:HG22	2.42	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:85:TRP:HA	1:B:88:TYR:CG	2.53	0.44
1:A:380:HIS:H	1:A:380:HIS:CD2	2.35	0.44
1:A:439:ILE:HD11	1:A:586:PHE:CG	2.53	0.44
1:A:537:LEU:CD1	1:A:585:TYR:HD1	2.31	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:455:LEU:O	1:A:456:PHE:C	2.60	0.44
1:A:256:MET:O	1:A:257:HIS:HB3	2.16	0.44
1:A:524:LYS:HE3	1:A:571:PHE:O	2.18	0.44
1:B:89:GLN:CD	1:B:89:GLN:N	2.72	0.44
1:B:353:GLN:NE2	1:B:355:THR:HG22	2.33	0.44
1:B:466:ASN:ND2	1:B:491:ASP:H	2.16	0.44
1:B:474:ASP:O	1:B:475:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:SER:OG	1:B:616:HIS:N	2.50	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:B:455:LEU:O	1:B:456:PHE:C	2.61	0.43
1:A:177:VAL:O	1:A:177:VAL:HG13	2.18	0.43
1:B:524:LYS:HE3	1:B:571:PHE:O	2.18	0.43
1:A:23:ILE:HG12	1:A:23:ILE:O	2.18	0.43
1:A:275:SER:HA	1:A:276:PRO:HD3	1.79	0.43
1:A:285:VAL:HG21	1:A:411:LEU:HD13	1.99	0.43
1:A:390:ASN:OD1	1:A:390:ASN:C	2.61	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:523:ILE:C	1:A:525:ALA:N	2.77	0.43
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:475:GLU:O	1:A:606:TRP:HH2	2.01	0.43
1:A:615:SER:OG	1:A:616:HIS:N	2.51	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:153:ILE:HG22	1:A:153:ILE:O	2.18	0.43
1:A:353:GLN:NE2	1:A:355:THR:HG22	2.34	0.43
1:A:392:GLY:HA3	1:A:509:VAL:HG21	2.01	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:B:327:LYS:CB	1:B:354:CYS:SG	3.07	0.43
1:B:334:LEU:HD22	1:B:335:VAL:C	2.44	0.43
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.54	0.43
1:B:177:VAL:HG13	1:B:177:VAL:O	2.17	0.43
1:A:313:THR:HB	1:A:373:GLN:HE22	1.84	0.42
1:B:523:ILE:C	1:B:525:ALA:H	2.26	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:A:337:HIS:O	1:A:338:ALA:C	2.62	0.42
1:B:382:PRO:O	1:B:383:PHE:C	2.61	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:A:153:ILE:O	1:A:260:GLY:HA2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:O	1:A:117:LEU:HG	2.19	0.42
1:A:541:ASP:C	1:A:543:TYR:N	2.75	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:423:ASP:O	1:B:424:ASP:HB2	2.20	0.42
1:B:143:LEU:HD22	1:B:148:GLU:HB3	2.02	0.42
1:B:146:ASP:CB	1:B:147:PRO:HD3	2.28	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:182:GLU:O	1:A:186:GLU:HG3	2.20	0.41
1:A:183:ARG:NH1	1:A:187:LEU:CD2	2.83	0.41
1:A:23:ILE:O	1:A:24:GLN:O	2.38	0.41
1:A:51:ARG:HD2	1:A:341:TRP:HZ2	1.84	0.41
1:A:84:GLN:O	1:A:88:TYR:CE1	2.74	0.41
1:A:250:GLU:O	1:A:251:THR:OG1	2.31	0.41
1:A:474:ASP:O	1:A:475:GLU:C	2.62	0.41
1:A:523:ILE:C	1:A:525:ALA:H	2.26	0.41
1:B:118:ASP:O	1:B:119:THR:C	2.61	0.41
1:A:529:ASP:O	1:A:531:ASP:N	2.54	0.41
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:A:292:GLN:O	1:A:293:ALA:HB3	2.21	0.41
1:B:528:TYR:OH	1:B:584:GLU:OE1	2.37	0.41
1:A:157:ARG:HA	1:A:243:TYR:HH	1.85	0.41
1:A:212:THR:O	1:A:216:GLN:HG3	2.20	0.41
1:A:423:ASP:O	1:A:424:ASP:HB2	2.20	0.41
1:B:337:HIS:O	1:B:338:ALA:C	2.63	0.41
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.79	0.41
1:A:366:HIS:O	1:A:367:HIS:C	2.63	0.41
1:A:449:ASP:OD2	1:A:452:ARG:NH2	2.47	0.41
1:B:390:ASN:OD1	1:B:390:ASN:C	2.64	0.41
1:B:610:ASN:HD22	1:B:610:ASN:HA	1.69	0.41
1:A:267:TRP:CE2	1:A:440:VAL:HG11	2.56	0.41
1:B:381:GLN:HE21	1:B:382:PRO:CD	2.34	0.41
1:B:613:VAL:HG23	1:B:614:SER:H	1.86	0.41
1:A:478:GLY:C	1:A:479:ILE:HD12	2.46	0.41
1:B:311:ASN:HD22	1:B:311:ASN:HA	1.57	0.41
1:A:109:PRO:CG	1:A:112:ASP:OD2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:CB	1:A:354:CYS:SG	3.09	0.40
1:A:381:GLN:HE21	1:A:382:PRO:CD	2.34	0.40
1:B:523:ILE:C	1:B:525:ALA:N	2.76	0.40
1:B:380:HIS:CD2	1:B:380:HIS:N	2.89	0.40
1:B:410:HIS:HD2	1:B:541:ASP:OD1	2.05	0.40
1:B:495:LYS:O	1:B:496:TYR:C	2.65	0.40
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.49	0.40
1:B:529:ASP:O	1:B:531:ASP:N	2.54	0.40
1:B:270:ILE:HG13	1:B:270:ILE:H	1.81	0.40
1:B:275:SER:HA	1:B:276:PRO:HD3	1.80	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	Interatomic distance (Å)	Clash overlap (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%)	3	4
1	B	596/607 (98%)	518 (87%)	56 (9%)	22 (4%)	2	3
All	All	1192/1214 (98%)	1035 (87%)	114 (10%)	43 (4%)	2	4

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	147	PRO

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Mol	Chain	Res	Type
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
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%)	484 (93%)	38 (7%)	13	29
1	B	522/530 (98%)	485 (93%)	37 (7%)	13	31
All	All	1044/1060 (98%)	969 (93%)	75 (7%)	13	30

All (75) 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	94	LYS
1	A	103	LEU
1	A	118	ASP
1	A	119	THR
1	A	134	ASP
1	A	151	GLU
1	A	154	SER
1	A	157	ARG
1	A	227	LEU
1	A	270	ILE
1	A	274	VAL
1	A	311	ASN
1	A	314	LYS
1	A	315	LEU
1	A	328	PRO
1	A	334	LEU
1	A	335	VAL
1	A	336	CYS
1	A	362	LEU
1	A	374	TYR
1	A	378	TYR
1	A	390	ASN
1	A	401	LEU

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Mol	Chain	Res	Type
1	A	404	SER
1	A	418	LYS
1	A	433	LEU
1	A	471	LYS
1	A	479	ILE
1	A	488	LYS
1	A	532	ASN
1	A	537	LEU
1	A	582	ILE
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	94	LYS
1	B	103	LEU
1	B	118	ASP
1	B	119	THR
1	B	134	ASP
1	B	151	GLU
1	B	154	SER
1	B	157	ARG
1	B	227	LEU
1	B	270	ILE
1	B	274	VAL
1	B	311	ASN
1	B	314	LYS
1	B	315	LEU
1	B	328	PRO
1	B	334	LEU
1	B	335	VAL
1	B	336	CYS
1	B	362	LEU
1	B	374	TYR
1	B	378	TYR
1	B	390	ASN
1	B	401	LEU
1	B	418	LYS
1	B	433	LEU
1	B	471	LYS
1	B	479	ILE

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Mol	Chain	Res	Type
1	B	488	LYS
1	B	532	ASN
1	B	537	LEU
1	B	582	ILE
1	B	606	TRP
1	B	612	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) 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	337	HIS
1	A	353	GLN
1	A	359	GLN
1	A	366	HIS
1	A	373	GLN
1	A	377	GLN
1	A	379	GLN
1	A	380	HIS
1	A	381	GLN
1	A	410	HIS
1	A	429	ASN
1	A	430	GLN
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	33	ASN
1	B	41	ASN
1	B	89	GLN
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	159	HIS
1	B	215	GLN
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	430	GLN
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 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 oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.