



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:37 am BST

PDB ID : 1J37
Title : Crystal Structure of Drosophila AnCE
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Deposited on : 2003-01-20
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

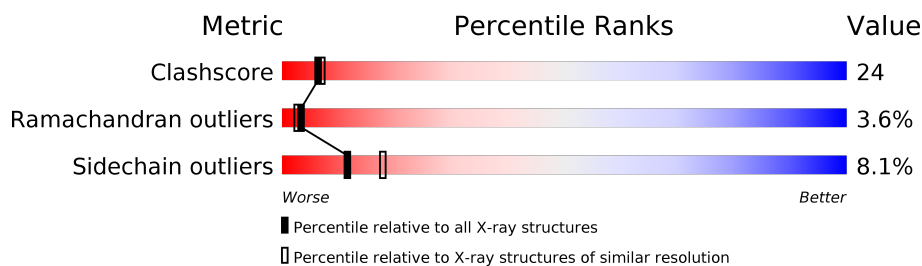
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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 9830 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			

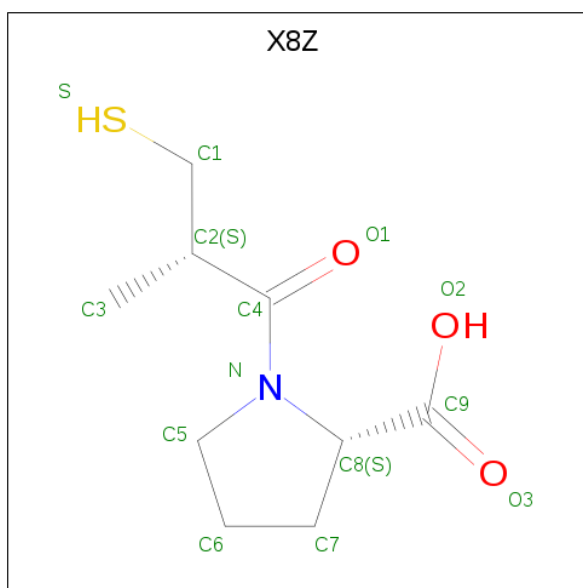
There are 16 discrepancies between the modelled and reference sequences:

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 (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 L-CAPTOPRIL (three-letter code: X8Z) (formula: $C_9H_{15}NO_3S$).



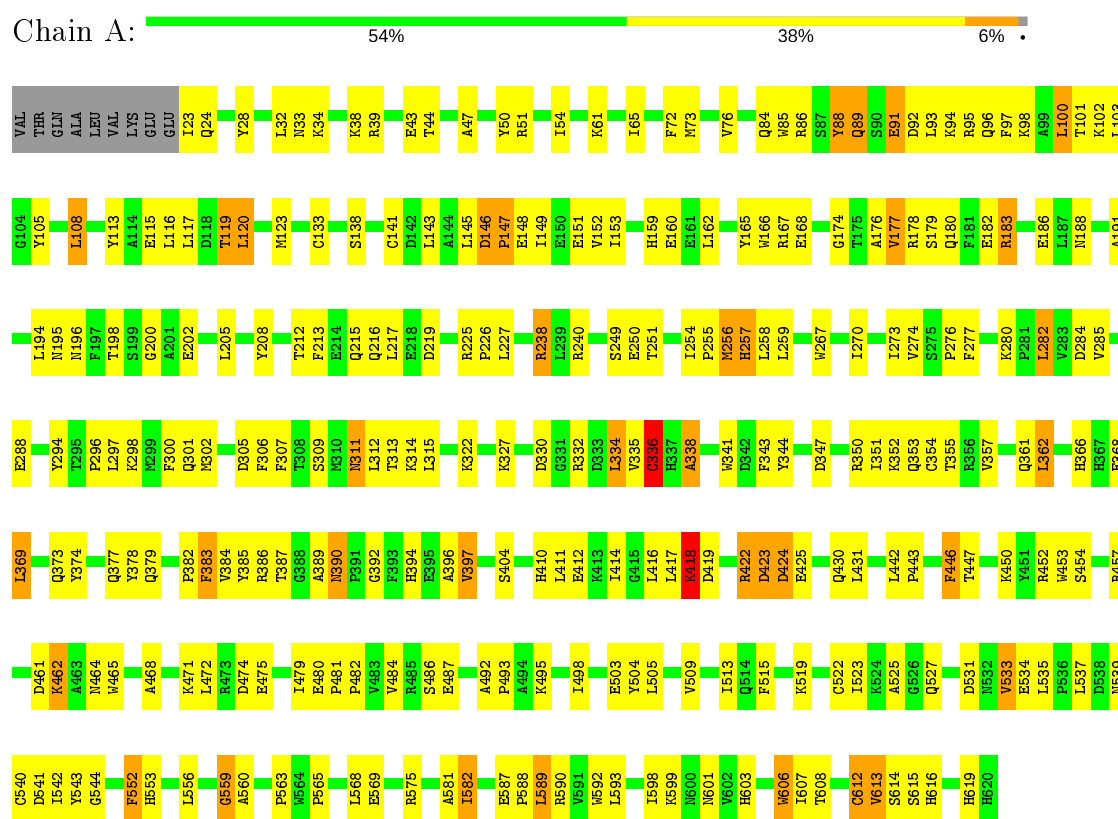
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

3 Residue-property plots

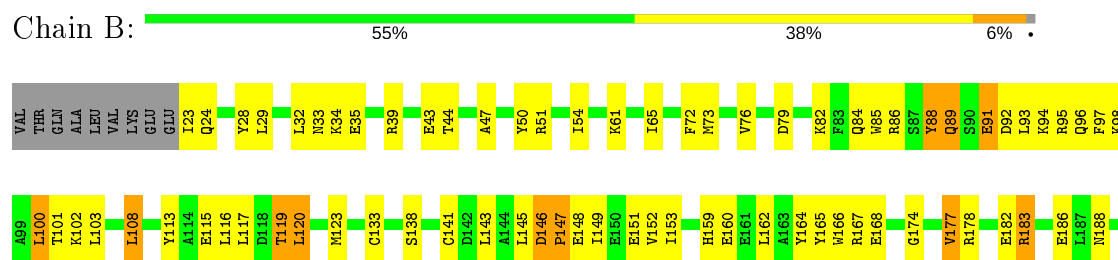
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



- Molecule 1: angiotensin converting enzyme



A191	E288	E368	L537
L194	M289	L369	D538
N195	Y294	Q373	N539
N196	T295	Y374	C540
F197	P296	K462	D641
T198	L297	A463	I542
S199	K298	N464	Y543
G200	M299	W465	G544
A201	F300	A468	F552
E202	Q301	H553	H553
Y208	M302	L556	L556
T212	D305	K471	G559
F213	F306	L472	A560
F213	F307	E473	P563
E214	T308	E475	P564
Q215	S309	I479	P565
Q216	M310	E480	L568
L217	N311	P481	E569
E218	L312	P482	R575
D219	T313	V483	A581
R225	K314	V484	I582
P226	L315	R485	E587
L227	K322	S486	P588
R238	K327	E487	I589
L239	K327	A492	R590
R240	D330	P493	V591
D245	G331	A494	L593
V248	R332	K495	M601
S249	D333	I498	V602
E250	L334	E503	H603
T251	G336	Y504	W606
I254	H337	L505	I607
P255	A338	V509	T608
M256	W341	I513	C612
H257	D342	Q514	V613
L258	F343	F515	S614
L259	Y344	Q516	S615
I270	D347	K519	H616
I273	R350	G522	H619
V274	I351	I523	H620
S275	Q353	K524	
P276	C354	A525	
F277	T355	G526	
K280	R356	Q527	
P281	V357	D531	
L282	Q361	M532	
V283	L362	V533	
D284	H366	E534	
V285	H367	L535	
		P536	

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 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: X8Z, 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	0.46	0/5031	0.67	1/6814 (0.0%)
1	B	0.46	0/5031	0.68	0/6814
All	All	0.46	0/10062	0.68	1/13628 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	CYS	CA-CB-SG	-5.93	103.33	114.00

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	222	0
1	B	4900	0	4696	231	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
All	All	9830	0	9418	450	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 24.

All (450) 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:533:VAL:HG22	1:A:534:GLU:H	1.20	1.06
1:B:533:VAL:HG22	1:B:534:GLU:H	1.21	1.04
1:B:418:LYS:HE3	1:B:418:LYS:H	1.29	0.95
1:A:347:ASP:H	1:A:379:GLN:HE22	1.14	0.91
1:A:418:LYS:H	1:A:418:LYS:HE3	1.34	0.91
1:B:347:ASP:H	1:B:379:GLN:HE22	1.12	0.90
1:B:347:ASP:H	1:B:379:GLN:NE2	1.70	0.88
1:A:115:GLU:O	1:A:119:THR:HG22	1.74	0.87
1:A:92:ASP:O	1:A:96:GLN:HG3	1.73	0.87
1:A:347:ASP:H	1:A:379:GLN:NE2	1.71	0.87
1:B:256:MET:O	1:B:258:LEU:N	2.08	0.86
1:B:115:GLU:O	1:B:119:THR:HG22	1.75	0.85
1:A:256:MET:O	1:A:258:LEU:N	2.10	0.84
1:B:92:ASP:O	1:B:96:GLN:HG3	1.79	0.82
1:B:613:VAL:HG23	1:B:614:SER:N	1.94	0.81
1:A:462:LYS:HB3	1:A:462:LYS:NZ	1.96	0.81
1:A:486:SER:HB2	1:A:614:SER:HA	1.63	0.80
1:A:174:GLY:HA2	1:A:493:PRO:HB2	1.63	0.80
1:B:541:ASP:O	1:B:543:TYR:N	2.15	0.80
1:A:541:ASP:O	1:A:543:TYR:N	2.15	0.80
1:A:613:VAL:HG23	1:A:614:SER:N	1.97	0.79
1:B:486:SER:HB2	1:B:614:SER:HA	1.64	0.78
1:A:133:CYS:HA	1:A:141:CYS:HA	1.66	0.78
1:B:133:CYS:HA	1:B:141:CYS:HA	1.66	0.77
1:B:174:GLY:HA2	1:B:493:PRO:HB2	1.66	0.77
1:A:344:TYR:HA	1:A:386:ARG:NH2	2.01	0.76
1:B:462:LYS:HB3	1:B:462:LYS:NZ	1.99	0.76
1:B:422:ARG:HD3	1:B:422:ARG:O	1.86	0.75
1:A:422:ARG:O	1:A:422:ARG:HD3	1.88	0.74
1:A:347:ASP:N	1:A:379:GLN:HE22	1.86	0.74
1:B:344:TYR:HA	1:B:386:ARG:NH2	2.03	0.73
1:B:330:ASP:OD1	1:B:332:ARG:HD3	1.89	0.73
1:B:347:ASP:N	1:B:379:GLN:HE22	1.86	0.73
1:A:270:ILE:O	1:A:274:VAL:HG12	1.90	0.72
1:B:613:VAL:HG23	1:B:614:SER:H	1.53	0.71
1:A:330:ASP:OD1	1:A:332:ARG:HD3	1.90	0.71
1:B:270:ILE:O	1:B:274:VAL:HG12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HB3	1:B:462:LYS:HZ3	1.56	0.71
1:B:251:THR:HG22	1:B:603:HIS:CD2	2.26	0.70
1:B:256:MET:C	1:B:258:LEU:H	1.93	0.70
1:B:533:VAL:HG22	1:B:534:GLU:N	2.03	0.70
1:A:147:PRO:HG2	1:A:148:GLU:OE1	1.92	0.70
1:A:47:ALA:O	1:A:51:ARG:HG3	1.92	0.70
1:B:47:ALA:O	1:B:51:ARG:HG3	1.92	0.70
1:A:256:MET:C	1:A:258:LEU:H	1.95	0.69
1:B:285:VAL:HG13	1:B:416:LEU:HB3	1.73	0.69
1:B:285:VAL:CG1	1:B:416:LEU:HB3	2.22	0.69
1:A:89:GLN:H	1:A:89:GLN:NE2	1.91	0.69
1:B:277:PHE:HB3	1:B:280:LYS:HB2	1.75	0.69
1:B:285:VAL:HG21	1:B:411:LEU:HD13	1.75	0.69
1:A:285:VAL:CG1	1:A:416:LEU:HB3	2.23	0.69
1:A:198:THR:HB	1:A:202:GLU:HG3	1.74	0.69
1:B:282:LEU:HB3	1:B:284:ASP:OD1	1.93	0.69
1:A:533:VAL:HG22	1:A:534:GLU:N	2.02	0.68
1:A:462:LYS:H	1:A:462:LYS:HD2	1.58	0.68
1:A:256:MET:O	1:A:257:HIS:ND1	2.26	0.68
1:B:198:THR:HB	1:B:202:GLU:HG3	1.74	0.68
1:A:285:VAL:HG13	1:A:416:LEU:HB3	1.75	0.68
1:A:285:VAL:HG21	1:A:411:LEU:HD13	1.75	0.67
1:B:147:PRO:HG2	1:B:148:GLU:OE1	1.93	0.67
1:A:251:THR:HG22	1:A:603:HIS:CD2	2.30	0.67
1:B:541:ASP:C	1:B:543:TYR:H	1.98	0.67
1:B:89:GLN:H	1:B:89:GLN:NE2	1.91	0.67
1:B:238:ARG:NH1	1:B:273:ILE:O	2.28	0.67
1:A:541:ASP:C	1:A:543:TYR:H	1.98	0.66
1:A:146:ASP:HB3	1:A:147:PRO:CD	2.25	0.66
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.61	0.66
1:A:277:PHE:HB3	1:A:280:LYS:HB2	1.77	0.66
1:A:613:VAL:HG23	1:A:614:SER:H	1.58	0.66
1:A:462:LYS:HB3	1:A:462:LYS:HZ3	1.60	0.66
1:B:256:MET:O	1:B:257:HIS:ND1	2.29	0.66
1:B:462:LYS:H	1:B:462:LYS:HD2	1.60	0.66
1:A:552:PHE:O	1:A:556:LEU:HG	1.97	0.65
1:A:254:ILE:HG21	1:A:259:LEU:HD21	1.77	0.65
1:B:254:ILE:HG21	1:B:259:LEU:HD21	1.79	0.64
1:A:282:LEU:HB3	1:A:284:ASP:OD1	1.97	0.64
1:A:315:LEU:HD21	1:A:369:LEU:HD11	1.80	0.64
1:B:51:ARG:HD2	1:B:341:TRP:CH2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:HD2	1:A:341:TRP:CH2	2.33	0.64
1:B:146:ASP:HB3	1:B:147:PRO:CD	2.28	0.64
1:B:527:GLN:HE21	1:B:540:CYS:HA	1.62	0.64
1:A:527:GLN:HE21	1:A:540:CYS:HA	1.62	0.64
1:A:72:PHE:O	1:A:76:VAL:HG23	1.97	0.63
1:A:533:VAL:CG2	1:A:534:GLU:H	2.02	0.63
1:A:116:LEU:O	1:A:120:LEU:HB2	1.99	0.62
1:B:51:ARG:HD2	1:B:341:TRP:HH2	1.64	0.62
1:A:51:ARG:HD2	1:A:341:TRP:HH2	1.64	0.62
1:B:178:ARG:HG2	1:B:178:ARG:HH11	1.64	0.61
1:B:85:TRP:HA	1:B:88:TYR:CD1	2.35	0.61
1:A:238:ARG:NH1	1:A:273:ILE:O	2.34	0.61
1:B:285:VAL:CG2	1:B:411:LEU:HD13	2.30	0.61
1:B:34:LYS:HB2	1:B:34:LYS:NZ	2.15	0.61
1:B:552:PHE:O	1:B:556:LEU:HG	1.99	0.61
1:B:322:LYS:HB3	1:B:350:ARG:HD3	1.83	0.61
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.54	0.61
1:B:72:PHE:O	1:B:76:VAL:HG23	2.01	0.61
1:A:285:VAL:CG2	1:A:411:LEU:HD13	2.31	0.60
1:A:474:ASP:O	1:A:606:TRP:CZ3	2.54	0.60
1:A:34:LYS:HB2	1:A:34:LYS:NZ	2.16	0.60
1:A:322:LYS:HB3	1:A:350:ARG:HD3	1.83	0.60
1:B:116:LEU:O	1:B:120:LEU:HB2	2.02	0.60
1:A:182:GLU:O	1:A:186:GLU:HG3	2.02	0.59
1:B:362:LEU:O	1:B:366:HIS:HD2	1.85	0.59
1:A:43:GLU:HA	1:A:65:ILE:HG21	1.84	0.59
1:A:85:TRP:HA	1:A:88:TYR:CD1	2.37	0.59
1:A:505:LEU:O	1:A:509:VAL:HG22	2.03	0.59
1:B:505:LEU:O	1:B:509:VAL:HG22	2.02	0.59
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.37	0.58
1:A:91:GLU:O	1:A:93:LEU:N	2.36	0.58
1:A:91:GLU:HA	1:A:94:LYS:HB3	1.85	0.58
1:B:335:VAL:O	1:B:352:LYS:NZ	2.36	0.58
1:B:389:ALA:O	1:B:390:ASN:HB3	2.03	0.58
1:A:464:ASN:HA	1:A:487:GLU:OE2	2.04	0.58
1:B:297:LEU:HG	1:B:301:GLN:NE2	2.18	0.58
1:B:182:GLU:O	1:B:186:GLU:HG3	2.03	0.58
1:B:294:TYR:O	1:B:357:VAL:HG11	2.03	0.57
1:B:315:LEU:HD21	1:B:369:LEU:HD11	1.85	0.57
1:A:177:VAL:HG13	1:A:177:VAL:O	2.05	0.57
1:A:471:LYS:O	1:A:475:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:O	1:A:357:VAL:HG11	2.05	0.57
1:B:613:VAL:CG2	1:B:614:SER:H	2.13	0.57
1:B:143:LEU:HD22	1:B:148:GLU:HG2	1.87	0.57
1:B:256:MET:HG3	1:B:480:GLU:O	2.05	0.57
1:B:43:GLU:HA	1:B:65:ILE:HG21	1.87	0.57
1:A:389:ALA:O	1:A:390:ASN:HB3	2.04	0.56
1:A:297:LEU:HG	1:A:301:GLN:NE2	2.20	0.56
1:A:335:VAL:O	1:A:352:LYS:NZ	2.38	0.56
1:A:148:GLU:H	1:A:148:GLU:CD	2.08	0.56
1:A:362:LEU:O	1:A:366:HIS:HD2	1.87	0.56
1:A:256:MET:HG3	1:A:480:GLU:O	2.05	0.56
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.41	0.55
1:B:513:ILE:HD11	1:B:568:LEU:HD13	1.88	0.55
1:A:613:VAL:CG2	1:A:614:SER:N	2.64	0.55
1:B:471:LYS:O	1:B:475:GLU:HG3	2.06	0.55
1:A:198:THR:HB	1:A:202:GLU:CG	2.36	0.55
1:B:91:GLU:O	1:B:93:LEU:N	2.37	0.55
1:B:91:GLU:HA	1:B:94:LYS:HB3	1.88	0.55
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.88	0.55
1:B:462:LYS:HA	1:B:465:TRP:CD1	2.42	0.55
1:B:178:ARG:NH2	1:B:465:TRP:HB2	2.22	0.55
1:B:387:THR:HG23	1:B:560:ALA:HB2	1.89	0.55
1:B:113:TYR:CE2	1:B:117:LEU:HD11	2.42	0.55
1:B:148:GLU:CD	1:B:148:GLU:H	2.11	0.55
1:B:442:LEU:HB2	1:B:443:PRO:CD	2.37	0.54
1:B:446:PHE:O	1:B:450:LYS:HG3	2.07	0.54
1:A:387:THR:HG23	1:A:560:ALA:HB2	1.89	0.54
1:B:464:ASN:HA	1:B:487:GLU:OE2	2.07	0.54
1:A:307:PHE:O	1:A:312:LEU:HB2	2.07	0.54
1:A:446:PHE:O	1:A:450:LYS:HG3	2.06	0.54
1:B:377:GLN:HE22	1:B:553:HIS:CD2	2.25	0.54
1:A:296:PRO:HB3	1:A:355:THR:OG1	2.08	0.54
1:A:44:THR:HG22	1:A:343:PHE:CE1	2.43	0.54
1:B:188:ASN:OD1	1:B:200:GLY:HA3	2.07	0.54
1:B:198:THR:HB	1:B:202:GLU:CG	2.37	0.54
1:B:123:MET:HG2	1:B:177:VAL:CG2	2.38	0.54
1:A:390:ASN:OD1	1:A:392:GLY:N	2.38	0.53
1:A:442:LEU:HB2	1:A:443:PRO:CD	2.38	0.53
1:A:115:GLU:O	1:A:119:THR:CG2	2.53	0.53
1:B:152:VAL:HG11	1:B:165:TYR:CD2	2.43	0.53
1:B:225:ARG:HB3	1:B:226:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:O	1:B:216:GLN:HG3	2.08	0.53
1:A:167:ARG:NH1	1:A:168:GLU:OE2	2.41	0.53
1:A:225:ARG:HB3	1:A:226:PRO:HD3	1.90	0.53
1:A:513:ILE:HD11	1:A:568:LEU:HD13	1.91	0.53
1:B:250:GLU:HA	1:B:250:GLU:OE1	2.09	0.53
1:B:177:VAL:O	1:B:177:VAL:HG13	2.08	0.53
1:A:188:ASN:OD1	1:A:200:GLY:HA3	2.08	0.52
1:A:178:ARG:NH2	1:A:465:TRP:HB2	2.24	0.52
1:A:28:TYR:CZ	1:A:32:LEU:HD22	2.45	0.52
1:B:146:ASP:HB3	1:B:147:PRO:HD3	1.90	0.52
1:A:123:MET:HG2	1:A:177:VAL:CG2	2.40	0.52
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.90	0.52
1:A:250:GLU:HA	1:A:250:GLU:OE1	2.09	0.52
1:A:377:GLN:HE22	1:A:553:HIS:CD2	2.27	0.52
1:B:377:GLN:HG3	1:B:556:LEU:HD12	1.92	0.52
1:B:251:THR:HG22	1:B:603:HIS:NE2	2.23	0.52
1:B:541:ASP:C	1:B:543:TYR:N	2.60	0.52
1:A:587:GLU:OE1	1:A:590:ARG:NH2	2.42	0.52
1:B:167:ARG:NH1	1:B:168:GLU:OE2	2.40	0.52
1:B:285:VAL:HG11	1:B:416:LEU:HD13	1.91	0.52
1:B:97:PHE:O	1:B:101:THR:HG23	2.10	0.52
1:B:296:PRO:HB3	1:B:355:THR:OG1	2.10	0.52
1:B:44:THR:HG22	1:B:343:PHE:CE1	2.45	0.52
1:B:527:GLN:HB3	1:B:540:CYS:HB3	1.91	0.52
1:A:285:VAL:HG11	1:A:416:LEU:HD13	1.92	0.52
1:B:280:LYS:NZ	1:B:425:GLU:HB2	2.25	0.52
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.45	0.51
1:A:91:GLU:HG3	1:A:94:LYS:CE	2.40	0.51
1:B:390:ASN:OD1	1:B:392:GLY:N	2.40	0.51
1:B:418:LYS:CE	1:B:418:LYS:H	2.12	0.51
1:B:443:PRO:O	1:B:447:THR:HG23	2.08	0.51
1:B:256:MET:C	1:B:257:HIS:HD1	2.13	0.51
1:B:385:TYR:O	1:B:559:GLY:O	2.27	0.51
1:A:97:PHE:O	1:A:101:THR:HG23	2.10	0.51
1:A:527:GLN:HB3	1:A:540:CYS:HB3	1.91	0.51
1:B:28:TYR:CZ	1:B:32:LEU:HD22	2.46	0.51
1:B:159:HIS:CE1	1:B:160:GLU:HG3	2.45	0.51
1:B:307:PHE:O	1:B:312:LEU:HB2	2.10	0.51
1:B:334:LEU:HD21	1:B:336:CYS:SG	2.51	0.51
1:A:607:ILE:HD12	1:A:608:THR:H	1.76	0.51
1:B:330:ASP:CG	1:B:332:ARG:HD3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PHE:CE2	1:A:217:LEU:HD11	2.47	0.50
1:A:541:ASP:OD2	1:A:541:ASP:O	2.29	0.50
1:A:612:CYS:O	1:A:612:CYS:SG	2.69	0.50
1:B:213:PHE:CE2	1:B:217:LEU:HD11	2.46	0.50
1:A:159:HIS:CE1	1:A:160:GLU:HG3	2.47	0.50
1:A:274:VAL:O	1:A:274:VAL:HG22	2.10	0.50
1:B:215:GLN:NE2	1:B:219:ASP:OD1	2.44	0.50
1:B:309:SER:HB3	1:B:544:GLY:HA2	1.92	0.50
1:A:418:LYS:H	1:A:418:LYS:CE	2.16	0.50
1:B:468:ALA:O	1:B:472:LEU:HB2	2.11	0.50
1:B:143:LEU:CD2	1:B:148:GLU:HG2	2.41	0.50
1:A:298:LYS:HE3	1:A:302:MET:SD	2.51	0.50
1:A:355:THR:HA	1:A:361:GLN:OE1	2.11	0.50
1:B:84:GLN:NE2	1:B:86:ARG:HB2	2.26	0.50
1:A:91:GLU:O	1:A:92:ASP:HB3	2.12	0.50
1:B:115:GLU:O	1:B:119:THR:CG2	2.54	0.50
1:B:34:LYS:HB2	1:B:34:LYS:HZ1	1.74	0.50
1:B:607:ILE:HD12	1:B:608:THR:H	1.77	0.50
1:A:309:SER:HB3	1:A:544:GLY:HA2	1.93	0.50
1:A:468:ALA:O	1:A:472:LEU:HB2	2.12	0.50
1:B:355:THR:HA	1:B:361:GLN:OE1	2.12	0.49
1:A:443:PRO:O	1:A:447:THR:HG23	2.11	0.49
1:A:599:LYS:HD2	1:B:79:ASP:HB3	1.94	0.49
1:B:147:PRO:O	1:B:151:GLU:HG3	2.11	0.49
1:B:178:ARG:HH21	1:B:465:TRP:HB2	1.77	0.49
1:B:563:PRO:HB2	1:B:565:PRO:HD2	1.94	0.49
1:A:240:ARG:HH11	1:A:249:SER:HA	1.76	0.49
1:A:280:LYS:NZ	1:A:425:GLU:HB2	2.27	0.49
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.33	0.49
1:A:240:ARG:NH1	1:A:249:SER:HA	2.27	0.49
1:A:385:TYR:O	1:A:559:GLY:O	2.30	0.49
1:B:587:GLU:OE1	1:B:590:ARG:NH2	2.45	0.49
1:A:569:GLU:HB2	1:A:575:ARG:HG2	1.95	0.49
1:B:255:PRO:O	1:B:256:MET:O	2.31	0.49
1:B:412:GLU:HG3	1:B:417:LEU:O	2.13	0.49
1:A:285:VAL:HG11	1:A:416:LEU:HB3	1.95	0.49
1:A:492:ALA:HB3	1:A:493:PRO:HD3	1.94	0.49
1:B:89:GLN:CD	1:B:89:GLN:H	2.13	0.49
1:A:527:GLN:HB3	1:A:540:CYS:CB	2.43	0.49
1:A:563:PRO:HB2	1:A:565:PRO:HD2	1.95	0.49
1:A:462:LYS:HB3	1:A:462:LYS:HZ2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LYS:HG2	1:A:419:ASP:H	1.78	0.49
1:B:541:ASP:O	1:B:541:ASP:OD2	2.31	0.49
1:B:91:GLU:HG3	1:B:94:LYS:CE	2.43	0.49
1:B:91:GLU:O	1:B:92:ASP:HB3	2.12	0.49
1:A:123:MET:HG2	1:A:177:VAL:HG21	1.95	0.48
1:B:240:ARG:NH1	1:B:249:SER:HA	2.28	0.48
1:B:162:LEU:HD13	1:B:257:HIS:O	2.13	0.48
1:A:215:GLN:NE2	1:A:219:ASP:OD1	2.46	0.48
1:B:123:MET:HG2	1:B:177:VAL:HG21	1.95	0.48
1:A:277:PHE:CE2	1:A:425:GLU:HB3	2.49	0.48
1:A:412:GLU:HG3	1:A:417:LEU:O	2.14	0.48
1:B:522:CYS:O	1:B:525:ALA:O	2.32	0.48
1:A:377:GLN:HG3	1:A:556:LEU:HD12	1.94	0.48
1:A:522:CYS:O	1:A:525:ALA:O	2.31	0.48
1:B:298:LYS:HE3	1:B:302:MET:SD	2.52	0.48
1:B:569:GLU:HB2	1:B:575:ARG:HG2	1.95	0.48
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.43	0.48
1:A:145:LEU:HA	1:A:149:ILE:HB	1.95	0.48
1:A:410:HIS:O	1:A:414:ILE:HG12	2.14	0.48
1:A:73:MET:HB3	1:A:103:LEU:HD11	1.95	0.48
1:B:285:VAL:HG11	1:B:416:LEU:HB3	1.95	0.48
1:B:418:LYS:HG2	1:B:419:ASP:H	1.78	0.48
1:B:240:ARG:HH11	1:B:249:SER:HA	1.78	0.47
1:B:276:PRO:HB3	1:B:592:TRP:CH2	2.49	0.47
1:B:327:LYS:HB2	1:B:354:CYS:SG	2.54	0.47
1:A:34:LYS:HB2	1:A:34:LYS:HZ1	1.79	0.47
1:B:452:ARG:HD3	1:B:498:ILE:HD12	1.96	0.47
1:B:612:CYS:SG	1:B:612:CYS:O	2.73	0.47
1:A:147:PRO:O	1:A:151:GLU:HG3	2.14	0.47
1:A:195:ASN:O	1:A:196:ASN:HB2	2.15	0.47
1:A:147:PRO:HG2	1:A:148:GLU:CD	2.35	0.47
1:A:178:ARG:HH21	1:A:465:TRP:HB2	1.79	0.47
1:B:96:GLN:O	1:B:100:LEU:HB2	2.15	0.47
1:A:166:TRP:CH2	1:A:481:PRO:HB3	2.49	0.47
1:B:166:TRP:CG	1:B:482:PRO:HG2	2.50	0.47
1:B:486:SER:CB	1:B:614:SER:HA	2.41	0.47
1:A:98:LYS:O	1:A:102:LYS:HG3	2.14	0.47
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.49	0.47
1:A:84:GLN:NE2	1:A:86:ARG:HB2	2.29	0.47
1:B:195:ASN:O	1:B:196:ASN:HB2	2.15	0.47
1:B:147:PRO:HG2	1:B:148:GLU:CD	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:THR:H	1:B:373:GLN:HE22	1.62	0.47
1:B:34:LYS:NZ	1:B:34:LYS:CB	2.77	0.47
1:B:474:ASP:O	1:B:606:TRP:CH2	2.67	0.47
1:A:166:TRP:CE3	1:A:482:PRO:HD2	2.50	0.46
1:B:98:LYS:O	1:B:102:LYS:HG3	2.15	0.46
1:A:212:THR:O	1:A:216:GLN:HG3	2.15	0.46
1:A:276:PRO:HB3	1:A:592:TRP:HH2	1.80	0.46
1:B:145:LEU:HA	1:B:149:ILE:HB	1.97	0.46
1:B:91:GLU:HG3	1:B:94:LYS:HE2	1.96	0.46
1:A:351:ILE:CD1	1:A:368:GLU:HB3	2.46	0.46
1:A:474:ASP:O	1:A:606:TRP:CH2	2.68	0.46
1:A:91:GLU:HG3	1:A:94:LYS:HE2	1.97	0.46
1:B:33:ASN:ND2	1:B:384:VAL:H	2.13	0.46
1:B:61:LYS:O	1:B:65:ILE:HG12	2.15	0.46
1:B:377:GLN:HG3	1:B:556:LEU:CD1	2.45	0.46
1:B:95:ARG:HD3	1:B:385:TYR:OH	2.15	0.46
1:A:147:PRO:HG2	1:A:148:GLU:H	1.80	0.46
1:A:322:LYS:CB	1:A:350:ARG:HD3	2.46	0.46
1:A:61:LYS:O	1:A:65:ILE:HG12	2.16	0.46
1:A:54:ILE:HG13	1:A:334:LEU:HA	1.98	0.46
1:A:208:TYR:HD1	1:A:390:ASN:ND2	2.14	0.46
1:B:256:MET:C	1:B:258:LEU:N	2.62	0.46
1:B:276:PRO:HB3	1:B:592:TRP:HH2	1.79	0.46
1:B:277:PHE:CE2	1:B:425:GLU:HB3	2.50	0.46
1:B:147:PRO:HG2	1:B:148:GLU:H	1.80	0.46
1:B:311:ASN:HA	1:B:311:ASN:HD22	1.54	0.46
1:B:569:GLU:OE1	1:B:575:ARG:NH1	2.46	0.46
1:B:73:MET:HB3	1:B:103:LEU:HD11	1.97	0.46
1:A:23:ILE:HG12	1:A:24:GLN:N	2.30	0.46
1:A:484:VAL:CG1	1:A:613:VAL:HG22	2.46	0.46
1:B:431:LEU:HD13	1:B:588:PRO:HG2	1.98	0.46
1:A:255:PRO:O	1:A:256:MET:O	2.34	0.45
1:A:351:ILE:HD13	1:A:368:GLU:HB3	1.97	0.45
1:B:351:ILE:HD13	1:B:368:GLU:HB3	1.98	0.45
1:B:613:VAL:CG2	1:B:614:SER:N	2.62	0.45
1:B:382:PRO:O	1:B:383:PHE:C	2.55	0.45
1:B:54:ILE:HG13	1:B:334:LEU:HA	1.98	0.45
1:B:23:ILE:HG12	1:B:24:GLN:N	2.31	0.45
1:B:492:ALA:HB3	1:B:493:PRO:HD3	1.99	0.45
1:A:143:LEU:CD2	1:A:148:GLU:HG2	2.46	0.45
1:A:256:MET:HG2	1:A:479:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:H	1:A:373:GLN:HE22	1.64	0.45
1:B:409:LYS:HE3	1:B:409:LYS:HB2	1.75	0.45
1:A:96:GLN:O	1:A:100:LEU:HB2	2.15	0.45
1:A:452:ARG:HD3	1:A:498:ILE:HD12	1.99	0.45
1:A:377:GLN:HG3	1:A:556:LEU:CD1	2.46	0.45
1:B:256:MET:HG2	1:B:479:ILE:HG23	1.98	0.45
1:B:389:ALA:O	1:B:390:ASN:O	2.35	0.45
1:A:34:LYS:CB	1:A:34:LYS:NZ	2.79	0.45
1:A:431:LEU:HD13	1:A:588:PRO:HG2	1.98	0.45
1:A:515:PHE:CE2	1:A:582:ILE:HG23	2.52	0.45
1:A:533:VAL:C	1:A:535:LEU:H	2.19	0.45
1:A:251:THR:HG22	1:A:603:HIS:NE2	2.32	0.45
1:A:95:ARG:HD3	1:A:385:TYR:OH	2.17	0.44
1:B:33:ASN:HD21	1:B:384:VAL:HB	1.81	0.44
1:B:410:HIS:O	1:B:414:ILE:HG12	2.17	0.44
1:A:33:ASN:HD21	1:A:384:VAL:HB	1.82	0.44
1:A:442:LEU:HB2	1:A:443:PRO:HD3	1.98	0.44
1:B:422:ARG:O	1:B:423:ASP:C	2.55	0.44
1:A:382:PRO:O	1:A:383:PHE:C	2.56	0.44
1:B:50:TYR:HD2	1:B:51:ARG:HG2	1.83	0.44
1:A:166:TRP:CG	1:A:482:PRO:HG2	2.52	0.44
1:A:327:LYS:HB2	1:A:354:CYS:SG	2.58	0.44
1:A:598:ILE:HD11	1:B:35:GLU:OE1	2.17	0.44
1:A:334:LEU:N	1:A:334:LEU:CD1	2.81	0.44
1:B:274:VAL:O	1:B:274:VAL:HG22	2.17	0.44
1:B:442:LEU:HB2	1:B:443:PRO:HD3	1.99	0.44
1:A:338:ALA:HB2	1:A:353:GLN:HG3	1.99	0.44
1:A:33:ASN:ND2	1:A:384:VAL:H	2.16	0.43
1:A:599:LYS:HE3	1:B:82:LYS:HD2	2.00	0.43
1:B:153:ILE:HA	1:B:162:LEU:CD2	2.48	0.43
1:A:334:LEU:HD22	1:A:335:VAL:C	2.39	0.43
1:B:410:HIS:HB2	1:B:541:ASP:CG	2.38	0.43
1:A:257:HIS:CE1	1:A:258:LEU:HG	2.53	0.43
1:A:300:PHE:HE2	1:A:355:THR:HG21	1.84	0.43
1:A:389:ALA:O	1:A:390:ASN:O	2.35	0.43
1:B:484:VAL:CG1	1:B:613:VAL:HG22	2.49	0.43
1:B:519:LYS:O	1:B:523:ILE:HG13	2.18	0.43
1:A:50:TYR:HD2	1:A:51:ARG:HG2	1.82	0.43
1:B:533:VAL:CG2	1:B:534:GLU:H	2.03	0.43
1:A:115:GLU:CD	1:A:183:ARG:HE	2.22	0.43
1:A:422:ARG:O	1:A:423:ASP:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HD22	1:B:335:VAL:C	2.39	0.43
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.88	0.43
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.39	0.43
1:A:454:SER:O	1:A:457:ARG:O	2.37	0.43
1:A:587:GLU:N	1:A:588:PRO:HD2	2.34	0.43
1:B:257:HIS:CE1	1:B:258:LEU:HG	2.53	0.43
1:B:533:VAL:C	1:B:535:LEU:H	2.21	0.43
1:B:515:PHE:CD2	1:B:582:ILE:HG23	2.53	0.43
1:B:351:ILE:CD1	1:B:368:GLU:HB3	2.49	0.43
1:A:116:LEU:HA	1:A:119:THR:HG23	2.00	0.43
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.28	0.43
1:A:38:LYS:HB2	1:A:38:LYS:HE2	1.86	0.43
1:A:589:LEU:HD22	1:A:593:LEU:CD1	2.49	0.42
1:B:95:ARG:HB3	1:B:385:TYR:OH	2.18	0.42
1:B:29:LEU:HD13	1:B:96:GLN:NE2	2.34	0.42
1:A:267:TRP:CD1	1:A:267:TRP:N	2.87	0.42
1:A:92:ASP:OD1	1:A:385:TYR:HE2	2.03	0.42
1:A:396:ALA:O	1:A:397:VAL:C	2.56	0.42
1:B:108:LEU:HD13	1:B:191:ALA:HB2	2.00	0.42
1:B:166:TRP:CH2	1:B:481:PRO:HB3	2.54	0.42
1:B:202:GLU:OE2	1:B:457:ARG:NE	2.46	0.42
1:B:422:ARG:C	1:B:422:ARG:HD3	2.39	0.42
1:B:515:PHE:CE2	1:B:582:ILE:HG23	2.54	0.42
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.86	0.42
1:A:541:ASP:C	1:A:543:TYR:N	2.61	0.42
1:B:116:LEU:HA	1:B:119:THR:HG23	2.01	0.42
1:B:115:GLU:CD	1:B:183:ARG:HE	2.23	0.42
1:B:383:PHE:HA	1:B:386:ARG:HD3	2.00	0.42
1:B:396:ALA:O	1:B:397:VAL:C	2.58	0.42
1:B:587:GLU:N	1:B:588:PRO:HD2	2.34	0.42
1:B:254:ILE:HA	1:B:255:PRO:HD3	1.90	0.42
1:B:208:TYR:HD1	1:B:390:ASN:ND2	2.17	0.42
1:B:240:ARG:HA	1:B:248:VAL:HB	2.02	0.42
1:B:330:ASP:OD2	1:B:332:ARG:HD3	2.19	0.42
1:A:105:TYR:O	1:A:108:LEU:HB2	2.20	0.42
1:B:288:GLU:HG3	1:B:418:LYS:HE2	2.01	0.42
1:A:108:LEU:HD13	1:A:191:ALA:HB2	2.02	0.42
1:A:334:LEU:HD21	1:A:336:CYS:SG	2.60	0.42
1:A:486:SER:CB	1:A:614:SER:HA	2.41	0.42
1:A:613:VAL:CG2	1:A:614:SER:H	2.17	0.41
1:A:39:ARG:CZ	1:A:72:PHE:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.84	0.41
1:A:431:LEU:CD1	1:A:588:PRO:HG2	2.51	0.41
1:A:515:PHE:CD2	1:A:582:ILE:HG23	2.54	0.41
1:B:166:TRP:CE3	1:B:482:PRO:HD2	2.55	0.41
1:B:251:THR:HG22	1:B:603:HIS:CE1	2.55	0.41
1:B:533:VAL:CG2	1:B:534:GLU:N	2.73	0.41
1:A:100:LEU:HA	1:A:100:LEU:HD12	1.80	0.41
1:A:422:ARG:C	1:A:422:ARG:HD3	2.41	0.41
1:A:452:ARG:NH2	1:A:504:TYR:HB2	2.35	0.41
1:B:178:ARG:CG	1:B:178:ARG:HH11	2.30	0.41
1:B:322:LYS:CB	1:B:350:ARG:HD3	2.50	0.41
1:B:92:ASP:OD1	1:B:385:TYR:HE2	2.02	0.41
1:A:153:ILE:HA	1:A:162:LEU:CD2	2.50	0.41
1:B:338:ALA:HB2	1:B:353:GLN:HG3	2.03	0.41
1:A:383:PHE:HA	1:A:386:ARG:HD3	2.02	0.41
1:A:95:ARG:HB3	1:A:385:TYR:OH	2.20	0.41
1:B:533:VAL:HG13	1:B:534:GLU:N	2.35	0.41
1:A:191:ALA:O	1:A:195:ASN:ND2	2.54	0.41
1:A:89:GLN:H	1:A:89:GLN:CD	2.15	0.41
1:B:285:VAL:HG12	1:B:289:MET:HG3	2.01	0.41
1:B:601:ASN:HA	1:B:601:ASN:HD22	1.62	0.41
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.85	0.41
1:A:179:SER:OG	1:A:180:GLN:N	2.53	0.41
1:B:300:PHE:HE2	1:B:355:THR:HG21	1.85	0.41
1:B:513:ILE:HA	1:B:516:GLN:HG3	2.02	0.41
1:B:589:LEU:HD22	1:B:593:LEU:CD1	2.51	0.41
1:A:288:GLU:HG3	1:A:418:LYS:HE2	2.02	0.40
1:A:256:MET:CG	1:A:479:ILE:HG23	2.51	0.40
1:A:533:VAL:HG13	1:A:534:GLU:N	2.36	0.40
1:B:164:TYR:O	1:B:168:GLU:HG2	2.21	0.40
1:B:416:LEU:HA	1:B:416:LEU:HD23	1.96	0.40
1:B:454:SER:O	1:B:457:ARG:O	2.39	0.40
1:A:519:LYS:O	1:A:523:ILE:HG13	2.20	0.40
1:B:191:ALA:O	1:B:195:ASN:ND2	2.54	0.40
1:B:123:MET:HG2	1:B:177:VAL:HG22	2.03	0.40
1:B:183:ARG:HA	1:B:186:GLU:OE1	2.22	0.40
1:A:311:ASN:HD22	1:A:311:ASN:HA	1.55	0.40
1:A:330:ASP:OD2	1:A:332:ARG:HD3	2.21	0.40
1:A:205:LEU:HD21	1:A:453:TRP:CZ2	2.56	0.40
1:B:100:LEU:HA	1:B:100:LEU:HD12	1.81	0.40
1:B:39:ARG:CZ	1:B:72:PHE:CD1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PHE:CZ	1:A:425:GLU:HB3	2.57	0.40
1:B:382:PRO:O	1:B:384:VAL:N	2.55	0.40
1:B:277:PHE:CZ	1:B:425:GLU:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/607 (98%)	532 (89%)	42 (7%)	22 (4%)	3	2
1	B	596/607 (98%)	535 (90%)	40 (7%)	21 (4%)	3	3
All	All	1192/1214 (98%)	1067 (90%)	82 (7%)	43 (4%)	3	3

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	256	MET
1	A	257	HIS
1	A	423	ASP
1	A	424	ASP
1	A	531	ASP
1	A	542	ILE
1	B	147	PRO
1	B	256	MET
1	B	257	HIS
1	B	423	ASP
1	B	424	ASP
1	B	542	ILE
1	A	88	TYR
1	A	383	PHE

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Mol	Chain	Res	Type
1	A	418	LYS
1	A	559	GLY
1	A	613	VAL
1	B	88	TYR
1	B	383	PHE
1	B	397	VAL
1	B	418	LYS
1	B	531	ASP
1	B	559	GLY
1	B	613	VAL
1	A	91	GLU
1	A	138	SER
1	A	146	ASP
1	A	338	ALA
1	A	390	ASN
1	A	581	ALA
1	B	91	GLU
1	B	338	ALA
1	B	390	ASN
1	B	581	ALA
1	A	397	VAL
1	B	146	ASP
1	B	616	HIS
1	A	176	ALA
1	A	616	HIS
1	B	138	SER
1	A	533	VAL
1	B	533	VAL

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%)	480 (92%)	42 (8%)	12	18
1	B	522/530 (98%)	479 (92%)	43 (8%)	11	17
All	All	1044/1060 (98%)	959 (92%)	85 (8%)	11	18

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	100	LEU
1	A	108	LEU
1	A	119	THR
1	A	120	LEU
1	A	177	VAL
1	A	183	ARG
1	A	194	LEU
1	A	227	LEU
1	A	238	ARG
1	A	282	LEU
1	A	305	ASP
1	A	306	PHE
1	A	311	ASN
1	A	314	LYS
1	A	334	LEU
1	A	336	CYS
1	A	362	LEU
1	A	369	LEU
1	A	374	TYR
1	A	378	TYR
1	A	394	HIS
1	A	404	SER
1	A	418	LYS
1	A	422	ARG
1	A	424	ASP
1	A	430	GLN
1	A	446	PHE
1	A	461	ASP
1	A	462	LYS
1	A	495	LYS
1	A	503	GLU
1	A	537	LEU
1	A	539	ASN
1	A	552	PHE
1	A	582	ILE
1	A	589	LEU
1	A	601	ASN
1	A	606	TRP
1	A	612	CYS
1	A	615	SER
1	A	619	HIS

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Mol	Chain	Res	Type
1	B	89	GLN
1	B	100	LEU
1	B	108	LEU
1	B	119	THR
1	B	120	LEU
1	B	177	VAL
1	B	183	ARG
1	B	194	LEU
1	B	227	LEU
1	B	238	ARG
1	B	245	ASP
1	B	282	LEU
1	B	305	ASP
1	B	306	PHE
1	B	311	ASN
1	B	314	LYS
1	B	334	LEU
1	B	336	CYS
1	B	362	LEU
1	B	369	LEU
1	B	374	TYR
1	B	378	TYR
1	B	394	HIS
1	B	404	SER
1	B	418	LYS
1	B	422	ARG
1	B	424	ASP
1	B	430	GLN
1	B	446	PHE
1	B	461	ASP
1	B	462	LYS
1	B	495	LYS
1	B	503	GLU
1	B	537	LEU
1	B	539	ASN
1	B	552	PHE
1	B	582	ILE
1	B	589	LEU
1	B	601	ASN
1	B	606	TRP
1	B	612	CYS
1	B	615	SER

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Mol	Chain	Res	Type
1	B	619	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	ASN
1	A	41	ASN
1	A	84	GLN
1	A	89	GLN
1	A	96	GLN
1	A	159	HIS
1	A	195	ASN
1	A	266	GLN
1	A	301	GLN
1	A	311	ASN
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	516	GLN
1	A	527	GLN
1	A	539	ASN
1	A	601	ASN
1	A	610	ASN
1	B	31	ASN
1	B	33	ASN
1	B	41	ASN
1	B	84	GLN
1	B	89	GLN
1	B	96	GLN
1	B	159	HIS
1	B	195	ASN
1	B	266	GLN

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Mol	Chain	Res	Type
1	B	301	GLN
1	B	311	ASN
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	516	GLN
1	B	527	GLN
1	B	539	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	X8Z	A	801	2	11,14,14	1.15	1 (9%)	14,19,19	1.25	1 (7%)
3	X8Z	B	802	2	11,14,14	1.28	1 (9%)	14,19,19	1.21	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X8Z	A	801	2	-	0/10/24/24	0/1/1/1
3	X8Z	B	802	2	-	0/10/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	X8Z	O1-C4	2.94	1.27	1.22
3	A	801	X8Z	O1-C4	2.62	1.27	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	X8Z	C7-C8-N	3.12	105.52	101.94
3	B	802	X8Z	C7-C8-N	2.90	105.27	101.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.