



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:02 AM UTC

PDB ID : 1J37 / pdb_00001j37
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

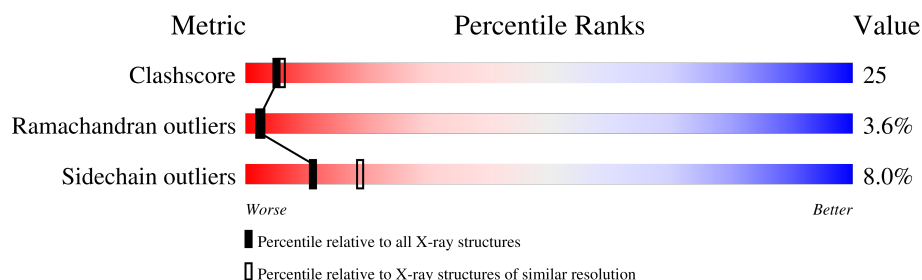
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	 52% 37% 8% ..
1	B	607	 53% 37% 8% ..

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 (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		

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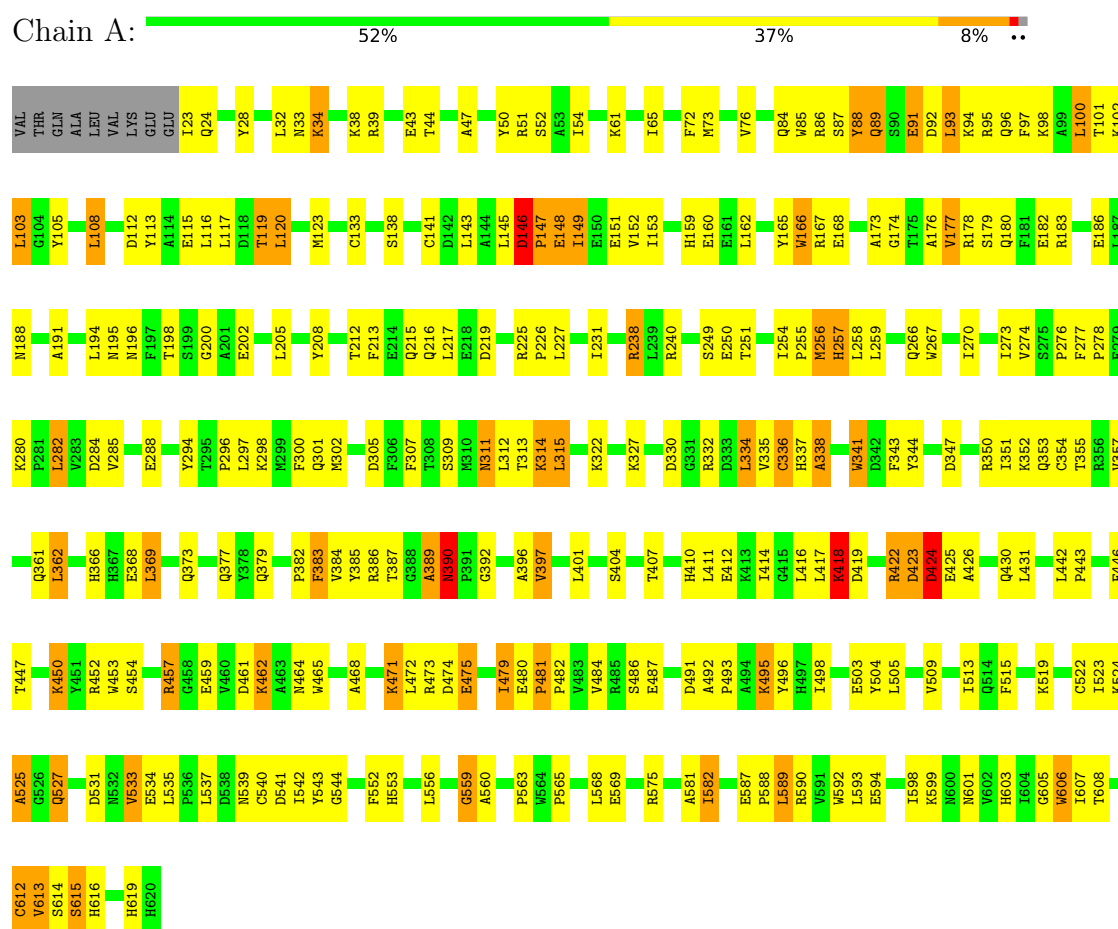
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 14	C 9	N 1	O 3	S 1	0	0
3	B	1	Total 14	C 9	N 1	O 3	S 1	0	0

3 Residue-property plots

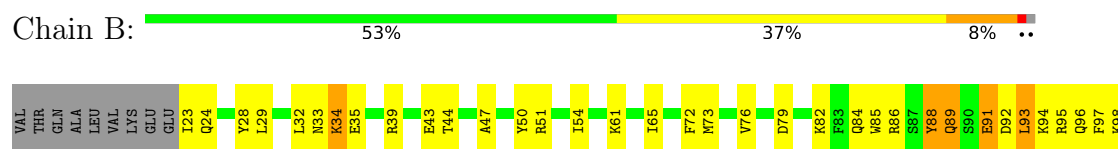
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

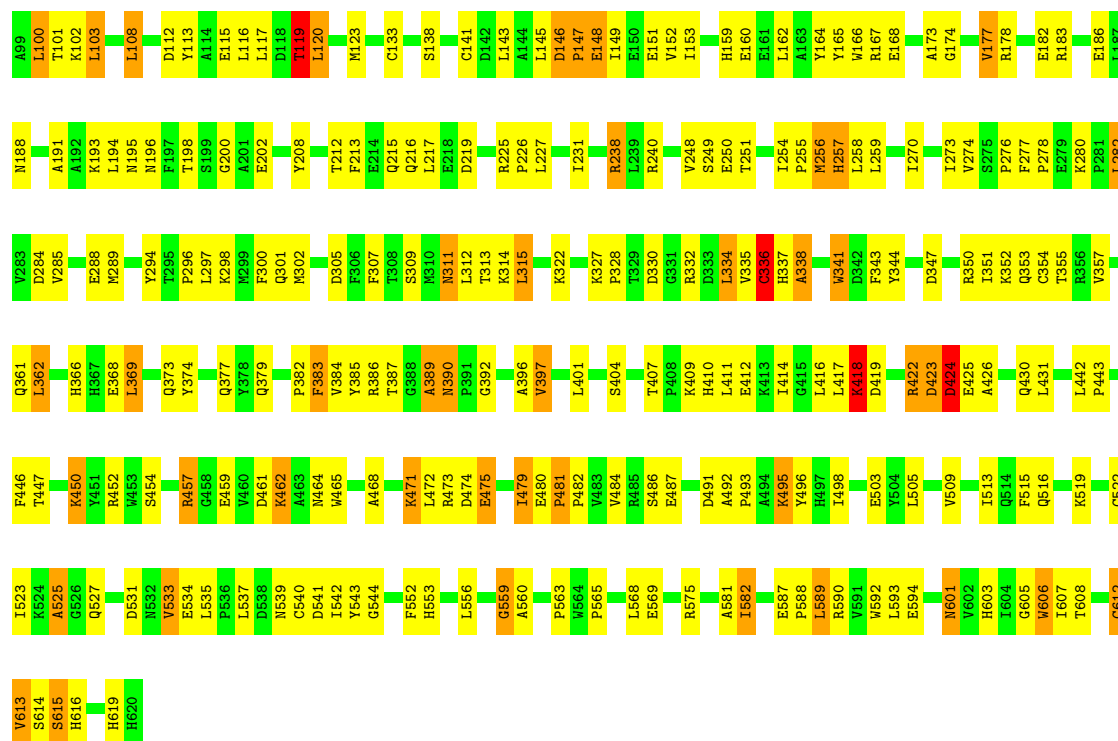
Note EDS was not executed.

- Molecule 1: angiotensin converting enzyme



- Molecule 1: angiotensin converting enzyme





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	0.54	0/5031	1.05	32/6814 (0.5%)
1	B	0.54	1/5031 (0.0%)	1.05	26/6814 (0.4%)
All	All	0.54	1/10062 (0.0%)	1.05	58/13628 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	THR	CA-CB	5.11	1.61	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	ARG	N-CA-C	-8.73	97.56	110.48
1	A	457	ARG	N-CA-C	-7.99	97.62	110.32
1	A	615	SER	N-CA-C	7.70	119.40	108.00
1	A	426	ALA	N-CA-C	-7.56	103.00	112.90
1	B	93	LEU	N-CA-C	-7.42	103.13	111.14
1	B	426	ALA	N-CA-C	-7.41	103.20	112.90
1	A	93	LEU	N-CA-C	-7.24	103.32	111.14
1	A	278	PRO	N-CA-C	-6.57	105.05	114.18
1	B	471	LYS	N-CA-C	-6.55	104.22	111.82
1	B	278	PRO	N-CA-C	-6.55	105.08	114.18
1	A	491	ASP	N-CA-C	6.41	121.30	112.90
1	B	481	PRO	CA-C-N	6.39	126.14	119.05
1	B	481	PRO	C-N-CA	6.39	126.14	119.05
1	A	481	PRO	CA-C-N	6.19	125.92	119.05
1	A	481	PRO	C-N-CA	6.19	125.92	119.05
1	A	231	ILE	N-CA-C	-6.11	104.34	111.00
1	B	231	ILE	N-CA-C	-6.05	104.41	111.00
1	A	471	LYS	N-CA-C	-6.00	104.86	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	TRP	N-CA-C	5.98	118.64	108.90
1	B	341	TRP	N-CA-C	5.86	118.45	108.90
1	B	389	ALA	N-CA-C	-5.82	100.77	109.15
1	B	407	THR	CA-C-N	5.80	127.08	119.84
1	B	407	THR	C-N-CA	5.80	127.08	119.84
1	A	459	GLU	N-CA-C	5.77	119.42	112.38
1	B	615	SER	N-CA-C	5.76	118.69	109.02
1	A	389	ALA	N-CA-C	-5.67	100.99	109.15
1	B	473	ARG	N-CA-C	-5.62	105.15	112.23
1	B	525	ALA	N-CA-C	-5.60	102.23	110.52
1	A	407	THR	CA-C-N	5.57	126.81	119.84
1	A	407	THR	C-N-CA	5.57	126.81	119.84
1	A	525	ALA	N-CA-C	-5.56	102.28	110.52
1	B	491	ASP	N-CA-C	5.51	120.11	112.90
1	B	450	LYS	N-CA-C	-5.47	105.32	111.28
1	A	615	SER	CB-CA-C	-5.46	108.69	116.34
1	A	166	TRP	N-CA-C	-5.42	105.01	111.03
1	B	615	SER	CB-CA-C	-5.34	108.84	115.89
1	A	52	SER	N-CA-C	-5.33	106.79	113.72
1	A	149	ILE	N-CA-C	5.27	115.48	110.42
1	B	424	ASP	N-CA-C	-5.19	99.74	110.80
1	A	148	GLU	N-CA-C	5.18	121.84	110.80
1	B	112	ASP	N-CA-C	5.18	117.01	111.36
1	B	475	GLU	N-CA-C	5.17	117.31	111.11
1	A	424	ASP	N-CA-C	-5.16	99.81	110.80
1	A	450	LYS	N-CA-C	-5.15	105.67	111.28
1	B	173	ALA	N-CA-C	5.14	117.78	111.82
1	B	148	GLU	N-CA-C	5.12	121.71	110.80
1	A	173	ALA	N-CA-C	5.11	117.75	111.82
1	A	146	ASP	CA-C-N	-5.10	113.46	119.84
1	A	146	ASP	C-N-CA	-5.10	113.46	119.84
1	A	524	LYS	N-CA-C	-5.06	105.95	111.82
1	A	475	GLU	N-CA-C	5.05	117.17	111.11
1	A	112	ASP	N-CA-C	5.04	116.85	111.36
1	A	407	THR	N-CA-C	5.03	116.17	109.93
1	A	473	ARG	N-CA-C	-5.03	105.89	112.23
1	B	336	CYS	N-CA-C	5.02	118.94	112.41
1	B	459	GLU	N-CA-C	5.01	118.66	112.54
1	B	193	LYS	N-CA-C	-5.01	106.68	112.89
1	A	527	GLN	N-CA-C	5.00	119.66	113.50

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	231	0
1	B	4900	0	4696	236	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	464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (464) 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:HE3	1:A:418:LYS:H	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:92:ASP:O	1:A:96:GLN:HG3	1.73	0.87
1:A:115:GLU:O	1:A:119:THR:HG22	1.74	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:NZ	1:A:462:LYS:HB3	1.96	0.81
1:A:174:GLY:HA2	1:A:493:PRO:HB2	1.63	0.80
1:A:486:SER:HB2	1:A:614:SER:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:422:ARG:HD3	1.86	0.75
1:B:256:MET:C	1:B:258:LEU:H	1.93	0.75
1:A:256:MET:C	1:A:258:LEU:H	1.95	0.74
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:541:ASP:C	1:B:543:TYR:H	1.98	0.71
1:B:613:VAL:HG23	1:B:614:SER:H	1.53	0.71
1:A:541:ASP:C	1:A:543:TYR:H	1.98	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
1:B:251:THR:HG22	1:B:603:HIS:CD2	2.26	0.70
1:B:533:VAL:HG22	1:B:534:GLU:N	2.03	0.70
1:A:47:ALA:O	1:A:51:ARG:HG3	1.92	0.70
1:A:147:PRO:HG2	1:A:148:GLU:OE1	1.92	0.70
1:B:47:ALA:O	1:B:51:ARG:HG3	1.92	0.70
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:A:285:VAL:CG1	1:A:416:LEU:HB3	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:146:ASP:HB3	1:A:147:PRO:CD	2.25	0.66
1:A:178:ARG:HG2	1:A:178:ARG:HH11	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
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:HH11	1:B:178:ARG:HG2	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:72:PHE:O	1:B:76:VAL:HG23	2.01	0.61
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.54	0.61
1:A:148:GLU:CD	1:A:148:GLU:H	2.08	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:O	1:A:186:GLU:HG3	2.02	0.59
1:B:148:GLU:CD	1:B:148:GLU:H	2.11	0.59
1:B:362:LEU:O	1:B:366:HIS:HD2	1.85	0.59
1:B:462:LYS:HB3	1:B:462:LYS:HZ3	1.68	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:91:GLU:O	1:A:93:LEU:N	2.36	0.58
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.37	0.58
1:A:533:VAL:HG22	1:A:534:GLU:N	2.02	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:A:34:LYS:HB2	1:A:34:LYS:HZ2	1.68	0.57
1:B:315:LEU:HD21	1:B:369:LEU:HD11	1.85	0.57
1:A:177:VAL:O	1:A:177:VAL:HG13	2.05	0.57
1:A:471:LYS:O	1:A:475:GLU:HG3	2.04	0.57
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:43:GLU:HA	1:B:65:ILE:HG21	1.87	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: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: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:B:256:MET:C	1:B:257:HIS:HD1	2.13	0.56
1:A:89:GLN:H	1:A:89:GLN:CD	2.15	0.55
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: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:330:ASP:CG	1:B:332:ARG:HD3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.88	0.55
1:B:89:GLN:H	1:B:89:GLN:CD	2.13	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:541:ASP:C	1:B:543:TYR:N	2.60	0.55
1:B:442:LEU:HB2	1:B:443:PRO:CD	2.37	0.54
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.33	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:44:THR:HG22	1:A:343:PHE:CE1	2.43	0.54
1:A:296:PRO:HB3	1:A:355:THR:OG1	2.08	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
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:177:VAL:HG13	1:B:177:VAL:O	2.08	0.53
1:A:188:ASN:OD1	1:A:200:GLY:HA3	2.08	0.52
1:A:28:TYR:CZ	1:A:32:LEU:HD22	2.45	0.52
1:A:178:ARG:NH2	1:A:465:TRP:HB2	2.24	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:B:250:GLU:HA	1:B: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:A:587:GLU:OE1	1:A:590:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PHE:O	1:B:101:THR:HG23	2.10	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:A:147:PRO:HG2	1:A:148:GLU:CD	2.35	0.52
1:B:44:THR:HG22	1:B:343:PHE:CE1	2.45	0.52
1:B:296:PRO:HB3	1:B:355:THR:OG1	2.10	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:91:GLU:HG3	1:A:94:LYS:CE	2.40	0.51
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.45	0.51
1:B:390:ASN:OD1	1:B:392:GLY:N	2.40	0.51
1:B:418:LYS:H	1:B:418:LYS:CE	2.12	0.51
1:B:443:PRO:O	1:B:447:THR:HG23	2.08	0.51
1:B:147:PRO:HG2	1:B:148:GLU:CD	2.35	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:A:250:GLU:OE1	1:A:250:GLU:HA	2.09	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:A:213:PHE:CE2	1:A:217:LEU:HD11	2.47	0.50
1:A:541:ASP:O	1:A:541:ASP:OD2	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:HG22	1:A:274:VAL:O	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:B:462:LYS:HB3	1:B:462:LYS:HZ2	1.73	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:B:382:PRO:O	1:B:383:PHE:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HB2	1:B:34:LYS:HZ2	1.74	0.50
1:B:115:GLU:O	1:B:119:THR:CG2	2.54	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: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:533:VAL:C	1:A:535:LEU:H	2.19	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: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:B:422:ARG:O	1:B:423:ASP:C	2.55	0.49
1:A:462:LYS:HB3	1:A:462:LYS:HZ2	1.75	0.49
1:A:418:LYS:HG2	1:A:419:ASP:H	1.78	0.49
1:B:91:GLU:O	1:B:92:ASP:HB3	2.12	0.49
1:B:91:GLU:HG3	1:B:94:LYS:CE	2.43	0.49
1:B:541:ASP:O	1:B:541:ASP:OD2	2.31	0.49
1:A:123:MET:HG2	1:A:177:VAL:HG21	1.95	0.48
1:B:162:LEU:HD13	1:B:257:HIS:O	2.13	0.48
1:B:240:ARG:NH1	1:B:249:SER:HA	2.28	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:334:LEU:HD22	1:A:335:VAL:C	2.39	0.48
1:A:412:GLU:HG3	1:A:417:LEU:O	2.14	0.48
1:A:382:PRO:O	1:A:383:PHE:C	2.56	0.48
1:B:410:HIS:HB2	1:B:541:ASP:CG	2.38	0.48
1:B:522:CYS:O	1:B:525:ALA:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:CD	1:A:183:ARG:HE	2.22	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:A:422:ARG:O	1:A:423:ASP:C	2.55	0.48
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.43	0.48
1:A:73:MET:HB3	1:A:103:LEU:HD11	1.95	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: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:533:VAL:C	1:B:535:LEU:H	2.21	0.48
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.39	0.47
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:B:452:ARG:HD3	1:B:498:ILE:HD12	1.96	0.47
1:B:612:CYS:O	1:B:612:CYS:SG	2.73	0.47
1:B:334:LEU:HD22	1:B:335:VAL:C	2.39	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: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:422:ARG:HD3	1:B:422:ARG:C	2.39	0.47
1:A:98:LYS:O	1:A:102:LYS:HG3	2.14	0.47
1:A:396:ALA:O	1:A:397:VAL:C	2.56	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:84:GLN:NE2	1:A:86:ARG:HB2	2.29	0.47
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.49	0.47
1:B:115:GLU:CD	1:B:183:ARG:HE	2.23	0.47
1:B:195:ASN:O	1:B:196:ASN:HB2	2.15	0.47
1:B:34:LYS:NZ	1:B:34:LYS:CB	2.77	0.47
1:B:313:THR:H	1:B:373:GLN:HE22	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:HG3	1:B:94:LYS:HE2	1.96	0.46
1:B:145:LEU:HA	1:B:149:ILE:HB	1.97	0.46
1:A:91:GLU:HG3	1:A:94:LYS:HE2	1.97	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: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:A:422:ARG:HD3	1:A:422:ARG:C	2.41	0.46
1:B:95:ARG:HD3	1:B:385:TYR:OH	2.15	0.46
1:B:377:GLN:HG3	1:B:556:LEU:CD1	2.45	0.46
1:A:61:LYS:O	1:A:65:ILE:HG12	2.16	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: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: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:73:MET:HB3	1:B:103:LEU:HD11	1.97	0.46
1:B:147:PRO:HG2	1:B:148:GLU:H	1.80	0.46
1:B:311:ASN:HD22	1:B:311:ASN:HA	1.54	0.46
1:B:569:GLU:OE1	1:B:575:ARG:NH1	2.46	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: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
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:377:GLN:HG3	1:A:556:LEU:CD1	2.46	0.45
1:A:452:ARG:HD3	1:A:498:ILE:HD12	1.99	0.45
1:B:256:MET:HG2	1:B:479:ILE:HG23	1.98	0.45
1:B:396:ALA:O	1:B:397:VAL:C	2.58	0.45
1:B:389:ALA:O	1:B:390:ASN:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:NZ	1:A:34:LYS:CB	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: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:541:ASP:C	1:A:543:TYR:N	2.61	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: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:HG22	1:B:274:VAL:O	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: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:256:MET:C	1:A:258:LEU:N	2.63	0.43
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.88	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: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:38:LYS:HB2	1:A:38:LYS:HE2	1.86	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:589:LEU:HD22	1:A:593:LEU:CD1	2.49	0.42
1:B:29:LEU:HD13	1:B:96:GLN:NE2	2.34	0.42
1:B:95:ARG:HB3	1:B:385:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:OD1	1:A:385:TYR:HE2	2.03	0.42
1:A:267:TRP:N	1:A:267:TRP:CD1	2.87	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: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:314:LYS:HD3	1:A:314:LYS:C	2.44	0.42
1:B:116:LEU:HA	1:B:119:THR:HG23	2.01	0.42
1:B:383:PHE:HA	1:B:386:ARG:HD3	2.00	0.42
1:B:587:GLU:N	1:B:588:PRO:HD2	2.34	0.42
1:A:91:GLU:C	1:A:93:LEU:N	2.78	0.42
1:B:254:ILE:HA	1:B:255:PRO:HD3	1.90	0.42
1:A:605:GLY:C	1:A:606:TRP:CD1	2.98	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:B:327:LYS:O	1:B:328:PRO:C	2.63	0.42
1:A:39:ARG:CZ	1:A:72:PHE:CD1	3.03	0.41
1:A:613:VAL:CG2	1:A:614:SER:H	2.17	0.41
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:A:100:LEU:HD12	1:A:100:LEU:HA	1.80	0.41
1:B:495:LYS:O	1:B:496:TYR:C	2.64	0.41
1:A:452:ARG:NH2	1:A:504:TYR:HB2	2.35	0.41
1:B:92:ASP:OD1	1:B:385:TYR:HE2	2.02	0.41
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.30	0.41
1:B:322:LYS:CB	1:B:350:ARG:HD3	2.50	0.41
1:A:153:ILE:HA	1:A:162:LEU:CD2	2.50	0.41
1:A:337:HIS:O	1:A:338:ALA:C	2.62	0.41
1:B:338:ALA:HB2	1:B:353:GLN:HG3	2.03	0.41
1:B:605:GLY:C	1:B:606:TRP:CD1	2.98	0.41
1:A:95:ARG:HB3	1:A:385:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLN:C	1:A:267:TRP:HD1	2.29	0.41
1:A:383:PHE:HA	1:A:386:ARG:HD3	2.02	0.41
1:A:495:LYS:O	1:A:496:TYR:C	2.63	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:266:GLN:C	1:A:267:TRP:CD1	2.99	0.41
1:A:474:ASP:OD2	1:A:474:ASP:C	2.61	0.41
1:B:285:VAL:HG12	1:B:289:MET:HG3	2.01	0.41
1:B:337:HIS:O	1:B:338:ALA:C	2.63	0.41
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.85	0.41
1:B:601:ASN:HD22	1:B:601:ASN:HA	1.62	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:256:MET:CG	1:A:479:ILE:HG23	2.51	0.40
1:A:288:GLU:HG3	1:A:418:LYS:HE2	2.02	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:HD23	1:B:416:LEU:HA	1.96	0.40
1:B:454:SER:O	1:B:457:ARG:O	2.39	0.40
1:B:474:ASP:C	1:B:474:ASP:OD2	2.62	0.40
1:A:519:LYS:O	1:A:523:ILE:HG13	2.20	0.40
1:B:91:GLU:C	1:B:93:LEU:N	2.78	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:85:TRP:C	1:A:87:SER:N	2.78	0.40
1:A:205:LEU:HD21	1:A:453:TRP:CZ2	2.56	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:B:39:ARG:CZ	1:B:72:PHE:CD1	3.04	0.40
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.81	0.40
1:A:277:PHE:CZ	1:A:425:GLU:HB3	2.57	0.40
1:B:277:PHE:CZ	1:B:425:GLU:HB3	2.56	0.40
1:B:382:PRO:O	1:B:384:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

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
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

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Mol	Chain	Res	Type
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%)	11	19
1	B	522/530 (98%)	480 (92%)	42 (8%)	11	19
All	All	1044/1060 (98%)	960 (92%)	84 (8%)	11	19

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	89	GLN
1	A	100	LEU
1	A	103	LEU
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	119	THR
1	A	120	LEU
1	A	177	VAL
1	A	194	LEU
1	A	227	LEU
1	A	238	ARG
1	A	282	LEU
1	A	305	ASP
1	A	311	ASN
1	A	314	LYS
1	A	315	LEU
1	A	334	LEU
1	A	336	CYS
1	A	362	LEU
1	A	369	LEU
1	A	390	ASN
1	A	401	LEU
1	A	404	SER
1	A	418	LYS
1	A	422	ARG
1	A	424	ASP
1	A	430	GLN
1	A	461	ASP
1	A	462	LYS
1	A	479	ILE
1	A	495	LYS
1	A	503	GLU
1	A	537	LEU
1	A	539	ASN
1	A	582	ILE
1	A	589	LEU
1	A	594	GLU
1	A	601	ASN
1	A	606	TRP
1	A	612	CYS
1	A	615	SER
1	A	619	HIS
1	B	34	LYS
1	B	89	GLN
1	B	100	LEU
1	B	103	LEU
1	B	108	LEU

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Mol	Chain	Res	Type
1	B	119	THR
1	B	120	LEU
1	B	177	VAL
1	B	194	LEU
1	B	227	LEU
1	B	238	ARG
1	B	282	LEU
1	B	305	ASP
1	B	311	ASN
1	B	314	LYS
1	B	315	LEU
1	B	334	LEU
1	B	336	CYS
1	B	362	LEU
1	B	369	LEU
1	B	374	TYR
1	B	401	LEU
1	B	404	SER
1	B	418	LYS
1	B	422	ARG
1	B	424	ASP
1	B	430	GLN
1	B	461	ASP
1	B	462	LYS
1	B	479	ILE
1	B	495	LYS
1	B	503	GLU
1	B	537	LEU
1	B	539	ASN
1	B	582	ILE
1	B	589	LEU
1	B	594	GLU
1	B	601	ASN
1	B	606	TRP
1	B	612	CYS
1	B	615	SER
1	B	619	HIS

Sometimes 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

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Mol	Chain	Res	Type
1	A	33	ASN
1	A	41	ASN
1	A	89	GLN
1	A	96	GLN
1	A	159	HIS
1	A	195	ASN
1	A	232	HIS
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	464	ASN
1	A	466	ASN
1	A	514	GLN
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	89	GLN
1	B	96	GLN
1	B	159	HIS
1	B	195	ASN
1	B	232	HIS
1	B	266	GLN
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

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Mol	Chain	Res	Type
1	B	380	HIS
1	B	381	GLN
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	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 oligosaccharides 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	14,14,14	1.06	1 (7%)	18,19,19	0.98	1 (5%)
3	X8Z	B	802	2	14,14,14	1.20	1 (7%)	18,19,19	0.99	1 (5%)

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	-	0/14/24/24	0/1/1/1
3	X8Z	B	802	2	-	0/14/24/24	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	2.93	1.27	1.22
3	A	801	X8Z	O1-C4	2.61	1.27	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	X8Z	C6-C7-C8	2.17	108.67	104.14
3	A	801	X8Z	C6-C7-C8	2.14	108.60	104.14

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.