Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 03:06 PM EST

PDB ID	:	1J37
Title	:	Crystal Structure of Drosophila AnCE
Authors	:	Kim, H.M.; Shin, D.R.; Yoo, O.J.; Lee, H.; Lee, J.-O.
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 (i) 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 (i)) were used in the production of this report:

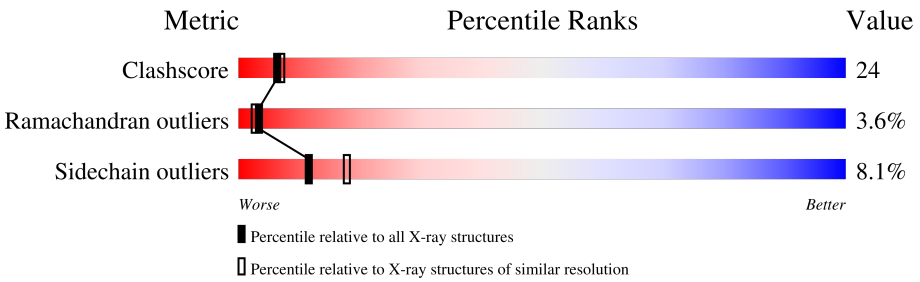
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	54% 38% 6% •
1	B	607	55% 38% 6% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	598	4900	3135	819	926	20	154	0	0
1	B	598	4900	3135	819	926	20	154	0	0

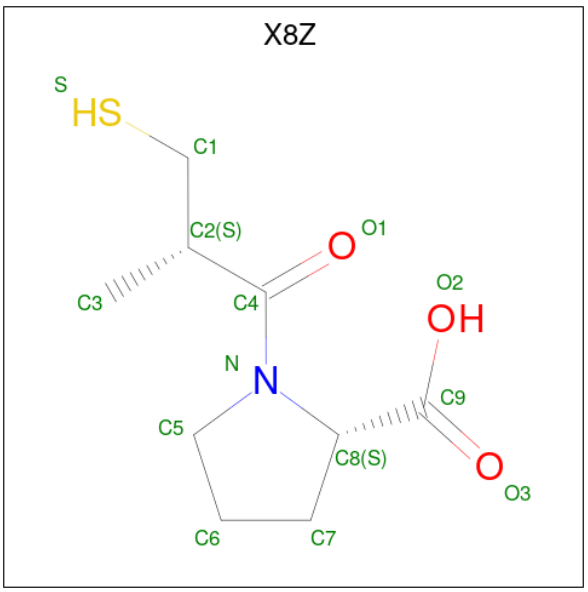
There are 16 discrepancies between the modelled and reference sequences:

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
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- 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		

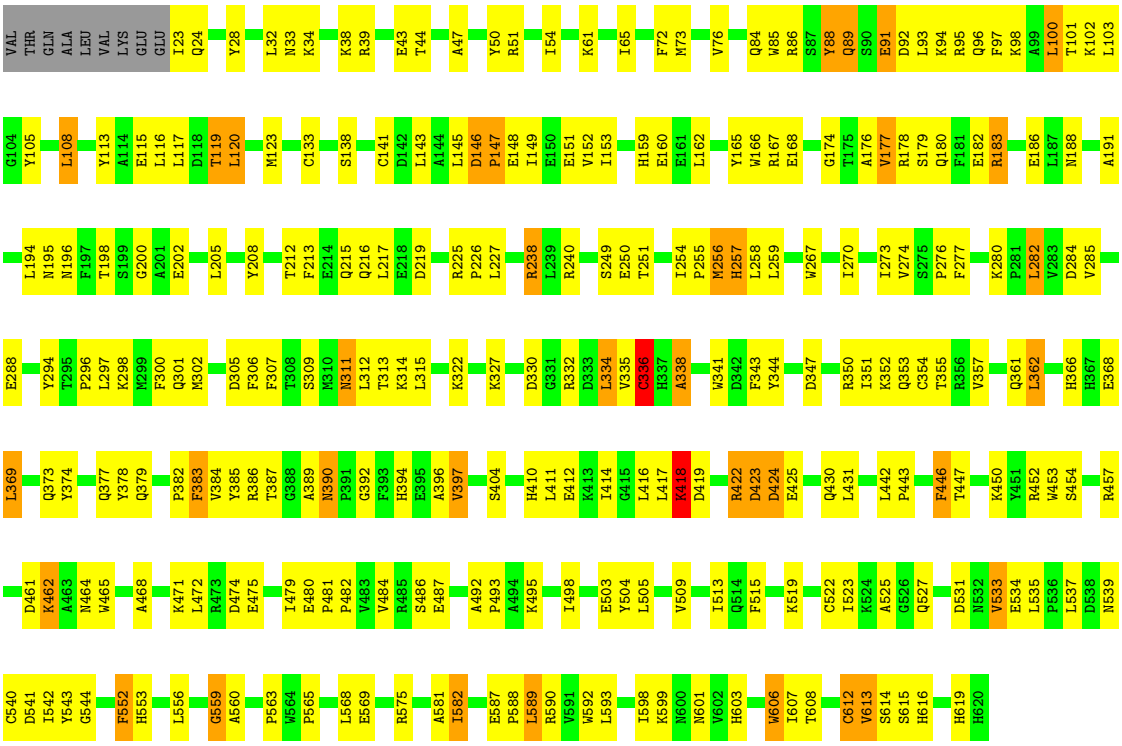
3 Residue-property plots (i)

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.

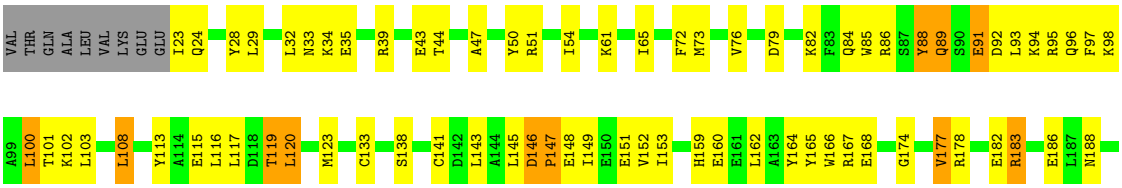
• Molecule 1: angiotensin converting enzyme

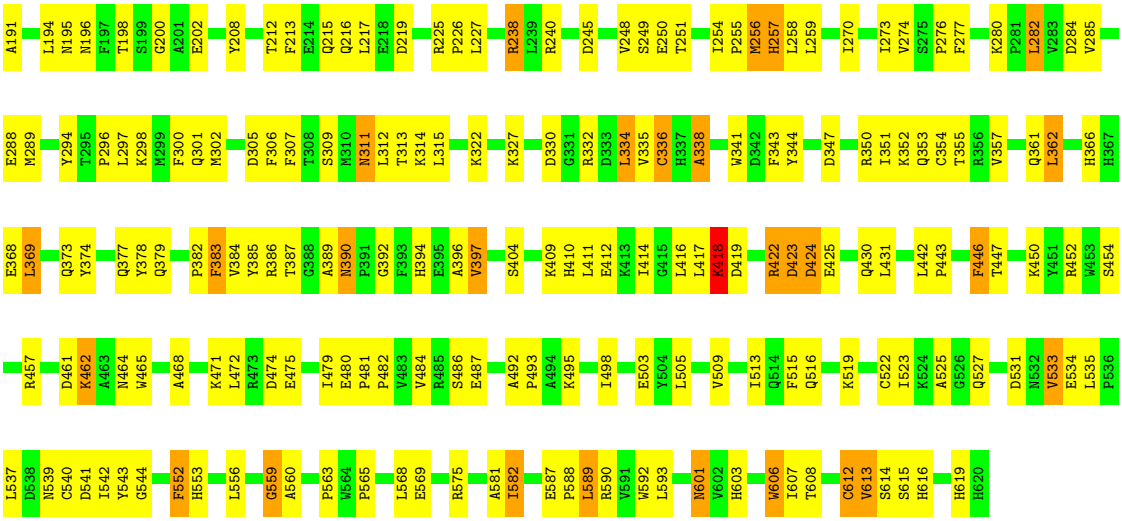
Chain A: 54% 38% 6% •



• Molecule 1: angiotensin converting enzyme

Chain B: 55% 38% 6% •




A191 L194 N195 N196 F197 T198 S199 G200 A201 E202 Y208 T212 F213 E214 Q215 Q216 L217 E218 D219 R225 P226 L227 R238 L239 R240 D245 V248 S249 E250 T251 I254 P255 M256 H257 L258 L259 I270 I273 V274 S275 P276 F277 K280 P281 L282 V283 D284 V285
E288 M289 Y294 T295 P296 L297 K298 M299 F300 Q301 M302 D305 F306 F307 T308 S309 M310 N311 L312 T313 K314 L315 K322 K327 D330 G331 R332 D333 L334 V335 C336 H337 A338 W341 D342 F343 Y344 D347 R350 I351 K352 Q353 C354 T355 R356 V357 Q361 L362 H366 H367
E368 L369 Q373 Y374 Q377 Y378 Q379 P382 F383 V384 Y385 R386 T387 G388 A389 N390 P391 G392 F393 H394 E395 A396 V397 S404 K409 H410 L411 E412 K413 I414 G415 L416 L417 K418 D419 R422 D423 D424 E425 Q430 L431 L442 P443 F446 T447 K450 Y451 R452 W453 S454
R457 D461 K462 A463 N464 W465 A468 K471 L472 R473 D474 E475 I479 E480 P481 P482 V483 V484 R485 S486 E487 A492 P493 A494 K495 I498 E503 Y504 L505 V509 I513 Q514 F515 Q516 K519 C522 I523 K524 A525 G526 Q527 D531 N532 V533 E534 L535 P536
L537 D538 N539 C540 D541 I542 Y543 G544 F552 H553 L556 G559 A560 P563 W564 P565 L568 E569 R575 A581 I582 E587 P588 L589 R590 V591 W592 L593 N601 V602 H603 W606 I607 T608 C612 V613 S614 S615 H616 H619 H620

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 (i)

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: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
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: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: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: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: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: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:89:GLN:H	1:B:89:GLN:NE2	1.91	0.67
1:B:541:ASP:C	1:B:543:TYR:H	1.98	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: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

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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: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: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: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: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:O	1:A:177:VAL:HG13	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: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:148:GLU:CD	1:A:148:GLU:H	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: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

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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: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:A:250:GLU:OE1	1:A:250:GLU:HA	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: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: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: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: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: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:34:LYS:HB2	1:B:34:LYS:HZ1	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: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:H	1:B:89:GLN:CD	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: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: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: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: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:O	1:B:612:CYS:SG	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:A:98:LYS:O	1:A:102:LYS:HG3	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PRO:HG2	1:B:148:GLU:CD	2.35	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
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: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: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: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:382:PRO:O	1:B:383:PHE:C	2.55	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: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:389:ALA:O	1:B:390:ASN:O	2.35	0.45
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:533:VAL:C	1:A:535:LEU:H	2.19	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: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: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:515:PHE:CD2	1:B:582:ILE:HG23	2.53	0.43
1:B:533:VAL:C	1:B:535:LEU:H	2.21	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
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: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:HD3	1:B:422:ARG:C	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:115:GLU:CD	1:B:183:ARG:HE	2.23	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: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: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

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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:HD12	1:A:100:LEU:HA	1.80	0.41
1:A:422:ARG:HD3	1:A:422:ARG:C	2.41	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:B:338:ALA:HB2	1:B:353:GLN:HG3	2.03	0.41
1:A:95:ARG:HB3	1:A:385:TYR:OH	2.20	0.41
1:A:383:PHE:HA	1:A:386:ARG:HD3	2.02	0.41
1:B:533:VAL:HG13	1:B:534:GLU:N	2.35	0.41
1:A:89:GLN:H	1:A:89:GLN:CD	2.15	0.41
1:A:191:ALA:O	1:A:195:ASN:ND2	2.54	0.41
1:B:285:VAL:HG12	1:B:289:MET:HG3	2.01	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: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: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

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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: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 (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 (i)

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	802	2	14,14,14	1.20	1 (7%)	18,19,19	0.98	1 (5%)
3	X8Z	A	801	2	14,14,14	1.05	1 (7%)	18,19,19	0.97	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	B	802	2	-	0/14/24/24	0/1/1/1
3	X8Z	A	801	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	2.94	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(^{o})	Ideal(^{o})
3	B	802	X8Z	C6-C7-C8	2.15	108.67	104.18
3	A	801	X8Z	C6-C7-C8	2.11	108.60	104.18

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.