Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

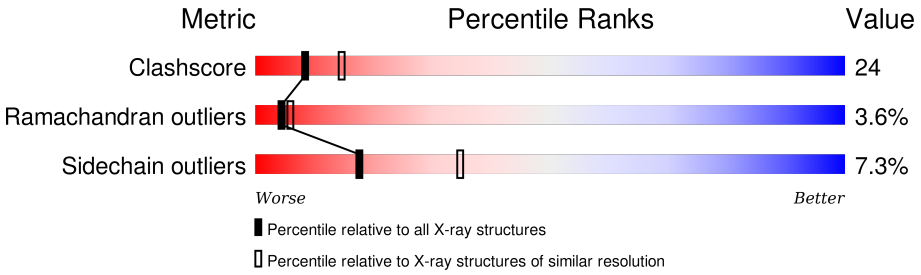
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	55% 37% 7%
1	B	607	56% 36% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9806 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called angiotensin converting enzyme.

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

There are 16 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is water.

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

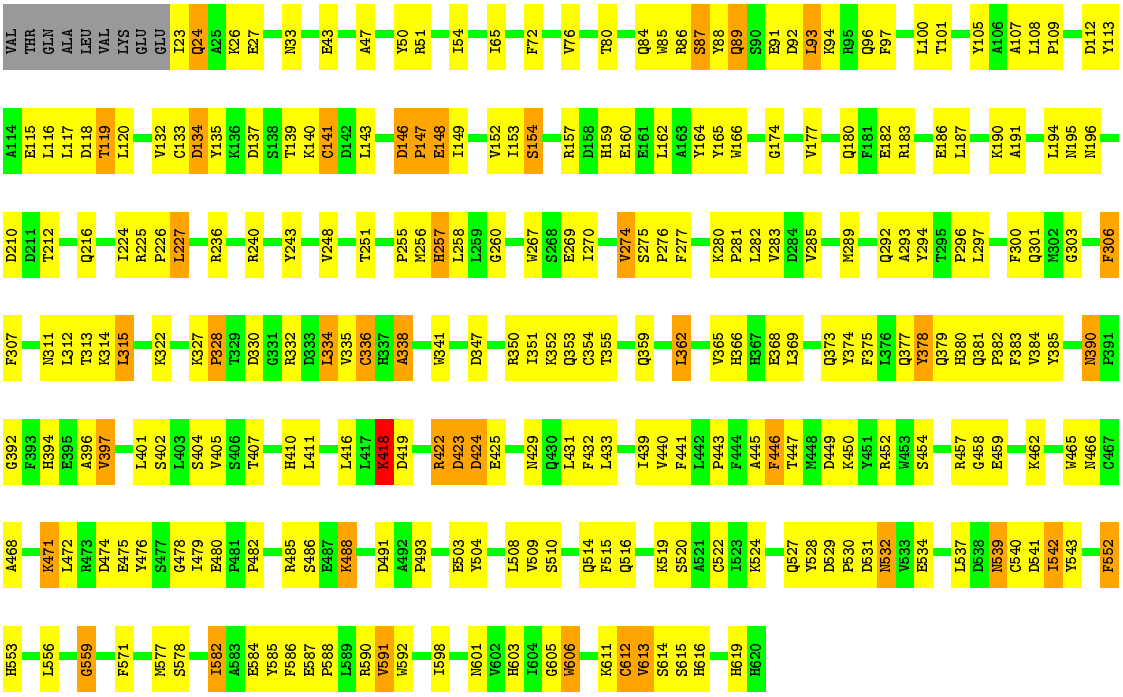
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

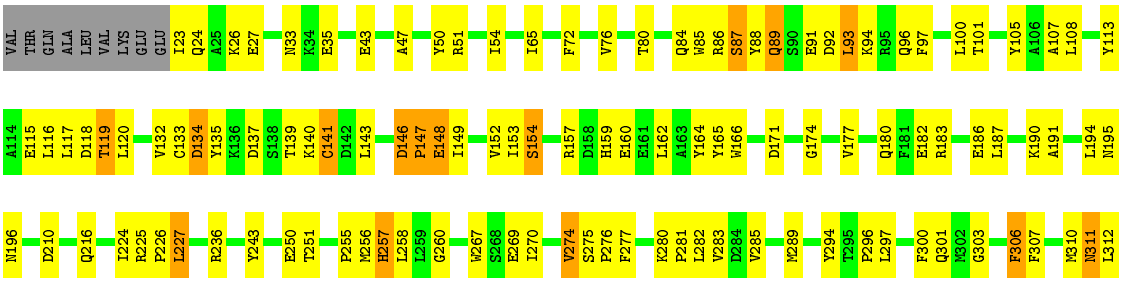
- Molecule 1: angiotensin converting enzyme

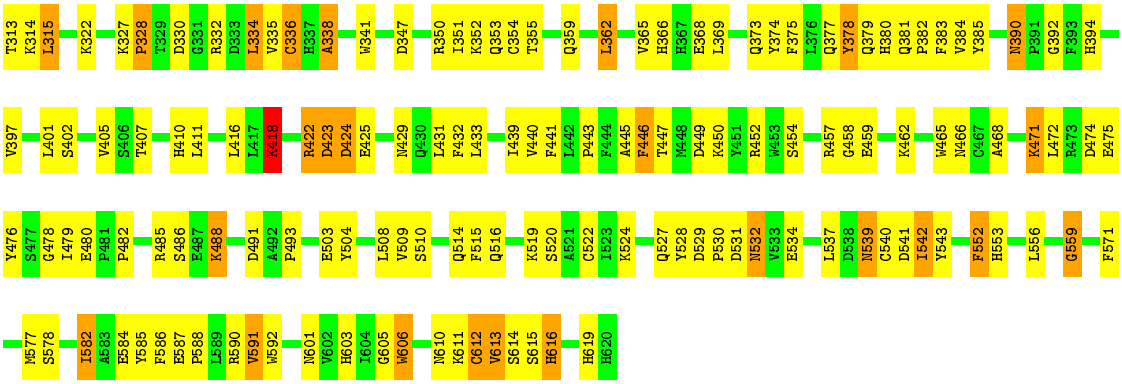
Chain A:



- Molecule 1: angiotensin converting enzyme

Chain B:




T313 K314 L315 K322 K327 P328 T329 D330 G331 R332 D333 L334 V335 C336 H337 A338 W341 D347 R350 I351 K352 Q353 C354 T355 Q359 L362 V365 H366 H367 E368 L369 Q373 Y374 F375 L376 Q377 Y378 Q379 H380 Q381 P382 F383 V384 Y385 N390 P391 G392 P393 H394
V397 L401 S402 V405 S406 T407 H410 L411 L416 L417 K418 R422 D423 D424 E425 N429 Q430 L431 F432 L433 I439 V440 F441 L442 P443 F444 A445 F446 T447 N448 D449 K450 Y451 R452 W453 S454 R457 G458 E459 K462 W465 N466 C467 A468 K471 L472 R473 D474 E475
Y476 S477 G478 I479 E480 P481 P482 R485 S486 E487 K488 D491 A492 P493 E503 Y504 L508 V509 S510 Q514 F515 Q516 K519 S520 A521 C522 I523 K524 Q527 Y528 D529 P530 D531 N532 V533 E534 L537 D538 N539 C540 D541 I542 Y543 F552 H553 L556 G559 F571
M577 S578 I582 A583 E584 Y585 F586 E587 P588 L589 R590 V591 W592 M601 V602 H603 I604 G605 W606 M610 K611 Q612 V613 S614 S615 H616 H619 H620

4 Data and refinement statistics (i)

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

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/5031	0.67	0/6814
1	B	0.45	0/5031	0.68	0/6814
All	All	0.44	0/10062	0.67	0/13628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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	221	2
1	B	4900	0	4696	230	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	9806	0	9392	450	2

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASN:HD22	1:B:534:GLU:H	1.38	0.71
1:B:108:LEU:HD13	1:B:191:ALA:HB2	1.73	0.70
1:A:516:GLN:NE2	1:A:578:SER:H	1.89	0.70
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.27	0.69
1:A:89:GLN:H	1:A:89:GLN:NE2	1.91	0.69
1:A:330:ASP:OD1	1:A:332:ARG:HB2	1.93	0.69
1:A:532:ASN:HD22	1:A:534:GLU:H	1.39	0.69
1:B:89:GLN:H	1:B:89:GLN:NE2	1.91	0.68
1:B:315:LEU:HD21	1:B:369:LEU:HD11	1.74	0.68
1:A:97:PHE:O	1:A:101:THR:HG23	1.94	0.68
1:A:443:PRO:O	1:A:447:THR:HG23	1.94	0.68
1:A:108:LEU:HD13	1:A:191:ALA:HB2	1.75	0.68
1:A:509:VAL:HB	1:A:577:MET:CE	2.24	0.68
1:A:322:LYS:CB	1:A:350:ARG:HD3	2.23	0.67
1:A:315:LEU:HD21	1:A:369:LEU:HD11	1.75	0.67
1:B:590:ARG:NH1	1:B:591:VAL:HG12	2.10	0.67
1:B:97:PHE:O	1:B:101:THR:HG23	1.95	0.67
1:A:590:ARG:NH1	1:A:591:VAL:HG12	2.09	0.66
1:A:166:TRP:HH2	1:A:485:ARG:HD2	1.61	0.66
1:B:285:VAL:CG1	1:B:416:LEU:HB3	2.25	0.65
1:A:516:GLN:HE22	1:A:578:SER:H	1.42	0.65
1:B:276:PRO:HB3	1:B:592:TRP:CH2	2.31	0.65
1:A:285:VAL:CG1	1:A:416:LEU:HB3	2.26	0.65
1:A:89:GLN:H	1:A:89:GLN:CD	2.00	0.65
1:B:509:VAL:HB	1:B:577:MET:CE	2.26	0.65
1:A:177:VAL:HG22	1:A:180:GLN:HB2	1.79	0.65
1:B:516:GLN:HE22	1:B:578:SER:H	1.41	0.65
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.31	0.65
1:B:89:GLN:H	1:B:89:GLN:CD	1.99	0.64
1:A:166:TRP:CH2	1:A:485:ARG:HD2	2.33	0.64
1:A:43:GLU:HA	1:A:65:ILE:HG21	1.79	0.64
1:B:177:VAL:HG22	1:B:180:GLN:HB2	1.78	0.63
1:B:225:ARG:HB3	1:B:226:PRO:HD3	1.80	0.63
1:B:152:VAL:HG11	1:B:165:TYR:CD2	2.34	0.63
1:B:322:LYS:CB	1:B:350:ARG:HD3	2.27	0.63
1:A:471:LYS:O	1:A:475:GLU:HG3	1.99	0.63
1:A:285:VAL:H	1:A:359:GLN:NE2	1.96	0.63
1:B:297:LEU:HG	1:B:301:GLN:NE2	2.13	0.63
1:A:148:GLU:H	1:A:148:GLU:CD	2.00	0.62
1:B:532:ASN:ND2	1:B:534:GLU:H	1.98	0.62
1:A:509:VAL:HB	1:A:577:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:H	1:B:359:GLN:NE2	1.98	0.61
1:A:297:LEU:HG	1:A:301:GLN:NE2	2.15	0.61
1:B:166:TRP:HH2	1:B:485:ARG:HD2	1.64	0.61
1:A:132:VAL:HG22	1:A:149:ILE:HD11	1.82	0.61
1:B:148:GLU:CD	1:B:148:GLU:H	2.04	0.61
1:B:296:PRO:HB3	1:B:355:THR:OG1	2.01	0.61
1:B:166:TRP:CH2	1:B:485:ARG:HD2	2.36	0.61
1:B:334:LEU:HD21	1:B:336:CYS:SG	2.41	0.60
1:A:296:PRO:HB3	1:A:355:THR:OG1	2.02	0.60
1:B:528:TYR:CE1	1:B:537:LEU:HB2	2.37	0.60
1:A:225:ARG:HB3	1:A:226:PRO:HD3	1.84	0.60
1:A:85:TRP:O	1:A:87:SER:N	2.35	0.60
1:A:532:ASN:ND2	1:A:534:GLU:H	1.99	0.59
1:A:598:ILE:CD1	1:B:35:GLU:HG2	2.33	0.59
1:A:365:VAL:O	1:A:369:LEU:HD23	2.03	0.59
1:B:96:GLN:O	1:B:100:LEU:HD23	2.03	0.59
1:A:613:VAL:HG23	1:A:614:SER:N	2.17	0.59
1:B:47:ALA:O	1:B:51:ARG:HG3	2.03	0.59
1:A:528:TYR:CE1	1:A:537:LEU:HB2	2.38	0.59
1:A:587:GLU:OE2	1:A:590:ARG:NH2	2.36	0.59
1:B:285:VAL:O	1:B:285:VAL:HG12	2.03	0.59
1:B:509:VAL:HB	1:B:577:MET:HE1	1.84	0.59
1:A:47:ALA:O	1:A:51:ARG:HG3	2.03	0.59
1:B:43:GLU:HA	1:B:65:ILE:HG21	1.84	0.59
1:B:552:PHE:O	1:B:556:LEU:HG	2.03	0.59
1:B:183:ARG:HH12	1:B:187:LEU:HD21	1.67	0.59
1:B:270:ILE:HD12	1:B:270:ILE:O	2.03	0.58
1:B:72:PHE:O	1:B:76:VAL:HG23	2.03	0.58
1:A:541:ASP:O	1:A:543:TYR:N	2.36	0.58
1:A:552:PHE:O	1:A:556:LEU:HG	2.02	0.58
1:B:520:SER:HB2	1:B:571:PHE:HE2	1.68	0.58
1:B:85:TRP:HA	1:B:88:TYR:CD1	2.38	0.58
1:A:162:LEU:HD13	1:A:257:HIS:O	2.02	0.58
1:B:537:LEU:O	1:B:537:LEU:HD13	2.03	0.58
1:A:183:ARG:HH12	1:A:187:LEU:HD21	1.69	0.58
1:A:270:ILE:HD12	1:A:270:ILE:O	2.03	0.58
1:A:251:THR:HG22	1:A:603:HIS:NE2	2.19	0.58
1:B:251:THR:HG22	1:B:603:HIS:NE2	2.19	0.58
1:A:72:PHE:O	1:A:76:VAL:HG23	2.04	0.58
1:A:520:SER:HB2	1:A:571:PHE:HE2	1.69	0.57
1:B:613:VAL:HG23	1:B:614:SER:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:O	1:A:100:LEU:HD23	2.04	0.57
1:B:91:GLU:HB3	1:B:94:LYS:NZ	2.20	0.57
1:B:446:PHE:O	1:B:450:LYS:HB2	2.03	0.57
1:B:365:VAL:O	1:B:369:LEU:HD23	2.04	0.57
1:A:277:PHE:H	1:A:429:ASN:HD21	1.52	0.57
1:A:488:LYS:HB2	1:A:488:LYS:HZ2	1.70	0.57
1:A:330:ASP:OD2	1:A:332:ARG:HD3	2.05	0.56
1:A:85:TRP:C	1:A:87:SER:H	2.08	0.56
1:B:257:HIS:ND1	1:B:482:PRO:HB3	2.21	0.56
1:A:537:LEU:HD13	1:A:537:LEU:O	2.05	0.56
1:B:385:TYR:HB3	1:B:559:GLY:O	2.04	0.56
1:A:256:MET:O	1:A:257:HIS:CB	2.53	0.56
1:A:257:HIS:ND1	1:A:482:PRO:HB3	2.20	0.56
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.40	0.56
1:A:85:TRP:HA	1:A:88:TYR:CD1	2.40	0.56
1:B:267:TRP:O	1:B:270:ILE:HG13	2.04	0.56
1:B:541:ASP:O	1:B:543:TYR:N	2.39	0.56
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.59	0.56
1:B:488:LYS:HZ2	1:B:488:LYS:HB2	1.70	0.56
1:A:251:THR:HG22	1:A:603:HIS:CE1	2.41	0.56
1:A:471:LYS:HD3	1:A:471:LYS:O	2.05	0.56
1:B:85:TRP:O	1:B:87:SER:N	2.38	0.56
1:B:162:LEU:HD13	1:B:257:HIS:O	2.04	0.56
1:A:105:TYR:O	1:A:108:LEU:HB2	2.05	0.56
1:B:587:GLU:OE2	1:B:590:ARG:NH2	2.38	0.56
1:B:280:LYS:HB3	1:B:281:PRO:HD2	1.88	0.56
1:B:105:TYR:O	1:B:108:LEU:HB2	2.05	0.56
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.41	0.56
1:A:91:GLU:HB3	1:A:94:LYS:NZ	2.20	0.56
1:A:116:LEU:O	1:A:120:LEU:HB2	2.05	0.56
1:B:277:PHE:H	1:B:429:ASN:HD21	1.53	0.56
1:A:446:PHE:O	1:A:450:LYS:HB2	2.06	0.56
1:B:85:TRP:C	1:B:87:SER:H	2.09	0.56
1:A:135:TYR:HB2	1:A:164:TYR:CD2	2.41	0.56
1:A:480:GLU:OE2	1:A:611:LYS:HE3	2.05	0.56
1:B:227:LEU:HD13	1:B:439:ILE:HD13	1.88	0.56
1:B:485:ARG:HD3	1:B:491:ASP:OD2	2.06	0.56
1:B:471:LYS:O	1:B:475:GLU:HG3	2.06	0.55
1:B:224:ILE:HG12	1:B:582:ILE:HD12	1.88	0.55
1:A:154:SER:HB2	1:A:269:GLU:CG	2.29	0.55
1:B:256:MET:O	1:B:257:HIS:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:PHE:HE2	1:B:355:THR:HG21	1.71	0.55
1:A:485:ARG:HD3	1:A:491:ASP:OD2	2.06	0.55
1:B:51:ARG:HD2	1:B:341:TRP:CZ2	2.42	0.55
1:A:107:ALA:O	1:A:194:LEU:HD23	2.06	0.55
1:A:280:LYS:HB3	1:A:281:PRO:HD2	1.88	0.55
1:A:510:SER:O	1:A:514:GLN:HB3	2.07	0.55
1:B:116:LEU:O	1:B:120:LEU:HB2	2.06	0.55
1:A:267:TRP:O	1:A:270:ILE:HG13	2.05	0.55
1:A:377:GLN:HE22	1:A:553:HIS:CD2	2.25	0.55
1:B:251:THR:HG22	1:B:603:HIS:CE1	2.41	0.55
1:B:183:ARG:HH12	1:B:187:LEU:CD2	2.19	0.55
1:A:457:ARG:O	1:A:459:GLU:N	2.38	0.55
1:A:474:ASP:O	1:A:606:TRP:CZ3	2.60	0.54
1:A:515:PHE:CD2	1:A:582:ILE:HG23	2.42	0.54
1:B:135:TYR:HB2	1:B:164:TYR:CD2	2.42	0.54
1:A:285:VAL:HG12	1:A:285:VAL:O	2.06	0.54
1:A:183:ARG:HH12	1:A:187:LEU:CD2	2.21	0.54
1:A:454:SER:O	1:A:457:ARG:O	2.25	0.54
1:B:480:GLU:OE2	1:B:611:LYS:HE3	2.08	0.54
1:A:385:TYR:HB3	1:A:559:GLY:O	2.07	0.54
1:A:256:MET:O	1:A:257:HIS:CG	2.60	0.54
1:A:51:ARG:HD2	1:A:341:TRP:CZ2	2.43	0.54
1:B:515:PHE:CD2	1:B:582:ILE:HG23	2.43	0.54
1:B:377:GLN:HE22	1:B:553:HIS:CD2	2.25	0.54
1:B:159:HIS:CE1	1:B:160:GLU:HG3	2.43	0.54
1:B:405:VAL:O	1:B:411:LEU:HD21	2.08	0.54
1:A:159:HIS:CE1	1:A:160:GLU:HG3	2.43	0.54
1:A:76:VAL:O	1:A:80:THR:HG23	2.08	0.54
1:B:510:SER:O	1:B:514:GLN:HB3	2.07	0.54
1:B:330:ASP:OD2	1:B:332:ARG:HD3	2.08	0.53
1:B:471:LYS:HD3	1:B:471:LYS:O	2.07	0.53
1:B:422:ARG:HD2	1:B:422:ARG:O	2.07	0.53
1:A:143:LEU:HB3	1:A:148:GLU:HB2	1.89	0.53
1:A:478:GLY:O	1:A:479:ILE:HD12	2.07	0.53
1:A:422:ARG:O	1:A:422:ARG:HD2	2.08	0.53
1:B:527:GLN:HB3	1:B:540:CYS:HB2	1.90	0.53
1:B:76:VAL:O	1:B:80:THR:HG23	2.08	0.53
1:B:508:LEU:O	1:B:508:LEU:HD12	2.09	0.53
1:B:457:ARG:O	1:B:459:GLU:N	2.41	0.53
1:A:289:MET:HE1	1:A:362:LEU:HG	1.89	0.53
1:B:251:THR:HG22	1:B:603:HIS:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:MET:HE1	1:B:362:LEU:HG	1.89	0.52
1:A:431:LEU:CD1	1:A:588:PRO:HG2	2.39	0.52
1:A:334:LEU:HD21	1:A:336:CYS:SG	2.50	0.52
1:A:152:VAL:HG11	1:A:165:TYR:CE2	2.44	0.52
1:A:300:PHE:HE2	1:A:355:THR:HG21	1.73	0.52
1:B:236:ARG:NH2	1:B:603:HIS:O	2.39	0.52
1:B:520:SER:HB2	1:B:571:PHE:CE2	2.44	0.52
1:B:478:GLY:O	1:B:479:ILE:HD12	2.10	0.52
1:B:327:LYS:HB2	1:B:354:CYS:SG	2.49	0.52
1:A:251:THR:HG22	1:A:603:HIS:CG	2.44	0.52
1:B:143:LEU:HB3	1:B:148:GLU:HB2	1.91	0.52
1:A:405:VAL:O	1:A:411:LEU:HD21	2.10	0.52
1:A:227:LEU:HD13	1:A:439:ILE:HD13	1.92	0.52
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.45	0.52
1:B:402:SER:HA	1:B:405:VAL:HG22	1.93	0.51
1:B:488:LYS:HB2	1:B:488:LYS:NZ	2.25	0.51
1:A:402:SER:HA	1:A:405:VAL:HG22	1.92	0.51
1:B:362:LEU:O	1:B:366:HIS:HD2	1.93	0.51
1:A:527:GLN:HB3	1:A:540:CYS:HB2	1.92	0.51
1:B:132:VAL:HG22	1:B:149:ILE:HD11	1.91	0.51
1:B:256:MET:O	1:B:257:HIS:CG	2.64	0.51
1:B:338:ALA:HB2	1:B:353:GLN:HG3	1.90	0.51
1:A:224:ILE:HG12	1:A:582:ILE:HD12	1.91	0.51
1:B:134:ASP:OD1	1:B:143:LEU:HD11	2.09	0.51
1:B:528:TYR:CG	1:B:537:LEU:HD23	2.46	0.51
1:B:96:GLN:O	1:B:100:LEU:CD2	2.58	0.51
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.31	0.51
1:B:537:LEU:HD13	1:B:585:TYR:HD1	1.76	0.51
1:A:541:ASP:OD2	1:A:541:ASP:O	2.29	0.51
1:A:133:CYS:HA	1:A:141:CYS:HA	1.91	0.51
1:A:338:ALA:HB2	1:A:353:GLN:HG3	1.92	0.51
1:B:154:SER:HB2	1:B:269:GLU:CG	2.33	0.51
1:B:152:VAL:HG11	1:B:165:TYR:CE2	2.45	0.51
1:B:454:SER:O	1:B:457:ARG:O	2.28	0.51
1:A:362:LEU:O	1:A:366:HIS:HD2	1.94	0.51
1:A:520:SER:HB2	1:A:571:PHE:CE2	2.46	0.51
1:A:33:ASN:HD22	1:A:383:PHE:HB3	1.75	0.50
1:B:190:LYS:O	1:B:194:LEU:HD13	2.11	0.50
1:A:134:ASP:OD1	1:A:143:LEU:HD11	2.10	0.50
1:B:113:TYR:CE2	1:B:117:LEU:HD11	2.46	0.50
1:A:541:ASP:C	1:A:543:TYR:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HA	1:A:243:TYR:OH	2.11	0.50
1:A:255:PRO:HB2	1:A:258:LEU:HD12	1.94	0.50
1:B:183:ARG:NH1	1:B:187:LEU:HD21	2.26	0.50
1:A:327:LYS:HB2	1:A:354:CYS:SG	2.52	0.50
1:B:255:PRO:HB2	1:B:258:LEU:HD12	1.93	0.50
1:B:392:GLY:HA3	1:B:509:VAL:CG2	2.41	0.50
1:A:537:LEU:HD13	1:A:585:TYR:HD1	1.76	0.50
1:B:157:ARG:HA	1:B:243:TYR:OH	2.10	0.50
1:A:528:TYR:CG	1:A:537:LEU:HD23	2.46	0.50
1:A:392:GLY:HA3	1:A:509:VAL:CG2	2.41	0.50
1:B:33:ASN:ND2	1:B:384:VAL:H	2.10	0.50
1:A:96:GLN:O	1:A:100:LEU:CD2	2.59	0.50
1:B:431:LEU:CD1	1:B:588:PRO:HG2	2.41	0.50
1:B:33:ASN:HD22	1:B:383:PHE:HB3	1.75	0.49
1:B:381:GLN:HE21	1:B:382:PRO:HD2	1.77	0.49
1:B:143:LEU:HD22	1:B:148:GLU:CB	2.42	0.49
1:B:153:ILE:HG22	1:B:153:ILE:O	2.12	0.49
1:A:307:PHE:O	1:A:312:LEU:HB2	2.11	0.49
1:B:410:HIS:HB2	1:B:541:ASP:CG	2.33	0.49
1:A:439:ILE:HD11	1:A:586:PHE:CD2	2.47	0.49
1:A:381:GLN:HE21	1:A:382:PRO:HD2	1.77	0.49
1:A:450:LYS:HE2	1:A:476:TYR:OH	2.12	0.49
1:A:190:LYS:O	1:A:194:LEU:HD13	2.12	0.49
1:A:275:SER:CB	1:A:282:LEU:HD21	2.41	0.49
1:A:303:GLY:HA2	1:A:366:HIS:CE1	2.47	0.49
1:A:431:LEU:HD13	1:A:588:PRO:HG2	1.94	0.49
1:A:509:VAL:HB	1:A:577:MET:HE2	1.94	0.49
1:B:441:PHE:CE2	1:B:445:ALA:HB2	2.47	0.49
1:B:285:VAL:HG23	1:B:359:GLN:NE2	2.27	0.49
1:A:210:ASP:OD1	1:A:216:GLN:NE2	2.44	0.49
1:B:107:ALA:O	1:B:194:LEU:HD23	2.13	0.49
1:B:210:ASP:OD1	1:B:216:GLN:NE2	2.42	0.49
1:B:133:CYS:HA	1:B:141:CYS:HA	1.93	0.49
1:A:195:ASN:O	1:A:196:ASN:HB2	2.13	0.48
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.34	0.48
1:A:183:ARG:NH1	1:A:187:LEU:HD21	2.28	0.48
1:A:236:ARG:NH2	1:A:603:HIS:O	2.40	0.48
1:B:50:TYR:CZ	1:B:54:ILE:HG23	2.49	0.48
1:A:306:PHE:CE2	1:A:543:TYR:HA	2.48	0.48
1:B:541:ASP:O	1:B:541:ASP:OD2	2.31	0.48
1:B:195:ASN:O	1:B:196:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:O	1:A:612:CYS:HA	2.13	0.48
1:A:471:LYS:HD3	1:A:475:GLU:HG3	1.96	0.48
1:A:351:ILE:HD13	1:A:368:GLU:HB3	1.96	0.48
1:B:471:LYS:HD3	1:B:475:GLU:HG3	1.96	0.48
1:B:439:ILE:HD11	1:B:586:PHE:CD2	2.49	0.48
1:B:250:GLU:O	1:B:251:THR:OG1	2.27	0.47
1:B:289:MET:O	1:B:294:TYR:HB2	2.14	0.47
1:B:275:SER:CB	1:B:282:LEU:HD21	2.44	0.47
1:B:276:PRO:HD3	1:B:432:PHE:CD1	2.49	0.47
1:A:33:ASN:ND2	1:A:384:VAL:H	2.11	0.47
1:A:441:PHE:CE2	1:A:445:ALA:HB2	2.48	0.47
1:A:407:THR:HB	1:A:539:ASN:HD22	1.79	0.47
1:B:537:LEU:CD1	1:B:585:TYR:HD1	2.28	0.47
1:B:532:ASN:HD22	1:B:532:ASN:C	2.18	0.47
1:A:276:PRO:HD2	1:A:429:ASN:ND2	2.30	0.47
1:A:532:ASN:HD22	1:A:532:ASN:C	2.18	0.47
1:B:335:VAL:O	1:B:352:LYS:NZ	2.44	0.47
1:A:276:PRO:HD3	1:A:432:PHE:CD1	2.50	0.47
1:B:509:VAL:HB	1:B:577:MET:HE2	1.95	0.47
1:A:418:LYS:N	1:A:418:LYS:HD2	2.29	0.47
1:B:380:HIS:H	1:B:380:HIS:CD2	2.33	0.47
1:A:137:ASP:C	1:A:139:THR:H	2.18	0.47
1:A:289:MET:O	1:A:294:TYR:HB2	2.14	0.47
1:B:418:LYS:HD2	1:B:418:LYS:N	2.29	0.47
1:B:303:GLY:HA2	1:B:366:HIS:CE1	2.49	0.47
1:B:468:ALA:O	1:B:472:LEU:HB2	2.15	0.47
1:B:541:ASP:C	1:B:543:TYR:H	2.18	0.47
1:B:307:PHE:O	1:B:312:LEU:HB2	2.15	0.47
1:B:407:THR:HB	1:B:539:ASN:HD22	1.80	0.47
1:A:488:LYS:HB2	1:A:488:LYS:NZ	2.29	0.46
1:B:485:ARG:O	1:B:612:CYS:HA	2.16	0.46
1:B:306:PHE:CE2	1:B:543:TYR:HA	2.50	0.46
1:A:285:VAL:HG23	1:A:359:GLN:NE2	2.30	0.46
1:B:137:ASP:C	1:B:139:THR:H	2.18	0.46
1:B:439:ILE:HD11	1:B:586:PHE:CG	2.51	0.46
1:B:351:ILE:HD13	1:B:368:GLU:HB3	1.97	0.46
1:B:50:TYR:OH	1:B:54:ILE:HG23	2.15	0.46
1:B:431:LEU:HD13	1:B:588:PRO:HG2	1.97	0.46
1:A:146:ASP:CB	1:A:147:PRO:HD3	2.28	0.46
1:B:285:VAL:HG21	1:B:411:LEU:HD13	1.98	0.46
1:A:328:PRO:HG2	1:A:332:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LYS:HE2	1:B:140:LYS:HB3	1.77	0.46
1:A:143:LEU:HD22	1:A:148:GLU:CB	2.45	0.45
1:B:277:PHE:CE2	1:B:425:GLU:HB3	2.52	0.45
1:B:100:LEU:HD21	1:B:384:VAL:HB	1.98	0.45
1:B:330:ASP:CG	1:B:332:ARG:HD3	2.37	0.45
1:B:276:PRO:HD2	1:B:429:ASN:ND2	2.30	0.45
1:B:171:ASP:OD1	1:B:485:ARG:NH2	2.36	0.45
1:B:328:PRO:HG2	1:B:332:ARG:NH2	2.31	0.45
1:A:277:PHE:CE2	1:A:425:GLU:HB3	2.51	0.45
1:B:153:ILE:O	1:B:260:GLY:HA2	2.16	0.45
1:A:519:LYS:HE3	1:A:584:GLU:OE2	2.16	0.45
1:B:614:SER:O	1:B:615:SER:HB3	2.17	0.45
1:B:450:LYS:HE2	1:B:476:TYR:OH	2.17	0.45
1:B:615:SER:OG	1:B:616:HIS:N	2.50	0.45
1:B:108:LEU:HD13	1:B:191:ALA:CB	2.42	0.45
1:B:275:SER:OG	1:B:282:LEU:HD11	2.17	0.45
1:B:54:ILE:HG13	1:B:334:LEU:HA	1.99	0.45
1:B:310:MET:HB2	1:B:312:LEU:HD12	1.99	0.45
1:B:274:VAL:O	1:B:274:VAL:HG13	2.16	0.45
1:A:275:SER:OG	1:A:282:LEU:HD11	2.17	0.44
1:A:108:LEU:HD13	1:A:191:ALA:CB	2.43	0.44
1:A:100:LEU:HD21	1:A:384:VAL:HB	1.99	0.44
1:A:375:PHE:HA	1:A:378:TYR:CE1	2.52	0.44
1:B:330:ASP:C	1:B:332:ARG:H	2.21	0.44
1:A:466:ASN:ND2	1:A:491:ASP:H	2.16	0.44
1:A:468:ALA:O	1:A:472:LEU:HB2	2.17	0.44
1:A:43:GLU:CA	1:A:65:ILE:HG21	2.46	0.44
1:B:256:MET:O	1:B:257:HIS:HB3	2.17	0.44
1:B:422:ARG:O	1:B:423:ASP:C	2.55	0.44
1:B:85:TRP:HA	1:B:88:TYR:CG	2.53	0.44
1:A:537:LEU:CD1	1:A:585:TYR:HD1	2.31	0.44
1:A:439:ILE:HD11	1:A:586:PHE:CG	2.53	0.44
1:A:380:HIS:H	1:A:380:HIS:CD2	2.35	0.44
1:A:274:VAL:O	1:A:274:VAL:HG13	2.17	0.44
1:A:452:ARG:NH2	1:A:504:TYR:HB2	2.32	0.44
1:A:256:MET:O	1:A:257:HIS:HB3	2.16	0.44
1:B:466:ASN:ND2	1:B:491:ASP:H	2.16	0.44
1:B:353:GLN:NE2	1:B:355:THR:HG22	2.33	0.44
1:A:524:LYS:HE3	1:A:571:PHE:O	2.18	0.44
1:A:422:ARG:O	1:A:423:ASP:C	2.56	0.44
1:A:522:CYS:SG	1:A:542:ILE:HG23	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CZ	1:A:54:ILE:HG23	2.53	0.43
1:A:177:VAL:HG13	1:A:177:VAL:O	2.18	0.43
1:B:524:LYS:HE3	1:B:571:PHE:O	2.18	0.43
1:A:285:VAL:HG21	1:A:411:LEU:HD13	1.99	0.43
1:A:275:SER:HA	1:A:276:PRO:HD3	1.79	0.43
1:A:330:ASP:C	1:A:332:ARG:H	2.22	0.43
1:B:84:GLN:O	1:B:88:TYR:CE1	2.72	0.43
1:B:462:LYS:HA	1:B:465:TRP:CD1	2.53	0.43
1:A:23:ILE:O	1:A:23:ILE:HG12	2.18	0.43
1:B:475:GLU:O	1:B:606:TRP:HH2	2.01	0.43
1:B:183:ARG:NH1	1:B:187:LEU:CD2	2.82	0.43
1:A:615:SER:OG	1:A:616:HIS:N	2.51	0.43
1:A:475:GLU:O	1:A:606:TRP:HH2	2.01	0.43
1:B:519:LYS:HE3	1:B:584:GLU:OE2	2.18	0.43
1:B:522:CYS:SG	1:B:542:ILE:HG23	2.58	0.43
1:A:392:GLY:HA3	1:A:509:VAL:HG21	2.01	0.43
1:A:353:GLN:NE2	1:A:355:THR:HG22	2.34	0.43
1:B:605:GLY:C	1:B:606:TRP:CD1	2.92	0.43
1:A:508:LEU:O	1:A:508:LEU:HD12	2.18	0.43
1:B:23:ILE:HG12	1:B:23:ILE:O	2.19	0.43
1:A:153:ILE:HG22	1:A:153:ILE:O	2.18	0.43
1:B:327:LYS:CB	1:B:354:CYS:SG	3.07	0.43
1:B:177:VAL:O	1:B:177:VAL:HG13	2.17	0.43
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.54	0.43
1:A:313:THR:HB	1:A:373:GLN:HE22	1.84	0.42
1:A:335:VAL:O	1:A:352:LYS:NZ	2.44	0.42
1:B:611:LYS:HD3	1:B:611:LYS:HA	1.86	0.42
1:A:85:TRP:HA	1:A:88:TYR:CG	2.55	0.42
1:B:392:GLY:HA3	1:B:509:VAL:HG21	2.01	0.42
1:B:375:PHE:HA	1:B:378:TYR:CE1	2.55	0.42
1:B:51:ARG:HD2	1:B:341:TRP:CH2	2.54	0.42
1:B:313:THR:HB	1:B:373:GLN:HE22	1.85	0.42
1:B:267:TRP:CE2	1:B:440:VAL:HG11	2.55	0.42
1:B:327:LYS:HG3	1:B:354:CYS:SG	2.59	0.42
1:A:153:ILE:O	1:A:260:GLY:HA2	2.19	0.42
1:B:423:ASP:O	1:B:424:ASP:HB2	2.20	0.42
1:A:113:TYR:O	1:A:117:LEU:HG	2.19	0.42
1:B:113:TYR:O	1:B:117:LEU:HG	2.20	0.42
1:B:182:GLU:O	1:B:186:GLU:HG3	2.19	0.42
1:B:146:ASP:CB	1:B:147:PRO:HD3	2.28	0.42
1:B:143:LEU:HD22	1:B:148:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASP:O	1:A:424:ASP:HB2	2.20	0.42
1:A:527:GLN:HB3	1:A:540:CYS:CB	2.50	0.42
1:B:449:ASP:OD2	1:B:452:ARG:NH2	2.48	0.42
1:A:115:GLU:OE1	1:A:183:ARG:NH2	2.53	0.41
1:A:183:ARG:NH1	1:A:187:LEU:CD2	2.83	0.41
1:A:182:GLU:O	1:A:186:GLU:HG3	2.20	0.41
1:A:84:GLN:O	1:A:88:TYR:CE1	2.74	0.41
1:A:51:ARG:HD2	1:A:341:TRP:HZ2	1.84	0.41
1:A:23:ILE:O	1:A:24:GLN:O	2.38	0.41
1:A:529:ASP:O	1:A:531:ASP:N	2.54	0.41
1:A:51:ARG:HD2	1:A:341:TRP:CH2	2.55	0.41
1:A:240:ARG:HA	1:A:248:VAL:HB	2.02	0.41
1:B:143:LEU:HD23	1:B:148:GLU:HG2	1.96	0.41
1:B:452:ARG:NH2	1:B:504:TYR:HB2	2.35	0.41
1:B:528:TYR:OH	1:B:584:GLU:OE1	2.37	0.41
1:A:292:GLN:O	1:A:293:ALA:HB3	2.21	0.41
1:A:471:LYS:HA	1:A:471:LYS:HZ3	1.86	0.41
1:A:212:THR:O	1:A:216:GLN:HG3	2.20	0.41
1:A:605:GLY:C	1:A:606:TRP:CD1	2.94	0.41
1:A:449:ASP:OD2	1:A:452:ARG:NH2	2.47	0.41
1:A:140:LYS:HE2	1:A:140:LYS:HB3	1.79	0.41
1:B:610:ASN:HD22	1:B:610:ASN:HA	1.69	0.41
1:B:613:VAL:HG23	1:B:614:SER:H	1.86	0.41
1:B:85:TRP:C	1:B:87:SER:N	2.75	0.41
1:A:267:TRP:CE2	1:A:440:VAL:HG11	2.56	0.41
1:B:471:LYS:HZ3	1:B:471:LYS:HA	1.86	0.41
1:B:381:GLN:HE21	1:B:382:PRO:CD	2.34	0.41
1:B:311:ASN:HA	1:B:311:ASN:HD22	1.57	0.41
1:B:89:GLN:N	1:B:89:GLN:CD	2.72	0.40
1:A:381:GLN:HE21	1:A:382:PRO:CD	2.34	0.40
1:A:327:LYS:CB	1:A:354:CYS:SG	3.09	0.40
1:A:109:PRO:CG	1:A:112:ASP:OD2	2.69	0.40
1:A:382:PRO:O	1:A:383:PHE:C	2.60	0.40
1:A:396:ALA:O	1:A:397:VAL:C	2.60	0.40
1:B:410:HIS:HD2	1:B:541:ASP:OD1	2.05	0.40
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.49	0.40
1:B:380:HIS:N	1:B:380:HIS:CD2	2.89	0.40
1:B:529:ASP:O	1:B:531:ASP:N	2.54	0.40
1:B:275:SER:HA	1:B:276:PRO:HD3	1.80	0.40
1:B:270:ILE:H	1:B:270:ILE:HG13	1.81	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:HIS:NE2	1:B:134:ASP:OD2[1_554]	2.07	0.13
1:A:134:ASP:OD2	1:B:619:HIS:NE2[1_554]	2.17	0.03

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

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	147	PRO
1	A	418	LYS
1	A	542	ILE
1	B	24	GLN
1	B	147	PRO
1	B	418	LYS
1	B	542	ILE
1	A	86	ARG
1	A	87	SER
1	A	338	ALA
1	A	423	ASP
1	A	424	ASP
1	A	613	VAL
1	B	86	ARG
1	B	87	SER
1	B	338	ALA

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Mol	Chain	Res	Type
1	B	423	ASP
1	B	424	ASP
1	B	613	VAL
1	A	559	GLY
1	B	141	CYS
1	B	283	VAL
1	B	559	GLY
1	A	141	CYS
1	A	257	HIS
1	A	283	VAL
1	A	390	ASN
1	B	257	HIS
1	B	390	ASN
1	A	148	GLU
1	A	397	VAL
1	A	458	GLY
1	B	148	GLU
1	B	397	VAL
1	B	616	HIS
1	B	146	ASP
1	A	530	PRO
1	A	591	VAL
1	B	458	GLY
1	B	530	PRO
1	B	591	VAL
1	A	146	ASP

5.3.2 Protein sidechains (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%)	483 (92%)	39 (8%)	17	33
1	B	522/530 (98%)	485 (93%)	37 (7%)	18	36
All	All	1044/1060 (98%)	968 (93%)	76 (7%)	17	35

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

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

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

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

Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	ASN
1	A	41	ASN
1	A	89	GLN
1	A	159	HIS

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	311	ASN
1	A	317	GLN
1	A	337	HIS
1	A	359	GLN
1	A	366	HIS
1	A	373	GLN
1	A	377	GLN
1	A	379	GLN
1	A	380	HIS
1	A	381	GLN
1	A	410	HIS
1	A	429	ASN
1	A	464	ASN
1	A	466	ASN
1	A	514	GLN
1	A	516	GLN
1	A	527	GLN
1	A	532	ASN
1	A	539	ASN
1	A	554	ASN
1	A	610	ASN
1	B	31	ASN
1	B	33	ASN
1	B	41	ASN
1	B	89	GLN
1	B	159	HIS
1	B	301	GLN
1	B	311	ASN
1	B	337	HIS
1	B	359	GLN
1	B	366	HIS
1	B	373	GLN
1	B	377	GLN
1	B	379	GLN
1	B	380	HIS
1	B	381	GLN
1	B	410	HIS
1	B	429	ASN
1	B	464	ASN
1	B	466	ASN
1	B	514	GLN

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Mol	Chain	Res	Type
1	B	516	GLN
1	B	527	GLN
1	B	532	ASN
1	B	539	ASN
1	B	554	ASN
1	B	601	ASN
1	B	610	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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