Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:45 PM GMT

PDB ID	:	1YIZ
Title	:	Aedes aegypti kynurenine aminotrasferase
Authors	:	Han, Q.; Gao, Y.G.; Robinson, H.; Ding, H.; Wilson, S.; Li, J.
Deposited on	:	2005-01-13
Resolution	:	1.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

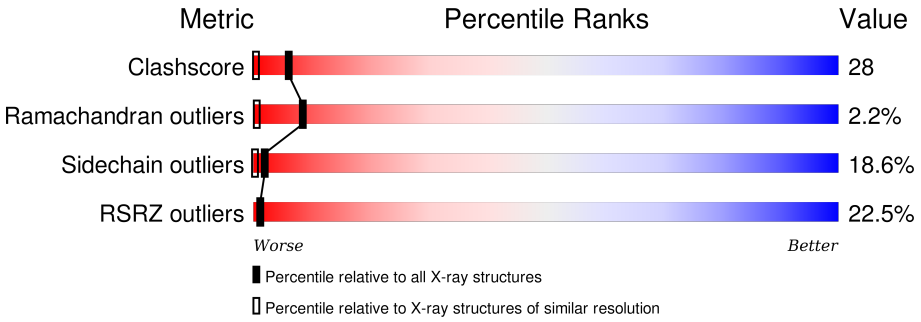
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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.

Mol	Chain	Length	Quality of chain
1	A	429	20% 53% 31% 12%
1	B	429	24% 52% 34% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	605	-	-	X	-
2	BR	B	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	B	604	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7105 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 kynurenine aminotransferase; glutamine transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	P	S	0	0	0
			3330	2141	550	618	1	20			
1	B	418	Total	C	N	O	P	S	0	0	0
			3330	2141	550	618	1	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LLP	LYS	MODIFIED RESIDUE	UNP Q95VY4
B	255	LLP	LYS	MODIFIED RESIDUE	UNP Q95VY4

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

- Molecule 3 is water.

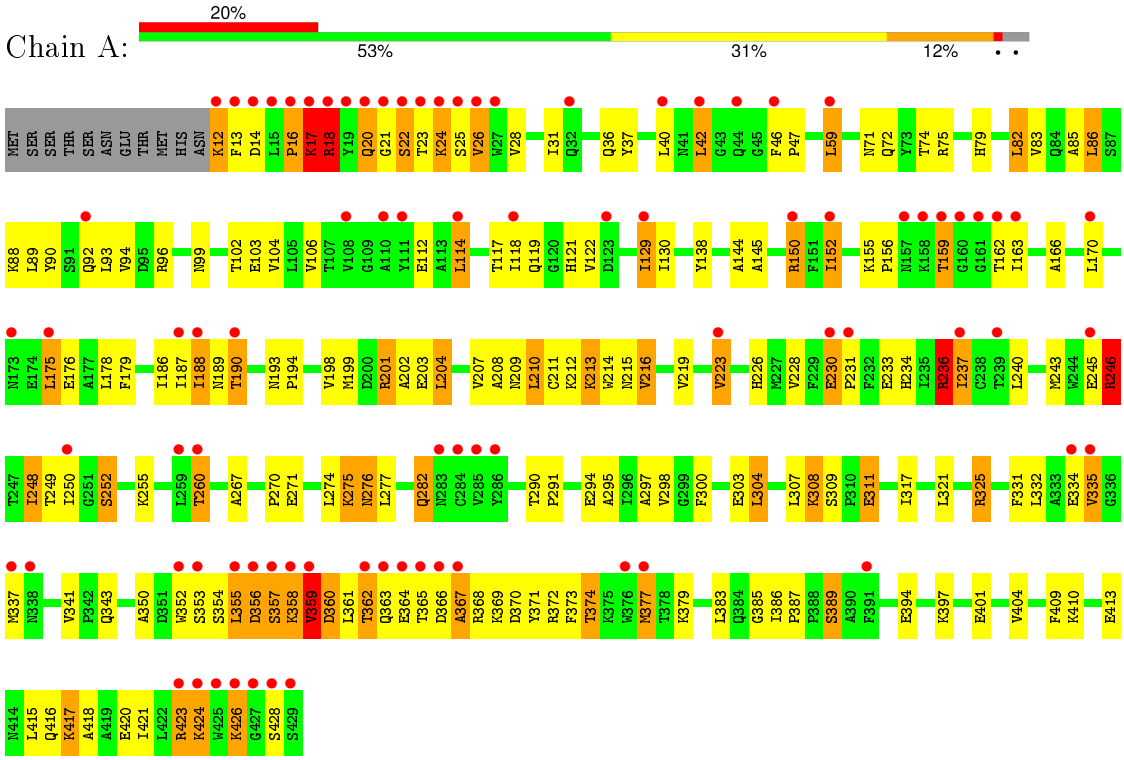
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	250	Total	O	0	0
			250	250		
3	B	190	Total	O	0	0
			190	190		

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.

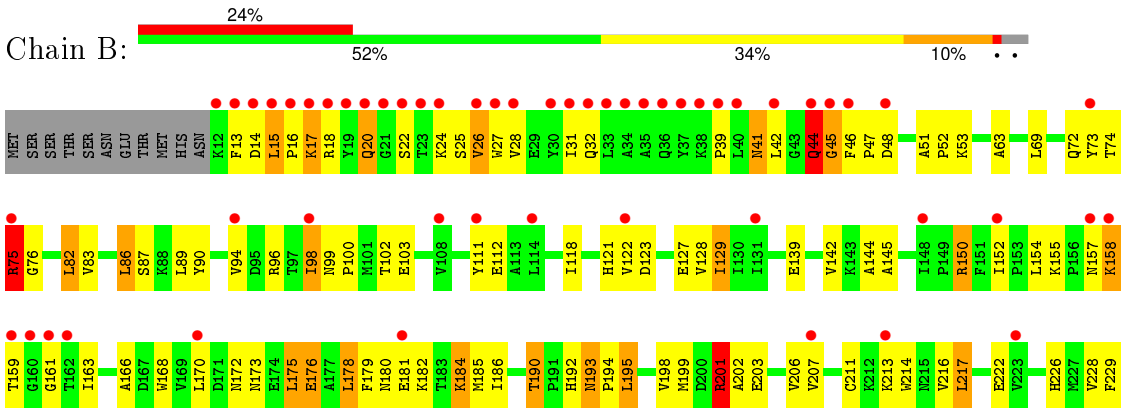
- Molecule 1: kynurenine aminotransferase; glutamine transaminase

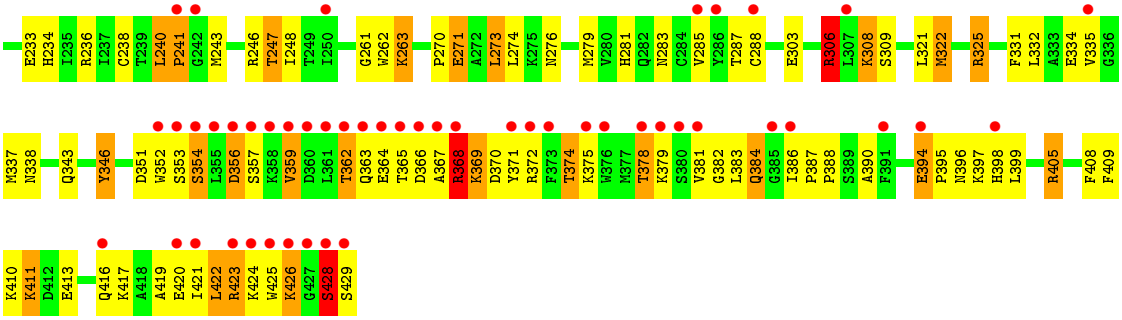
Chain A:



- Molecule 1: kynurenine aminotransferase; glutamine transaminase

Chain B:




E233 H234 I235 R236 I237 C238 T239 L240 P241 G242 M243 R246 T247 I248 T249 I250 G261 W262 K263 P270 E271 A272 L273 L274 K275 N276 M279 Y280 H281 Q282 N283 C284 V285 Y286 T287 C288 E303 R306 L307 K308 S309 L321 M322 R325 F331 L332 A333 E334 V335 G336
M337 N338 Q343 Y346 D351 W352 S353 S354 L355 D356 S357 K358 V359 D360 L361 T362 Q363 E364 T365 D366 A367 R368 K369 D370 Y371 R372 F373 T374 K375 W376 M377 T378 K379 S380 V381 G382 L383 Q384 G385 I386 P387 P388 S389 A390 F391 E394 P395 N396 K397 H398 L399 R405 F408 F409
K410 K411 D412 E413 Q416 K417 A418 A419 E420 I421 L422 R423 K424 W425 K426 G427 S428 S429

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.29Å 94.98Å 167.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.55 39.30 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-1.55) 95.7 (39.30-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.43 (at 1.55Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.254 , (Not available) 0.279 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 123988 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7105	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.44	1/3393 (0.0%)	0.93	7/4604 (0.2%)
1	B	0.41	0/3393	0.93	13/4604 (0.3%)
All	All	0.42	1/6786 (0.0%)	0.93	20/9208 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	ARG	CZ-NH1	9.52	1.45	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	ARG	NE-CZ-NH1	16.07	128.34	120.30
1	A	246	ARG	NE-CZ-NH2	8.65	124.63	120.30
1	A	18	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	325	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	374	THR	CA-CB-CG2	-7.28	102.20	112.40
1	A	246	ARG	CD-NE-CZ	7.12	133.57	123.60
1	B	405	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	236	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	A	325	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	201	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	325	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	75	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	247	THR	CA-CB-CG2	-5.95	104.06	112.40
1	B	325	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	236	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	B	201	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	325	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	306	ARG	NE-CZ-NH1	5.51	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	306	ARG	CD-NE-CZ	5.43	131.21	123.60
1	B	346	TYR	CB-CG-CD1	5.17	124.10	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3278	213	0
1	B	3330	0	3278	180	0
2	A	3	0	0	6	0
2	B	2	0	0	0	0
3	A	250	0	0	45	0
3	B	190	0	0	16	0
All	All	7105	0	6556	375	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 28.

All (375) 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:234:HIS:N	2:A:605:BR:BR	2.42	1.06
1:A:228:VAL:HG21	2:A:605:BR:BR	2.12	1.05
1:A:187:ILE:HG21	3:A:777:HOH:O	1.63	0.96
1:A:248:ILE:HD11	1:A:267:ALA:HB1	1.51	0.91
1:A:129:ILE:HD12	1:A:152:ILE:HD11	1.50	0.91
1:A:357:SER:HA	1:A:361:LEU:HB2	1.53	0.91
1:B:14:ASP:O	1:B:16:PRO:HD3	1.73	0.88
1:A:24:LYS:HE3	1:A:24:LYS:H	1.38	0.86
1:A:211:CYS:HA	1:A:216:VAL:HG13	1.58	0.85
1:B:42:LEU:HD22	1:B:383:LEU:HD11	1.59	0.84
1:B:180:ASN:HD21	1:B:182:LYS:HB2	1.42	0.83
1:A:71:ASN:HD22	1:B:262:TRP:HE1	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HB1	1:A:243:MET:HE3	1.60	0.82
1:B:331:PHE:HA	1:B:334:GLU:HG2	1.62	0.81
1:A:355:LEU:HA	1:A:358:LYS:NZ	1.95	0.81
1:A:82:LEU:HD22	1:A:86:LEU:HD22	1.63	0.81
1:A:297:ALA:HA	3:A:792:HOH:O	1.81	0.80
1:A:228:VAL:CG2	2:A:605:BR:BR	2.84	0.80
1:A:413:GLU:O	1:A:417:LYS:HD2	1.82	0.80
1:B:193:ASN:HD21	1:B:405:ARG:HH11	1.30	0.79
1:A:187:ILE:HB	3:A:772:HOH:O	1.82	0.78
1:A:155:LYS:HD2	1:A:156:PRO:HD2	1.64	0.78
1:A:72:GLN:O	1:A:290:THR:HG21	1.84	0.78
1:B:353:SER:HA	1:B:356:ASP:OD2	1.84	0.78
1:A:89:LEU:O	1:A:93:LEU:HD13	1.84	0.77
1:B:261:GLY:HA2	1:B:263:LYS:HE3	1.66	0.77
1:A:367:ALA:HB1	3:A:738:HOH:O	1.86	0.76
1:B:378:THR:HG22	1:B:384:GLN:HA	1.68	0.74
1:B:198:VAL:HB	3:B:765:HOH:O	1.86	0.74
1:B:367:ALA:H	1:B:372:ARG:HH22	1.35	0.74
1:B:180:ASN:ND2	1:B:182:LYS:H	1.86	0.73
1:B:217:LEU:HD11	1:B:248:ILE:HD12	1.70	0.73
1:A:228:VAL:HG22	3:A:751:HOH:O	1.89	0.72
1:A:130:ILE:HG12	1:A:187:ILE:HD11	1.72	0.72
1:B:118:ILE:O	1:B:122:VAL:HG13	1.90	0.71
1:A:117:THR:HA	1:A:277:LEU:HD22	1.72	0.71
1:B:394:GLU:HG2	3:B:691:HOH:O	1.91	0.70
1:A:25:SER:O	1:A:28:VAL:HG12	1.93	0.69
1:A:187:ILE:HG13	3:A:754:HOH:O	1.91	0.69
1:B:413:GLU:O	1:B:416:GLN:HG3	1.93	0.69
1:A:362:THR:HG22	3:A:838:HOH:O	1.93	0.68
1:B:121:HIS:O	1:B:184:LYS:HE2	1.92	0.68
1:B:332:LEU:O	1:B:335:VAL:HG12	1.93	0.68
1:B:180:ASN:HD22	1:B:182:LYS:H	1.39	0.68
1:B:190:THR:HG21	1:B:199:MET:H	1.57	0.68
1:A:355:LEU:HB2	1:A:360:ASP:OD2	1.93	0.68
1:A:355:LEU:HA	1:A:358:LYS:HZ3	1.57	0.67
1:A:31:ILE:HD12	1:B:75:ARG:NH2	2.11	0.67
1:A:357:SER:HB3	3:A:720:HOH:O	1.94	0.66
1:A:18:ARG:HA	1:A:18:ARG:NE	2.10	0.66
1:A:112:GLU:HB2	1:B:285:VAL:HG22	1.77	0.66
1:A:28:VAL:HA	1:B:75:ARG:NH2	2.12	0.65
1:A:118:ILE:HG21	3:A:752:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:SER:HA	1:B:98:ILE:HD11	1.79	0.64
1:B:26:VAL:HG21	1:B:390:ALA:HB1	1.79	0.64
1:B:170:LEU:HD23	3:B:648:HOH:O	1.96	0.64
1:B:383:LEU:HB2	1:B:421:ILE:HD12	1.78	0.64
1:A:364:GLU:O	1:A:367:ALA:HB3	1.97	0.64
1:A:223:VAL:HG23	1:A:252:SER:HB3	1.80	0.64
1:B:285:VAL:HB	3:B:715:HOH:O	1.98	0.64
1:B:192:HIS:HD2	1:B:195:LEU:HB2	1.63	0.63
1:A:22:SER:HA	1:A:24:LYS:NZ	2.13	0.63
1:A:21:GLY:HA2	1:B:279:MET:HG3	1.80	0.63
1:A:249:THR:HG23	3:A:764:HOH:O	1.98	0.63
1:B:170:LEU:HD23	1:B:170:LEU:H	1.62	0.62
1:A:215:ASN:HA	1:A:246:ARG:HH21	1.63	0.62
1:B:201:ARG:HG2	1:B:201:ARG:HH11	1.64	0.62
1:A:423:ARG:HH12	1:A:426:LYS:HD3	1.65	0.62
1:A:250:ILE:HG22	3:A:753:HOH:O	1.98	0.62
1:B:367:ALA:N	1:B:372:ARG:HH22	1.97	0.62
1:A:353:SER:HB3	3:A:791:HOH:O	1.99	0.62
1:B:24:LYS:HB2	1:B:28:VAL:HG23	1.82	0.62
1:A:93:LEU:HD23	1:A:236:ARG:NH2	2.14	0.62
1:A:20:GLN:HE22	1:A:144:ALA:HB2	1.64	0.62
1:A:114:LEU:O	1:A:118:ILE:HG13	1.99	0.62
1:B:90:TYR:O	1:B:94:VAL:HG12	2.00	0.62
1:B:367:ALA:H	1:B:372:ARG:NH2	1.97	0.62
1:B:270:PRO:HG2	1:B:273:LEU:HD22	1.82	0.62
1:B:127:GLU:OE2	1:B:150:ARG:HD2	1.99	0.61
1:B:193:ASN:HD22	1:B:194:PRO:CA	2.14	0.61
1:A:90:TYR:HD1	3:A:612:HOH:O	1.83	0.61
1:A:355:LEU:HA	1:A:358:LYS:HZ2	1.65	0.61
1:B:192:HIS:CD2	1:B:195:LEU:HB2	2.36	0.61
1:B:193:ASN:HD22	1:B:194:PRO:HA	1.66	0.61
1:B:378:THR:HG21	1:B:384:GLN:OE1	2.01	0.61
1:B:180:ASN:ND2	1:B:182:LYS:HB2	2.13	0.61
1:A:290:THR:OG1	1:A:291:PRO:HD3	2.01	0.61
1:A:223:VAL:CG2	1:A:252:SER:HB3	2.31	0.61
1:A:230:GLU:HB2	2:A:602:BR:BR	2.55	0.61
1:B:383:LEU:HD13	1:B:421:ILE:HD11	1.82	0.60
1:A:12:LYS:O	1:A:12:LYS:HG3	2.00	0.60
1:A:337:MET:HE3	1:A:352:TRP:HB3	1.83	0.60
1:A:92:GLN:HG3	3:A:832:HOH:O	2.01	0.60
1:A:166:ALA:HB2	1:A:343:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HG2	3:A:805:HOH:O	2.01	0.59
1:B:152:ILE:HG12	1:B:178:LEU:HD22	1.83	0.59
1:A:24:LYS:HB2	1:A:24:LYS:NZ	2.17	0.59
1:A:190:THR:CG2	1:A:199:MET:H	2.15	0.59
1:B:362:THR:O	1:B:363:GLN:HG3	2.02	0.59
1:B:190:THR:CG2	1:B:199:MET:H	2.14	0.59
1:A:59:LEU:HD13	1:B:63:ALA:HB2	1.85	0.59
1:B:44:GLN:HE22	1:B:410:LYS:NZ	2.01	0.59
1:A:361:LEU:O	1:A:362:THR:HB	2.03	0.58
1:B:424:LYS:HE2	1:B:425:TRP:N	2.18	0.58
1:A:250:ILE:HD11	3:A:837:HOH:O	2.02	0.58
1:A:40:LEU:HD13	3:A:779:HOH:O	2.01	0.58
1:B:192:HIS:HD2	1:B:195:LEU:H	1.52	0.58
1:A:423:ARG:HA	1:A:423:ARG:HH11	1.69	0.58
1:A:337:MET:HE1	1:A:350:ALA:HB3	1.86	0.58
1:A:367:ALA:HB2	3:A:839:HOH:O	2.04	0.58
1:A:28:VAL:HA	1:B:75:ARG:HH21	1.69	0.58
1:A:352:TRP:CD1	1:A:404:VAL:HG23	2.38	0.58
1:A:190:THR:HG21	1:A:199:MET:H	1.69	0.57
1:A:118:ILE:HD12	1:A:119:GLN:N	2.19	0.57
1:B:102:THR:HG23	1:B:103:GLU:HG3	1.86	0.57
1:B:166:ALA:HB2	1:B:343:GLN:NE2	2.19	0.57
1:B:308:LYS:H	1:B:308:LYS:HE3	1.69	0.57
1:A:130:ILE:HG12	1:A:187:ILE:CD1	2.34	0.57
1:A:79:HIS:HE1	1:A:294:GLU:OE1	1.87	0.57
1:A:22:SER:HA	1:A:24:LYS:HZ3	1.68	0.57
1:A:377:MET:HG3	3:A:769:HOH:O	2.04	0.57
1:B:381:VAL:HG13	1:B:424:LYS:NZ	2.20	0.57
1:A:17:LYS:HE3	3:A:827:HOH:O	2.04	0.57
1:A:16:PRO:HA	1:B:276:ASN:ND2	2.19	0.57
1:B:168:TRP:CE3	1:B:195:LEU:HD21	2.40	0.57
1:A:99:ASN:HB3	1:A:103:GLU:HG3	1.88	0.56
1:A:309:SER:HB3	1:A:311:GLU:OE2	2.05	0.56
1:A:186:ILE:HG12	1:A:188:ILE:HD12	1.86	0.56
1:A:417:LYS:O	1:A:420:GLU:HG2	2.05	0.56
1:A:226:HIS:HD2	3:A:793:HOH:O	1.87	0.56
1:A:226:HIS:HE1	3:A:745:HOH:O	1.88	0.56
1:A:421:ILE:HA	1:A:424:LYS:HD3	1.86	0.56
1:B:226:HIS:HE1	3:B:728:HOH:O	1.88	0.55
1:B:381:VAL:HG21	1:B:425:TRP:CD1	2.41	0.55
1:B:159:THR:HG21	3:B:770:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:HD2	3:B:622:HOH:O	1.88	0.55
1:A:373:PHE:O	1:A:377:MET:HG2	2.05	0.55
1:A:74:THR:OG1	1:A:79:HIS:HD2	1.89	0.55
1:B:15:LEU:HD12	3:B:734:HOH:O	2.07	0.55
1:A:362:THR:O	1:A:362:THR:HG23	2.07	0.55
1:A:356:ASP:N	1:A:358:LYS:HD2	2.22	0.55
1:A:365:THR:HA	1:A:372:ARG:CZ	2.37	0.55
1:A:386:ILE:HG23	1:A:387:PRO:HD2	1.90	0.54
1:A:37:TYR:CZ	1:A:379:LYS:HG2	2.43	0.54
1:A:354:SER:O	1:A:356:ASP:OD2	2.25	0.54
1:A:198:VAL:HG23	3:A:732:HOH:O	2.07	0.54
1:A:260:THR:HG22	1:B:72:GLN:HA	1.89	0.54
1:A:260:THR:CG2	1:B:73:TYR:H	2.21	0.54
1:A:83:VAL:HG12	3:A:758:HOH:O	2.08	0.54
1:A:211:CYS:HA	1:A:216:VAL:CG1	2.35	0.54
1:B:26:VAL:HG23	3:B:760:HOH:O	2.06	0.54
1:A:373:PHE:CE2	1:A:404:VAL:HG21	2.43	0.54
3:A:831:HOH:O	1:B:69:LEU:HD12	2.06	0.54
1:A:155:LYS:CD	1:A:156:PRO:HD2	2.36	0.53
1:B:152:ILE:CD1	1:B:175:LEU:HA	2.38	0.53
1:A:190:THR:OG1	1:A:199:MET:HE3	2.08	0.53
1:A:104:VAL:HG12	3:A:789:HOH:O	2.08	0.53
1:A:219:VAL:HG22	1:A:248:ILE:CG2	2.38	0.53
1:A:24:LYS:CE	1:A:24:LYS:H	2.15	0.53
1:A:104:VAL:HG12	3:A:758:HOH:O	2.09	0.53
1:A:71:ASN:ND2	1:B:262:TRP:HE1	2.01	0.53
1:A:234:HIS:HB3	2:A:605:BR:BR	2.63	0.53
1:A:209:ASN:O	1:A:213:LYS:HD2	2.07	0.53
1:B:15:LEU:HD13	1:B:15:LEU:H	1.73	0.53
1:B:170:LEU:HD21	3:B:638:HOH:O	2.09	0.53
1:B:397:LYS:HD2	3:B:720:HOH:O	2.08	0.53
1:A:85:ALA:HB3	3:A:792:HOH:O	2.08	0.53
1:B:386:ILE:HD11	1:B:405:ARG:NE	2.24	0.53
1:B:352:TRP:O	1:B:356:ASP:OD1	2.27	0.53
1:B:75:ARG:HG3	3:B:659:HOH:O	2.10	0.52
1:A:102:THR:HB	1:A:271:GLU:HG3	1.90	0.52
1:B:152:ILE:HD13	1:B:175:LEU:HA	1.91	0.52
1:B:243:MET:O	1:B:247:THR:HG22	2.09	0.52
1:B:193:ASN:HD21	1:B:405:ARG:NH1	2.01	0.52
1:A:93:LEU:HD23	1:A:236:ARG:HH22	1.75	0.52
1:B:374:THR:O	1:B:378:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HH11	1:B:76:GLY:H	1.57	0.52
1:B:238:CYS:HB2	1:B:247:THR:HG21	1.92	0.52
1:B:337:MET:HG2	1:B:352:TRP:HA	1.91	0.52
1:A:234:HIS:CB	2:A:605:BR:BR	3.13	0.52
1:A:145:ALA:O	1:B:17:LYS:HE2	2.09	0.51
1:B:383:LEU:HB2	1:B:421:ILE:CD1	2.39	0.51
1:A:294:GLU:O	1:A:298:VAL:HG13	2.09	0.51
1:B:152:ILE:HD11	1:B:175:LEU:HD23	1.92	0.51
1:B:82:LEU:HD22	1:B:86:LEU:HD22	1.91	0.51
1:B:211:CYS:HA	1:B:216:VAL:HG22	1.92	0.51
1:B:172:ASN:O	1:B:176:GLU:HG2	2.11	0.51
1:B:367:ALA:N	1:B:372:ARG:NH2	2.58	0.51
1:B:139:GLU:O	1:B:142:VAL:HG22	2.10	0.51
1:A:219:VAL:HA	1:A:248:ILE:HG23	1.92	0.51
1:A:356:ASP:N	1:A:356:ASP:OD2	2.44	0.51
1:A:198:VAL:O	1:A:198:VAL:HG23	2.11	0.51
1:B:99:ASN:HB3	1:B:102:THR:HG22	1.93	0.51
1:B:375:LYS:O	1:B:379:LYS:HG2	2.10	0.51
1:B:374:THR:HG21	1:B:387:PRO:HD3	1.94	0.50
1:B:14:ASP:C	1:B:16:PRO:HD3	2.30	0.50
1:B:367:ALA:O	1:B:368:ARG:O	2.29	0.50
1:B:368:ARG:O	1:B:368:ARG:HG2	2.11	0.50
1:B:157:ASN:O	1:B:158:LYS:O	2.30	0.50
1:B:411:LYS:HZ2	1:B:413:GLU:H	1.59	0.50
1:B:129:ILE:HG12	1:B:186:ILE:HD12	1.93	0.50
1:A:260:THR:HG22	1:B:72:GLN:OE1	2.12	0.50
1:A:71:ASN:ND2	1:A:291:PRO:HG3	2.26	0.50
1:A:114:LEU:HA	1:A:117:THR:HG22	1.93	0.50
1:A:418:ALA:HA	3:A:779:HOH:O	2.12	0.50
1:A:114:LEU:HD23	3:A:623:HOH:O	2.12	0.49
1:A:248:ILE:HG12	3:A:837:HOH:O	2.12	0.49
1:A:22:SER:HA	1:A:24:LYS:CE	2.42	0.49
1:A:369:LYS:HA	1:A:372:ARG:HD3	1.93	0.49
1:B:154:LEU:HD21	1:B:170:LEU:HD22	1.94	0.49
1:A:74:THR:HB	1:A:290:THR:HG22	1.94	0.49
1:B:229:PHE:HB3	1:B:322:MET:HE3	1.93	0.49
1:A:117:THR:HB	3:A:837:HOH:O	2.11	0.49
1:A:24:LYS:HE3	1:A:24:LYS:N	2.18	0.49
1:B:74:THR:O	1:B:287:THR:HG21	2.11	0.49
1:A:96:ARG:HD3	3:A:721:HOH:O	2.12	0.49
1:B:17:LYS:O	1:B:17:LYS:HG3	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:HD22	1:A:276:ASN:N	2.11	0.48
1:A:150:ARG:HE	1:A:178:LEU:HD11	1.78	0.48
1:A:114:LEU:HD13	1:A:250:ILE:CD1	2.43	0.48
1:A:208:ALA:CB	1:A:243:MET:HE3	2.37	0.48
1:B:27:TRP:O	1:B:31:ILE:HB	2.13	0.48
1:B:17:LYS:HE3	1:B:17:LYS:HB2	1.64	0.48
1:B:240:LEU:HB3	1:B:241:PRO:HD2	1.95	0.48
1:B:198:VAL:O	1:B:198:VAL:HG13	2.13	0.48
1:A:121:HIS:HD2	3:A:807:HOH:O	1.95	0.48
1:A:334:GLU:OE1	1:A:423:ARG:NH1	2.46	0.48
1:A:159:THR:HG23	1:A:159:THR:O	2.12	0.48
1:A:21:GLY:O	1:A:24:LYS:HE2	2.12	0.48
1:A:423:ARG:NH1	1:A:426:LYS:HD3	2.28	0.48
1:B:152:ILE:CD1	1:B:175:LEU:HD23	2.43	0.48
1:B:44:GLN:HE22	1:B:410:LYS:HZ3	1.59	0.48
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.14	0.48
1:A:188:ILE:CD1	1:A:207:VAL:HG11	2.43	0.48
1:B:199:MET:HA	1:B:203:GLU:OE1	2.14	0.48
1:A:373:PHE:HE2	1:A:404:VAL:HG21	1.79	0.48
1:A:26:VAL:HG13	1:A:371:TYR:OH	2.14	0.48
1:A:199:MET:HG2	1:A:203:GLU:CB	2.44	0.47
1:B:128:VAL:HG11	1:B:185:MET:HE3	1.97	0.47
1:A:223:VAL:HG22	1:A:255:LLP:HG2	1.96	0.47
1:A:199:MET:HG2	1:A:203:GLU:HB2	1.96	0.47
1:A:199:MET:HB3	1:A:204:LEU:HD13	1.95	0.47
1:A:421:ILE:O	1:A:424:LYS:HE2	2.15	0.47
1:A:90:TYR:O	1:A:94:VAL:HG22	2.14	0.47
1:B:428:SER:O	1:B:429:SER:HB3	2.14	0.47
1:A:246:ARG:NH1	3:A:618:HOH:O	2.48	0.47
1:A:17:LYS:HE2	1:B:123:ASP:CG	2.35	0.47
1:A:374:THR:HG21	1:A:385:GLY:O	2.15	0.47
1:A:46:PHE:HB2	1:A:47:PRO:HD2	1.96	0.47
1:B:381:VAL:HG13	1:B:424:LYS:HZ3	1.80	0.46
1:B:112:GLU:OE2	1:B:281:HIS:HD2	1.98	0.46
1:A:210:LEU:HD22	3:A:741:HOH:O	2.15	0.46
1:A:212:LYS:HG3	1:A:243:MET:CE	2.45	0.46
1:B:202:ALA:O	1:B:206:VAL:HG23	2.16	0.46
1:B:17:LYS:O	1:B:18:ARG:HB2	2.16	0.46
1:A:275:LYS:NZ	3:A:725:HOH:O	2.48	0.46
1:A:357:SER:HB3	1:A:372:ARG:NH2	2.31	0.46
1:B:331:PHE:CA	1:B:334:GLU:HG2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:CYS:CB	1:B:247:THR:HG21	2.45	0.46
1:B:22:SER:HA	3:B:753:HOH:O	2.15	0.46
1:A:150:ARG:HA	1:A:150:ARG:HD2	1.36	0.46
1:B:369:LYS:HD3	3:B:681:HOH:O	2.16	0.46
1:B:270:PRO:CG	1:B:273:LEU:HD22	2.45	0.45
1:A:295:ALA:O	1:A:298:VAL:HG22	2.17	0.45
1:B:192:HIS:CD2	1:B:195:LEU:H	2.31	0.45
1:B:41:ASN:ND2	1:B:44:GLN:HG3	2.31	0.45
1:B:381:VAL:O	1:B:381:VAL:HG12	2.17	0.45
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.98	0.45
1:B:287:THR:HG22	1:B:288:CYS:H	1.82	0.45
1:A:179:PHE:HB3	1:A:214:TRP:CD1	2.51	0.45
1:B:353:SER:HA	1:B:356:ASP:CG	2.36	0.45
1:A:366:ASP:O	1:A:367:ALA:O	2.35	0.45
1:A:368:ARG:HB3	1:A:401:GLU:HG2	1.98	0.45
1:B:261:GLY:CA	1:B:263:LYS:HE3	2.42	0.45
1:A:248:ILE:HD13	1:A:277:LEU:HD11	1.98	0.44
1:A:423:ARG:NH2	1:A:428:SER:OG	2.50	0.44
1:B:367:ALA:O	1:B:368:ARG:HG2	2.18	0.44
1:B:44:GLN:CD	1:B:45:GLY:H	2.20	0.44
1:A:17:LYS:O	1:A:17:LYS:NZ	2.46	0.44
1:B:303:GLU:OE1	1:B:306:ARG:HD2	2.17	0.44
1:A:208:ALA:O	1:A:243:MET:HE1	2.17	0.44
1:B:370:ASP:O	1:B:374:THR:HB	2.17	0.44
1:B:18:ARG:NH1	1:B:20:GLN:NE2	2.66	0.44
1:A:332:LEU:O	1:A:335:VAL:HG23	2.17	0.44
1:A:308:LYS:HG2	1:A:308:LYS:H	1.54	0.44
1:A:114:LEU:O	1:A:117:THR:HG22	2.18	0.44
1:A:248:ILE:CD1	1:A:277:LEU:HD11	2.47	0.44
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.31	0.44
1:A:248:ILE:HD11	1:A:267:ALA:CB	2.36	0.44
1:A:212:LYS:HG3	1:A:243:MET:HE2	2.00	0.44
1:B:308:LYS:HD2	1:B:308:LYS:C	2.38	0.44
1:B:213:LYS:HB3	3:B:727:HOH:O	2.16	0.44
1:B:179:PHE:HB3	1:B:214:TRP:CD1	2.52	0.44
1:A:356:ASP:O	1:A:358:LYS:N	2.50	0.44
1:A:421:ILE:HD12	3:A:779:HOH:O	2.18	0.44
1:B:378:THR:CG2	1:B:384:GLN:HA	2.41	0.44
1:B:163:ILE:HD11	1:B:168:TRP:HE1	1.83	0.44
1:A:189:ASN:ND2	1:A:193:ASN:H	2.15	0.44
1:A:129:ILE:HG13	1:A:186:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:N	1:A:277:LEU:HD23	2.33	0.43
1:B:411:LYS:NZ	1:B:413:GLU:H	2.16	0.43
1:B:24:LYS:HB2	1:B:28:VAL:CG2	2.48	0.43
1:B:46:PHE:HB2	1:B:47:PRO:HD2	1.99	0.43
1:B:419:ALA:O	1:B:423:ARG:NH2	2.51	0.43
1:A:20:GLN:NE2	1:A:144:ALA:N	2.66	0.43
1:B:44:GLN:NE2	1:B:410:LYS:NZ	2.64	0.43
1:A:231:PRO:HG2	3:A:757:HOH:O	2.18	0.43
1:B:18:ARG:HB2	1:B:144:ALA:HA	2.00	0.43
1:A:201:ARG:HG3	1:A:202:ALA:N	2.34	0.43
1:A:228:VAL:HG11	1:A:234:HIS:HB2	2.01	0.43
1:A:129:ILE:HD11	1:A:186:ILE:HD12	2.01	0.43
1:A:138:TYR:CG	1:A:187:ILE:HD12	2.54	0.43
1:A:106:VAL:HG23	3:A:758:HOH:O	2.18	0.43
1:A:193:ASN:HA	1:A:194:PRO:HA	1.83	0.43
1:A:129:ILE:HD11	1:A:186:ILE:CD1	2.49	0.43
1:B:364:GLU:N	1:B:364:GLU:OE2	2.46	0.43
1:B:122:VAL:HG22	1:B:145:ALA:HB1	2.01	0.43
1:A:198:VAL:HG22	1:A:343:GLN:CD	2.39	0.43
1:B:15:LEU:HD13	1:B:15:LEU:N	2.32	0.43
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.84	0.42
1:B:83:VAL:HG13	1:B:100:PRO:HB2	2.01	0.42
1:A:129:ILE:CD1	1:A:152:ILE:HD11	2.36	0.42
1:B:99:ASN:CG	1:B:102:THR:HG22	2.40	0.42
1:B:338:ASN:HB2	1:B:351:ASP:HB3	2.02	0.42
1:A:170:LEU:HD23	1:A:175:LEU:HG	2.01	0.42
1:A:270:PRO:HD2	3:A:782:HOH:O	2.19	0.42
1:A:300:PHE:HB2	3:A:792:HOH:O	2.19	0.42
1:A:423:ARG:HH12	1:A:426:LYS:HB3	1.85	0.42
1:B:271:GLU:HG2	1:B:271:GLU:H	1.50	0.42
1:B:325:ARG:HB2	1:B:408:PHE:CZ	2.55	0.42
1:A:359:VAL:HG22	1:A:360:ASP:N	2.34	0.42
1:B:287:THR:HG22	1:B:288:CYS:N	2.34	0.42
1:A:307:LEU:HB3	1:A:308:LYS:HE3	2.00	0.42
1:A:370:ASP:OD1	1:A:389:SER:HB2	2.20	0.42
1:B:129:ILE:HG13	1:B:186:ILE:HG13	2.01	0.42
1:B:150:ARG:HH11	1:B:150:ARG:HG2	1.84	0.41
1:A:260:THR:HG23	1:B:73:TYR:H	1.84	0.41
1:B:368:ARG:HG3	1:B:371:TYR:CD1	2.55	0.41
1:B:411:LYS:HE3	1:B:413:GLU:OE2	2.20	0.41
1:A:106:VAL:CG2	3:A:789:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	3:A:792:HOH:O	2.21	0.41
1:A:237:ILE:HG13	3:A:765:HOH:O	2.19	0.41
1:A:188:ILE:HD13	1:A:207:VAL:HG11	2.01	0.41
1:A:356:ASP:C	1:A:358:LYS:HG3	2.41	0.41
1:A:416:GLN:HG2	1:A:417:LYS:HE3	2.03	0.41
1:A:31:ILE:HD12	1:B:75:ARG:CZ	2.50	0.41
1:B:18:ARG:HH12	1:B:20:GLN:NE2	2.19	0.41
1:B:306:ARG:HB2	1:B:309:SER:HB3	2.02	0.41
1:A:325:ARG:HD3	1:A:341:VAL:HG13	2.03	0.41
1:A:209:ASN:O	1:A:213:LYS:CD	2.69	0.41
1:B:83:VAL:CG1	1:B:100:PRO:HB2	2.50	0.41
1:A:394:GLU:HA	1:A:397:LYS:HD2	2.02	0.41
1:B:39:PRO:HB3	1:B:382:GLY:HA2	2.03	0.41
1:A:282:GLN:NE2	1:B:25:SER:H	2.18	0.41
1:A:22:SER:HB2	1:B:283:ASN:HD21	1.85	0.41
1:A:355:LEU:HG	1:A:355:LEU:H	1.67	0.41
1:B:386:ILE:HD11	1:B:405:ARG:CD	2.51	0.41
1:B:394:GLU:HG3	1:B:395:PRO:HD3	2.02	0.41
1:B:416:GLN:HG3	1:B:417:LYS:N	2.36	0.41
1:B:128:VAL:CG1	1:B:185:MET:HE3	2.51	0.41
1:B:161:GLY:O	1:B:338:ASN:HB3	2.21	0.41
1:A:118:ILE:O	1:A:122:VAL:HB	2.21	0.41
1:A:360:ASP:N	1:A:360:ASP:OD1	2.50	0.41
1:A:74:THR:CG2	1:A:290:THR:HG22	2.51	0.40
1:B:127:GLU:CD	1:B:150:ARG:HD2	2.40	0.40
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.87	0.40
1:A:42:LEU:HA	1:A:42:LEU:HD12	1.95	0.40
1:B:222:GLU:OE1	1:B:234:HIS:HE1	2.04	0.40
1:B:228:VAL:HG22	3:B:765:HOH:O	2.20	0.40
1:A:331:PHE:O	1:A:334:GLU:HB3	2.21	0.40
1:A:230:GLU:HB3	1:A:231:PRO:HD3	2.02	0.40
1:B:396:ASN:O	1:B:399:LEU:HB2	2.21	0.40
1:A:364:GLU:HB2	1:A:367:ALA:HB3	2.03	0.40
1:B:386:ILE:HD11	1:B:405:ARG:HD3	2.03	0.40
1:B:387:PRO:HA	1:B:388:PRO:HD3	1.90	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	415/429 (97%)	386 (93%)	20 (5%)	9 (2%)	8	0
1	B	415/429 (97%)	383 (92%)	23 (6%)	9 (2%)	8	0
All	All	830/858 (97%)	769 (93%)	43 (5%)	18 (2%)	8	0

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	159	THR
1	A	362	THR
1	A	367	ALA
1	B	44	GLN
1	B	158	LYS
1	B	354	SER
1	B	359	VAL
1	B	368	ARG
1	A	17	LYS
1	B	426	LYS
1	B	241	PRO
1	B	428	SER
1	A	14	ASP
1	A	357	SER
1	A	16	PRO
1	A	359	VAL
1	B	45	GLY

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	355/366 (97%)	288 (81%)	67 (19%)	2 0
1	B	355/366 (97%)	290 (82%)	65 (18%)	2 0
All	All	710/732 (97%)	578 (81%)	132 (19%)	2 0

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	PHE
1	A	17	LYS
1	A	18	ARG
1	A	20	GLN
1	A	22	SER
1	A	23	THR
1	A	24	LYS
1	A	26	VAL
1	A	36	GLN
1	A	42	LEU
1	A	59	LEU
1	A	82	LEU
1	A	86	LEU
1	A	88	LYS
1	A	114	LEU
1	A	129	ILE
1	A	150	ARG
1	A	152	ILE
1	A	162	THR
1	A	163	ILE
1	A	175	LEU
1	A	176	GLU
1	A	188	ILE
1	A	190	THR
1	A	201	ARG
1	A	204	LEU
1	A	210	LEU
1	A	213	LYS
1	A	216	VAL
1	A	223	VAL
1	A	230	GLU
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	236	ARG
1	A	237	ILE
1	A	240	LEU
1	A	245	GLU
1	A	246	ARG
1	A	248	ILE
1	A	252	SER
1	A	260	THR
1	A	274	LEU
1	A	275	LYS
1	A	276	ASN
1	A	282	GLN
1	A	304	LEU
1	A	308	LYS
1	A	311	GLU
1	A	317	ILE
1	A	321	LEU
1	A	335	VAL
1	A	355	LEU
1	A	356	ASP
1	A	358	LYS
1	A	359	VAL
1	A	360	ASP
1	A	363	GLN
1	A	377	MET
1	A	383	LEU
1	A	389	SER
1	A	409	PHE
1	A	410	LYS
1	A	415	LEU
1	A	417	LYS
1	A	423	ARG
1	A	424	LYS
1	A	426	LYS
1	B	13	PHE
1	B	15	LEU
1	B	17	LYS
1	B	20	GLN
1	B	26	VAL
1	B	32	GLN
1	B	41	ASN
1	B	44	GLN

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Mol	Chain	Res	Type
1	B	48	ASP
1	B	53	LYS
1	B	75	ARG
1	B	82	LEU
1	B	86	LEU
1	B	89	LEU
1	B	96	ARG
1	B	98	ILE
1	B	111	TYR
1	B	129	ILE
1	B	150	ARG
1	B	155	LYS
1	B	173	ASN
1	B	175	LEU
1	B	176	GLU
1	B	178	LEU
1	B	181	GLU
1	B	184	LYS
1	B	190	THR
1	B	193	ASN
1	B	195	LEU
1	B	201	ARG
1	B	207	VAL
1	B	217	LEU
1	B	233	GLU
1	B	240	LEU
1	B	246	ARG
1	B	263	LYS
1	B	271	GLU
1	B	273	LEU
1	B	274	LEU
1	B	306	ARG
1	B	308	LYS
1	B	321	LEU
1	B	322	MET
1	B	346	TYR
1	B	354	SER
1	B	356	ASP
1	B	357	SER
1	B	359	VAL
1	B	362	THR
1	B	365	THR

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Mol	Chain	Res	Type
1	B	366	ASP
1	B	368	ARG
1	B	369	LYS
1	B	374	THR
1	B	378	THR
1	B	384	GLN
1	B	394	GLU
1	B	398	HIS
1	B	409	PHE
1	B	411	LYS
1	B	420	GLU
1	B	422	LEU
1	B	423	ARG
1	B	426	LYS
1	B	428	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	36	GLN
1	A	57	ASN
1	A	71	ASN
1	A	79	HIS
1	A	92	GLN
1	A	121	HIS
1	A	157	ASN
1	A	189	ASN
1	A	226	HIS
1	A	276	ASN
1	A	282	GLN
1	A	283	ASN
1	A	363	GLN
1	B	20	GLN
1	B	41	ASN
1	B	44	GLN
1	B	50	HIS
1	B	84	GLN
1	B	119	GLN
1	B	172	ASN
1	B	180	ASN
1	B	192	HIS

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Mol	Chain	Res	Type
1	B	193	ASN
1	B	226	HIS
1	B	234	HIS
1	B	278	GLN
1	B	282	GLN
1	B	283	ASN
1	B	414	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	LLP	A	255	1	23,24,25	1.60	3 (13%)	28,32,34	1.87	7 (25%)
1	LLP	B	255	1	23,24,25	1.65	4 (17%)	28,32,34	1.69	6 (21%)

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
1	LLP	A	255	1	-	0/15/17/19	0/1/1/1
1	LLP	B	255	1	-	0/15/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	LLP	C3-C2	-2.42	1.39	1.40
1	B	255	LLP	C3-C2	-2.29	1.39	1.40
1	B	255	LLP	P-OP3	-2.04	1.47	1.54
1	B	255	LLP	C4'-NZ	2.67	1.35	1.27
1	A	255	LLP	C4'-NZ	2.83	1.36	1.27
1	A	255	LLP	C4-C4'	4.86	1.55	1.46
1	B	255	LLP	C4-C4'	5.13	1.55	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	255	LLP	C4-C4'-NZ	-3.90	103.37	125.06
1	A	255	LLP	C4-C4'-NZ	-3.45	105.85	125.06
1	A	255	LLP	OP4-P-OP1	-2.98	99.56	107.14
1	A	255	LLP	C3-C2-N1	-2.07	117.76	120.61
1	A	255	LLP	C3-C4-C5	-2.05	116.57	118.11
1	B	255	LLP	CD-CE-NZ	2.15	114.50	110.98
1	B	255	LLP	C3-C4-C4'	2.43	123.31	120.16
1	A	255	LLP	C3-C4-C4'	2.50	123.40	120.16
1	B	255	LLP	CE-NZ-C4'	2.53	126.26	118.97
1	B	255	LLP	C2'-C2-C3	3.30	125.02	121.04
1	B	255	LLP	OP4-C5'-C5	3.58	114.92	108.99
1	A	255	LLP	OP4-C5'-C5	4.46	116.36	108.99
1	A	255	LLP	C2'-C2-C3	5.05	127.12	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	255	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	417/429 (97%)	1.68	85 (20%) 1 1	6, 13, 63, 91	0
1	B	417/429 (97%)	2.06	103 (24%) 1 1	7, 17, 66, 95	0
All	All	834/858 (97%)	1.87	188 (22%) 1 1	6, 15, 64, 95	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	THR	29.8
1	B	359	VAL	26.0
1	B	365	THR	23.2
1	B	428	SER	22.1
1	A	159	THR	19.8
1	B	355	LEU	18.3
1	B	361	LEU	18.2
1	A	13	PHE	17.5
1	B	16	PRO	16.7
1	A	160	GLY	15.8
1	B	363	GLN	15.2
1	B	22	SER	14.7
1	A	359	VAL	14.4
1	A	428	SER	13.9
1	B	357	SER	13.3
1	A	366	ASP	13.1
1	B	23	THR	13.1
1	A	161	GLY	12.7
1	A	365	THR	12.6
1	B	13	PHE	12.4
1	A	427	GLY	11.8
1	A	19	TYR	11.6
1	B	425	TRP	11.5
1	A	20	GLN	11.2

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Mol	Chain	Res	Type	RSRZ
1	B	366	ASP	11.2
1	A	21	GLY	11.0
1	A	429	SER	10.9
1	A	12	LYS	10.9
1	B	429	SER	10.4
1	A	23	THR	10.2
1	B	364	GLU	10.1
1	B	358	LYS	10.0
1	A	22	SER	9.9
1	B	14	ASP	9.8
1	B	159	THR	9.6
1	B	15	LEU	9.2
1	A	18	ARG	9.0
1	A	355	LEU	9.0
1	A	16	PRO	9.0
1	A	14	ASP	8.8
1	B	356	ASP	8.7
1	A	15	LEU	8.4
1	A	358	LYS	8.3
1	B	18	ARG	8.1
1	B	360	ASP	7.9
1	B	158	LYS	7.8
1	A	24	LYS	7.4
1	B	12	LYS	6.8
1	B	376	TRP	6.8
1	B	160	GLY	6.7
1	A	357	SER	6.6
1	B	427	GLY	6.5
1	A	162	THR	6.5
1	B	35	ALA	6.3
1	B	37	TYR	6.0
1	B	21	GLY	5.6
1	A	362	THR	5.5
1	B	17	LYS	5.5
1	B	20	GLN	5.4
1	A	367	ALA	5.3
1	B	367	ALA	5.2
1	B	157	ASN	5.1
1	A	17	LYS	5.0
1	B	19	TYR	4.9
1	A	353	SER	4.8
1	B	353	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	26	VAL	4.6
1	B	398	HIS	4.5
1	B	44	GLN	4.5
1	B	423	ARG	4.5
1	B	352	TRP	4.5
1	A	25	SER	4.4
1	B	28	VAL	4.3
1	A	158	LYS	4.2
1	A	187	ILE	4.2
1	B	161	GLY	4.2
1	B	379	LYS	4.0
1	A	356	ASP	4.0
1	B	354	SER	3.9
1	B	335	VAL	3.9
1	B	421	ILE	3.9
1	B	241	PRO	3.8
1	B	424	LYS	3.8
1	B	307	LEU	3.7
1	B	381	VAL	3.7
1	B	373	PHE	3.7
1	A	129	ILE	3.6
1	A	231	PRO	3.6
1	A	364	GLU	3.6
1	B	207	VAL	3.5
1	A	163	ILE	3.5
1	A	157	ASN	3.4
1	B	26	VAL	3.4
1	B	386	ILE	3.4
1	B	27	TRP	3.4
1	A	230	GLU	3.3
1	A	108	VAL	3.3
1	B	242	GLY	3.3
1	A	425	TRP	3.3
1	A	237	ILE	3.2
1	B	75	ARG	3.2
1	A	285	VAL	3.1
1	B	32	GLN	3.1
1	B	378	THR	3.1
1	B	39	PRO	3.0
1	B	34	ALA	3.0
1	B	98	ILE	3.0
1	B	24	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	46	PHE	3.0
1	B	40	LEU	2.9
1	B	162	THR	2.9
1	A	118	ILE	2.9
1	A	377	MET	2.9
1	B	30	TYR	2.9
1	B	48	ASP	2.9
1	B	426	LYS	2.9
1	B	31	ILE	2.9
1	A	423	ARG	2.8
1	A	188	ILE	2.8
1	B	108	VAL	2.8
1	B	122	VAL	2.8
1	A	391	PHE	2.8
1	A	426	LYS	2.7
1	A	190	THR	2.7
1	A	260	THR	2.7
1	B	368	ARG	2.7
1	B	420	GLU	2.7
1	A	114	LEU	2.7
1	B	45	GLY	2.7
1	B	33	LEU	2.7
1	A	424	LYS	2.7
1	B	148	ILE	2.7
1	B	372	ARG	2.7
1	B	380	SER	2.6
1	A	92	GLN	2.6
1	A	152	ILE	2.6
1	A	363	GLN	2.6
1	B	170	LEU	2.5
1	B	375	LYS	2.5
1	A	27	TRP	2.5
1	A	123	ASP	2.5
1	A	40	LEU	2.4
1	A	59	LEU	2.4
1	A	283	ASN	2.4
1	B	42	LEU	2.4
1	A	239	THR	2.4
1	B	213	LYS	2.4
1	B	94	VAL	2.4
1	A	150	ARG	2.4
1	B	371	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	2.4
1	B	152	ILE	2.4
1	A	245	GLU	2.4
1	A	42	LEU	2.3
1	B	38	LYS	2.3
1	A	334	GLU	2.3
1	B	394	GLU	2.3
1	A	338	ASN	2.3
1	B	385	GLY	2.3
1	A	284	CYS	2.3
1	A	175	LEU	2.3
1	A	259	LEU	2.3
1	B	416	GLN	2.3
1	A	337	MET	2.2
1	B	73	TYR	2.2
1	A	173	ASN	2.2
1	B	391	PHE	2.2
1	A	44	GLN	2.2
1	A	352	TRP	2.2
1	B	111	TYR	2.2
1	B	286	TYR	2.2
1	B	181	GLU	2.1
1	B	223	VAL	2.1
1	B	131	ILE	2.1
1	A	111	TYR	2.1
1	A	110	ALA	2.1
1	A	335	VAL	2.1
1	A	32	GLN	2.1
1	A	170	LEU	2.1
1	B	36	GLN	2.1
1	A	376	TRP	2.1
1	A	223	VAL	2.1
1	B	114	LEU	2.1
1	B	288	CYS	2.0
1	A	46	PHE	2.0
1	A	286	TYR	2.0
1	B	285	VAL	2.0
1	B	250	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	B	255	24/25	0.92	0.18	-	11,16,31,38	0
1	LLP	A	255	24/25	0.91	0.20	-	10,14,22,26	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BR	B	601	1/1	0.99	0.30	5.37	0,0,0,0	0
2	BR	B	604	1/1	0.96	0.35	2.91	3,3,3,3	0
2	BR	A	602	1/1	0.97	0.30	1.85	1,1,1,1	0
2	BR	A	605	1/1	0.69	0.44	-	9,9,9,9	1
2	BR	A	603	1/1	0.98	0.33	-	0,0,0,0	0

6.5 Other polymers (i)

There are no such residues in this entry.