Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 09:21 PM EST

PDB ID	:	3QDK
Title	:	Structural insight on mechanism and diverse substrate selection strategy of ribulokinase
Authors	:	Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-01-18
Resolution	:	2.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

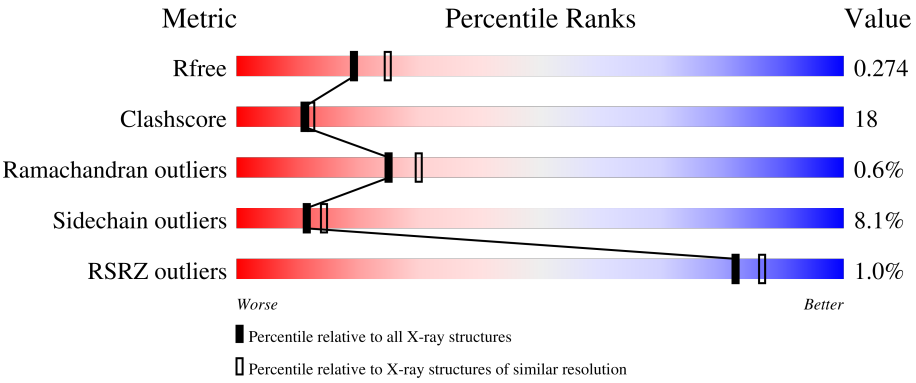
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.31 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))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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% 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	572	2% 61% 31% • 5%
1	B	572	% 60% 31% • 5%
1	C	572	64% 29% • •
1	D	572	65% 28% • • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17164 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 Ribulokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4163	2646	709	786	22			
1	B	543	Total	C	N	O	S	0	0	0
			4155	2642	705	786	22			
1	C	549	Total	C	N	O	S	0	0	0
			4202	2670	717	793	22			
1	D	554	Total	C	N	O	S	0	0	0
			4239	2690	724	803	22			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9KBQ3
A	2	SER	-	expression tag	UNP Q9KBQ3
A	3	LEU	-	expression tag	UNP Q9KBQ3
A	565	GLU	-	expression tag	UNP Q9KBQ3
A	566	GLY	-	expression tag	UNP Q9KBQ3
A	567	HIS	-	expression tag	UNP Q9KBQ3
A	568	HIS	-	expression tag	UNP Q9KBQ3
A	569	HIS	-	expression tag	UNP Q9KBQ3
A	570	HIS	-	expression tag	UNP Q9KBQ3
A	571	HIS	-	expression tag	UNP Q9KBQ3
A	572	HIS	-	expression tag	UNP Q9KBQ3
B	1	MET	-	expression tag	UNP Q9KBQ3
B	2	SER	-	expression tag	UNP Q9KBQ3
B	3	LEU	-	expression tag	UNP Q9KBQ3
B	565	GLU	-	expression tag	UNP Q9KBQ3
B	566	GLY	-	expression tag	UNP Q9KBQ3
B	567	HIS	-	expression tag	UNP Q9KBQ3
B	568	HIS	-	expression tag	UNP Q9KBQ3
B	569	HIS	-	expression tag	UNP Q9KBQ3
B	570	HIS	-	expression tag	UNP Q9KBQ3
B	571	HIS	-	expression tag	UNP Q9KBQ3

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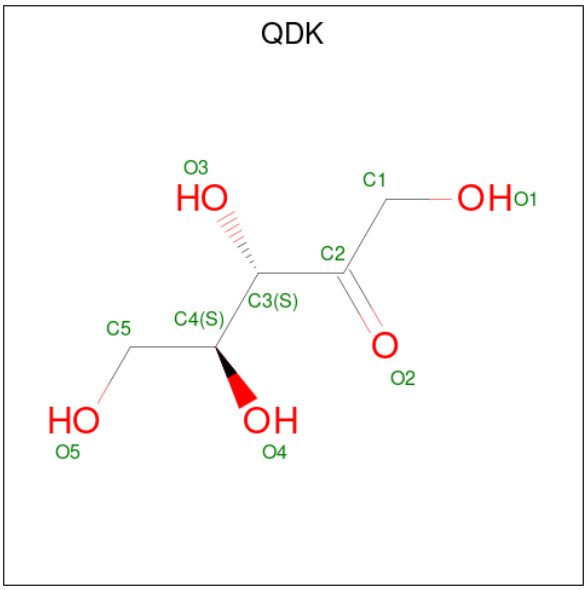
Chain	Residue	Modelled	Actual	Comment	Reference
B	572	HIS	-	expression tag	UNP Q9KBQ3
C	1	MET	-	expression tag	UNP Q9KBQ3
C	2	SER	-	expression tag	UNP Q9KBQ3
C	3	LEU	-	expression tag	UNP Q9KBQ3
C	565	GLU	-	expression tag	UNP Q9KBQ3
C	566	GLY	-	expression tag	UNP Q9KBQ3
C	567	HIS	-	expression tag	UNP Q9KBQ3
C	568	HIS	-	expression tag	UNP Q9KBQ3
C	569	HIS	-	expression tag	UNP Q9KBQ3
C	570	HIS	-	expression tag	UNP Q9KBQ3
C	571	HIS	-	expression tag	UNP Q9KBQ3
C	572	HIS	-	expression tag	UNP Q9KBQ3
D	1	MET	-	expression tag	UNP Q9KBQ3
D	2	SER	-	expression tag	UNP Q9KBQ3
D	3	LEU	-	expression tag	UNP Q9KBQ3
D	565	GLU	-	expression tag	UNP Q9KBQ3
D	566	GLY	-	expression tag	UNP Q9KBQ3
D	567	HIS	-	expression tag	UNP Q9KBQ3
D	568	HIS	-	expression tag	UNP Q9KBQ3
D	569	HIS	-	expression tag	UNP Q9KBQ3
D	570	HIS	-	expression tag	UNP Q9KBQ3
D	571	HIS	-	expression tag	UNP Q9KBQ3
D	572	HIS	-	expression tag	UNP Q9KBQ3

- Molecule 2 is L-ribulose (three-letter code: QDK) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0

- Molecule 3 is water.

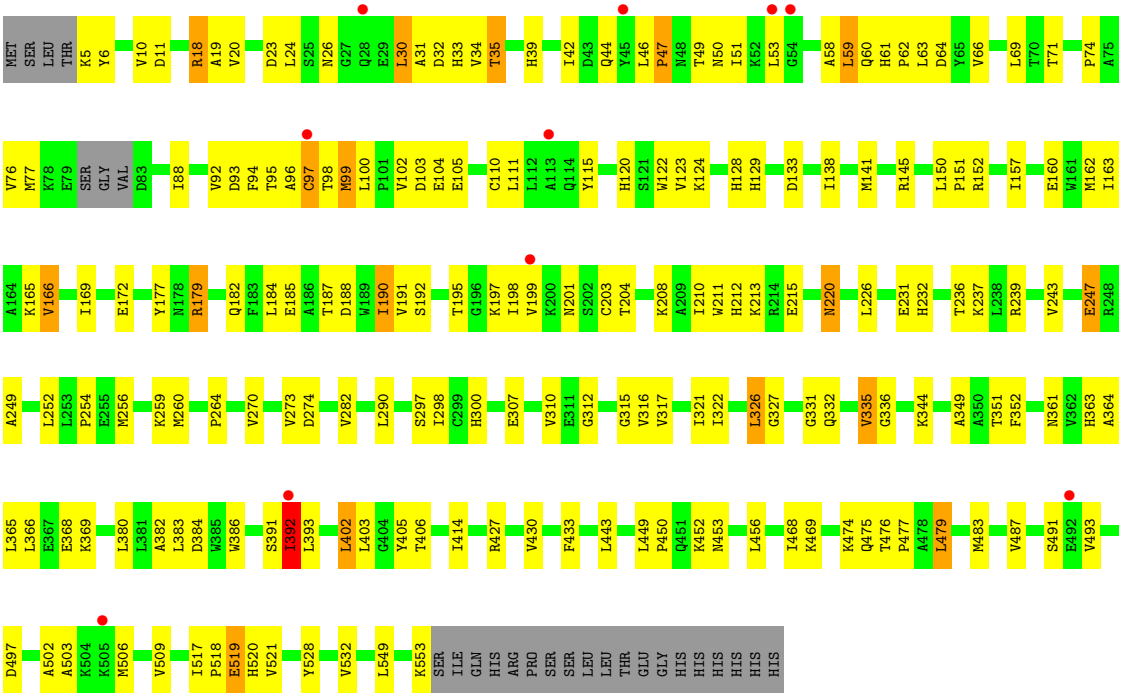
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	76	Total O 76 76	0	0
3	B	77	Total O 77 77	0	0
3	C	100	Total O 100 100	0	0
3	D	142	Total O 142 142	0	0

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 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.

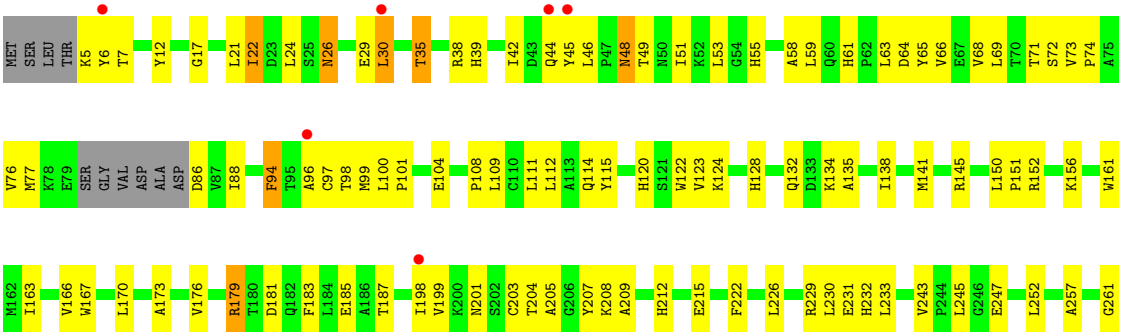
• Molecule 1: Ribulokinase

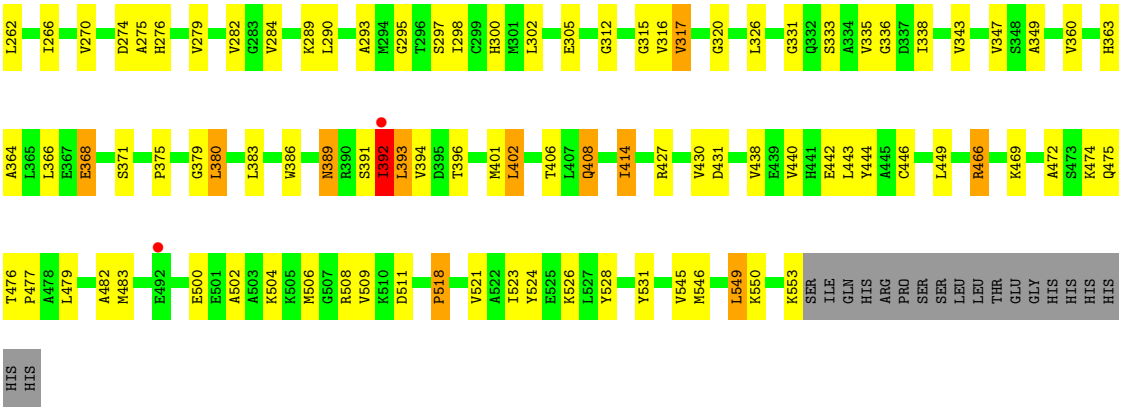
Chain A:



• Molecule 1: Ribulokinase

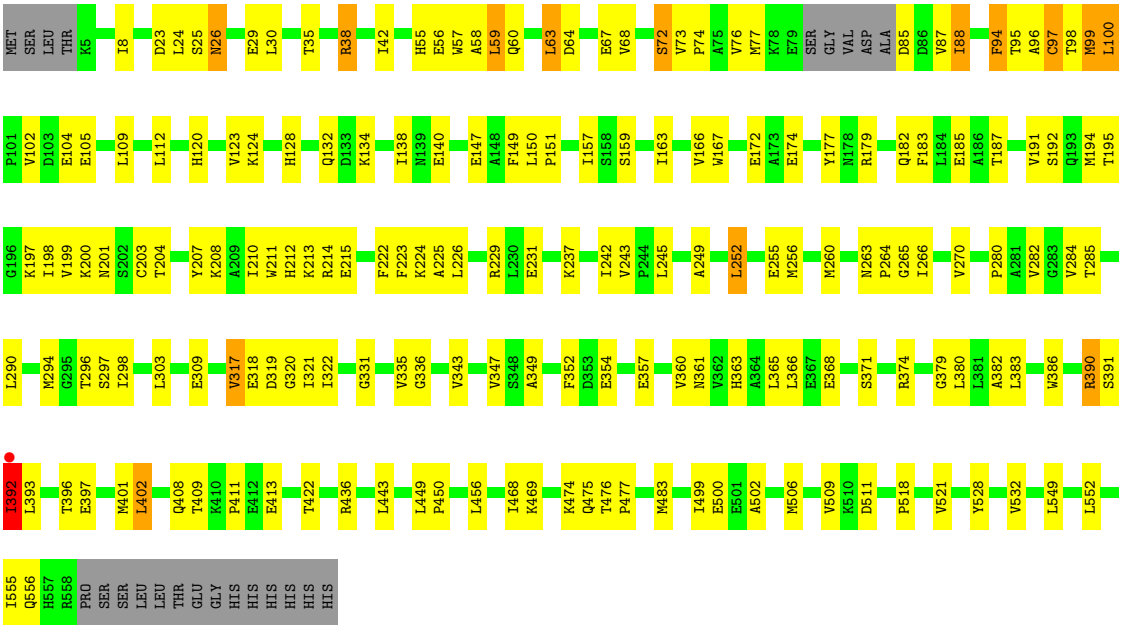
Chain B:





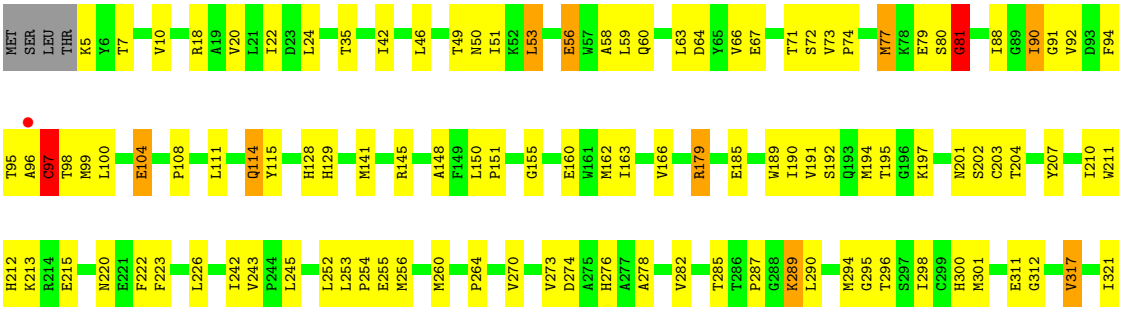
• Molecule 1: Ribulokinase

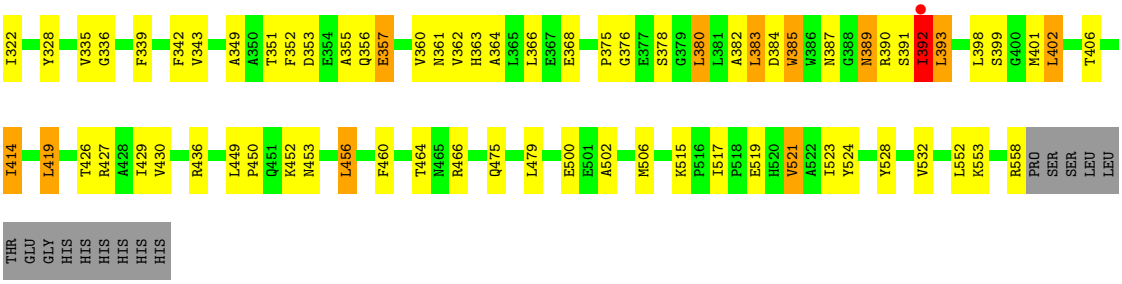
Chain C:



• Molecule 1: Ribulokinase

Chain D:




I322 Y328 V335 G336 F339 F342 V343 A349 A350 T351 F352 D353 E354 A355 Q356 E357 V360 N361 V362 H363 A364 L365 L366 E367 E368 P375 G376 E377 S378 G379 L380 L381 A382 L383 D384 W385 W386 N387 G388 N389 R390 S391 I392 L393 L398 S399 G400 M401 L402 T406
I414 L419 T426 R427 A428 I429 V430 R436 L449 P450 Q451 K452 N453 L456 F460 T464 N465 R466 Q475 L479 E500 E501 A502 M506 K515 P516 I517 P518 E519 H520 V521 A522 I523 Y524 Y528 V532 L552 K553 R558 PRO SER SER LEU LEU
THR GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.68Å 88.84Å 230.53Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	48.31 – 2.31 48.31 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.31-2.31) 96.3 (48.31-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.92 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1, CCP4	Depositor
R, R_{free}	0.224 , 0.274 0.226 , 0.274	Depositor DCC
R_{free} test set	2940 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17164	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: QDK

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	0.42	0/4255	0.67	2/5776 (0.0%)
1	B	0.42	0/4246	0.66	1/5762 (0.0%)
1	C	0.42	0/4295	0.65	1/5826 (0.0%)
1	D	0.46	0/4333	0.71	4/5880 (0.1%)
All	All	0.43	0/17129	0.67	8/23244 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	97	CYS	CA-CB-SG	-9.99	96.02	114.00
1	A	97	CYS	CA-CB-SG	-6.70	101.93	114.00
1	A	98	THR	N-CA-C	-6.47	93.53	111.00
1	B	98	THR	N-CA-C	-6.07	94.62	111.00
1	C	98	THR	N-CA-C	-5.89	95.10	111.00
1	D	98	THR	N-CA-C	-5.79	95.38	111.00
1	D	81	GLY	N-CA-C	5.21	126.13	113.10
1	D	385	TRP	N-CA-C	5.12	124.82	111.00

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	4163	0	4066	161	0
1	B	4155	0	4069	155	0
1	C	4202	0	4107	141	0
1	D	4239	0	4140	153	0
2	A	10	0	10	3	0
3	A	76	0	0	4	0
3	B	77	0	0	6	0
3	C	100	0	0	5	0
3	D	142	0	0	4	0
All	All	17164	0	16392	594	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 18.

All (594) 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:D:195:THR:HG23	1:D:197:LYS:H	1.30	0.96
1:A:69:LEU:HD11	1:A:190:ILE:HD11	1.45	0.96
1:B:389:ASN:HD21	1:B:393:LEU:HB3	1.31	0.94
1:C:195:THR:HG23	1:C:197:LYS:H	1.37	0.87
1:B:61:HIS:HD1	1:B:122:TRP:HZ3	1.22	0.86
1:B:298:ILE:HG13	1:B:335:VAL:HG11	1.57	0.85
1:D:356:GLN:O	1:D:357:GLU:HB3	1.77	0.85
1:A:63:LEU:HD11	1:A:111:LEU:HD21	1.59	0.85
1:B:108:PRO:HG2	1:B:111:LEU:HD13	1.61	0.82
1:B:170:LEU:HD11	1:B:229:ARG:HE	1.42	0.82
1:D:56:GLU:HG3	1:D:129:HIS:HB2	1.61	0.82
1:C:97:CYS:HB2	1:C:208:LYS:HG2	1.60	0.82
1:D:212:HIS:HD2	1:D:215:GLU:H	1.29	0.80
1:D:335:VAL:HG23	1:D:336:GLY:H	1.47	0.78
1:C:252:LEU:HD22	1:C:266:ILE:HG12	1.63	0.78
1:A:6:TYR:HD1	1:A:23:ASP:HA	1.49	0.78
1:D:356:GLN:O	1:D:357:GLU:CB	2.31	0.78
1:A:195:THR:HG23	1:A:197:LYS:H	1.48	0.77
1:A:185:GLU:HG2	1:A:204:THR:HG21	1.67	0.77
1:A:46:LEU:O	1:A:49:THR:HG22	1.84	0.77
1:C:298:ILE:HG13	1:C:335:VAL:HG11	1.65	0.76
1:C:303:LEU:HD11	1:C:322:ILE:HD12	1.67	0.76
1:C:150:LEU:HB3	1:C:151:PRO:HD3	1.67	0.76
1:C:97:CYS:HA	1:C:185:GLU:OE2	1.85	0.76
1:A:35:THR:HG21	1:A:71:THR:HB	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:HIS:HD2	1:B:215:GLU:H	1.33	0.74
1:B:502:ALA:HB1	1:B:506:MET:HE3	1.68	0.74
1:B:389:ASN:ND2	1:B:393:LEU:HB3	2.02	0.74
1:D:49:THR:HG23	1:D:51:ILE:H	1.52	0.74
1:D:185:GLU:HG2	1:D:204:THR:HG21	1.69	0.74
1:C:212:HIS:HD2	1:C:215:GLU:H	1.34	0.73
1:C:285:THR:HA	1:C:322:ILE:HD13	1.70	0.72
1:B:63:LEU:HD21	1:B:111:LEU:HD21	1.70	0.72
1:C:185:GLU:HG2	1:C:204:THR:HG21	1.69	0.72
1:D:185:GLU:HG3	3:D:1053:HOH:O	1.89	0.72
1:A:104:GLU:CD	1:A:104:GLU:H	1.93	0.71
1:C:163:ILE:HA	1:C:166:VAL:HG12	1.72	0.71
1:C:361:ASN:ND2	1:C:363:HIS:HB2	2.06	0.71
1:D:391:SER:HB3	1:D:429:ILE:HD12	1.71	0.71
1:D:35:THR:HG23	1:D:72:SER:OG	1.90	0.70
1:D:361:ASN:ND2	1:D:363:HIS:HB2	2.06	0.70
1:D:252:LEU:HD11	1:D:260:MET:HE3	1.72	0.70
1:D:252:LEU:HD21	1:D:260:MET:HE3	1.72	0.70
1:B:35:THR:HG21	1:B:68:VAL:HA	1.73	0.70
1:D:108:PRO:HG2	1:D:111:LEU:HD22	1.73	0.70
1:A:298:ILE:HG13	1:A:335:VAL:HG11	1.74	0.69
1:C:42:ILE:HD13	1:C:60:GLN:HA	1.73	0.69
1:B:545:VAL:HG22	1:B:549:LEU:HD22	1.75	0.69
1:B:100:LEU:HD12	1:B:108:PRO:HB3	1.74	0.68
1:B:46:LEU:HD13	1:B:53:LEU:HD11	1.73	0.68
1:B:7:THR:HG23	1:B:24:LEU:HD21	1.74	0.68
1:A:210:ILE:HD13	3:A:576:HOH:O	1.94	0.68
1:B:44:GLN:HG2	1:B:45:TYR:CD2	2.29	0.68
1:D:201:ASN:HD22	1:D:203:CYS:H	1.42	0.68
1:B:252:LEU:HD22	1:B:266:ILE:HD11	1.76	0.68
1:B:257:ALA:HB1	1:B:262:LEU:O	1.94	0.67
1:D:35:THR:HG21	1:D:71:THR:HB	1.77	0.67
1:C:192:SER:HA	1:C:195:THR:HG22	1.75	0.67
1:B:96:ALA:HB1	1:B:208:LYS:HE3	1.77	0.67
1:B:335:VAL:HG13	1:B:336:GLY:H	1.61	0.66
1:B:35:THR:HG22	1:B:72:SER:OG	1.95	0.66
1:B:201:ASN:HD21	1:B:204:THR:H	1.43	0.66
1:D:335:VAL:HG23	1:D:336:GLY:N	2.11	0.66
1:B:472:ALA:HB3	1:B:508:ARG:HB3	1.77	0.66
1:C:256:MET:HB3	1:C:260:MET:HE2	1.77	0.66
1:D:104:GLU:H	1:D:104:GLU:CD	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:THR:HG23	1:C:397:GLU:OE2	1.95	0.66
1:B:134:LYS:O	1:B:138:ILE:HG12	1.95	0.66
1:A:124:LYS:HZ3	1:A:169:ILE:HD11	1.61	0.66
1:B:141:MET:HG2	1:B:226:LEU:HD12	1.77	0.66
1:D:96:ALA:HB2	1:D:273:VAL:HG13	1.78	0.66
1:A:96:ALA:HB3	2:A:573:QDK:O2	1.95	0.65
1:C:30:LEU:HD23	1:C:30:LEU:H	1.61	0.65
1:C:469:LYS:HB3	1:C:509:VAL:HG11	1.77	0.65
1:B:474:LYS:HG3	1:B:475:GLN:HG2	1.76	0.65
1:A:518:PRO:HA	1:A:521:VAL:HG22	1.78	0.65
1:B:7:THR:HG23	1:B:24:LEU:HD11	1.77	0.65
1:B:282:VAL:HG13	1:B:284:VAL:HG23	1.79	0.65
1:A:163:ILE:HD13	1:A:210:ILE:HG12	1.78	0.64
1:A:361:ASN:ND2	1:A:363:HIS:HB2	2.13	0.64
1:A:502:ALA:HB1	1:A:506:MET:HE2	1.79	0.64
1:C:502:ALA:HB1	1:C:506:MET:CE	2.28	0.64
1:A:115:TYR:CZ	1:A:179:ARG:HG3	2.32	0.64
1:B:185:GLU:HG2	1:B:204:THR:HG21	1.79	0.64
1:D:252:LEU:HD11	1:D:260:MET:CE	2.28	0.64
1:B:5:LYS:HE2	1:B:88:ILE:HD11	1.80	0.64
1:A:96:ALA:HB1	1:A:208:LYS:HD2	1.80	0.64
1:C:163:ILE:HD12	1:C:210:ILE:HG13	1.79	0.64
1:A:391:SER:O	1:A:392:ILE:HG23	1.98	0.64
1:C:100:LEU:HB3	1:C:123:VAL:HG22	1.81	0.63
1:A:254:PRO:HA	1:A:264:PRO:HB3	1.79	0.63
1:A:58:ALA:H	1:A:128:HIS:HD1	1.47	0.63
1:D:519:GLU:O	1:D:523:ILE:HD13	1.99	0.63
1:D:97:CYS:HA	1:D:185:GLU:OE2	1.99	0.63
1:B:500:GLU:O	1:B:504:LYS:HG2	2.00	0.62
1:A:553:LYS:HE2	1:B:379:GLY:HA3	1.81	0.62
1:A:212:HIS:HD2	1:A:215:GLU:H	1.43	0.62
1:D:212:HIS:CD2	1:D:215:GLU:H	2.14	0.62
1:B:222:PHE:O	1:B:226:LEU:HD13	1.99	0.62
1:B:312:GLY:HA3	1:B:392:ILE:HA	1.82	0.62
1:A:96:ALA:HB2	1:A:273:VAL:HG13	1.82	0.61
1:C:134:LYS:O	1:C:138:ILE:HG12	2.00	0.61
1:D:90:ILE:HD13	1:D:91:GLY:N	2.15	0.61
1:D:58:ALA:H	1:D:128:HIS:HD1	1.48	0.61
1:D:201:ASN:HD21	1:D:204:THR:H	1.47	0.61
1:C:335:VAL:HG13	1:C:336:GLY:H	1.66	0.61
1:D:150:LEU:HG	1:D:155:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:TYR:HA	1:B:24:LEU:HD13	1.82	0.61
1:A:361:ASN:ND2	1:A:363:HIS:H	1.99	0.60
1:A:99:MET:HE2	1:A:124:LYS:HB2	1.83	0.60
1:C:149:PHE:HE2	1:C:157:ILE:HD11	1.66	0.60
1:D:49:THR:C	1:D:50:ASN:HD22	2.05	0.60
1:D:223:PHE:HA	1:D:226:LEU:HD23	1.83	0.60
1:D:189:TRP:O	1:D:192:SER:HB3	2.01	0.60
1:A:502:ALA:HB1	1:A:506:MET:CE	2.32	0.60
1:A:282:VAL:O	1:A:282:VAL:HG12	2.02	0.60
1:A:427:ARG:HA	1:A:430:VAL:HG22	1.84	0.60
1:D:150:LEU:HB3	1:D:151:PRO:HD3	1.83	0.60
1:C:391:SER:O	1:C:392:ILE:HG23	2.02	0.59
1:A:364:ALA:O	1:A:368:GLU:HG2	2.02	0.59
1:B:392:ILE:HG12	3:B:608:HOH:O	2.01	0.59
1:A:100:LEU:HB3	1:A:123:VAL:HG22	1.82	0.59
1:B:124:LYS:HE2	3:B:580:HOH:O	2.00	0.59
1:A:316:VAL:HA	1:A:327:GLY:O	2.01	0.59
1:B:156:LYS:HD3	1:B:394:VAL:HG12	1.83	0.59
1:D:321:ILE:O	1:D:322:ILE:HD12	2.03	0.59
1:A:349:ALA:HA	1:B:349:ALA:HB2	1.84	0.59
1:A:252:LEU:HD11	1:A:260:MET:HE3	1.84	0.59
1:D:115:TYR:OH	1:D:179:ARG:HG3	2.03	0.59
1:D:163:ILE:HA	1:D:166:VAL:HG12	1.85	0.59
1:D:380:LEU:HD23	1:D:414:ILE:HA	1.85	0.59
1:A:62:PRO:HG3	1:A:123:VAL:HG23	1.84	0.59
1:A:231:GLU:O	1:A:232:HIS:HB2	2.03	0.58
1:C:63:LEU:O	1:C:67:GLU:HG2	2.03	0.58
1:C:132:GLN:NE2	1:C:159:SER:HB3	2.17	0.58
1:D:46:LEU:O	1:D:49:THR:HG22	2.02	0.58
1:D:191:VAL:O	1:D:195:THR:HG22	2.03	0.58
1:A:69:LEU:HD11	1:A:190:ILE:CD1	2.27	0.58
1:D:42:ILE:HD12	1:D:42:ILE:N	2.18	0.58
1:A:150:LEU:HB3	1:A:151:PRO:HD3	1.86	0.58
1:C:382:ALA:HB2	1:C:402:LEU:HD22	1.85	0.58
1:D:298:ILE:HG13	1:D:335:VAL:HG21	1.85	0.58
1:A:124:LYS:NZ	1:A:169:ILE:HD11	2.18	0.57
1:C:349:ALA:HA	1:D:349:ALA:HB2	1.85	0.57
1:A:479:LEU:O	1:A:483:MET:HG3	2.04	0.57
1:C:256:MET:HB3	1:C:260:MET:CE	2.33	0.57
1:D:414:ILE:C	1:D:414:ILE:HD13	2.24	0.57
1:A:476:THR:HB	1:A:477:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:HIS:HE1	1:D:160:GLU:OE2	1.88	0.57
1:C:502:ALA:HB1	1:C:506:MET:HE2	1.86	0.57
1:D:63:LEU:O	1:D:66:VAL:HG12	2.04	0.57
1:C:280:PRO:HB2	1:C:483:MET:HE2	1.86	0.57
1:B:22:ILE:CD1	1:B:482:ALA:HB1	2.35	0.57
1:C:391:SER:C	1:C:392:ILE:HG23	2.25	0.57
1:A:382:ALA:HB2	1:A:402:LEU:HD22	1.85	0.57
1:D:99:MET:HE2	1:D:162:MET:HE1	1.87	0.57
1:D:42:ILE:HD13	1:D:60:GLN:HA	1.86	0.56
1:A:312:GLY:HA3	1:A:392:ILE:H	1.71	0.56
1:A:141:MET:O	1:A:145:ARG:HB2	2.05	0.56
1:B:73:VAL:O	1:B:76:VAL:HG12	2.06	0.56
1:C:392:ILE:HG12	3:C:590:HOH:O	2.06	0.56
1:D:255:GLU:H	1:D:255:GLU:CD	2.08	0.56
1:A:321:ILE:HG22	1:A:322:ILE:HG12	1.86	0.56
1:A:190:ILE:HD13	1:A:190:ILE:O	2.05	0.56
1:A:97:CYS:HB2	1:A:208:LYS:HD3	1.86	0.56
1:C:555:ILE:HG22	1:C:556:GLN:HE21	1.70	0.56
1:A:10:VAL:HB	1:A:92:VAL:HG12	1.87	0.56
1:C:201:ASN:HD22	1:C:203:CYS:H	1.54	0.56
1:C:255:GLU:CD	1:C:255:GLU:H	2.09	0.56
1:D:342:PHE:CE1	1:D:414:ILE:HD12	2.41	0.56
1:B:380:LEU:HD23	1:B:414:ILE:HA	1.87	0.56
1:C:201:ASN:HD21	1:C:204:THR:H	1.52	0.56
1:B:293:ALA:HA	1:B:446:CYS:HB2	1.87	0.56
1:D:502:ALA:HB1	1:D:506:MET:CE	2.36	0.56
1:A:449:LEU:HB3	1:A:450:PRO:HD3	1.88	0.55
1:B:368:GLU:O	1:B:371:SER:HB3	2.06	0.55
1:D:500:GLU:HB2	3:D:1026:HOH:O	2.05	0.55
1:B:49:THR:OG1	1:B:51:ILE:HG12	2.07	0.55
1:C:163:ILE:HD13	1:C:223:PHE:HE2	1.71	0.55
1:D:426:THR:O	1:D:430:VAL:HG12	2.05	0.55
1:C:23:ASP:HB3	1:C:26:ASN:HD21	1.72	0.55
1:D:99:MET:CE	1:D:162:MET:HE1	2.35	0.55
1:B:100:LEU:HB3	1:B:123:VAL:HG22	1.89	0.55
1:D:285:THR:O	1:D:285:THR:HG22	2.06	0.55
1:A:96:ALA:N	2:A:573:QDK:O3	2.38	0.55
1:B:152:ARG:O	1:B:315:GLY:HA2	2.05	0.55
1:A:162:MET:O	1:A:166:VAL:HG12	2.07	0.55
1:C:210:ILE:HD13	3:C:616:HOH:O	2.06	0.55
1:B:338:ILE:CD1	1:B:386:TRP:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ARG:HA	1:D:430:VAL:CG1	2.37	0.55
1:A:30:LEU:HD23	1:A:30:LEU:N	2.22	0.55
1:A:307:GLU:HB2	1:A:326:LEU:HD21	1.88	0.55
1:A:469:LYS:HB3	1:A:509:VAL:HG11	1.89	0.55
1:B:96:ALA:HB1	1:B:208:LYS:CE	2.36	0.55
1:D:282:VAL:O	1:D:282:VAL:HG12	2.07	0.55
1:B:295:GLY:HA2	1:B:449:LEU:HD23	1.88	0.54
1:A:491:SER:HB2	1:A:497:ASP:OD2	2.07	0.54
1:B:312:GLY:HA3	1:B:392:ILE:CA	2.36	0.54
1:B:201:ASN:ND2	1:B:203:CYS:HB3	2.21	0.54
1:A:61:HIS:HD2	1:A:63:LEU:H	1.54	0.54
1:A:120:HIS:HD2	1:A:124:LYS:NZ	2.05	0.54
1:A:179:ARG:O	1:A:179:ARG:HD3	2.08	0.54
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.89	0.54
1:B:290:LEU:HD21	1:B:300:HIS:HD2	1.73	0.54
1:A:406:THR:HA	1:B:386:TRP:O	2.08	0.54
1:C:374:ARG:NH2	1:D:558:ARG:HB2	2.22	0.54
1:B:427:ARG:HA	1:B:430:VAL:HG22	1.89	0.54
1:D:104:GLU:OE2	1:D:179:ARG:NH2	2.41	0.54
1:A:192:SER:HA	1:A:195:THR:HG22	1.90	0.54
1:C:552:LEU:HD11	1:D:376:GLY:HA3	1.89	0.54
1:D:528:TYR:O	1:D:532:VAL:HG23	2.08	0.54
1:A:247:GLU:OE1	1:A:247:GLU:HA	2.06	0.53
1:A:20:VAL:HG12	1:A:32:ASP:HB2	1.90	0.53
1:B:401:MET:HG2	1:B:402:LEU:N	2.23	0.53
1:B:469:LYS:HB3	1:B:509:VAL:HG11	1.89	0.53
1:A:103:ASP:HB2	1:A:104:GLU:OE2	2.08	0.53
1:B:232:HIS:HA	3:B:578:HOH:O	2.08	0.53
1:C:321:ILE:HG22	1:C:322:ILE:HG13	1.89	0.53
1:A:96:ALA:HB2	1:A:273:VAL:CG1	2.37	0.53
1:A:349:ALA:HB2	1:B:349:ALA:HA	1.91	0.53
1:B:440:VAL:O	1:B:466:ARG:HD3	2.09	0.53
1:B:38:ARG:HB3	1:B:64:ASP:OD1	2.09	0.53
1:D:201:ASN:ND2	1:D:203:CYS:HB3	2.24	0.53
1:D:35:THR:HG23	1:D:72:SER:HG	1.72	0.53
1:B:170:LEU:HD11	1:B:229:ARG:NE	2.20	0.53
1:C:294:MET:HB2	1:C:450:PRO:HD3	1.90	0.53
1:D:311:GLU:H	1:D:436:ARG:HH12	1.57	0.53
1:A:236:THR:O	1:A:239:ARG:HG2	2.09	0.53
1:A:71:THR:C	1:A:74:PRO:HD2	2.29	0.53
1:D:148:ALA:O	1:D:151:PRO:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HA	1:A:165:LYS:NZ	2.24	0.52
1:B:518:PRO:O	1:B:521:VAL:HG22	2.09	0.52
1:C:68:VAL:O	1:C:72:SER:HB2	2.09	0.52
1:D:64:ASP:O	1:D:67:GLU:HB2	2.09	0.52
1:A:365:LEU:HD11	1:A:369:LYS:HD2	1.90	0.52
1:C:443:LEU:HB2	1:C:468:ILE:HG12	1.91	0.52
1:B:104:GLU:HA	1:B:181:ASP:OD1	2.08	0.52
1:B:185:GLU:HG3	1:B:187:THR:HG22	1.91	0.52
1:C:174:GLU:HB2	3:C:630:HOH:O	2.08	0.52
1:B:120:HIS:HD2	1:B:124:LYS:NZ	2.08	0.52
1:B:201:ASN:ND2	1:B:204:THR:H	2.07	0.52
1:C:35:THR:HG23	1:C:72:SER:OG	2.10	0.52
1:A:312:GLY:HA3	1:A:392:ILE:HA	1.91	0.52
1:B:243:VAL:CG2	1:B:270:VAL:HG11	2.40	0.52
1:B:71:THR:C	1:B:74:PRO:HD2	2.30	0.52
1:A:259:LYS:HE3	1:C:38:ARG:NH2	2.25	0.52
1:A:120:HIS:HD2	1:A:124:LYS:HZ3	1.57	0.52
1:A:391:SER:C	1:A:392:ILE:HG23	2.31	0.52
1:A:60:GLN:O	1:A:123:VAL:HB	2.09	0.52
1:C:212:HIS:CD2	1:C:215:GLU:H	2.20	0.52
1:D:391:SER:O	1:D:392:ILE:HG23	2.10	0.51
1:A:120:HIS:HE1	1:A:172:GLU:HB3	1.75	0.51
1:B:297:SER:HA	1:B:335:VAL:HG12	1.91	0.51
1:D:141:MET:O	1:D:141:MET:HE2	2.10	0.51
1:A:386:TRP:O	1:B:406:THR:HA	2.11	0.51
1:A:198:ILE:O	1:A:198:ILE:HG13	2.11	0.51
1:A:165:LYS:O	1:A:169:ILE:HD13	2.10	0.51
1:D:253:LEU:HB3	1:D:255:GLU:OE2	2.11	0.51
1:B:205:ALA:O	1:B:208:LYS:O	2.28	0.51
1:B:208:LYS:O	1:B:209:ALA:HB3	2.10	0.51
1:A:307:GLU:HB2	1:A:326:LEU:CD2	2.41	0.51
1:B:73:VAL:O	1:B:77:MET:HG2	2.11	0.51
1:C:331:GLY:O	1:C:391:SER:HB2	2.11	0.51
1:C:401:MET:HG2	1:C:402:LEU:N	2.26	0.51
1:C:552:LEU:CD1	1:D:376:GLY:HA3	2.41	0.51
1:A:256:MET:HB3	1:A:260:MET:CE	2.41	0.51
1:B:120:HIS:HA	1:B:124:LYS:HZ1	1.76	0.51
1:B:173:ALA:HB1	1:B:176:VAL:HG23	1.92	0.50
1:C:361:ASN:HD22	1:C:363:HIS:HB2	1.76	0.50
1:D:278:ALA:O	1:D:282:VAL:HG23	2.11	0.50
1:C:518:PRO:O	1:C:521:VAL:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:THR:HG22	3:B:634:HOH:O	2.10	0.50
1:A:49:THR:HG23	1:A:51:ILE:H	1.76	0.50
1:C:282:VAL:HG13	1:C:284:VAL:HG23	1.94	0.50
1:C:318:GLU:O	1:C:319:ASP:HB2	2.11	0.50
1:B:231:GLU:O	1:B:232:HIS:HB2	2.12	0.50
1:A:259:LYS:HE3	1:C:38:ARG:CZ	2.41	0.50
1:D:361:ASN:HD22	1:D:363:HIS:HB2	1.76	0.50
1:B:156:LYS:HB3	1:B:394:VAL:HG11	1.93	0.50
1:C:185:GLU:HG2	1:C:204:THR:CG2	2.40	0.50
1:C:317:VAL:HG22	1:C:320:GLY:HA3	1.94	0.50
1:C:55:HIS:O	1:C:56:GLU:HB2	2.11	0.50
1:D:243:VAL:CG2	1:D:270:VAL:HG11	2.42	0.50
1:B:207:TYR:CZ	1:B:317:VAL:HG13	2.46	0.50
1:D:382:ALA:HB2	1:D:402:LEU:HD13	1.93	0.50
1:D:202:SER:HA	1:D:242:ILE:CG2	2.42	0.50
1:A:46:LEU:HB2	1:A:49:THR:HG21	1.94	0.49
1:C:386:TRP:O	1:D:406:THR:HA	2.12	0.49
1:A:104:GLU:HG2	1:A:105:GLU:OE1	2.12	0.49
1:A:231:GLU:HG2	1:A:232:HIS:CD2	2.47	0.49
1:A:23:ASP:HB3	1:A:26:ASN:OD1	2.12	0.49
1:C:134:LYS:HD2	1:C:167:TRP:CD2	2.47	0.49
1:C:97:CYS:HB2	1:C:208:LYS:CG	2.39	0.49
1:D:343:VAL:HG13	1:D:362:VAL:HG11	1.94	0.49
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.94	0.49
1:C:252:LEU:HD21	1:C:264:PRO:HA	1.94	0.49
1:D:163:ILE:HA	1:D:166:VAL:CG1	2.43	0.49
1:A:403:LEU:HD11	1:B:546:MET:CE	2.42	0.49
1:D:517:ILE:O	1:D:521:VAL:HG13	2.13	0.49
1:A:88:ILE:HD11	1:A:493:VAL:HB	1.95	0.49
1:B:94:PHE:HB2	1:B:187:THR:HB	1.95	0.49
1:B:63:LEU:HA	1:B:66:VAL:HG12	1.94	0.49
1:C:157:ILE:HD12	1:C:157:ILE:N	2.28	0.49
1:A:33:HIS:CE1	1:A:35:THR:HG23	2.48	0.49
1:C:102:VAL:HG22	1:C:182:GLN:O	2.13	0.48
1:D:18:ARG:HD2	1:D:475:GLN:HG2	1.95	0.48
1:A:188:ASP:O	1:A:191:VAL:HG22	2.14	0.48
1:D:79:GLU:O	1:D:80:SER:C	2.52	0.48
1:A:185:GLU:CG	1:A:204:THR:HG21	2.41	0.48
1:C:109:LEU:HA	1:C:112:LEU:HD13	1.96	0.48
1:D:141:MET:HE2	1:D:145:ARG:HG3	1.94	0.48
1:D:392:ILE:HG23	1:D:429:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:MET:O	1:C:252:LEU:HA	2.14	0.48
1:D:452:LYS:NZ	1:D:453:ASN:HD22	2.11	0.48
1:A:335:VAL:HG22	1:A:336:GLY:N	2.28	0.48
1:C:72:SER:O	1:C:76:VAL:HG23	2.14	0.48
1:D:335:VAL:CG2	1:D:336:GLY:H	2.23	0.48
1:D:391:SER:C	1:D:392:ILE:HG23	2.34	0.48
1:A:152:ARG:O	1:A:315:GLY:HA2	2.13	0.48
1:A:331:GLY:O	1:A:391:SER:HB2	2.13	0.48
1:B:305:GLU:O	1:B:326:LEU:HD23	2.13	0.48
1:B:343:VAL:HG21	1:B:363:HIS:NE2	2.29	0.48
1:C:223:PHE:HA	1:C:226:LEU:HD23	1.95	0.48
1:C:298:ILE:CG1	1:C:335:VAL:HG11	2.41	0.48
1:D:20:VAL:HG23	1:D:22:ILE:HG13	1.96	0.48
1:C:379:GLY:HA3	1:D:553:LYS:HE3	1.94	0.48
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.96	0.48
1:B:476:THR:HB	1:B:477:PRO:HD3	1.95	0.48
1:B:58:ALA:H	1:B:128:HIS:HD1	1.62	0.48
1:A:199:VAL:O	1:A:199:VAL:HG13	2.14	0.48
1:D:5:LYS:HD2	1:D:5:LYS:N	2.29	0.48
1:A:18:ARG:HD2	1:A:475:GLN:HG2	1.95	0.48
1:A:518:PRO:O	1:A:521:VAL:HG22	2.13	0.48
1:B:44:GLN:HG2	1:B:45:TYR:CE2	2.49	0.48
1:B:64:ASP:O	1:B:68:VAL:HG23	2.14	0.48
1:A:138:ILE:CD1	1:A:163:ILE:HG22	2.43	0.47
1:B:331:GLY:O	1:B:391:SER:HB2	2.14	0.47
1:C:38:ARG:HB2	1:C:64:ASP:OD1	2.14	0.47
1:C:88:ILE:O	1:C:266:ILE:HB	2.14	0.47
1:D:452:LYS:HD3	1:D:453:ASN:HB2	1.96	0.47
1:B:141:MET:HE3	1:B:145:ARG:HG3	1.96	0.47
1:D:10:VAL:HB	1:D:92:VAL:HG12	1.96	0.47
1:A:380:LEU:HD23	1:A:414:ILE:HA	1.97	0.47
1:C:163:ILE:HD12	1:C:210:ILE:CG1	2.45	0.47
1:D:114:GLN:HG3	1:D:115:TYR:CE1	2.49	0.47
1:D:294:MET:HB3	1:D:298:ILE:HG12	1.96	0.47
1:B:22:ILE:H	1:B:22:ILE:HD13	1.79	0.47
1:B:29:GLU:OE2	1:B:474:LYS:HG2	2.14	0.47
1:C:318:GLU:HG2	1:C:319:ASP:OD1	2.13	0.47
1:C:35:THR:OG1	1:C:68:VAL:HG22	2.14	0.47
1:D:378:SER:O	1:D:380:LEU:HD13	2.14	0.47
1:A:182:GLN:HG3	3:A:604:HOH:O	2.14	0.47
1:A:6:TYR:CD1	1:A:23:ASP:HA	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HD12	1:B:482:ALA:HB1	1.96	0.47
1:B:257:ALA:O	1:B:261:GLY:N	2.48	0.47
1:D:99:MET:CE	1:D:162:MET:CE	2.93	0.47
1:B:141:MET:HG2	1:B:226:LEU:CD1	2.43	0.47
1:C:42:ILE:N	1:C:42:ILE:HD12	2.30	0.47
1:B:71:THR:O	1:B:74:PRO:HD2	2.15	0.47
1:C:26:ASN:H	1:C:26:ASN:HD22	1.63	0.47
1:C:297:SER:HA	1:C:335:VAL:HG12	1.97	0.47
1:C:476:THR:HB	1:C:477:PRO:HD3	1.96	0.47
1:D:385:TRP:CE3	1:D:398:LEU:HB3	2.49	0.47
1:D:77:MET:O	1:D:81:GLY:HA2	2.15	0.47
1:A:392:ILE:HG12	3:A:582:HOH:O	2.13	0.47
1:A:443:LEU:HB2	1:A:468:ILE:HG12	1.97	0.47
1:D:114:GLN:HG3	1:D:115:TYR:CD1	2.50	0.47
1:A:483:MET:HA	1:A:506:MET:HE1	1.97	0.47
1:A:274:ASP:OD1	2:A:573:QDK:H3	2.15	0.46
1:C:207:TYR:CZ	1:C:317:VAL:HG13	2.50	0.46
1:A:129:HIS:HE1	1:A:160:GLU:OE2	1.98	0.46
1:A:290:LEU:HD22	1:A:430:VAL:HG12	1.97	0.46
1:D:222:PHE:CE2	1:D:226:LEU:HD21	2.50	0.46
1:D:285:THR:HG21	1:D:500:GLU:HA	1.97	0.46
1:C:317:VAL:HG22	1:C:320:GLY:CA	2.46	0.46
1:D:22:ILE:CD1	1:D:479:LEU:HA	2.44	0.46
1:A:157:ILE:N	1:A:157:ILE:HD12	2.31	0.46
1:B:109:LEU:HD12	1:B:112:LEU:HD22	1.97	0.46
1:B:22:ILE:HD11	1:B:482:ALA:HB1	1.97	0.46
1:C:411:PRO:HB3	3:C:594:HOH:O	2.15	0.46
1:D:222:PHE:O	1:D:226:LEU:HD22	2.16	0.46
1:A:63:LEU:CD1	1:A:111:LEU:HD11	2.45	0.46
1:C:252:LEU:HD21	1:C:263:ASN:O	2.16	0.46
1:D:210:ILE:HG22	1:D:210:ILE:O	2.16	0.46
1:A:88:ILE:HG13	1:A:88:ILE:O	2.15	0.46
1:B:161:TRP:CD1	1:B:161:TRP:N	2.84	0.46
1:D:414:ILE:HD13	1:D:414:ILE:O	2.16	0.46
1:B:523:ILE:O	1:B:526:LYS:HB2	2.15	0.46
1:D:195:THR:HG23	1:D:197:LYS:N	2.14	0.46
1:B:550:LYS:O	1:B:553:LYS:HB2	2.16	0.45
1:B:86:ASP:HA	3:B:633:HOH:O	2.15	0.45
1:A:62:PRO:HG3	1:A:123:VAL:CG2	2.47	0.45
1:A:95:THR:HA	1:A:274:ASP:OD2	2.16	0.45
1:B:163:ILE:O	1:B:166:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:HB3	1:B:509:VAL:CG1	2.45	0.45
1:C:354:GLU:HB3	1:C:365:LEU:HD21	1.96	0.45
1:C:469:LYS:HB3	1:C:509:VAL:CG1	2.45	0.45
1:D:71:THR:C	1:D:74:PRO:HD2	2.36	0.45
1:B:120:HIS:O	1:B:176:VAL:HG11	2.16	0.45
1:B:26:ASN:HD22	1:B:26:ASN:C	2.19	0.45
1:D:452:LYS:HE2	3:D:1097:HOH:O	2.16	0.45
1:A:483:MET:O	1:A:487:VAL:HG23	2.16	0.45
1:B:65:TYR:O	1:B:68:VAL:HB	2.17	0.45
1:D:46:LEU:CD1	1:D:53:LEU:HD11	2.46	0.45
1:B:12:TYR:HA	1:B:17:GLY:HA2	1.99	0.45
1:B:39:HIS:HB3	1:B:42:ILE:HD11	1.99	0.45
1:C:203:CYS:HB2	1:C:245:LEU:HD11	1.98	0.45
1:A:312:GLY:HA3	1:A:392:ILE:CA	2.47	0.45
1:B:243:VAL:HG21	1:B:270:VAL:HG11	1.99	0.45
1:B:375:PRO:HB3	1:B:524:TYR:CZ	2.52	0.45
1:D:95:THR:HA	1:D:274:ASP:OD2	2.17	0.45
1:D:96:ALA:HB2	1:D:273:VAL:CG1	2.46	0.45
1:A:115:TYR:CE2	1:A:179:ARG:HG3	2.50	0.45
1:B:101:PRO:HB3	1:B:183:PHE:CE1	2.52	0.45
1:A:469:LYS:HB3	1:A:509:VAL:CG1	2.46	0.45
1:C:96:ALA:HB1	1:C:208:LYS:HE3	1.98	0.45
1:C:23:ASP:HB3	1:C:26:ASN:ND2	2.32	0.45
1:C:343:VAL:HG21	1:C:363:HIS:CD2	2.52	0.45
1:D:99:MET:HE3	1:D:162:MET:CE	2.47	0.45
1:A:187:THR:O	1:A:190:ILE:HG22	2.17	0.45
1:D:383:LEU:HD12	1:D:383:LEU:HA	1.88	0.45
1:A:553:LYS:CE	1:B:379:GLY:HA3	2.47	0.45
1:A:66:VAL:HA	1:A:69:LEU:HD12	1.98	0.45
1:C:166:VAL:HG23	1:C:183:PHE:CE2	2.52	0.45
1:C:298:ILE:HG13	1:C:335:VAL:CG1	2.44	0.45
1:D:353:ASP:O	1:D:356:GLN:O	2.35	0.45
1:D:383:LEU:HB2	1:D:401:MET:HB3	1.98	0.45
1:B:279:VAL:O	1:B:282:VAL:HG12	2.17	0.44
1:D:361:ASN:HD21	1:D:363:HIS:HB2	1.82	0.44
1:D:312:GLY:HA3	1:D:392:ILE:HA	1.99	0.44
1:A:49:THR:OG1	1:A:50:ASN:N	2.50	0.44
1:B:391:SER:C	1:B:392:ILE:HG23	2.37	0.44
1:B:97:CYS:HA	1:B:185:GLU:OE2	2.18	0.44
1:C:347:VAL:HG13	1:C:347:VAL:O	2.17	0.44
1:A:19:ALA:O	1:A:32:ASP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:VAL:HG13	1:C:336:GLY:N	2.31	0.44
1:D:223:PHE:HA	1:D:226:LEU:CD2	2.47	0.44
1:C:361:ASN:ND2	1:C:363:HIS:H	2.16	0.44
1:D:339:PHE:CZ	1:D:419:LEU:HD12	2.52	0.44
1:A:300:HIS:HE1	1:A:332:GLN:HB2	1.83	0.44
1:B:101:PRO:HB2	1:B:109:LEU:HD23	2.00	0.44
1:D:194:MET:HB3	1:D:252:LEU:HD12	2.00	0.44
1:A:100:LEU:N	1:A:100:LEU:HD23	2.33	0.44
1:C:201:ASN:ND2	1:C:203:CYS:HB3	2.33	0.44
1:C:252:LEU:CD2	1:C:264:PRO:HA	2.48	0.44
1:C:26:ASN:N	1:C:26:ASN:ND2	2.66	0.44
1:D:50:ASN:HD22	1:D:50:ASN:N	2.15	0.44
1:C:99:MET:HG3	1:C:124:LYS:HB2	1.99	0.44
1:D:114:GLN:HE21	1:D:114:GLN:HB2	1.57	0.44
1:A:62:PRO:HG2	1:A:110:CYS:SG	2.58	0.44
1:B:335:VAL:HG13	1:B:336:GLY:N	2.32	0.44
1:C:309:GLU:O	1:C:436:ARG:NE	2.51	0.44
1:D:211:TRP:CZ2	1:D:213:LYS:HA	2.53	0.44
1:A:243:VAL:CG2	1:A:270:VAL:HG11	2.48	0.43
1:A:63:LEU:O	1:A:66:VAL:HG22	2.18	0.43
1:B:53:LEU:H	1:B:53:LEU:HD22	1.83	0.43
1:C:242:ILE:N	1:C:242:ILE:HD12	2.32	0.43
1:C:528:TYR:O	1:C:532:VAL:HG23	2.18	0.43
1:A:100:LEU:HD23	1:A:184:LEU:O	2.18	0.43
1:B:446:CYS:SG	1:B:476:THR:HG21	2.59	0.43
1:C:198:ILE:HG13	1:C:198:ILE:O	2.17	0.43
1:A:483:MET:HE1	1:A:503:ALA:HA	2.00	0.43
1:B:289:LYS:HB3	1:B:444:TYR:CE2	2.53	0.43
1:C:199:VAL:HG11	1:C:249:ALA:HB1	1.99	0.43
1:A:104:GLU:CD	1:A:104:GLU:N	2.67	0.43
1:B:156:LYS:HE3	3:B:634:HOH:O	2.18	0.43
1:D:56:GLU:CG	1:D:129:HIS:HB2	2.42	0.43
1:D:375:PRO:HB3	1:D:524:TYR:CZ	2.53	0.43
1:A:212:HIS:CD2	1:A:215:GLU:H	2.30	0.43
1:A:69:LEU:O	1:A:74:PRO:HD3	2.18	0.43
1:B:185:GLU:CG	1:B:187:THR:HG22	2.47	0.43
1:B:69:LEU:O	1:B:74:PRO:HD3	2.18	0.43
1:C:147:GLU:HG3	3:C:629:HOH:O	2.18	0.43
1:B:96:ALA:HB1	1:B:208:LYS:NZ	2.33	0.43
1:D:99:MET:HE3	1:D:162:MET:HE3	1.99	0.43
1:B:391:SER:O	1:B:392:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASN:ND2	1:D:204:THR:H	2.14	0.43
1:D:220:ASN:HD22	1:D:220:ASN:N	2.16	0.43
1:D:321:ILE:HG22	1:D:322:ILE:HD13	2.01	0.43
1:B:545:VAL:O	1:B:549:LEU:HB2	2.19	0.43
1:C:57:TRP:HE3	1:C:59:LEU:HD11	1.84	0.43
1:C:8:ILE:HD13	1:C:73:VAL:HG13	2.00	0.43
1:D:389:ASN:C	1:D:389:ASN:HD22	2.22	0.43
1:A:201:ASN:HD21	1:A:203:CYS:HB3	1.84	0.43
1:A:310:VAL:HG21	1:A:433:PHE:CD1	2.53	0.43
1:B:360:VAL:HG22	1:B:364:ALA:HB3	2.01	0.43
1:B:479:LEU:O	1:B:483:MET:HG3	2.19	0.43
1:B:528:TYR:O	1:B:531:TYR:HB3	2.19	0.43
1:C:224:LYS:HB2	1:C:231:GLU:HG3	2.00	0.43
1:C:335:VAL:HG23	1:C:422:THR:HG21	2.01	0.43
1:A:47:PRO:HG2	1:A:122:TRP:CH2	2.55	0.42
1:B:343:VAL:O	1:B:347:VAL:HG12	2.19	0.42
1:B:430:VAL:HG23	1:B:431:ASP:N	2.34	0.42
1:C:243:VAL:HG21	1:C:270:VAL:HG11	2.01	0.42
1:B:48:ASN:OD1	1:B:48:ASN:O	2.37	0.42
1:D:360:VAL:HG22	1:D:364:ALA:HB3	2.01	0.42
1:A:199:VAL:HG11	1:A:249:ALA:HA	2.01	0.42
1:A:30:LEU:H	1:A:30:LEU:HD23	1.84	0.42
1:A:517:ILE:HG22	1:A:519:GLU:HG2	2.02	0.42
1:B:115:TYR:OH	1:B:179:ARG:HG3	2.18	0.42
1:B:274:ASP:OD1	1:B:275:ALA:N	2.50	0.42
1:A:120:HIS:HE1	1:A:172:GLU:CB	2.32	0.42
1:A:31:ALA:HB3	1:A:76:VAL:HG13	2.01	0.42
1:B:21:LEU:O	1:B:30:LEU:HD13	2.19	0.42
1:D:254:PRO:HA	1:D:264:PRO:HB3	2.02	0.42
1:D:295:GLY:O	1:D:335:VAL:HG23	2.19	0.42
1:D:449:LEU:N	1:D:450:PRO:CD	2.82	0.42
1:A:160:GLU:HA	1:A:165:LYS:HZ3	1.84	0.42
1:A:211:TRP:CZ2	1:A:213:LYS:HA	2.54	0.42
1:D:207:TYR:CZ	1:D:317:VAL:HG13	2.55	0.42
1:B:290:LEU:HD22	1:B:430:VAL:HG12	2.01	0.42
1:C:211:TRP:CZ2	1:C:213:LYS:HA	2.55	0.42
1:A:403:LEU:HD11	1:B:546:MET:HE2	2.00	0.42
1:C:195:THR:HG23	1:C:197:LYS:N	2.19	0.42
1:D:7:THR:HG23	1:D:24:LEU:HD11	2.02	0.42
1:C:26:ASN:N	1:C:26:ASN:HD22	2.18	0.42
1:C:390:ARG:HD3	1:C:390:ARG:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:LEU:CD1	1:D:260:MET:HE3	2.47	0.42
1:A:316:VAL:HG22	1:A:326:LEU:HD23	2.02	0.42
1:B:408:GLN:HE21	1:B:408:GLN:HB2	1.58	0.42
1:C:112:LEU:HD12	1:C:112:LEU:N	2.34	0.42
1:C:252:LEU:HD23	1:C:252:LEU:O	2.19	0.42
1:D:456:LEU:HD22	1:D:460:PHE:CE2	2.55	0.42
1:A:220:ASN:HD22	1:A:220:ASN:HA	1.57	0.41
1:B:276:HIS:CD2	1:B:276:HIS:H	2.36	0.41
1:C:343:VAL:HG21	1:C:363:HIS:NE2	2.35	0.41
1:C:502:ALA:HB1	1:C:506:MET:HE3	2.01	0.41
1:A:39:HIS:HB2	1:A:64:ASP:OD2	2.19	0.41
1:A:491:SER:HB2	1:A:497:ASP:CG	2.41	0.41
1:C:174:GLU:OE1	1:C:229:ARG:NH1	2.53	0.41
1:B:290:LEU:HD12	1:B:302:LEU:HB2	2.02	0.41
1:C:252:LEU:HD23	1:C:265:GLY:H	1.84	0.41
1:C:252:LEU:HD23	1:C:265:GLY:N	2.35	0.41
1:C:26:ASN:H	1:C:26:ASN:ND2	2.18	0.41
1:C:282:VAL:O	1:C:282:VAL:HG22	2.20	0.41
1:C:55:HIS:ND1	1:C:56:GLU:HG2	2.35	0.41
1:C:94:PHE:HD2	1:C:95:THR:H	1.68	0.41
1:D:256:MET:HB3	1:D:260:MET:CE	2.49	0.41
1:B:97:CYS:HA	1:B:185:GLU:OE1	2.20	0.41
1:D:273:VAL:HB	1:D:276:HIS:HD2	1.84	0.41
1:B:317:VAL:HG22	1:B:320:GLY:CA	2.51	0.41
1:C:163:ILE:HD13	1:C:223:PHE:CE2	2.53	0.41
1:C:222:PHE:O	1:C:225:ALA:HB3	2.20	0.41
1:C:77:MET:HE1	1:C:87:VAL:HG21	2.02	0.41
1:D:22:ILE:HD13	1:D:479:LEU:HD13	2.03	0.41
1:D:301:MET:HA	1:D:328:TYR:O	2.19	0.41
1:A:297:SER:HA	1:A:335:VAL:HG13	2.02	0.41
1:A:61:HIS:HB3	1:A:64:ASP:OD2	2.21	0.41
1:B:35:THR:CG2	1:B:68:VAL:HA	2.47	0.41
1:C:42:ILE:H	1:C:42:ILE:HD12	1.84	0.41
1:D:321:ILE:HG22	1:D:322:ILE:CD1	2.51	0.41
1:D:464:THR:O	1:D:466:ARG:HD2	2.20	0.41
1:A:402:LEU:HD12	1:A:405:TYR:CE2	2.55	0.41
1:A:452:LYS:HE2	1:A:453:ASN:HB2	2.02	0.41
1:B:231:GLU:HG2	1:B:232:HIS:CD2	2.56	0.41
1:C:449:LEU:HD12	1:C:449:LEU:HA	1.90	0.41
1:D:22:ILE:HD13	1:D:479:LEU:CD1	2.51	0.41
1:D:256:MET:HB3	1:D:260:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:MET:HG2	1:D:402:LEU:N	2.34	0.41
1:A:201:ASN:ND2	1:A:203:CYS:HB3	2.35	0.41
1:B:199:VAL:O	1:B:199:VAL:HG23	2.20	0.41
1:B:201:ASN:HD22	1:B:203:CYS:HB3	1.86	0.41
1:B:230:LEU:HD22	1:B:233:LEU:HD22	2.02	0.41
1:D:355:ALA:HB1	1:D:360:VAL:O	2.20	0.41
1:D:393:LEU:HA	1:D:393:LEU:HD12	1.86	0.41
1:A:59:LEU:HA	1:A:123:VAL:O	2.21	0.41
1:A:102:VAL:HG22	1:A:182:GLN:O	2.21	0.41
1:A:177:TYR:CZ	1:A:237:LYS:HD3	2.56	0.41
1:A:185:GLU:HG3	3:A:588:HOH:O	2.20	0.41
1:A:528:TYR:O	1:A:532:VAL:HG23	2.21	0.41
1:B:134:LYS:HD2	1:B:167:TRP:CG	2.56	0.41
1:C:58:ALA:H	1:C:128:HIS:HD1	1.67	0.41
1:C:120:HIS:CE1	1:C:172:GLU:HB2	2.56	0.41
1:C:187:THR:O	1:C:191:VAL:HG13	2.20	0.41
1:C:409:THR:HA	1:C:413:GLU:OE1	2.21	0.41
1:D:201:ASN:HD22	1:D:203:CYS:N	2.14	0.41
1:D:287:PRO:O	1:D:289:LYS:HD2	2.21	0.41
1:D:475:GLN:HG3	3:D:1119:HOH:O	2.19	0.41
1:B:442:GLU:O	1:B:443:LEU:HD12	2.21	0.41
1:D:290:LEU:HD11	1:D:300:HIS:HB3	2.03	0.41
1:D:452:LYS:HZ3	1:D:453:ASN:HD22	1.69	0.41
1:B:132:GLN:O	1:B:135:ALA:HB3	2.21	0.40
1:B:198:ILE:HG13	1:B:198:ILE:O	2.21	0.40
1:D:141:MET:CE	1:D:145:ARG:HG3	2.50	0.40
1:A:44:GLN:C	1:A:53:LEU:HD23	2.41	0.40
1:B:63:LEU:CD2	1:B:111:LEU:HD11	2.52	0.40
1:A:42:ILE:HB	1:A:59:LEU:HB2	2.04	0.40
1:A:97:CYS:N	1:A:185:GLU:OE2	2.54	0.40
1:B:316:VAL:HG13	1:B:316:VAL:O	2.22	0.40
1:C:177:TYR:O	1:C:237:LYS:HE3	2.20	0.40
1:C:285:THR:HA	1:C:322:ILE:CD1	2.43	0.40
1:A:11:ASP:OD1	1:A:93:ASP:OD1	2.40	0.40
1:A:88:ILE:CD1	1:A:493:VAL:HB	2.52	0.40
1:C:552:LEU:HD13	1:C:552:LEU:O	2.22	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	542/572 (95%)	508 (94%)	31 (6%)	3 (1%)	25	30
1	B	539/572 (94%)	499 (93%)	36 (7%)	4 (1%)	22	26
1	C	545/572 (95%)	509 (93%)	34 (6%)	2 (0%)	34	41
1	D	552/572 (96%)	523 (95%)	24 (4%)	5 (1%)	17	19
All	All	2178/2288 (95%)	2039 (94%)	125 (6%)	14 (1%)	25	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	384	ASP
1	B	55	HIS
1	D	357	GLU
1	D	392	ILE
1	B	48	ASN
1	B	392	ILE
1	D	81	GLY
1	D	97	CYS
1	A	47	PRO
1	A	392	ILE
1	A	384	ASP
1	C	97	CYS
1	C	392	ILE
1	B	518	PRO

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	425/461 (92%)	391 (92%)	34 (8%)	12 15
1	B	426/461 (92%)	399 (94%)	27 (6%)	18 24
1	C	430/461 (93%)	387 (90%)	43 (10%)	7 8
1	D	434/461 (94%)	399 (92%)	35 (8%)	11 14
All	All	1715/1844 (93%)	1576 (92%)	139 (8%)	11 14

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	18	ARG
1	A	24	LEU
1	A	30	LEU
1	A	34	VAL
1	A	35	THR
1	A	59	LEU
1	A	77	MET
1	A	94	PHE
1	A	99	MET
1	A	133	ASP
1	A	166	VAL
1	A	179	ARG
1	A	190	ILE
1	A	220	ASN
1	A	226	LEU
1	A	247	GLU
1	A	317	VAL
1	A	326	LEU
1	A	335	VAL
1	A	344	LYS
1	A	351	THR
1	A	352	PHE
1	A	366	LEU
1	A	383	LEU
1	A	392	ILE
1	A	393	LEU
1	A	402	LEU
1	A	456	LEU
1	A	474	LYS
1	A	479	LEU
1	A	519	GLU
1	A	520	HIS

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Mol	Chain	Res	Type
1	A	549	LEU
1	B	22	ILE
1	B	26	ASN
1	B	30	LEU
1	B	35	THR
1	B	59	LEU
1	B	94	PHE
1	B	99	MET
1	B	114	GLN
1	B	179	ARG
1	B	245	LEU
1	B	247	GLU
1	B	317	VAL
1	B	333	SER
1	B	366	LEU
1	B	368	GLU
1	B	380	LEU
1	B	383	LEU
1	B	389	ASN
1	B	392	ILE
1	B	393	LEU
1	B	402	LEU
1	B	408	GLN
1	B	414	ILE
1	B	438	VAL
1	B	466	ARG
1	B	511	ASP
1	B	549	LEU
1	C	24	LEU
1	C	25	SER
1	C	26	ASN
1	C	29	GLU
1	C	38	ARG
1	C	59	LEU
1	C	63	LEU
1	C	72	SER
1	C	85	ASP
1	C	88	ILE
1	C	94	PHE
1	C	99	MET
1	C	100	LEU
1	C	104	GLU

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Mol	Chain	Res	Type
1	C	105	GLU
1	C	140	GLU
1	C	179	ARG
1	C	200	LYS
1	C	214	ARG
1	C	252	LEU
1	C	290	LEU
1	C	296	THR
1	C	317	VAL
1	C	352	PHE
1	C	357	GLU
1	C	360	VAL
1	C	366	LEU
1	C	368	GLU
1	C	371	SER
1	C	380	LEU
1	C	383	LEU
1	C	390	ARG
1	C	392	ILE
1	C	393	LEU
1	C	402	LEU
1	C	408	GLN
1	C	456	LEU
1	C	474	LYS
1	C	475	GLN
1	C	499	ILE
1	C	500	GLU
1	C	511	ASP
1	C	549	LEU
1	D	53	LEU
1	D	56	GLU
1	D	59	LEU
1	D	77	MET
1	D	88	ILE
1	D	90	ILE
1	D	94	PHE
1	D	100	LEU
1	D	104	GLU
1	D	114	GLN
1	D	179	ARG
1	D	190	ILE
1	D	245	LEU

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Mol	Chain	Res	Type
1	D	289	LYS
1	D	296	THR
1	D	317	VAL
1	D	351	THR
1	D	352	PHE
1	D	366	LEU
1	D	368	GLU
1	D	380	LEU
1	D	383	LEU
1	D	387	ASN
1	D	389	ASN
1	D	390	ARG
1	D	392	ILE
1	D	393	LEU
1	D	399	SER
1	D	402	LEU
1	D	414	ILE
1	D	419	LEU
1	D	456	LEU
1	D	515	LYS
1	D	521	VAL
1	D	552	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	48	ASN
1	A	61	HIS
1	A	120	HIS
1	A	129	HIS
1	A	168	GLN
1	A	178	ASN
1	A	201	ASN
1	A	212	HIS
1	A	220	ASN
1	A	232	HIS
1	A	263	ASN
1	A	276	HIS
1	A	300	HIS
1	A	308	GLN
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	520	HIS
1	B	26	ASN
1	B	48	ASN
1	B	50	ASN
1	B	114	GLN
1	B	120	HIS
1	B	129	HIS
1	B	132	GLN
1	B	168	GLN
1	B	178	ASN
1	B	201	ASN
1	B	212	HIS
1	B	220	ASN
1	B	276	HIS
1	B	300	HIS
1	B	389	ASN
1	B	408	GLN
1	C	26	ASN
1	C	39	HIS
1	C	120	HIS
1	C	129	HIS
1	C	132	GLN
1	C	168	GLN
1	C	201	ASN
1	C	212	HIS
1	C	220	ASN
1	C	263	ASN
1	C	276	HIS
1	C	300	HIS
1	C	361	ASN
1	C	408	GLN
1	C	556	GLN
1	D	48	ASN
1	D	50	ASN
1	D	114	GLN
1	D	120	HIS
1	D	129	HIS
1	D	132	GLN
1	D	168	GLN
1	D	178	ASN
1	D	201	ASN
1	D	212	HIS

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Mol	Chain	Res	Type
1	D	220	ASN
1	D	276	HIS
1	D	300	HIS
1	D	361	ASN
1	D	387	ASN
1	D	389	ASN
1	D	453	ASN
1	D	556	GLN

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)

1 ligand is 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	$\#\|Z\| > 2$
2	QDK	A	573	-	7,9,9	1.43	1 (14%)	5,11,11	1.37	0

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
2	QDK	A	573	-	-	5/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	573	QDK	O1-C1	2.37	1.49	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	573	QDK	O1-C1-C2-C3
2	A	573	QDK	C1-C2-C3-C4
2	A	573	QDK	O1-C1-C2-O2
2	A	573	QDK	O2-C2-C3-C4
2	A	573	QDK	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	573	QDK	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	546/572 (95%)	0.09	10 (1%)	68	75	25, 39, 49, 54	0
1	B	543/572 (94%)	-0.03	8 (1%)	73	79	21, 38, 48, 55	0
1	C	549/572 (95%)	-0.14	1 (0%)	95	97	20, 36, 47, 53	0
1	D	554/572 (96%)	-0.09	2 (0%)	92	95	20, 30, 42, 50	0
All	All	2192/2288 (95%)	-0.04	21 (0%)	82	86	20, 36, 48, 55	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	4.6
1	C	392	ILE	3.9
1	A	97	CYS	2.7
1	A	505	LYS	2.7
1	B	96	ALA	2.5
1	D	96	ALA	2.5
1	B	30	LEU	2.4
1	B	198	ILE	2.4
1	D	392	ILE	2.3
1	A	53	LEU	2.3
1	B	492	GLU	2.3
1	B	44	GLN	2.3
1	A	199	VAL	2.3
1	A	28	GLN	2.3
1	A	45	TYR	2.2
1	A	113	ALA	2.2
1	A	392	ILE	2.2
1	A	492	GLU	2.2
1	B	6	TYR	2.2
1	B	392	ILE	2.1
1	A	54	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	QDK	A	573	10/10	0.79	0.21	22,23,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.