Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:54 AM EDT

PDB ID	:	6QVI
Title	:	Crystal structure of competence-associated pilin ComZ from Thermus thermophilus
Authors	:	Karuppiah, V.; Derrick, J.P.
Deposited on	:	2019-03-01
Resolution	:	2.72 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

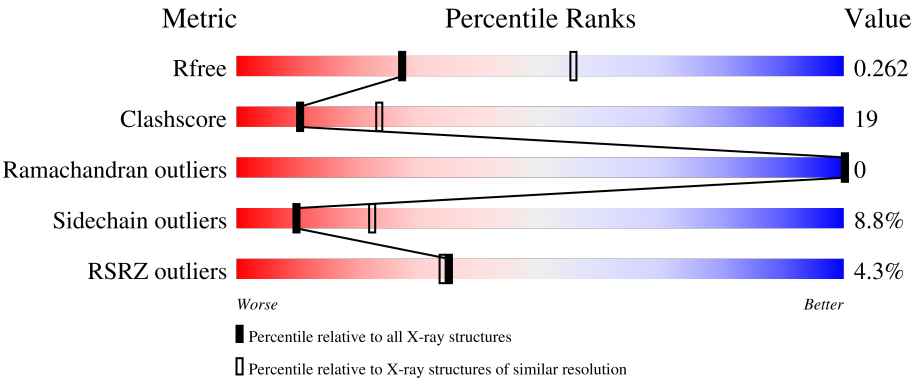
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	534	2% 70% 25%
1	B	534	7% 63% 26% 7%
1	C	534	4% 62% 30% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11520 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 ComZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3933	2457	699	763	14			
1	B	498	Total	C	N	O	S	0	0	0
			3761	2348	662	737	14			
1	C	507	Total	C	N	O	S	0	0	0
			3811	2390	664	743	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q72JC1
A	0	ALA	-	expression tag	UNP Q72JC1
A	525	LEU	-	expression tag	UNP Q72JC1
A	526	GLU	-	expression tag	UNP Q72JC1
A	527	HIS	-	expression tag	UNP Q72JC1
A	528	HIS	-	expression tag	UNP Q72JC1
A	529	HIS	-	expression tag	UNP Q72JC1
A	530	HIS	-	expression tag	UNP Q72JC1
A	531	HIS	-	expression tag	UNP Q72JC1
A	532	HIS	-	expression tag	UNP Q72JC1
B	-1	MET	-	initiating methionine	UNP Q72JC1
B	0	ALA	-	expression tag	UNP Q72JC1
B	525	LEU	-	expression tag	UNP Q72JC1
B	526	GLU	-	expression tag	UNP Q72JC1
B	527	HIS	-	expression tag	UNP Q72JC1
B	528	HIS	-	expression tag	UNP Q72JC1
B	529	HIS	-	expression tag	UNP Q72JC1
B	530	HIS	-	expression tag	UNP Q72JC1
B	531	HIS	-	expression tag	UNP Q72JC1
B	532	HIS	-	expression tag	UNP Q72JC1
C	-1	MET	-	initiating methionine	UNP Q72JC1
C	0	ALA	-	expression tag	UNP Q72JC1
C	525	LEU	-	expression tag	UNP Q72JC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	526	GLU	-	expression tag	UNP Q72JC1
C	527	HIS	-	expression tag	UNP Q72JC1
C	528	HIS	-	expression tag	UNP Q72JC1
C	529	HIS	-	expression tag	UNP Q72JC1
C	530	HIS	-	expression tag	UNP Q72JC1
C	531	HIS	-	expression tag	UNP Q72JC1
C	532	HIS	-	expression tag	UNP Q72JC1

- Molecule 2 is water.

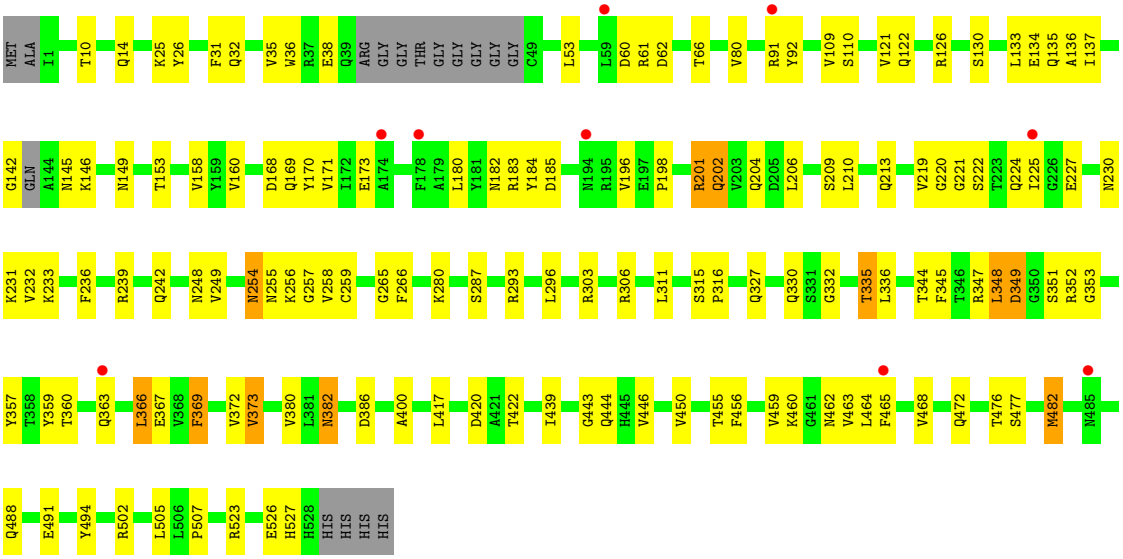
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	4	Total O 4 4	0	0
2	C	4	Total O 4 4	0	0

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.

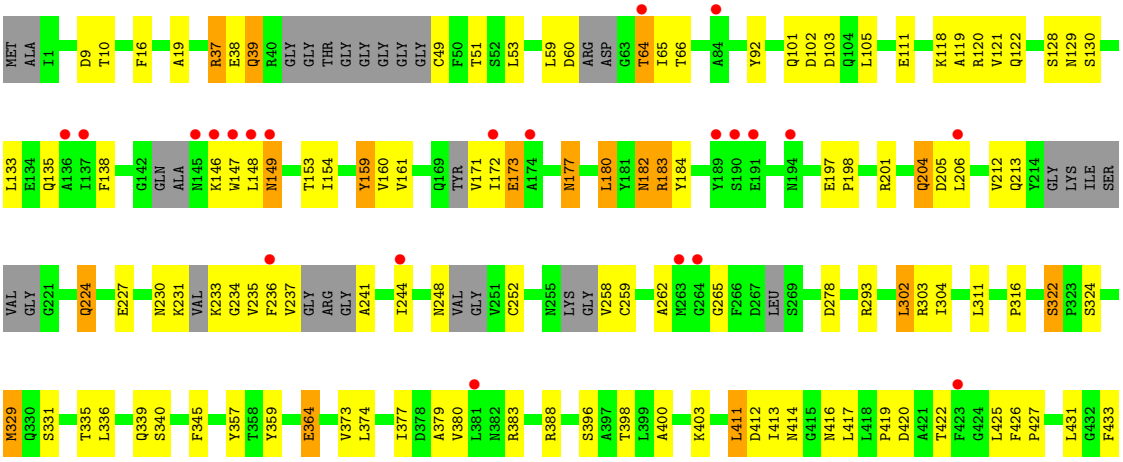
• Molecule 1: ComZ

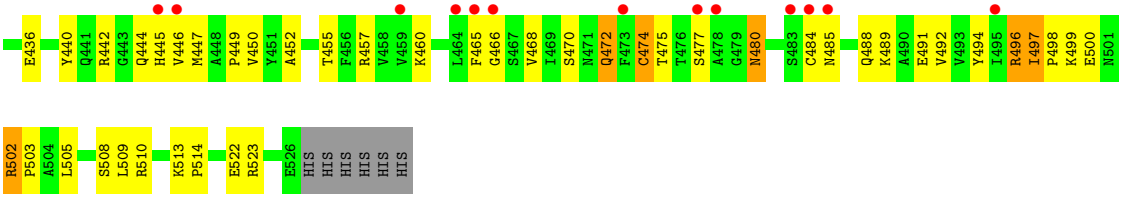
Chain A:



• Molecule 1: ComZ

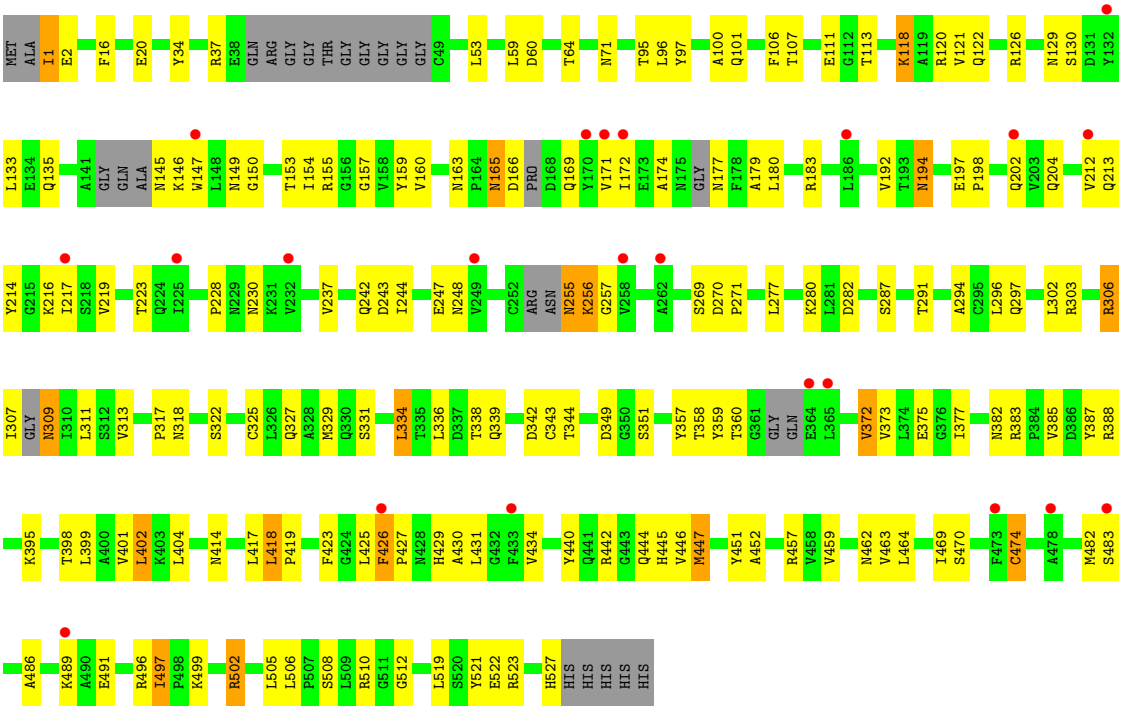
Chain B:





- Molecule 1: ComZ

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.86Å 121.86Å 212.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.79 – 2.72 58.79 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.79-2.72) 99.9 (58.79-2.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.267 0.211 , 0.262	Depositor DCC
R_{free} test set	2515 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11520	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

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	0.79	0/4006	0.81	0/5439
1	B	0.66	0/3821	0.77	0/5182
1	C	0.76	0/3877	0.81	0/5266
All	All	0.74	0/11704	0.80	0/15887

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	3933	0	3830	106	0
1	B	3761	0	3634	154	0
1	C	3811	0	3676	162	0
2	A	7	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
All	All	11520	0	11140	422	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 19.

All (422) 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:C:256:LYS:HG3	1:C:257:GLY:H	1.07	1.12
1:C:372:VAL:HG22	1:C:399:LEU:HD22	1.33	1.05
1:C:256:LYS:CG	1:C:257:GLY:H	1.73	1.01
1:B:496:ARG:HH11	1:B:496:ARG:HG2	1.24	1.01
1:B:153:THR:CG2	1:B:489:LYS:HD2	1.92	0.99
1:C:256:LYS:CG	1:C:257:GLY:N	2.23	0.96
1:C:414:ASN:HD21	1:C:442:ARG:HH11	1.09	0.96
1:B:497:ILE:HD12	1:B:497:ILE:H	1.31	0.95
1:B:455:THR:HG23	1:B:472:GLN:HB3	1.49	0.93
1:C:160:VAL:HG11	1:C:171:VAL:HG21	1.51	0.93
1:A:248:ASN:HB3	1:A:257:GLY:HA2	1.51	0.93
1:C:306:ARG:HG2	1:C:306:ARG:HH11	1.34	0.91
1:C:256:LYS:HG3	1:C:257:GLY:N	1.84	0.91
1:C:296:LEU:HD23	1:C:505:LEU:HD23	1.53	0.91
1:B:329:MET:HE2	1:B:377:ILE:HD13	1.56	0.87
1:B:182:ASN:O	1:B:182:ASN:ND2	2.07	0.87
1:A:373:VAL:HB	1:A:400:ALA:HB3	1.57	0.87
1:B:183:ARG:HG2	1:B:183:ARG:HH11	1.40	0.86
1:B:431:LEU:HD23	1:B:433:PHE:CE2	2.11	0.85
1:B:153:THR:HG23	1:B:489:LYS:HD2	1.55	0.85
1:C:497:ILE:HD12	1:C:497:ILE:H	1.40	0.85
1:C:446:VAL:CG2	1:C:464:LEU:HD13	2.06	0.84
1:A:335:THR:HB	1:A:380:VAL:HG22	1.60	0.82
1:A:347:ARG:HG3	1:A:347:ARG:HH11	1.43	0.82
1:B:227:GLU:O	1:B:230:ASN:O	1.97	0.81
1:B:414:ASN:HD21	1:B:442:ARG:HH11	1.29	0.81
1:C:113:THR:HG22	1:C:118:LYS:HG3	1.65	0.79
1:A:349:ASP:OD2	1:A:349:ASP:N	2.12	0.79
1:B:496:ARG:HG2	1:B:496:ARG:NH1	1.96	0.79
1:A:348:LEU:HD23	1:A:348:LEU:H	1.47	0.79
1:C:334:LEU:HD23	1:C:334:LEU:O	1.83	0.78
1:B:153:THR:HG23	1:B:489:LYS:CD	2.14	0.77
1:C:426:PHE:HE2	1:C:430:ALA:CB	1.97	0.77
1:B:153:THR:CG2	1:B:489:LYS:CD	2.63	0.76
1:A:336:LEU:HB3	1:A:357:TYR:CE2	2.20	0.76
1:C:372:VAL:HG22	1:C:399:LEU:CD2	2.13	0.75
1:C:256:LYS:HG2	1:C:257:GLY:N	2.02	0.75
1:C:342:ASP:OD1	1:C:344:THR:HG22	1.86	0.75
1:A:347:ARG:HG3	1:A:347:ARG:NH1	2.02	0.74
1:B:154:ILE:HG23	1:B:492:VAL:HG13	1.69	0.74
1:B:120:ARG:NH2	1:B:122:GLN:OE1	2.21	0.74
1:C:174:ALA:HB1	1:C:223:THR:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG12	1:A:248:ASN:HB2	1.69	0.73
1:B:224:GLN:O	1:B:224:GLN:HG2	1.88	0.73
1:B:416:ASN:HD21	1:B:444:GLN:H	1.36	0.73
1:C:414:ASN:ND2	1:C:442:ARG:HH11	1.84	0.72
1:C:446:VAL:HG23	1:C:464:LEU:HD13	1.71	0.72
1:C:256:LYS:HB3	1:C:256:LYS:HZ2	1.55	0.72
1:B:278:ASP:OD1	1:B:293:ARG:NH1	2.23	0.72
1:B:177:ASN:OD1	1:B:177:ASN:N	2.20	0.71
1:B:480:ASN:N	1:B:480:ASN:OD1	2.19	0.71
1:C:96:LEU:HD11	1:C:106:PHE:HB3	1.71	0.71
1:C:414:ASN:HD21	1:C:442:ARG:NH1	1.85	0.70
1:B:248:ASN:HB3	1:B:258:VAL:HG12	1.73	0.70
1:C:194:ASN:OD1	1:C:194:ASN:N	2.18	0.70
1:C:426:PHE:CE2	1:C:430:ALA:HB2	2.27	0.70
1:A:446:VAL:HG13	1:A:464:LEU:HD13	1.74	0.70
1:B:180:LEU:HD12	1:B:180:LEU:O	1.92	0.70
1:B:414:ASN:ND2	1:B:442:ARG:HH11	1.90	0.70
1:C:426:PHE:HE2	1:C:430:ALA:HB2	1.55	0.69
1:B:416:ASN:HD21	1:B:444:GLN:HB2	1.57	0.69
1:B:146:LYS:HZ2	1:B:173:GLU:HG3	1.58	0.69
1:C:497:ILE:HD12	1:C:497:ILE:N	2.08	0.69
1:B:65:ILE:N	1:B:65:ILE:HD12	2.07	0.69
1:B:180:LEU:HD12	1:B:180:LEU:C	2.13	0.69
1:A:231:LYS:HD2	1:A:259:CYS:HB3	1.74	0.69
1:B:447:MET:HG2	1:B:465:PHE:HB2	1.73	0.69
1:B:497:ILE:HD12	1:B:497:ILE:N	2.07	0.68
1:C:256:LYS:HB3	1:C:256:LYS:NZ	2.07	0.68
1:B:121:VAL:HG12	1:B:523:ARG:HG3	1.76	0.68
1:B:147:TRP:CE3	1:B:171:VAL:HG23	2.27	0.68
1:A:348:LEU:HD23	1:A:348:LEU:N	2.07	0.68
1:B:183:ARG:HB2	1:B:204:GLN:HA	1.75	0.68
1:C:197:GLU:HG3	1:C:198:PRO:HD2	1.74	0.68
1:B:359:TYR:HA	1:B:364:GLU:HG3	1.76	0.68
1:A:280:LYS:NZ	1:A:287:SER:O	2.27	0.67
1:B:452:ALA:HB3	1:B:470:SER:HB2	1.77	0.67
1:C:204:GLN:O	1:C:230:ASN:ND2	2.25	0.67
1:B:65:ILE:HD12	1:B:65:ILE:H	1.58	0.67
1:C:130:SER:OG	1:C:510:ARG:NH2	2.27	0.66
1:B:153:THR:OG1	1:B:491:GLU:HB2	1.95	0.66
1:B:183:ARG:HH11	1:B:183:ARG:CG	2.09	0.66
1:C:426:PHE:CE1	1:C:447:MET:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ARG:HH11	1:C:306:ARG:CG	2.09	0.65
1:A:198:PRO:HA	1:A:201:ARG:HE	1.61	0.65
1:B:234:GLY:HA2	1:B:262:ALA:O	1.97	0.65
1:A:38:GLU:OE2	1:A:130:SER:N	2.30	0.64
1:A:221:GLY:HA2	1:A:248:ASN:HD21	1.62	0.64
1:B:500:GLU:O	1:B:500:GLU:HG2	1.95	0.64
1:A:204:GLN:O	1:A:230:ASN:ND2	2.27	0.64
1:A:296:LEU:HD23	1:A:505:LEU:HD13	1.78	0.64
1:B:146:LYS:NZ	1:B:173:GLU:HG3	2.13	0.64
1:B:426:PHE:HB2	1:B:447:MET:HE1	1.80	0.63
1:A:366:LEU:HD12	1:A:366:LEU:C	2.16	0.63
1:C:372:VAL:CG2	1:C:399:LEU:HD22	2.20	0.63
1:B:398:THR:HG21	1:B:505:LEU:HB2	1.80	0.63
1:B:102:ASP:HB3	1:B:105:LEU:HG	1.81	0.63
1:B:322:SER:HG	1:B:324:SER:HG	1.45	0.63
1:B:339:GLN:HE21	1:B:340:SER:H	1.47	0.63
1:A:463:VAL:HG23	1:A:491:GLU:HG2	1.81	0.62
1:B:147:TRP:CD2	1:B:171:VAL:HG23	2.34	0.62
1:B:403:LYS:HD2	1:B:436:GLU:HG2	1.80	0.62
1:B:431:LEU:HD23	1:B:433:PHE:HE2	1.65	0.62
1:C:302:LEU:C	1:C:302:LEU:HD13	2.20	0.62
1:C:426:PHE:CD1	1:C:447:MET:CG	2.83	0.62
1:A:348:LEU:H	1:A:348:LEU:CD2	2.05	0.62
1:C:334:LEU:HD23	1:C:334:LEU:C	2.19	0.62
1:C:248:ASN:ND2	1:C:256:LYS:HD2	2.15	0.61
1:C:242:GLN:HG2	1:C:243:ASP:OD1	1.99	0.61
1:C:280:LYS:NZ	1:C:287:SER:O	2.34	0.61
1:A:160:VAL:HG11	1:A:171:VAL:CG1	2.30	0.60
1:C:146:LYS:HG3	1:C:149:ASN:HD21	1.65	0.60
1:C:457:ARG:NH1	1:C:482:MET:O	2.34	0.60
1:A:502:ARG:NH2	1:A:507:PRO:O	2.34	0.60
1:B:416:ASN:HD21	1:B:444:GLN:N	1.99	0.60
1:B:9:ASP:N	1:B:9:ASP:OD1	2.34	0.60
1:B:16:PHE:CE1	1:B:523:ARG:HG2	2.36	0.60
1:B:101:GLN:HG2	1:B:102:ASP:N	2.16	0.60
1:C:388:ARG:HB3	1:C:423:PHE:CD2	2.36	0.60
1:B:416:ASN:ND2	1:B:444:GLN:H	1.99	0.59
1:B:419:PRO:CD	1:B:447:MET:HE2	2.31	0.59
1:C:434:VAL:HG13	1:C:451:TYR:CD2	2.37	0.59
1:B:426:PHE:HB2	1:B:447:MET:CE	2.32	0.59
1:C:418:LEU:HD22	1:C:418:LEU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ALA:HB3	1:C:470:SER:HB2	1.83	0.59
1:C:329:MET:HB3	1:C:377:ILE:HD13	1.84	0.59
1:C:426:PHE:CD1	1:C:447:MET:HG3	2.37	0.59
1:A:335:THR:HB	1:A:380:VAL:CG2	2.31	0.59
1:A:36:TRP:HB2	1:A:61:ARG:NH2	2.17	0.59
1:B:431:LEU:CD2	1:B:433:PHE:CZ	2.86	0.59
1:C:388:ARG:NE	1:C:423:PHE:HD2	2.01	0.59
1:C:401:VAL:O	1:C:401:VAL:HG23	2.03	0.59
1:C:172:ILE:HG22	1:C:172:ILE:O	2.02	0.58
1:B:426:PHE:CG	1:B:447:MET:HE3	2.39	0.58
1:A:227:GLU:O	1:A:231:LYS:HB3	2.02	0.58
1:C:418:LEU:HB3	1:C:419:PRO:HD2	1.85	0.58
1:C:388:ARG:HE	1:C:423:PHE:HD2	1.51	0.57
1:B:146:LYS:NZ	1:B:173:GLU:CG	2.67	0.57
1:A:158:VAL:HG13	1:A:180:LEU:HD11	1.85	0.57
1:A:168:ASP:OD1	1:A:239:ARG:NH2	2.29	0.57
1:A:204:GLN:N	1:A:204:GLN:OE1	2.38	0.57
1:B:447:MET:CG	1:B:465:PHE:HB2	2.35	0.57
1:A:158:VAL:HG22	1:A:210:LEU:HD13	1.87	0.56
1:C:96:LEU:HD12	1:C:107:THR:O	2.05	0.56
1:C:150:GLY:HA2	1:C:486:ALA:HB3	1.87	0.56
1:C:338:THR:HG23	1:C:338:THR:O	2.04	0.56
1:C:497:ILE:HD13	1:C:502:ARG:NH1	2.19	0.56
1:B:133:LEU:CD1	1:B:159:TYR:CE1	2.89	0.56
1:C:327:GLN:OE1	1:C:327:GLN:HA	2.06	0.56
1:B:146:LYS:HZ1	1:B:173:GLU:CG	2.19	0.56
1:A:369:PHE:CD1	1:A:369:PHE:N	2.73	0.56
1:B:241:ALA:HA	1:B:244:ILE:HG22	1.87	0.56
1:B:153:THR:HG22	1:B:489:LYS:HD2	1.87	0.56
1:B:118:LYS:HG2	1:B:119:ALA:N	2.20	0.55
1:C:111:GLU:HG3	1:C:120:ARG:HG3	1.88	0.55
1:B:447:MET:HG3	1:B:465:PHE:HD1	1.72	0.55
1:B:60:ASP:HA	1:B:64:THR:HG23	1.87	0.55
1:B:302:LEU:HD21	1:B:304:ILE:HD13	1.89	0.55
1:B:419:PRO:HD3	1:B:447:MET:HE2	1.89	0.55
1:C:177:ASN:O	1:C:489:LYS:HE3	2.07	0.55
1:A:220:GLY:O	1:A:248:ASN:ND2	2.40	0.55
1:A:417:LEU:HB3	1:A:446:VAL:HG23	1.88	0.55
1:B:431:LEU:HD23	1:B:433:PHE:CZ	2.41	0.55
1:A:145:ASN:O	1:A:146:LYS:HD3	2.07	0.55
1:B:130:SER:HB3	1:B:510:ARG:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:CD1	1:B:159:TYR:HE1	2.19	0.55
1:B:414:ASN:HD21	1:B:442:ARG:NH1	2.03	0.55
1:C:34:TYR:HD2	1:C:129:ASN:HD21	1.53	0.55
1:C:155:ARG:NH1	1:C:183:ARG:O	2.37	0.55
1:B:417:LEU:O	1:B:446:VAL:HA	2.05	0.55
1:A:446:VAL:O	1:A:464:LEU:HD12	2.05	0.54
1:B:379:ALA:HB3	1:B:411:LEU:HD12	1.89	0.54
1:C:171:VAL:O	1:C:171:VAL:HG22	2.06	0.54
1:C:217:ILE:HG13	1:C:217:ILE:O	2.07	0.54
1:C:60:ASP:OD1	1:C:60:ASP:N	2.41	0.54
1:C:126:ARG:HB2	1:C:519:LEU:HD11	1.88	0.54
1:B:38:GLU:HG2	1:B:129:ASN:OD1	2.07	0.54
1:C:248:ASN:HD21	1:C:256:LYS:HD2	1.73	0.54
1:B:241:ALA:HA	1:B:244:ILE:CG2	2.37	0.54
1:C:375:GLU:HG2	1:C:402:LEU:HD12	1.90	0.54
1:A:32:GLN:HG2	1:A:61:ARG:NH2	2.23	0.54
1:C:329:MET:HB3	1:C:377:ILE:CD1	2.37	0.54
1:B:235:VAL:HG23	1:B:235:VAL:O	2.07	0.54
1:B:450:VAL:CG2	1:B:468:VAL:HG23	2.38	0.54
1:B:502:ARG:HG3	1:B:503:PRO:HD2	1.89	0.54
1:A:142:GLY:HA2	1:A:472:GLN:HG3	1.89	0.54
1:C:216:LYS:HE3	1:C:243:ASP:HA	1.90	0.54
1:C:247:GLU:OE2	1:C:247:GLU:N	2.32	0.54
1:C:183:ARG:CB	1:C:204:GLN:HA	2.37	0.54
1:C:291:THR:HG23	1:C:294:ALA:H	1.72	0.54
1:B:427:PRO:HG2	1:B:498:PRO:HD3	1.90	0.53
1:A:249:VAL:HA	1:A:258:VAL:HG22	1.89	0.53
1:C:219:VAL:HG13	1:C:219:VAL:O	2.09	0.53
1:C:306:ARG:HG2	1:C:306:ARG:NH1	2.13	0.53
1:B:160:VAL:HB	1:B:212:VAL:HG22	1.90	0.53
1:A:306:ARG:CZ	1:A:332:GLY:CA	2.87	0.53
1:A:184:TYR:CD1	1:A:206:LEU:HD21	2.44	0.53
1:C:395:LYS:HB3	1:C:429:HIS:HD2	1.74	0.53
1:A:444:GLN:HA	1:A:462:ASN:ND2	2.23	0.52
1:B:227:GLU:N	1:B:230:ASN:O	2.42	0.52
1:C:313:VAL:HG12	1:C:313:VAL:O	2.09	0.52
1:B:183:ARG:CG	1:B:183:ARG:NH1	2.72	0.52
1:B:39:GLN:O	1:B:39:GLN:HG2	2.10	0.52
1:A:347:ARG:HH11	1:A:347:ARG:CG	2.18	0.52
1:B:146:LYS:HZ1	1:B:173:GLU:H	1.56	0.52
1:C:446:VAL:HG22	1:C:464:LEU:HD13	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:THR:HG21	1:C:97:TYR:CE2	2.46	0.51
1:C:372:VAL:CG2	1:C:399:LEU:CD2	2.84	0.51
1:B:171:VAL:HG13	1:B:172:ILE:HD12	1.93	0.51
1:B:431:LEU:HD21	1:B:433:PHE:CZ	2.45	0.51
1:A:306:ARG:NH2	1:A:332:GLY:HA3	2.25	0.51
1:C:135:GLN:HB2	1:C:157:GLY:O	2.10	0.51
1:C:163:ASN:HB3	1:C:166:ASP:HB3	1.92	0.51
1:A:225:ILE:HD12	1:A:258:VAL:HG12	1.93	0.51
1:B:153:THR:HG22	1:B:489:LYS:CD	2.39	0.51
1:B:161:VAL:HG13	1:B:213:GLN:HE21	1.76	0.51
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.11	0.51
1:C:213:GLN:HG2	1:C:214:TYR:CD1	2.46	0.51
1:A:306:ARG:CZ	1:A:332:GLY:HA3	2.41	0.51
1:B:431:LEU:CD2	1:B:433:PHE:CE2	2.87	0.51
1:C:447:MET:O	1:C:447:MET:HG2	2.10	0.51
1:C:418:LEU:HD12	1:C:447:MET:HE3	1.91	0.51
1:C:446:VAL:HG23	1:C:464:LEU:CD1	2.39	0.51
1:A:316:PRO:HG3	1:A:345:PHE:CD1	2.46	0.50
1:B:135:GLN:NE2	1:B:138:PHE:HD2	2.10	0.50
1:B:236:PHE:HB3	1:B:265:GLY:O	2.11	0.50
1:B:447:MET:HG3	1:B:465:PHE:CD1	2.46	0.50
1:C:336:LEU:HD22	1:C:357:TYR:CD2	2.47	0.50
1:C:417:LEU:HB3	1:C:446:VAL:HG12	1.93	0.50
1:A:460:LYS:HG3	1:A:476:THR:O	2.12	0.50
1:C:192:VAL:HG12	1:C:192:VAL:O	2.09	0.50
1:B:413:ILE:HG21	1:B:446:VAL:HG11	1.93	0.50
1:A:303:ARG:HB3	1:A:315:SER:HB2	1.93	0.50
1:A:439:ILE:HD12	1:A:450:VAL:HG13	1.94	0.50
1:B:416:ASN:ND2	1:B:445:HIS:H	2.10	0.50
1:A:10:THR:O	1:A:14:GLN:HG3	2.12	0.50
1:A:185:ASP:OD1	1:A:202:GLN:HB3	2.12	0.50
1:B:316:PRO:HG3	1:B:345:PHE:CG	2.46	0.49
1:C:145:ASN:C	1:C:146:LYS:HD3	2.32	0.49
1:A:60:ASP:OD1	1:A:62:ASP:HB3	2.13	0.49
1:B:184:TYR:CD1	1:B:184:TYR:C	2.85	0.49
1:B:509:LEU:HD12	1:B:509:LEU:H	1.77	0.49
1:A:196:VAL:HG23	1:A:201:ARG:HD3	1.94	0.49
1:C:153:THR:HG22	1:C:489:LYS:NZ	2.27	0.49
1:A:184:TYR:CE1	1:A:206:LEU:HD21	2.47	0.49
1:C:306:ARG:CG	1:C:306:ARG:NH1	2.72	0.49
1:A:463:VAL:HG13	1:A:465:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HG23	1:B:468:VAL:HG23	1.94	0.49
1:C:165:ASN:OD1	1:C:165:ASN:N	2.46	0.49
1:B:227:GLU:O	1:B:231:LYS:HB3	2.13	0.48
1:A:160:VAL:HG11	1:A:171:VAL:HG11	1.95	0.48
1:A:456:PHE:CD2	1:A:456:PHE:C	2.85	0.48
1:C:497:ILE:N	1:C:497:ILE:CD1	2.73	0.48
1:A:158:VAL:HG13	1:A:180:LEU:CD1	2.43	0.48
1:B:388:ARG:NH1	1:B:420:ASP:OD2	2.46	0.48
1:C:359:TYR:CD2	1:C:359:TYR:C	2.86	0.48
1:B:198:PRO:HA	1:B:201:ARG:HG3	1.95	0.48
1:C:1:ILE:HD12	1:C:2:GLU:H	1.78	0.48
1:A:359:TYR:CD1	1:A:360:THR:N	2.82	0.48
1:C:426:PHE:CD2	1:C:427:PRO:HA	2.49	0.48
1:A:169:GLN:O	1:A:171:VAL:HG23	2.13	0.48
1:C:130:SER:HA	1:C:512:GLY:O	2.13	0.48
1:C:426:PHE:CD1	1:C:447:MET:SD	3.07	0.48
1:B:133:LEU:HD11	1:B:159:TYR:HE1	1.78	0.48
1:C:213:GLN:HG2	1:C:214:TYR:CE1	2.49	0.48
1:B:416:ASN:ND2	1:B:444:GLN:N	2.61	0.47
1:B:426:PHE:CD1	1:B:427:PRO:HA	2.49	0.47
1:B:460:LYS:HD2	1:B:488:GLN:HB3	1.95	0.47
1:C:237:VAL:CG2	1:C:244:ILE:HG13	2.44	0.47
1:A:198:PRO:CA	1:A:201:ARG:HE	2.26	0.47
1:B:135:GLN:HE22	1:B:138:PHE:HD2	1.61	0.47
1:B:304:ILE:HD12	1:B:304:ILE:N	2.29	0.47
1:B:237:VAL:HG12	1:B:237:VAL:O	2.14	0.47
1:C:34:TYR:CD2	1:C:129:ASN:ND2	2.82	0.47
1:A:444:GLN:HA	1:A:462:ASN:HD22	1.80	0.47
1:B:359:TYR:HE2	1:B:383:ARG:HD3	1.80	0.47
1:C:37:ARG:CB	1:C:129:ASN:OD1	2.62	0.47
1:C:383:ARG:CZ	1:C:383:ARG:HB3	2.45	0.47
1:A:236:PHE:HB3	1:A:265:GLY:O	2.15	0.47
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.28	0.47
1:B:303:ARG:C	1:B:304:ILE:HD12	2.35	0.47
1:B:336:LEU:HB3	1:B:357:TYR:CE2	2.50	0.47
1:C:219:VAL:HG13	1:C:248:ASN:HB2	1.97	0.47
1:A:170:TYR:HB3	1:A:173:GLU:HG2	1.96	0.47
1:C:153:THR:HG22	1:C:489:LYS:HZ3	1.78	0.47
1:C:228:PRO:HG2	1:C:255:ASN:HD21	1.80	0.46
1:B:502:ARG:HG3	1:B:503:PRO:CD	2.46	0.46
1:C:64:THR:O	1:C:64:THR:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLN:HB3	1:C:303:ARG:CZ	2.45	0.46
1:B:234:GLY:HA3	1:B:236:PHE:CZ	2.51	0.46
1:B:329:MET:HE1	1:B:374:LEU:HD13	1.97	0.46
1:A:254:ASN:O	1:A:255:ASN:HB3	2.15	0.46
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.47	0.46
1:C:434:VAL:HG13	1:C:451:TYR:HD2	1.79	0.46
1:A:209:SER:HA	1:A:232:VAL:HG22	1.97	0.46
1:B:153:THR:OG1	1:B:153:THR:O	2.27	0.46
1:C:146:LYS:HD3	1:C:146:LYS:N	2.30	0.46
1:C:121:VAL:HG12	1:C:523:ARG:HB3	1.98	0.46
1:B:133:LEU:HD13	1:B:159:TYR:CD1	2.51	0.45
1:A:142:GLY:HA2	1:A:472:GLN:CG	2.47	0.45
1:C:121:VAL:HG12	1:C:523:ARG:CB	2.47	0.45
1:A:31:PHE:O	1:A:35:VAL:HG13	2.16	0.45
1:A:455:THR:HG22	1:A:472:GLN:HB2	1.98	0.45
1:C:53:LEU:HD12	1:C:53:LEU:HA	1.63	0.45
1:A:443:GLY:C	1:A:462:ASN:HD22	2.20	0.45
1:B:184:TYR:CD1	1:B:184:TYR:O	2.70	0.45
1:B:339:GLN:HE21	1:B:340:SER:N	2.13	0.45
1:A:233:LYS:HE3	1:A:233:LYS:HB3	1.59	0.45
1:A:446:VAL:HG13	1:A:464:LEU:CD1	2.44	0.45
1:C:426:PHE:HE2	1:C:430:ALA:HB1	1.81	0.45
1:B:302:LEU:CD2	1:B:304:ILE:HD13	2.46	0.45
1:B:420:ASP:OD1	1:B:422:THR:HG22	2.17	0.45
1:B:502:ARG:HA	1:B:503:PRO:HD3	1.78	0.45
1:C:508:SER:O	1:C:508:SER:OG	2.33	0.45
1:B:431:LEU:O	1:B:449:PRO:HD2	2.17	0.45
1:B:457:ARG:HG2	1:B:474:CYS:SG	2.57	0.45
1:C:302:LEU:C	1:C:302:LEU:CD1	2.85	0.45
1:A:136:ALA:HB2	1:A:494:TYR:HB2	1.99	0.45
1:C:357:TYR:O	1:C:357:TYR:CG	2.69	0.45
1:C:463:VAL:HA	1:C:491:GLU:O	2.17	0.45
1:B:133:LEU:HD13	1:B:159:TYR:CE1	2.51	0.44
1:B:231:LYS:HB2	1:B:259:CYS:HB3	1.99	0.44
1:C:248:ASN:CG	1:C:256:LYS:HD2	2.37	0.44
1:A:92:TYR:CD1	1:A:92:TYR:C	2.91	0.44
1:B:466:GLY:O	1:B:494:TYR:HA	2.17	0.44
1:C:329:MET:HG2	1:C:377:ILE:HD13	2.00	0.44
1:A:36:TRP:HB2	1:A:61:ARG:HH21	1.82	0.44
1:A:456:PHE:CD2	1:A:456:PHE:O	2.70	0.44
1:C:497:ILE:HD13	1:C:502:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:HG12	1:A:523:ARG:CB	2.48	0.44
1:B:303:ARG:HA	1:B:373:VAL:O	2.18	0.44
1:B:505:LEU:N	1:B:505:LEU:HD22	2.33	0.44
1:C:426:PHE:HA	1:C:427:PRO:HA	1.73	0.44
1:A:146:LYS:HB3	1:A:149:ASN:HD21	1.83	0.44
1:A:316:PRO:HG3	1:A:345:PHE:CG	2.52	0.44
1:B:153:THR:HG23	1:B:489:LYS:HD3	1.99	0.44
1:B:329:MET:HE3	1:B:329:MET:HB3	1.64	0.44
1:C:317:PRO:C	1:C:318:ASN:HD22	2.20	0.44
1:A:460:LYS:CE	1:A:488:GLN:HB2	2.47	0.44
1:A:482:MET:HE3	1:A:482:MET:HB3	1.69	0.44
1:A:53:LEU:HA	1:A:53:LEU:HD12	1.74	0.44
1:C:237:VAL:HG22	1:C:244:ILE:HG13	1.99	0.44
1:A:196:VAL:CG2	1:A:201:ARG:HD3	2.48	0.44
1:A:222:SER:H	1:A:256:LYS:HG3	1.83	0.43
1:B:497:ILE:H	1:B:497:ILE:CD1	2.12	0.43
1:C:444:GLN:C	1:C:445:HIS:HD2	2.21	0.43
1:A:182:ASN:O	1:A:182:ASN:ND2	2.51	0.43
1:B:146:LYS:HZ1	1:B:173:GLU:HG2	1.83	0.43
1:B:233:LYS:O	1:B:233:LYS:HG2	2.18	0.43
1:C:387:TYR:CD1	1:C:387:TYR:C	2.91	0.43
1:C:440:TYR:CE2	1:C:442:ARG:HG2	2.54	0.43
1:A:231:LYS:CD	1:A:259:CYS:HB3	2.44	0.43
1:B:197:GLU:HG2	1:B:425:LEU:HB2	2.00	0.43
1:B:335:THR:HA	1:B:380:VAL:HG22	2.01	0.43
1:C:212:VAL:HB	1:C:237:VAL:HB	2.01	0.43
1:A:201:ARG:HB2	1:A:202:GLN:OE1	2.18	0.43
1:A:344:THR:HA	1:A:353:GLY:O	2.18	0.43
1:B:122:GLN:HG2	1:B:522:GLU:HG2	2.00	0.43
1:C:71:ASN:OD1	1:C:100:ALA:HB2	2.18	0.43
1:C:277:LEU:O	1:C:291:THR:OG1	2.36	0.43
1:A:366:LEU:HD12	1:A:367:GLU:N	2.34	0.43
1:A:459:VAL:HG23	1:A:462:ASN:OD1	2.19	0.43
1:C:147:TRP:HB2	1:C:171:VAL:HG23	2.01	0.43
1:C:248:ASN:OD1	1:C:256:LYS:HD2	2.19	0.43
1:A:231:LYS:HD2	1:A:259:CYS:C	2.40	0.43
1:A:137:ILE:HG12	1:A:468:VAL:HG22	2.00	0.43
1:A:224:GLN:NE2	1:A:227:GLU:HG2	2.34	0.43
1:C:133:LEU:N	1:C:133:LEU:HD23	2.32	0.42
1:A:134:GLU:HB3	1:A:494:TYR:CE1	2.54	0.42
1:B:103:ASP:OD1	1:B:103:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ASN:OD1	1:C:309:ASN:N	2.51	0.42
1:B:182:ASN:HD21	1:B:206:LEU:H	1.68	0.42
1:C:154:ILE:O	1:C:180:LEU:HA	2.20	0.42
1:C:339:GLN:O	1:C:339:GLN:HG3	2.18	0.42
1:C:146:LYS:CG	1:C:149:ASN:HD21	2.32	0.42
1:C:306:ARG:HD2	1:C:311:LEU:HD11	2.02	0.42
1:A:306:ARG:O	1:A:306:ARG:HG2	2.20	0.42
1:A:460:LYS:HE3	1:A:477:SER:HA	2.01	0.42
1:C:349:ASP:OD1	1:C:351:SER:HB3	2.19	0.42
1:A:526:GLU:O	1:A:527:HIS:ND1	2.53	0.41
1:C:297:GLN:HA	1:C:303:ARG:HD2	2.02	0.41
1:C:440:TYR:CD1	1:C:457:ARG:HG3	2.55	0.41
1:A:133:LEU:HB3	1:A:135:GLN:OE1	2.20	0.41
1:B:19:ALA:HB1	1:B:121:VAL:HG22	2.02	0.41
1:B:180:LEU:C	1:B:180:LEU:CD1	2.85	0.41
1:C:296:LEU:CD2	1:C:505:LEU:HD23	2.35	0.41
1:B:474:CYS:HB2	1:B:484:CYS:HB3	1.93	0.41
1:C:447:MET:HE2	1:C:447:MET:HB2	1.71	0.41
1:A:25:LYS:HD3	1:A:26:TYR:CE1	2.55	0.41
1:B:92:TYR:HA	1:B:111:GLU:O	2.21	0.41
1:B:128:SER:O	1:B:514:PRO:HA	2.21	0.41
1:B:380:VAL:HG12	1:B:412:ASP:HB2	2.02	0.41
1:A:382:ASN:O	1:A:382:ASN:ND2	2.47	0.41
1:B:153:THR:HG1	1:B:491:GLU:HB2	1.83	0.41
1:C:20:GLU:OE1	1:C:521:TYR:OH	2.32	0.41
1:A:213:GLN:HA	1:A:266:PHE:CD1	2.56	0.41
1:B:373:VAL:HG22	1:B:400:ALA:HB3	2.03	0.41
1:C:179:ALA:HB3	1:C:489:LYS:HZ3	1.85	0.41
1:C:325:CYS:HB2	1:C:343:CYS:HA	2.03	0.41
1:C:459:VAL:HG22	1:C:462:ASN:ND2	2.36	0.41
1:C:499:LYS:HA	1:C:499:LYS:HD2	1.74	0.41
1:A:360:THR:HG21	1:A:363:GLN:O	2.21	0.41
1:B:135:GLN:HE21	1:B:159:TYR:HD1	1.68	0.41
1:B:148:LEU:HD22	1:B:149:ASN:H	1.86	0.41
1:C:1:ILE:HD12	1:C:1:ILE:HA	1.75	0.41
1:C:150:GLY:CA	1:C:486:ALA:HB3	2.50	0.41
1:C:197:GLU:HG3	1:C:198:PRO:CD	2.47	0.41
1:C:497:ILE:H	1:C:497:ILE:CD1	2.22	0.41
1:B:59:LEU:H	1:B:59:LEU:HD12	1.86	0.40
1:C:111:GLU:CG	1:C:120:ARG:HG3	2.51	0.40
1:C:271:PRO:O	1:C:271:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:VAL:O	1:C:192:VAL:CG1	2.70	0.40
1:C:457:ARG:HA	1:C:474:CYS:O	2.21	0.40
1:A:109:VAL:HG22	1:A:122:GLN:HB2	2.03	0.40
1:C:451:TYR:HA	1:C:469:ILE:O	2.20	0.40
1:A:158:VAL:O	1:A:158:VAL:CG2	2.70	0.40
1:A:327:GLN:OE1	1:A:330:GLN:NE2	2.55	0.40
1:B:39:GLN:O	1:B:39:GLN:CG	2.70	0.40
1:C:122:GLN:HG2	1:C:522:GLU:HG2	2.03	0.40
1:C:219:VAL:O	1:C:219:VAL:CG1	2.69	0.40
1:C:360:THR:O	1:C:360:THR:CG2	2.69	0.40
1:C:426:PHE:CE2	1:C:430:ALA:CB	2.86	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	512/534 (96%)	478 (93%)	34 (7%)	0	100	100
1	B	476/534 (89%)	441 (93%)	35 (7%)	0	100	100
1	C	491/534 (92%)	460 (94%)	31 (6%)	0	100	100
All	All	1479/1602 (92%)	1379 (93%)	100 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	415/424 (98%)	388 (94%)	27 (6%)	17 37
1	B	396/424 (93%)	357 (90%)	39 (10%)	8 18
1	C	399/424 (94%)	358 (90%)	41 (10%)	7 16
All	All	1210/1272 (95%)	1103 (91%)	107 (9%)	10 22

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	80	VAL
1	A	91	ARG
1	A	110	SER
1	A	126	ARG
1	A	153	THR
1	A	183	ARG
1	A	201	ARG
1	A	202	GLN
1	A	242	GLN
1	A	254	ASN
1	A	293	ARG
1	A	311	LEU
1	A	335	THR
1	A	348	LEU
1	A	349	ASP
1	A	351	SER
1	A	352	ARG
1	A	366	LEU
1	A	369	PHE
1	A	372	VAL
1	A	373	VAL
1	A	382	ASN
1	A	386	ASP
1	A	420	ASP
1	A	422	THR
1	A	482	MET
1	B	10	THR
1	B	37	ARG
1	B	39	GLN
1	B	49	CYS
1	B	51	THR

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Mol	Chain	Res	Type
1	B	64	THR
1	B	66	THR
1	B	149	ASN
1	B	159	TYR
1	B	173	GLU
1	B	177	ASN
1	B	180	LEU
1	B	182	ASN
1	B	183	ARG
1	B	204	GLN
1	B	205	ASP
1	B	224	GLN
1	B	252	CYS
1	B	302	LEU
1	B	311	LEU
1	B	322	SER
1	B	329	MET
1	B	331	SER
1	B	364	GLU
1	B	396	SER
1	B	411	LEU
1	B	440	TYR
1	B	472	GLN
1	B	474	CYS
1	B	475	THR
1	B	477	SER
1	B	480	ASN
1	B	485	ASN
1	B	496	ARG
1	B	497	ILE
1	B	499	LYS
1	B	502	ARG
1	B	508	SER
1	B	513	LYS
1	C	1	ILE
1	C	16	PHE
1	C	59	LEU
1	C	101	GLN
1	C	118	LYS
1	C	159	TYR
1	C	165	ASN
1	C	169	GLN

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	202	GLN
1	C	255	ASN
1	C	256	LYS
1	C	269	SER
1	C	270	ASP
1	C	282	ASP
1	C	306	ARG
1	C	307	ILE
1	C	309	ASN
1	C	322	SER
1	C	331	SER
1	C	334	LEU
1	C	358	THR
1	C	372	VAL
1	C	373	VAL
1	C	382	ASN
1	C	385	VAL
1	C	398	THR
1	C	402	LEU
1	C	404	LEU
1	C	418	LEU
1	C	425	LEU
1	C	426	PHE
1	C	431	LEU
1	C	447	MET
1	C	474	CYS
1	C	483	SER
1	C	496	ARG
1	C	497	ILE
1	C	502	ARG
1	C	506	LEU
1	C	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	248	ASN
1	A	444	GLN
1	B	70	ASN
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	175	ASN
1	B	339	GLN
1	B	414	ASN
1	B	416	ASN
1	B	445	HIS
1	B	471	ASN
1	B	488	GLN
1	C	129	ASN
1	C	255	ASN
1	C	318	ASN
1	C	390	GLN
1	C	414	ASN
1	C	416	ASN
1	C	445	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	518/534 (97%)	0.25	9 (1%)	70	72	45, 82, 133, 186	0
1	B	498/534 (93%)	0.45	35 (7%)	16	15	53, 95, 163, 197	0
1	C	507/534 (94%)	0.27	22 (4%)	35	34	67, 102, 145, 177	0
All	All	1523/1602 (95%)	0.32	66 (4%)	35	34	45, 94, 148, 197	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	VAL	5.0
1	C	217	ILE	4.9
1	B	465	PHE	4.9
1	B	206	LEU	4.9
1	B	473	PHE	4.8
1	B	145	ASN	4.5
1	B	147	TRP	4.4
1	B	172	ILE	4.2
1	B	466	GLY	4.2
1	B	484	CYS	4.2
1	C	172	ILE	4.0
1	A	178	PHE	4.0
1	C	364	GLU	3.9
1	B	191	GLU	3.8
1	C	147	TRP	3.6
1	B	137	ILE	3.3
1	B	445	HIS	3.3
1	C	225	ILE	3.3
1	B	190	SER	3.3
1	B	495	ILE	3.1
1	B	423	PHE	3.1
1	A	363	GLN	3.0
1	C	202	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	ILE	3.0
1	A	465	PHE	2.9
1	B	148	LEU	2.9
1	B	483	SER	2.9
1	B	464	LEU	2.9
1	C	489	LYS	2.8
1	C	212	VAL	2.8
1	C	473	PHE	2.7
1	B	446	VAL	2.7
1	B	264	GLY	2.7
1	B	189	TYR	2.6
1	C	478	ALA	2.5
1	C	433	PHE	2.5
1	A	225	ILE	2.5
1	B	477	SER	2.4
1	C	426	PHE	2.4
1	A	174	ALA	2.4
1	C	365	LEU	2.4
1	B	194	ASN	2.4
1	B	381	LEU	2.4
1	A	194	ASN	2.3
1	B	149	ASN	2.3
1	B	459	VAL	2.2
1	C	186	LEU	2.2
1	B	146	LYS	2.2
1	C	170	TYR	2.2
1	A	485	ASN	2.2
1	B	84	ALA	2.2
1	B	174	ALA	2.2
1	C	232	VAL	2.2
1	C	132	TYR	2.1
1	A	91	ARG	2.1
1	B	485	ASN	2.1
1	B	64	THR	2.1
1	C	483	SER	2.1
1	B	136	ALA	2.1
1	B	263	MET	2.1
1	C	249	VAL	2.0
1	C	258	VAL	2.0
1	B	478	ALA	2.0
1	C	262	ALA	2.0
1	B	236	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	59	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.