Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:16 PM EDT

PDB ID	:	3R2W
Title	:	Crystal Structure of UDP-glucose Pyrophosphorylase of Homo Sapiens
Authors	:	Zheng, X.; Yu, Q.
Deposited on	:	2011-03-14
Resolution	:	3.60 Å(reported)

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

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

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

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

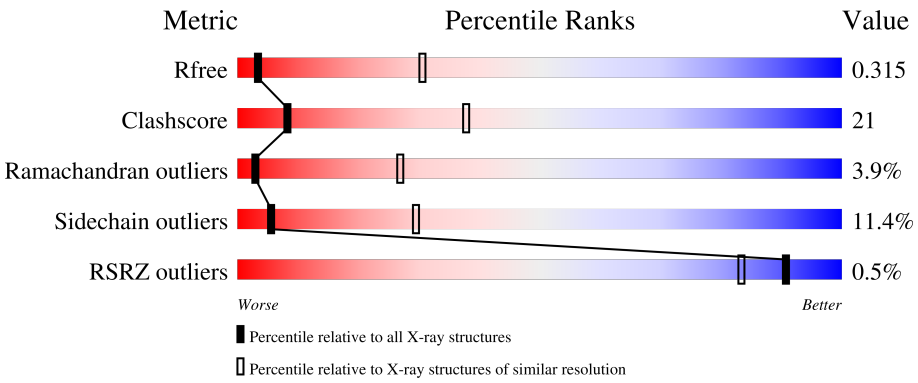
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	528	51% 32% 5% • 12%
1	B	528	47% 34% 6% • 12%
1	C	528	% 55% 26% • 15%
1	D	528	46% 36% 6% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13938 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3539	2253	604	672	10	0	0	0
1	B	467	3534	2251	605	667	11	0	0	0
1	C	450	3299	2088	557	646	8	0	0	0
1	D	468	3566	2275	608	672	11	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	expression tag	UNP Q16851
A	-29	GLY	-	expression tag	UNP Q16851
A	-28	SER	-	expression tag	UNP Q16851
A	-27	SER	-	expression tag	UNP Q16851
A	-26	HIS	-	expression tag	UNP Q16851
A	-25	HIS	-	expression tag	UNP Q16851
A	-24	HIS	-	expression tag	UNP Q16851
A	-23	HIS	-	expression tag	UNP Q16851
A	-22	HIS	-	expression tag	UNP Q16851
A	-21	HIS	-	expression tag	UNP Q16851
A	-20	SER	-	expression tag	UNP Q16851
A	-19	SER	-	expression tag	UNP Q16851
A	-18	GLY	-	expression tag	UNP Q16851
A	-17	LEU	-	expression tag	UNP Q16851
A	-16	VAL	-	expression tag	UNP Q16851
A	-15	PRO	-	expression tag	UNP Q16851
A	-14	ARG	-	expression tag	UNP Q16851
A	-13	GLY	-	expression tag	UNP Q16851
A	-12	SER	-	expression tag	UNP Q16851
A	-11	HIS	-	expression tag	UNP Q16851
B	-30	MET	-	expression tag	UNP Q16851

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	GLY	-	expression tag	UNP Q16851
B	-28	SER	-	expression tag	UNP Q16851
B	-27	SER	-	expression tag	UNP Q16851
B	-26	HIS	-	expression tag	UNP Q16851
B	-25	HIS	-	expression tag	UNP Q16851
B	-24	HIS	-	expression tag	UNP Q16851
B	-23	HIS	-	expression tag	UNP Q16851
B	-22	HIS	-	expression tag	UNP Q16851
B	-21	HIS	-	expression tag	UNP Q16851
B	-20	SER	-	expression tag	UNP Q16851
B	-19	SER	-	expression tag	UNP Q16851
B	-18	GLY	-	expression tag	UNP Q16851
B	-17	LEU	-	expression tag	UNP Q16851
B	-16	VAL	-	expression tag	UNP Q16851
B	-15	PRO	-	expression tag	UNP Q16851
B	-14	ARG	-	expression tag	UNP Q16851
B	-13	GLY	-	expression tag	UNP Q16851
B	-12	SER	-	expression tag	UNP Q16851
B	-11	HIS	-	expression tag	UNP Q16851
C	-30	MET	-	expression tag	UNP Q16851
C	-29	GLY	-	expression tag	UNP Q16851
C	-28	SER	-	expression tag	UNP Q16851
C	-27	SER	-	expression tag	UNP Q16851
C	-26	HIS	-	expression tag	UNP Q16851
C	-25	HIS	-	expression tag	UNP Q16851
C	-24	HIS	-	expression tag	UNP Q16851
C	-23	HIS	-	expression tag	UNP Q16851
C	-22	HIS	-	expression tag	UNP Q16851
C	-21	HIS	-	expression tag	UNP Q16851
C	-20	SER	-	expression tag	UNP Q16851
C	-19	SER	-	expression tag	UNP Q16851
C	-18	GLY	-	expression tag	UNP Q16851
C	-17	LEU	-	expression tag	UNP Q16851
C	-16	VAL	-	expression tag	UNP Q16851
C	-15	PRO	-	expression tag	UNP Q16851
C	-14	ARG	-	expression tag	UNP Q16851
C	-13	GLY	-	expression tag	UNP Q16851
C	-12	SER	-	expression tag	UNP Q16851
C	-11	HIS	-	expression tag	UNP Q16851
D	-30	MET	-	expression tag	UNP Q16851
D	-29	GLY	-	expression tag	UNP Q16851
D	-28	SER	-	expression tag	UNP Q16851

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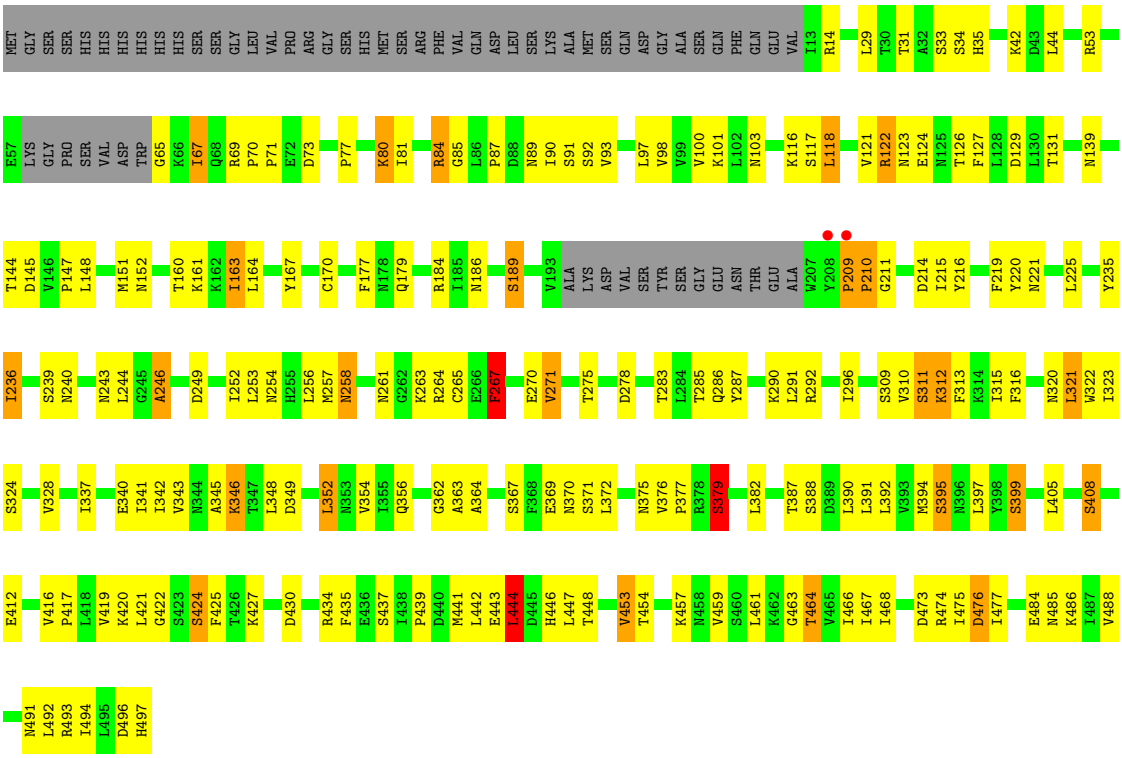
Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	SER	-	expression tag	UNP Q16851
D	-26	HIS	-	expression tag	UNP Q16851
D	-25	HIS	-	expression tag	UNP Q16851
D	-24	HIS	-	expression tag	UNP Q16851
D	-23	HIS	-	expression tag	UNP Q16851
D	-22	HIS	-	expression tag	UNP Q16851
D	-21	HIS	-	expression tag	UNP Q16851
D	-20	SER	-	expression tag	UNP Q16851
D	-19	SER	-	expression tag	UNP Q16851
D	-18	GLY	-	expression tag	UNP Q16851
D	-17	LEU	-	expression tag	UNP Q16851
D	-16	VAL	-	expression tag	UNP Q16851
D	-15	PRO	-	expression tag	UNP Q16851
D	-14	ARG	-	expression tag	UNP Q16851
D	-13	GLY	-	expression tag	UNP Q16851
D	-12	SER	-	expression tag	UNP Q16851
D	-11	HIS	-	expression tag	UNP Q16851

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.

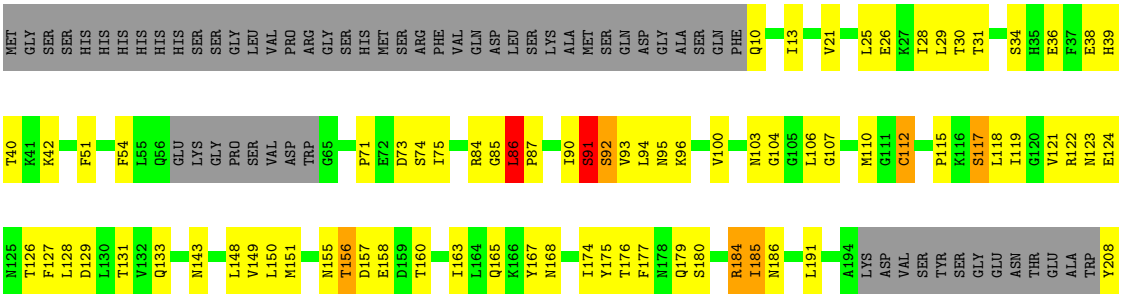
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

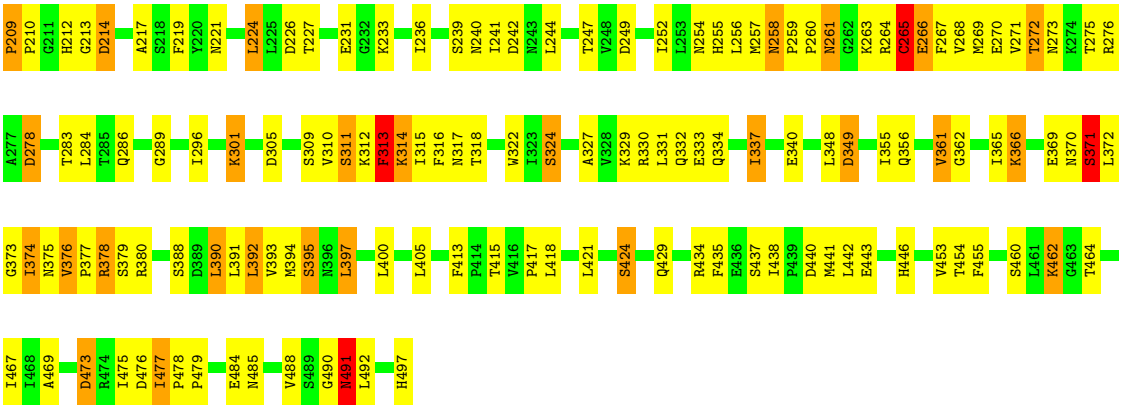
Chain A: 51% 32% 5% • 12%



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

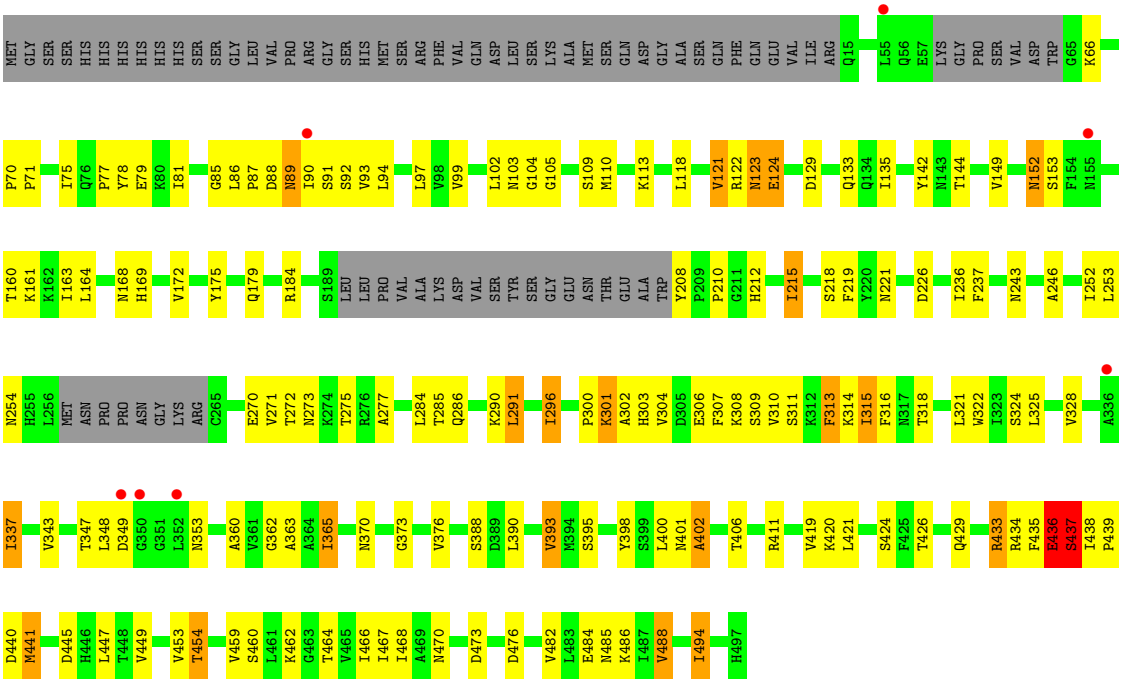
Chain B: 47% 34% 6% • 12%





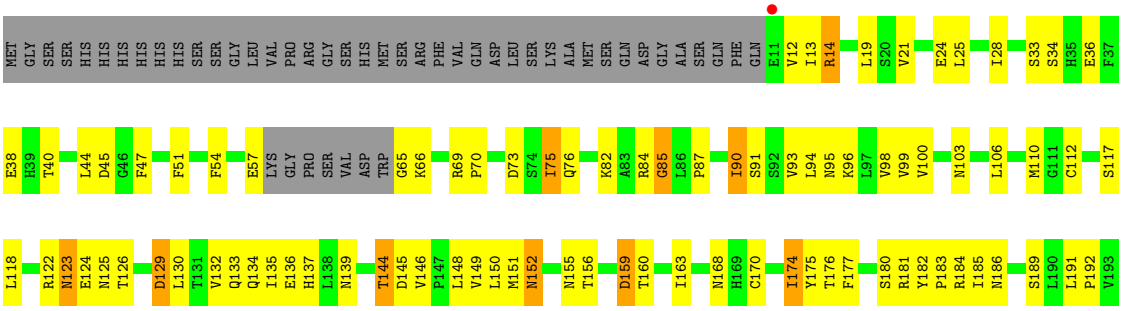
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

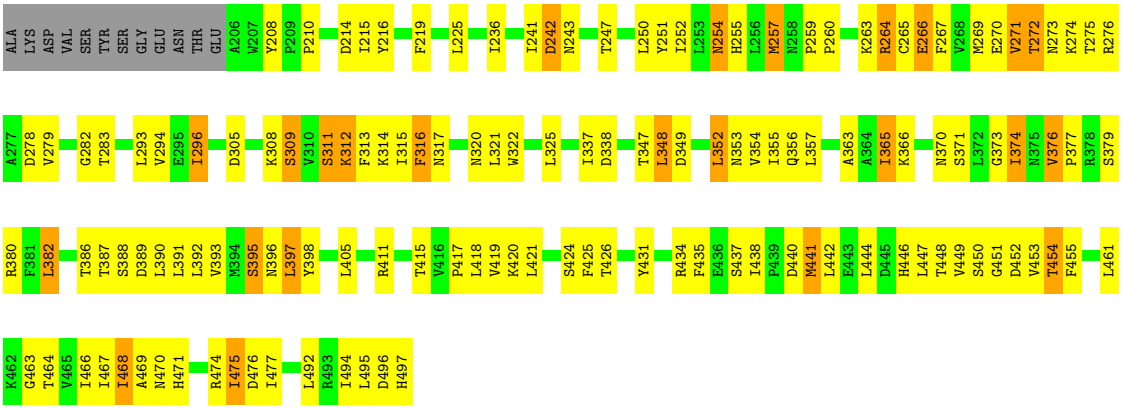
Chain C:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain D:




ALA LYS ASP VAL SER TYR SER GLY GLU ASN THR GLU A206 W207 Y208 P209 P210 D214 I215 Y216 F219 L225 I236 I241 D242 N243 T247 L250 Y251 I252 L253 N254 H255 L256 M257 N258 P259 P260 K263 R264 C265 E266 F267 V268 M269 E270 V271 T272 N273 K274 T275 R276
A277 D278 V279 G282 T283 L293 V294 E295 I296 D305 K308 S309 V310 S311 K312 F313 K314 I315 F316 N317 N320 L321 W322 L325 I337 D338 T347 L348 D349 L352 N353 V354 I355 Q356 L357 A363 A364 I365 K366 N370 S371 L372 G373 I374 N375 V376 P377 R378 S379
R380 F381 L382 T386 T387 S388 D389 L390 L391 L392 V393 M394 S395 N396 L397 Y398 L405 R411 T415 Y416 P417 L418 V419 K420 L421 S424 F425 T426 Y431 R434 F435 E436 S437 I438 P439 D440 M441 L442 E443 L444 D445 H446 L447 T448 V449 S450 G451 D452 V453 T454 F455 L461
K462 G463 T464 V465 I466 I467 I468 A469 N470 H471 R474 I475 D476 I477 L492 R493 I494 L495 D496 H497

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.44Å 140.44Å 311.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.60) 94.0 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.247 , 0.304 0.267 , 0.315	Depositor DCC
R_{free} test set	1985 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	113.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 (i)

5.1 Standard geometry (i)

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	0.61	2/3602 (0.1%)	0.72	1/4894 (0.0%)
1	B	0.58	0/3596	0.79	1/4889 (0.0%)
1	C	0.51	0/3353	0.66	0/4578
1	D	0.67	0/3630	0.83	3/4936 (0.1%)
All	All	0.60	2/14181 (0.0%)	0.75	5/19297 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	SER	CB-OG	10.91	1.56	1.42
1	A	379	SER	CB-OG	7.32	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	382	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	33	SER	N-CA-C	-5.80	95.35	111.00
1	A	444	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	86	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	33	SER	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	91	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	3474	134	0
1	B	3534	0	3471	171	0
1	C	3299	0	3094	104	0
1	D	3566	0	3511	184	0
All	All	13938	0	13550	581	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 21.

All (581) 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:B:265:CYS:HA	1:B:266:GLU:CB	1.83	1.07
1:C:218:SER:HA	1:C:221:ASN:HB2	1.37	1.02
1:C:91:SER:H	1:C:92:SER:HA	1.19	1.00
1:D:87:PRO:HG3	1:D:254:ASN:HB2	1.47	0.96
1:D:129:ASP:O	1:D:133:GLN:HG3	1.64	0.95
1:B:265:CYS:HA	1:B:266:GLU:HB2	1.50	0.94
1:A:446:HIS:HB3	1:A:464:THR:HG22	1.49	0.93
1:B:273:ASN:HA	1:B:314:LYS:O	1.69	0.92
1:B:84:ARG:H	1:B:85:GLY:HA2	1.34	0.92
1:D:186:ASN:HB3	1:D:189:SER:HB2	1.52	0.92
1:A:454:THR:HG23	1:A:476:ASP:HB3	1.52	0.92
1:A:309:SER:HA	1:A:310:VAL:C	1.89	0.92
1:B:90:ILE:H	1:B:91:SER:HA	1.35	0.91
1:D:90:ILE:N	1:D:91:SER:HA	1.85	0.91
1:A:126:THR:HG22	1:A:129:ASP:OD2	1.71	0.90
1:A:91:SER:HA	1:A:92:SER:HB3	1.54	0.89
1:B:100:VAL:HG22	1:B:149:VAL:HB	1.54	0.89
1:D:454:THR:HG22	1:D:476:ASP:HA	1.56	0.88
1:C:92:SER:H	1:C:93:VAL:HB	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HD12	1:B:438:ILE:H	1.40	0.87
1:B:126:THR:HG23	1:B:129:ASP:H	1.40	0.86
1:C:91:SER:N	1:C:92:SER:HA	1.87	0.85
1:B:265:CYS:HA	1:B:266:GLU:HB3	1.59	0.84
1:B:337:ILE:HD12	1:B:337:ILE:H	1.40	0.84
1:C:436:GLU:O	1:C:437:SER:HB2	1.77	0.83
1:B:309:SER:HB2	1:B:310:VAL:HA	1.62	0.82
1:A:387:THR:HG21	1:A:425:PHE:O	1.80	0.82
1:D:148:LEU:HD21	1:D:150:LEU:HD21	1.63	0.80
1:A:90:ILE:H	1:A:91:SER:HA	1.44	0.80
1:B:90:ILE:N	1:B:91:SER:HA	1.97	0.80
1:B:392:LEU:HD11	1:B:417:PRO:HG2	1.64	0.80
1:A:123:ASN:N	1:A:124:GLU:HA	1.97	0.80
1:B:129:ASP:O	1:B:133:GLN:HG2	1.82	0.78
1:D:90:ILE:H	1:D:91:SER:HA	1.46	0.78
1:D:444:LEU:HD12	1:D:461:LEU:HB2	1.63	0.78
1:B:469:ALA:HB2	1:B:475:ILE:HG13	1.64	0.77
1:B:376:VAL:HG12	1:B:377:PRO:HD2	1.64	0.77
1:D:411:ARG:NH2	1:D:417:PRO:HD3	1.98	0.77
1:D:149:VAL:HG22	1:D:175:TYR:HB2	1.67	0.77
1:D:106:LEU:HD21	1:D:155:ASN:HB3	1.67	0.77
1:C:103:ASN:HD22	1:C:152:ASN:HD22	1.32	0.77
1:A:167:TYR:O	1:A:170:CYS:HB2	1.85	0.76
1:B:115:PRO:HB3	1:B:156:THR:HG22	1.67	0.75
1:C:494:ILE:O	1:C:494:ILE:HG22	1.86	0.75
1:B:123:ASN:N	1:B:124:GLU:HA	2.02	0.75
1:D:272:THR:HG22	1:D:316:PHE:CD2	2.21	0.75
1:C:70:PRO:HG3	1:C:285:THR:HG22	1.67	0.75
1:D:122:ARG:C	1:D:124:GLU:HA	2.07	0.74
1:A:420:LYS:HE2	1:D:496:ASP:O	1.87	0.74
1:C:122:ARG:HD2	1:C:400:LEU:HD13	1.68	0.74
1:B:84:ARG:H	1:B:85:GLY:CA	2.01	0.74
1:B:267:PHE:CE2	1:B:365:ILE:HG12	2.22	0.73
1:D:129:ASP:O	1:D:133:GLN:CG	2.34	0.73
1:A:324:SER:O	1:A:328:VAL:HG23	1.87	0.73
1:D:449:VAL:HG12	1:D:467:ILE:HB	1.69	0.73
1:D:265:CYS:HB3	1:D:370:ASN:HB3	1.70	0.73
1:B:454:THR:HG22	1:B:476:ASP:HA	1.70	0.72
1:A:264:ARG:HB3	1:A:265:CYS:HA	1.70	0.72
1:D:395:SER:HB2	1:D:397:LEU:H	1.55	0.71
1:D:139:ASN:OD1	1:D:146:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ALA:HB2	1:D:475:ILE:HD11	1.72	0.71
1:A:91:SER:HA	1:A:92:SER:CB	2.20	0.71
1:B:75:ILE:HA	1:B:373:GLY:O	1.90	0.71
1:C:77:PRO:C	1:C:79:GLU:H	1.94	0.71
1:D:382:LEU:HD21	1:D:398:TYR:HE1	1.54	0.71
1:D:450:SER:HB3	1:D:468:ILE:HD12	1.71	0.71
1:D:263:LYS:HA	1:D:264:ARG:CB	2.21	0.71
1:A:42:LYS:HE3	1:A:221:ASN:HD22	1.55	0.70
1:C:215:ILE:O	1:C:219:PHE:HB2	1.92	0.70
1:D:419:VAL:HG22	1:D:447:LEU:HB3	1.73	0.70
1:A:388:SER:HA	1:A:421:LEU:HD12	1.72	0.70
1:D:90:ILE:N	1:D:91:SER:CA	2.54	0.70
1:B:337:ILE:HD12	1:B:337:ILE:N	2.06	0.69
1:A:90:ILE:N	1:A:91:SER:HA	2.07	0.69
1:C:92:SER:N	1:C:93:VAL:HB	2.06	0.69
1:A:434:ARG:HD2	1:A:453:VAL:O	1.93	0.69
1:C:275:THR:HG22	1:C:277:ALA:H	1.57	0.69
1:B:497:HIS:O	1:C:420:LYS:HD3	1.92	0.68
1:A:90:ILE:H	1:A:92:SER:HB3	1.58	0.68
1:D:87:PRO:HG3	1:D:254:ASN:CB	2.24	0.68
1:A:91:SER:HB2	1:A:93:VAL:H	1.58	0.67
1:D:271:VAL:CG1	1:D:315:ILE:HG23	2.24	0.67
1:B:310:VAL:HB	1:B:312:LYS:HG3	1.77	0.67
1:B:441:MET:O	1:B:443:GLU:N	2.25	0.67
1:A:290:LYS:HE2	1:A:369:GLU:HA	1.76	0.67
1:D:122:ARG:O	1:D:123:ASN:HB3	1.94	0.67
1:B:184:ARG:H	1:B:184:ARG:HD2	1.59	0.67
1:D:47:PHE:HD1	1:D:182:TYR:HD1	1.43	0.67
1:D:123:ASN:N	1:D:124:GLU:HA	2.09	0.66
1:B:84:ARG:N	1:B:85:GLY:HA2	2.00	0.66
1:C:419:VAL:HG12	1:C:447:LEU:HB3	1.77	0.66
1:D:276:ARG:HA	1:D:279:VAL:HG23	1.77	0.66
1:A:496:ASP:O	1:A:497:HIS:HB3	1.96	0.66
1:B:184:ARG:H	1:B:184:ARG:CD	2.08	0.66
1:D:186:ASN:CB	1:D:189:SER:HB2	2.24	0.66
1:B:272:THR:HG22	1:B:273:ASN:H	1.60	0.66
1:C:301:LYS:O	1:C:304:VAL:HG23	1.95	0.66
1:A:494:ILE:HG22	1:A:494:ILE:O	1.96	0.66
1:C:324:SER:O	1:C:328:VAL:HG23	1.95	0.66
1:B:265:CYS:CA	1:B:266:GLU:CB	2.67	0.65
1:C:488:VAL:HG12	1:D:492:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ILE:HG23	1:D:355:ILE:HB	1.78	0.65
1:B:313:PHE:H	1:B:313:PHE:HD2	1.45	0.65
1:D:156:THR:O	1:D:160:THR:HG23	1.97	0.65
1:A:448:THR:HG23	1:A:466:ILE:HG23	1.78	0.64
1:C:464:THR:O	1:C:485:ASN:HA	1.98	0.64
1:B:117:SER:OG	1:B:241:ILE:HG21	1.96	0.64
1:D:438:ILE:HD12	1:D:438:ILE:H	1.63	0.64
1:B:397:LEU:HD11	1:B:417:PRO:HG3	1.77	0.64
1:D:118:LEU:HA	1:D:126:THR:OG1	1.97	0.64
1:D:75:ILE:HA	1:D:373:GLY:O	1.97	0.64
1:D:421:LEU:HD23	1:D:449:VAL:CG2	2.28	0.64
1:B:270:GLU:HB3	1:B:376:VAL:HG21	1.79	0.63
1:D:185:ILE:O	1:D:354:VAL:HG22	1.98	0.63
1:A:243:ASN:HD22	1:A:246:ALA:HB2	1.64	0.63
1:C:161:LYS:HA	1:C:164:LEU:HD12	1.79	0.63
1:B:128:LEU:HD23	1:B:167:TYR:HE2	1.63	0.63
1:A:345:ALA:O	1:A:346:LYS:HB2	1.96	0.63
1:C:462:LYS:O	1:C:484:GLU:HA	1.98	0.63
1:B:91:SER:HB3	1:B:93:VAL:H	1.63	0.63
1:B:283:THR:HG22	1:B:315:ILE:O	1.98	0.63
1:C:460:SER:HB3	1:C:482:VAL:HG13	1.79	0.63
1:D:311:SER:HA	1:D:313:PHE:H	1.64	0.62
1:D:47:PHE:CD1	1:D:183:PRO:HD2	2.35	0.62
1:D:151:MET:HG3	1:D:177:PHE:CZ	2.35	0.62
1:A:399:SER:HB2	1:A:408:SER:OG	1.99	0.62
1:C:252:ILE:HG21	1:C:322:TRP:CZ3	2.34	0.62
1:D:36:GLU:O	1:D:40:THR:HB	1.99	0.62
1:C:494:ILE:O	1:C:494:ILE:CG2	2.47	0.62
1:A:184:ARG:HB3	1:A:354:VAL:HG11	1.82	0.62
1:A:437:SER:HB3	1:A:457:LYS:HA	1.80	0.62
1:B:265:CYS:HB2	1:B:370:ASN:HB2	1.82	0.62
1:A:270:GLU:HB2	1:A:320:ASN:HB2	1.82	0.61
1:A:453:VAL:HG22	1:A:475:ILE:HB	1.81	0.61
1:A:179:GLN:NE2	1:A:211:GLY:O	2.27	0.61
1:A:243:ASN:ND2	1:A:246:ALA:HB2	2.16	0.61
1:A:291:LEU:HD12	1:A:371:SER:O	2.00	0.61
1:C:303:HIS:ND1	1:C:306:GLU:OE1	2.34	0.61
1:D:271:VAL:HG11	1:D:315:ILE:HG23	1.80	0.61
1:B:395:SER:HB2	1:B:397:LEU:H	1.66	0.61
1:B:497:HIS:O	1:C:420:LYS:NZ	2.27	0.61
1:B:21:VAL:HG12	1:B:25:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ILE:CG2	1:D:355:ILE:HB	2.30	0.60
1:B:257:MET:O	1:B:258:ASN:C	2.39	0.60
1:A:235:TYR:CE1	1:A:256:LEU:HD22	2.36	0.60
1:D:25:LEU:HD22	1:D:44:LEU:HD13	1.84	0.60
1:A:271:VAL:O	1:A:375:ASN:HA	2.01	0.59
1:D:424:SER:OG	1:D:434:ARG:NH2	2.35	0.59
1:B:151:MET:HG3	1:B:177:PHE:CZ	2.36	0.59
1:A:444:LEU:HD12	1:A:461:LEU:HB2	1.85	0.59
1:A:103:ASN:HD21	1:A:160:THR:HG21	1.67	0.59
1:A:163:ILE:HG22	1:A:163:ILE:O	2.01	0.59
1:B:467:ILE:HG23	1:B:488:VAL:HB	1.83	0.59
1:D:265:CYS:HA	1:D:266:GLU:CB	2.32	0.59
1:D:397:LEU:HD22	1:D:398:TYR:HE2	1.67	0.59
1:A:65:GLY:N	1:A:287:TYR:HH	2.01	0.58
1:A:446:HIS:HB3	1:A:464:THR:CG2	2.29	0.58
1:D:271:VAL:O	1:D:376:VAL:HG23	2.04	0.58
1:C:184:ARG:HA	1:C:208:TYR:HE2	1.68	0.58
1:A:151:MET:HG3	1:A:177:PHE:CZ	2.38	0.58
1:A:337:ILE:O	1:A:337:ILE:HG22	2.03	0.58
1:A:390:LEU:O	1:A:394:MET:HG2	2.03	0.58
1:B:361:VAL:HG12	1:B:362:GLY:N	2.18	0.58
1:A:484:GLU:O	1:A:486:LYS:HG3	2.03	0.58
1:B:395:SER:HB3	1:B:441:MET:HG3	1.85	0.58
1:D:148:LEU:HD21	1:D:150:LEU:CD2	2.33	0.57
1:A:441:MET:O	1:A:443:GLU:N	2.36	0.57
1:B:240:ASN:HB3	1:B:242:ASP:OD2	2.04	0.57
1:B:376:VAL:HG12	1:B:377:PRO:CD	2.35	0.57
1:C:434:ARG:HD2	1:C:453:VAL:O	2.04	0.57
1:D:469:ALA:HB2	1:D:475:ILE:CD1	2.35	0.57
1:D:274:LYS:NZ	1:D:308:LYS:HA	2.19	0.57
1:B:186:ASN:HB2	1:B:191:LEU:H	1.69	0.57
1:D:386:THR:O	1:D:389:ASP:HB2	2.04	0.57
1:A:377:PRO:HB2	1:A:379:SER:HB2	1.85	0.57
1:B:376:VAL:CG1	1:B:377:PRO:HD2	2.32	0.57
1:D:185:ILE:HG13	1:D:186:ASN:H	1.69	0.57
1:D:469:ALA:HB2	1:D:475:ILE:CG1	2.35	0.57
1:A:313:PHE:HA	1:A:315:ILE:HD12	1.85	0.56
1:B:252:ILE:HD11	1:B:374:ILE:HG12	1.86	0.56
1:A:492:LEU:HD13	1:B:492:LEU:HD12	1.87	0.56
1:B:128:LEU:HD23	1:B:167:TYR:CE2	2.40	0.56
1:B:217:ALA:O	1:B:221:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ASP:HB3	1:B:460:SER:HA	1.86	0.56
1:B:490:GLY:O	1:B:491:ASN:HB3	2.04	0.56
1:D:47:PHE:CD1	1:D:182:TYR:HD1	2.21	0.56
1:B:126:THR:OG1	1:B:127:PHE:N	2.38	0.56
1:B:94:LEU:C	1:B:96:LYS:H	2.09	0.56
1:B:266:GLU:OE1	1:B:369:GLU:HG2	2.06	0.56
1:B:10:GLN:HA	1:B:13:ILE:HD12	1.88	0.56
1:B:332:GLN:C	1:B:334:GLN:H	2.09	0.56
1:D:265:CYS:HA	1:D:266:GLU:HB2	1.86	0.56
1:D:126:THR:HG23	1:D:129:ASP:H	1.71	0.56
1:B:263:LYS:HA	1:B:264:ARG:CB	2.37	0.55
1:A:309:SER:HA	1:A:311:SER:N	2.21	0.55
1:C:454:THR:CG2	1:C:476:ASP:OD1	2.55	0.55
1:B:264:ARG:O	1:B:265:CYS:CB	2.55	0.55
1:B:149:VAL:HG22	1:B:175:TYR:HB2	1.89	0.55
1:B:443:GLU:HB2	1:B:462:LYS:HB3	1.88	0.55
1:D:382:LEU:HD21	1:D:398:TYR:CE1	2.40	0.55
1:B:473:ASP:HB2	1:B:491:ASN:HB2	1.87	0.55
1:A:69:ARG:HH21	1:A:312:LYS:HE3	1.71	0.55
1:A:118:LEU:HD21	1:A:163:ILE:HD12	1.89	0.55
1:B:21:VAL:HG12	1:B:25:LEU:CD1	2.36	0.55
1:B:265:CYS:CA	1:B:266:GLU:HB3	2.34	0.54
1:D:387:THR:HG21	1:D:426:THR:HA	1.88	0.54
1:B:374:ILE:O	1:B:374:ILE:HG13	2.08	0.54
1:A:362:GLY:C	1:A:364:ALA:H	2.09	0.54
1:D:272:THR:HG22	1:D:316:PHE:CE2	2.41	0.54
1:B:71:PRO:HG2	1:B:74:SER:OG	2.07	0.54
1:B:397:LEU:CD1	1:B:417:PRO:HG3	2.37	0.54
1:D:215:ILE:O	1:D:219:PHE:HB2	2.08	0.54
1:B:129:ASP:O	1:B:133:GLN:CG	2.52	0.54
1:B:490:GLY:O	1:B:491:ASN:CB	2.56	0.54
1:D:444:LEU:CD1	1:D:461:LEU:HB2	2.35	0.54
1:D:448:THR:HG22	1:D:466:ILE:HG12	1.90	0.54
1:A:121:VAL:O	1:A:122:ARG:HB2	2.07	0.54
1:A:71:PRO:HD3	1:A:286:GLN:HB2	1.89	0.53
1:B:267:PHE:CE2	1:B:365:ILE:CG1	2.89	0.53
1:C:75:ILE:HA	1:C:373:GLY:O	2.09	0.53
1:B:185:ILE:HG22	1:B:355:ILE:O	2.08	0.53
1:D:440:ASP:C	1:D:441:MET:HG2	2.29	0.53
1:C:236:ILE:HD11	1:C:325:LEU:HG	1.90	0.53
1:A:236:ILE:HG22	1:A:323:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:CD1	1:B:374:ILE:HG12	2.38	0.53
1:D:103:ASN:HB3	1:D:152:ASN:HB3	1.91	0.53
1:A:90:ILE:N	1:A:91:SER:CA	2.71	0.53
1:A:309:SER:CA	1:A:310:VAL:C	2.70	0.53
1:B:446:HIS:HB3	1:B:464:THR:HG22	1.90	0.53
1:A:287:TYR:HB3	1:A:292:ARG:HG3	1.90	0.53
1:B:267:PHE:CD2	1:B:365:ILE:HG12	2.43	0.53
1:D:180:SER:HB2	1:D:182:TYR:HE2	1.74	0.53
1:D:446:HIS:HB2	1:D:464:THR:HG22	1.91	0.53
1:C:360:ALA:HB3	1:C:363:ALA:HB2	1.91	0.53
1:D:84:ARG:H	1:D:85:GLY:CA	2.22	0.53
1:B:268:VAL:HA	1:B:372:LEU:O	2.09	0.53
1:B:226:ASP:OD1	1:B:329:LYS:HE3	2.09	0.52
1:B:435:PHE:CE1	1:B:455:PHE:CD2	2.97	0.52
1:B:148:LEU:HD23	1:B:149:VAL:N	2.24	0.52
1:D:185:ILE:HG13	1:D:186:ASN:N	2.22	0.52
1:D:272:THR:HG22	1:D:316:PHE:HD2	1.70	0.52
1:A:270:GLU:HG3	1:A:322:TRP:HZ3	1.75	0.52
1:A:271:VAL:HG22	1:A:316:PHE:O	2.08	0.52
1:B:264:ARG:O	1:B:265:CYS:HB3	2.09	0.52
1:D:236:ILE:HG23	1:D:325:LEU:HD21	1.92	0.52
1:B:42:LYS:HD3	1:B:221:ASN:HD21	1.75	0.52
1:C:121:VAL:HG12	1:C:122:ARG:N	2.24	0.52
1:D:126:THR:N	1:D:129:ASP:HB2	2.25	0.52
1:D:25:LEU:HD23	1:D:28:ILE:HD12	1.92	0.52
1:B:115:PRO:HD2	1:B:118:LEU:HD12	1.92	0.51
1:B:438:ILE:H	1:B:438:ILE:CD1	2.13	0.51
1:D:448:THR:CG2	1:D:466:ILE:HG12	2.40	0.51
1:D:494:ILE:C	1:D:495:LEU:HG	2.30	0.51
1:C:77:PRO:C	1:C:79:GLU:N	2.63	0.51
1:D:93:VAL:HG22	1:D:257:MET:HG3	1.92	0.51
1:D:271:VAL:HG13	1:D:315:ILE:HG23	1.91	0.51
1:D:132:VAL:HG12	1:D:148:LEU:HD13	1.93	0.51
1:A:447:LEU:HD13	1:A:461:LEU:HD13	1.91	0.51
1:B:313:PHE:O	1:B:315:ILE:N	2.43	0.51
1:D:87:PRO:CG	1:D:254:ASN:HB2	2.32	0.51
1:A:322:TRP:O	1:A:323:ILE:HG12	2.11	0.51
1:A:492:LEU:HB2	1:B:492:LEU:HG	1.92	0.51
1:B:446:HIS:CB	1:B:464:THR:HG22	2.41	0.51
1:C:286:GLN:HE21	1:C:291:LEU:HD23	1.75	0.51
1:B:278:ASP:OD2	1:B:378:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASN:HA	1:C:314:LYS:O	2.10	0.51
1:A:53:ARG:HB3	1:A:341:ILE:HD11	1.92	0.51
1:B:36:GLU:HG2	1:B:39:HIS:HE1	1.76	0.51
1:C:92:SER:HB2	1:C:93:VAL:CG2	2.41	0.51
1:A:352:LEU:O	1:A:354:VAL:HG23	2.10	0.50
1:B:497:HIS:C	1:C:420:LYS:HD3	2.30	0.50
1:C:401:ASN:O	1:C:402:ALA:HB3	2.11	0.50
1:A:215:ILE:HG23	1:A:216:TYR:N	2.26	0.50
1:B:208:TYR:CD1	1:B:356:GLN:HG3	2.46	0.50
1:D:265:CYS:CB	1:D:370:ASN:HB3	2.40	0.50
1:D:444:LEU:HD12	1:D:461:LEU:CB	2.37	0.50
1:C:92:SER:HB2	1:C:93:VAL:HG23	1.93	0.50
1:C:395:SER:OG	1:C:441:MET:HG3	2.10	0.50
1:D:448:THR:HG23	1:D:466:ILE:HG23	1.92	0.50
1:B:150:LEU:HB2	1:B:176:THR:HG22	1.93	0.50
1:D:100:VAL:HA	1:D:149:VAL:O	2.12	0.50
1:D:47:PHE:HD1	1:D:182:TYR:CD1	2.28	0.50
1:B:313:PHE:N	1:B:313:PHE:CD2	2.78	0.50
1:C:153:SER:HA	1:C:179:GLN:HG2	1.92	0.50
1:A:103:ASN:ND2	1:A:160:THR:HG21	2.26	0.50
1:B:418:LEU:HD11	1:B:446:HIS:CE1	2.47	0.50
1:A:184:ARG:HH11	1:A:356:GLN:HE21	1.58	0.50
1:B:424:SER:HB2	1:B:434:ARG:HH21	1.76	0.50
1:B:464:THR:O	1:B:485:ASN:HA	2.12	0.50
1:A:139:ASN:OD1	1:A:144:THR:HG23	2.12	0.49
1:C:307:PHE:O	1:C:308:LYS:HG2	2.13	0.49
1:A:117:SER:HA	1:A:127:PHE:HB2	1.95	0.49
1:A:184:ARG:HH11	1:A:356:GLN:NE2	2.11	0.49
1:B:86:LEU:HD23	1:B:86:LEU:H	1.78	0.49
1:B:256:LEU:HD21	1:B:268:VAL:CG2	2.43	0.49
1:B:369:GLU:C	1:B:371:SER:H	2.16	0.49
1:D:13:ILE:HD12	1:D:14:ARG:HG3	1.95	0.49
1:D:126:THR:HG22	1:D:129:ASP:OD2	2.13	0.49
1:D:283:THR:HG21	1:D:313:PHE:HD1	1.77	0.49
1:B:272:THR:HG21	1:B:378:ARG:HG2	1.95	0.49
1:C:272:THR:O	1:C:316:PHE:HB3	2.12	0.49
1:D:73:ASP:O	1:D:76:GLN:NE2	2.46	0.49
1:D:388:SER:HB3	1:D:419:VAL:HG12	1.94	0.49
1:A:91:SER:HB2	1:A:93:VAL:N	2.26	0.48
1:C:449:VAL:HG13	1:C:467:ILE:HB	1.95	0.48
1:D:444:LEU:HD21	1:D:447:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:C	1:A:124:GLU:HA	2.33	0.48
1:D:93:VAL:CG2	1:D:257:MET:HG3	2.44	0.48
1:C:454:THR:HG21	1:C:476:ASP:OD1	2.12	0.48
1:D:308:LYS:O	1:D:309:SER:HB3	2.13	0.48
1:B:284:LEU:H	1:B:315:ILE:HD12	1.77	0.48
1:D:267:PHE:CE2	1:D:321:LEU:HD23	2.49	0.48
1:C:435:PHE:O	1:C:436:GLU:C	2.51	0.48
1:D:135:ILE:HG13	1:D:148:LEU:HD12	1.94	0.48
1:D:273:ASN:HA	1:D:314:LYS:O	2.14	0.48
1:D:396:ASN:ND2	1:D:442:LEU:HG	2.29	0.48
1:A:215:ILE:O	1:A:219:PHE:HB2	2.13	0.48
1:D:122:ARG:O	1:D:123:ASN:CB	2.62	0.48
1:D:168:ASN:C	1:D:170:CYS:H	2.16	0.48
1:B:413:PHE:N	1:B:413:PHE:CD2	2.81	0.48
1:C:92:SER:CA	1:C:93:VAL:HB	2.43	0.48
1:A:340:GLU:O	1:A:342:ILE:HD12	2.14	0.48
1:B:51:PHE:O	1:B:54:PHE:N	2.44	0.48
1:C:470:ASN:O	1:C:473:ASP:HB2	2.13	0.48
1:A:209:PRO:HA	1:A:210:PRO:HD2	1.65	0.47
1:A:91:SER:HB2	1:A:93:VAL:HG22	1.96	0.47
1:A:249:ASP:HB3	1:A:252:ILE:HD12	1.96	0.47
1:A:256:LEU:HD23	1:A:265:CYS:HB2	1.95	0.47
1:C:87:PRO:HG3	1:C:254:ASN:HB2	1.97	0.47
1:D:387:THR:HG21	1:D:425:PHE:O	2.14	0.47
1:A:71:PRO:C	1:A:73:ASP:H	2.16	0.47
1:A:463:GLY:HA3	1:A:485:ASN:OD1	2.14	0.47
1:C:90:ILE:HA	1:C:91:SER:HA	1.58	0.47
1:D:75:ILE:HD12	1:D:315:ILE:HG12	1.95	0.47
1:B:453:VAL:HG12	1:B:454:THR:N	2.30	0.47
1:A:264:ARG:HB3	1:A:265:CYS:CA	2.41	0.47
1:B:260:PRO:O	1:B:261:ASN:HB2	2.15	0.47
1:B:269:MET:O	1:B:269:MET:HG2	2.14	0.47
1:C:347:THR:HB	1:C:353:ASN:HA	1.96	0.47
1:C:362:GLY:O	1:C:365:ILE:HG13	2.15	0.47
1:D:274:LYS:HZ1	1:D:308:LYS:HA	1.78	0.47
1:D:397:LEU:HD22	1:D:398:TYR:CE2	2.47	0.47
1:A:33:SER:O	1:A:35:HIS:N	2.48	0.47
1:B:438:ILE:HD12	1:B:438:ILE:N	2.20	0.47
1:D:269:MET:O	1:D:269:MET:HG2	2.15	0.47
1:B:93:VAL:O	1:B:257:MET:HE3	2.15	0.47
1:B:184:ARG:HG3	1:B:208:TYR:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:OD1	1:B:318:THR:N	2.48	0.47
1:C:92:SER:H	1:C:93:VAL:CB	2.19	0.47
1:D:130:LEU:O	1:D:133:GLN:HB2	2.15	0.47
1:A:454:THR:CG2	1:A:476:ASP:HB3	2.35	0.47
1:C:484:GLU:O	1:C:486:LYS:HG3	2.15	0.47
1:D:75:ILE:CD1	1:D:315:ILE:HG12	2.44	0.47
1:D:267:PHE:HE2	1:D:321:LEU:HD23	1.80	0.47
1:C:88:ASP:HA	1:C:89:ASN:HA	1.69	0.46
1:C:436:GLU:OE2	1:C:436:GLU:HA	2.16	0.46
1:B:110:MET:CE	1:B:119:ILE:HD13	2.45	0.46
1:B:90:ILE:N	1:B:91:SER:CA	2.74	0.46
1:B:272:THR:HG23	1:B:376:VAL:O	2.15	0.46
1:C:440:ASP:HB3	1:C:460:SER:HA	1.97	0.46
1:A:267:PHE:C	1:A:267:PHE:CD2	2.89	0.46
1:C:337:ILE:H	1:C:337:ILE:HG13	1.56	0.46
1:C:92:SER:N	1:C:94:LEU:H	2.14	0.46
1:D:470:ASN:O	1:D:471:HIS:C	2.53	0.46
1:A:97:LEU:HG	1:A:98:VAL:N	2.28	0.46
1:C:99:VAL:HG13	1:C:237:PHE:HD2	1.80	0.46
1:B:390:LEU:HD22	1:B:394:MET:HE2	1.98	0.46
1:D:265:CYS:HB2	1:D:266:GLU:HB3	1.98	0.46
1:A:84:ARG:HA	1:A:85:GLY:HA3	1.47	0.46
1:B:327:ALA:O	1:B:331:LEU:HD12	2.15	0.46
1:C:270:GLU:HB3	1:C:376:VAL:HG21	1.98	0.46
1:D:420:LYS:HD3	1:D:448:THR:OG1	2.15	0.46
1:B:219:PHE:HE1	1:B:224:LEU:HD13	1.79	0.46
1:D:100:VAL:HG11	1:D:215:ILE:HD11	1.98	0.46
1:D:435:PHE:CE1	1:D:455:PHE:CD2	3.05	0.45
1:A:161:LYS:HA	1:A:164:LEU:HD12	1.99	0.45
1:B:126:THR:HG22	1:B:129:ASP:CG	2.36	0.45
1:B:131:THR:HG22	1:B:148:LEU:HD11	1.97	0.45
1:B:149:VAL:HA	1:B:175:TYR:O	2.17	0.45
1:D:208:TYR:CE1	1:D:356:GLN:HG3	2.50	0.45
1:A:420:LYS:HG3	1:D:497:HIS:C	2.36	0.45
1:B:26:GLU:HA	1:B:29:LEU:HD12	1.98	0.45
1:B:87:PRO:HD3	1:B:254:ASN:HB2	1.98	0.45
1:B:477:ILE:HA	1:B:478:PRO:HD3	1.73	0.45
1:D:98:VAL:O	1:D:236:ILE:HA	2.17	0.45
1:D:182:TYR:CE2	1:D:210:PRO:HG3	2.51	0.45
1:D:363:ALA:O	1:D:366:LYS:HG2	2.17	0.45
1:A:264:ARG:NH2	1:A:265:CYS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HB3	1:A:493:ARG:HE	1.82	0.45
1:D:91:SER:C	1:D:93:VAL:H	2.19	0.45
1:D:184:ARG:HD3	1:D:354:VAL:HG11	1.99	0.45
1:D:270:GLU:OE2	1:D:376:VAL:HG11	2.17	0.45
1:A:473:ASP:CG	1:A:491:ASN:HB2	2.37	0.45
1:D:21:VAL:HA	1:D:24:GLU:HB3	1.99	0.45
1:D:65:GLY:HA3	1:D:66:LYS:HA	1.62	0.45
1:D:126:THR:H	1:D:129:ASP:HB2	1.81	0.45
1:A:453:VAL:HG21	1:A:467:ILE:HG22	1.99	0.45
1:B:311:SER:N	1:B:312:LYS:HB2	2.32	0.45
1:C:129:ASP:O	1:C:133:GLN:CG	2.65	0.45
1:C:462:LYS:HB2	1:C:484:GLU:HG3	1.99	0.45
1:D:126:THR:HG22	1:D:129:ASP:CG	2.37	0.45
1:D:159:ASP:O	1:D:163:ILE:HD12	2.17	0.45
1:D:270:GLU:HB3	1:D:376:VAL:HG21	1.98	0.45
1:C:348:LEU:HA	1:C:349:ASP:HA	1.72	0.44
1:A:89:ASN:HA	1:A:90:ILE:HA	1.46	0.44
1:D:219:PHE:CD2	1:D:225:LEU:HD13	2.52	0.44
1:D:352:LEU:HD23	1:D:353:ASN:H	1.82	0.44
1:D:376:VAL:HG12	1:D:377:PRO:HD2	1.99	0.44
1:C:129:ASP:O	1:C:133:GLN:HG2	2.18	0.44
1:C:388:SER:HA	1:C:421:LEU:HD12	1.99	0.44
1:D:293:LEU:O	1:D:294:VAL:HG23	2.17	0.44
1:D:313:PHE:C	1:D:315:ILE:H	2.19	0.44
1:C:70:PRO:HA	1:C:71:PRO:HD3	1.89	0.44
1:B:259:PRO:HA	1:B:260:PRO:HD3	1.77	0.44
1:C:286:GLN:HG3	1:C:290:LYS:O	2.18	0.44
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.74	0.44
1:A:320:ASN:C	1:A:321:LEU:HG	2.38	0.44
1:A:179:GLN:HE21	1:A:214:ASP:HB3	1.82	0.44
1:A:220:TYR:HD1	1:A:225:LEU:HD23	1.82	0.44
1:B:388:SER:OG	1:B:421:LEU:HB2	2.18	0.44
1:A:42:LYS:CE	1:A:221:ASN:HD22	2.28	0.44
1:B:122:ARG:C	1:B:124:GLU:HA	2.36	0.44
1:B:272:THR:HG22	1:B:273:ASN:N	2.30	0.44
1:B:275:THR:HG22	1:B:276:ARG:H	1.82	0.44
1:C:91:SER:N	1:C:92:SER:CA	2.69	0.44
1:A:468:ILE:HD12	1:C:468:ILE:HD12	2.00	0.43
1:B:391:LEU:HG	1:B:392:LEU:N	2.32	0.43
1:C:462:LYS:CB	1:C:484:GLU:HG3	2.48	0.43
1:D:125:ASN:HB3	1:D:129:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:H	1:D:85:GLY:HA2	1.81	0.43
1:D:452:ASP:OD2	1:D:474:ARG:HD2	2.18	0.43
1:A:116:LYS:C	1:A:118:LEU:H	2.21	0.43
1:A:491:ASN:O	1:B:491:ASN:N	2.52	0.43
1:D:451:GLY:O	1:D:453:VAL:HG23	2.18	0.43
1:A:467:ILE:HG12	1:A:488:VAL:HB	2.00	0.43
1:C:118:LEU:HD22	1:C:163:ILE:HD12	1.98	0.43
1:C:123:ASN:HA	1:C:124:GLU:HA	1.65	0.43
1:C:393:VAL:HA	1:C:398:TYR:CD2	2.54	0.43
1:D:94:LEU:C	1:D:96:LYS:H	2.22	0.43
1:D:208:TYR:CD1	1:D:356:GLN:HG3	2.53	0.43
1:D:283:THR:HG21	1:D:313:PHE:CD1	2.53	0.43
1:C:424:SER:HB2	1:C:434:ARG:NH2	2.33	0.43
1:D:82:LYS:HA	1:D:251:TYR:CD1	2.53	0.43
1:A:77:PRO:HG2	1:A:80:LYS:HG2	2.00	0.43
1:A:98:VAL:HG13	1:A:147:PRO:HG2	2.01	0.43
1:A:270:GLU:OE1	1:A:320:ASN:HB3	2.17	0.43
1:B:256:LEU:HD21	1:B:268:VAL:HG21	2.01	0.43
1:A:101:LYS:NZ	1:A:131:THR:HG21	2.34	0.43
1:A:424:SER:HB2	1:A:434:ARG:HH21	1.82	0.43
1:B:332:GLN:C	1:B:334:GLN:N	2.72	0.43
1:D:144:THR:OG1	1:D:145:ASP:N	2.51	0.43
1:D:397:LEU:CD2	1:D:398:TYR:CE2	3.01	0.43
1:D:421:LEU:HD23	1:D:449:VAL:HG21	2.01	0.43
1:A:264:ARG:CB	1:A:265:CYS:HA	2.40	0.43
1:A:271:VAL:H	1:A:376:VAL:HG23	1.83	0.43
1:C:243:ASN:HD22	1:C:246:ALA:HB2	1.83	0.43
1:D:444:LEU:HA	1:D:463:GLY:H	1.84	0.43
1:C:212:HIS:CD2	1:C:212:HIS:H	2.35	0.43
1:C:252:ILE:HG21	1:C:322:TRP:CH2	2.53	0.43
1:C:438:ILE:HA	1:C:439:PRO:HD3	1.75	0.42
1:D:449:VAL:HA	1:D:467:ILE:O	2.19	0.42
1:A:256:LEU:O	1:A:258:ASN:N	2.53	0.42
1:A:494:ILE:HG12	1:B:488:VAL:HG22	2.01	0.42
1:B:271:VAL:O	1:B:375:ASN:HA	2.19	0.42
1:D:398:TYR:N	1:D:398:TYR:CD2	2.86	0.42
1:A:87:PRO:HB3	1:A:254:ASN:ND2	2.35	0.42
1:B:96:LYS:HA	1:B:233:LYS:HA	1.99	0.42
1:D:126:THR:O	1:D:129:ASP:HB2	2.20	0.42
1:D:388:SER:HA	1:D:421:LEU:HD12	2.01	0.42
1:B:378:ARG:O	1:B:380:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:HD22	1:C:152:ASN:HB3	1.83	0.42
1:D:184:ARG:NE	1:D:356:GLN:OE1	2.51	0.42
1:D:270:GLU:HB2	1:D:320:ASN:HB2	2.01	0.42
1:B:366:LYS:HB2	1:B:366:LYS:HE3	1.78	0.42
1:B:478:PRO:O	1:B:479:PRO:C	2.58	0.42
1:C:311:SER:HA	1:C:313:PHE:N	2.35	0.42
1:D:272:THR:HG23	1:D:273:ASN:O	2.20	0.42
1:D:296:ILE:HD12	1:D:296:ILE:H	1.83	0.42
1:D:312:LYS:HD3	1:D:313:PHE:CD2	2.54	0.42
1:A:391:LEU:HD13	1:A:435:PHE:CE2	2.55	0.42
1:A:416:VAL:HA	1:A:417:PRO:HD3	1.84	0.42
1:B:244:LEU:HD12	1:B:393:VAL:HG21	2.02	0.42
1:D:21:VAL:HG12	1:D:25:LEU:HD12	2.02	0.42
1:A:100:VAL:HG23	1:A:236:ILE:HG13	2.02	0.42
1:A:184:ARG:NH1	1:A:356:GLN:NE2	2.68	0.42
1:A:186:ASN:HB3	1:A:189:SER:H	1.85	0.42
1:A:264:ARG:CZ	1:A:265:CYS:HB3	2.49	0.42
1:A:264:ARG:NH1	1:A:265:CYS:HB3	2.35	0.42
1:B:301:LYS:HE3	1:B:301:LYS:HA	2.02	0.42
1:C:149:VAL:HA	1:C:175:TYR:O	2.19	0.42
1:A:70:PRO:HB3	1:A:285:THR:HA	2.01	0.42
1:A:101:LYS:HE2	1:A:239:SER:OG	2.19	0.42
1:C:454:THR:HG23	1:C:476:ASP:OD1	2.19	0.42
1:D:122:ARG:O	1:D:124:GLU:HA	2.19	0.42
1:A:65:GLY:HA2	1:A:67:ILE:HG13	2.02	0.42
1:A:348:LEU:HA	1:A:349:ASP:HA	1.84	0.42
1:B:25:LEU:HD23	1:B:28:ILE:HD12	2.01	0.42
1:B:103:ASN:HD21	1:B:160:THR:HG21	1.84	0.42
1:B:313:PHE:C	1:B:315:ILE:H	2.21	0.42
1:D:210:PRO:HG2	1:D:214:ASP:HB2	2.01	0.42
1:B:266:GLU:HA	1:B:324:SER:HB3	2.02	0.42
1:C:168:ASN:O	1:C:169:HIS:HB2	2.20	0.42
1:D:392:LEU:O	1:D:395:SER:OG	2.32	0.42
1:D:469:ALA:HB2	1:D:475:ILE:HG13	2.01	0.42
1:A:439:PRO:HB3	1:A:459:VAL:HB	2.01	0.41
1:C:296:ILE:H	1:C:296:ILE:HG13	1.70	0.41
1:C:440:ASP:C	1:C:441:MET:HG2	2.39	0.41
1:D:51:PHE:O	1:D:54:PHE:HB3	2.20	0.41
1:D:174:ILE:O	1:D:174:ILE:HG23	2.20	0.41
1:A:417:PRO:HB3	1:A:444:LEU:HD23	2.01	0.41
1:B:378:ARG:C	1:B:380:ARG:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:SER:HB2	1:C:93:VAL:HB	2.02	0.41
1:D:255:HIS:O	1:D:259:PRO:HB3	2.20	0.41
1:A:101:LYS:HZ2	1:A:131:THR:HG21	1.85	0.41
1:B:157:ASP:O	1:B:158:GLU:C	2.57	0.41
1:B:212:HIS:O	1:B:214:ASP:N	2.52	0.41
1:B:270:GLU:HB3	1:B:376:VAL:CG2	2.49	0.41
1:B:348:LEU:HA	1:B:349:ASP:HA	1.67	0.41
1:C:135:ILE:HG21	1:C:172:VAL:HG13	2.03	0.41
1:C:271:VAL:HA	1:C:318:THR:HG1	1.85	0.41
1:C:308:LYS:HG3	1:C:309:SER:OG	2.20	0.41
1:D:374:ILE:O	1:D:374:ILE:HG13	2.20	0.41
1:A:362:GLY:O	1:A:364:ALA:N	2.52	0.41
1:B:266:GLU:OE2	1:B:330:ARG:NH2	2.52	0.41
1:B:271:VAL:O	1:B:376:VAL:HG23	2.19	0.41
1:C:103:ASN:O	1:C:105:GLY:N	2.48	0.41
1:C:271:VAL:HG12	1:C:316:PHE:O	2.20	0.41
1:D:134:GLN:O	1:D:137:HIS:N	2.54	0.41
1:C:488:VAL:HG13	1:D:494:ILE:HG12	2.01	0.41
1:D:216:TYR:CD2	1:D:337:ILE:HG21	2.54	0.41
1:B:208:TYR:HE1	1:B:210:PRO:HA	1.85	0.41
1:B:271:VAL:HG11	1:B:315:ILE:HB	2.02	0.41
1:B:104:GLY:HA3	1:B:179:GLN:NE2	2.35	0.41
1:C:142:TYR:HB2	1:C:144:THR:HG22	2.03	0.41
1:C:243:ASN:ND2	1:C:246:ALA:HB2	2.35	0.41
1:C:309:SER:HA	1:C:310:VAL:HA	1.78	0.41
1:C:284:LEU:O	1:C:315:ILE:HD13	2.21	0.41
1:C:390:LEU:O	1:C:393:VAL:N	2.54	0.41
1:D:99:VAL:HG21	1:D:135:ILE:CD1	2.50	0.41
1:D:257:MET:H	1:D:257:MET:HG2	1.63	0.41
1:A:395:SER:C	1:A:397:LEU:H	2.25	0.41
1:A:427:LYS:O	1:A:430:ASP:HB2	2.20	0.41
1:B:107:GLY:O	1:B:112:CYS:N	2.54	0.41
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.84	0.41
1:B:208:TYR:HA	1:B:209:PRO:HD3	1.90	0.41
1:B:209:PRO:HA	1:B:210:PRO:HD3	1.99	0.41
1:B:268:VAL:HB	1:B:322:TRP:HB2	2.02	0.41
1:B:462:LYS:O	1:B:484:GLU:HA	2.21	0.41
1:C:97:LEU:HD22	1:C:253:LEU:HD21	2.02	0.41
1:C:103:ASN:HD21	1:C:160:THR:HG21	1.85	0.41
1:D:69:ARG:HA	1:D:70:PRO:HD3	1.93	0.41
1:D:191:LEU:HG	1:D:192:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:GLU:OE1	1:D:380:ARG:NH2	2.54	0.41
1:D:390:LEU:O	1:D:391:LEU:C	2.59	0.41
1:A:278:ASP:OD2	1:A:316:PHE:CE2	2.74	0.41
1:D:348:LEU:HA	1:D:349:ASP:HA	1.78	0.41
1:A:29:LEU:HG	1:A:44:LEU:HD12	2.03	0.40
1:C:300:PRO:O	1:C:302:ALA:N	2.54	0.40
1:C:429:GLN:HG2	1:C:433:ARG:NH1	2.37	0.40
1:D:84:ARG:N	1:D:85:GLY:CA	2.83	0.40
1:C:236:ILE:CD1	1:C:325:LEU:HG	2.51	0.40
1:D:242:ASP:N	1:D:242:ASP:OD1	2.54	0.40
1:D:265:CYS:CA	1:D:266:GLU:CB	2.99	0.40
1:D:272:THR:HG23	1:D:273:ASN:N	2.35	0.40
1:D:397:LEU:CD2	1:D:398:TYR:HE2	2.34	0.40
1:B:71:PRO:HD3	1:B:286:GLN:HB2	2.03	0.40
1:B:106:LEU:HD21	1:B:155:ASN:HB3	2.01	0.40
1:B:365:ILE:O	1:B:366:LYS:C	2.60	0.40
1:B:378:ARG:C	1:B:380:ARG:H	2.24	0.40
1:D:174:ILE:O	1:D:174:ILE:CG2	2.69	0.40
1:A:388:SER:HB3	1:A:419:VAL:HG12	2.03	0.40
1:B:227:THR:HG22	1:B:231:GLU:OE2	2.22	0.40
1:B:255:HIS:O	1:B:255:HIS:CD2	2.75	0.40
1:D:134:GLN:C	1:D:136:GLU:N	2.75	0.40
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.80	0.40
1:A:392:LEU:O	1:A:395:SER:OG	2.40	0.40
1:B:28:ILE:H	1:B:28:ILE:HG13	1.77	0.40
1:B:249:ASP:HB3	1:B:252:ILE:HG22	2.03	0.40
1:D:282:GLY:O	1:D:317:ASN:N	2.52	0.40
1:D:347:THR:HB	1:D:353:ASN:HA	2.03	0.40
1:D:392:LEU:HD12	1:D:392:LEU:HA	1.84	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	459/528 (87%)	376 (82%)	64 (14%)	19 (4%)	3	26
1	B	461/528 (87%)	377 (82%)	58 (13%)	26 (6%)	2	19
1	C	442/528 (84%)	363 (82%)	65 (15%)	14 (3%)	4	31
1	D	462/528 (88%)	384 (83%)	65 (14%)	13 (3%)	5	34
All	All	1824/2112 (86%)	1500 (82%)	252 (14%)	72 (4%)	3	27

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	257	MET
1	A	263	LYS
1	B	265	CYS
1	B	266	GLU
1	B	313	PHE
1	B	491	ASN
1	C	121	VAL
1	C	437	SER
1	D	34	SER
1	D	371	SER
1	A	84	ARG
1	A	346	LYS
1	A	363	ALA
1	A	370	ASN
1	A	379	SER
1	B	143	ASN
1	B	314	LYS
1	B	379	SER
1	B	442	LEU
1	C	78	TYR
1	C	301	LYS
1	C	343	VAL
1	C	370	ASN
1	C	436	GLU
1	D	38	GLU
1	D	254	ASN
1	D	264	ARG
1	D	266	GLU
1	D	365	ILE
1	A	210	PRO
1	A	246	ALA
1	A	261	ASN

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Mol	Chain	Res	Type
1	A	267	PHE
1	A	442	LEU
1	B	92	SER
1	B	95	ASN
1	B	261	ASN
1	B	333	GLU
1	B	371	SER
1	B	415	THR
1	B	437	SER
1	C	113	LYS
1	C	411	ARG
1	D	309	SER
1	A	122	ARG
1	A	258	ASN
1	A	412	GLU
1	B	34	SER
1	B	165	GLN
1	B	224	LEU
1	B	392	LEU
1	D	85	GLY
1	A	209	PRO
1	B	38	GLU
1	B	117	SER
1	B	213	GLY
1	C	210	PRO
1	C	402	ALA
1	D	117	SER
1	D	123	ASN
1	D	129	ASP
1	D	379	SER
1	B	209	PRO
1	C	104	GLY
1	B	121	VAL
1	B	258	ASN
1	A	163	ILE
1	B	289	GLY
1	C	85	GLY
1	C	215	ILE
1	A	422	GLY

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	381/470 (81%)	345 (91%)	36 (9%)	8	38
1	B	380/470 (81%)	331 (87%)	49 (13%)	4	24
1	C	341/470 (73%)	310 (91%)	31 (9%)	9	39
1	D	385/470 (82%)	331 (86%)	54 (14%)	3	21
All	All	1487/1880 (79%)	1317 (89%)	170 (11%)	5	29

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	31	THR
1	A	67	ILE
1	A	80	LYS
1	A	81	ILE
1	A	118	LEU
1	A	145	ASP
1	A	148	LEU
1	A	152	ASN
1	A	189	SER
1	A	236	ILE
1	A	240	ASN
1	A	253	LEU
1	A	267	PHE
1	A	271	VAL
1	A	275	THR
1	A	283	THR
1	A	296	ILE
1	A	312	LYS
1	A	321	LEU
1	A	343	VAL
1	A	352	LEU
1	A	367	SER
1	A	372	LEU

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Mol	Chain	Res	Type
1	A	379	SER
1	A	382	LEU
1	A	395	SER
1	A	399	SER
1	A	405	LEU
1	A	408	SER
1	A	424	SER
1	A	444	LEU
1	A	453	VAL
1	A	464	THR
1	A	476	ASP
1	A	477	ILE
1	B	30	THR
1	B	31	THR
1	B	40	THR
1	B	73	ASP
1	B	86	LEU
1	B	91	SER
1	B	92	SER
1	B	112	CYS
1	B	156	THR
1	B	163	ILE
1	B	168	ASN
1	B	174	ILE
1	B	180	SER
1	B	184	ARG
1	B	185	ILE
1	B	214	ASP
1	B	236	ILE
1	B	239	SER
1	B	247	THR
1	B	265	CYS
1	B	272	THR
1	B	278	ASP
1	B	296	ILE
1	B	301	LYS
1	B	305	ASP
1	B	311	SER
1	B	313	PHE
1	B	316	PHE
1	B	324	SER
1	B	337	ILE

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Mol	Chain	Res	Type
1	B	340	GLU
1	B	349	ASP
1	B	361	VAL
1	B	366	LYS
1	B	371	SER
1	B	374	ILE
1	B	376	VAL
1	B	378	ARG
1	B	390	LEU
1	B	395	SER
1	B	397	LEU
1	B	400	LEU
1	B	405	LEU
1	B	424	SER
1	B	429	GLN
1	B	462	LYS
1	B	473	ASP
1	B	477	ILE
1	B	491	ASN
1	C	66	LYS
1	C	81	ILE
1	C	86	LEU
1	C	89	ASN
1	C	102	LEU
1	C	109	SER
1	C	110	MET
1	C	123	ASN
1	C	124	GLU
1	C	152	ASN
1	C	226	ASP
1	C	291	LEU
1	C	296	ILE
1	C	313	PHE
1	C	315	ILE
1	C	321	LEU
1	C	337	ILE
1	C	365	ILE
1	C	393	VAL
1	C	406	THR
1	C	426	THR
1	C	433	ARG
1	C	436	GLU

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Mol	Chain	Res	Type
1	C	437	SER
1	C	441	MET
1	C	445	ASP
1	C	454	THR
1	C	459	VAL
1	C	466	ILE
1	C	488	VAL
1	C	494	ILE
1	D	12	VAL
1	D	14	ARG
1	D	19	LEU
1	D	45	ASP
1	D	57	GLU
1	D	75	ILE
1	D	90	ILE
1	D	95	ASN
1	D	110	MET
1	D	112	CYS
1	D	144	THR
1	D	152	ASN
1	D	159	ASP
1	D	174	ILE
1	D	176	THR
1	D	181	ARG
1	D	241	ILE
1	D	242	ASP
1	D	243	ASN
1	D	247	THR
1	D	250	LEU
1	D	252	ILE
1	D	257	MET
1	D	260	PRO
1	D	271	VAL
1	D	272	THR
1	D	275	THR
1	D	278	ASP
1	D	296	ILE
1	D	305	ASP
1	D	311	SER
1	D	312	LYS
1	D	316	PHE
1	D	322	TRP

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Mol	Chain	Res	Type
1	D	338	ASP
1	D	348	LEU
1	D	352	LEU
1	D	357	LEU
1	D	365	ILE
1	D	374	ILE
1	D	376	VAL
1	D	393	VAL
1	D	395	SER
1	D	397	LEU
1	D	405	LEU
1	D	415	THR
1	D	418	LEU
1	D	431	TYR
1	D	437	SER
1	D	441	MET
1	D	454	THR
1	D	468	ILE
1	D	475	ILE
1	D	477	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	221	ASN
1	A	254	ASN
1	A	286	GLN
1	A	320	ASN
1	A	356	GLN
1	A	470	ASN
1	B	39	HIS
1	B	179	GLN
1	B	221	ASN
1	B	255	HIS
1	B	258	ASN
1	B	320	ASN
1	B	446	HIS
1	C	152	ASN
1	C	179	GLN
1	C	286	GLN
1	C	319	ASN

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Mol	Chain	Res	Type
1	C	429	GLN
1	D	125	ASN
1	D	254	ASN
1	D	258	ASN
1	D	320	ASN
1	D	334	GLN
1	D	446	HIS

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	465/528 (88%)	-0.41	2 (0%) 92 86	80, 145, 200, 335	0
1	B	467/528 (88%)	-0.52	0 100 100	72, 130, 184, 231	0
1	C	450/528 (85%)	-0.24	7 (1%) 72 57	85, 190, 241, 272	0
1	D	468/528 (88%)	-0.60	1 (0%) 95 91	58, 114, 164, 227	0
All	All	1850/2112 (87%)	-0.44	10 (0%) 91 83	58, 135, 218, 335	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ASP	3.0
1	A	208	TYR	2.7
1	C	55	LEU	2.7
1	C	336	ALA	2.5
1	A	209	PRO	2.4
1	C	352	LEU	2.4
1	D	11	GLU	2.2
1	C	155	ASN	2.1
1	C	90	ILE	2.1
1	C	350	GLY	2.1

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.