



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:03 PM UTC

PDB ID : 3R2W / pdb_00003r2w
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

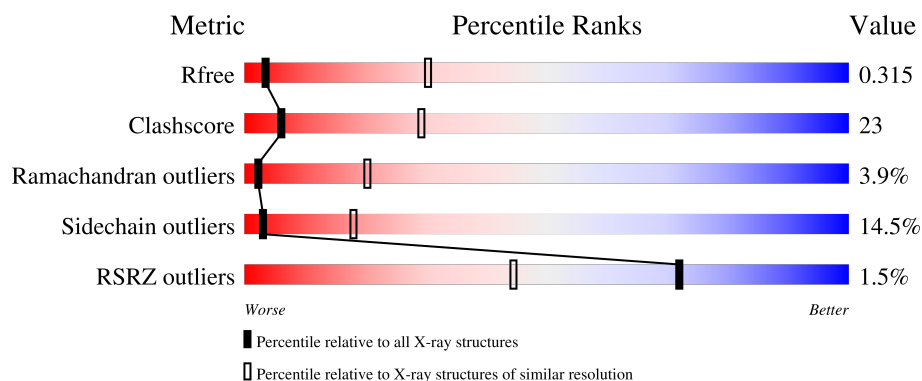
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 $\leq 5\%$. 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	% 47% 33% 7% • 12%
1	B	528	44% 34% 9% • 12%
1	C	528	3% 53% 27% 5% 15%
1	D	528	% 43% 36% 9% • 11%

2 Entry composition

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

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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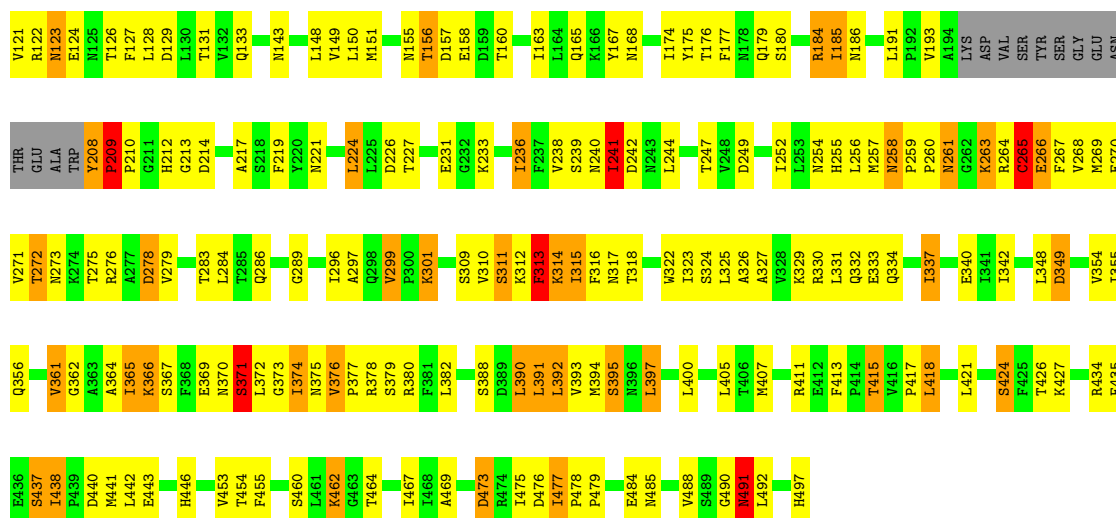
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	GLY	-	expression tag	UNP Q16851
B	-28	SER	-	expression tag	UNP Q16851
B	-27	SER	-	expression tag	UNP Q16851
B	-26	HIS	-	expression tag	UNP Q16851
B	-25	HIS	-	expression tag	UNP Q16851
B	-24	HIS	-	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

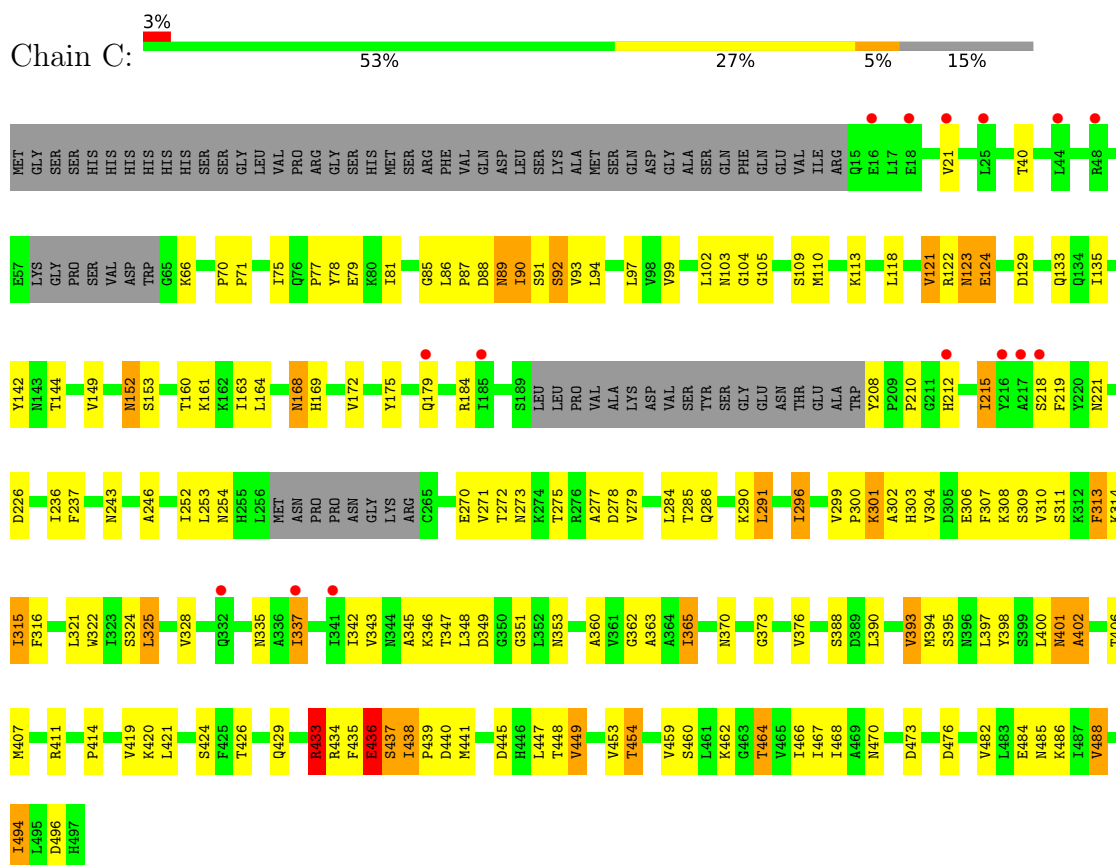
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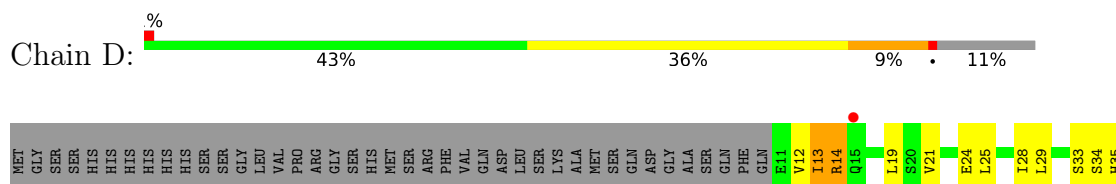
Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	SER	-	expression tag	UNP Q16851
D	-26	HIS	-	expression tag	UNP Q16851
D	-25	HIS	-	expression tag	UNP Q16851
D	-24	HIS	-	expression tag	UNP Q16851
D	-23	HIS	-	expression tag	UNP Q16851
D	-22	HIS	-	expression tag	UNP Q16851
D	-21	HIS	-	expression tag	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

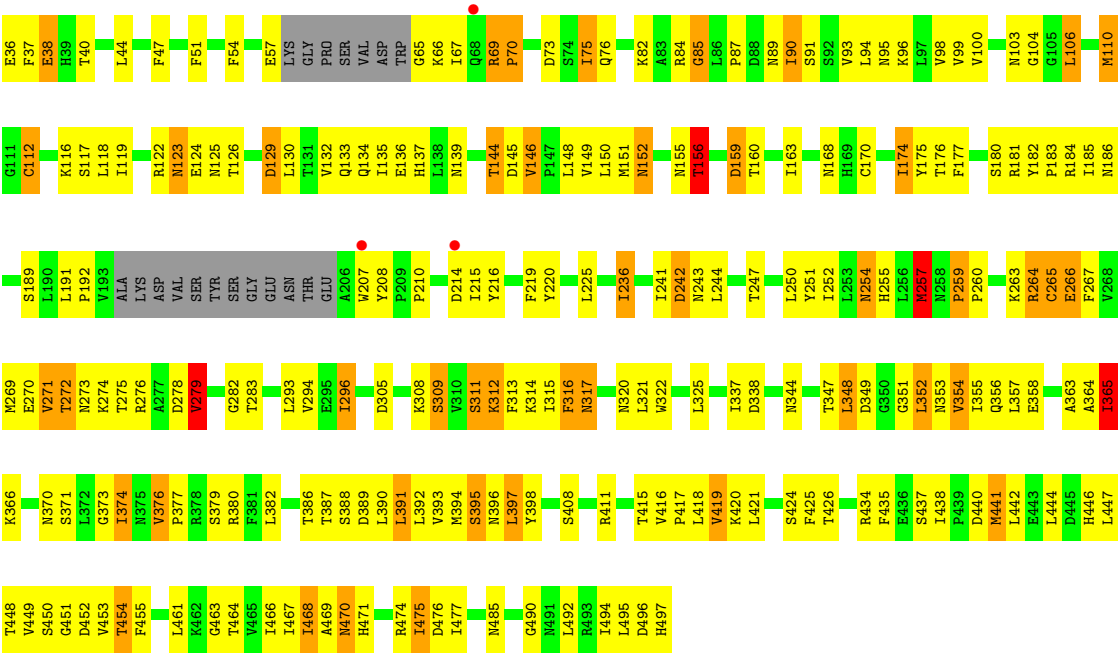


• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



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





4 Data and refinement statistics

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) 93.3 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.24 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.75	1/3602 (0.0%)	1.08	17/4894 (0.3%)
1	B	0.76	1/3596 (0.0%)	1.15	17/4889 (0.3%)
1	C	0.70	1/3353 (0.0%)	0.97	8/4578 (0.2%)
1	D	0.86	1/3630 (0.0%)	1.20	20/4936 (0.4%)
All	All	0.77	4/14181 (0.0%)	1.11	62/19297 (0.3%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	SER	CB-OG	7.14	1.56	1.42
1	C	90	ILE	CA-CB	6.21	1.60	1.53
1	B	209	PRO	CA-C	5.39	1.57	1.52
1	D	279	VAL	CA-CB	5.23	1.60	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	SER	N-CA-C	-9.69	95.35	109.59
1	A	114	GLY	CA-C-N	8.52	130.48	119.84
1	A	114	GLY	C-N-CA	8.52	130.48	119.84
1	A	209	PRO	CA-C-N	8.22	130.12	119.84
1	A	209	PRO	C-N-CA	8.22	130.12	119.84
1	B	209	PRO	CA-C-N	8.00	129.83	119.84
1	B	209	PRO	C-N-CA	8.00	129.83	119.84
1	B	68	GLN	N-CA-C	7.15	119.04	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	CYS	CA-C-N	6.89	134.09	121.70
1	D	265	CYS	C-N-CA	6.89	134.09	121.70
1	D	33	SER	CA-C-N	6.75	134.43	121.54
1	D	33	SER	C-N-CA	6.75	134.43	121.54
1	D	244	LEU	N-CA-C	-6.64	105.00	113.23
1	B	208	TYR	CA-C-N	6.32	126.89	120.38
1	B	208	TYR	C-N-CA	6.32	126.89	120.38
1	B	114	GLY	CA-C-N	6.18	126.51	119.83
1	B	114	GLY	C-N-CA	6.18	126.51	119.83
1	C	438	ILE	CA-C-N	6.08	126.92	120.11
1	C	438	ILE	C-N-CA	6.08	126.92	120.11
1	C	279	VAL	N-CA-C	6.08	116.25	110.42
1	A	68	GLN	N-CA-C	6.07	119.14	110.10
1	D	70	PRO	N-CA-C	6.07	118.10	110.70
1	A	475	ILE	CB-CA-C	-6.05	103.12	110.99
1	D	259	PRO	CA-C-N	5.94	127.27	119.84
1	D	259	PRO	C-N-CA	5.94	127.27	119.84
1	B	123	ASN	N-CA-C	5.93	122.11	113.40
1	C	433	ARG	N-CA-C	-5.92	104.91	111.36
1	D	470	ASN	N-CA-C	5.88	118.29	110.53
1	B	426	THR	N-CA-C	5.87	117.36	110.97
1	A	123	ASN	N-CA-C	5.80	121.93	113.40
1	A	299	VAL	CA-C-N	5.78	127.07	119.84
1	A	299	VAL	C-N-CA	5.78	127.07	119.84
1	D	490	GLY	N-CA-C	5.75	117.93	110.45
1	D	69	ARG	CA-C-N	5.75	126.30	120.38
1	D	69	ARG	C-N-CA	5.75	126.30	120.38
1	C	496	ASP	N-CA-C	5.71	122.96	110.80
1	D	344	ASN	N-CA-C	5.65	117.90	108.02
1	D	317	ASN	N-CA-C	5.59	117.81	109.25
1	D	156	THR	CB-CA-C	-5.57	101.31	110.72
1	C	448	THR	CB-CA-C	5.50	118.61	110.14
1	A	455	PHE	N-CA-C	5.49	118.93	110.42
1	A	146	VAL	CB-CA-C	-5.43	104.90	110.71
1	B	263	LYS	CA-C-N	5.42	131.46	121.70
1	B	263	LYS	C-N-CA	5.42	131.46	121.70
1	B	299	VAL	CA-C-N	5.41	126.26	119.98
1	B	299	VAL	C-N-CA	5.41	126.26	119.98
1	A	416	VAL	CA-C-N	5.30	125.22	119.76
1	A	416	VAL	C-N-CA	5.30	125.22	119.76
1	D	408	SER	N-CA-C	5.25	117.37	109.23
1	B	415	THR	CA-C-N	-5.25	118.81	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	THR	C-N-CA	-5.25	118.81	122.59
1	D	112	CYS	N-CA-C	5.22	117.19	108.99
1	B	236	ILE	CB-CA-C	-5.21	103.63	110.98
1	A	110	MET	N-CA-C	-5.16	106.98	113.28
1	C	92	SER	CA-C-N	5.14	130.96	121.70
1	C	92	SER	C-N-CA	5.14	130.96	121.70
1	A	372	LEU	N-CA-C	5.14	116.55	107.61
1	A	229	ILE	N-CA-C	-5.13	105.39	110.62
1	B	241	ILE	N-CA-C	-5.05	106.44	113.00
1	D	257	MET	N-CA-C	-5.02	103.06	110.48
1	D	419	VAL	N-CA-C	5.01	115.19	107.77
1	A	235	TYR	N-CA-C	5.00	117.06	108.90

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 ⓘ

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	145	0
1	B	3534	0	3471	182	0
1	C	3299	0	3094	107	0
1	D	3566	0	3511	198	0
All	All	13938	0	13550	620	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 23.

All (620) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:309:SER:HA	1:A:310:VAL:C	1.89	0.96
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:110:MET:HE2	1:B:119:ILE:HD13	1.51	0.92
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: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
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:D:122:ARG:C	1:D:124:GLU:HA	2.07	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:77:PRO:C	1:C:79:GLU:H	1.94	0.75
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
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: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:D:110:MET:HE3	1:D:119:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:390:LEU:HB3	1:A:394:MET:HE3	1.75	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: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:B:269:MET:HE3	1:B:317:ASN:CG	2.21	0.65
1:C:488:VAL:HG12	1:D:492:LEU:HD11	1.78	0.65
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:B:257:MET:O	1:B:258:ASN:C	2.39	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:D:123:ASN:N	1:D:124:GLU:HA	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:269:MET:HE2	1:A:317:ASN:OD1	1.99	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:94:LEU:C	1:B:96:LYS:H	2.09	0.61
1:B:395:SER:HB2	1:B:397:LEU:H	1.66	0.61
1:B:21:VAL:HG12	1:B:25:LEU:HD12	1.83	0.60
1:B:332:GLN:C	1:B:334:GLN:H	2.09	0.60
1:D:185:ILE:CG2	1:D:355:ILE:HB	2.30	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:A:269:MET:HE1	1:A:293:LEU:HD13	1.85	0.59
1:A:362:GLY:C	1:A:364:ALA:H	2.09	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	2.02	0.58
1:A:446:HIS:HB3	1:A:464:THR:CG2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:440:ASP:C	1:D:441:MET:HG2	2.29	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:D:274:LYS:HZ3	1:D:308:LYS:HA	1.68	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:309:SER:CA	1:A:310:VAL:C	2.70	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
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:D:494:ILE:C	1:D:495:LEU:HG	2.30	0.56
1:B:266:GLU:OE1	1:B:369:GLU:HG2	2.06	0.56
1:B:497:HIS:C	1:C:420:LYS:HD3	2.30	0.56
1:B:10:GLN:HA	1:B:13:ILE:HD12	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:497:HIS:O	1:C:420:LYS:NZ	2.27	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:B:390:LEU:HD22	1:B:394:MET:HE2	1.89	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:B:369:GLU:C	1:B:371:SER:H	2.16	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:C:236:ILE:HD11	1:C:325:LEU:HG	1.90	0.53
1:A:122:ARG:C	1:A:124:GLU:HA	2.33	0.53
1:A:236:ILE:HG22	1:A:323:ILE:HB	1.89	0.53
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: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:C:435:PHE:O	1:C:436:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:71:PRO:C	1:A:73:ASP:H	2.16	0.52
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:D:168:ASN:C	1:D:170:CYS:H	2.16	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:A:267:PHE:C	1:A:267:PHE:CD2	2.89	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
1:D:470:ASN:O	1:D:471:HIS:C	2.53	0.51
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:420:LYS:HG3	1:D:497:HIS:C	2.36	0.50
1:B:126:THR:HG22	1:B:129:ASP:CG	2.36	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:A:473:ASP:CG	1:A:491:ASN:HB2	2.37	0.49
1:C:307:PHE:O	1:C:308:LYS:HG2	2.13	0.49
1:D:126:THR:HG22	1:D:129:ASP:CG	2.37	0.49
1:D:181:ARG:HH21	1:D:207:TRP:CD1	2.30	0.49
1:D:91:SER:C	1:D:93:VAL:H	2.19	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: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:D:313:PHE:C	1:D:315:ILE:H	2.19	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:A:320:ASN:C	1:A:321:LEU:HG	2.38	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
1:B:122:ARG:C	1:B:124:GLU:HA	2.36	0.48
1:D:93:VAL:CG2	1:D:257:MET:HG3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:94:LEU:C	1:D:96:LYS:H	2.22	0.48
1:D:396:ASN:ND2	1:D:442:LEU:HG	2.29	0.48
1:A:116:LYS:C	1:A:118:LEU:H	2.21	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:B:332:GLN:C	1:B:334:GLN:N	2.72	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:C:77:PRO:C	1:C:79:GLU:N	2.63	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:463:GLY:HA3	1:A:485:ASN:OD1	2.14	0.47
1:B:93:VAL:O	1:B:257:MET:HE3	2.15	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:B:478:PRO:O	1:B:479:PRO:C	2.58	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:C:390:LEU:HB3	1:C:394:MET:HE3	1.96	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: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: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:B:378:ARG:C	1:B:380:ARG:N	2.73	0.46
1:C:440:ASP:HB3	1:C:460:SER:HA	1.97	0.46
1:B:157:ASP:O	1:B:158:GLU:C	2.57	0.46
1:B:313:PHE:C	1:B:315:ILE:H	2.21	0.46
1:C:337:ILE:H	1:C:337:ILE:HG13	1.56	0.46
1:C:440:ASP:C	1:C:441:MET:HG2	2.39	0.46
1:C:92:SER:N	1:C:94:LEU:H	2.14	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:D:269:MET:HE3	1:D:317:ASN:CG	2.40	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:390:LEU:O	1:D:391:LEU:C	2.59	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:A:395:SER:C	1:A:397:LEU:H	2.25	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: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:B:365:ILE:O	1:B:366:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ARG:C	1:B:380:ARG:H	2.24	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
1:A:474:ARG:HB3	1:A:493:ARG:HE	1.82	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: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:362:GLY:C	1:A:364:ALA:N	2.75	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: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:A:411:ARG:O	1:A:412:GLU:C	2.59	0.44
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:A:168:ASN:C	1:A:170:CYS:H	2.25	0.44
1:B:94:LEU:C	1:B:96:LYS:N	2.74	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:A:267:PHE:C	1:A:267:PHE:HD2	2.26	0.44
1:B:212:HIS:C	1:B:214:ASP:H	2.25	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: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:C:407:MET:HE1	1:C:414:PRO:HA	1.99	0.44
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.74	0.44
1:C:345:ALA:C	1:C:346:LYS:HG3	2.43	0.44
1:D:269:MET:O	1:D:270:GLU:C	2.61	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:312:LYS:C	1:B:314:LYS:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:491:ASN:O	1:B:491:ASN:N	2.52	0.43
1:D:219:PHE:O	1:D:220:TYR:C	2.62	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: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:A:264:ARG:HE	1:A:370:ASN:C	2.22	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:D:134:GLN:C	1:D:136:GLU:N	2.75	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: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:B:325:LEU:O	1:B:326:ALA:C	2.62	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:D:390:LEU:HB3	1:D:394:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:103:ASN:HD22	1:C:152:ASN:HB3	1.83	0.42
1:D:93:VAL:O	1:D:257:MET:HE3	2.20	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:A:311:SER:C	1:A:313:PHE:H	2.25	0.42
1:B:366:LYS:HB2	1:B:366:LYS:HE3	1.78	0.42
1:B:391:LEU:HG	1:B:392:LEU:N	2.32	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:D:364:ALA:O	1:D:365:ILE:C	2.62	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:D:103:ASN:O	1:D:104:GLY:C	2.62	0.42
1:D:210:PRO:HG2	1:D:214:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLU:HA	1:B:324:SER:HB3	2.02	0.42
1:B:364:ALA:O	1:B:365:ILE:C	2.63	0.42
1:B:370:ASN:O	1:B:371:SER:C	2.63	0.42
1:B:435:PHE:C	1:B:437:SER:H	2.27	0.42
1:C:168:ASN:O	1:C:169:HIS:HB2	2.20	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: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:C:92:SER:HB2	1:C:93:VAL:HB	2.02	0.41
1:D:89:ASN:C	1:D:91:SER:HB3	2.45	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: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: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:116:LYS:C	1:D:118:LEU:H	2.28	0.41
1:D:168:ASN:C	1:D:170:CYS:N	2.78	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:A:168:ASN:C	1:A:170:CYS:N	2.79	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:D:349:ASP:C	1:D:351:GLY:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:297:ALA:C	1:B:299:VAL:H	2.27	0.41
1:B:391:LEU:O	1:B:392:LEU:C	2.64	0.41
1:B:407:MET:HE3	1:B:411:ARG:HG2	2.03	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
1:D:270:GLU:OE1	1:D:380:ARG:NH2	2.54	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:A:441:MET:C	1:A:443:GLU:N	2.79	0.40
1:C:300:PRO:O	1:C:302:ALA:N	2.54	0.40
1:C:347:THR:OG1	1:C:351:GLY:O	2.35	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:37:PHE:O	1:D:38:GLU:C	2.64	0.40
1:D:210:PRO:C	1:D:358:GLU:HG2	2.45	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/528 (87%)	376 (82%)	64 (14%)	19 (4%)	2	19
1	B	461/528 (87%)	377 (82%)	58 (13%)	26 (6%)	1	14
1	C	442/528 (84%)	363 (82%)	65 (15%)	14 (3%)	3	24
1	D	462/528 (88%)	384 (83%)	65 (14%)	13 (3%)	4	26
All	All	1824/2112 (86%)	1500 (82%)	252 (14%)	72 (4%)	2	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	332 (87%)	49 (13%)	4	22
1	B	380/470 (81%)	318 (84%)	62 (16%)	2	15
1	C	341/470 (73%)	300 (88%)	41 (12%)	5	24
1	D	385/470 (82%)	322 (84%)	63 (16%)	2	14
All	All	1487/1880 (79%)	1272 (86%)	215 (14%)	3	18

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	31	THR

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Mol	Chain	Res	Type
1	A	67	ILE
1	A	80	LYS
1	A	81	ILE
1	A	118	LEU
1	A	132	VAL
1	A	145	ASP
1	A	148	LEU
1	A	152	ASN
1	A	163	ILE
1	A	184	ARG
1	A	189	SER
1	A	215	ILE
1	A	236	ILE
1	A	240	ASN
1	A	241	ILE
1	A	253	LEU
1	A	266	GLU
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	334	GLN
1	A	342	ILE
1	A	343	VAL
1	A	352	LEU
1	A	367	SER
1	A	372	LEU
1	A	374	ILE
1	A	376	VAL
1	A	379	SER
1	A	382	LEU
1	A	395	SER
1	A	399	SER
1	A	401	ASN
1	A	405	LEU
1	A	408	SER
1	A	424	SER
1	A	444	LEU
1	A	447	LEU
1	A	449	VAL

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Mol	Chain	Res	Type
1	A	453	VAL
1	A	459	VAL
1	A	464	THR
1	A	476	ASP
1	A	477	ILE
1	B	28	ILE
1	B	30	THR
1	B	31	THR
1	B	40	THR
1	B	67	ILE
1	B	75	ILE
1	B	86	LEU
1	B	90	ILE
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	193	VAL
1	B	236	ILE
1	B	238	VAL
1	B	239	SER
1	B	241	ILE
1	B	247	THR
1	B	265	CYS
1	B	272	THR
1	B	278	ASP
1	B	279	VAL
1	B	296	ILE
1	B	301	LYS
1	B	311	SER
1	B	313	PHE
1	B	315	ILE
1	B	316	PHE
1	B	323	ILE
1	B	337	ILE
1	B	340	GLU

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Mol	Chain	Res	Type
1	B	342	ILE
1	B	349	ASP
1	B	354	VAL
1	B	361	VAL
1	B	365	ILE
1	B	366	LYS
1	B	367	SER
1	B	371	SER
1	B	374	ILE
1	B	376	VAL
1	B	382	LEU
1	B	390	LEU
1	B	391	LEU
1	B	395	SER
1	B	397	LEU
1	B	400	LEU
1	B	405	LEU
1	B	418	LEU
1	B	424	SER
1	B	427	LYS
1	B	438	ILE
1	B	462	LYS
1	B	473	ASP
1	B	477	ILE
1	B	491	ASN
1	C	21	VAL
1	C	40	THR
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	168	ASN
1	C	226	ASP
1	C	278	ASP
1	C	291	LEU
1	C	296	ILE

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Mol	Chain	Res	Type
1	C	299	VAL
1	C	313	PHE
1	C	315	ILE
1	C	321	LEU
1	C	325	LEU
1	C	335	ASN
1	C	337	ILE
1	C	342	ILE
1	C	365	ILE
1	C	393	VAL
1	C	397	LEU
1	C	401	ASN
1	C	406	THR
1	C	426	THR
1	C	433	ARG
1	C	436	GLU
1	C	445	ASP
1	C	449	VAL
1	C	454	THR
1	C	459	VAL
1	C	464	THR
1	C	466	ILE
1	C	488	VAL
1	C	494	ILE
1	D	12	VAL
1	D	13	ILE
1	D	14	ARG
1	D	19	LEU
1	D	29	LEU
1	D	35	HIS
1	D	57	GLU
1	D	67	ILE
1	D	75	ILE
1	D	90	ILE
1	D	95	ASN
1	D	106	LEU
1	D	110	MET
1	D	112	CYS
1	D	144	THR
1	D	146	VAL
1	D	152	ASN
1	D	156	THR

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Mol	Chain	Res	Type
1	D	159	ASP
1	D	174	ILE
1	D	176	THR
1	D	236	ILE
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	279	VAL
1	D	296	ILE
1	D	305	ASP
1	D	311	SER
1	D	312	LYS
1	D	316	PHE
1	D	322	TRP
1	D	338	ASP
1	D	348	LEU
1	D	352	LEU
1	D	354	VAL
1	D	357	LEU
1	D	365	ILE
1	D	374	ILE
1	D	376	VAL
1	D	391	LEU
1	D	393	VAL
1	D	395	SER
1	D	397	LEU
1	D	415	THR
1	D	416	VAL
1	D	418	LEU
1	D	437	SER
1	D	441	MET
1	D	454	THR
1	D	468	ILE

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Mol	Chain	Res	Type
1	D	475	ILE
1	D	477	ILE
1	D	485	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	52	HIS
1	A	137	HIS
1	A	221	ASN
1	A	254	ASN
1	A	286	GLN
1	A	320	ASN
1	A	356	GLN
1	B	39	HIS
1	B	152	ASN
1	B	179	GLN
1	B	221	ASN
1	B	255	HIS
1	B	258	ASN
1	B	320	ASN
1	B	334	GLN
1	B	335	ASN
1	B	375	ASN
1	B	446	HIS
1	B	458	ASN
1	C	152	ASN
1	C	179	GLN
1	C	286	GLN
1	C	429	GLN
1	D	125	ASN
1	D	137	HIS
1	D	221	ASN
1	D	254	ASN
1	D	258	ASN
1	D	320	ASN
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 oligosaccharides 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

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, 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%)	-0.10	7 (1%) 72 44	80, 145, 200, 335	0
1	B	467/528 (88%)	-0.26	1 (0%) 91 80	72, 130, 184, 231	0
1	C	450/528 (85%)	0.06	15 (3%) 49 28	85, 190, 241, 272	0
1	D	468/528 (88%)	-0.24	4 (0%) 81 56	58, 114, 164, 227	0
All	All	1850/2112 (87%)	-0.14	27 (1%) 72 44	58, 135, 218, 335	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	PRO	7.3
1	A	209	PRO	7.3
1	A	208	TYR	4.3
1	C	179	GLN	4.1
1	C	217	ALA	3.6
1	C	216	TYR	3.3
1	C	212	HIS	2.9
1	C	25	LEU	2.8
1	A	412	GLU	2.7
1	C	44	LEU	2.6
1	A	387	THR	2.5
1	C	341	ILE	2.5
1	C	218	SER	2.5
1	A	207	TRP	2.5
1	C	16	GLU	2.4
1	D	207	TRP	2.4
1	C	332	GLN	2.3
1	D	214	ASP	2.3
1	D	68	GLN	2.3
1	C	48	ARG	2.3
1	C	185	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	CYS	2.2
1	B	73	ASP	2.1
1	C	337	ILE	2.1
1	D	15	GLN	2.1
1	C	18	GLU	2.1
1	C	21	VAL	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 oligosaccharides 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.