



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:15 PM UTC

PDB ID : 1Y1U / pdb_00001y1u
Title : Structure of unphosphorylated STAT5a
Authors : Neculai, D.; Neculai, A.M.; Verrier, S.; Straub, K.; Klumpp, K.; Pfitzner, E.;
Becker, S.
Deposited on : 2004-11-19
Resolution : 3.21 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

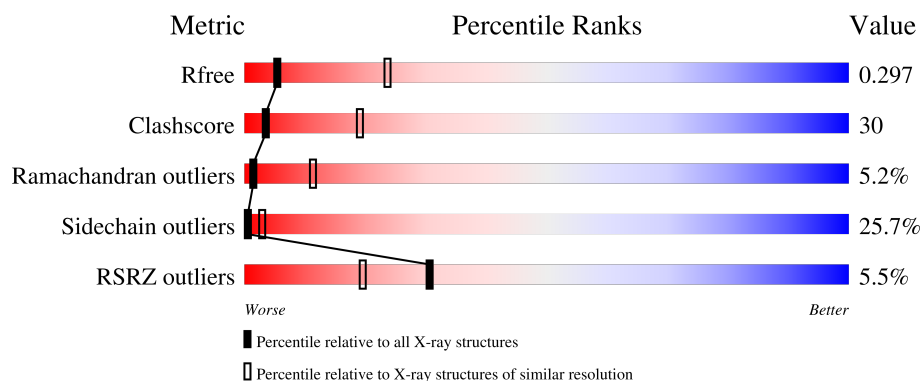
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	585	
1	B	585	
1	C	585	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13293 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.

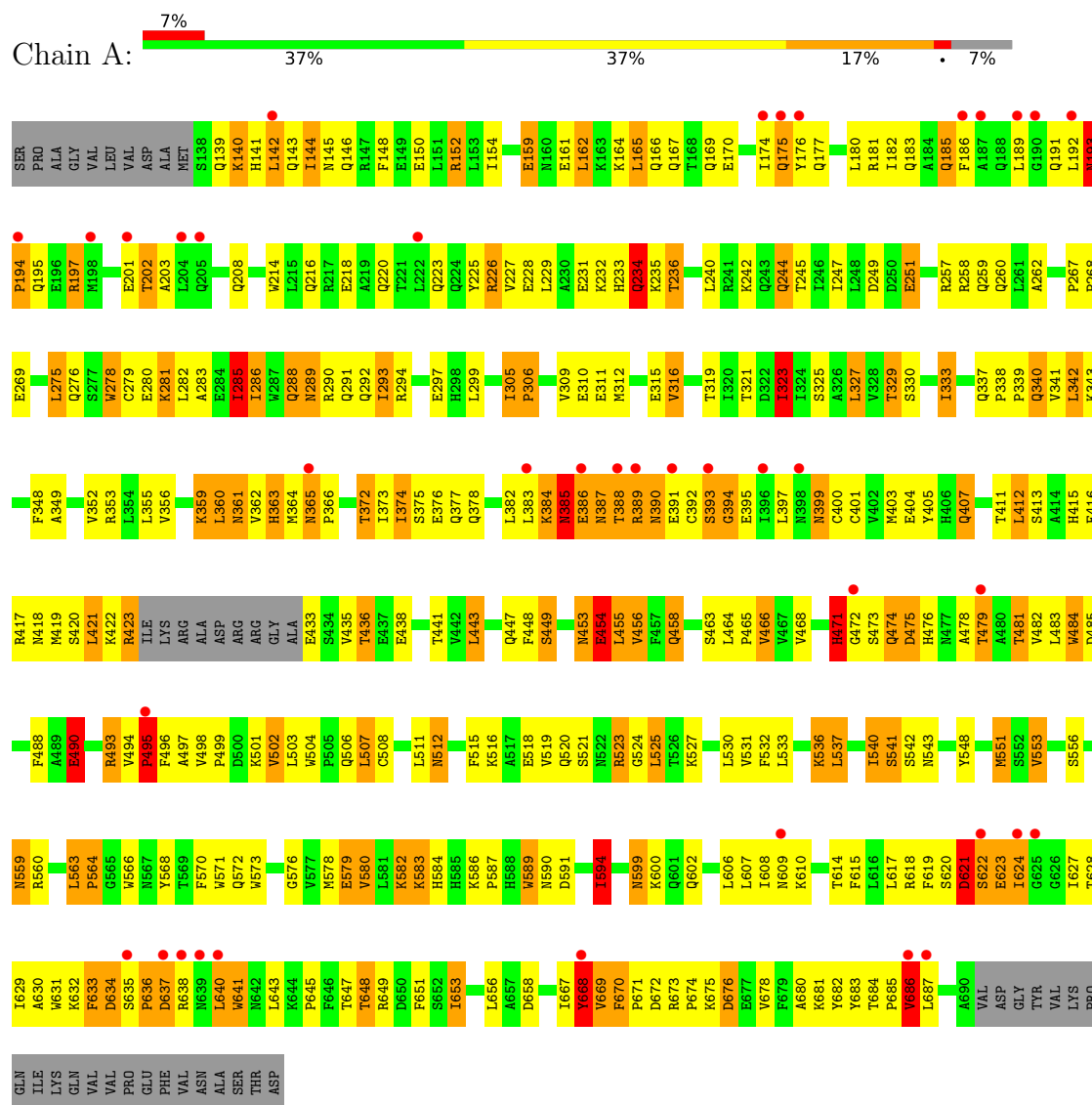
- Molecule 1 is a protein called Signal transducer and activator of transcription 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total 4431	C 2818	N 778	O 821	S 14	0	0	0
1	B	544	Total 4431	C 2818	N 778	O 821	S 14	0	0	0
1	C	544	Total 4431	C 2818	N 778	O 821	S 14	0	0	0

3 Residue-property plots

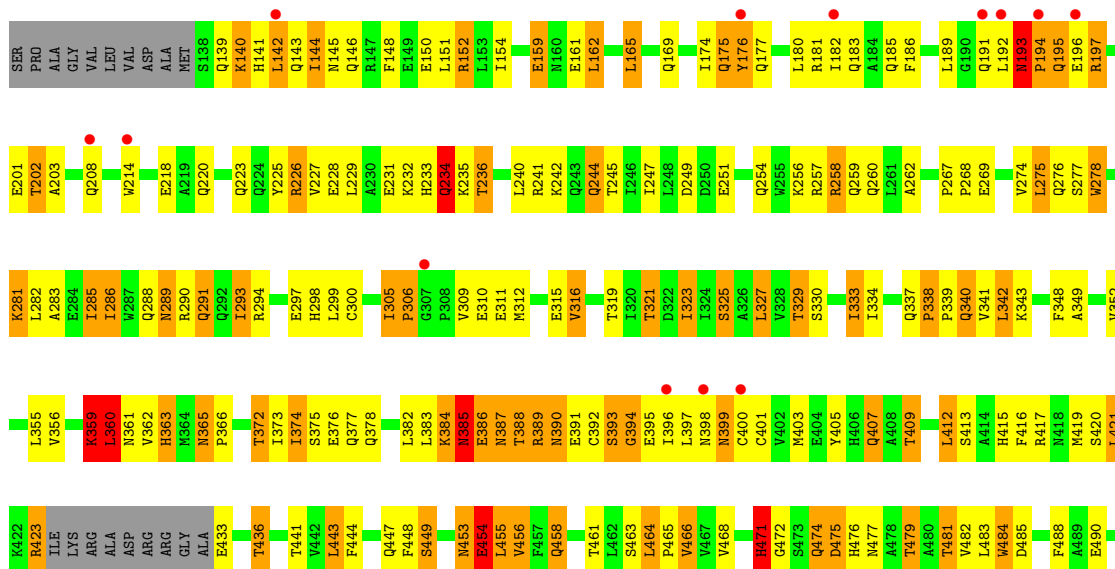
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

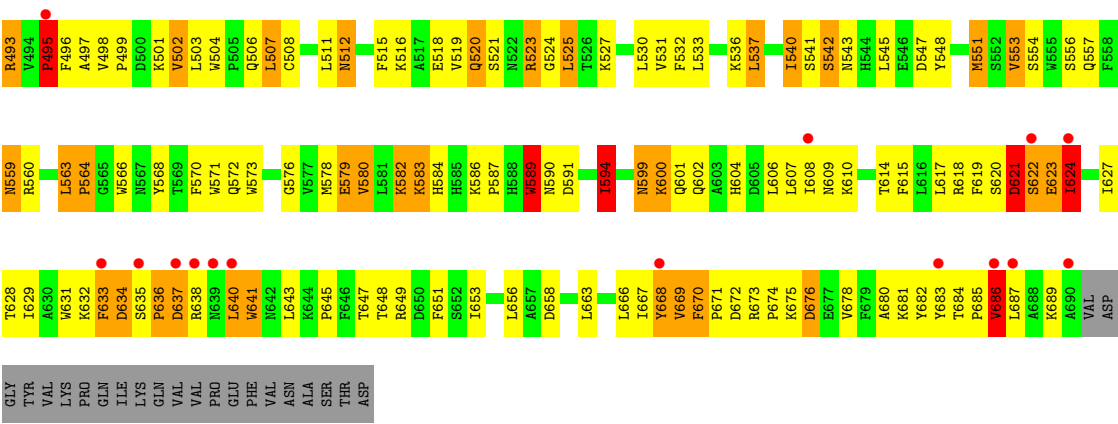
- Molecule 1: Signal transducer and activator of transcription 5A



- Molecule 1: Signal transducer and activator of transcription 5A







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.02Å 235.43Å 111.42Å 90.00° 108.76° 90.00°	Depositor
Resolution (Å)	78.56 – 3.21 78.56 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (78.56-3.21) 98.6 (78.56-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.266 , 0.299 0.264 , 0.297	Depositor DCC
R_{free} test set	5010 reflections (8.82%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13293	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.43% 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	0.82	4/4527 (0.1%)	1.16	25/6134 (0.4%)
1	B	0.82	1/4527 (0.0%)	1.15	24/6134 (0.4%)
1	C	0.81	2/4527 (0.0%)	1.14	25/6134 (0.4%)
All	All	0.81	7/13581 (0.1%)	1.15	74/18402 (0.4%)

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	A	0	5
1	B	0	6
1	C	0	5
All	All	0	16

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	594	ILE	CA-CB	6.12	1.61	1.53
1	A	594	ILE	CA-CB	5.71	1.60	1.53
1	A	285	ILE	CA-CB	5.64	1.62	1.54
1	C	396	ILE	CA-CB	5.46	1.59	1.54
1	A	653	ILE	CA-CB	5.43	1.61	1.54
1	B	653	ILE	CA-CB	5.43	1.61	1.54
1	A	323	ILE	CA-CB	5.21	1.61	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ASN	CA-C-N	-8.12	109.69	119.84
1	B	193	ASN	C-N-CA	-8.12	109.69	119.84
1	A	365	ASN	CA-C-N	7.69	128.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ASN	C-N-CA	7.69	128.30	120.38
1	A	193	ASN	CA-C-N	-7.50	110.47	119.84
1	A	193	ASN	C-N-CA	-7.50	110.47	119.84
1	C	193	ASN	CA-C-N	-7.47	110.50	119.84
1	C	193	ASN	C-N-CA	-7.47	110.50	119.84
1	B	365	ASN	CA-C-N	7.16	127.76	120.38
1	B	365	ASN	C-N-CA	7.16	127.76	120.38
1	B	621	ASP	N-CA-C	-7.15	103.52	111.82
1	A	634	ASP	N-CA-C	6.94	119.87	111.82
1	A	624	ILE	N-CA-C	6.93	120.73	111.17
1	C	201	GLU	N-CA-C	-6.92	103.75	111.71
1	B	201	GLU	N-CA-C	-6.85	103.83	111.71
1	A	563	LEU	CA-C-N	6.69	128.21	119.84
1	A	563	LEU	C-N-CA	6.69	128.21	119.84
1	B	490	GLU	CA-C-N	-6.66	112.91	119.90
1	B	490	GLU	C-N-CA	-6.66	112.91	119.90
1	C	689	LYS	N-CA-C	6.51	120.25	109.96
1	A	201	GLU	N-CA-C	-6.47	104.27	111.71
1	C	563	LEU	CA-C-N	6.44	127.89	119.84
1	C	563	LEU	C-N-CA	6.44	127.89	119.84
1	B	687	LEU	N-CA-C	-6.43	102.75	111.55
1	A	472	GLY	N-CA-C	-6.36	98.10	113.18
1	C	365	ASN	CA-C-N	6.29	126.86	120.38
1	C	365	ASN	C-N-CA	6.29	126.86	120.38
1	A	687	LEU	N-CA-C	-6.29	102.94	111.55
1	C	495	PRO	CA-C-N	-6.26	113.85	123.17
1	C	495	PRO	C-N-CA	-6.26	113.85	123.17
1	B	495	PRO	CA-C-N	-6.21	113.92	123.17
1	B	495	PRO	C-N-CA	-6.21	113.92	123.17
1	B	634	ASP	N-CA-C	6.10	118.90	111.82
1	C	634	ASP	N-CA-C	6.09	119.97	112.54
1	B	563	LEU	CA-C-N	6.09	127.45	119.84
1	B	563	LEU	C-N-CA	6.09	127.45	119.84
1	C	472	GLY	N-CA-C	-5.92	99.14	113.18
1	A	401	CYS	N-CA-C	5.84	118.72	110.14
1	A	668	TYR	N-CA-C	5.81	118.24	109.23
1	A	471	HIS	N-CA-C	5.73	115.67	108.45
1	C	687	LEU	N-CA-C	-5.72	103.71	111.55
1	C	476	HIS	N-CA-C	5.62	117.08	111.07
1	C	401	CYS	N-CA-C	5.60	118.37	110.14
1	B	472	GLY	N-CA-C	-5.57	99.98	113.18
1	C	621	ASP	N-CA-C	-5.55	105.32	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	GLU	CA-C-N	-5.51	114.12	119.90
1	A	490	GLU	C-N-CA	-5.51	114.12	119.90
1	A	476	HIS	N-CA-C	5.47	116.92	111.07
1	B	624	ILE	N-CA-C	5.42	118.64	111.17
1	B	176	TYR	CA-CB-CG	5.41	123.63	113.90
1	B	668	TYR	N-CA-C	5.40	117.60	109.23
1	A	495	PRO	CA-C-N	-5.39	115.13	123.17
1	A	495	PRO	C-N-CA	-5.39	115.13	123.17
1	B	471	HIS	N-CA-C	5.36	115.20	108.45
1	C	471	HIS	N-CA-C	5.34	115.18	108.45
1	B	338	PRO	CA-C-N	5.32	126.49	119.84
1	B	338	PRO	C-N-CA	5.32	126.49	119.84
1	A	251	GLU	N-CA-C	5.32	117.49	111.11
1	B	401	CYS	N-CA-C	5.21	117.78	109.81
1	A	279	CYS	N-CA-C	5.17	117.00	111.36
1	C	176	TYR	CA-CB-CG	5.16	123.18	113.90
1	C	464	LEU	CA-C-N	-5.15	114.93	120.03
1	C	464	LEU	C-N-CA	-5.15	114.93	120.03
1	A	621	ASP	N-CA-C	-5.13	105.81	111.71
1	A	361	ASN	N-CA-C	5.12	117.01	107.99
1	A	167	GLN	N-CA-C	-5.12	105.60	111.07
1	C	589	TRP	N-CA-C	5.11	116.71	111.03
1	B	673	ARG	N-CA-C	5.11	115.85	109.57
1	C	409	THR	N-CA-C	-5.11	99.92	110.80
1	C	338	PRO	CA-C-N	5.11	126.22	119.84
1	C	338	PRO	C-N-CA	5.11	126.22	119.84
1	B	409	THR	N-CA-C	-5.08	99.98	110.80
1	A	404	GLU	N-CA-C	5.03	116.79	108.13
1	C	624	ILE	N-CA-C	5.02	119.77	109.34

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Peptide
1	A	360	LEU	Peptide
1	A	387	ASN	Peptide
1	A	471	HIS	Peptide
1	A	623	GLU	Peptide
1	B	197	ARG	Peptide
1	B	360	LEU	Peptide
1	B	387	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	471	HIS	Peptide
1	B	565	GLY	Peptide
1	B	623	GLU	Peptide
1	C	197	ARG	Peptide
1	C	360	LEU	Peptide
1	C	387	ASN	Peptide
1	C	471	HIS	Peptide
1	C	623	GLU	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	4431	0	4415	270	0
1	B	4431	0	4415	267	0
1	C	4431	0	4415	264	0
All	All	13293	0	13245	786	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 30.

All (786) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:TYR:HB3	1:A:674:PRO:HA	1.21	1.14
1:C:668:TYR:HB3	1:C:674:PRO:HA	1.19	1.13
1:A:226:ARG:HH12	1:A:305:ILE:HG12	1.04	1.13
1:B:668:TYR:HB3	1:B:674:PRO:HA	1.21	1.13
1:C:226:ARG:HH12	1:C:305:ILE:HG12	0.96	1.12
1:B:226:ARG:HH12	1:B:305:ILE:HG12	1.04	1.08
1:C:186:PHE:HE1	1:C:208:GLN:HE22	1.04	1.01
1:A:361:ASN:HD22	1:B:361:ASN:HD22	1.00	0.99
1:B:399:ASN:O	1:B:400:CYS:SG	2.21	0.98
1:C:226:ARG:NH1	1:C:305:ILE:HG12	1.78	0.97
1:B:186:PHE:HE1	1:B:208:GLN:HE22	0.98	0.96
1:A:226:ARG:NH1	1:A:305:ILE:HG12	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PHE:HE1	1:A:208:GLN:HE22	0.96	0.93
1:B:226:ARG:NH1	1:B:305:ILE:HG12	1.81	0.93
1:B:523:ARG:HB3	1:B:589:TRP:CZ3	2.03	0.92
1:C:668:TYR:HB3	1:C:674:PRO:CA	2.01	0.91
1:A:364:MET:HG3	1:B:361:ASN:ND2	1.85	0.90
1:A:361:ASN:ND2	1:B:364:MET:HG3	1.85	0.90
1:A:523:ARG:HB3	1:A:589:TRP:CZ3	2.06	0.90
1:C:523:ARG:HB3	1:C:589:TRP:CZ3	2.06	0.89
1:A:361:ASN:HD22	1:B:361:ASN:ND2	1.71	0.88
1:B:668:TYR:HB3	1:B:674:PRO:CA	2.04	0.87
1:A:385:ASN:N	1:A:385:ASN:HD22	1.72	0.87
1:B:378:GLN:HE22	1:B:393:SER:H	1.21	0.87
1:A:361:ASN:ND2	1:B:361:ASN:HD22	1.73	0.86
1:B:186:PHE:HE1	1:B:208:GLN:NE2	1.74	0.86
1:A:668:TYR:HB3	1:A:674:PRO:CA	2.04	0.85
1:B:523:ARG:HB3	1:B:589:TRP:HZ3	1.39	0.85
1:A:214:TRP:NE1	1:A:218:GLU:OE1	2.09	0.85
1:C:399:ASN:O	1:C:400:CYS:SG	2.35	0.84
1:C:385:ASN:N	1:C:385:ASN:HD22	1.75	0.84
1:A:378:GLN:HE22	1:A:393:SER:H	1.24	0.84
1:B:281:LYS:O	1:B:285:ILE:HG22	1.76	0.84
1:A:385:ASN:ND2	1:A:385:ASN:H	1.72	0.84
1:B:385:ASN:N	1:B:385:ASN:HD22	1.74	0.84
1:A:186:PHE:HE1	1:A:208:GLN:NE2	1.75	0.84
1:B:214:TRP:NE1	1:B:218:GLU:OE1	2.10	0.84
1:B:385:ASN:H	1:B:385:ASN:ND2	1.75	0.83
1:C:281:LYS:O	1:C:285:ILE:HG22	1.77	0.83
1:C:523:ARG:HB3	1:C:589:TRP:HZ3	1.42	0.83
1:B:670:PHE:HB3	1:B:671:PRO:HD3	1.60	0.83
1:A:186:PHE:CE1	1:A:208:GLN:NE2	2.47	0.83
1:A:523:ARG:HB3	1:A:589:TRP:HZ3	1.44	0.83
1:C:378:GLN:HE22	1:C:393:SER:H	1.23	0.83
1:C:385:ASN:ND2	1:C:385:ASN:H	1.74	0.82
1:B:602:GLN:O	1:B:606:LEU:HG	1.80	0.82
1:A:399:ASN:HB3	1:A:419:MET:HG2	1.61	0.82
1:C:214:TRP:NE1	1:C:218:GLU:OE1	2.12	0.82
1:C:602:GLN:O	1:C:606:LEU:HG	1.80	0.81
1:A:670:PHE:HB3	1:A:671:PRO:HD3	1.60	0.80
1:B:186:PHE:CE1	1:B:208:GLN:NE2	2.48	0.80
1:B:599:ASN:ND2	1:B:602:GLN:H	1.79	0.80
1:A:281:LYS:O	1:A:285:ILE:HG22	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:SER:OG	1:B:628:THR:HG23	1.81	0.80
1:C:670:PHE:HB3	1:C:671:PRO:HD3	1.64	0.80
1:C:399:ASN:HB3	1:C:419:MET:HG2	1.64	0.80
1:C:503:LEU:O	1:C:506:GLN:HG2	1.83	0.79
1:C:186:PHE:HE1	1:C:208:GLN:NE2	1.79	0.79
1:C:634:ASP:O	1:C:636:PRO:HD3	1.82	0.78
1:A:634:ASP:O	1:A:636:PRO:HD3	1.83	0.78
1:B:140:LYS:H	1:B:140:LYS:HZ2	1.31	0.78
1:B:378:GLN:NE2	1:B:393:SER:H	1.80	0.78
1:A:385:ASN:N	1:A:385:ASN:ND2	2.30	0.78
1:A:418:ASN:HD21	1:B:170:GLU:HG3	1.49	0.77
1:B:634:ASP:O	1:B:636:PRO:HD3	1.84	0.77
1:C:681:LYS:HD2	1:C:682:TYR:CZ	2.19	0.77
1:B:399:ASN:HB3	1:B:419:MET:HG2	1.65	0.77
1:C:378:GLN:NE2	1:C:393:SER:H	1.83	0.77
1:A:170:GLU:HG3	1:B:418:ASN:HD21	1.51	0.76
1:B:503:LEU:O	1:B:506:GLN:HG2	1.85	0.76
1:B:385:ASN:N	1:B:385:ASN:ND2	2.32	0.75
1:C:186:PHE:CE1	1:C:208:GLN:NE2	2.51	0.75
1:C:599:ASN:ND2	1:C:602:GLN:H	1.84	0.75
1:B:193:ASN:HB2	1:B:194:PRO:CD	2.16	0.75
1:A:193:ASN:HB2	1:A:194:PRO:CD	2.16	0.75
1:A:602:GLN:O	1:A:606:LEU:HG	1.87	0.75
1:A:378:GLN:NE2	1:A:393:SER:H	1.84	0.75
1:B:623:GLU:HB3	1:B:645:PRO:HG2	1.69	0.74
1:A:556:SER:HA	1:A:560:ARG:HB3	1.70	0.74
1:B:251:GLU:OE2	1:B:251:GLU:HA	1.87	0.74
1:C:587:PRO:O	1:C:591:ASP:HB2	1.88	0.74
1:B:556:SER:HA	1:B:560:ARG:HB3	1.69	0.73
1:C:251:GLU:HA	1:C:251:GLU:OE2	1.87	0.73
1:C:620:SER:OG	1:C:628:THR:HG23	1.88	0.73
1:B:193:ASN:HB2	1:B:194:PRO:HD3	1.70	0.73
1:A:548:TYR:HA	1:A:551:MET:HG3	1.70	0.73
1:C:392:CYS:O	1:C:394:GLY:N	2.22	0.73
1:A:503:LEU:O	1:A:506:GLN:HG2	1.88	0.73
1:B:490:GLU:O	1:B:493:ARG:HG3	1.88	0.73
1:A:620:SER:OG	1:A:628:THR:HG23	1.88	0.73
1:A:490:GLU:O	1:A:493:ARG:HG3	1.89	0.72
1:A:471:HIS:CD2	1:A:474:GLN:HB2	2.24	0.72
1:C:193:ASN:HB2	1:C:194:PRO:CD	2.19	0.72
1:A:386:GLU:O	1:A:386:GLU:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ASN:ND2	1:A:602:GLN:H	1.88	0.72
1:A:193:ASN:HB2	1:A:194:PRO:HD3	1.71	0.72
1:B:392:CYS:O	1:B:394:GLY:N	2.23	0.72
1:C:548:TYR:HA	1:C:551:MET:HG3	1.72	0.71
1:B:386:GLU:O	1:B:386:GLU:HG2	1.90	0.71
1:C:386:GLU:O	1:C:386:GLU:HG2	1.90	0.71
1:C:471:HIS:CD2	1:C:474:GLN:HB2	2.26	0.71
1:A:392:CYS:O	1:A:394:GLY:N	2.25	0.70
1:A:251:GLU:OE2	1:A:251:GLU:HA	1.90	0.70
1:C:140:LYS:H	1:C:140:LYS:HZ2	1.39	0.70
1:C:680:ALA:HA	1:C:683:TYR:CD1	2.27	0.70
1:A:587:PRO:O	1:A:591:ASP:HB2	1.92	0.70
1:B:399:ASN:C	1:B:400:CYS:SG	2.74	0.70
1:B:582:LYS:HA	1:B:586:LYS:HG2	1.74	0.70
1:A:140:LYS:H	1:A:140:LYS:HZ2	1.39	0.69
1:A:399:ASN:O	1:A:400:CYS:SG	2.47	0.69
1:C:385:ASN:N	1:C:385:ASN:ND2	2.32	0.69
1:C:490:GLU:O	1:C:493:ARG:HG3	1.91	0.69
1:A:139:GLN:HG3	1:A:140:LYS:HD3	1.73	0.69
1:A:175:GLN:HE21	1:A:175:GLN:HA	1.57	0.69
1:A:620:SER:HB3	1:A:622:SER:HB2	1.74	0.69
1:C:193:ASN:HB2	1:C:194:PRO:HD3	1.74	0.69
1:C:225:TYR:HA	1:C:228:GLU:HG3	1.74	0.69
1:A:202:THR:CG2	1:A:203:ALA:N	2.56	0.69
1:A:523:ARG:HA	1:A:523:ARG:HH11	1.58	0.69
1:B:471:HIS:CD2	1:B:474:GLN:HB2	2.28	0.69
1:A:559:ASN:OD1	1:A:571:TRP:HB3	1.91	0.68
1:C:556:SER:HA	1:C:560:ARG:HB3	1.73	0.68
1:B:139:GLN:HG3	1:B:140:LYS:HD3	1.74	0.68
1:C:399:ASN:C	1:C:400:CYS:SG	2.76	0.68
1:B:620:SER:HB3	1:B:622:SER:HB2	1.76	0.68
1:C:139:GLN:HG3	1:C:140:LYS:HD3	1.75	0.68
1:B:548:TYR:HA	1:B:551:MET:HG3	1.75	0.68
1:B:286:ILE:HG13	1:B:323:ILE:HD11	1.76	0.67
1:C:374:ILE:HG22	1:C:441:THR:HG23	1.77	0.67
1:C:527:LYS:H	1:C:527:LYS:HD3	1.59	0.67
1:A:582:LYS:HA	1:A:586:LYS:HG2	1.76	0.67
1:A:623:GLU:HB3	1:A:645:PRO:HG2	1.77	0.67
1:C:610:LYS:O	1:C:632:LYS:HE2	1.95	0.67
1:C:623:GLU:HB3	1:C:645:PRO:HG2	1.77	0.67
1:B:681:LYS:HD2	1:B:682:TYR:CZ	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:HD2	1:A:682:TYR:CZ	2.30	0.66
1:B:395:GLU:CB	1:B:423:ARG:HD3	2.26	0.66
1:A:361:ASN:ND2	1:B:361:ASN:ND2	2.37	0.66
1:B:191:GLN:O	1:B:197:ARG:HD2	1.96	0.66
1:B:202:THR:CG2	1:B:203:ALA:N	2.59	0.66
1:A:680:ALA:HA	1:A:683:TYR:CD1	2.31	0.66
1:C:305:ILE:O	1:C:306:PRO:C	2.39	0.66
1:B:395:GLU:OE1	1:B:423:ARG:NH1	2.29	0.65
1:C:537:LEU:HD23	1:C:570:PHE:CG	2.31	0.65
1:A:305:ILE:O	1:A:306:PRO:C	2.37	0.65
1:B:610:LYS:O	1:B:632:LYS:HE2	1.97	0.65
1:C:631:TRP:CE2	1:C:641:TRP:HB3	2.32	0.64
1:A:475:ASP:O	1:A:479:THR:HB	1.97	0.64
1:A:527:LYS:HD3	1:A:527:LYS:H	1.62	0.64
1:B:225:TYR:HA	1:B:228:GLU:HG3	1.78	0.64
1:C:340:GLN:HG2	1:C:482:VAL:HG13	1.80	0.64
1:C:582:LYS:HA	1:C:586:LYS:HG2	1.80	0.64
1:A:202:THR:HG22	1:A:203:ALA:H	1.62	0.64
1:A:275:LEU:O	1:A:278:TRP:HB2	1.96	0.64
1:B:275:LEU:O	1:B:278:TRP:HB2	1.97	0.64
1:B:599:ASN:HD22	1:B:602:GLN:H	1.44	0.64
1:A:610:LYS:O	1:A:632:LYS:HE2	1.98	0.64
1:B:523:ARG:HA	1:B:523:ARG:HH11	1.62	0.64
1:B:186:PHE:O	1:B:189:LEU:HG	1.97	0.64
1:A:225:TYR:HA	1:A:228:GLU:HG3	1.80	0.63
1:A:556:SER:CA	1:A:560:ARG:HB3	2.28	0.63
1:B:475:ASP:O	1:B:479:THR:HB	1.98	0.63
1:C:202:THR:CG2	1:C:203:ALA:N	2.60	0.63
1:A:186:PHE:O	1:A:189:LEU:HG	1.99	0.63
1:B:305:ILE:O	1:B:306:PRO:C	2.42	0.63
1:C:186:PHE:O	1:C:189:LEU:HG	1.97	0.63
1:A:340:GLN:HG2	1:A:482:VAL:HG13	1.81	0.63
1:A:537:LEU:HD23	1:A:570:PHE:CG	2.34	0.63
1:B:340:GLN:HG2	1:B:482:VAL:HG13	1.79	0.63
1:B:587:PRO:O	1:B:591:ASP:HB2	1.98	0.63
1:C:372:THR:HG23	1:C:443:LEU:HD23	1.79	0.63
1:C:512:ASN:HA	1:C:525:LEU:HD22	1.81	0.63
1:C:325:SER:O	1:C:329:THR:OG1	2.15	0.63
1:A:319:THR:O	1:A:323:ILE:HG23	1.99	0.63
1:B:530:LEU:HA	1:B:533:LEU:HD12	1.81	0.63
1:C:395:GLU:CB	1:C:423:ARG:HD3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:SER:HB3	1:C:622:SER:HB2	1.80	0.63
1:C:286:ILE:HG13	1:C:323:ILE:HD11	1.80	0.62
1:B:185:GLN:HE21	1:B:185:GLN:HA	1.65	0.62
1:B:374:ILE:HG22	1:B:441:THR:HG23	1.80	0.62
1:A:286:ILE:HD13	1:A:286:ILE:C	2.25	0.62
1:B:436:THR:O	1:B:481:THR:HG21	1.99	0.62
1:A:374:ILE:HG22	1:A:441:THR:HG23	1.81	0.62
1:B:142:LEU:HD13	1:B:145:ASN:HD22	1.65	0.62
1:B:631:TRP:CE2	1:B:641:TRP:HB3	2.35	0.62
1:B:372:THR:HG23	1:B:443:LEU:HD23	1.81	0.62
1:B:385:ASN:HD22	1:B:385:ASN:H	1.39	0.62
1:B:413:SER:HB3	1:B:415:HIS:CE1	2.33	0.62
1:B:521:SER:OG	1:B:590:ASN:HB3	1.98	0.62
1:C:668:TYR:CB	1:C:674:PRO:HA	2.14	0.62
1:A:395:GLU:CB	1:A:423:ARG:HD3	2.29	0.61
1:A:413:SER:HB3	1:A:415:HIS:CE1	2.35	0.61
1:B:537:LEU:HD23	1:B:570:PHE:CG	2.34	0.61
1:A:372:THR:HG23	1:A:443:LEU:HD23	1.81	0.61
1:B:680:ALA:HA	1:B:683:TYR:CD1	2.36	0.61
1:C:530:LEU:HA	1:C:533:LEU:HD12	1.81	0.61
1:C:223:GLN:O	1:C:227:VAL:HG23	2.00	0.61
1:C:436:THR:O	1:C:481:THR:HG21	2.01	0.61
1:B:556:SER:CA	1:B:560:ARG:HB3	2.30	0.61
1:C:556:SER:CA	1:C:560:ARG:HB3	2.29	0.61
1:B:175:GLN:HE21	1:B:175:GLN:HA	1.66	0.60
1:A:631:TRP:CE2	1:A:641:TRP:HB3	2.36	0.60
1:A:276:GLN:HE21	1:A:355:LEU:HA	1.66	0.60
1:B:293:ILE:O	1:B:297:GLU:HG2	2.01	0.60
1:B:523:ARG:HB3	1:B:589:TRP:CE3	2.37	0.60
1:A:399:ASN:CB	1:A:419:MET:HG2	2.32	0.60
1:A:436:THR:O	1:A:481:THR:HG21	2.01	0.60
1:C:175:GLN:HA	1:C:175:GLN:HE21	1.67	0.60
1:A:339:PRO:HG2	1:A:348:PHE:HB2	1.84	0.60
1:C:559:ASN:OD1	1:C:571:TRP:HB3	2.02	0.60
1:C:599:ASN:HD22	1:C:602:GLN:H	1.50	0.60
1:A:395:GLU:OE1	1:A:423:ARG:NH1	2.34	0.60
1:C:202:THR:HG22	1:C:203:ALA:H	1.66	0.60
1:B:640:LEU:HD23	1:B:641:TRP:H	1.67	0.59
1:A:521:SER:OG	1:A:590:ASN:HB3	2.02	0.59
1:C:502:VAL:HG13	1:C:506:GLN:HG3	1.84	0.59
1:C:681:LYS:HD2	1:C:682:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:PRO:HG2	1:B:348:PHE:HB2	1.84	0.59
1:A:512:ASN:HA	1:A:525:LEU:HD22	1.83	0.59
1:B:191:GLN:C	1:B:197:ARG:HH11	2.10	0.59
1:B:375:SER:HB3	1:B:393:SER:HB2	1.85	0.59
1:C:413:SER:HB3	1:C:415:HIS:CE1	2.37	0.59
1:C:286:ILE:HD13	1:C:286:ILE:C	2.28	0.59
1:C:475:ASP:O	1:C:479:THR:HB	2.02	0.59
1:C:521:SER:OG	1:C:590:ASN:HB3	2.03	0.59
1:C:293:ILE:O	1:C:297:GLU:HG2	2.02	0.59
1:A:405:TYR:CE2	1:A:407:GLN:HA	2.38	0.59
1:A:502:VAL:HG13	1:A:506:GLN:HG3	1.85	0.58
1:A:530:LEU:HA	1:A:533:LEU:HD12	1.85	0.58
1:A:651:PHE:CE2	1:A:656:LEU:HB2	2.38	0.58
1:C:191:GLN:O	1:C:197:ARG:HD2	2.04	0.58
1:B:527:LYS:H	1:B:527:LYS:HD3	1.68	0.58
1:B:286:ILE:C	1:B:286:ILE:HD13	2.28	0.58
1:B:566:TRP:HB3	1:B:568:TYR:CE1	2.38	0.58
1:A:142:LEU:HD13	1:A:145:ASN:HD22	1.69	0.58
1:C:337:GLN:HE21	1:C:338:PRO:HD2	1.67	0.58
1:B:559:ASN:OD1	1:B:571:TRP:HB3	2.04	0.57
1:B:576:GLY:O	1:B:580:VAL:HG22	2.04	0.57
1:B:202:THR:HG22	1:B:203:ALA:H	1.69	0.57
1:A:233:HIS:O	1:A:234:GLN:C	2.47	0.57
1:A:576:GLY:O	1:A:580:VAL:HG22	2.04	0.57
1:A:584:HIS:HE1	1:A:648:THR:OG1	1.87	0.57
1:A:640:LEU:HD23	1:A:641:TRP:H	1.68	0.57
1:B:502:VAL:HG13	1:B:506:GLN:HG3	1.87	0.57
1:A:286:ILE:HG13	1:A:323:ILE:HD11	1.85	0.57
1:B:259:GLN:HB2	1:B:269:GLU:HG2	1.87	0.57
1:C:395:GLU:OE1	1:C:423:ARG:NH1	2.37	0.57
1:C:504:TRP:NE1	1:C:508:CYS:SG	2.77	0.57
1:B:397:LEU:HA	1:B:420:SER:O	2.04	0.57
1:C:319:THR:O	1:C:323:ILE:HG23	2.04	0.57
1:A:293:ILE:O	1:A:297:GLU:HG2	2.04	0.57
1:A:337:GLN:HE21	1:A:338:PRO:HD2	1.70	0.57
1:B:378:GLN:HE22	1:B:393:SER:N	1.99	0.57
1:C:527:LYS:H	1:C:527:LYS:CD	2.17	0.57
1:A:671:PRO:HG2	1:A:673:ARG:NH1	2.20	0.57
1:A:599:ASN:HD22	1:A:602:GLN:H	1.52	0.57
1:C:159:GLU:HA	1:C:162:LEU:HB2	1.87	0.57
1:A:566:TRP:HB3	1:A:568:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD22	1:A:285:ILE:CD1	2.35	0.56
1:A:512:ASN:C	1:A:512:ASN:HD22	2.13	0.56
1:C:584:HIS:HE1	1:C:648:THR:OG1	1.87	0.56
1:C:640:LEU:HD23	1:C:641:TRP:H	1.70	0.56
1:A:174:ILE:HA	1:A:177:GLN:NE2	2.19	0.56
1:B:518:GLU:HG2	1:B:578:MET:HB3	1.86	0.56
1:B:516:LYS:HD3	1:B:524:GLY:CA	2.35	0.56
1:B:405:TYR:CE2	1:B:407:GLN:HA	2.41	0.56
1:A:191:GLN:O	1:A:197:ARG:HD2	2.06	0.56
1:A:312:MET:O	1:A:316:VAL:HB	2.05	0.56
1:A:515:PHE:O	1:A:519:VAL:HG22	2.06	0.56
1:A:599:ASN:HD22	1:A:599:ASN:C	2.13	0.56
1:A:337:GLN:HE21	1:A:463:SER:HB2	1.71	0.56
1:A:685:PRO:O	1:A:686:VAL:HG22	2.06	0.56
1:A:399:ASN:C	1:A:400:CYS:SG	2.90	0.55
1:A:594:ILE:HG13	1:A:594:ILE:O	2.05	0.55
1:B:340:GLN:HG2	1:B:482:VAL:CG1	2.36	0.55
1:C:523:ARG:HH11	1:C:523:ARG:HA	1.72	0.55
1:A:202:THR:HG22	1:A:203:ALA:N	2.21	0.55
1:C:342:LEU:HD11	1:C:466:VAL:HG11	1.88	0.55
1:C:566:TRP:HB3	1:C:568:TYR:CE1	2.42	0.55
1:B:141:HIS:C	1:B:143:GLN:H	2.13	0.55
1:C:141:HIS:C	1:C:143:GLN:H	2.14	0.55
1:C:142:LEU:HD13	1:C:145:ASN:HD22	1.70	0.55
1:A:375:SER:HB3	1:A:393:SER:HB2	1.88	0.55
1:A:633:PHE:H	1:A:641:TRP:HD1	1.55	0.55
1:A:671:PRO:HG2	1:A:673:ARG:HH12	1.72	0.55
1:C:185:GLN:HE21	1:C:185:GLN:HA	1.71	0.55
1:A:518:GLU:HG2	1:A:578:MET:HB3	1.89	0.55
1:C:191:GLN:C	1:C:197:ARG:HH11	2.15	0.55
1:C:516:LYS:HD3	1:C:524:GLY:CA	2.35	0.55
1:B:312:MET:O	1:B:316:VAL:HB	2.07	0.55
1:B:319:THR:O	1:B:323:ILE:HG23	2.07	0.55
1:B:512:ASN:C	1:B:512:ASN:HD22	2.15	0.55
1:B:579:GLU:O	1:B:583:LYS:HB2	2.07	0.55
1:B:584:HIS:HE1	1:B:648:THR:OG1	1.90	0.55
1:B:675:LYS:O	1:B:676:ASP:C	2.50	0.55
1:A:282:LEU:O	1:A:286:ILE:HG22	2.07	0.55
1:A:340:GLN:HG2	1:A:482:VAL:CG1	2.36	0.55
1:A:579:GLU:O	1:A:583:LYS:HB2	2.07	0.55
1:A:681:LYS:HD2	1:A:682:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.71	0.55
1:B:607:LEU:CD2	1:B:614:THR:HG22	2.37	0.54
1:C:399:ASN:CB	1:C:419:MET:HG2	2.35	0.54
1:A:337:GLN:NE2	1:A:463:SER:HB2	2.22	0.54
1:A:523:ARG:HB3	1:A:589:TRP:CE3	2.42	0.54
1:B:174:ILE:HA	1:B:177:GLN:NE2	2.23	0.54
1:B:640:LEU:CD2	1:B:641:TRP:H	2.20	0.54
1:B:259:GLN:HA	1:B:269:GLU:HG3	1.89	0.54
1:C:276:GLN:HE21	1:C:355:LEU:HA	1.72	0.54
1:C:285:ILE:C	1:C:285:ILE:HD13	2.32	0.54
1:C:576:GLY:O	1:C:580:VAL:HG22	2.07	0.54
1:B:395:GLU:HB3	1:B:423:ARG:HD3	1.90	0.54
1:C:668:TYR:HB2	1:C:673:ARG:O	2.08	0.54
1:A:636:PRO:HB2	1:A:640:LEU:HG	1.90	0.54
1:B:276:GLN:HE21	1:B:355:LEU:HA	1.71	0.54
1:C:507:LEU:HD22	1:C:511:LEU:HG	1.89	0.54
1:B:202:THR:HG22	1:B:203:ALA:N	2.23	0.54
1:B:633:PHE:H	1:B:641:TRP:HD1	1.55	0.54
1:C:174:ILE:HA	1:C:177:GLN:NE2	2.22	0.54
1:C:586:LYS:HB2	1:C:587:PRO:HD3	1.89	0.54
1:A:527:LYS:H	1:A:527:LYS:CD	2.20	0.54
1:B:165:LEU:HD11	1:B:226:ARG:HD2	1.89	0.54
1:B:599:ASN:HD22	1:B:599:ASN:C	2.16	0.54
1:A:141:HIS:C	1:A:143:GLN:H	2.15	0.53
1:C:512:ASN:C	1:C:512:ASN:HD22	2.16	0.53
1:B:140:LYS:H	1:B:140:LYS:NZ	2.04	0.53
1:B:681:LYS:HD2	1:B:682:TYR:CE1	2.44	0.53
1:C:599:ASN:HD22	1:C:599:ASN:C	2.17	0.53
1:B:325:SER:O	1:B:329:THR:OG1	2.18	0.53
1:C:373:ILE:HD13	1:C:421:LEU:HD11	1.90	0.53
1:C:493:ARG:HB2	1:C:497:ALA:HB3	1.90	0.53
1:B:512:ASN:HA	1:B:525:LEU:HD22	1.90	0.53
1:C:202:THR:HG22	1:C:203:ALA:N	2.23	0.53
1:C:508:CYS:SG	1:C:530:LEU:HD22	2.49	0.53
1:A:165:LEU:HD11	1:A:226:ARG:HD2	1.90	0.53
1:A:516:LYS:HD3	1:A:524:GLY:CA	2.39	0.53
1:C:339:PRO:HG2	1:C:348:PHE:HB2	1.89	0.53
1:B:185:GLN:HA	1:B:185:GLN:NE2	2.22	0.53
1:C:165:LEU:HD11	1:C:226:ARG:HD2	1.91	0.53
1:C:671:PRO:HG2	1:C:673:ARG:NH1	2.24	0.53
1:B:399:ASN:CB	1:B:419:MET:HG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:PRO:O	1:B:686:VAL:HG22	2.09	0.53
1:B:636:PRO:HB2	1:B:640:LEU:HG	1.91	0.52
1:A:285:ILE:HD13	1:A:285:ILE:C	2.34	0.52
1:C:312:MET:O	1:C:316:VAL:HB	2.09	0.52
1:C:340:GLN:HG3	1:C:465:PRO:O	2.10	0.52
1:C:618:ARG:HG2	1:C:618:ARG:HH21	1.74	0.52
1:A:675:LYS:O	1:A:676:ASP:C	2.52	0.52
1:B:586:LYS:HB2	1:B:587:PRO:HD3	1.90	0.52
1:A:259:GLN:HB2	1:A:269:GLU:HG2	1.92	0.52
1:A:337:GLN:NE2	1:A:338:PRO:HD2	2.24	0.52
1:B:515:PHE:O	1:B:519:VAL:HG22	2.09	0.52
1:C:405:TYR:CE2	1:C:407:GLN:HA	2.44	0.52
1:C:515:PHE:O	1:C:519:VAL:HG22	2.08	0.52
1:A:403:MET:HB3	1:A:412:LEU:CD2	2.39	0.52
1:B:159:GLU:HA	1:B:162:LEU:HB2	1.92	0.52
1:C:337:GLN:HE21	1:C:463:SER:HB2	1.75	0.52
1:C:337:GLN:NE2	1:C:338:PRO:HD2	2.25	0.52
1:B:337:GLN:HE21	1:B:338:PRO:HD2	1.75	0.52
1:C:152:ARG:HH21	1:C:285:ILE:HB	1.75	0.52
1:C:233:HIS:O	1:C:234:GLN:C	2.52	0.52
1:C:375:SER:HB3	1:C:393:SER:HB2	1.92	0.52
1:A:507:LEU:HD22	1:A:511:LEU:HG	1.92	0.52
1:A:607:LEU:CD2	1:A:614:THR:HG22	2.39	0.52
1:B:447:GLN:O	1:B:448:PHE:HB3	2.09	0.52
1:C:340:GLN:HG2	1:C:482:VAL:CG1	2.40	0.52
1:A:504:TRP:NE1	1:A:508:CYS:SG	2.83	0.51
1:B:493:ARG:HB2	1:B:497:ALA:HB3	1.92	0.51
1:C:579:GLU:O	1:C:583:LYS:HB2	2.10	0.51
1:A:191:GLN:C	1:A:197:ARG:HH11	2.17	0.51
1:C:337:GLN:NE2	1:C:463:SER:HB2	2.26	0.51
1:C:518:GLU:HG2	1:C:578:MET:HB3	1.92	0.51
1:C:633:PHE:H	1:C:641:TRP:HD1	1.58	0.51
1:A:342:LEU:HD11	1:A:466:VAL:HG11	1.92	0.51
1:B:563:LEU:HD11	1:B:570:PHE:HA	1.93	0.51
1:C:685:PRO:O	1:C:686:VAL:HG22	2.11	0.51
1:B:259:GLN:CA	1:B:269:GLU:HG3	2.41	0.51
1:B:373:ILE:HD13	1:B:421:LEU:HD11	1.92	0.51
1:A:573:TRP:HE1	1:A:621:ASP:HA	1.76	0.51
1:A:678:VAL:HG12	1:A:678:VAL:O	2.11	0.51
1:B:233:HIS:O	1:B:234:GLN:C	2.53	0.51
1:B:651:PHE:CE2	1:B:656:LEU:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:ARG:HB3	1:C:589:TRP:CE3	2.46	0.51
1:C:678:VAL:HG12	1:C:678:VAL:O	2.11	0.51
1:A:159:GLU:HA	1:A:162:LEU:HB2	1.93	0.50
1:B:349:ALA:HA	1:B:416:PHE:O	2.11	0.50
1:B:527:LYS:H	1:B:527:LYS:CD	2.23	0.50
1:B:537:LEU:HB2	1:B:570:PHE:CE2	2.46	0.50
1:B:670:PHE:CB	1:B:671:PRO:HD3	2.36	0.50
1:C:150:GLU:O	1:C:154:ILE:HG22	2.11	0.50
1:C:254:GLN:HG2	1:C:258:ARG:HH21	1.77	0.50
1:C:668:TYR:CB	1:C:673:ARG:O	2.59	0.50
1:B:618:ARG:HG2	1:B:618:ARG:HH21	1.76	0.50
1:C:594:ILE:O	1:C:594:ILE:HG13	2.11	0.50
1:C:453:ASN:O	1:C:454:GLU:C	2.54	0.50
1:A:170:GLU:HG3	1:B:418:ASN:ND2	2.23	0.50
1:A:484:TRP:HZ3	1:A:499:PRO:O	1.95	0.50
1:C:181:ARG:C	1:C:183:GLN:H	2.20	0.50
1:A:465:PRO:HG2	1:A:485:ASP:OD1	2.12	0.50
1:A:531:VAL:O	1:A:532:PHE:C	2.53	0.50
1:C:449:SER:HA	1:C:456:VAL:HA	1.94	0.50
1:B:465:PRO:HG2	1:B:485:ASP:CG	2.37	0.50
1:C:397:LEU:HA	1:C:420:SER:O	2.12	0.50
1:A:231:GLU:HA	1:A:234:GLN:HB2	1.94	0.50
1:A:244:GLN:HE22	1:A:327:LEU:HG	1.76	0.50
1:A:340:GLN:HG3	1:A:465:PRO:O	2.11	0.49
1:B:285:ILE:HD13	1:B:285:ILE:C	2.37	0.49
1:A:140:LYS:H	1:A:140:LYS:NZ	2.09	0.49
1:A:183:GLN:C	1:A:185:GLN:H	2.18	0.49
1:C:282:LEU:O	1:C:286:ILE:HG22	2.13	0.49
1:A:586:LYS:HB2	1:A:587:PRO:HD3	1.95	0.49
1:C:245:THR:HG23	1:C:249:ASP:OD2	2.12	0.49
1:C:594:ILE:HD11	1:C:619:PHE:CE2	2.47	0.49
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.26	0.49
1:A:327:LEU:HD22	1:A:356:VAL:HG11	1.93	0.49
1:B:658:ASP:OD1	1:B:684:THR:HG22	2.12	0.49
1:C:523:ARG:HD2	1:C:523:ARG:N	2.26	0.49
1:A:259:GLN:CA	1:A:269:GLU:HG3	2.42	0.49
1:A:373:ILE:HD13	1:A:421:LEU:HD11	1.92	0.49
1:C:636:PRO:HB2	1:C:640:LEU:HG	1.94	0.49
1:B:150:GLU:O	1:B:154:ILE:HG22	2.12	0.49
1:B:231:GLU:HA	1:B:234:GLN:HB2	1.94	0.49
1:B:449:SER:HA	1:B:456:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLN:HA	1:C:185:GLN:NE2	2.27	0.49
1:C:231:GLU:HA	1:C:234:GLN:HB2	1.95	0.49
1:C:259:GLN:HA	1:C:269:GLU:HG3	1.94	0.49
1:C:670:PHE:O	1:C:671:PRO:C	2.55	0.49
1:A:260:GLN:HG3	1:A:464:LEU:HD22	1.95	0.49
1:B:260:GLN:HG3	1:B:464:LEU:HD22	1.95	0.49
1:C:403:MET:HB3	1:C:412:LEU:CD2	2.43	0.49
1:B:223:GLN:O	1:B:227:VAL:HG23	2.13	0.49
1:A:290:ARG:HH12	1:A:455:LEU:HD22	1.78	0.48
1:C:537:LEU:HB2	1:C:570:PHE:CE2	2.48	0.48
1:B:152:ARG:HH21	1:B:285:ILE:HB	1.78	0.48
1:C:527:LYS:HD3	1:C:527:LYS:N	2.27	0.48
1:B:342:LEU:HD11	1:B:466:VAL:HG11	1.95	0.48
1:B:541:SER:O	1:B:542:SER:C	2.57	0.48
1:C:140:LYS:H	1:C:140:LYS:NZ	2.07	0.48
1:A:259:GLN:HA	1:A:269:GLU:HG3	1.94	0.48
1:A:397:LEU:HA	1:A:420:SER:O	2.13	0.48
1:A:465:PRO:HG2	1:A:485:ASP:CG	2.37	0.48
1:B:141:HIS:O	1:B:144:ILE:HG12	2.13	0.48
1:B:507:LEU:HD22	1:B:511:LEU:HG	1.94	0.48
1:C:241:ARG:NH1	1:C:244:GLN:HG2	2.28	0.48
1:A:493:ARG:HB2	1:A:497:ALA:HB3	1.96	0.48
1:A:527:LYS:HD3	1:A:527:LYS:N	2.27	0.48
1:A:670:PHE:CB	1:A:671:PRO:HD3	2.38	0.48
1:B:340:GLN:HG3	1:B:465:PRO:O	2.13	0.48
1:C:141:HIS:O	1:C:144:ILE:HG12	2.13	0.48
1:C:175:GLN:C	1:C:177:GLN:N	2.70	0.48
1:C:247:ILE:O	1:C:251:GLU:HB2	2.13	0.48
1:B:259:GLN:O	1:B:262:ALA:HB3	2.14	0.48
1:B:327:LEU:HD22	1:B:356:VAL:HG11	1.95	0.48
1:B:508:CYS:SG	1:B:530:LEU:HD22	2.54	0.48
1:A:175:GLN:C	1:A:177:GLN:N	2.69	0.48
1:B:233:HIS:HA	1:B:236:THR:HG23	1.96	0.48
1:B:671:PRO:HG2	1:B:673:ARG:NH1	2.29	0.48
1:A:618:ARG:HG2	1:A:618:ARG:HH21	1.78	0.48
1:B:162:LEU:HD23	1:B:229:LEU:HD11	1.95	0.48
1:C:365:ASN:HA	1:C:366:PRO:HD2	1.62	0.48
1:C:395:GLU:HB3	1:C:423:ARG:HD3	1.94	0.48
1:B:247:ILE:HD12	1:B:278:TRP:HB3	1.95	0.48
1:C:563:LEU:HD11	1:C:570:PHE:HA	1.95	0.48
1:A:395:GLU:HB3	1:A:423:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:PHE:O	1:A:671:PRO:C	2.56	0.47
1:C:372:THR:CG2	1:C:443:LEU:HD23	2.44	0.47
1:C:629:ILE:HB	1:C:643:LEU:CD2	2.44	0.47
1:A:378:GLN:HE22	1:A:393:SER:N	2.01	0.47
1:B:537:LEU:HD11	1:B:553:VAL:HG13	1.96	0.47
1:B:183:GLN:C	1:B:185:GLN:H	2.22	0.47
1:B:241:ARG:NH1	1:B:244:GLN:HG2	2.30	0.47
1:B:453:ASN:O	1:B:454:GLU:C	2.57	0.47
1:C:233:HIS:HA	1:C:236:THR:HG23	1.95	0.47
1:A:233:HIS:C	1:A:235:LYS:N	2.71	0.47
1:A:516:LYS:HD3	1:A:524:GLY:HA3	1.96	0.47
1:A:337:GLN:HG2	1:A:464:LEU:HD12	1.97	0.47
1:C:378:GLN:HE22	1:C:393:SER:N	2.01	0.47
1:C:259:GLN:HB2	1:C:269:GLU:HG2	1.97	0.47
1:A:361:ASN:HD21	1:B:364:MET:HG3	1.74	0.47
1:A:382:LEU:HD23	1:A:387:ASN:OD1	2.14	0.47
1:B:337:GLN:HE21	1:B:463:SER:HB2	1.79	0.47
1:C:465:PRO:HG2	1:C:485:ASP:CG	2.39	0.47
1:C:488:PHE:HB3	1:C:499:PRO:HG2	1.97	0.47
1:B:181:ARG:C	1:B:183:GLN:H	2.23	0.47
1:B:384:LYS:O	1:B:386:GLU:N	2.47	0.47
1:B:504:TRP:NE1	1:B:508:CYS:SG	2.87	0.47
1:C:151:LEU:HD13	1:C:240:LEU:HD13	1.97	0.47
1:A:152:ARG:HH21	1:A:285:ILE:HB	1.80	0.47
1:A:259:GLN:O	1:A:262:ALA:HB3	2.15	0.47
1:A:418:ASN:ND2	1:B:170:GLU:HG3	2.24	0.47
1:B:413:SER:CB	1:B:415:HIS:CE1	2.96	0.47
1:B:573:TRP:HE1	1:B:621:ASP:HA	1.80	0.47
1:C:259:GLN:O	1:C:262:ALA:HB3	2.14	0.47
1:C:669:VAL:HG22	1:C:673:ARG:HG3	1.96	0.47
1:A:453:ASN:O	1:A:454:GLU:C	2.58	0.47
1:B:453:ASN:C	1:B:453:ASN:ND2	2.73	0.47
1:C:275:LEU:O	1:C:278:TRP:HB2	2.15	0.47
1:C:340:GLN:O	1:C:466:VAL:HA	2.15	0.47
1:A:220:GLN:C	1:A:220:GLN:CD	2.82	0.46
1:A:349:ALA:HA	1:A:416:PHE:O	2.16	0.46
1:A:540:ILE:HD12	1:A:540:ILE:HA	1.84	0.46
1:A:670:PHE:HB3	1:A:671:PRO:CD	2.39	0.46
1:A:678:VAL:O	1:A:678:VAL:CG1	2.63	0.46
1:B:282:LEU:O	1:B:286:ILE:HG22	2.15	0.46
1:B:629:ILE:HB	1:B:643:LEU:CD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:PHE:O	1:B:671:PRO:C	2.58	0.46
1:C:233:HIS:C	1:C:235:LYS:N	2.72	0.46
1:A:183:GLN:C	1:A:185:GLN:N	2.72	0.46
1:A:413:SER:CB	1:A:415:HIS:CE1	2.98	0.46
1:A:617:LEU:HB3	1:A:627:ILE:HG21	1.98	0.46
1:B:342:LEU:O	1:B:468:VAL:HA	2.15	0.46
1:A:594:ILE:HD11	1:A:619:PHE:CE2	2.51	0.46
1:B:254:GLN:HG2	1:B:258:ARG:HH21	1.81	0.46
1:C:516:LYS:HD3	1:C:524:GLY:HA3	1.96	0.46
1:A:247:ILE:HD12	1:A:278:TRP:HB3	1.97	0.46
1:A:523:ARG:HD2	1:A:523:ARG:N	2.29	0.46
1:B:533:LEU:O	1:B:536:LYS:N	2.48	0.46
1:A:294:ARG:NH1	1:A:454:GLU:OE2	2.49	0.46
1:B:365:ASN:HA	1:B:366:PRO:HD2	1.60	0.46
1:A:629:ILE:HB	1:A:643:LEU:CD2	2.45	0.46
1:B:531:VAL:O	1:B:532:PHE:C	2.59	0.46
1:C:675:LYS:O	1:C:676:ASP:C	2.59	0.46
1:A:541:SER:O	1:A:542:SER:C	2.57	0.46
1:A:640:LEU:CD2	1:A:641:TRP:H	2.29	0.46
1:C:220:GLN:C	1:C:220:GLN:CD	2.84	0.46
1:B:363:HIS:CD2	1:B:363:HIS:N	2.84	0.46
1:C:465:PRO:HG2	1:C:485:ASP:OD1	2.15	0.46
1:C:573:TRP:HE1	1:C:621:ASP:HA	1.80	0.46
1:A:141:HIS:O	1:A:144:ILE:HG12	2.15	0.46
1:B:337:GLN:NE2	1:B:338:PRO:HD2	2.31	0.46
1:C:640:LEU:CD2	1:C:641:TRP:H	2.29	0.46
1:A:259:GLN:HB2	1:A:269:GLU:CG	2.46	0.46
1:A:294:ARG:HA	1:A:297:GLU:HG2	1.98	0.46
1:A:364:MET:HG3	1:B:361:ASN:HD21	1.70	0.46
1:B:471:HIS:NE2	1:B:474:GLN:HB2	2.31	0.46
1:C:670:PHE:HB3	1:C:671:PRO:CD	2.42	0.46
1:A:348:PHE:CE1	1:A:419:MET:HE3	2.50	0.45
1:A:658:ASP:OD1	1:A:684:THR:HG22	2.16	0.45
1:B:175:GLN:C	1:B:177:GLN:N	2.71	0.45
1:C:382:LEU:HD23	1:C:387:ASN:OD1	2.16	0.45
1:C:651:PHE:CE2	1:C:656:LEU:HB2	2.51	0.45
1:A:223:GLN:O	1:A:227:VAL:HG23	2.16	0.45
1:B:276:GLN:O	1:B:277:SER:C	2.60	0.45
1:B:632:LYS:HG3	1:B:640:LEU:HD11	1.99	0.45
1:C:349:ALA:HA	1:C:416:PHE:O	2.15	0.45
1:A:388:THR:O	1:A:390:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:HIS:CD2	1:B:363:HIS:H	2.35	0.45
1:B:516:LYS:HD3	1:B:524:GLY:HA3	1.98	0.45
1:B:337:GLN:HE22	1:B:463:SER:HA	1.82	0.45
1:B:340:GLN:O	1:B:466:VAL:HA	2.17	0.45
1:B:382:LEU:HD23	1:B:387:ASN:OD1	2.17	0.45
1:B:523:ARG:HD2	1:B:523:ARG:N	2.32	0.45
1:B:183:GLN:HE21	1:B:208:GLN:CD	2.24	0.45
1:B:378:GLN:CD	1:B:393:SER:H	2.22	0.45
1:B:527:LYS:HD3	1:B:527:LYS:N	2.31	0.45
1:A:181:ARG:C	1:A:183:GLN:H	2.25	0.45
1:A:216:GLN:HE22	1:C:686:VAL:HG13	1.82	0.45
1:A:471:HIS:NE2	1:A:474:GLN:HB2	2.31	0.45
1:A:537:LEU:HB2	1:A:570:PHE:CE2	2.51	0.45
1:B:220:GLN:CD	1:B:220:GLN:C	2.83	0.45
1:B:474:GLN:HG2	1:B:477:ASN:HD22	1.82	0.45
1:B:537:LEU:HB2	1:B:570:PHE:CD2	2.51	0.45
1:C:259:GLN:CA	1:C:269:GLU:HG3	2.46	0.45
1:C:384:LYS:O	1:C:386:GLU:N	2.49	0.45
1:C:288:GLN:O	1:C:290:ARG:N	2.50	0.45
1:C:327:LEU:HD22	1:C:356:VAL:HG11	1.97	0.45
1:A:364:MET:HE3	1:B:361:ASN:HB3	1.98	0.45
1:B:403:MET:HB3	1:B:412:LEU:CD2	2.47	0.45
1:B:668:TYR:HB2	1:B:673:ARG:O	2.16	0.45
1:C:363:HIS:O	1:C:366:PRO:HD3	2.17	0.45
1:C:531:VAL:O	1:C:532:PHE:C	2.60	0.45
1:C:556:SER:HA	1:C:560:ARG:CB	2.44	0.45
1:A:289:ASN:O	1:A:293:ILE:HG23	2.17	0.45
1:A:449:SER:HA	1:A:456:VAL:HA	1.98	0.45
1:A:363:HIS:N	1:A:363:HIS:CD2	2.85	0.44
1:A:556:SER:HA	1:A:560:ARG:CB	2.44	0.44
1:A:563:LEU:HD11	1:A:570:PHE:HA	1.99	0.44
1:A:384:LYS:O	1:A:386:GLU:N	2.51	0.44
1:B:609:ASN:HD22	1:B:609:ASN:C	2.25	0.44
1:B:669:VAL:O	1:B:670:PHE:C	2.61	0.44
1:C:474:GLN:HG2	1:C:477:ASN:HD22	1.82	0.44
1:A:146:GLN:C	1:A:148:PHE:N	2.75	0.44
1:A:325:SER:O	1:A:329:THR:OG1	2.25	0.44
1:B:224:GLN:O	1:B:228:GLU:HG2	2.18	0.44
1:B:290:ARG:HH12	1:B:455:LEU:HD22	1.82	0.44
1:B:465:PRO:HG2	1:B:485:ASP:OD1	2.17	0.44
1:B:594:ILE:O	1:B:594:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LYS:O	1:C:360:LEU:C	2.60	0.44
1:C:484:TRP:HZ3	1:C:499:PRO:O	2.00	0.44
1:A:286:ILE:HD13	1:A:286:ILE:O	2.16	0.44
1:A:669:VAL:O	1:A:670:PHE:C	2.60	0.44
1:B:678:VAL:HG12	1:B:678:VAL:O	2.17	0.44
1:C:658:ASP:OD1	1:C:684:THR:HG22	2.17	0.44
1:A:478:ALA:O	1:A:481:THR:HG23	2.18	0.44
1:B:413:SER:CB	1:B:415:HIS:HE1	2.30	0.44
1:B:670:PHE:CB	1:B:671:PRO:CD	2.96	0.44
1:C:183:GLN:C	1:C:185:GLN:H	2.24	0.44
1:C:260:GLN:HG3	1:C:464:LEU:HD22	1.98	0.44
1:C:618:ARG:HG2	1:C:618:ARG:NH2	2.32	0.44
1:A:519:VAL:C	1:A:586:LYS:NZ	2.76	0.44
1:A:615:PHE:HB2	1:A:630:ALA:O	2.17	0.44
1:B:240:LEU:HD22	1:B:285:ILE:CD1	2.47	0.44
1:A:193:ASN:CB	1:A:194:PRO:CD	2.94	0.44
1:B:193:ASN:CB	1:B:194:PRO:CD	2.94	0.44
1:B:363:HIS:O	1:B:366:PRO:HD3	2.17	0.44
1:B:372:THR:CG2	1:B:443:LEU:HD23	2.48	0.44
1:B:395:GLU:HB2	1:B:423:ARG:HB2	1.99	0.44
1:C:140:LYS:HD3	1:C:140:LYS:N	2.33	0.44
1:C:251:GLU:OE2	1:C:251:GLU:CA	2.59	0.44
1:C:288:GLN:C	1:C:290:ARG:N	2.76	0.44
1:C:376:GLU:HG3	1:C:496:PHE:HD1	1.83	0.44
1:C:447:GLN:O	1:C:448:PHE:HB3	2.18	0.44
1:C:678:VAL:O	1:C:678:VAL:CG1	2.65	0.44
1:B:337:GLN:NE2	1:B:464:LEU:H	2.16	0.44
1:C:146:GLN:C	1:C:148:PHE:N	2.73	0.44
1:A:471:HIS:HD2	1:A:474:GLN:N	2.16	0.43
1:C:162:LEU:HD23	1:C:229:LEU:HD11	2.00	0.43
1:C:226:ARG:NH2	1:C:300:CYS:HA	2.33	0.43
1:C:541:SER:O	1:C:542:SER:C	2.60	0.43
1:A:247:ILE:O	1:A:251:GLU:HB2	2.17	0.43
1:A:283:ALA:HA	1:A:286:ILE:HG22	2.00	0.43
1:B:161:GLU:O	1:B:162:LEU:C	2.61	0.43
1:C:617:LEU:HB3	1:C:627:ILE:HG21	1.99	0.43
1:A:488:PHE:HB3	1:A:499:PRO:HG2	2.00	0.43
1:B:283:ALA:HA	1:B:286:ILE:HG22	2.00	0.43
1:B:668:TYR:CB	1:B:673:ARG:O	2.66	0.43
1:C:183:GLN:C	1:C:185:GLN:N	2.76	0.43
1:C:471:HIS:NE2	1:C:474:GLN:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:LEU:CD2	1:C:614:THR:HG22	2.47	0.43
1:B:141:HIS:C	1:B:143:GLN:N	2.75	0.43
1:B:146:GLN:C	1:B:148:PHE:N	2.76	0.43
1:B:256:LYS:O	1:B:259:GLN:HB3	2.18	0.43
1:B:233:HIS:C	1:B:235:LYS:N	2.76	0.43
1:B:671:PRO:HG2	1:B:673:ARG:HH12	1.83	0.43
1:C:512:ASN:C	1:C:512:ASN:ND2	2.76	0.43
1:A:223:GLN:HE21	1:C:685:PRO:HG3	1.84	0.43
1:B:618:ARG:HG2	1:B:618:ARG:NH2	2.33	0.43
1:C:399:ASN:HB2	1:C:419:MET:HA	2.01	0.43
1:A:294:ARG:CZ	1:A:454:GLU:OE2	2.66	0.43
1:B:658:ASP:CG	1:B:684:THR:HG22	2.44	0.43
1:A:162:LEU:HD23	1:A:229:LEU:HD11	2.01	0.43
1:A:629:ILE:HD12	1:A:643:LEU:HD21	2.01	0.43
1:B:376:GLU:HG3	1:B:496:PHE:HD1	1.84	0.43
1:B:480:ALA:HB2	1:B:571:TRP:CD1	2.54	0.43
1:B:518:GLU:HG3	1:B:582:LYS:HG2	2.01	0.43
1:B:647:THR:HG21	1:B:649:ARG:HH22	1.84	0.43
1:C:537:LEU:HD11	1:C:553:VAL:HG13	2.01	0.43
1:B:183:GLN:C	1:B:185:GLN:N	2.75	0.43
1:B:195:GLN:HB2	1:B:196:GLU:OE2	2.19	0.43
1:B:257:ARG:O	1:B:258:ARG:C	2.62	0.43
1:B:484:TRP:HZ3	1:B:499:PRO:O	2.01	0.43
1:B:447:GLN:HG3	1:B:458:GLN:HB3	2.01	0.43
1:B:488:PHE:HB3	1:B:499:PRO:HG2	2.00	0.43
1:B:594:ILE:HD11	1:B:619:PHE:CE2	2.54	0.43
1:C:397:LEU:HB2	1:C:420:SER:O	2.19	0.43
1:C:599:ASN:O	1:C:600:LYS:C	2.62	0.43
1:A:233:HIS:HA	1:A:236:THR:HG23	2.01	0.42
1:B:503:LEU:O	1:B:504:TRP:C	2.61	0.42
1:C:413:SER:CB	1:C:415:HIS:CE1	3.01	0.42
1:A:342:LEU:O	1:A:468:VAL:HA	2.19	0.42
1:A:376:GLU:HG3	1:A:496:PHE:HD1	1.83	0.42
1:C:283:ALA:HA	1:C:286:ILE:HG22	2.01	0.42
1:C:337:GLN:HG2	1:C:464:LEU:HD12	1.99	0.42
1:C:537:LEU:HB2	1:C:570:PHE:CD2	2.53	0.42
1:A:288:GLN:O	1:A:290:ARG:N	2.52	0.42
1:A:338:PRO:HA	1:A:339:PRO:HD2	1.82	0.42
1:A:372:THR:CG2	1:A:443:LEU:HD23	2.47	0.42
1:A:471:HIS:HD2	1:A:474:GLN:HB2	1.81	0.42
1:A:512:ASN:C	1:A:512:ASN:ND2	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ARG:CZ	1:C:454:GLU:OE2	2.67	0.42
1:A:150:GLU:O	1:A:154:ILE:HG22	2.19	0.42
1:A:378:GLN:CD	1:A:393:SER:H	2.26	0.42
1:A:458:GLN:HE21	1:A:458:GLN:HB3	1.68	0.42
1:A:537:LEU:HD13	1:A:537:LEU:C	2.44	0.42
1:A:327:LEU:HD22	1:A:356:VAL:CG1	2.49	0.42
1:C:294:ARG:NH2	1:C:454:GLU:OE2	2.51	0.42
1:C:632:LYS:HG3	1:C:640:LEU:HD11	2.01	0.42
1:C:670:PHE:CB	1:C:671:PRO:HD3	2.42	0.42
1:A:340:GLN:O	1:A:466:VAL:HA	2.20	0.42
1:A:447:GLN:O	1:A:448:PHE:HB3	2.19	0.42
1:A:503:LEU:O	1:A:504:TRP:C	2.63	0.42
1:A:537:LEU:HD11	1:A:553:VAL:HG13	2.01	0.42
1:B:162:LEU:HD23	1:B:229:LEU:CD1	2.49	0.42
1:B:388:THR:O	1:B:390:ASN:N	2.52	0.42
1:B:507:LEU:HD21	1:B:558:PHE:CE1	2.55	0.42
1:A:141:HIS:C	1:A:143:GLN:N	2.77	0.42
1:A:290:ARG:O	1:A:293:ILE:HD13	2.19	0.42
1:B:259:GLN:HB2	1:B:269:GLU:CG	2.49	0.42
1:B:519:VAL:C	1:B:586:LYS:HZ2	2.27	0.42
1:C:142:LEU:HD13	1:C:145:ASN:ND2	2.34	0.42
1:C:289:ASN:O	1:C:293:ILE:HG23	2.20	0.42
1:C:333:ILE:HD13	1:C:355:LEU:HD11	2.00	0.42
1:C:388:THR:O	1:C:390:ASN:N	2.53	0.42
1:C:631:TRP:CZ2	1:C:641:TRP:HB3	2.54	0.42
1:A:202:THR:HG23	1:A:203:ALA:N	2.32	0.42
1:A:363:HIS:O	1:A:366:PRO:HD3	2.20	0.42
1:A:447:GLN:HG3	1:A:458:GLN:HB3	2.00	0.42
1:B:142:LEU:HD13	1:B:145:ASN:ND2	2.32	0.42
1:B:267:PRO:HA	1:B:268:PRO:HD3	1.88	0.42
1:B:337:GLN:NE2	1:B:463:SER:HB2	2.35	0.42
1:C:193:ASN:CB	1:C:194:PRO:CD	2.96	0.42
1:C:267:PRO:HA	1:C:268:PRO:HD3	1.93	0.42
1:B:327:LEU:HD22	1:B:356:VAL:CG1	2.50	0.42
1:B:359:LYS:O	1:B:360:LEU:C	2.62	0.42
1:C:518:GLU:HG3	1:C:582:LYS:HG2	2.02	0.42
1:A:164:LYS:C	1:A:166:GLN:N	2.78	0.42
1:A:618:ARG:HG2	1:A:618:ARG:NH2	2.35	0.42
1:C:247:ILE:HD12	1:C:278:TRP:HB3	2.01	0.42
1:C:294:ARG:HA	1:C:297:GLU:HG2	2.02	0.42
1:C:540:ILE:HD12	1:C:540:ILE:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:GLU:CD	1:C:624:ILE:H	2.27	0.42
1:A:376:GLU:OE1	1:A:496:PHE:HB2	2.20	0.41
1:B:286:ILE:HD13	1:B:286:ILE:O	2.20	0.41
1:C:600:LYS:O	1:C:600:LYS:HE2	2.20	0.41
1:A:365:ASN:HA	1:A:366:PRO:HD2	1.60	0.41
1:B:615:PHE:HB2	1:B:630:ALA:O	2.20	0.41
1:C:240:LEU:HD22	1:C:285:ILE:CD1	2.49	0.41
1:C:636:PRO:HA	1:C:641:TRP:NE1	2.35	0.41
1:A:280:GLU:HB2	1:A:359:LYS:HD3	2.02	0.41
1:A:337:GLN:HE22	1:A:463:SER:HA	1.85	0.41
1:A:453:ASN:ND2	1:A:453:ASN:C	2.78	0.41
1:A:333:ILE:HD13	1:A:355:LEU:HD11	2.03	0.41
1:B:505:PRO:O	1:B:508:CYS:HB2	2.20	0.41
1:C:195:GLN:HB2	1:C:196:GLU:OE2	2.20	0.41
1:C:244:GLN:HE22	1:C:327:LEU:HG	1.85	0.41
1:C:274:VAL:O	1:C:277:SER:OG	2.39	0.41
1:C:363:HIS:CD2	1:C:363:HIS:N	2.88	0.41
1:C:601:GLN:O	1:C:604:HIS:HB3	2.21	0.41
1:C:621:ASP:O	1:C:622:SER:C	2.63	0.41
1:C:680:ALA:HA	1:C:683:TYR:CE1	2.53	0.41
1:A:142:LEU:HD13	1:A:145:ASN:ND2	2.33	0.41
1:C:321:THR:HG22	1:C:455:LEU:HD21	2.03	0.41
1:C:615:PHE:HB3	1:C:631:TRP:CB	2.51	0.41
1:A:140:LYS:HD3	1:A:140:LYS:N	2.35	0.41
1:A:288:GLN:C	1:A:290:ARG:N	2.79	0.41
1:A:435:VAL:HA	1:A:438:GLU:OE2	2.20	0.41
1:B:140:LYS:HD3	1:B:140:LYS:N	2.36	0.41
1:B:478:ALA:O	1:B:481:THR:HG23	2.21	0.41
1:C:554:SER:HB3	1:C:557:GLN:HG3	2.03	0.41
1:A:240:LEU:HD22	1:A:285:ILE:HD13	2.02	0.41
1:A:395:GLU:HB2	1:A:423:ARG:HB2	2.02	0.41
1:A:397:LEU:HB2	1:A:420:SER:O	2.21	0.41
1:A:502:VAL:HG13	1:A:506:GLN:CG	2.49	0.41
1:A:537:LEU:HB2	1:A:570:PHE:CD2	2.56	0.41
1:A:632:LYS:HG3	1:A:640:LEU:HD11	2.03	0.41
1:B:615:PHE:HB3	1:B:631:TRP:CB	2.51	0.41
1:B:669:VAL:HG22	1:B:673:ARG:HG3	2.02	0.41
1:B:670:PHE:HB3	1:B:671:PRO:CD	2.38	0.41
1:C:276:GLN:O	1:C:277:SER:C	2.63	0.41
1:C:361:ASN:OD1	1:C:361:ASN:N	2.38	0.41
1:C:395:GLU:HB2	1:C:423:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:SER:CB	1:C:560:ARG:HB3	2.51	0.41
1:C:671:PRO:HG2	1:C:673:ARG:HH12	1.84	0.41
1:A:292:GLN:HE21	1:A:292:GLN:HB3	1.70	0.41
1:A:353:ARG:NH1	1:A:411:THR:HG22	2.36	0.41
1:B:244:GLN:HE22	1:B:327:LEU:HG	1.86	0.41
1:B:573:TRP:CZ3	1:B:577:VAL:HG21	2.56	0.41
1:C:141:HIS:C	1:C:143:GLN:N	2.78	0.41
1:C:519:VAL:C	1:C:586:LYS:HZ2	2.29	0.41
1:A:519:VAL:C	1:A:586:LYS:HZ2	2.28	0.40
1:B:470:VAL:HG13	1:B:470:VAL:O	2.21	0.40
1:A:245:THR:HG23	1:A:249:ASP:OD2	2.21	0.40
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.91	0.40
1:A:361:ASN:OD1	1:A:361:ASN:N	2.40	0.40
1:A:363:HIS:CD2	1:A:363:HIS:H	2.39	0.40
1:B:240:LEU:HD22	1:B:285:ILE:HD13	2.04	0.40
1:B:471:HIS:HD2	1:B:474:GLN:N	2.20	0.40
1:B:678:VAL:O	1:B:678:VAL:CG1	2.69	0.40
1:C:291:GLN:HE21	1:C:291:GLN:HB3	1.50	0.40
1:C:663:LEU:HB2	1:C:666:LEU:HD12	2.03	0.40
1:A:162:LEU:HD23	1:A:229:LEU:CD1	2.51	0.40
1:A:533:LEU:O	1:A:536:LYS:N	2.54	0.40
1:B:308:PRO:O	1:B:312:MET:HG3	2.21	0.40
1:C:256:LYS:O	1:C:259:GLN:HB3	2.22	0.40
1:C:337:GLN:HE22	1:C:463:SER:HA	1.85	0.40
1:C:342:LEU:O	1:C:468:VAL:HA	2.22	0.40
1:A:421:LEU:O	1:A:422:LYS:HG3	2.21	0.40
1:B:376:GLU:OE1	1:B:496:PHE:HB2	2.21	0.40
1:B:523:ARG:CB	1:B:589:TRP:CE3	3.04	0.40
1:C:241:ARG:HH12	1:C:244:GLN:HG2	1.86	0.40
1:C:297:GLU:O	1:C:298:HIS:C	2.64	0.40
1:C:458:GLN:HE21	1:C:458:GLN:HB3	1.72	0.40
1:C:520:GLN:HE21	1:C:586:LYS:HE2	1.86	0.40
1:C:545:LEU:O	1:C:547:ASP:N	2.55	0.40
1:C:378:GLN:CD	1:C:393:SER:H	2.29	0.40
1:C:444:PHE:HB2	1:C:461:THR:CG2	2.51	0.40
1:C:465:PRO:HG3	1:C:496:PHE:CD2	2.56	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	540/585 (92%)	434 (80%)	78 (14%)	28 (5%)	1	11
1	B	540/585 (92%)	430 (80%)	84 (16%)	26 (5%)	2	13
1	C	540/585 (92%)	440 (82%)	69 (13%)	31 (6%)	1	10
All	All	1620/1755 (92%)	1304 (80%)	231 (14%)	85 (5%)	1	11

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	194	PRO
1	A	359	LYS
1	A	385	ASN
1	A	389	ARG
1	A	393	SER
1	A	495	PRO
1	A	636	PRO
1	A	670	PHE
1	B	193	ASN
1	B	194	PRO
1	B	359	LYS
1	B	385	ASN
1	B	389	ARG
1	B	393	SER
1	B	495	PRO
1	B	636	PRO
1	B	670	PHE
1	C	193	ASN
1	C	194	PRO
1	C	359	LYS
1	C	385	ASN
1	C	389	ARG
1	C	393	SER

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Mol	Chain	Res	Type
1	C	495	PRO
1	C	636	PRO
1	C	670	PHE
1	A	176	TYR
1	A	289	ASN
1	A	390	ASN
1	A	454	GLU
1	A	637	ASP
1	A	672	ASP
1	A	686	VAL
1	B	289	ASN
1	B	390	ASN
1	B	454	GLU
1	B	635	SER
1	B	637	ASP
1	B	672	ASP
1	C	176	TYR
1	C	289	ASN
1	C	390	ASN
1	C	454	GLU
1	C	637	ASP
1	C	672	ASP
1	C	686	VAL
1	A	182	ILE
1	A	306	PRO
1	A	453	ASN
1	A	635	SER
1	B	142	LEU
1	B	176	TYR
1	B	182	ILE
1	B	306	PRO
1	B	453	ASN
1	B	686	VAL
1	C	142	LEU
1	C	182	ILE
1	C	306	PRO
1	C	453	ASN
1	A	142	LEU
1	A	234	GLN
1	A	622	SER
1	A	641	TRP
1	A	649	ARG

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Mol	Chain	Res	Type
1	B	641	TRP
1	C	363	HIS
1	C	622	SER
1	C	635	SER
1	C	641	TRP
1	C	649	ARG
1	A	288	GLN
1	C	409	THR
1	B	409	THR
1	B	542	SER
1	C	234	GLN
1	C	398	ASN
1	C	542	SER
1	B	564	PRO
1	A	564	PRO
1	B	394	GLY
1	C	394	GLY
1	C	564	PRO
1	A	394	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	490/523 (94%)	362 (74%)	128 (26%)	0	3
1	B	490/523 (94%)	364 (74%)	126 (26%)	0	3
1	C	490/523 (94%)	366 (75%)	124 (25%)	0	3
All	All	1470/1569 (94%)	1092 (74%)	378 (26%)	0	3

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	144	ILE
1	A	152	ARG

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Mol	Chain	Res	Type
1	A	159	GLU
1	A	161	GLU
1	A	162	LEU
1	A	165	LEU
1	A	169	GLN
1	A	175	GLN
1	A	180	LEU
1	A	185	GLN
1	A	192	LEU
1	A	195	GLN
1	A	202	THR
1	A	226	ARG
1	A	232	LYS
1	A	234	GLN
1	A	236	THR
1	A	242	LYS
1	A	244	GLN
1	A	257	ARG
1	A	258	ARG
1	A	275	LEU
1	A	278	TRP
1	A	281	LYS
1	A	285	ILE
1	A	286	ILE
1	A	291	GLN
1	A	293	ILE
1	A	299	LEU
1	A	305	ILE
1	A	309	VAL
1	A	310	GLU
1	A	311	GLU
1	A	315	GLU
1	A	316	VAL
1	A	321	THR
1	A	323	ILE
1	A	327	LEU
1	A	329	THR
1	A	330	SER
1	A	333	ILE
1	A	340	GLN
1	A	341	VAL
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	343	LYS
1	A	352	VAL
1	A	360	LEU
1	A	362	VAL
1	A	363	HIS
1	A	372	THR
1	A	374	ILE
1	A	377	GLN
1	A	383	LEU
1	A	384	LYS
1	A	385	ASN
1	A	386	GLU
1	A	388	THR
1	A	389	ARG
1	A	391	GLU
1	A	399	ASN
1	A	407	GLN
1	A	412	LEU
1	A	417	ARG
1	A	421	LEU
1	A	423	ARG
1	A	433	GLU
1	A	436	THR
1	A	443	LEU
1	A	449	SER
1	A	454	GLU
1	A	455	LEU
1	A	456	VAL
1	A	458	GLN
1	A	466	VAL
1	A	473	SER
1	A	474	GLN
1	A	475	ASP
1	A	479	THR
1	A	481	THR
1	A	483	LEU
1	A	484	TRP
1	A	490	GLU
1	A	493	ARG
1	A	494	VAL
1	A	495	PRO
1	A	498	VAL

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Mol	Chain	Res	Type
1	A	501	LYS
1	A	502	VAL
1	A	507	LEU
1	A	512	ASN
1	A	520	GLN
1	A	523	ARG
1	A	525	LEU
1	A	536	LYS
1	A	537	LEU
1	A	540	ILE
1	A	541	SER
1	A	543	ASN
1	A	551	MET
1	A	553	VAL
1	A	559	ASN
1	A	564	PRO
1	A	572	GLN
1	A	579	GLU
1	A	580	VAL
1	A	582	LYS
1	A	583	LYS
1	A	589	TRP
1	A	594	ILE
1	A	599	ASN
1	A	600	LYS
1	A	608	ILE
1	A	609	ASN
1	A	621	ASP
1	A	624	ILE
1	A	633	PHE
1	A	637	ASP
1	A	638	ARG
1	A	640	LEU
1	A	647	THR
1	A	648	THR
1	A	653	ILE
1	A	667	ILE
1	A	668	TYR
1	A	669	VAL
1	A	676	ASP
1	A	686	VAL
1	B	140	LYS

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Mol	Chain	Res	Type
1	B	144	ILE
1	B	152	ARG
1	B	159	GLU
1	B	161	GLU
1	B	162	LEU
1	B	165	LEU
1	B	169	GLN
1	B	175	GLN
1	B	180	LEU
1	B	185	GLN
1	B	192	LEU
1	B	195	GLN
1	B	202	THR
1	B	221	THR
1	B	226	ARG
1	B	232	LYS
1	B	234	GLN
1	B	236	THR
1	B	242	LYS
1	B	244	GLN
1	B	257	ARG
1	B	258	ARG
1	B	275	LEU
1	B	278	TRP
1	B	281	LYS
1	B	285	ILE
1	B	286	ILE
1	B	291	GLN
1	B	293	ILE
1	B	299	LEU
1	B	305	ILE
1	B	309	VAL
1	B	310	GLU
1	B	311	GLU
1	B	315	GLU
1	B	316	VAL
1	B	321	THR
1	B	323	ILE
1	B	325	SER
1	B	327	LEU
1	B	329	THR
1	B	330	SER

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Mol	Chain	Res	Type
1	B	333	ILE
1	B	340	GLN
1	B	341	VAL
1	B	342	LEU
1	B	343	LYS
1	B	352	VAL
1	B	360	LEU
1	B	362	VAL
1	B	363	HIS
1	B	372	THR
1	B	374	ILE
1	B	377	GLN
1	B	383	LEU
1	B	384	LYS
1	B	385	ASN
1	B	386	GLU
1	B	388	THR
1	B	389	ARG
1	B	391	GLU
1	B	399	ASN
1	B	407	GLN
1	B	412	LEU
1	B	421	LEU
1	B	423	ARG
1	B	433	GLU
1	B	443	LEU
1	B	449	SER
1	B	454	GLU
1	B	455	LEU
1	B	456	VAL
1	B	458	GLN
1	B	466	VAL
1	B	474	GLN
1	B	475	ASP
1	B	479	THR
1	B	481	THR
1	B	483	LEU
1	B	484	TRP
1	B	493	ARG
1	B	494	VAL
1	B	495	PRO
1	B	498	VAL

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Mol	Chain	Res	Type
1	B	501	LYS
1	B	502	VAL
1	B	507	LEU
1	B	512	ASN
1	B	523	ARG
1	B	525	LEU
1	B	536	LYS
1	B	537	LEU
1	B	540	ILE
1	B	541	SER
1	B	543	ASN
1	B	551	MET
1	B	553	VAL
1	B	559	ASN
1	B	564	PRO
1	B	572	GLN
1	B	579	GLU
1	B	580	VAL
1	B	582	LYS
1	B	583	LYS
1	B	589	TRP
1	B	594	ILE
1	B	598	VAL
1	B	599	ASN
1	B	600	LYS
1	B	608	ILE
1	B	609	ASN
1	B	621	ASP
1	B	624	ILE
1	B	633	PHE
1	B	637	ASP
1	B	638	ARG
1	B	640	LEU
1	B	647	THR
1	B	653	ILE
1	B	667	ILE
1	B	668	TYR
1	B	669	VAL
1	B	676	ASP
1	B	686	VAL
1	B	687	LEU
1	C	140	LYS

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Mol	Chain	Res	Type
1	C	144	ILE
1	C	152	ARG
1	C	159	GLU
1	C	161	GLU
1	C	162	LEU
1	C	165	LEU
1	C	169	GLN
1	C	175	GLN
1	C	180	LEU
1	C	192	LEU
1	C	195	GLN
1	C	202	THR
1	C	226	ARG
1	C	232	LYS
1	C	234	GLN
1	C	236	THR
1	C	242	LYS
1	C	244	GLN
1	C	257	ARG
1	C	258	ARG
1	C	275	LEU
1	C	278	TRP
1	C	281	LYS
1	C	285	ILE
1	C	286	ILE
1	C	291	GLN
1	C	293	ILE
1	C	299	LEU
1	C	305	ILE
1	C	309	VAL
1	C	310	GLU
1	C	311	GLU
1	C	315	GLU
1	C	316	VAL
1	C	321	THR
1	C	323	ILE
1	C	325	SER
1	C	327	LEU
1	C	329	THR
1	C	330	SER
1	C	333	ILE
1	C	334	ILE

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Mol	Chain	Res	Type
1	C	340	GLN
1	C	341	VAL
1	C	342	LEU
1	C	343	LYS
1	C	352	VAL
1	C	359	LYS
1	C	360	LEU
1	C	362	VAL
1	C	372	THR
1	C	374	ILE
1	C	377	GLN
1	C	383	LEU
1	C	384	LYS
1	C	385	ASN
1	C	386	GLU
1	C	388	THR
1	C	389	ARG
1	C	391	GLU
1	C	399	ASN
1	C	407	GLN
1	C	412	LEU
1	C	417	ARG
1	C	421	LEU
1	C	423	ARG
1	C	433	GLU
1	C	436	THR
1	C	443	LEU
1	C	449	SER
1	C	454	GLU
1	C	455	LEU
1	C	456	VAL
1	C	458	GLN
1	C	466	VAL
1	C	474	GLN
1	C	475	ASP
1	C	479	THR
1	C	481	THR
1	C	483	LEU
1	C	484	TRP
1	C	493	ARG
1	C	495	PRO
1	C	498	VAL

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Mol	Chain	Res	Type
1	C	501	LYS
1	C	502	VAL
1	C	507	LEU
1	C	512	ASN
1	C	520	GLN
1	C	523	ARG
1	C	525	LEU
1	C	536	LYS
1	C	537	LEU
1	C	540	ILE
1	C	543	ASN
1	C	551	MET
1	C	553	VAL
1	C	559	ASN
1	C	564	PRO
1	C	572	GLN
1	C	579	GLU
1	C	580	VAL
1	C	582	LYS
1	C	583	LYS
1	C	589	TRP
1	C	594	ILE
1	C	599	ASN
1	C	600	LYS
1	C	608	ILE
1	C	609	ASN
1	C	621	ASP
1	C	624	ILE
1	C	633	PHE
1	C	637	ASP
1	C	638	ARG
1	C	640	LEU
1	C	647	THR
1	C	653	ILE
1	C	667	ILE
1	C	668	TYR
1	C	669	VAL
1	C	676	ASP
1	C	686	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	167	GLN
1	A	175	GLN
1	A	177	GLN
1	A	183	GLN
1	A	185	GLN
1	A	216	GLN
1	A	223	GLN
1	A	244	GLN
1	A	276	GLN
1	A	291	GLN
1	A	292	GLN
1	A	298	HIS
1	A	302	GLN
1	A	317	ASN
1	A	337	GLN
1	A	340	GLN
1	A	361	ASN
1	A	363	HIS
1	A	368	GLN
1	A	385	ASN
1	A	399	ASN
1	A	415	HIS
1	A	418	ASN
1	A	458	GLN
1	A	471	HIS
1	A	474	GLN
1	A	477	ASN
1	A	486	ASN
1	A	512	ASN
1	A	520	GLN
1	A	529	ASN
1	A	544	HIS
1	A	584	HIS
1	A	599	ASN
1	A	602	GLN
1	A	609	ASN
1	B	145	ASN
1	B	167	GLN
1	B	175	GLN
1	B	177	GLN
1	B	183	GLN
1	B	185	GLN

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Mol	Chain	Res	Type
1	B	216	GLN
1	B	244	GLN
1	B	276	GLN
1	B	291	GLN
1	B	292	GLN
1	B	298	HIS
1	B	302	GLN
1	B	317	ASN
1	B	337	GLN
1	B	340	GLN
1	B	363	HIS
1	B	368	GLN
1	B	385	ASN
1	B	399	ASN
1	B	415	HIS
1	B	418	ASN
1	B	458	GLN
1	B	471	HIS
1	B	474	GLN
1	B	477	ASN
1	B	486	ASN
1	B	512	ASN
1	B	520	GLN
1	B	544	HIS
1	B	584	HIS
1	B	599	ASN
1	B	602	GLN
1	B	609	ASN
1	C	145	ASN
1	C	167	GLN
1	C	175	GLN
1	C	177	GLN
1	C	183	GLN
1	C	185	GLN
1	C	216	GLN
1	C	244	GLN
1	C	291	GLN
1	C	292	GLN
1	C	298	HIS
1	C	302	GLN
1	C	317	ASN
1	C	337	GLN

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Mol	Chain	Res	Type
1	C	340	GLN
1	C	363	HIS
1	C	365	ASN
1	C	368	GLN
1	C	385	ASN
1	C	399	ASN
1	C	415	HIS
1	C	458	GLN
1	C	474	GLN
1	C	477	ASN
1	C	486	ASN
1	C	512	ASN
1	C	520	GLN
1	C	544	HIS
1	C	584	HIS
1	C	599	ASN
1	C	602	GLN
1	C	609	ASN

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 ⓘ

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	544/585 (92%)	0.57	39 (7%)	21 14	31, 53, 77, 94	0
1	B	544/585 (92%)	0.48	22 (4%)	42 26	31, 53, 77, 94	0
1	C	544/585 (92%)	0.48	28 (5%)	33 21	31, 53, 77, 94	0
All	All	1632/1755 (92%)	0.51	89 (5%)	30 19	31, 53, 77, 94	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	686	VAL	5.1
1	C	192	LEU	4.9
1	B	640	LEU	4.9
1	A	187	ALA	4.7
1	A	189	LEU	4.6
1	C	640	LEU	4.4
1	B	192	LEU	4.4
1	B	196	GLU	4.2
1	A	640	LEU	4.1
1	C	176	TYR	4.0
1	A	686	VAL	3.8
1	C	396	ILE	3.8
1	C	687	LEU	3.8
1	A	393	SER	3.7
1	C	194	PRO	3.5
1	C	686	VAL	3.5
1	A	687	LEU	3.5
1	A	176	TYR	3.4
1	C	495	PRO	3.4
1	B	197	ARG	3.3
1	B	176	TYR	3.2
1	C	622	SER	3.2
1	A	637	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	LEU	3.2
1	C	637	ASP	3.2
1	A	609	ASN	3.1
1	A	198	MET	3.1
1	C	142	LEU	3.1
1	A	622	SER	3.1
1	A	190	GLY	3.1
1	B	194	PRO	3.1
1	C	638	ARG	3.0
1	C	639	ASN	3.0
1	B	687	LEU	2.9
1	C	690	ALA	2.9
1	B	495	PRO	2.9
1	B	639	ASN	2.9
1	A	194	PRO	2.7
1	C	196	GLU	2.7
1	A	201	GLU	2.7
1	B	625	GLY	2.7
1	B	668	TYR	2.7
1	A	472	GLY	2.6
1	A	635	SER	2.6
1	A	174	ILE	2.6
1	A	186	PHE	2.6
1	A	204	LEU	2.6
1	B	142	LEU	2.6
1	B	195	GLN	2.5
1	B	637	ASP	2.5
1	B	622	SER	2.5
1	A	625	GLY	2.5
1	A	479	THR	2.5
1	C	307	GLY	2.5
1	A	222	LEU	2.4
1	A	388	THR	2.4
1	A	396	ILE	2.3
1	C	608	ILE	2.3
1	B	396	ILE	2.3
1	C	398	ASN	2.3
1	B	649	ARG	2.3
1	A	639	ASN	2.3
1	B	193	ASN	2.3
1	A	495	PRO	2.3
1	C	635	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	ARG	2.3
1	B	472	GLY	2.2
1	A	668	TYR	2.2
1	C	683	TYR	2.2
1	A	205	GLN	2.2
1	C	214	TRP	2.1
1	A	386	GLU	2.1
1	A	398	ASN	2.1
1	C	633	PHE	2.1
1	C	624	ILE	2.1
1	A	365	ASN	2.1
1	A	383	LEU	2.1
1	A	175	GLN	2.1
1	C	400	CYS	2.1
1	A	391	GLU	2.1
1	A	638	ARG	2.0
1	B	436	THR	2.0
1	C	668	TYR	2.0
1	C	208	GLN	2.0
1	A	624	ILE	2.0
1	B	636	PRO	2.0
1	C	191	GLN	2.0
1	A	142	LEU	2.0
1	C	182	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.