



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 3V9F / pdb_00003v9f
Title : Crystal Structure of the extracellular domain of the putative hybrid two component system BT3049 from *B. thetaiotaomicron*
Authors : Zhang, Z.; Liu, Q.; Hendrickson, W.A.
Deposited on : 2011-12-27
Resolution : 3.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

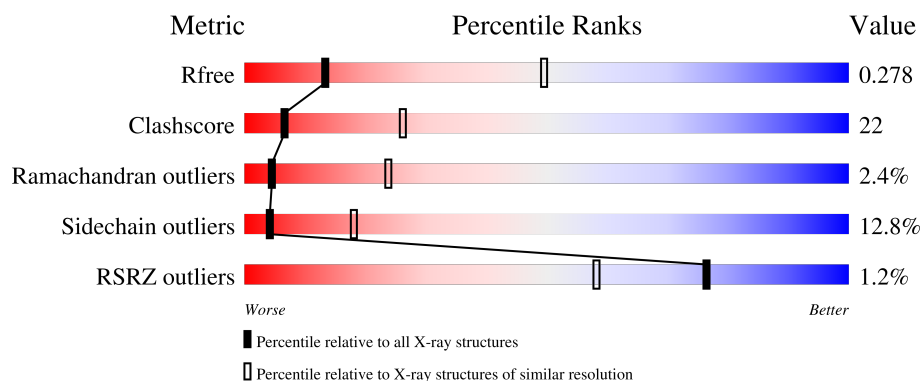
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	781	52%33%8% • 6%
1	B	781	52%35%6% • 6%
1	C	781	52%34%8% • 6%
1	D	781	53%34%7% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23560 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 Two-component system sensor histidine kinase/response regulator, hybrid (One-component system).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	Se	0	0	0
			5890	3751	990	1134	10	5			
1	B	736	Total	C	N	O	S	Se	0	0	0
			5890	3751	990	1134	10	5			
1	C	736	Total	C	N	O	S	Se	0	0	0
			5890	3751	990	1134	10	5			
1	D	736	Total	C	N	O	S	Se	0	0	0
			5890	3751	990	1134	10	5			

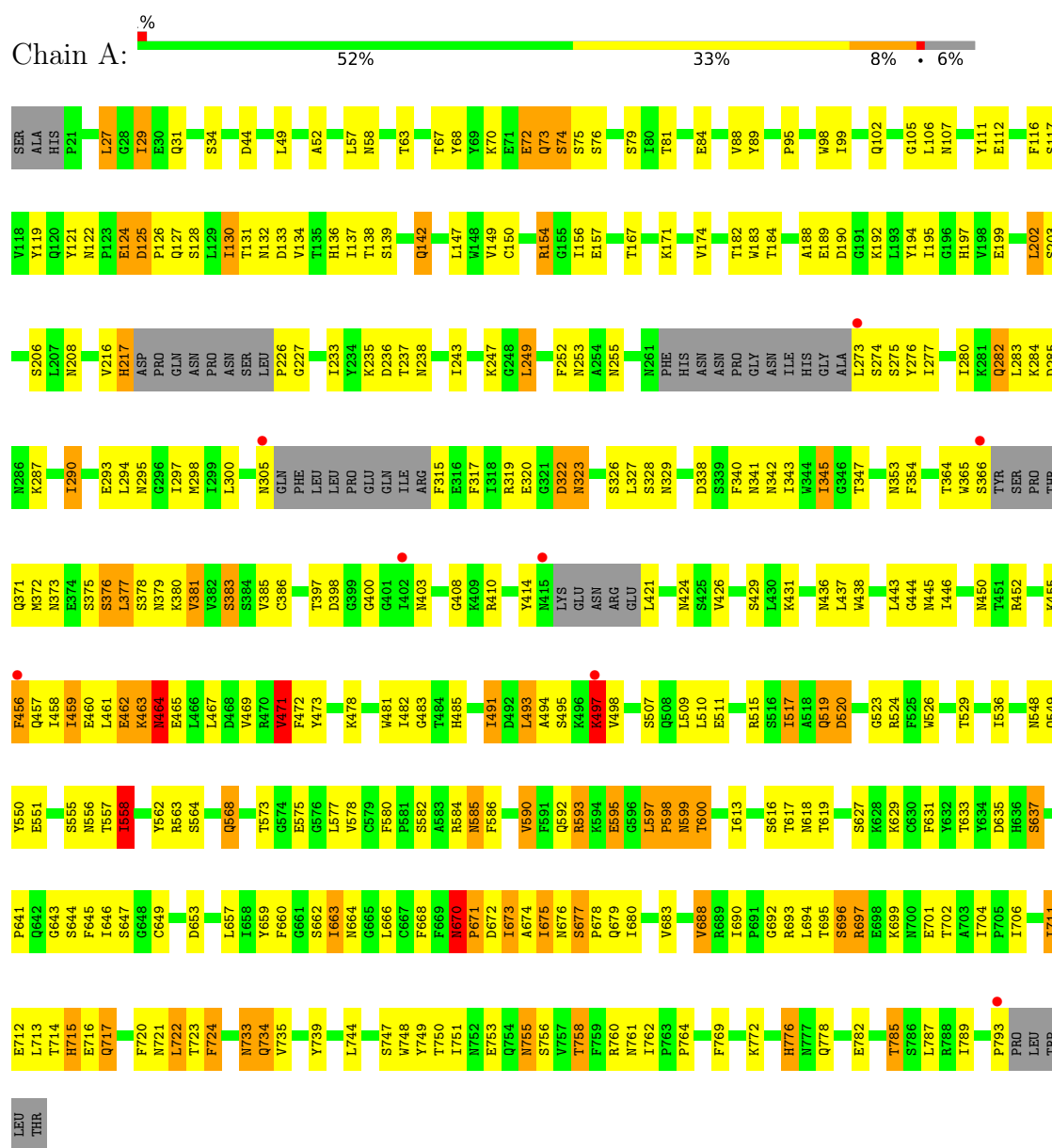
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP Q8A3A5
B	18	SER	-	expression tag	UNP Q8A3A5
C	18	SER	-	expression tag	UNP Q8A3A5
D	18	SER	-	expression tag	UNP Q8A3A5

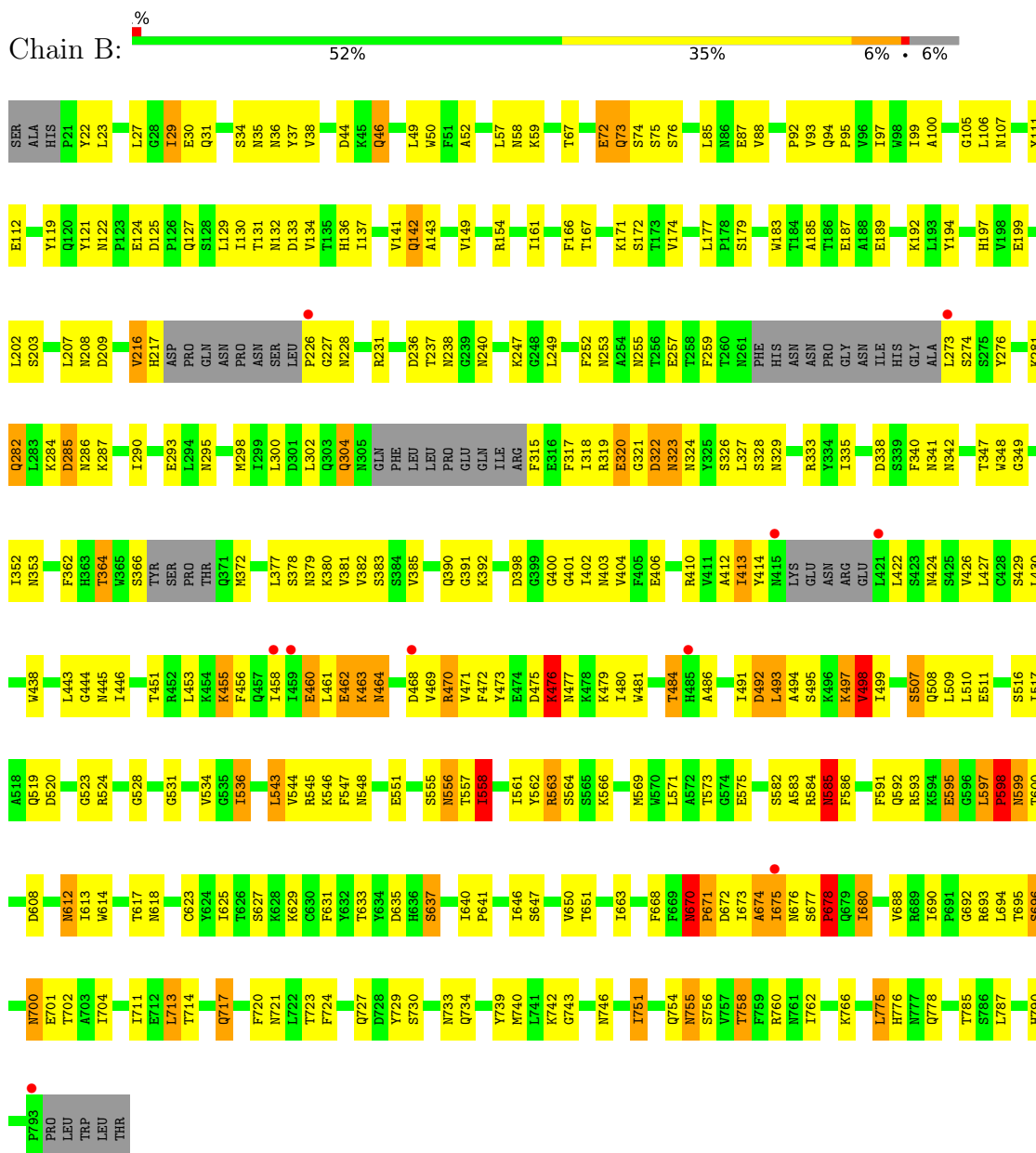
3 Residue-property plots

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.

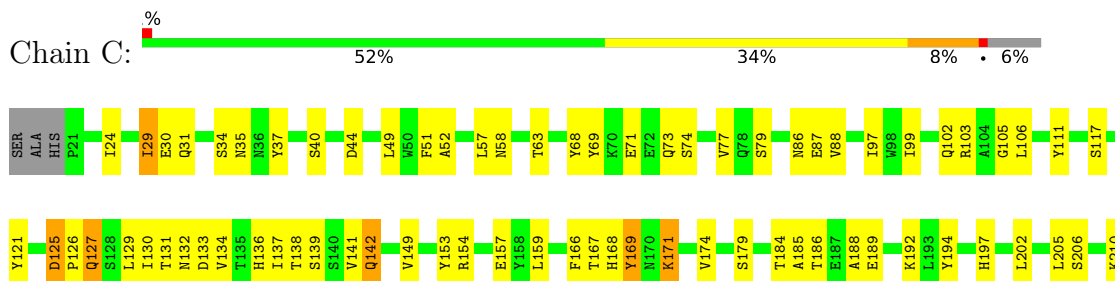
- Molecule 1: Two-component system sensor histidine kinase/response regulator, hybrid (One-component system)

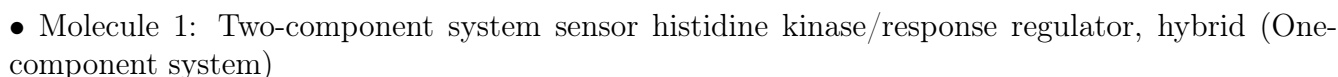


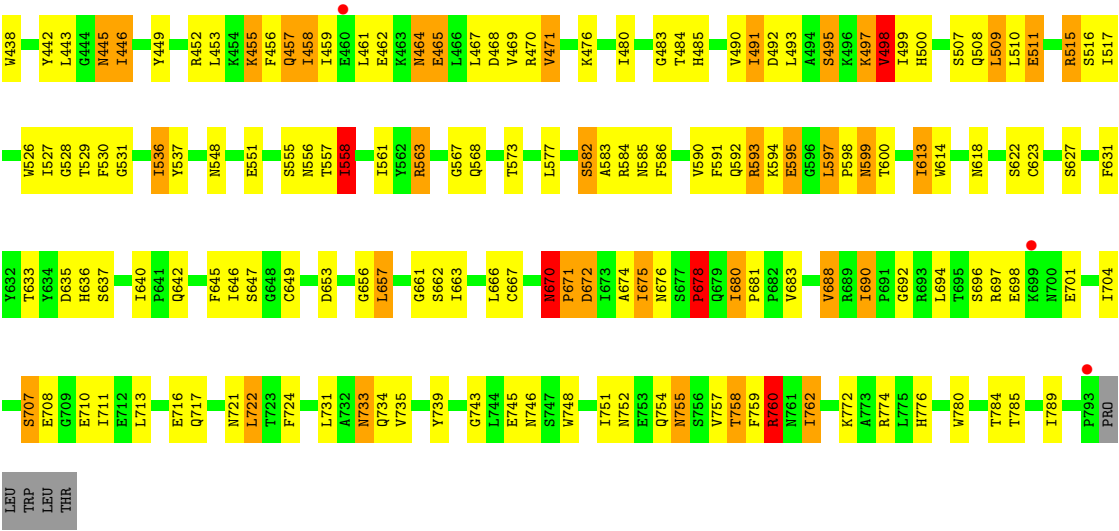
- Molecule 1: Two-component system sensor histidine kinase/response regulator, hybrid (One-component system)



- Molecule 1: Two-component system sensor histidine kinase/response regulator, hybrid (One-component system)







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.93Å 114.12Å 487.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.83 – 3.30 39.83 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.83-3.30) 99.6 (39.83-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.277 0.228 , 0.278	Depositor DCC
R_{free} test set	3459 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23560	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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	0.88	3/6026 (0.0%)	1.06	20/8167 (0.2%)
1	B	0.86	1/6026 (0.0%)	1.06	18/8167 (0.2%)
1	C	0.92	7/6026 (0.1%)	1.09	18/8167 (0.2%)
1	D	0.82	2/6026 (0.0%)	1.04	18/8167 (0.2%)
All	All	0.87	13/24104 (0.1%)	1.06	74/32668 (0.2%)

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	3
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	9

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	ARG	CZ-NH1	19.16	1.59	1.32
1	A	456	PHE	CG-CD2	11.39	1.62	1.38
1	C	670	ASN	CA-C	7.00	1.61	1.52
1	A	305	ASN	CA-C	6.73	1.67	1.52
1	C	210	LYS	C-N	6.37	1.42	1.33
1	B	670	ASN	CA-C	6.16	1.60	1.52
1	D	636	HIS	CG-CD2	5.93	1.42	1.35
1	D	670	ASN	CA-C	5.80	1.60	1.52
1	C	210	LYS	CD-CE	-5.57	1.35	1.52
1	C	636	HIS	CG-CD2	5.32	1.41	1.35
1	C	776	HIS	CG-CD2	5.32	1.41	1.35
1	A	670	ASN	CA-C	5.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	485	HIS	CG-CD2	5.05	1.41	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	PHE	CA-CB-CG	-9.76	104.04	113.80
1	B	497	LYS	N-CA-C	8.34	122.77	112.59
1	B	597	LEU	CA-C-N	-8.31	111.60	120.66
1	B	597	LEU	C-N-CA	-8.31	111.60	120.66
1	B	558	ILE	CB-CA-C	7.95	122.24	111.19
1	D	697	ARG	N-CA-C	-7.61	102.06	112.03
1	C	670	ASN	N-CA-C	6.98	125.23	109.81
1	C	640	ILE	CB-CA-C	-6.97	104.46	110.94
1	B	670	ASN	N-CA-C	6.91	125.08	109.81
1	C	339	SER	N-CA-C	-6.63	105.05	113.01
1	A	414	TYR	N-CA-C	6.45	119.51	108.02
1	C	530	PHE	N-CA-C	-6.35	98.84	109.07
1	A	497	LYS	N-CA-C	6.34	120.47	112.87
1	C	452	ARG	N-CA-C	-6.29	105.46	112.57
1	A	702	THR	N-CA-C	6.27	119.13	110.35
1	A	444	GLY	N-CA-C	-6.25	101.34	110.90
1	C	754	GLN	N-CA-C	6.23	118.65	108.55
1	B	598	PRO	N-CA-C	-6.08	101.61	111.77
1	D	752	ASN	N-CA-C	6.08	118.81	108.90
1	D	228	ASN	N-CA-C	6.05	119.86	112.23
1	D	760	ARG	N-CA-C	6.00	118.90	108.76
1	D	670	ASN	N-CA-C	5.99	123.04	109.81
1	A	762	ILE	CA-C-N	5.96	126.52	120.38
1	A	762	ILE	C-N-CA	5.96	126.52	120.38
1	D	558	ILE	CB-CA-C	5.95	119.65	110.96
1	B	413	ILE	CB-CG1-CD1	5.95	126.29	113.80
1	D	75	SER	N-CA-C	-5.95	106.37	113.21
1	C	646	ILE	CB-CA-C	5.84	119.22	110.98
1	A	619	THR	CA-C-N	-5.84	115.82	122.42
1	A	619	THR	C-N-CA	-5.84	115.82	122.42
1	B	228	ASN	N-CA-C	5.80	120.50	112.90
1	B	75	SER	N-CA-C	-5.79	106.56	113.21
1	A	776	HIS	N-CA-C	5.78	118.32	111.33
1	C	444	GLY	N-CA-C	-5.77	101.97	111.38
1	C	400	GLY	N-CA-C	-5.76	103.15	112.31
1	D	598	PRO	N-CA-C	-5.75	100.64	112.47
1	D	339	SER	N-CA-C	-5.72	106.14	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASN	N-CA-C	5.69	121.11	114.62
1	C	169	TYR	CD1-CG-CD2	-5.64	109.64	118.10
1	A	597	LEU	CA-C-N	-5.64	114.52	120.66
1	A	597	LEU	C-N-CA	-5.64	114.52	120.66
1	D	42	THR	CB-CA-C	-5.63	102.21	114.10
1	A	670	ASN	N-CA-C	5.58	122.14	109.81
1	C	458	ILE	CB-CA-C	5.58	120.44	111.29
1	B	443	LEU	CA-C-N	5.58	125.90	121.61
1	B	443	LEU	C-N-CA	5.58	125.90	121.61
1	B	612	ASN	N-CA-C	5.57	118.09	110.24
1	D	491	ILE	N-CA-C	5.53	116.08	108.12
1	B	668	PHE	N-CA-C	5.53	117.47	109.07
1	B	73	GLN	N-CA-C	-5.52	107.20	114.04
1	C	558	ILE	CB-CA-C	5.47	118.95	110.96
1	A	580	PHE	CA-C-N	5.46	125.80	119.47
1	A	580	PHE	C-N-CA	5.46	125.80	119.47
1	D	597	LEU	CA-C-N	-5.46	113.02	119.84
1	D	597	LEU	C-N-CA	-5.46	113.02	119.84
1	B	720	PHE	N-CA-C	5.41	116.64	108.46
1	D	240	ASN	CA-C-N	-5.33	116.34	122.95
1	D	240	ASN	C-N-CA	-5.33	116.34	122.95
1	C	228	ASN	N-CA-C	5.29	119.84	112.90
1	C	672	ASP	CB-CA-C	5.29	120.22	111.23
1	A	677	SER	CA-C-N	-5.28	113.25	119.84
1	A	677	SER	C-N-CA	-5.28	113.25	119.84
1	A	471	VAL	CB-CA-C	-5.20	103.80	111.80
1	A	519	GLN	N-CA-C	5.17	117.32	108.90
1	C	498	VAL	N-CA-CB	5.16	119.75	111.23
1	A	485	HIS	N-CA-C	-5.14	106.84	113.01
1	D	497	LYS	N-CA-C	5.12	116.94	108.49
1	C	153	TYR	N-CA-C	5.09	119.23	112.72
1	C	575	GLU	N-CA-C	5.09	119.06	108.53
1	B	444	GLY	N-CA-C	-5.07	103.11	111.38
1	A	558	ILE	CB-CA-C	5.06	117.18	110.91
1	D	154	ARG	N-CA-C	5.05	116.93	110.61
1	D	465	GLU	N-CA-C	5.03	117.19	110.35
1	C	169	TYR	CB-CG-CD2	5.00	128.30	120.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	PRO	Peptide
1	A	672	ASP	Peptide
1	A	74	SER	Peptide
1	B	598	PRO	Peptide
1	B	670	ASN	Peptide
1	B	672	ASP	Peptide
1	C	303	GLN	Peptide
1	C	672	ASP	Peptide
1	D	672	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5890	0	5669	277	0
1	B	5890	0	5669	250	0
1	C	5890	0	5669	254	0
1	D	5890	0	5669	243	0
All	All	23560	0	22676	997	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 22.

All (997) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LYS:O	1:C:498:VAL:HG22	1.23	1.32
1:C:491:ILE:HD12	1:C:497:LYS:HB2	1.31	1.11
1:A:450:ASN:HD21	1:A:452:ARG:HB3	0.97	1.10
1:B:29:ILE:H	1:B:29:ILE:HD12	1.00	1.10
1:B:329:ASN:HB3	1:B:347:THR:CG2	1.84	1.07
1:D:323:ASN:HD21	1:D:326:SER:HB2	1.13	1.06
1:A:450:ASN:ND2	1:A:452:ARG:HB3	1.69	1.05
1:C:29:ILE:H	1:C:29:ILE:HD12	0.89	1.05
1:A:73:GLN:OE1	1:A:73:GLN:HA	1.53	1.04
1:C:446:ILE:HB	1:C:458:ILE:HG23	1.36	1.04
1:B:476:LYS:NZ	1:B:563:ARG:HH22	1.56	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:HD12	1:C:29:ILE:N	1.72	1.00
1:B:285:ASP:HB2	1:B:287:LYS:HG3	1.44	1.00
1:C:29:ILE:H	1:C:29:ILE:CD1	1.65	0.99
1:A:446:ILE:HB	1:A:458:ILE:HG23	1.44	0.97
1:B:29:ILE:H	1:B:29:ILE:CD1	1.76	0.97
1:C:497:LYS:O	1:C:498:VAL:CG2	2.11	0.97
1:C:328:SER:H	1:C:353:ASN:HD21	1.06	0.97
1:D:29:ILE:HD12	1:D:29:ILE:H	1.26	0.97
1:A:329:ASN:HB3	1:A:347:THR:CG2	1.94	0.96
1:A:189:GLU:HB2	1:A:192:LYS:HB2	1.46	0.96
1:A:142:GLN:H	1:A:142:GLN:HE21	1.14	0.95
1:A:723:THR:HG22	1:A:756:SER:HB3	1.50	0.94
1:A:462:GLU:HG3	1:A:463:LYS:H	1.31	0.94
1:D:329:ASN:HB3	1:D:347:THR:HG21	1.48	0.93
1:D:323:ASN:ND2	1:D:326:SER:HB2	1.82	0.93
1:B:328:SER:H	1:B:353:ASN:HD21	1.00	0.93
1:A:280:ILE:HG12	1:A:290:ILE:HG23	1.48	0.93
1:B:29:ILE:HG12	1:D:642:GLN:HE21	1.32	0.93
1:C:216:VAL:HG12	1:C:217:HIS:H	1.34	0.92
1:B:216:VAL:HG12	1:B:217:HIS:H	1.28	0.92
1:A:188:ALA:O	1:A:235:LYS:HE3	1.68	0.92
1:D:338:ASP:HB3	1:D:340:PHE:H	1.33	0.92
1:B:29:ILE:HD12	1:B:29:ILE:N	1.85	0.91
1:B:323:ASN:HD21	1:B:326:SER:HB2	1.36	0.91
1:A:338:ASP:HB3	1:A:340:PHE:H	1.35	0.90
1:B:338:ASP:HB3	1:B:340:PHE:H	1.36	0.90
1:B:754:GLN:NE2	1:D:754:GLN:HE22	1.68	0.90
1:D:328:SER:H	1:D:353:ASN:HD21	1.19	0.90
1:C:227:GLY:HA3	1:C:247:LYS:HB2	1.53	0.90
1:A:697:ARG:HA	1:A:697:ARG:HH11	1.36	0.88
1:D:635:ASP:OD1	1:D:637:SER:HB3	1.73	0.88
1:B:476:LYS:HZ1	1:B:563:ARG:HH22	0.93	0.88
1:D:378:SER:H	1:D:403:ASN:HD21	1.20	0.88
1:A:329:ASN:HB3	1:A:347:THR:HG21	1.52	0.88
1:D:125:ASP:HB3	1:D:127:GLN:N	1.89	0.87
1:A:378:SER:H	1:A:403:ASN:HD21	1.22	0.87
1:D:329:ASN:HB3	1:D:347:THR:CG2	2.05	0.86
1:C:189:GLU:HB2	1:C:192:LYS:HB2	1.57	0.86
1:B:476:LYS:NZ	1:B:563:ARG:NH2	2.23	0.86
1:B:754:GLN:HE22	1:D:754:GLN:HE22	1.21	0.85
1:C:470:ARG:HD3	1:C:515:ARG:CZ	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ASN:HB3	1:D:319:ARG:NH1	1.91	0.85
1:B:723:THR:HG22	1:B:756:SER:HB3	1.59	0.85
1:A:721:ASN:HB2	1:A:758:THR:HB	1.59	0.84
1:A:72:GLU:OE2	1:C:593:ARG:HD2	1.76	0.84
1:A:125:ASP:CB	1:A:126:PRO:HA	2.08	0.83
1:B:329:ASN:HB3	1:B:347:THR:HG21	1.60	0.83
1:B:476:LYS:HZ1	1:B:563:ARG:NH2	1.76	0.83
1:C:338:ASP:HB3	1:C:340:PHE:H	1.45	0.82
1:A:676:ASN:HA	1:A:778:GLN:HE21	1.43	0.82
1:C:449:TYR:HD1	1:C:455:LYS:HB2	1.45	0.81
1:A:673:ILE:C	1:A:675:ILE:H	1.88	0.81
1:A:462:GLU:HG3	1:A:463:LYS:N	1.93	0.80
1:B:216:VAL:HG12	1:B:217:HIS:N	1.95	0.80
1:D:622:SER:OG	1:D:633:THR:HG22	1.81	0.80
1:B:323:ASN:ND2	1:B:326:SER:HB2	1.96	0.80
1:C:635:ASP:OD1	1:C:637:SER:HB3	1.81	0.80
1:A:95:PRO:CB	1:A:112:GLU:HG3	2.12	0.80
1:A:295:ASN:HB3	1:A:319:ARG:HH11	1.47	0.79
1:A:373:ASN:H	1:A:376:SER:HB2	1.46	0.79
1:A:659:TYR:HB3	1:A:666:LEU:HD11	1.64	0.79
1:C:283:LEU:HD22	1:C:289:TRP:CD1	2.18	0.79
1:D:446:ILE:HB	1:D:458:ILE:HG23	1.63	0.79
1:B:125:ASP:HB3	1:B:127:GLN:N	1.97	0.78
1:A:74:SER:C	1:A:76:SER:H	1.91	0.78
1:A:676:ASN:HA	1:A:778:GLN:NE2	1.97	0.78
1:D:422:LEU:HG	1:D:457:GLN:HE22	1.47	0.78
1:A:704:ILE:HG22	1:A:711:ILE:HD11	1.64	0.78
1:A:29:ILE:HD11	1:C:642:GLN:HE21	1.49	0.78
1:D:592:GLN:H	1:D:595:GLU:HG2	1.48	0.77
1:B:592:GLN:H	1:B:595:GLU:HG2	1.49	0.77
1:C:548:ASN:HB2	1:C:551:GLU:HB2	1.67	0.77
1:D:125:ASP:HB3	1:D:127:GLN:H	1.46	0.77
1:D:452:ARG:O	1:D:452:ARG:HG2	1.83	0.77
1:D:386:CYS:HB2	1:D:429:SER:OG	1.85	0.77
1:A:125:ASP:HB3	1:A:126:PRO:CA	2.14	0.77
1:A:450:ASN:HD21	1:A:452:ARG:CB	1.88	0.77
1:B:134:VAL:HG13	1:B:149:VAL:HG13	1.65	0.77
1:C:30:GLU:HB2	1:C:31:GLN:NE2	2.00	0.77
1:C:188:ALA:O	1:C:235:LYS:HE3	1.83	0.77
1:A:297:ILE:HD11	1:A:345:ILE:HG12	1.66	0.76
1:D:327:LEU:HD22	1:D:353:ASN:HD22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ALA:HB2	1:C:88:VAL:HG13	1.66	0.76
1:B:693:ARG:NH1	1:D:745:GLU:OE1	2.18	0.76
1:C:125:ASP:HB3	1:C:127:GLN:N	1.99	0.76
1:D:298:MSE:HB3	1:D:317:PHE:CE1	2.20	0.76
1:B:142:GLN:H	1:B:142:GLN:HE21	1.34	0.76
1:A:125:ASP:HB3	1:A:127:GLN:N	2.00	0.75
1:B:721:ASN:HD21	1:B:756:SER:HB2	1.49	0.75
1:D:63:THR:HG21	1:D:755:ASN:HD21	1.50	0.75
1:A:491:ILE:HB	1:A:497:LYS:O	1.86	0.75
1:D:282:GLN:O	1:D:282:GLN:HG3	1.84	0.75
1:A:52:ALA:HB2	1:A:88:VAL:HG13	1.67	0.75
1:C:511:GLU:HB2	1:C:529:THR:HG21	1.67	0.75
1:A:298:MSE:HE2	1:A:317:PHE:CE1	2.21	0.75
1:C:558:ILE:HD13	1:C:558:ILE:O	1.87	0.74
1:A:295:ASN:HB3	1:A:319:ARG:NH1	2.02	0.74
1:B:675:ILE:HG13	1:B:678:PRO:HG2	1.70	0.74
1:D:461:LEU:O	1:D:464:ASN:HA	1.88	0.74
1:D:130:ILE:HG12	1:D:157:GLU:OE1	1.87	0.74
1:C:515:ARG:HG2	1:C:530:PHE:HB2	1.68	0.74
1:B:429:SER:HA	1:B:438:TRP:O	1.88	0.73
1:D:582:SER:OG	1:D:584:ARG:HG2	1.87	0.73
1:B:557:THR:HG23	1:D:103:ARG:HH12	1.53	0.73
1:D:216:VAL:HG12	1:D:217:HIS:N	2.03	0.73
1:D:381:VAL:HG23	1:D:398:ASP:HB3	1.71	0.73
1:D:23:LEU:HD12	1:D:324:ASN:HB3	1.69	0.73
1:C:253:ASN:ND2	1:C:255:ASN:HB3	2.03	0.72
1:A:635:ASP:OD1	1:A:637:SER:HB3	1.88	0.72
1:B:189:GLU:HB2	1:B:192:LYS:HB2	1.70	0.72
1:C:327:LEU:HD22	1:C:353:ASN:HD22	1.53	0.72
1:D:216:VAL:HG12	1:D:217:HIS:H	1.55	0.72
1:B:298:MSE:HB3	1:B:317:PHE:CE1	2.25	0.72
1:A:548:ASN:HB2	1:A:551:GLU:HB2	1.69	0.72
1:A:645:PHE:CD1	1:A:662:SER:HB3	2.25	0.72
1:C:382:VAL:O	1:C:646:ILE:HG21	1.90	0.71
1:A:459:ILE:HG21	1:A:464:ASN:HB2	1.72	0.71
1:B:58:ASN:ND2	1:B:67:THR:HG22	2.05	0.71
1:C:298:MSE:HE2	1:C:317:PHE:HE1	1.55	0.71
1:B:328:SER:N	1:B:353:ASN:HD21	1.83	0.71
1:C:378:SER:H	1:C:403:ASN:HD21	1.36	0.71
1:D:694:LEU:HG	1:D:694:LEU:O	1.91	0.71
1:A:478:LYS:O	1:A:493:LEU:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:548:ASN:HB2	1:D:551:GLU:HB2	1.73	0.70
1:B:105:GLY:CA	1:B:132:ASN:HB2	2.22	0.69
1:C:74:SER:OG	1:C:77:VAL:HB	1.91	0.69
1:A:715:HIS:CE1	1:A:764:PRO:HG3	2.28	0.69
1:B:561:ILE:HG22	1:B:569:MSE:CE	2.22	0.69
1:C:599:ASN:OD1	1:C:618:ASN:HB2	1.92	0.69
1:A:125:ASP:CB	1:A:126:PRO:CA	2.69	0.69
1:D:491:ILE:HG22	1:D:498:VAL:HA	1.74	0.69
1:A:27:LEU:HD23	1:A:31:GLN:HG2	1.75	0.69
1:B:329:ASN:HB3	1:B:347:THR:HG22	1.74	0.69
1:B:754:GLN:HE22	1:D:754:GLN:NE2	1.91	0.69
1:B:561:ILE:HG22	1:B:569:MSE:HE2	1.75	0.68
1:D:29:ILE:HD12	1:D:29:ILE:N	2.05	0.68
1:A:130:ILE:HG12	1:A:157:GLU:OE1	1.93	0.68
1:B:73:GLN:HA	1:B:73:GLN:OE1	1.94	0.68
1:C:402:ILE:HG13	1:C:426:VAL:HG21	1.74	0.68
1:D:427:LEU:HD11	1:D:442:TYR:HB2	1.75	0.68
1:A:338:ASP:OD2	1:A:342:ASN:HB2	1.94	0.68
1:C:125:ASP:HB3	1:C:127:GLN:H	1.57	0.68
1:C:492:ASP:HB3	1:C:496:LYS:O	1.94	0.68
1:C:676:ASN:HA	1:C:778:GLN:HE21	1.58	0.68
1:B:378:SER:H	1:B:403:ASN:HD21	1.41	0.68
1:D:459:ILE:HB	1:D:464:ASN:HB3	1.76	0.68
1:C:460:GLU:HB2	1:C:467:LEU:HD12	1.75	0.68
1:D:63:THR:HG21	1:D:755:ASN:ND2	2.07	0.67
1:A:73:GLN:OE1	1:A:73:GLN:CA	2.36	0.67
1:A:298:MSE:HB3	1:A:317:PHE:CE1	2.29	0.67
1:C:460:GLU:CB	1:C:467:LEU:HD12	2.25	0.67
1:A:280:ILE:HG12	1:A:290:ILE:CG2	2.25	0.66
1:A:446:ILE:HB	1:A:458:ILE:CG2	2.21	0.66
1:C:460:GLU:HA	1:C:460:GLU:OE2	1.94	0.66
1:D:192:LYS:HD3	1:D:206:SER:HB3	1.78	0.66
1:D:275:SER:HB2	1:D:294:LEU:HD12	1.78	0.66
1:C:142:GLN:H	1:C:142:GLN:HE21	1.41	0.66
1:A:462:GLU:O	1:A:463:LYS:C	2.38	0.66
1:A:721:ASN:HD21	1:A:756:SER:HB2	1.60	0.66
1:B:492:ASP:HB3	1:B:499:ILE:HD11	1.77	0.66
1:D:29:ILE:H	1:D:29:ILE:CD1	2.01	0.66
1:C:462:GLU:O	1:C:463:LYS:C	2.38	0.66
1:D:528:GLY:HA3	1:D:558:ILE:HD12	1.78	0.66
1:A:673:ILE:C	1:A:675:ILE:N	2.52	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:HG12	1:D:642:GLN:NE2	2.09	0.65
1:D:236:ASP:HB2	1:D:240:ASN:HB2	1.79	0.65
1:B:125:ASP:HB3	1:B:127:GLN:H	1.61	0.65
1:B:670:ASN:CG	1:B:671:PRO:HD2	2.22	0.65
1:C:227:GLY:CA	1:C:247:LYS:HB2	2.24	0.65
1:D:163:THR:HB	1:D:165:LYS:HD2	1.77	0.65
1:A:511:GLU:HB2	1:A:529:THR:HG21	1.78	0.65
1:D:275:SER:CB	1:D:294:LEU:HD12	2.27	0.65
1:B:520:ASP:OD2	1:B:524:ARG:NH1	2.29	0.65
1:A:130:ILE:HG12	1:A:157:GLU:CD	2.22	0.64
1:C:438:TRP:CH2	1:C:491:ILE:HD11	2.32	0.64
1:B:253:ASN:ND2	1:B:255:ASN:HB3	2.13	0.64
1:A:125:ASP:HB3	1:A:126:PRO:HA	1.79	0.64
1:A:520:ASP:OD2	1:A:524:ARG:NH1	2.30	0.64
1:C:721:ASN:HD21	1:C:756:SER:HB2	1.62	0.64
1:C:297:ILE:HD11	1:C:345:ILE:HG12	1.80	0.64
1:C:662:SER:C	1:C:664:ASN:H	2.05	0.64
1:D:52:ALA:HB2	1:D:88:VAL:HG13	1.78	0.64
1:B:328:SER:H	1:B:353:ASN:ND2	1.85	0.64
1:B:555:SER:HB3	1:B:573:THR:HB	1.79	0.64
1:B:561:ILE:CG2	1:B:569:MSE:HE2	2.27	0.64
1:C:63:THR:HG21	1:C:755:ASN:HD21	1.63	0.64
1:B:460:GLU:OE2	1:B:460:GLU:HA	1.97	0.64
1:A:253:ASN:ND2	1:A:255:ASN:HB3	2.13	0.63
1:B:635:ASP:OD1	1:B:637:SER:HB3	1.98	0.63
1:C:329:ASN:HB3	1:C:347:THR:HG21	1.78	0.63
1:A:673:ILE:O	1:A:675:ILE:N	2.32	0.63
1:B:458:ILE:HD11	1:B:497:LYS:HB2	1.78	0.63
1:A:298:MSE:HE2	1:A:317:PHE:HE1	1.63	0.63
1:D:711:ILE:HG22	1:D:789:ILE:HA	1.80	0.63
1:C:362:PHE:CD1	1:C:640:ILE:HD11	2.33	0.63
1:B:582:SER:C	1:B:584:ARG:H	2.06	0.63
1:B:711:ILE:HB	1:B:787:LEU:HD11	1.79	0.63
1:B:462:GLU:HG3	1:B:463:LYS:HG2	1.80	0.63
1:C:134:VAL:HG13	1:C:149:VAL:HG13	1.81	0.63
1:A:57:LEU:HB3	1:A:68:TYR:HB2	1.80	0.63
1:A:106:LEU:HB3	1:A:119:TYR:HB2	1.81	0.63
1:C:74:SER:HG	1:C:77:VAL:HB	1.62	0.63
1:A:276:TYR:HB3	1:A:293:GLU:HB2	1.80	0.62
1:A:366:SER:HA	1:A:377:LEU:HB2	1.81	0.62
1:B:743:GLY:H	1:B:746:ASN:HD21	1.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:TRP:HB3	1:A:517:ILE:HD11	1.81	0.62
1:C:130:ILE:HG12	1:C:157:GLU:OE1	1.99	0.62
1:D:599:ASN:OD1	1:D:618:ASN:HB2	2.00	0.62
1:D:73:GLN:HA	1:D:73:GLN:OE1	1.99	0.62
1:A:386:CYS:HB2	1:A:429:SER:OG	2.00	0.62
1:A:724:PHE:O	1:A:755:ASN:HB2	1.99	0.62
1:B:534:VAL:HG12	1:B:547:PHE:HB2	1.81	0.62
1:D:526:TRP:CD2	1:D:536:ILE:HD12	2.35	0.62
1:B:462:GLU:O	1:B:463:LYS:C	2.43	0.62
1:B:733:ASN:HD22	1:B:734:GLN:HE21	1.47	0.62
1:A:373:ASN:N	1:A:376:SER:HB2	2.15	0.62
1:B:174:VAL:HB	1:B:177:LEU:HD12	1.80	0.62
1:B:599:ASN:HD21	1:B:618:ASN:H	1.47	0.62
1:D:378:SER:H	1:D:403:ASN:ND2	1.96	0.62
1:B:322:ASP:OD1	1:B:322:ASP:N	2.33	0.61
1:D:295:ASN:HB3	1:D:319:ARG:HH11	1.63	0.61
1:A:192:LYS:NZ	1:A:206:SER:HB3	2.15	0.61
1:C:378:SER:N	1:C:403:ASN:HD21	1.98	0.61
1:A:549:GLN:H	1:A:556:ASN:HD21	1.49	0.61
1:C:673:ILE:C	1:C:675:ILE:H	2.08	0.61
1:C:421:LEU:HD12	1:C:455:LYS:HD3	1.82	0.61
1:B:473:TYR:OH	1:B:519:GLN:HB2	2.00	0.61
1:C:364:THR:HG21	1:C:641:PRO:HG3	1.82	0.61
1:D:642:GLN:O	1:D:642:GLN:HG2	2.01	0.61
1:B:558:ILE:HG13	1:B:571:LEU:HD23	1.81	0.61
1:D:591:PHE:HA	1:D:595:GLU:HG3	1.83	0.61
1:A:98:TRP:CE2	1:A:147:LEU:HD21	2.36	0.61
1:C:491:ILE:CD1	1:C:497:LYS:HB2	2.20	0.61
1:A:400:GLY:O	1:A:424:ASN:HB2	2.01	0.60
1:B:366:SER:HA	1:B:377:LEU:HB2	1.83	0.60
1:A:29:ILE:CD1	1:C:642:GLN:HE21	2.14	0.60
1:B:531:GLY:HA2	1:D:103:ARG:HH11	1.67	0.60
1:C:57:LEU:HB3	1:C:68:TYR:HB2	1.82	0.60
1:D:452:ARG:O	1:D:452:ARG:CG	2.49	0.60
1:B:692:GLY:HA3	1:B:701:GLU:HG3	1.83	0.60
1:D:106:LEU:HB3	1:D:119:TYR:HB2	1.83	0.60
1:B:676:ASN:HA	1:B:778:GLN:HE21	1.67	0.60
1:A:562:TYR:CE2	1:A:564:SER:HA	2.37	0.60
1:D:467:LEU:HD13	1:D:484:THR:HG21	1.84	0.60
1:A:58:ASN:ND2	1:A:67:THR:HG22	2.16	0.60
1:A:373:ASN:CB	1:A:376:SER:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:VAL:O	1:A:785:THR:HG21	2.02	0.60
1:B:99:ILE:HB	1:B:107:ASN:HB2	1.83	0.60
1:D:675:ILE:C	1:D:678:PRO:HD2	2.27	0.60
1:A:722:LEU:CD2	1:A:787:LEU:HD23	2.32	0.59
1:A:782:GLU:OE1	1:A:782:GLU:HA	2.02	0.59
1:B:528:GLY:HA3	1:B:558:ILE:HD12	1.85	0.59
1:C:379:ASN:HD22	1:C:381:VAL:H	1.50	0.59
1:C:438:TRP:HH2	1:C:491:ILE:HD11	1.67	0.59
1:B:285:ASP:O	1:B:286:ASN:HB2	2.02	0.59
1:C:366:SER:HA	1:C:377:LEU:HB2	1.84	0.59
1:C:528:GLY:HA3	1:C:558:ILE:HD12	1.84	0.59
1:D:511:GLU:CB	1:D:529:THR:HG21	2.32	0.59
1:B:458:ILE:HD11	1:B:497:LYS:CB	2.32	0.59
1:B:557:THR:HG23	1:D:103:ARG:NH1	2.16	0.59
1:A:711:ILE:HG23	1:A:713:LEU:HD23	1.83	0.59
1:A:557:THR:HG23	1:C:103:ARG:HH12	1.67	0.59
1:C:484:THR:HG22	1:C:486:ALA:H	1.67	0.59
1:D:429:SER:HA	1:D:438:TRP:O	2.03	0.59
1:A:438:TRP:HH2	1:A:491:ILE:HD11	1.66	0.59
1:A:526:TRP:CE2	1:A:536:ILE:HD12	2.38	0.58
1:B:29:ILE:CG1	1:D:642:GLN:HE21	2.12	0.58
1:C:429:SER:HA	1:C:438:TRP:O	2.03	0.58
1:B:591:PHE:HA	1:B:595:GLU:HG3	1.84	0.58
1:C:373:ASN:HB3	1:C:376:SER:HB2	1.83	0.58
1:B:185:ALA:HA	1:B:194:TYR:O	2.03	0.58
1:C:298:MSE:HE2	1:C:317:PHE:CE1	2.37	0.58
1:C:446:ILE:HB	1:C:458:ILE:CG2	2.24	0.58
1:B:236:ASP:HB3	1:B:240:ASN:H	1.68	0.58
1:C:73:GLN:OE1	1:C:73:GLN:HA	2.03	0.58
1:C:497:LYS:C	1:C:498:VAL:HG22	2.21	0.58
1:A:142:GLN:H	1:A:142:GLN:NE2	1.94	0.58
1:A:491:ILE:O	1:A:491:ILE:HG13	2.02	0.58
1:B:766:LYS:HE3	1:B:790:HIS:CE1	2.39	0.58
1:B:558:ILE:HD11	1:B:561:ILE:HG13	1.84	0.58
1:B:740:MSE:HE3	1:B:742:LYS:HG3	1.86	0.58
1:B:100:ALA:HB2	1:B:137:ILE:HD11	1.84	0.58
1:A:298:MSE:HE2	1:A:317:PHE:CZ	2.38	0.57
1:A:365:TRP:CZ2	1:A:408:GLY:HA2	2.39	0.57
1:C:30:GLU:HB2	1:C:31:GLN:HE22	1.68	0.57
1:C:561:ILE:HG22	1:C:569:MSE:HE3	1.86	0.57
1:D:372:MSE:CE	1:D:410:ARG:HD3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ASP:HB2	1:D:657:LEU:HB2	1.85	0.57
1:C:105:GLY:CA	1:C:132:ASN:HB2	2.34	0.57
1:D:125:ASP:CB	1:D:126:PRO:HA	2.34	0.57
1:D:142:GLN:H	1:D:142:GLN:HE21	1.53	0.57
1:D:278:PHE:HE2	1:D:293:GLU:HB2	1.69	0.57
1:A:130:ILE:HD12	1:A:154:ARG:O	2.04	0.57
1:A:643:GLY:HA3	1:A:664:ASN:HD22	1.69	0.57
1:C:511:GLU:HB2	1:C:529:THR:CG2	2.33	0.57
1:B:484:THR:HB	1:B:486:ALA:H	1.70	0.57
1:D:731:LEU:O	1:D:735:VAL:HG23	2.03	0.57
1:A:131:THR:HG21	1:A:154:ARG:HB2	1.87	0.57
1:C:324:ASN:H	1:C:324:ASN:ND2	2.02	0.57
1:B:382:VAL:O	1:B:646:ILE:HG21	2.04	0.57
1:D:372:MSE:HE2	1:D:410:ARG:HD3	1.85	0.57
1:B:599:ASN:ND2	1:B:617:THR:HB	2.20	0.57
1:B:733:ASN:ND2	1:B:734:GLN:HE21	2.02	0.57
1:C:526:TRP:CD2	1:C:536:ILE:HD12	2.40	0.57
1:D:237:THR:OG1	1:D:282:GLN:NE2	2.37	0.57
1:A:74:SER:C	1:A:76:SER:N	2.61	0.57
1:B:714:THR:H	1:B:717:GLN:HG3	1.70	0.57
1:C:105:GLY:N	1:C:132:ASN:HB2	2.20	0.57
1:C:236:ASP:OD1	1:C:282:GLN:NE2	2.38	0.57
1:C:770:LEU:HD23	1:C:786:SER:HB3	1.87	0.56
1:D:137:ILE:HG23	1:D:147:LEU:HD13	1.87	0.56
1:D:402:ILE:HG12	1:D:426:VAL:HG21	1.86	0.56
1:C:216:VAL:HG12	1:C:217:HIS:N	2.14	0.56
1:A:29:ILE:HD11	1:C:642:GLN:NE2	2.20	0.56
1:A:481:TRP:CB	1:A:517:ILE:HD11	2.36	0.56
1:A:526:TRP:CD2	1:A:536:ILE:HD12	2.41	0.56
1:B:74:SER:C	1:B:76:SER:H	2.11	0.56
1:B:295:ASN:HB3	1:B:319:ARG:NH1	2.20	0.56
1:B:593:ARG:HB2	1:D:72:GLU:OE2	2.05	0.56
1:C:35:ASN:ND2	1:C:37:TYR:HB2	2.20	0.56
1:C:237:THR:H	1:C:282:GLN:HE21	1.53	0.56
1:D:688:VAL:HG12	1:D:722:LEU:HG	1.86	0.56
1:A:125:ASP:HB2	1:A:126:PRO:HA	1.85	0.56
1:B:329:ASN:CB	1:B:347:THR:HG21	2.35	0.56
1:C:480:ILE:HD12	1:C:493:LEU:HG	1.87	0.56
1:D:285:ASP:HB2	1:D:287:LYS:HG3	1.88	0.56
1:C:388:ASP:C	1:C:390:GLN:H	2.14	0.56
1:D:35:ASN:HD21	1:D:54:GLU:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:CD1	1:A:195:ILE:HG12	2.36	0.56
1:B:468:ASP:OD2	1:B:470:ARG:NH2	2.39	0.56
1:C:328:SER:H	1:C:353:ASN:ND2	1.88	0.56
1:C:473:TYR:OH	1:C:519:GLN:HB2	2.06	0.56
1:D:722:LEU:HD12	1:D:722:LEU:H	1.71	0.56
1:C:379:ASN:HB3	1:C:397:THR:HB	1.88	0.56
1:B:520:ASP:HB3	1:B:523:GLY:H	1.71	0.56
1:C:381:VAL:HG22	1:C:398:ASP:HB3	1.88	0.56
1:C:782:GLU:OE1	1:C:782:GLU:HA	2.05	0.56
1:C:502:TYR:CD2	1:C:541:MSE:HG3	2.41	0.56
1:C:528:GLY:HA3	1:C:558:ILE:CD1	2.36	0.56
1:D:71:GLU:OE1	1:D:74:SER:HB3	2.06	0.56
1:B:383:SER:HB2	1:B:426:VAL:O	2.06	0.55
1:B:430:LEU:HD22	1:B:472:PHE:HB3	1.88	0.55
1:C:642:GLN:O	1:C:642:GLN:HG2	2.06	0.55
1:D:558:ILE:HD13	1:D:558:ILE:C	2.31	0.55
1:B:94:GLN:HE22	1:B:161:ILE:HG21	1.72	0.55
1:B:226:PRO:HD3	1:B:259:PHE:CD2	2.41	0.55
1:A:105:GLY:HA2	1:A:132:ASN:HB2	1.87	0.55
1:B:216:VAL:CG1	1:B:217:HIS:N	2.68	0.55
1:B:475:ASP:C	1:B:477:ASN:H	2.14	0.55
1:B:536:ILE:HG13	1:B:586:PHE:CE1	2.41	0.55
1:C:723:THR:HG22	1:C:756:SER:HB3	1.89	0.55
1:D:333:ARG:HG2	1:D:348:TRP:HB2	1.88	0.55
1:A:599:ASN:HD21	1:A:618:ASN:H	1.55	0.55
1:B:402:ILE:O	1:B:413:ILE:HA	2.06	0.55
1:C:740:MSE:HE3	1:C:770:LEU:HD12	1.89	0.55
1:D:675:ILE:CG1	1:D:678:PRO:HG2	2.36	0.55
1:B:92:PRO:HG2	1:B:143:ALA:HB1	1.87	0.55
1:B:131:THR:HG22	1:B:154:ARG:HB2	1.87	0.55
1:B:694:LEU:O	1:B:696:SER:HB2	2.07	0.55
1:A:105:GLY:CA	1:A:132:ASN:HB2	2.37	0.55
1:C:670:ASN:CG	1:C:671:PRO:HD3	2.32	0.55
1:A:95:PRO:CB	1:A:112:GLU:CG	2.85	0.55
1:A:322:ASP:N	1:A:322:ASP:OD1	2.39	0.55
1:A:598:PRO:HD2	1:A:633:THR:HG21	1.89	0.55
1:B:122:ASN:C	1:B:124:GLU:H	2.15	0.55
1:B:673:ILE:C	1:B:675:ILE:N	2.64	0.55
1:C:333:ARG:HG2	1:C:348:TRP:HB2	1.88	0.55
1:D:87:GLU:OE2	1:D:136:HIS:ND1	2.40	0.55
1:D:121:TYR:HA	1:D:129:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG23	1:A:483:GLY:HA3	1.89	0.54
1:B:304:GLN:OE1	1:B:315:PHE:N	2.39	0.54
1:C:638:ASN:O	1:C:639:ASN:CB	2.54	0.54
1:D:383:SER:OG	1:D:398:ASP:HB2	2.07	0.54
1:D:563:ARG:HH11	1:D:563:ARG:HB3	1.71	0.54
1:A:70:LYS:HD2	1:A:81:THR:O	2.07	0.54
1:A:715:HIS:HE1	1:A:764:PRO:HG3	1.71	0.54
1:D:471:VAL:HG23	1:D:483:GLY:HA3	1.90	0.54
1:A:95:PRO:CG	1:A:112:GLU:HG3	2.37	0.54
1:A:555:SER:HB2	1:A:575:GLU:HG2	1.90	0.54
1:B:614:TRP:CE3	1:B:623:CYS:HB2	2.43	0.54
1:A:134:VAL:CG1	1:A:149:VAL:HG13	2.36	0.54
1:B:46:GLN:O	1:B:727:GLN:NE2	2.40	0.54
1:B:551:GLU:OE1	1:B:551:GLU:HA	2.07	0.54
1:C:342:ASN:HB3	1:C:354:PHE:CE1	2.42	0.54
1:D:422:LEU:HG	1:D:457:GLN:NE2	2.18	0.54
1:A:692:GLY:HA3	1:A:701:GLU:HG3	1.90	0.54
1:A:644:SER:H	1:A:663:ILE:HD11	1.73	0.54
1:B:673:ILE:C	1:B:675:ILE:H	2.14	0.54
1:C:44:ASP:HB3	1:C:97:ILE:HD11	1.89	0.54
1:D:774:ARG:HG2	1:D:780:TRP:CZ3	2.43	0.54
1:A:95:PRO:HB2	1:A:112:GLU:HG3	1.90	0.54
1:C:86:ASN:ND2	1:C:102:GLN:HB3	2.23	0.54
1:A:95:PRO:HB2	1:A:112:GLU:CG	2.38	0.54
1:A:125:ASP:HB3	1:A:126:PRO:C	2.33	0.54
1:A:670:ASN:CB	1:A:671:PRO:CD	2.86	0.54
1:B:383:SER:HA	1:B:646:ILE:HD13	1.90	0.54
1:A:217:HIS:HB2	1:A:226:PRO:HD2	1.90	0.53
1:A:327:LEU:HD22	1:A:353:ASN:HD22	1.73	0.53
1:A:381:VAL:HG12	1:A:663:ILE:HA	1.89	0.53
1:A:121:TYR:H	1:A:132:ASN:HD22	1.56	0.53
1:C:484:THR:HG22	1:C:485:HIS:N	2.24	0.53
1:A:694:LEU:O	1:A:696:SER:N	2.41	0.53
1:A:706:ILE:HA	1:A:711:ILE:HD13	1.90	0.53
1:C:614:TRP:HZ2	1:C:673:ILE:CG2	2.22	0.53
1:D:278:PHE:CE2	1:D:293:GLU:HB2	2.43	0.53
1:A:44:ASP:HB2	1:A:111:TYR:CZ	2.44	0.53
1:A:125:ASP:HB3	1:A:127:GLN:H	1.71	0.53
1:B:105:GLY:HA2	1:B:132:ASN:HB2	1.89	0.53
1:C:131:THR:HG21	1:C:154:ARG:H	1.74	0.53
1:D:722:LEU:HD12	1:D:722:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:GLY:H	1:D:746:ASN:HD21	1.56	0.53
1:B:52:ALA:HB2	1:B:88:VAL:HG13	1.91	0.53
1:C:136:HIS:ND1	1:C:184:THR:HG22	2.24	0.53
1:B:650:VAL:HG22	1:B:651:THR:N	2.24	0.53
1:B:739:TYR:OH	1:D:760:ARG:HD2	2.09	0.53
1:D:558:ILE:HD13	1:D:558:ILE:O	2.08	0.53
1:A:188:ALA:HB3	1:A:194:TYR:CD1	2.44	0.53
1:A:300:LEU:HD12	1:A:315:PHE:CE1	2.44	0.53
1:B:27:LEU:HD23	1:B:31:GLN:HG2	1.91	0.53
1:B:281:LYS:HD2	1:B:335:ILE:O	2.09	0.53
1:D:156:ILE:CD1	1:D:195:ILE:HG12	2.39	0.53
1:A:283:LEU:HD23	1:A:343:ILE:CD1	2.39	0.52
1:D:125:ASP:HB3	1:D:126:PRO:CA	2.38	0.52
1:D:323:ASN:ND2	1:D:326:SER:CB	2.65	0.52
1:A:429:SER:HA	1:A:438:TRP:O	2.09	0.52
1:B:558:ILE:HD13	1:B:558:ILE:O	2.09	0.52
1:B:724:PHE:CZ	1:B:751:ILE:HD11	2.45	0.52
1:D:381:VAL:CG2	1:D:398:ASP:HB3	2.37	0.52
1:D:422:LEU:CG	1:D:457:GLN:HE22	2.18	0.52
1:D:199:GLU:OE2	1:D:229:ASP:HB2	2.09	0.52
1:A:323:ASN:HD21	1:A:326:SER:HB2	1.74	0.52
1:A:446:ILE:HD13	1:A:469:VAL:HG21	1.91	0.52
1:B:555:SER:HB2	1:B:575:GLU:HG3	1.91	0.52
1:D:284:LYS:HB2	1:D:337:GLN:HE22	1.74	0.52
1:D:288:LEU:O	1:D:299:ILE:HA	2.10	0.52
1:C:670:ASN:CG	1:C:671:PRO:CD	2.83	0.52
1:A:134:VAL:HG11	1:A:149:VAL:HG13	1.92	0.52
1:B:44:ASP:HB3	1:B:97:ILE:HD11	1.92	0.52
1:B:72:GLU:OE2	1:D:593:ARG:HD2	2.09	0.52
1:B:372:MSE:HE2	1:B:410:ARG:HH11	1.75	0.52
1:B:404:VAL:HB	1:B:412:ALA:HB3	1.92	0.52
1:C:446:ILE:HD12	1:C:472:PHE:CE1	2.44	0.52
1:C:670:ASN:CB	1:C:671:PRO:CD	2.88	0.52
1:D:582:SER:C	1:D:584:ARG:H	2.17	0.52
1:B:516:SER:O	1:B:528:GLY:N	2.34	0.52
1:C:492:ASP:HB2	1:C:499:ILE:HD11	1.91	0.52
1:A:670:ASN:HB3	1:A:671:PRO:HD2	1.91	0.52
1:C:24:ILE:HD11	1:C:318:ILE:HG21	1.92	0.52
1:C:383:SER:HB2	1:C:426:VAL:O	2.10	0.52
1:D:373:ASN:HB3	1:D:376:SER:HB2	1.92	0.52
1:D:675:ILE:HG12	1:D:678:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ILE:HG21	1:A:717:GLN:HB2	1.92	0.52
1:B:675:ILE:C	1:B:678:PRO:HD2	2.34	0.52
1:A:680:ILE:HD12	1:A:680:ILE:O	2.10	0.52
1:B:379:ASN:HD21	1:B:381:VAL:HG22	1.74	0.52
1:B:401:GLY:HA3	1:B:414:TYR:O	2.10	0.52
1:B:598:PRO:HD2	1:B:633:THR:HG21	1.92	0.52
1:C:379:ASN:ND2	1:C:381:VAL:H	2.07	0.51
1:C:445:ASN:ND2	1:C:467:LEU:H	2.08	0.51
1:D:379:ASN:HB2	1:D:400:GLY:H	1.75	0.51
1:A:473:TYR:OH	1:A:519:GLN:HB2	2.09	0.51
1:D:243:ILE:HD12	1:D:252:PHE:HB3	1.90	0.51
1:D:558:ILE:HD11	1:D:561:ILE:HG13	1.91	0.51
1:A:149:VAL:HB	1:A:157:GLU:HB2	1.92	0.51
1:C:273:LEU:HD12	1:C:274:SER:OG	2.11	0.51
1:A:136:HIS:ND1	1:A:184:THR:HG22	2.26	0.51
1:A:693:ARG:NH2	1:C:747:SER:OG	2.44	0.51
1:C:179:SER:HB3	1:C:197:HIS:CD2	2.45	0.51
1:C:323:ASN:HD22	1:C:325:TYR:H	1.57	0.51
1:C:364:THR:HA	1:C:666:LEU:O	2.11	0.51
1:D:74:SER:C	1:D:76:SER:H	2.18	0.51
1:D:511:GLU:HB3	1:D:529:THR:HG21	1.91	0.51
1:D:688:VAL:HG23	1:D:704:ILE:O	2.11	0.51
1:D:708:GLU:HB3	1:D:710:GLU:HG2	1.92	0.51
1:D:772:LYS:HB3	1:D:784:THR:HG22	1.91	0.51
1:A:373:ASN:H	1:A:376:SER:CB	2.20	0.51
1:A:460:GLU:HB2	1:A:467:LEU:HD12	1.92	0.51
1:C:670:ASN:HB3	1:C:671:PRO:CD	2.41	0.51
1:A:378:SER:H	1:A:403:ASN:ND2	2.00	0.51
1:C:327:LEU:CD2	1:C:353:ASN:HD22	2.23	0.51
1:A:520:ASP:HB3	1:A:523:GLY:H	1.76	0.51
1:B:479:LYS:HG2	1:B:492:ASP:HA	1.92	0.51
1:C:762:ILE:HG22	1:C:791:ILE:HD12	1.93	0.51
1:A:653:ASP:HB2	1:A:657:LEU:HB2	1.93	0.50
1:B:531:GLY:HA2	1:D:103:ARG:NH1	2.25	0.50
1:C:87:GLU:OE2	1:C:136:HIS:HA	2.11	0.50
1:B:320:GLU:HG2	1:B:321:GLY:N	2.26	0.50
1:D:515:ARG:HG3	1:D:530:PHE:HB2	1.92	0.50
1:D:724:PHE:O	1:D:755:ASN:HB2	2.11	0.50
1:A:99:ILE:HB	1:A:107:ASN:HB2	1.93	0.50
1:D:242:TRP:CZ3	1:D:251:LEU:HB2	2.46	0.50
1:D:428:CYS:SG	1:D:470:ARG:HA	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ASP:O	1:B:477:ASN:N	2.44	0.50
1:C:34:SER:H	1:C:58:ASN:HD21	1.57	0.50
1:A:142:GLN:HE21	1:A:142:GLN:N	1.96	0.50
1:D:531:GLY:N	1:D:557:THR:HG22	2.27	0.50
1:A:670:ASN:HB3	1:A:671:PRO:CD	2.41	0.50
1:B:723:THR:HG22	1:B:756:SER:CB	2.37	0.50
1:A:197:HIS:HE1	1:A:203:SER:HB2	1.77	0.50
1:D:80:ILE:HD12	1:D:82:GLY:O	2.11	0.50
1:D:592:GLN:H	1:D:595:GLU:CG	2.20	0.50
1:A:323:ASN:ND2	1:A:326:SER:HB2	2.27	0.49
1:B:44:ASP:HB2	1:B:111:TYR:CZ	2.47	0.49
1:C:592:GLN:H	1:C:595:GLU:HG2	1.77	0.49
1:C:670:ASN:HB3	1:C:671:PRO:HD2	1.94	0.49
1:A:616:SER:HB3	1:A:660:PHE:CD1	2.47	0.49
1:B:237:THR:OG1	1:B:282:GLN:NE2	2.45	0.49
1:C:340:PHE:O	1:C:341:ASN:HB2	2.12	0.49
1:B:34:SER:H	1:B:58:ASN:HD21	1.60	0.49
1:C:328:SER:N	1:C:353:ASN:HD21	1.90	0.49
1:C:731:LEU:O	1:C:735:VAL:HG23	2.11	0.49
1:B:338:ASP:HB2	1:B:342:ASN:H	1.77	0.49
1:B:378:SER:H	1:B:403:ASN:ND2	2.10	0.49
1:C:51:PHE:HB2	1:C:58:ASN:HB2	1.94	0.49
1:C:635:ASP:O	1:C:638:ASN:N	2.39	0.49
1:A:237:THR:OG1	1:A:282:GLN:NE2	2.45	0.49
1:D:125:ASP:CB	1:D:126:PRO:CA	2.91	0.49
1:A:379:ASN:HB3	1:A:397:THR:HB	1.93	0.49
1:B:35:ASN:HD21	1:B:37:TYR:HB2	1.78	0.49
1:C:713:LEU:HB2	1:C:791:ILE:HG12	1.94	0.49
1:D:577:LEU:HD21	1:D:613:ILE:HD11	1.95	0.49
1:B:739:TYR:C	1:B:739:TYR:CD2	2.90	0.49
1:C:496:LYS:NZ	1:C:496:LYS:HB3	2.28	0.49
1:C:509:LEU:HD22	1:C:511:GLU:H	1.78	0.49
1:D:298:MSE:HB3	1:D:317:PHE:CD1	2.47	0.49
1:A:670:ASN:CG	1:A:671:PRO:HD2	2.38	0.49
1:B:236:ASP:OD2	1:B:238:ASN:HB2	2.12	0.49
1:B:713:LEU:HD12	1:B:717:GLN:HB2	1.95	0.49
1:C:324:ASN:H	1:C:324:ASN:HD22	1.60	0.49
1:B:38:VAL:HG21	1:B:352:ILE:HG13	1.93	0.49
1:B:381:VAL:HG12	1:B:663:ILE:HA	1.95	0.49
1:C:44:ASP:HB2	1:C:111:TYR:CE2	2.48	0.49
1:C:284:LYS:C	1:C:286:ASN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:O	1:C:495:SER:N	2.46	0.49
1:D:724:PHE:CZ	1:D:751:ILE:HD11	2.48	0.49
1:A:562:TYR:HE2	1:A:564:SER:HA	1.77	0.49
1:B:543:LEU:HD11	1:B:546:LYS:HB3	1.93	0.49
1:C:470:ARG:CD	1:C:515:ARG:CZ	2.86	0.49
1:C:558:ILE:HD13	1:C:558:ILE:C	2.37	0.49
1:D:404:VAL:HB	1:D:412:ALA:HB3	1.94	0.49
1:D:517:ILE:HG22	1:D:527:ILE:HG23	1.93	0.49
1:C:555:SER:HB3	1:C:573:THR:HB	1.95	0.48
1:A:694:LEU:HD11	1:C:780:TRP:CE2	2.49	0.48
1:B:37:TYR:CE2	1:B:349:GLY:HA2	2.47	0.48
1:D:188:ALA:HB3	1:D:194:TYR:CD1	2.48	0.48
1:D:445:ASN:ND2	1:D:467:LEU:H	2.12	0.48
1:B:468:ASP:OD2	1:B:470:ARG:NE	2.46	0.48
1:B:492:ASP:CB	1:B:499:ILE:HD11	2.44	0.48
1:C:189:GLU:HB2	1:C:192:LYS:CB	2.37	0.48
1:C:393:LEU:HD11	1:C:659:TYR:CZ	2.49	0.48
1:D:148:TRP:CZ3	1:D:158:TYR:HB2	2.47	0.48
1:D:585:ASN:O	1:D:586:PHE:HB2	2.13	0.48
1:A:130:ILE:CD1	1:A:154:ARG:O	2.61	0.48
1:B:582:SER:C	1:B:584:ARG:N	2.72	0.48
1:B:721:ASN:HB2	1:B:758:THR:HB	1.95	0.48
1:C:450:ASN:HD21	1:C:452:ARG:HE	1.59	0.48
1:C:592:GLN:O	1:C:593:ARG:C	2.56	0.48
1:D:170:ASN:ND2	1:D:172:SER:OG	2.46	0.48
1:D:446:ILE:HD13	1:D:469:VAL:HG21	1.94	0.48
1:A:558:ILE:HD13	1:A:558:ILE:C	2.38	0.48
1:A:688:VAL:CG2	1:A:704:ILE:HB	2.44	0.48
1:C:378:SER:H	1:C:403:ASN:ND2	2.09	0.48
1:D:592:GLN:O	1:D:593:ARG:C	2.56	0.48
1:C:366:SER:HA	1:C:377:LEU:HD22	1.95	0.48
1:C:482:ILE:HD12	1:C:491:ILE:HG23	1.94	0.48
1:C:559:ASN:HD21	1:C:601:HIS:HE1	1.61	0.48
1:D:491:ILE:HA	1:D:499:ILE:HG12	1.96	0.48
1:D:692:GLY:HA3	1:D:701:GLU:OE1	2.14	0.48
1:A:328:SER:H	1:A:353:ASN:HD21	1.61	0.48
1:C:676:ASN:HA	1:C:778:GLN:NE2	2.26	0.48
1:D:442:TYR:CE2	1:D:443:LEU:HD13	2.48	0.48
1:A:79:SER:HA	1:A:116:PHE:CD2	2.49	0.48
1:A:131:THR:CG2	1:A:154:ARG:HB2	2.42	0.48
1:B:29:ILE:CD1	1:B:29:ILE:N	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:TRP:CE2	1:C:536:ILE:HD12	2.48	0.48
1:D:400:GLY:O	1:D:424:ASN:HB2	2.14	0.48
1:D:721:ASN:HB2	1:D:758:THR:HB	1.96	0.48
1:A:70:LYS:NZ	1:C:575:GLU:OE1	2.47	0.48
1:B:189:GLU:HB2	1:B:192:LYS:CB	2.43	0.48
1:C:171:LYS:HA	1:C:174:VAL:O	2.14	0.48
1:C:470:ARG:HD3	1:C:515:ARG:NH1	2.29	0.48
1:A:122:ASN:HD21	1:A:124:GLU:HB2	1.78	0.47
1:A:520:ASP:HB3	1:A:523:GLY:N	2.29	0.47
1:A:578:VAL:HG22	1:A:590:VAL:HG13	1.95	0.47
1:B:227:GLY:HA3	1:B:247:LYS:HB2	1.96	0.47
1:B:276:TYR:HB3	1:B:293:GLU:HB2	1.95	0.47
1:C:129:LEU:HD12	1:C:157:GLU:HG3	1.96	0.47
1:D:110:ASN:OD1	1:D:112:GLU:HB2	2.13	0.47
1:D:555:SER:HB3	1:D:573:THR:HB	1.95	0.47
1:B:282:GLN:HG3	1:B:282:GLN:O	2.13	0.47
1:D:29:ILE:HD11	1:D:36:ASN:HD21	1.79	0.47
1:A:327:LEU:HD22	1:A:353:ASN:ND2	2.28	0.47
1:A:662:SER:C	1:A:664:ASN:H	2.22	0.47
1:A:577:LEU:HD21	1:A:613:ILE:HD11	1.96	0.47
1:A:670:ASN:CB	1:A:671:PRO:HD2	2.45	0.47
1:B:724:PHE:HZ	1:B:751:ILE:CD1	2.27	0.47
1:B:468:ASP:CG	1:B:470:ARG:HH21	2.22	0.47
1:C:643:GLY:HA3	1:C:664:ASN:HD22	1.78	0.47
1:D:363:HIS:O	1:D:667:CYS:HA	2.14	0.47
1:A:134:VAL:HG13	1:A:149:VAL:CG1	2.45	0.47
1:A:137:ILE:HG23	1:A:147:LEU:HD13	1.97	0.47
1:A:711:ILE:HG22	1:A:789:ILE:HG12	1.97	0.47
1:B:340:PHE:O	1:B:341:ASN:HB2	2.15	0.47
1:B:381:VAL:CG2	1:B:398:ASP:HB3	2.44	0.47
1:B:766:LYS:HG3	1:B:790:HIS:ND1	2.30	0.47
1:C:381:VAL:CG2	1:C:398:ASP:HB3	2.45	0.47
1:C:520:ASP:HB3	1:C:523:GLY:H	1.78	0.47
1:C:597:LEU:HD13	1:C:631:PHE:CD2	2.49	0.47
1:C:650:VAL:HG22	1:C:651:THR:N	2.28	0.47
1:D:99:ILE:HB	1:D:107:ASN:HB2	1.96	0.47
1:D:197:HIS:HE1	1:D:203:SER:HB2	1.80	0.47
1:D:509:LEU:HA	1:D:537:TYR:OH	2.15	0.47
1:D:733:ASN:HD22	1:D:734:GLN:HB3	1.80	0.47
1:C:706:ILE:HA	1:C:711:ILE:CD1	2.45	0.47
1:A:249:LEU:CD1	1:A:249:LEU:C	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD23	1:A:343:ILE:HD11	1.97	0.47
1:A:298:MSE:HB3	1:A:317:PHE:CD1	2.50	0.47
1:B:23:LEU:HD12	1:B:324:ASN:HB3	1.96	0.47
1:B:106:LEU:HB3	1:B:119:TYR:HB2	1.96	0.47
1:B:122:ASN:C	1:B:124:GLU:N	2.73	0.47
1:C:24:ILE:HD11	1:C:318:ILE:CG2	2.45	0.47
1:C:599:ASN:HD21	1:C:618:ASN:H	1.62	0.47
1:A:714:THR:OG1	1:A:717:GLN:HG2	2.15	0.47
1:B:724:PHE:CZ	1:B:751:ILE:CD1	2.98	0.47
1:A:131:THR:HB	1:A:154:ARG:HD3	1.97	0.46
1:A:131:THR:HB	1:A:154:ARG:HH11	1.79	0.46
1:B:507:SER:OG	1:B:508:GLN:N	2.49	0.46
1:D:136:HIS:ND1	1:D:184:THR:HG22	2.29	0.46
1:D:388:ASP:C	1:D:390:GLN:H	2.22	0.46
1:A:34:SER:H	1:A:58:ASN:HD21	1.62	0.46
1:A:192:LYS:HZ3	1:A:206:SER:HB3	1.79	0.46
1:B:22:TYR:CD2	1:B:318:ILE:HD11	2.50	0.46
1:D:35:ASN:HB3	1:D:53:THR:HB	1.98	0.46
1:D:751:ILE:HD13	1:D:757:VAL:HG23	1.95	0.46
1:A:74:SER:OG	1:A:76:SER:HB2	2.15	0.46
1:A:459:ILE:HG21	1:A:464:ASN:CB	2.42	0.46
1:A:714:THR:H	1:A:717:GLN:CG	2.28	0.46
1:A:722:LEU:HD23	1:A:787:LEU:CD2	2.46	0.46
1:A:748:TRP:CH2	1:A:772:LYS:HE3	2.50	0.46
1:B:136:HIS:HB2	1:B:183:TRP:O	2.15	0.46
1:C:690:ILE:HG23	1:C:704:ILE:HD11	1.97	0.46
1:D:338:ASP:HB3	1:D:340:PHE:N	2.15	0.46
1:D:759:PHE:HB3	1:D:762:ILE:HD13	1.96	0.46
1:A:373:ASN:HB3	1:A:376:SER:HB2	1.97	0.46
1:A:711:ILE:HD12	1:A:711:ILE:HA	1.84	0.46
1:B:438:TRP:CH2	1:B:491:ILE:HD11	2.51	0.46
1:D:322:ASP:OD1	1:D:322:ASP:N	2.48	0.46
1:D:657:LEU:HD23	1:D:670:ASN:OD1	2.15	0.46
1:A:340:PHE:O	1:A:341:ASN:HB2	2.14	0.46
1:A:670:ASN:CG	1:A:671:PRO:CD	2.89	0.46
1:A:739:TYR:HB2	1:A:769:PHE:CE1	2.50	0.46
1:C:71:GLU:HB3	1:C:74:SER:HB3	1.98	0.46
1:C:739:TYR:CD2	1:C:739:TYR:C	2.93	0.46
1:A:473:TYR:CZ	1:A:519:GLN:HB2	2.50	0.46
1:B:58:ASN:HD22	1:B:67:THR:HG22	1.80	0.46
1:B:378:SER:N	1:B:403:ASN:HD21	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ALA:C	1:B:676:ASN:H	2.24	0.46
1:D:711:ILE:CG2	1:D:789:ILE:HG12	2.46	0.46
1:A:722:LEU:O	1:A:756:SER:HA	2.16	0.46
1:B:558:ILE:HD13	1:B:558:ILE:C	2.40	0.46
1:D:30:GLU:O	1:D:64:ARG:NH2	2.49	0.46
1:D:243:ILE:HD12	1:D:252:PHE:CB	2.45	0.46
1:A:84:GLU:O	1:A:102:GLN:HG2	2.16	0.46
1:A:95:PRO:HG3	1:A:112:GLU:HG3	1.98	0.46
1:B:95:PRO:CB	1:B:112:GLU:HG3	2.46	0.46
1:B:548:ASN:HA	1:B:556:ASN:HD21	1.80	0.46
1:B:690:ILE:HG23	1:B:704:ILE:HD11	1.98	0.46
1:C:430:LEU:HG	1:C:431:LYS:N	2.31	0.46
1:D:381:VAL:HG12	1:D:663:ILE:HA	1.97	0.46
1:D:490:VAL:HB	1:D:500:HIS:HB2	1.98	0.46
1:D:649:CYS:SG	1:D:661:GLY:HA3	2.56	0.46
1:A:378:SER:N	1:A:403:ASN:HD21	2.03	0.46
1:B:362:PHE:CD1	1:B:640:ILE:HD11	2.51	0.46
1:B:675:ILE:HA	1:B:678:PRO:HD2	1.98	0.46
1:B:724:PHE:O	1:B:755:ASN:HB2	2.16	0.46
1:C:275:SER:HB2	1:C:294:LEU:HD13	1.98	0.46
1:D:78:GLN:NE2	1:D:79:SER:O	2.48	0.46
1:D:614:TRP:CE3	1:D:623:CYS:HB2	2.51	0.46
1:A:29:ILE:HD12	1:A:29:ILE:H	1.80	0.46
1:A:461:LEU:HB3	1:A:465:GLU:HB2	1.98	0.46
1:B:593:ARG:NH2	1:B:599:ASN:HB2	2.31	0.46
1:C:386:CYS:HB2	1:C:429:SER:OG	2.15	0.46
1:D:492:ASP:HB3	1:D:499:ILE:HD11	1.97	0.46
1:A:711:ILE:HG22	1:A:789:ILE:HA	1.98	0.45
1:C:192:LYS:NZ	1:C:206:SER:HB3	2.31	0.45
1:C:393:LEU:HD11	1:C:659:TYR:CE1	2.51	0.45
1:A:585:ASN:O	1:A:586:PHE:HB2	2.16	0.45
1:B:524:ARG:HD2	1:B:536:ILE:HG22	1.96	0.45
1:B:692:GLY:CA	1:B:701:GLU:HG3	2.46	0.45
1:B:252:PHE:CE1	1:B:257:GLU:HA	2.52	0.45
1:B:364:THR:HG21	1:B:641:PRO:HG3	1.98	0.45
1:C:338:ASP:HB3	1:C:340:PHE:N	2.24	0.45
1:C:459:ILE:HG21	1:C:464:ASN:HA	1.97	0.45
1:C:462:GLU:O	1:C:465:GLU:N	2.34	0.45
1:B:524:ARG:HD2	1:B:536:ILE:CG2	2.47	0.45
1:C:275:SER:HB2	1:C:294:LEU:CD1	2.47	0.45
1:C:363:HIS:O	1:C:667:CYS:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:CG1	1:C:426:VAL:HG21	2.44	0.45
1:A:556:ASN:HD22	1:A:556:ASN:HA	1.57	0.45
1:A:592:GLN:H	1:A:595:GLU:HG2	1.81	0.45
1:B:562:TYR:CE2	1:B:564:SER:HA	2.51	0.45
1:C:724:PHE:O	1:C:755:ASN:HB2	2.17	0.45
1:D:733:ASN:C	1:D:733:ASN:ND2	2.74	0.45
1:A:697:ARG:HA	1:A:697:ARG:NH1	2.16	0.45
1:A:722:LEU:HD23	1:A:787:LEU:HD23	1.98	0.45
1:B:582:SER:O	1:B:584:ARG:N	2.49	0.45
1:B:680:ILE:H	1:B:680:ILE:HG13	1.55	0.45
1:D:449:TYR:CD1	1:D:455:LYS:HB2	2.51	0.45
1:B:237:THR:H	1:B:282:GLN:HE21	1.64	0.45
1:B:338:ASP:C	1:B:340:PHE:H	2.25	0.45
1:B:690:ILE:O	1:B:690:ILE:HG13	2.16	0.45
1:C:605:ILE:CG2	1:C:613:ILE:HD13	2.46	0.45
1:D:599:ASN:HD22	1:D:599:ASN:H	1.65	0.45
1:A:72:GLU:OE2	1:C:593:ARG:HB2	2.17	0.45
1:A:156:ILE:HD11	1:A:195:ILE:HG12	1.99	0.45
1:B:57:LEU:HB2	1:B:85:LEU:HD11	1.99	0.45
1:B:129:LEU:HD13	1:B:166:PHE:CE1	2.52	0.45
1:C:329:ASN:HB3	1:C:347:THR:CG2	2.44	0.45
1:C:748:TRP:CZ3	1:C:772:LYS:HG2	2.52	0.45
1:D:670:ASN:CB	1:D:671:PRO:CD	2.94	0.45
1:B:410:ARG:HD2	1:B:413:ILE:HD11	1.99	0.45
1:C:401:GLY:HA3	1:C:414:TYR:O	2.17	0.45
1:D:298:MSE:HE2	1:D:317:PHE:HE1	1.82	0.45
1:A:688:VAL:HG23	1:A:704:ILE:HB	1.99	0.45
1:C:337:GLN:HG2	1:C:341:ASN:HA	1.99	0.45
1:C:520:ASP:HB3	1:C:523:GLY:N	2.32	0.45
1:D:125:ASP:HB3	1:D:126:PRO:C	2.42	0.45
1:D:449:TYR:HD1	1:D:455:LYS:HB2	1.82	0.45
1:C:121:TYR:HA	1:C:129:LEU:O	2.17	0.44
1:C:320:GLU:HG3	1:C:329:ASN:C	2.42	0.44
1:C:638:ASN:O	1:C:639:ASN:HB3	2.17	0.44
1:D:683:VAL:O	1:D:785:THR:HG21	2.17	0.44
1:B:545:ARG:HG2	1:B:546:LYS:H	1.82	0.44
1:B:724:PHE:HZ	1:B:751:ILE:HD13	1.82	0.44
1:C:138:THR:HG22	1:C:139:SER:O	2.17	0.44
1:C:382:VAL:O	1:C:646:ILE:CG2	2.64	0.44
1:C:601:HIS:CE1	1:C:603:ARG:NH1	2.85	0.44
1:D:96:VAL:HA	1:D:109:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:O	1:D:286:ASN:HB2	2.16	0.44
1:A:364:THR:CG2	1:A:641:PRO:HG3	2.47	0.44
1:A:714:THR:H	1:A:717:GLN:HG3	1.82	0.44
1:B:592:GLN:O	1:B:593:ARG:C	2.60	0.44
1:D:273:LEU:HD12	1:D:274:SER:OG	2.18	0.44
1:B:290:ILE:HB	1:B:298:MSE:HG3	2.00	0.44
1:B:300:LEU:HD22	1:B:302:LEU:HD23	1.99	0.44
1:C:549:GLN:H	1:C:556:ASN:ND2	2.15	0.44
1:D:670:ASN:HB3	1:D:671:PRO:CD	2.46	0.44
1:D:672:ASP:HA	1:D:674:ALA:H	1.82	0.44
1:A:285:ASP:HB3	1:A:287:LYS:HE3	1.99	0.44
1:A:381:VAL:CG2	1:A:398:ASP:HB3	2.47	0.44
1:A:597:LEU:HD22	1:A:631:PHE:CZ	2.53	0.44
1:B:544:VAL:O	1:C:372:MSE:HB2	2.18	0.44
1:C:246:SER:HB3	1:C:276:TYR:CZ	2.53	0.44
1:C:287:LYS:HE2	1:C:301:ASP:OD2	2.17	0.44
1:C:473:TYR:CZ	1:C:519:GLN:HB2	2.53	0.44
1:A:197:HIS:HE1	1:A:203:SER:CB	2.30	0.44
1:B:520:ASP:HB3	1:B:523:GLY:N	2.33	0.44
1:B:608:ASP:OD2	1:B:612:ASN:HB2	2.18	0.44
1:C:71:GLU:HG2	1:C:79:SER:CB	2.48	0.44
1:C:484:THR:HG22	1:C:485:HIS:H	1.81	0.44
1:D:404:VAL:HG12	1:D:411:VAL:HG23	1.99	0.44
1:D:645:PHE:CD1	1:D:662:SER:HB3	2.53	0.44
1:A:227:GLY:HA3	1:A:247:LYS:HB2	2.00	0.44
1:A:438:TRP:CH2	1:A:491:ILE:HD11	2.50	0.44
1:A:690:ILE:O	1:A:690:ILE:HG13	2.18	0.44
1:A:704:ILE:N	1:A:704:ILE:HD12	2.32	0.44
1:A:715:HIS:CG	1:A:793:PRO:HA	2.53	0.44
1:A:733:ASN:HB3	1:A:734:GLN:HG2	1.99	0.44
1:A:739:TYR:CE1	1:A:749:TYR:HB2	2.52	0.44
1:D:672:ASP:C	1:D:674:ALA:H	2.25	0.44
1:D:192:LYS:CD	1:D:206:SER:HB3	2.47	0.44
1:D:510:LEU:N	1:D:537:TYR:OH	2.50	0.44
1:A:711:ILE:CG2	1:A:789:ILE:HG12	2.48	0.43
1:A:750:THR:HG22	1:A:751:ILE:N	2.32	0.43
1:B:592:GLN:H	1:B:595:GLU:CG	2.23	0.43
1:A:236:ASP:OD2	1:A:238:ASN:HB2	2.17	0.43
1:A:592:GLN:O	1:A:593:ARG:C	2.61	0.43
1:B:491:ILE:HG22	1:B:498:VAL:HA	1.99	0.43
1:C:298:MSE:HB3	1:C:317:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:LEU:O	1:C:694:LEU:HG	2.18	0.43
1:D:670:ASN:HB3	1:D:671:PRO:HD2	2.00	0.43
1:B:231:ARG:NH1	1:B:276:TYR:OH	2.52	0.43
1:B:333:ARG:HD3	1:B:333:ARG:HA	1.72	0.43
1:D:35:ASN:ND2	1:D:37:TYR:HB2	2.33	0.43
1:D:492:ASP:CB	1:D:499:ILE:HD11	2.47	0.43
1:A:379:ASN:HB2	1:A:400:GLY:H	1.83	0.43
1:A:431:LYS:HA	1:A:437:LEU:HD23	1.99	0.43
1:A:720:PHE:CE2	1:A:722:LEU:HD11	2.54	0.43
1:A:747:SER:OG	1:C:693:ARG:NH1	2.52	0.43
1:B:481:TRP:HB3	1:B:517:ILE:HD12	2.00	0.43
1:C:63:THR:HG21	1:C:755:ASN:ND2	2.30	0.43
1:C:662:SER:C	1:C:664:ASN:N	2.72	0.43
1:D:146:GLY:HA2	1:D:161:ILE:HG13	2.01	0.43
1:D:507:SER:OG	1:D:508:GLN:N	2.52	0.43
1:B:327:LEU:HD22	1:B:353:ASN:HD22	1.84	0.43
1:B:400:GLY:O	1:B:424:ASN:HB2	2.18	0.43
1:B:585:ASN:O	1:B:586:PHE:HB2	2.18	0.43
1:C:99:ILE:O	1:C:106:LEU:HD12	2.19	0.43
1:D:328:SER:N	1:D:353:ASN:HD21	2.00	0.43
1:D:680:ILE:HA	1:D:681:PRO:HD3	1.89	0.43
1:C:515:ARG:HA	1:C:515:ARG:HD3	1.62	0.43
1:D:236:ASP:CB	1:D:240:ASN:HB2	2.47	0.43
1:D:721:ASN:HD22	1:D:758:THR:HB	1.83	0.43
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.83	0.43
1:A:659:TYR:CD1	1:A:668:PHE:HB3	2.53	0.43
1:B:536:ILE:HG13	1:B:586:PHE:CZ	2.54	0.43
1:D:692:GLY:HA3	1:D:701:GLU:HG3	1.99	0.43
1:A:253:ASN:HD22	1:A:255:ASN:HB3	1.82	0.43
1:A:282:GLN:O	1:A:282:GLN:HG3	2.19	0.43
1:B:455:LYS:NZ	1:B:455:LYS:HB2	2.34	0.43
1:B:650:VAL:CG2	1:B:651:THR:N	2.82	0.43
1:C:599:ASN:C	1:C:599:ASN:ND2	2.74	0.43
1:C:650:VAL:CG2	1:C:651:THR:N	2.82	0.43
1:A:280:ILE:CG1	1:A:290:ILE:HG23	2.35	0.43
1:B:187:GLU:HA	1:B:192:LYS:O	2.19	0.43
1:B:379:ASN:ND2	1:B:381:VAL:HG22	2.34	0.43
1:B:391:GLY:O	1:B:406:GLU:HG3	2.18	0.43
1:D:690:ILE:O	1:D:690:ILE:HG13	2.18	0.43
1:D:759:PHE:HB3	1:D:762:ILE:CD1	2.49	0.43
1:A:593:ARG:NH1	1:A:600:THR:CG2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:GLN:OE1	1:C:581:PRO:HA	2.18	0.43
1:D:382:VAL:HG11	1:D:666:LEU:HD13	2.01	0.43
1:D:711:ILE:HG21	1:D:789:ILE:HG12	2.01	0.43
1:D:733:ASN:ND2	1:D:734:GLN:HB3	2.34	0.43
1:D:743:GLY:H	1:D:746:ASN:ND2	2.16	0.43
1:B:329:ASN:CB	1:B:347:THR:CG2	2.75	0.42
1:C:659:TYR:CD1	1:C:668:PHE:HB3	2.54	0.42
1:C:750:THR:HG22	1:C:751:ILE:N	2.34	0.42
1:D:207:LEU:C	1:D:209:ASP:H	2.26	0.42
1:A:599:ASN:ND2	1:A:617:THR:HB	2.34	0.42
1:B:74:SER:C	1:B:76:SER:N	2.76	0.42
1:B:729:TYR:O	1:B:730:SER:C	2.60	0.42
1:C:159:LEU:HD13	1:C:166:PHE:CE1	2.54	0.42
1:C:236:ASP:HB2	1:C:240:ASN:O	2.19	0.42
1:C:446:ILE:HD12	1:C:472:PHE:CZ	2.54	0.42
1:C:770:LEU:HD23	1:C:786:SER:CB	2.48	0.42
1:D:237:THR:H	1:D:282:GLN:NE2	2.17	0.42
1:D:672:ASP:C	1:D:674:ALA:N	2.77	0.42
1:A:320:GLU:HB2	1:A:329:ASN:C	2.44	0.42
1:A:373:ASN:HB3	1:A:376:SER:N	2.34	0.42
1:B:536:ILE:HG13	1:B:586:PHE:HE1	1.83	0.42
1:D:298:MSE:HE2	1:D:317:PHE:CE1	2.54	0.42
1:D:563:ARG:HD3	1:D:567:GLY:HA2	2.02	0.42
1:A:126:PRO:C	1:A:128:SER:H	2.28	0.42
1:A:354:PHE:CD2	1:A:354:PHE:C	2.97	0.42
1:B:693:ARG:C	1:B:695:THR:H	2.28	0.42
1:C:34:SER:HB2	1:C:69:TYR:OH	2.19	0.42
1:C:470:ARG:CD	1:C:515:ARG:NH1	2.83	0.42
1:D:253:ASN:ND2	1:D:255:ASN:HB3	2.35	0.42
1:D:421:LEU:HG	1:D:421:LEU:O	2.19	0.42
1:A:329:ASN:CB	1:A:347:THR:HG21	2.37	0.42
1:A:472:PHE:CD1	1:A:482:ILE:HG12	2.54	0.42
1:B:640:ILE:HG23	1:B:641:PRO:HD2	2.02	0.42
1:D:40:SER:CB	1:D:87:GLU:HA	2.50	0.42
1:B:451:THR:C	1:B:453:LEU:H	2.26	0.42
1:B:593:ARG:NH1	1:B:600:THR:HG22	2.35	0.42
1:B:597:LEU:HD22	1:B:631:PHE:CZ	2.55	0.42
1:D:30:GLU:HB2	1:D:31:GLN:NE2	2.34	0.42
1:A:722:LEU:HD12	1:A:722:LEU:H	1.84	0.42
1:B:29:ILE:HG13	1:B:36:ASN:HD21	1.84	0.42
1:B:125:ASP:C	1:B:127:GLN:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ARG:HG2	1:B:546:LYS:N	2.34	0.42
1:B:688:VAL:HG22	1:B:704:ILE:O	2.20	0.42
1:C:338:ASP:C	1:C:340:PHE:H	2.28	0.42
1:D:109:TYR:OH	1:D:114:GLN:HG2	2.20	0.42
1:D:690:ILE:HG23	1:D:704:ILE:HD11	2.00	0.42
1:D:707:SER:OG	1:D:708:GLU:N	2.51	0.42
1:A:675:ILE:HA	1:A:678:PRO:HD2	2.02	0.42
1:C:497:LYS:C	1:C:498:VAL:CG2	2.84	0.42
1:D:158:TYR:O	1:D:166:PHE:HA	2.19	0.42
1:D:290:ILE:HB	1:D:298:MSE:HG3	2.02	0.42
1:D:468:ASP:HB3	1:D:485:HIS:HB3	2.01	0.42
1:D:516:SER:O	1:D:528:GLY:N	2.40	0.42
1:D:599:ASN:HD22	1:D:599:ASN:N	2.18	0.42
1:A:555:SER:HB3	1:A:573:THR:HB	2.02	0.42
1:A:646:ILE:HG23	1:A:649:CYS:HB3	2.02	0.42
1:A:677:SER:O	1:A:678:PRO:C	2.61	0.42
1:B:599:ASN:HD21	1:B:617:THR:HB	1.84	0.42
1:A:208:ASN:HD22	1:A:208:ASN:H	1.68	0.42
1:A:283:LEU:CD2	1:A:343:ILE:HD13	2.50	0.42
1:B:35:ASN:ND2	1:B:37:TYR:H	2.17	0.42
1:B:544:VAL:HA	1:C:371:GLN:HB2	2.01	0.42
1:C:381:VAL:CG2	1:C:398:ASP:CB	2.98	0.42
1:D:34:SER:H	1:D:58:ASN:HD21	1.68	0.42
1:D:674:ALA:C	1:D:676:ASN:H	2.27	0.42
1:A:383:SER:HB2	1:A:426:VAL:O	2.20	0.41
1:A:462:GLU:C	1:A:464:ASN:N	2.75	0.41
1:B:87:GLU:OE2	1:B:136:HIS:ND1	2.52	0.41
1:B:121:TYR:HA	1:B:129:LEU:O	2.20	0.41
1:B:473:TYR:CZ	1:B:519:GLN:HB2	2.54	0.41
1:C:40:SER:CB	1:C:87:GLU:HA	2.50	0.41
1:C:278:PHE:HE2	1:C:293:GLU:HB2	1.85	0.41
1:C:338:ASP:C	1:C:340:PHE:N	2.76	0.41
1:A:63:THR:HG21	1:A:755:ASN:HD21	1.84	0.41
1:A:253:ASN:C	1:A:255:ASN:H	2.27	0.41
1:A:761:ASN:HB2	1:C:744:LEU:HD11	2.02	0.41
1:C:131:THR:CG2	1:C:154:ARG:HB2	2.50	0.41
1:D:531:GLY:H	1:D:557:THR:HG22	1.85	0.41
1:A:136:HIS:HB2	1:A:183:TRP:O	2.19	0.41
1:A:194:TYR:HB3	1:A:233:ILE:HD13	2.01	0.41
1:A:704:ILE:HG22	1:A:711:ILE:CD1	2.41	0.41
1:C:283:LEU:HB3	1:C:285:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ILE:HD12	1:C:497:LYS:CB	2.23	0.41
1:A:720:PHE:HE2	1:A:722:LEU:HD11	1.84	0.41
1:C:157:GLU:CD	1:C:168:HIS:HD1	2.27	0.41
1:C:284:LYS:C	1:C:286:ASN:N	2.78	0.41
1:C:320:GLU:HB2	1:C:330:ALA:HA	2.02	0.41
1:C:762:ILE:HA	1:C:763:PRO:HD3	1.87	0.41
1:D:202:LEU:HD12	1:D:202:LEU:C	2.45	0.41
1:D:739:TYR:CD2	1:D:739:TYR:C	2.98	0.41
1:A:372:MSE:CE	1:A:410:ARG:HD3	2.51	0.41
1:B:197:HIS:CE1	1:B:203:SER:OG	2.74	0.41
1:B:458:ILE:HG13	1:B:497:LYS:HD2	2.02	0.41
1:B:677:SER:O	1:B:678:PRO:C	2.62	0.41
1:C:575:GLU:HA	1:C:600:THR:HG23	2.01	0.41
1:D:748:TRP:HH2	1:D:784:THR:HG21	1.86	0.41
1:A:150:CYS:HB3	1:A:182:THR:OG1	2.20	0.41
1:A:462:GLU:CG	1:A:463:LYS:H	2.17	0.41
1:C:185:ALA:HA	1:C:194:TYR:O	2.21	0.41
1:D:40:SER:HB3	1:D:52:ALA:HB3	2.03	0.41
1:D:216:VAL:CG1	1:D:217:HIS:N	2.74	0.41
1:D:290:ILE:HD12	1:D:298:MSE:HG3	2.02	0.41
1:D:597:LEU:HD13	1:D:631:PHE:CD2	2.55	0.41
1:A:568:GLN:H	1:A:568:GLN:HG2	1.74	0.41
1:C:559:ASN:HD21	1:C:601:HIS:CE1	2.38	0.41
1:D:383:SER:CB	1:D:426:VAL:O	2.69	0.41
1:D:388:ASP:OD2	1:D:394:TRP:NE1	2.49	0.41
1:D:653:ASP:HB3	1:D:656:GLY:H	1.85	0.41
1:A:58:ASN:HD22	1:A:67:THR:HG22	1.85	0.41
1:A:364:THR:OG1	1:A:641:PRO:HD3	2.21	0.41
1:A:364:THR:HG21	1:A:641:PRO:HG3	2.02	0.41
1:A:383:SER:HA	1:A:646:ILE:HG21	2.03	0.41
1:A:646:ILE:CG2	1:A:649:CYS:HB3	2.51	0.41
1:C:283:LEU:HD22	1:C:289:TRP:CG	2.56	0.41
1:C:470:ARG:CZ	1:C:470:ARG:HB3	2.50	0.41
1:D:287:LYS:HE2	1:D:301:ASP:OD2	2.21	0.41
1:A:89:TYR:OH	1:A:139:SER:HB2	2.21	0.41
1:A:338:ASP:HB2	1:A:342:ASN:N	2.36	0.41
1:A:482:ILE:HD12	1:A:491:ILE:HG23	2.02	0.41
1:A:582:SER:C	1:A:584:ARG:H	2.29	0.41
1:B:50:TRP:CE3	1:B:59:LYS:HB2	2.55	0.41
1:B:724:PHE:CE2	1:B:751:ILE:HD11	2.56	0.41
1:C:125:ASP:HB3	1:C:126:PRO:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:ILE:O	1:C:680:ILE:HD12	2.21	0.41
1:D:457:GLN:HE21	1:D:457:GLN:HB3	1.72	0.41
1:A:130:ILE:HG13	1:A:131:THR:HG22	2.02	0.41
1:A:677:SER:O	1:A:679:GLN:N	2.54	0.41
1:A:723:THR:HA	1:A:756:SER:HA	2.02	0.41
1:D:79:SER:OG	1:D:80:ILE:N	2.54	0.41
1:A:575:GLU:HA	1:A:600:THR:HG23	2.02	0.40
1:B:95:PRO:CG	1:B:112:GLU:HG3	2.50	0.40
1:B:179:SER:HB3	1:B:197:HIS:CD2	2.56	0.40
1:B:236:ASP:CB	1:B:240:ASN:HB2	2.51	0.40
1:B:556:ASN:HD22	1:B:556:ASN:HA	1.57	0.40
1:C:229:ASP:O	1:C:245:THR:HA	2.21	0.40
1:C:285:ASP:OD1	1:C:285:ASP:N	2.51	0.40
1:C:635:ASP:O	1:C:636:HIS:C	2.63	0.40
1:D:515:ARG:HH11	1:D:515:ARG:HG2	1.86	0.40
1:A:558:ILE:HD13	1:A:558:ILE:O	2.21	0.40
1:B:207:LEU:C	1:B:209:ASP:H	2.30	0.40
1:B:377:LEU:HA	1:B:403:ASN:ND2	2.36	0.40
1:D:43:GLN:HB2	1:D:49:LEU:HD22	2.03	0.40
1:D:338:ASP:OD2	1:D:342:ASN:HB2	2.21	0.40
1:A:192:LYS:HZ2	1:A:206:SER:HB3	1.84	0.40
1:B:510:LEU:HD11	1:B:546:LYS:HD2	2.03	0.40
1:C:297:ILE:HG12	1:C:335:ILE:HD11	2.02	0.40
1:C:380:LYS:HE3	1:C:663:ILE:O	2.21	0.40
1:C:488:VAL:HG22	1:C:514:VAL:HG21	2.03	0.40
1:C:706:ILE:HG13	1:C:711:ILE:HD13	2.03	0.40
1:D:138:THR:HG22	1:D:139:SER:N	2.36	0.40
1:A:202:LEU:HD12	1:A:202:LEU:C	2.47	0.40
1:A:277:ILE:HG23	1:A:290:ILE:HG22	2.03	0.40
1:B:208:ASN:H	1:B:208:ASN:HD22	1.69	0.40
1:C:237:THR:H	1:C:282:GLN:NE2	2.19	0.40
1:C:290:ILE:N	1:C:298:MSE:O	2.49	0.40
1:C:322:ASP:OD1	1:C:322:ASP:N	2.53	0.40
1:C:427:LEU:HD13	1:C:470:ARG:NH2	2.37	0.40
1:D:378:SER:N	1:D:403:ASN:HD21	2.02	0.40
1:A:243:ILE:HD12	1:A:252:PHE:HB2	2.02	0.40
1:A:253:ASN:C	1:A:255:ASN:N	2.79	0.40
1:B:446:ILE:HD13	1:B:469:VAL:HG21	2.03	0.40
1:B:678:PRO:HB2	1:B:775:LEU:HD12	2.03	0.40
1:C:449:TYR:CD1	1:C:455:LYS:HB2	2.37	0.40
1:C:462:GLU:O	1:C:464:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:LEU:HB2	1:C:578:VAL:HB	2.03	0.40
1:D:95:PRO:HG3	1:D:112:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/781 (93%)	632 (87%)	76 (10%)	16 (2%)	5	26
1	B	724/781 (93%)	634 (88%)	71 (10%)	19 (3%)	4	23
1	C	724/781 (93%)	638 (88%)	69 (10%)	17 (2%)	5	25
1	D	724/781 (93%)	637 (88%)	69 (10%)	18 (2%)	4	23
All	All	2896/3124 (93%)	2541 (88%)	285 (10%)	70 (2%)	4	24

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	670	ASN
1	A	671	PRO
1	B	637	SER
1	B	670	ASN
1	C	125	ASP
1	C	445	ASN
1	C	464	ASN
1	C	498	VAL
1	C	670	ASN
1	D	464	ASN
1	D	493	LEU
1	D	498	VAL

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Mol	Chain	Res	Type
1	D	670	ASN
1	A	445	ASN
1	A	462	GLU
1	A	464	ASN
1	A	674	ALA
1	A	753	GLU
1	B	445	ASN
1	B	463	LYS
1	B	476	LYS
1	B	498	VAL
1	C	285	ASP
1	C	462	GLU
1	C	463	LYS
1	C	494	ALA
1	C	495	SER
1	C	671	PRO
1	C	753	GLU
1	D	445	ASN
1	D	671	PRO
1	A	190	ASP
1	A	695	THR
1	B	422	LEU
1	B	462	GLU
1	B	464	ASN
1	B	583	ALA
1	B	702	THR
1	C	493	LEU
1	C	583	ALA
1	C	585	ASN
1	D	125	ASP
1	D	199	GLU
1	D	462	GLU
1	D	583	ALA
1	A	463	LYS
1	A	637	SER
1	B	493	LEU
1	B	674	ALA
1	C	637	SER
1	D	162	ALA
1	D	495	SER
1	A	495	SER
1	B	494	ALA

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Mol	Chain	Res	Type
1	B	675	ILE
1	C	598	PRO
1	D	178	PRO
1	D	208	ASN
1	D	216	VAL
1	D	422	LEU
1	A	75	SER
1	A	494	ALA
1	B	678	PRO
1	B	700	ASN
1	B	216	VAL
1	D	675	ILE
1	D	678	PRO
1	B	671	PRO
1	A	663	ILE

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	649/685 (95%)	558 (86%)	91 (14%)	3	15
1	B	649/685 (95%)	573 (88%)	76 (12%)	5	20
1	C	649/685 (95%)	562 (87%)	87 (13%)	4	16
1	D	649/685 (95%)	571 (88%)	78 (12%)	5	20
All	All	2596/2740 (95%)	2264 (87%)	332 (13%)	4	18

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	ILE
1	A	49	LEU
1	A	72	GLU
1	A	73	GLN
1	A	117	SER

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Mol	Chain	Res	Type
1	A	124	GLU
1	A	130	ILE
1	A	133	ASP
1	A	138	THR
1	A	142	GLN
1	A	154	ARG
1	A	167	THR
1	A	171	LYS
1	A	174	VAL
1	A	199	GLU
1	A	202	LEU
1	A	216	VAL
1	A	217	HIS
1	A	249	LEU
1	A	273	LEU
1	A	274	SER
1	A	275	SER
1	A	282	GLN
1	A	284	LYS
1	A	290	ILE
1	A	294	LEU
1	A	322	ASP
1	A	323	ASN
1	A	345	ILE
1	A	371	GLN
1	A	375	SER
1	A	376	SER
1	A	377	LEU
1	A	380	LYS
1	A	381	VAL
1	A	383	SER
1	A	385	VAL
1	A	421	LEU
1	A	436	ASN
1	A	443	LEU
1	A	455	LYS
1	A	456	PHE
1	A	457	GLN
1	A	459	ILE
1	A	464	ASN
1	A	471	VAL
1	A	491	ILE

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Mol	Chain	Res	Type
1	A	493	LEU
1	A	497	LYS
1	A	498	VAL
1	A	507	SER
1	A	509	LEU
1	A	510	LEU
1	A	517	ILE
1	A	520	ASP
1	A	550	TYR
1	A	558	ILE
1	A	563	ARG
1	A	568	GLN
1	A	585	ASN
1	A	590	VAL
1	A	593	ARG
1	A	595	GLU
1	A	599	ASN
1	A	600	THR
1	A	627	SER
1	A	629	LYS
1	A	647	SER
1	A	673	ILE
1	A	675	ILE
1	A	688	VAL
1	A	696	SER
1	A	697	ARG
1	A	699	LYS
1	A	711	ILE
1	A	712	GLU
1	A	715	HIS
1	A	716	GLU
1	A	717	GLN
1	A	722	LEU
1	A	724	PHE
1	A	733	ASN
1	A	734	GLN
1	A	735	VAL
1	A	744	LEU
1	A	755	ASN
1	A	758	THR
1	A	760	ARG
1	A	776	HIS

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Mol	Chain	Res	Type
1	A	785	THR
1	B	29	ILE
1	B	30	GLU
1	B	46	GLN
1	B	49	LEU
1	B	72	GLU
1	B	93	VAL
1	B	130	ILE
1	B	133	ASP
1	B	141	VAL
1	B	142	GLN
1	B	167	THR
1	B	171	LYS
1	B	172	SER
1	B	199	GLU
1	B	202	LEU
1	B	249	LEU
1	B	273	LEU
1	B	274	SER
1	B	282	GLN
1	B	284	LYS
1	B	285	ASP
1	B	304	GLN
1	B	320	GLU
1	B	322	ASP
1	B	323	ASN
1	B	348	TRP
1	B	364	THR
1	B	380	LYS
1	B	385	VAL
1	B	390	GLN
1	B	392	LYS
1	B	427	LEU
1	B	455	LYS
1	B	460	GLU
1	B	461	LEU
1	B	464	ASN
1	B	470	ARG
1	B	471	VAL
1	B	476	LYS
1	B	480	ILE
1	B	484	THR

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Mol	Chain	Res	Type
1	B	492	ASP
1	B	493	LEU
1	B	495	SER
1	B	498	VAL
1	B	507	SER
1	B	509	LEU
1	B	511	GLU
1	B	536	ILE
1	B	543	LEU
1	B	556	ASN
1	B	558	ILE
1	B	563	ARG
1	B	566	LYS
1	B	585	ASN
1	B	595	GLU
1	B	599	ASN
1	B	613	ILE
1	B	625	ILE
1	B	627	SER
1	B	629	LYS
1	B	647	SER
1	B	678	PRO
1	B	680	ILE
1	B	696	SER
1	B	700	ASN
1	B	713	LEU
1	B	717	GLN
1	B	751	ILE
1	B	755	ASN
1	B	758	THR
1	B	760	ARG
1	B	762	ILE
1	B	775	LEU
1	B	776	HIS
1	B	785	THR
1	C	29	ILE
1	C	49	LEU
1	C	117	SER
1	C	127	GLN
1	C	133	ASP
1	C	137	ILE
1	C	141	VAL

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Mol	Chain	Res	Type
1	C	142	GLN
1	C	167	THR
1	C	169	TYR
1	C	171	LYS
1	C	186	THR
1	C	202	LEU
1	C	205	LEU
1	C	231	ARG
1	C	249	LEU
1	C	273	LEU
1	C	276	TYR
1	C	282	GLN
1	C	283	LEU
1	C	285	ASP
1	C	288	LEU
1	C	292	THR
1	C	299	ILE
1	C	305	ASN
1	C	324	ASN
1	C	326	SER
1	C	347	THR
1	C	372	MSE
1	C	376	SER
1	C	381	VAL
1	C	385	VAL
1	C	392	LYS
1	C	421	LEU
1	C	423	SER
1	C	427	LEU
1	C	451	THR
1	C	455	LYS
1	C	457	GLN
1	C	459	ILE
1	C	461	LEU
1	C	464	ASN
1	C	471	VAL
1	C	480	ILE
1	C	491	ILE
1	C	495	SER
1	C	496	LYS
1	C	497	LYS
1	C	498	VAL

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Mol	Chain	Res	Type
1	C	499	ILE
1	C	501	HIS
1	C	509	LEU
1	C	515	ARG
1	C	517	ILE
1	C	550	TYR
1	C	551	GLU
1	C	556	ASN
1	C	558	ILE
1	C	593	ARG
1	C	595	GLU
1	C	599	ASN
1	C	600	THR
1	C	613	ILE
1	C	627	SER
1	C	642	GLN
1	C	647	SER
1	C	652	LYS
1	C	673	ILE
1	C	675	ILE
1	C	680	ILE
1	C	687	LYS
1	C	696	SER
1	C	697	ARG
1	C	701	GLU
1	C	710	GLU
1	C	711	ILE
1	C	713	LEU
1	C	717	GLN
1	C	730	SER
1	C	746	ASN
1	C	751	ILE
1	C	755	ASN
1	C	758	THR
1	C	760	ARG
1	C	762	ILE
1	C	776	HIS
1	C	778	GLN
1	D	23	LEU
1	D	29	ILE
1	D	49	LEU
1	D	66	ILE

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Mol	Chain	Res	Type
1	D	130	ILE
1	D	133	ASP
1	D	141	VAL
1	D	142	GLN
1	D	167	THR
1	D	172	SER
1	D	202	LEU
1	D	205	LEU
1	D	249	LEU
1	D	273	LEU
1	D	274	SER
1	D	276	TYR
1	D	282	GLN
1	D	285	ASP
1	D	290	ILE
1	D	300	LEU
1	D	322	ASP
1	D	323	ASN
1	D	326	SER
1	D	385	VAL
1	D	410	ARG
1	D	411	VAL
1	D	430	LEU
1	D	446	ILE
1	D	453	LEU
1	D	455	LYS
1	D	456	PHE
1	D	457	GLN
1	D	458	ILE
1	D	465	GLU
1	D	471	VAL
1	D	476	LYS
1	D	480	ILE
1	D	495	SER
1	D	497	LYS
1	D	498	VAL
1	D	509	LEU
1	D	511	GLU
1	D	515	ARG
1	D	536	ILE
1	D	556	ASN
1	D	558	ILE

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Mol	Chain	Res	Type
1	D	563	ARG
1	D	568	GLN
1	D	582	SER
1	D	590	VAL
1	D	593	ARG
1	D	594	LYS
1	D	595	GLU
1	D	599	ASN
1	D	600	THR
1	D	613	ILE
1	D	627	SER
1	D	640	ILE
1	D	646	ILE
1	D	647	SER
1	D	657	LEU
1	D	678	PRO
1	D	680	ILE
1	D	688	VAL
1	D	690	ILE
1	D	696	SER
1	D	698	GLU
1	D	707	SER
1	D	713	LEU
1	D	716	GLU
1	D	717	GLN
1	D	722	LEU
1	D	733	ASN
1	D	755	ASN
1	D	758	THR
1	D	760	ARG
1	D	762	ILE
1	D	776	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	58	ASN
1	A	94	GLN
1	A	102	GLN
1	A	132	ASN
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	HIS
1	A	208	ASN
1	A	240	ASN
1	A	282	GLN
1	A	304	GLN
1	A	323	ASN
1	A	341	ASN
1	A	353	ASN
1	A	403	ASN
1	A	424	ASN
1	A	450	ASN
1	A	477	ASN
1	A	556	ASN
1	A	599	ASN
1	A	601	HIS
1	A	664	ASN
1	A	715	HIS
1	A	717	GLN
1	A	721	ASN
1	A	725	ASN
1	A	733	ASN
1	A	734	GLN
1	A	752	ASN
1	A	755	ASN
1	A	778	GLN
1	B	35	ASN
1	B	58	ASN
1	B	94	GLN
1	B	142	GLN
1	B	197	HIS
1	B	208	ASN
1	B	240	ASN
1	B	255	ASN
1	B	261	ASN
1	B	282	GLN
1	B	286	ASN
1	B	304	GLN
1	B	323	ASN
1	B	341	ASN
1	B	353	ASN
1	B	371	GLN

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Mol	Chain	Res	Type
1	B	379	ASN
1	B	390	GLN
1	B	403	ASN
1	B	556	ASN
1	B	585	ASN
1	B	589	GLN
1	B	599	ASN
1	B	601	HIS
1	B	638	ASN
1	B	639	ASN
1	B	676	ASN
1	B	717	GLN
1	B	721	ASN
1	B	725	ASN
1	B	734	GLN
1	B	746	ASN
1	B	752	ASN
1	B	754	GLN
1	B	778	GLN
1	B	792	ASN
1	C	25	GLN
1	C	35	ASN
1	C	58	ASN
1	C	94	GLN
1	C	102	GLN
1	C	132	ASN
1	C	142	GLN
1	C	170	ASN
1	C	240	ASN
1	C	253	ASN
1	C	282	GLN
1	C	323	ASN
1	C	324	ASN
1	C	341	ASN
1	C	353	ASN
1	C	373	ASN
1	C	379	ASN
1	C	403	ASN
1	C	436	ASN
1	C	445	ASN
1	C	464	ASN
1	C	500	HIS

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Mol	Chain	Res	Type
1	C	556	ASN
1	C	601	HIS
1	C	638	ASN
1	C	642	GLN
1	C	654	HIS
1	C	664	ASN
1	C	676	ASN
1	C	700	ASN
1	C	717	GLN
1	C	721	ASN
1	C	725	ASN
1	C	752	ASN
1	C	754	GLN
1	C	755	ASN
1	C	778	GLN
1	D	35	ASN
1	D	36	ASN
1	D	58	ASN
1	D	78	GLN
1	D	94	GLN
1	D	107	ASN
1	D	132	ASN
1	D	142	GLN
1	D	170	ASN
1	D	197	HIS
1	D	217	HIS
1	D	240	ASN
1	D	253	ASN
1	D	282	GLN
1	D	323	ASN
1	D	341	ASN
1	D	353	ASN
1	D	371	GLN
1	D	403	ASN
1	D	415	ASN
1	D	424	ASN
1	D	445	ASN
1	D	457	GLN
1	D	506	ASN
1	D	542	GLN
1	D	556	ASN
1	D	568	GLN

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Mol	Chain	Res	Type
1	D	585	ASN
1	D	599	ASN
1	D	601	HIS
1	D	639	ASN
1	D	642	GLN
1	D	679	GLN
1	D	721	ASN
1	D	733	ASN
1	D	746	ASN
1	D	752	ASN
1	D	755	ASN
1	D	778	GLN
1	D	792	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 [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	731/781 (93%)	-0.31	8 (1%) 78 60	39, 71, 121, 177	0
1	B	731/781 (93%)	-0.27	10 (1%) 73 55	44, 75, 135, 210	0
1	C	731/781 (93%)	-0.20	8 (1%) 78 60	38, 80, 147, 221	0
1	D	731/781 (93%)	-0.30	8 (1%) 78 60	43, 77, 149, 219	0
All	All	2924/3124 (93%)	-0.27	34 (1%) 76 58	38, 76, 139, 221	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	LYS	4.9
1	A	415	ASN	4.7
1	D	793	PRO	4.5
1	B	415	ASN	4.3
1	D	226	PRO	3.9
1	A	273	LEU	3.6
1	B	273	LEU	3.5
1	B	226	PRO	3.5
1	C	415	ASN	3.3
1	D	273	LEU	3.3
1	C	273	LEU	3.2
1	D	699	LYS	3.1
1	C	675	ILE	3.0
1	B	468	ASP	2.9
1	D	305	ASN	2.8
1	A	305	ASN	2.7
1	B	485	HIS	2.5
1	B	421	LEU	2.5
1	D	261	ASN	2.5
1	D	415	ASN	2.5
1	B	459	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	458	ILE	2.3
1	C	252	PHE	2.3
1	C	461	LEU	2.3
1	B	675	ILE	2.3
1	C	226	PRO	2.3
1	C	583	ALA	2.3
1	A	402	ILE	2.2
1	C	257	GLU	2.2
1	D	460	GLU	2.2
1	A	793	PRO	2.2
1	B	793	PRO	2.0
1	A	366	SER	2.0
1	A	456	PHE	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.