Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:53 PM GMT

PDB ID	:	3V9F
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

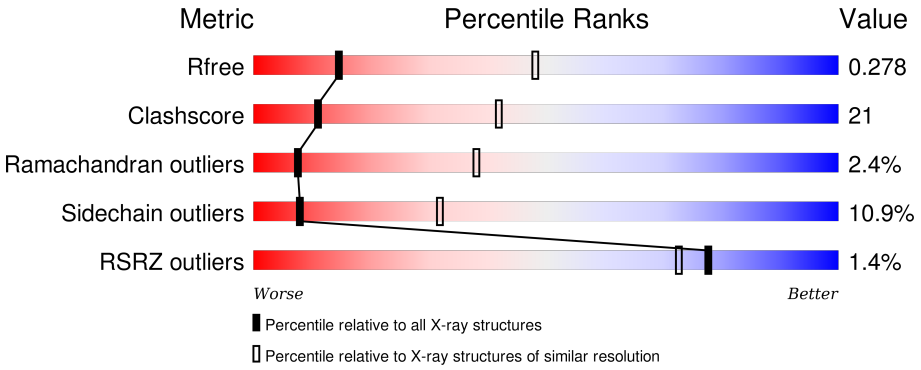
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	781	55% 33% 6% • 6%
1	B	781	% 54% 34% 6% • 6%
1	C	781	2% 54% 34% 6% • 6%
1	D	781	2% 54% 33% 7% • 6%

2 Entry composition (i)

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:

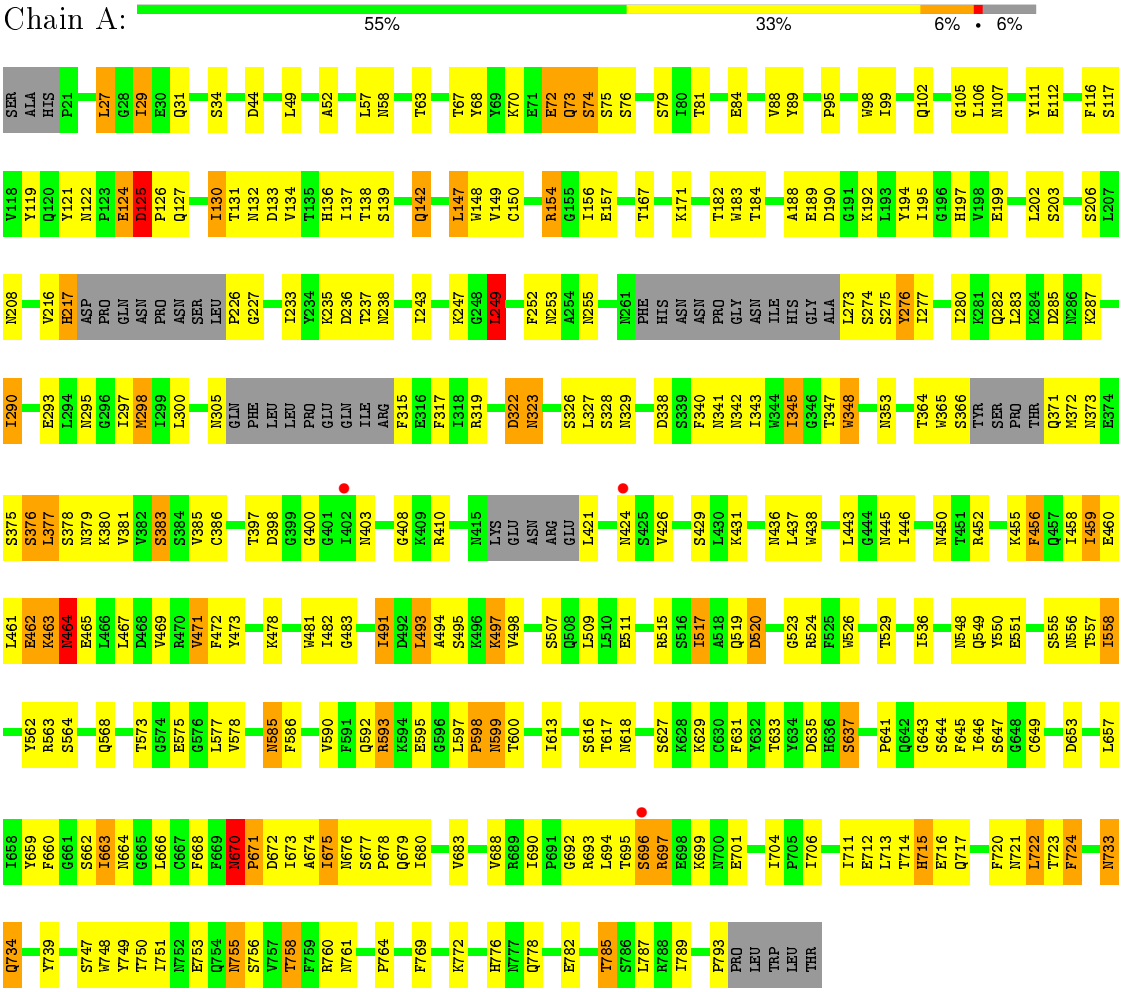
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	EXPRESSION TAG	UNP Q8A3A5
B	18	SER	-	EXPRESSION TAG	UNP Q8A3A5
C	18	SER	-	EXPRESSION TAG	UNP Q8A3A5
D	18	SER	-	EXPRESSION TAG	UNP Q8A3A5

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

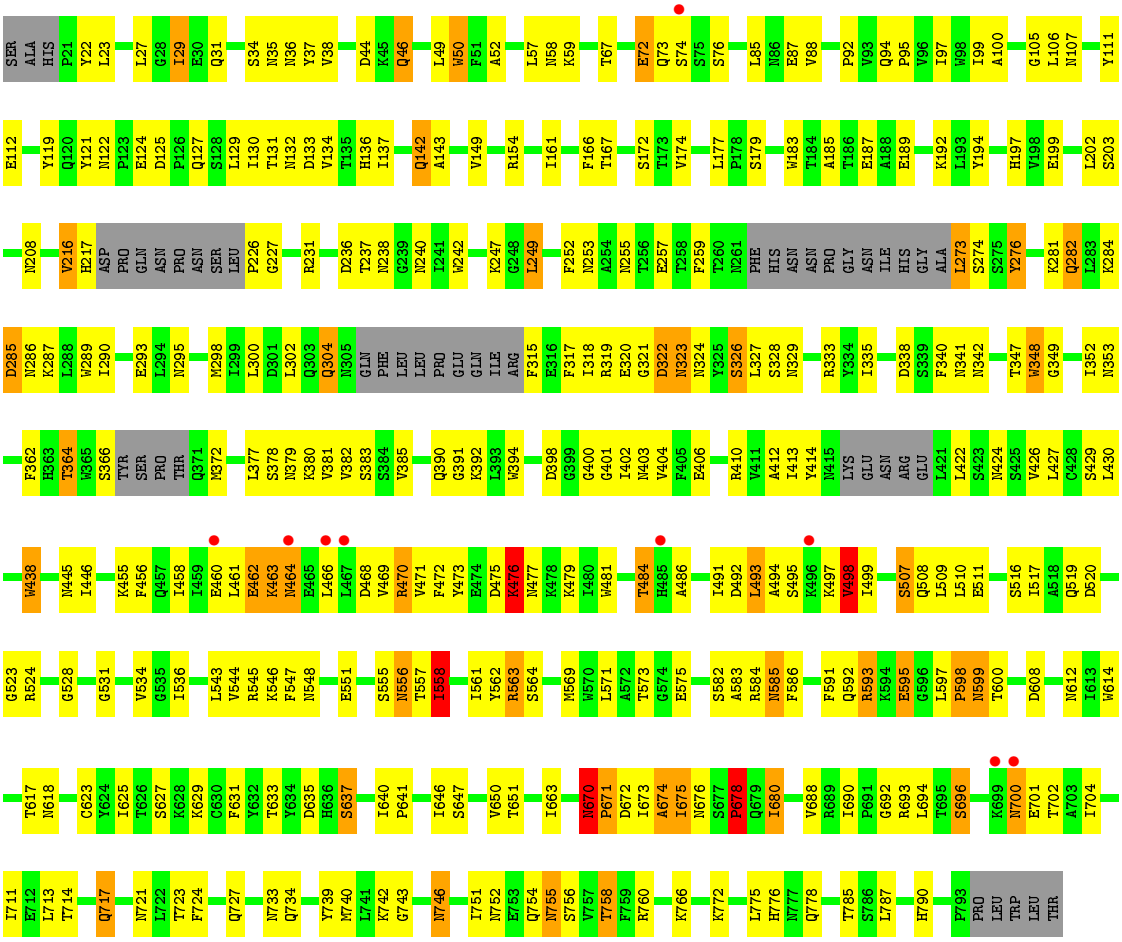
• Molecule 1: Two-component system sensor histidine kinase/response regulator, hybrid (One-component system)

Chain A:



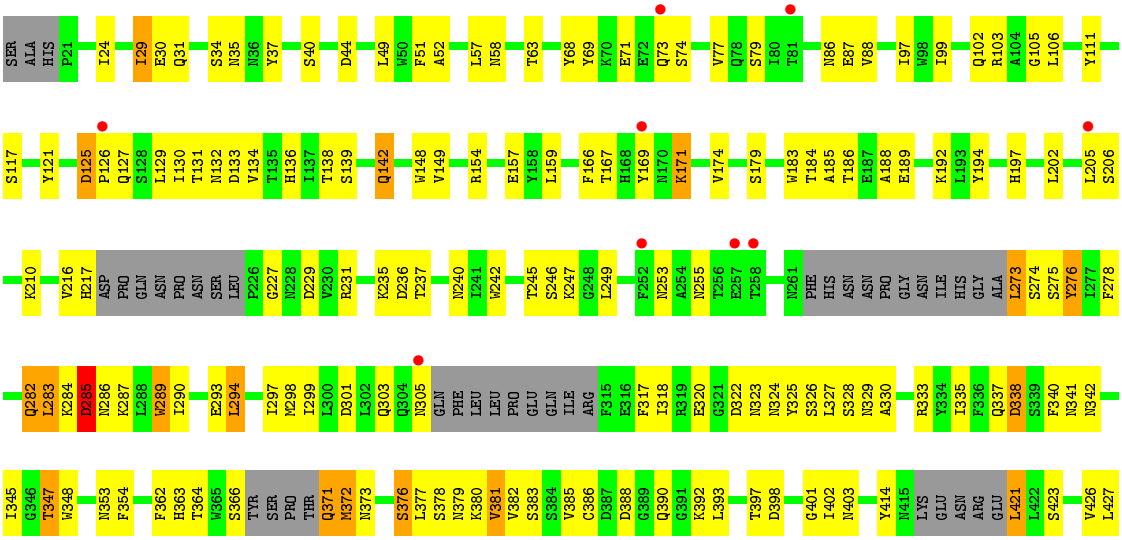
• Molecule 1: Two-component system sensor histidine kinase/response regulator, hybrid (One-component system)

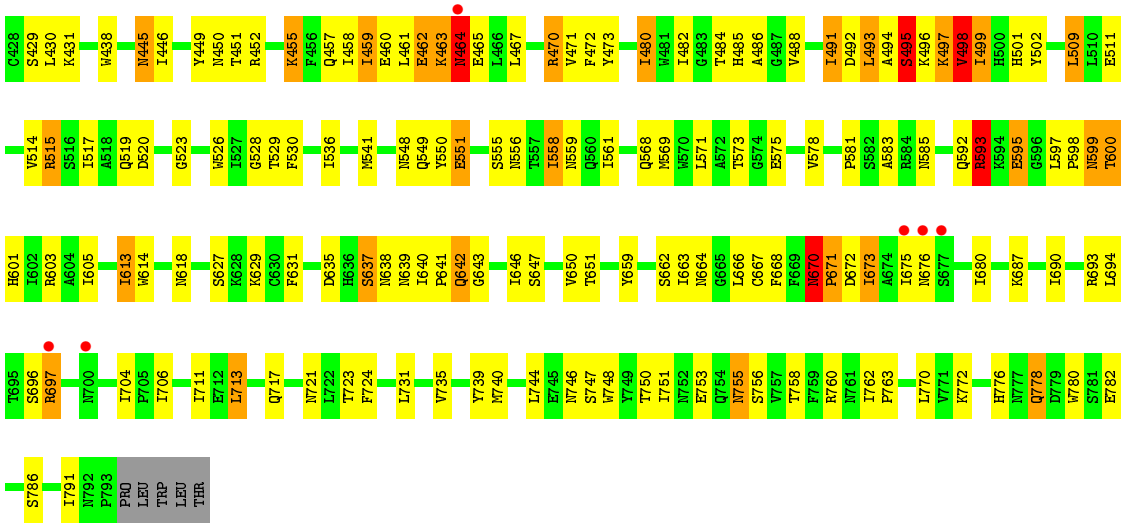
Chain B:



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

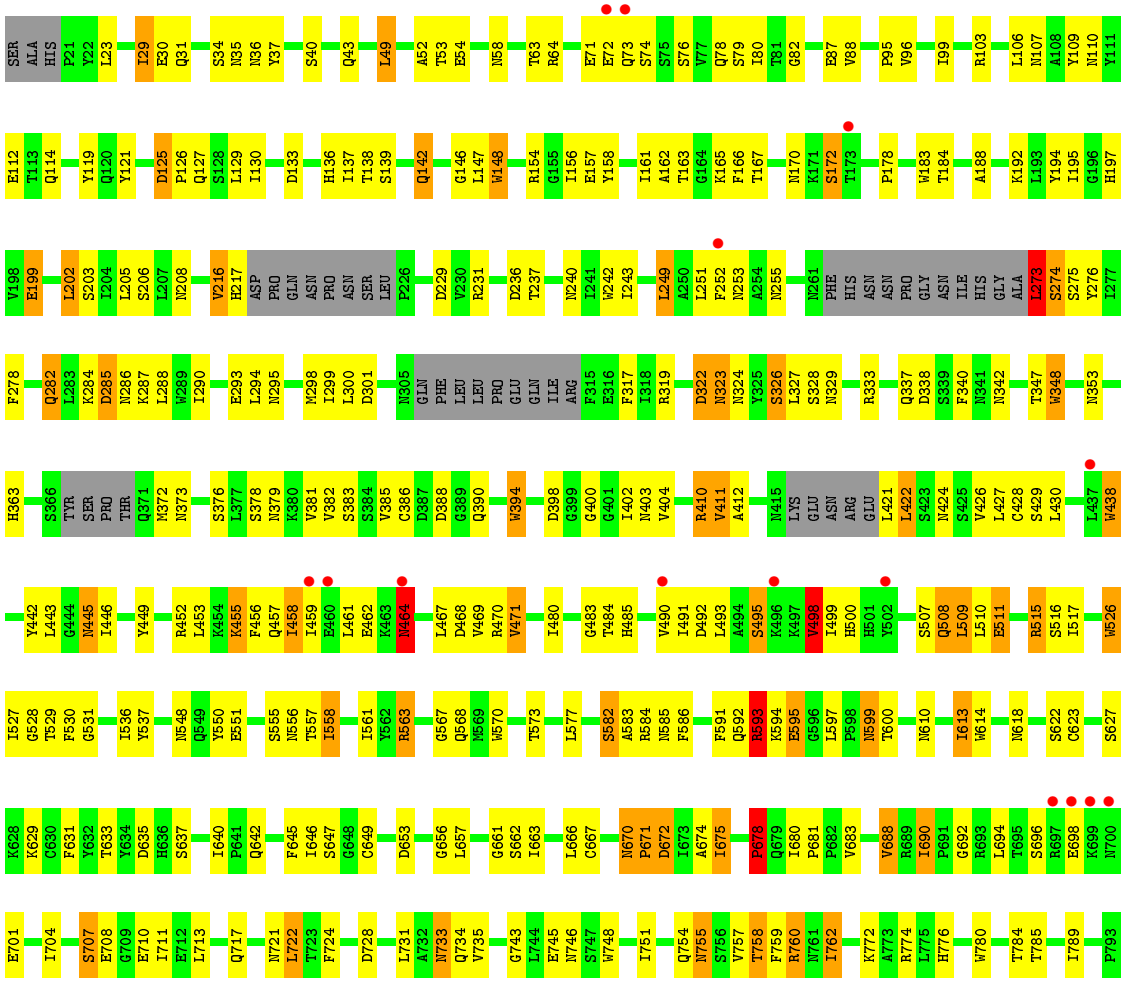
Chain C:





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

Chain D:




PRO
LEU
TRP
LEU
THR

4 Data and refinement statistics (i)

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) 99.7 (39.83-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.277 0.228 , 0.278	Depositor DCC
R_{free} test set	3459 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 68230 reflections	Xtriage
F_o,F_c correlation	0.90	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.72	6/6026 (0.1%)	0.80	4/8167 (0.0%)
1	B	0.69	6/6026 (0.1%)	0.80	7/8167 (0.1%)
1	C	0.75	10/6026 (0.2%)	0.84	12/8167 (0.1%)
1	D	0.65	7/6026 (0.1%)	0.77	5/8167 (0.1%)
All	All	0.70	29/24104 (0.1%)	0.80	28/32668 (0.1%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	ARG	CZ-NH1	20.40	1.59	1.33
1	A	456	PHE	CG-CD2	16.02	1.62	1.38
1	C	169	TYR	CD1-CE1	7.43	1.50	1.39
1	A	456	PHE	CE2-CZ	7.00	1.50	1.37
1	A	348	TRP	CD2-CE2	6.55	1.49	1.41
1	C	169	TYR	CD2-CE2	6.53	1.49	1.39
1	B	348	TRP	CD2-CE2	6.43	1.49	1.41
1	C	210	LYS	CD-CE	-6.20	1.35	1.51
1	D	348	TRP	CD2-CE2	5.81	1.48	1.41
1	C	148	TRP	CD2-CE2	5.63	1.48	1.41
1	B	394	TRP	CD2-CE2	5.58	1.48	1.41
1	C	183	TRP	CD2-CE2	5.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	ASN	CA-C	5.43	1.67	1.52
1	D	148	TRP	CD2-CE2	5.36	1.47	1.41
1	B	242	TRP	CD2-CE2	5.35	1.47	1.41
1	D	526	TRP	CD2-CE2	5.32	1.47	1.41
1	B	50	TRP	CD2-CE2	5.32	1.47	1.41
1	D	394	TRP	CD2-CE2	5.31	1.47	1.41
1	C	169	TYR	CZ-OH	5.29	1.46	1.37
1	B	438	TRP	CD2-CE2	5.28	1.47	1.41
1	A	456	PHE	CB-CG	5.27	1.60	1.51
1	C	242	TRP	CD2-CE2	5.17	1.47	1.41
1	D	438	TRP	CD2-CE2	5.15	1.47	1.41
1	B	289	TRP	CD2-CE2	5.11	1.47	1.41
1	D	570	TRP	CD2-CE2	5.11	1.47	1.41
1	C	169	TYR	CE1-CZ	-5.08	1.31	1.38
1	C	289	TRP	CD2-CE2	5.06	1.47	1.41
1	A	148	TRP	CD2-CE2	5.04	1.47	1.41
1	D	183	TRP	CD2-CE2	5.03	1.47	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	TYR	CB-CG-CD2	12.17	128.30	121.00
1	B	249	LEU	CA-CB-CG	7.99	133.69	115.30
1	C	169	TYR	CG-CD1-CE1	7.71	127.47	121.30
1	B	456	PHE	CB-CG-CD1	-7.51	115.54	120.80
1	C	169	TYR	CD1-CG-CD2	-7.51	109.64	117.90
1	A	249	LEU	CA-CB-CG	7.06	131.54	115.30
1	C	593	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	470	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	202	LEU	CA-CB-CG	6.64	130.58	115.30
1	D	249	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	456	PHE	CB-CG-CD2	-6.55	116.22	120.80
1	C	169	TYR	CZ-CE2-CD2	6.16	125.35	119.80
1	D	593	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	273	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	456	PHE	CZ-CE2-CD2	-5.83	113.10	120.10
1	C	697	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	B	466	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	147	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	697	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	558	ILE	CB-CA-C	5.32	122.24	111.60
1	B	593	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	273	LEU	CA-CB-CG	5.28	127.43	115.30
1	C	670	ASN	N-CA-C	5.27	125.23	111.00
1	B	670	ASN	N-CA-C	5.21	125.08	111.00
1	C	470	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	273	LEU	CA-CB-CG	5.10	127.04	115.30
1	C	461	LEU	CA-CB-CG	5.03	126.86	115.30
1	D	728	ASP	CB-CG-OD1	5.02	122.81	118.30

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	267	0
1	B	5890	0	5669	242	0
1	C	5890	0	5669	246	0
1	D	5890	0	5669	236	0
All	All	23560	0	22676	964	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (964) 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:HD12	1:C:29:ILE:H	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
1:C:29:ILE:N	1:C:29:ILE:HD12	1.72	1.00
1:B:285:ASP:HB2	1:B:287:LYS:HG3	1.44	1.00
1:C:29:ILE:CD1	1:C:29:ILE:H	1.65	0.99
1:B:29:ILE:CD1	1:B:29:ILE:H	1.76	0.97
1:A:446:ILE:HB	1:A:458:ILE:HG23	1.44	0.97
1:C:497:LYS:O	1:C:498:VAL:CG2	2.11	0.97
1:D:29:ILE:H	1:D:29:ILE:HD12	1.26	0.97
1:C:328:SER:H	1:C:353:ASN:HD21	1.06	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:HE21	1:A:142:GLN:H	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:B:29:ILE:HG12	1:D:642:GLN:HE21	1.32	0.93
1:A:280:ILE:HG12	1:A:290:ILE:HG23	1.48	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:N	1:B:29:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:295:ASN:HB3	1:D:319:ARG:NH1	1.91	0.85
1:C:470:ARG:HD3	1:C:515:ARG:CZ	2.05	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: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:C:283:LEU:HD22	1:C:289:TRP:CD1	2.18	0.79
1:A:659:TYR:HB3	1:A:666:LEU:HD11	1.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:CYS:HB2	1:D:429:SER:OG	1.85	0.77
1:A:450:ASN:HD21	1:A:452:ARG:CB	1.88	0.77
1:A:125:ASP:HB3	1:A:126:PRO:CA	2.14	0.77
1:B:134:VAL:HG13	1:B:149:VAL:HG13	1.65	0.77
1:C:188:ALA:O	1:C:235:LYS:HE3	1.83	0.77
1:C:30:GLU:HB2	1:C:31:GLN:NE2	2.00	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
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:A:673:ILE:C	1:A:675:ILE:H	1.88	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:D:282:GLN:HG3	1:D:282:GLN:O	1.84	0.75
1:A:491:ILE:HB	1:A:497:LYS:O	1.86	0.75
1:C:511:GLU:HB2	1:C:529:THR:HG21	1.67	0.75
1:A:52:ALA:HB2	1:A:88:VAL:HG13	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:A:74:SER:C	1:A:76:SER:H	1.91	0.74
1:D:582:SER:OG	1:D:584:ARG:HG2	1.87	0.73
1:B:429:SER:HA	1:B:438:TRP:O	1.88	0.73
1:B:557:THR:HG23	1:D:103:ARG:HH12	1.53	0.73
1:D:381:VAL:HG23	1:D:398:ASP:HB3	1.71	0.73
1:D:216:VAL:HG12	1:D:217:HIS:N	2.03	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:C:327:LEU:HD22	1:C:353:ASN:HD22	1.53	0.72
1:B:189:GLU:HB2	1:B:192:LYS:HB2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:PHE:CD1	1:A:662:SER:HB3	2.25	0.72
1:A:548:ASN:HB2	1:A:551:GLU:HB2	1.69	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:O	1:D:694:LEU:HG	1.91	0.71
1:A:478:LYS:O	1:A:493:LEU:HB2	1.90	0.71
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: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:715:HIS:CE1	1:A:764:PRO:HG3	2.28	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:D:29:ILE:N	1:D:29:ILE:HD12	2.05	0.68
1:B:561:ILE:HG22	1:B:569:MSE:HE2	1.75	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:D:427:LEU:HD11	1:D:442:TYR:HB2	1.75	0.68
1:C:402:ILE:HG13	1:C:426:VAL:HG21	1.74	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:676:ASN:HA	1:C:778:GLN:HE21	1.58	0.68
1:C:492:ASP:HB3	1:C:496:LYS:O	1.94	0.68
1:D:459:ILE:HB	1:D:464:ASN:HB3	1.76	0.68
1:B:378:SER:H	1:B:403:ASN:HD21	1.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:SER:HB2	1:D:294:LEU:HD12	1.78	0.66
1:D:192:LYS:HD3	1:D:206:SER:HB3	1.78	0.66
1:C:142:GLN:HE21	1:C:142:GLN:H	1.41	0.66
1:D:29:ILE:H	1:D:29:ILE:CD1	2.01	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:528:GLY:HA3	1:D:558:ILE:HD12	1.78	0.66
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:C:227:GLY:CA	1:C:247:LYS:HB2	2.24	0.65
1:B:125:ASP:HB3	1:B:127:GLN:H	1.61	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: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: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: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:555:SER:HB3	1:B:573:THR:HB	1.79	0.64
1:B:460:GLU:HA	1:B:460:GLU:OE2	1.97	0.64
1:A:253:ASN:ND2	1:A:255:ASN:HB3	2.13	0.63
1:C:329:ASN:HB3	1:C:347:THR:HG21	1.78	0.63
1:B:635:ASP:OD1	1:B:637:SER:HB3	1.98	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:711:ILE:HB	1:B:787:LEU:HD11	1.79	0.63
1:C:134:VAL:HG13	1:C:149:VAL:HG13	1.81	0.63
1:B:462:GLU:HG3	1:B:463:LYS:HG2	1.80	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:A:276:TYR:HB3	1:A:293:GLU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:130:ILE:HG12	1:C:157:GLU:OE1	1.99	0.62
1:A:481:TRP:HB3	1:A:517:ILE:HD11	1.81	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:673:ILE:C	1:A:675:ILE:N	2.52	0.62
1:A:386:CYS:HB2	1:A:429:SER:OG	2.00	0.62
1:D:526:TRP:CD2	1:D:536:ILE:HD12	2.35	0.62
1:B:534:VAL:HG12	1:B:547:PHE:HB2	1.81	0.62
1:A:724:PHE:O	1:A:755:ASN:HB2	1.99	0.62
1:B:733:ASN:HD22	1:B:734:GLN:HE21	1.47	0.62
1:D:378:SER:H	1:D:403:ASN:ND2	1.96	0.62
1:A:373:ASN:N	1:A:376:SER:HB2	2.15	0.62
1:B:599:ASN:HD21	1:B:618:ASN:H	1.47	0.62
1:B:174:VAL:HB	1:B:177:LEU:HD12	1.80	0.62
1:D:295:ASN:HB3	1:D:319:ARG:HH11	1.63	0.61
1:B:322:ASP:OD1	1:B:322:ASP:N	2.33	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:A:462:GLU:O	1:A:463:LYS:C	2.38	0.61
1:C:421:LEU:HD12	1:C:455:LYS:HD3	1.82	0.61
1:D:642:GLN:O	1:D:642:GLN:HG2	2.01	0.61
1:C:462:GLU:O	1:C:463:LYS:C	2.38	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: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:C:491:ILE:CD1	1:C:497:LYS:HB2	2.20	0.61
1:A:98:TRP:CE2	1:A:147:LEU:HD21	2.36	0.61
1:B:366:SER:HA	1:B:377:LEU:HB2	1.83	0.60
1:A:400:GLY:O	1:A:424:ASN:HB2	2.01	0.60
1:B:670:ASN:CG	1:B:671:PRO:HD2	2.22	0.60
1:A:29:ILE:CD1	1:C:642:GLN:HE21	2.14	0.60
1:D:452:ARG:CG	1:D:452:ARG:O	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:373:ASN:CB	1:A:376:SER:HB2	2.31	0.60
1:A:130:ILE:HG12	1:A:157:GLU:CD	2.22	0.60
1:A:58:ASN:ND2	1:A:67:THR:HG22	2.16	0.60
1:B:99:ILE:HB	1:B:107:ASN:HB2	1.83	0.60
1:A:683:VAL:O	1:A:785:THR:HG21	2.02	0.60
1:A:722:LEU:CD2	1:A:787:LEU:HD23	2.32	0.59
1:C:662:SER:C	1:C:664:ASN:H	2.05	0.59
1:C:438:TRP:HH2	1:C:491:ILE:HD11	1.67	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:A:782:GLU:HA	1:A:782:GLU:OE1	2.02	0.59
1:B:285:ASP:O	1:B:286:ASN:HB2	2.02	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:C:366:SER:HA	1:C:377:LEU:HB2	1.84	0.59
1:B:557:THR:HG23	1:D:103:ARG:NH1	2.16	0.59
1:B:458:ILE:HD11	1:B:497:LYS:CB	2.32	0.59
1:A:711:ILE:HG23	1:A:713:LEU:HD23	1.83	0.59
1:C:484:THR:HG22	1:C:486:ALA:H	1.67	0.59
1:A:557:THR:HG23	1:C:103:ARG:HH12	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:C:429:SER:HA	1:C:438:TRP:O	2.03	0.58
1:B:29:ILE:CG1	1:D:642:GLN:HE21	2.12	0.58
1:A:491:ILE:HG13	1:A:491:ILE:O	2.02	0.58
1:A:526:TRP:CE2	1:A:536:ILE:HD12	2.38	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:C:446:ILE:HB	1:C:458:ILE:CG2	2.24	0.58
1:C:298:MSE:HE2	1:C:317:PHE:CE1	2.37	0.58
1:B:185:ALA:HA	1:B:194:TYR:O	2.03	0.58
1:B:236:ASP:HB3	1:B:240:ASN:H	1.68	0.58
1:C:73:GLN:HA	1:C:73:GLN:OE1	2.03	0.58
1:B:582:SER:C	1:B:584:ARG:H	2.06	0.58
1:A:142:GLN:NE2	1:A:142:GLN:H	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:HB2	1:C:31:GLN:HE22	1.68	0.57
1:A:298:MSE:HE2	1:A:317:PHE:CZ	2.38	0.57
1:D:653:ASP:HB2	1:D:657:LEU:HB2	1.85	0.57
1:A:365:TRP:CZ2	1:A:408:GLY:HA2	2.39	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
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:278:PHE:HE2	1:D:293:GLU:HB2	1.69	0.57
1:D:142:GLN:HE21	1:D:142:GLN:H	1.53	0.57
1:C:511:GLU:HB2	1:C:529:THR:CG2	2.33	0.57
1:A:643:GLY:HA3	1:A:664:ASN:HD22	1.69	0.57
1:A:130:ILE:HD12	1:A:154:ARG:O	2.04	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:B:462:GLU:O	1:B:463:LYS:C	2.43	0.57
1:C:782:GLU:HA	1:C:782:GLU:OE1	2.05	0.57
1:C:324:ASN:ND2	1:C:324:ASN:H	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:D:237:THR:OG1	1:D:282:GLN:NE2	2.37	0.57
1:B:733:ASN:ND2	1:B:734:GLN:HE21	2.02	0.57
1:B:599:ASN:ND2	1:B:617:THR:HB	2.20	0.57
1:C:526:TRP:CD2	1:C:536:ILE:HD12	2.40	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:B:714:THR:H	1:B:717:GLN:HG3	1.70	0.57
1:D:402:ILE:HG12	1:D:426:VAL:HG21	1.86	0.56
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: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:B:593:ARG:HB2	1:D:72:GLU:OE2	2.05	0.56
1:A:526:TRP:CD2	1:A:536:ILE:HD12	2.41	0.56
1:B:295:ASN:HB3	1:B:319:ARG:NH1	2.20	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:B:329:ASN:CB	1:B:347:THR:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:HB2	1:A:126:PRO:HA	1.85	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:D:35:ASN:HD21	1:D:54:GLU:HB2	1.69	0.56
1:C:328:SER:H	1:C:353:ASN:ND2	1.88	0.56
1:D:722:LEU:H	1:D:722:LEU:HD12	1.71	0.56
1:A:156:ILE:CD1	1:A:195:ILE:HG12	2.36	0.56
1:C:473:TYR:OH	1:C:519:GLN:HB2	2.06	0.56
1:B:468:ASP:OD2	1:B:470:ARG:NH2	2.39	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: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:C:502:TYR:CD2	1:C:541:MSE:HG3	2.41	0.56
1:C:642:GLN:O	1:C:642:GLN:HG2	2.06	0.55
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:673:ILE:C	1:C:675:ILE:H	2.08	0.55
1:B:226:PRO:HD3	1:B:259:PHE:CD2	2.41	0.55
1:B:94:GLN:HE22	1:B:161:ILE:HG21	1.72	0.55
1:B:216:VAL:CG1	1:B:217:HIS:N	2.68	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:A:105:GLY:HA2	1:A:132:ASN:HB2	1.87	0.55
1:D:333:ARG:HG2	1:D:348:TRP:HB2	1.88	0.55
1:B:551:GLU:OE1	1:B:551:GLU:HA	2.07	0.55
1:C:740:MSE:HE3	1:C:770:LEU:HD12	1.89	0.55
1:B:402:ILE:O	1:B:413:ILE:HA	2.06	0.55
1:D:675:ILE:CG1	1:D:678:PRO:HG2	2.36	0.55
1:D:675:ILE:C	1:D:678:PRO:HD2	2.27	0.55
1:A:599:ASN:HD21	1:A:618:ASN:H	1.55	0.55
1:B:131:THR:HG22	1:B:154:ARG:HB2	1.87	0.55
1:B:92:PRO:HG2	1:B:143:ALA:HB1	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:A:95:PRO:CB	1:A:112:GLU:CG	2.85	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
1:C:333:ARG:HG2	1:C:348:TRP:HB2	1.88	0.55
1:A:598:PRO:HD2	1:A:633:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:OD1	1:A:322:ASP:N	2.39	0.55
1:A:471:VAL:HG23	1:A:483:GLY:HA3	1.89	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:B:304:GLN:OE1	1:B:315:PHE:N	2.39	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:70:LYS:HD2	1:A:81:THR:O	2.07	0.54
1:A:95:PRO:CG	1:A:112:GLU:HG3	2.37	0.54
1:B:614:TRP:CE3	1:B:623:CYS:HB2	2.43	0.54
1:A:555:SER:HB2	1:A:575:GLU:HG2	1.90	0.54
1:D:422:LEU:HG	1:D:457:GLN:NE2	2.18	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:C:342:ASN:HB3	1:C:354:PHE:CE1	2.42	0.54
1:A:692:GLY:HA3	1:A:701:GLU:HG3	1.90	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:644:SER:H	1:A:663:ILE:HD11	1.73	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:B:383:SER:HA	1:B:646:ILE:HD13	1.90	0.54
1:A:670:ASN:CB	1:A:671:PRO:CD	2.86	0.54
1:A:327:LEU:HD22	1:A:353:ASN:HD22	1.73	0.53
1:A:217:HIS:HB2	1:A:226:PRO:HD2	1.90	0.53
1:A:381:VAL:HG12	1:A:663:ILE:HA	1.89	0.53
1:C:484:THR:HG22	1:C:485:HIS:N	2.24	0.53
1:A:121:TYR:H	1:A:132:ASN:HD22	1.56	0.53
1:A:706:ILE:HA	1:A:711:ILE:HD13	1.90	0.53
1:D:278:PHE:CE2	1:D:293:GLU:HB2	2.43	0.53
1:C:614:TRP:HZ2	1:C:673:ILE:CG2	2.22	0.53
1:A:694:LEU:O	1:A:696:SER:N	2.41	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:D:722:LEU:N	1:D:722:LEU:HD12	2.24	0.53
1:D:743:GLY:H	1:D:746:ASN:HD21	1.56	0.53
1:C:131:THR:HG21	1:C:154:ARG:H	1.74	0.53
1:C:136:HIS:ND1	1:C:184:THR:HG22	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ALA:HB2	1:B:88:VAL:HG13	1.91	0.53
1:D:558:ILE:O	1:D:558:ILE:HD13	2.08	0.53
1:B:739:TYR:OH	1:D:760:ARG:HD2	2.09	0.53
1:B:650:VAL:HG22	1:B:651:THR:N	2.24	0.53
1:A:188:ALA:HB3	1:A:194:TYR:CD1	2.44	0.53
1:B:27:LEU:HD23	1:B:31:GLN:HG2	1.91	0.53
1:D:156:ILE:CD1	1:D:195:ILE:HG12	2.39	0.53
1:B:281:LYS:HD2	1:B:335:ILE:O	2.09	0.53
1:A:300:LEU:HD12	1:A:315:PHE:CE1	2.44	0.53
1:D:323:ASN:ND2	1:D:326:SER:CB	2.65	0.52
1:D:125:ASP:HB3	1:D:126:PRO:CA	2.38	0.52
1:A:283:LEU:HD23	1:A:343:ILE:CD1	2.39	0.52
1:D:422:LEU:CG	1:D:457:GLN:HE22	2.18	0.52
1:A:429:SER:HA	1:A:438:TRP:O	2.09	0.52
1:D:381:VAL:CG2	1:D:398:ASP:HB3	2.37	0.52
1:B:558:ILE:O	1:B:558:ILE:HD13	2.09	0.52
1:B:724:PHE:CZ	1:B:751:ILE:HD11	2.45	0.52
1:D:199:GLU:OE2	1:D:229:ASP:HB2	2.09	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:288:LEU:O	1:D:299:ILE:HA	2.10	0.52
1:A:323:ASN:HD21	1:A:326:SER:HB2	1.74	0.52
1:D:284:LYS:HB2	1:D:337:GLN:HE22	1.74	0.52
1:A:74:SER:C	1:A:76:SER:N	2.61	0.52
1:C:446:ILE:HD12	1:C:472:PHE:CE1	2.44	0.52
1:B:72:GLU:OE2	1:D:593:ARG:HD2	2.09	0.52
1:A:134:VAL:HG11	1:A:149:VAL:HG13	1.92	0.52
1:B:372:MSE:HE2	1:B:410:ARG:HH11	1.75	0.52
1:C:670:ASN:CB	1:C:671:PRO:CD	2.88	0.52
1:B:404:VAL:HB	1:B:412:ALA:HB3	1.92	0.52
1:B:44:ASP:HB3	1:B:97:ILE:HD11	1.92	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:B:74:SER:C	1:B:76:SER:H	2.11	0.52
1:C:383:SER:HB2	1:C:426:VAL:O	2.10	0.52
1:D:675:ILE:HG12	1:D:678:PRO:HG2	1.92	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:D:373:ASN:HB3	1:D:376:SER:HB2	1.92	0.52
1:A:690:ILE:HG21	1:A:717:GLN:HB2	1.92	0.52
1:B:401:GLY:HA3	1:B:414:TYR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:PRO:HD2	1:B:633:THR:HG21	1.92	0.52
1:B:379:ASN:HD21	1:B:381:VAL:HG22	1.74	0.52
1:A:680:ILE:O	1:A:680:ILE:HD12	2.10	0.52
1:C:445:ASN:ND2	1:C:467:LEU:H	2.08	0.51
1:C:379:ASN:ND2	1:C:381:VAL:H	2.07	0.51
1:D:379:ASN:HB2	1:D:400:GLY:H	1.75	0.51
1:D:558:ILE:HD11	1:D:561:ILE:HG13	1.91	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:C:388:ASP:C	1:C:390:GLN:H	2.14	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:C:364:THR:HA	1:C:666:LEU:O	2.11	0.51
1:D:511:GLU:HB3	1:D:529:THR:HG21	1.91	0.51
1:C:323:ASN:HD22	1:C:325:TYR:H	1.57	0.51
1:C:179:SER:HB3	1:C:197:HIS:CD2	2.45	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: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:C:670:ASN:HB3	1:C:671:PRO:CD	2.41	0.51
1:A:460:GLU:HB2	1:A:467:LEU:HD12	1.92	0.51
1:C:327:LEU:CD2	1:C:353:ASN:HD22	2.23	0.51
1:A:378:SER:H	1:A:403:ASN:ND2	2.00	0.51
1:B:479:LYS:HG2	1:B:492:ASP:HA	1.92	0.51
1:A:520:ASP:HB3	1:A:523:GLY:H	1.76	0.51
1:B:122:ASN:C	1:B:124:GLU:H	2.15	0.51
1:C:762:ILE:HG22	1:C:791:ILE:HD12	1.93	0.51
1:B:531:GLY:HA2	1:D:103:ARG:NH1	2.25	0.50
1:D:558:ILE:C	1:D:558:ILE:HD13	2.31	0.50
1:C:87:GLU:OE2	1:C:136:HIS:HA	2.11	0.50
1:A:653:ASP:HB2	1:A:657:LEU:HB2	1.93	0.50
1:B:475:ASP:C	1:B:477:ASN:H	2.14	0.50
1:D:724:PHE:O	1:D:755:ASN:HB2	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:428:CYS:SG	1:D:470:ARG:HA	2.51	0.50
1:D:242:TRP:CZ3	1:D:251:LEU:HB2	2.46	0.50
1:A:99:ILE:HB	1:A:107:ASN:HB2	1.93	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:C:670:ASN:CG	1:C:671:PRO:HD3	2.32	0.50
1:B:723:THR:HG22	1:B:756:SER:CB	2.37	0.50
1:B:673:ILE:C	1:B:675:ILE:N	2.64	0.50
1:A:670:ASN:HB3	1:A:671:PRO:CD	2.41	0.50
1:C:340:PHE:O	1:C:341:ASN:HB2	2.12	0.50
1:D:592:GLN:H	1:D:595:GLU:CG	2.20	0.50
1:D:80:ILE:HD12	1:D:82:GLY:O	2.11	0.50
1:A:197:HIS:HE1	1:A:203:SER:HB2	1.77	0.50
1:C:592:GLN:H	1:C:595:GLU:HG2	1.77	0.49
1:A:323:ASN:ND2	1:A:326:SER:HB2	2.27	0.49
1:C:670:ASN:HB3	1:C:671:PRO:HD2	1.94	0.49
1:B:44:ASP:HB2	1:B:111:TYR:CZ	2.47	0.49
1:B:237:THR:OG1	1:B:282:GLN:NE2	2.45	0.49
1:A:616:SER:HB3	1:A:660:PHE:CD1	2.47	0.49
1:C:328:SER:N	1:C:353:ASN:HD21	1.90	0.49
1:B:673:ILE:C	1:B:675:ILE:H	2.14	0.49
1:B:34:SER:H	1:B:58:ASN:HD21	1.60	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:C:635:ASP:O	1:C:638:ASN:N	2.39	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:D:125:ASP:CB	1:D:126:PRO:CA	2.91	0.49
1:A:237:THR:OG1	1:A:282:GLN:NE2	2.45	0.49
1:A:379:ASN:HB3	1:A:397:THR:HB	1.93	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:35:ASN:HD21	1:B:37:TYR:HB2	1.78	0.49
1:D:298:MSE:HB3	1:D:317:PHE:CD1	2.47	0.49
1:C:509:LEU:HD22	1:C:511:GLU:H	1.78	0.49
1:C:496:LYS:HB3	1:C:496:LYS:NZ	2.28	0.49
1:B:236:ASP:OD2	1:B:238:ASN:HB2	2.12	0.49
1:C:324:ASN:HD22	1:C:324:ASN:H	1.60	0.49
1:B:713:LEU:HD12	1:B:717:GLN:HB2	1.95	0.49
1:A:125:ASP:HB3	1:A:126:PRO:C	2.33	0.49
1:D:724:PHE:CZ	1:D:751:ILE:HD11	2.48	0.49
1:C:493:LEU:O	1:C:495:SER:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASP:HB2	1:C:111:TYR:CE2	2.48	0.49
1:B:381:VAL:HG12	1:B:663:ILE:HA	1.95	0.49
1:B:38:VAL:HG21	1:B:352:ILE:HG13	1.93	0.49
1:C:470:ARG:CD	1:C:515:ARG:CZ	2.86	0.49
1:A:562:TYR:HE2	1:A:564:SER:HA	1.77	0.49
1:D:404:VAL:HB	1:D:412:ALA:HB3	1.94	0.49
1:B:543:LEU:HD11	1:B:546:LYS:HB3	1.93	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:D:445:ASN:ND2	1:D:467:LEU:H	2.12	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:C:189:GLU:HB2	1:C:192:LYS:CB	2.37	0.48
1:B:492:ASP:CB	1:B:499:ILE:HD11	2.44	0.48
1:B:468:ASP:OD2	1:B:470:ARG:NE	2.46	0.48
1:D:585:ASN:O	1:D:586:PHE:HB2	2.13	0.48
1:D:148:TRP:CZ3	1:D:158:TYR:HB2	2.47	0.48
1:C:393:LEU:HD11	1:C:659:TYR:CZ	2.49	0.48
1:B:721:ASN:HB2	1:B:758:THR:HB	1.95	0.48
1:D:446:ILE:HD13	1:D:469:VAL:HG21	1.94	0.48
1:A:130:ILE:CD1	1:A:154:ARG:O	2.61	0.48
1:C:450:ASN:HD21	1:C:452:ARG:HE	1.59	0.48
1:D:170:ASN:ND2	1:D:172:SER:OG	2.46	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:C:482:ILE:HD12	1:C:491:ILE:HG23	1.94	0.48
1:D:491:ILE:HA	1:D:499:ILE:HG12	1.96	0.48
1:C:366:SER:HA	1:C:377:LEU:HD22	1.95	0.48
1:C:559:ASN:HD21	1:C:601:HIS:HE1	1.61	0.48
1:D:692:GLY:HA3	1:D:701:GLU:OE1	2.14	0.48
1:D:442:TYR:CE2	1:D:443:LEU:HD13	2.48	0.48
1:C:676:ASN:HA	1:C:778:GLN:NE2	2.26	0.48
1:A:328:SER:H	1:A:353:ASN:HD21	1.61	0.48
1:B:29:ILE:CD1	1:B:29:ILE:N	2.57	0.48
1:A:131:THR:CG2	1:A:154:ARG:HB2	2.42	0.48
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:79:SER:HA	1:A:116:PHE:CD2	2.49	0.48
1:C:470:ARG:HD3	1:C:515:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:HB2	1:B:192:LYS:CB	2.43	0.48
1:A:70:LYS:NZ	1:C:575:GLU:OE1	2.47	0.48
1:C:171:LYS:HA	1:C:174:VAL:O	2.14	0.48
1:A:520:ASP:HB3	1:A:523:GLY:N	2.29	0.47
1:C:129:LEU:HD12	1:C:157:GLU:HG3	1.96	0.47
1:B:227:GLY:HA3	1:B:247:LYS:HB2	1.96	0.47
1:D:555:SER:HB3	1:D:573:THR:HB	1.95	0.47
1:D:110:ASN:OD1	1:D:112:GLU:HB2	2.13	0.47
1:A:122:ASN:HD21	1:A:124:GLU:HB2	1.78	0.47
1:B:276:TYR:HB3	1:B:293:GLU:HB2	1.95	0.47
1:A:578:VAL:HG22	1:A:590:VAL:HG13	1.95	0.47
1:D:29:ILE:HD11	1:D:36:ASN:HD21	1.79	0.47
1:B:282:GLN:O	1:B:282:GLN:HG3	2.13	0.47
1:A:327:LEU:HD22	1:A:353:ASN:ND2	2.28	0.47
1:C:670:ASN:CG	1:C:671:PRO:CD	2.83	0.47
1:D:582:SER:C	1:D:584:ARG:H	2.17	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:A:577:LEU:HD21	1:A:613:ILE:HD11	1.96	0.47
1:B:675:ILE:C	1:B:678:PRO:HD2	2.34	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:B:340:PHE:O	1:B:341:ASN:HB2	2.15	0.47
1:A:711:ILE:HG22	1:A:789:ILE:HG12	1.97	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:C:381:VAL:CG2	1:C:398:ASP:HB3	2.45	0.47
1:B:766:LYS:HG3	1:B:790:HIS:ND1	2.30	0.47
1:B:381:VAL:CG2	1:B:398:ASP:HB3	2.44	0.47
1:D:197:HIS:HE1	1:D:203:SER:HB2	1.80	0.47
1:C:520:ASP:HB3	1:C:523:GLY:H	1.78	0.47
1:D:99:ILE:HB	1:D:107:ASN:HB2	1.96	0.47
1:D:509:LEU:HA	1:D:537:TYR:OH	2.15	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: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:298:MSE:HB3	1:A:317:PHE:CD1	2.50	0.47
1:C:599:ASN:HD21	1:C:618:ASN:H	1.62	0.47
1:A:283:LEU:HD23	1:A:343:ILE:HD11	1.97	0.47
1:C:24:ILE:HD11	1:C:318:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:724:PHE:CZ	1:B:751:ILE:CD1	2.98	0.47
1:A:714:THR:OG1	1:A:717:GLN:HG2	2.15	0.47
1:A:131:THR:HB	1:A:154:ARG:HH11	1.79	0.46
1:A:131:THR:HB	1:A:154:ARG:HD3	1.97	0.46
1:D:136:HIS:ND1	1:D:184:THR:HG22	2.29	0.46
1:B:507:SER:OG	1:B:508:GLN:N	2.49	0.46
1:A:192:LYS:HZ3	1:A:206:SER:HB3	1.79	0.46
1:D:751:ILE:HD13	1:D:757:VAL:HG23	1.95	0.46
1:A:34:SER:H	1:A:58:ASN:HD21	1.62	0.46
1:D:35:ASN:HB3	1:D:53:THR:HB	1.98	0.46
1:D:74:SER:C	1:D:76:SER:H	2.18	0.46
1:B:22:TYR:CD2	1:B:318:ILE:HD11	2.50	0.46
1:A:722:LEU:HD23	1:A:787:LEU:CD2	2.46	0.46
1:D:338:ASP:HB3	1:D:340:PHE:N	2.15	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:B:136:HIS:HB2	1:B:183:TRP:O	2.15	0.46
1:D:759:PHE:HB3	1:D:762:ILE:HD13	1.96	0.46
1:C:690:ILE:HG23	1:C:704:ILE:HD11	1.97	0.46
1:A:748:TRP:CH2	1:A:772:LYS:HE3	2.50	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:657:LEU:HD23	1:D:670:ASN:OD1	2.15	0.46
1:D:322:ASP:OD1	1:D:322:ASP:N	2.48	0.46
1:A:340:PHE:O	1:A:341:ASN:HB2	2.14	0.46
1:C:71:GLU:HB3	1:C:74:SER:HB3	1.98	0.46
1:A:739:TYR:HB2	1:A:769:PHE:CE1	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
1:D:711:ILE:CG2	1:D:789:ILE:HG12	2.46	0.46
1:A:473:TYR:CZ	1:A:519:GLN:HB2	2.50	0.46
1:A:722:LEU:O	1:A:756:SER:HA	2.16	0.46
1:D:243:ILE:HD12	1:D:252:PHE:CB	2.45	0.46
1:D:30:GLU:O	1:D:64:ARG:NH2	2.49	0.46
1:A:95:PRO:HG3	1:A:112:GLU:HG3	1.98	0.46
1:D:381:VAL:HG12	1:D:663:ILE:HA	1.97	0.46
1:D:649:CYS:SG	1:D:661:GLY:HA3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:ILE:HG23	1:B:704:ILE:HD11	1.98	0.46
1:D:490:VAL:HB	1:D:500:HIS:HB2	1.98	0.46
1:C:430:LEU:HG	1:C:431:LYS:N	2.31	0.46
1:B:548:ASN:HA	1:B:556:ASN:HD21	1.80	0.46
1:A:84:GLU:O	1:A:102:GLN:HG2	2.16	0.46
1:B:95:PRO:CB	1:B:112:GLU:HG3	2.46	0.46
1:A:378:SER:N	1:A:403:ASN:HD21	2.03	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:D:78:GLN:NE2	1:D:79:SER:O	2.48	0.46
1:B:362:PHE:CD1	1:B:640:ILE:HD11	2.51	0.46
1:D:614:TRP:CE3	1:D:623:CYS:HB2	2.51	0.46
1:C:275:SER:HB2	1:C:294:LEU:HD13	1.98	0.46
1:C:386:CYS:HB2	1:C:429:SER:OG	2.15	0.46
1:A:29:ILE:HD12	1:A:29:ILE:H	1.80	0.46
1:D:492:ASP:HB3	1:D:499:ILE:HD11	1.97	0.46
1:B:593:ARG:NH2	1:B:599:ASN:HB2	2.31	0.46
1:A:461:LEU:HB3	1:A:465:GLU:HB2	1.98	0.46
1:C:192:LYS:NZ	1:C:206:SER:HB3	2.31	0.45
1:A:711:ILE:HG22	1:A:789:ILE:HA	1.98	0.45
1:C:393:LEU:HD11	1:C:659:TYR:CE1	2.51	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:A:585:ASN:O	1:A:586:PHE:HB2	2.16	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:364:THR:HG21	1:B:641:PRO:HG3	1.98	0.45
1:B:252:PHE:CE1	1:B:257:GLU:HA	2.52	0.45
1:C:402:ILE:CG1	1:C:426:VAL:HG21	2.44	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
1:C:724:PHE:O	1:C:755:ASN:HB2	2.17	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:A:722:LEU:HD23	1:A:787:LEU:HD23	1.98	0.45
1:A:697:ARG:NH1	1:A:697:ARG:HA	2.16	0.45
1:B:582:SER:O	1:B:584:ARG:N	2.49	0.45
1:B:680:ILE:HG13	1:B:680:ILE:H	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:TYR:CD1	1:D:455:LYS:HB2	2.51	0.45
1:D:599:ASN:HD22	1:D:599:ASN:H	1.65	0.45
1:B:237:THR:H	1:B:282:GLN:HE21	1.64	0.45
1:B:690:ILE:HG13	1:B:690:ILE:O	2.16	0.45
1:C:605:ILE:CG2	1:C:613:ILE:HD13	2.46	0.45
1:A:72:GLU:OE2	1:C:593:ARG:HB2	2.17	0.45
1:C:329:ASN:HB3	1:C:347:THR:CG2	2.44	0.45
1:D:670:ASN:CB	1:D:671:PRO:CD	2.94	0.45
1:A:156:ILE:HD11	1:A:195:ILE:HG12	1.99	0.45
1:B:129:LEU:HD13	1:B:166:PHE:CE1	2.52	0.45
1:B:57:LEU:HB2	1:B:85:LEU:HD11	1.99	0.45
1:C:748:TRP:CZ3	1:C:772:LYS:HG2	2.52	0.45
1:D:298:MSE:HE2	1:D:317:PHE:HE1	1.82	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:C:337:GLN:HG2	1:C:341:ASN:HA	1.99	0.45
1:A:688:VAL:HG23	1:A:704:ILE:HB	1.99	0.45
1:C:520:ASP:HB3	1:C:523:GLY:N	2.32	0.45
1:D:449:TYR:HD1	1:D:455:LYS:HB2	1.82	0.45
1:C:638:ASN:O	1:C:639:ASN:HB3	2.17	0.44
1:C:121:TYR:HA	1:C:129:LEU:O	2.17	0.44
1:D:683:VAL:O	1:D:785:THR:HG21	2.17	0.44
1:C:382:VAL:O	1:C:646:ILE:CG2	2.64	0.44
1:D:285:ASP:O	1:D:286:ASN:HB2	2.16	0.44
1:B:739:TYR:C	1:B:739:TYR:CD2	2.90	0.44
1:B:724:PHE:HZ	1:B:751:ILE:HD13	1.82	0.44
1:B:545:ARG:HG2	1:B:546:LYS:H	1.82	0.44
1:C:601:HIS:CE1	1:C:603:ARG:NH1	2.85	0.44
1:C:138:THR:HG22	1:C:139:SER:O	2.17	0.44
1:D:96:VAL:HA	1:D:109:TYR:O	2.17	0.44
1:A:670:ASN:CG	1:A:671:PRO:HD2	2.38	0.44
1:A:714:THR:H	1:A:717:GLN:HG3	1.82	0.44
1:A:364:THR:CG2	1:A:641:PRO:HG3	2.47	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:D:670:ASN:HB3	1:D:671:PRO:CD	2.46	0.44
1:C:549:GLN:H	1:C:556:ASN:ND2	2.15	0.44
1:D:672:ASP:HA	1:D:674:ALA:H	1.82	0.44
1:C:284:LYS:C	1:C:286:ASN:H	2.20	0.44
1:B:300:LEU:HD22	1:B:302:LEU:HD23	1.99	0.44
1:C:473:TYR:CZ	1:C:519:GLN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:CG2	1:A:398:ASP:HB3	2.47	0.44
1:C:287:LYS:HE2	1:C:301:ASP:OD2	2.17	0.44
1:C:246:SER:HB3	1:C:276:TYR:CZ	2.53	0.44
1:A:285:ASP:HB3	1:A:287:LYS:HE3	1.99	0.44
1:B:544:VAL:O	1:C:372:MSE:HB2	2.18	0.44
1:A:597:LEU:HD22	1:A:631:PHE:CZ	2.53	0.44
1:C:558:ILE:HD13	1:C:558:ILE:C	2.37	0.44
1:C:71:GLU:HG2	1:C:79:SER:CB	2.48	0.44
1:B:520:ASP:HB3	1:B:523:GLY:N	2.33	0.44
1:C:484:THR:HG22	1:C:485:HIS:H	1.81	0.44
1:A:197:HIS:HE1	1:A:203:SER:CB	2.30	0.44
1:D:404:VAL:HG12	1:D:411:VAL:HG23	1.99	0.44
1:B:608:ASP:OD2	1:B:612:ASN:HB2	2.18	0.44
1:D:645:PHE:CD1	1:D:662:SER:HB3	2.53	0.44
1:A:704:ILE:HD12	1:A:704:ILE:N	2.32	0.44
1:A:438:TRP:CH2	1:A:491:ILE:HD11	2.50	0.44
1:A:715:HIS:CG	1:A:793:PRO:HA	2.53	0.44
1:A:690:ILE:O	1:A:690:ILE:HG13	2.18	0.44
1:A:739:TYR:CE1	1:A:749:TYR:HB2	2.52	0.44
1:A:227:GLY:HA3	1:A:247:LYS:HB2	2.00	0.44
1:A:733:ASN:HB3	1:A:734:GLN:HG2	1.99	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:C:497:LYS:C	1:C:498:VAL:HG22	2.21	0.43
1:A:711:ILE:CG2	1:A:789:ILE:HG12	2.48	0.43
1:B:592:GLN:H	1:B:595:GLU:CG	2.23	0.43
1:A:750:THR:HG22	1:A:751:ILE:N	2.32	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
1:B:582:SER:C	1:B:584:ARG:N	2.72	0.43
1:D:670:ASN:HB3	1:D:671:PRO:HD2	2.00	0.43
1:A:236:ASP:OD2	1:A:238:ASN:HB2	2.17	0.43
1:C:694:LEU:O	1:C:694:LEU:HG	2.18	0.43
1:C:592:GLN:O	1:C:593:ARG:C	2.56	0.43
1:D:592:GLN:O	1:D:593:ARG:C	2.56	0.43
1:D:492:ASP:CB	1:D:499:ILE:HD11	2.47	0.43
1:D:35:ASN:ND2	1:D:37:TYR:HB2	2.33	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:A:558:ILE:HD13	1:A:558:ILE:C	2.38	0.43
1:A:720:PHE:CE2	1:A:722:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:THR:HG21	1:C:755:ASN:ND2	2.30	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: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:D:507:SER:OG	1:D:508:GLN:N	2.52	0.43
1:D:146:GLY:HA2	1:D:161:ILE:HG13	2.01	0.43
1:B:327:LEU:HD22	1:B:353:ASN:HD22	1.84	0.43
1:D:328:SER:N	1:D:353:ASN:HD21	2.00	0.43
1:B:585:ASN:O	1:B:586:PHE:HB2	2.18	0.43
1:B:400:GLY:O	1:B:424:ASN:HB2	2.18	0.43
1:D:680:ILE:HA	1:D:681:PRO:HD3	1.89	0.43
1:C:99:ILE:O	1:C:106:LEU:HD12	2.19	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: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:515:ARG:HG2	1:A:515:ARG:HH11	1.83	0.43
1:A:662:SER:C	1:A:664:ASN:H	2.22	0.43
1:A:253:ASN:HD22	1:A:255:ASN:HB3	1.82	0.43
1:B:650:VAL:CG2	1:B:651:THR:N	2.82	0.43
1:A:282:GLN:O	1:A:282:GLN:HG3	2.19	0.43
1:C:650:VAL:CG2	1:C:651:THR:N	2.82	0.43
1:B:455:LYS:HB2	1:B:455:LYS:NZ	2.34	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:C:662:SER:C	1:C:664:ASN:N	2.72	0.43
1:D:690:ILE:HG13	1:D:690:ILE:O	2.18	0.43
1:B:379:ASN:ND2	1:B:381:VAL:HG22	2.34	0.43
1:D:759:PHE:HB3	1:D:762:ILE:CD1	2.49	0.43
1:B:391:GLY:O	1:B:406:GLU:HG3	2.18	0.43
1:D:711:ILE:HG21	1:D:789:ILE:HG12	2.01	0.43
1:A:593:ARG:NH1	1:A:600:THR:CG2	2.82	0.43
1:D:743:GLY:H	1:D:746:ASN:ND2	2.16	0.43
1:D:733:ASN:ND2	1:D:734:GLN:HB3	2.34	0.43
1:D:382:VAL:HG11	1:D:666:LEU:HD13	2.01	0.43
1:C:568:GLN:OE1	1:C:581:PRO:HA	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:THR:HG22	1:C:751:ILE:N	2.34	0.42
1:C:446:ILE:HD12	1:C:472:PHE:CZ	2.54	0.42
1:D:237:THR:H	1:D:282:GLN:NE2	2.17	0.42
1:C:236:ASP:HB2	1:C:240:ASN:O	2.19	0.42
1:C:770:LEU:HD23	1:C:786:SER:CB	2.48	0.42
1:A:599:ASN:ND2	1:A:617:THR:HB	2.34	0.42
1:C:159:LEU:HD13	1:C:166:PHE:CE1	2.54	0.42
1:A:373:ASN:HB3	1:A:376:SER:N	2.34	0.42
1:D:298:MSE:HE2	1:D:317:PHE:CE1	2.54	0.42
1:B:536:ILE:HG13	1:B:586:PHE:HE1	1.83	0.42
1:B:468:ASP:CG	1:B:470:ARG:HH21	2.22	0.42
1:D:563:ARG:HD3	1:D:567:GLY:HA2	2.02	0.42
1:C:470:ARG:CD	1:C:515:ARG:NH1	2.83	0.42
1:C:34:SER:HB2	1:C:69:TYR:OH	2.19	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:D:40:SER:CB	1:D:87:GLU:HA	2.50	0.42
1:B:640:ILE:HG23	1:B:641:PRO:HD2	2.02	0.42
1:B:593:ARG:NH1	1:B:600:THR:HG22	2.35	0.42
1:D:30:GLU:HB2	1:D:31:GLN:NE2	2.34	0.42
1:B:597:LEU:HD22	1:B:631:PHE:CZ	2.55	0.42
1:B:29:ILE:HG13	1:B:36:ASN:HD21	1.84	0.42
1:A:722:LEU:HD12	1:A:722:LEU:H	1.84	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: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:D:109:TYR:OH	1:D:114:GLN:HG2	2.20	0.42
1:A:675:ILE:HA	1:A:678:PRO:HD2	2.02	0.42
1:D:290:ILE:HB	1:D:298:MSE:HG3	2.02	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:D:158:TYR:O	1:D:166:PHE:HA	2.19	0.42
1:A:249:LEU:C	1:A:249:LEU:CD1	2.88	0.42
1:C:322:ASP:N	1:C:322:ASP:OD1	2.53	0.42
1:D:468:ASP:HB3	1:D:485:HIS:HB3	2.01	0.42
1:B:599:ASN:HD21	1:B:617:THR:HB	1.84	0.42
1:A:555:SER:HB3	1:A:573:THR:HB	2.02	0.42
1:D:388:ASP:C	1:D:390:GLN:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ILE:HG23	1:A:649:CYS:HB3	2.02	0.42
1:C:381:VAL:CG2	1:C:398:ASP:CB	2.98	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:D:34:SER:H	1:D:58:ASN:HD21	1.68	0.42
1:A:208:ASN:H	1:A:208:ASN:HD22	1.68	0.42
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: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:A:383:SER:HB2	1:A:426:VAL:O	2.20	0.41
1:C:278:PHE:HE2	1:C:293:GLU:HB2	1.85	0.41
1:A:63:THR:HG21	1:A:755:ASN:HD21	1.84	0.41
1:C:131:THR:CG2	1:C:154:ARG:HB2	2.50	0.41
1:B:122:ASN:C	1:B:124:GLU:N	2.73	0.41
1:D:531:GLY:H	1:D:557:THR:HG22	1.85	0.41
1:A:761:ASN:HB2	1:C:744:LEU:HD11	2.02	0.41
1:C:491:ILE:HD12	1:C:497:LYS:CB	2.23	0.41
1:A:194:TYR:HB3	1:A:233:ILE:HD13	2.01	0.41
1:C:283:LEU:HB3	1:C:285:ASP:OD1	2.20	0.41
1:A:704:ILE:HG22	1:A:711:ILE:CD1	2.41	0.41
1:A:670:ASN:CG	1:A:671:PRO:CD	2.89	0.41
1:A:136:HIS:HB2	1:A:183:TRP:O	2.19	0.41
1:C:739:TYR:C	1:C:739:TYR:CD2	2.93	0.41
1:A:720:PHE:HE2	1:A:722:LEU:HD11	1.84	0.41
1:C:320:GLU:HB2	1:C:330:ALA:HA	2.02	0.41
1:B:674:ALA:C	1:B:676:ASN:H	2.24	0.41
1:C:762:ILE:HA	1:C:763:PRO:HD3	1.87	0.41
1:B:558:ILE:C	1:B:558:ILE:HD13	2.40	0.41
1:B:458:ILE:HG13	1:B:497:LYS:HD2	2.02	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: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:A:462:GLU:CG	1:A:463:LYS:H	2.17	0.41
1:D:290:ILE:HD12	1:D:298:MSE:HG3	2.02	0.41
1:D:216:VAL:CG1	1:D:217:HIS:N	2.74	0.41
1:D:40:SER:HB3	1:D:52:ALA:HB3	2.03	0.41
1:A:150:CYS:HB3	1:A:182:THR:OG1	2.20	0.41
1:D:597:LEU:HD13	1:D:631:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ALA:HA	1:C:194:TYR:O	2.21	0.41
1:D:383:SER:CB	1:D:426:VAL:O	2.69	0.41
1:D:653:ASP:HB3	1:D:656:GLY:H	1.85	0.41
1:C:559:ASN:HD21	1:C:601:HIS:CE1	2.38	0.41
1:D:388:ASP:OD2	1:D:394:TRP:NE1	2.49	0.41
1:A:568:GLN:H	1:A:568:GLN:HG2	1.74	0.41
1:C:470:ARG:CZ	1:C:470:ARG:HB3	2.50	0.41
1:C:283:LEU:HD22	1:C:289:TRP:CG	2.56	0.41
1:A:58:ASN:HD22	1:A:67:THR:HG22	1.85	0.41
1:D:287:LYS:HE2	1:D:301:ASP:OD2	2.21	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:A:338:ASP:HB2	1:A:342:ASN:N	2.36	0.41
1:D:457:GLN:HB3	1:D:457:GLN:HE21	1.72	0.41
1:C:125:ASP:HB3	1:C:126:PRO:CA	2.51	0.41
1:A:482:ILE:HD12	1:A:491:ILE:HG23	2.02	0.41
1:B:724:PHE:CE2	1:B:751:ILE:HD11	2.56	0.41
1:C:680:ILE:O	1:C:680:ILE:HD12	2.21	0.41
1:A:89:TYR:OH	1:A:139:SER:HB2	2.21	0.41
1:B:50:TRP:CE3	1:B:59:LYS:HB2	2.55	0.41
1:A:723:THR:HA	1:A:756:SER:HA	2.02	0.41
1:A:130:ILE:HG13	1:A:131:THR:HG22	2.02	0.41
1:D:79:SER:OG	1:D:80:ILE:N	2.54	0.41
1:A:677:SER:O	1:A:679:GLN:N	2.54	0.41
1:C:285:ASP:OD1	1:C:285:ASP:N	2.51	0.40
1:B:236:ASP:CB	1:B:240:ASN:HB2	2.51	0.40
1:A:575:GLU:HA	1:A:600:THR:HG23	2.02	0.40
1:D:515:ARG:HH11	1:D:515:ARG:HG2	1.86	0.40
1:B:556:ASN:HA	1:B:556:ASN:HD22	1.57	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:C:229:ASP:O	1:C:245:THR:HA	2.21	0.40
1:D:338:ASP:OD2	1:D:342:ASN:HB2	2.21	0.40
1:B:377:LEU:HA	1:B:403:ASN:ND2	2.36	0.40
1:D:733:ASN:ND2	1:D:733:ASN:C	2.74	0.40
1:A:558:ILE:HD13	1:A:558:ILE:O	2.21	0.40
1:D:43:GLN:HB2	1:D:49:LEU:HD22	2.03	0.40
1:A:192:LYS:HZ2	1:A:206:SER:HB3	1.84	0.40
1:C:297:ILE:HG12	1:C:335:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:LEU:HD11	1:B:546:LYS:HD2	2.03	0.40
1:C:706:ILE:HG13	1:C:711:ILE:HD13	2.03	0.40
1:C:488:VAL:HG22	1:C:514:VAL:HG21	2.03	0.40
1:D:138:THR:HG22	1:D:139:SER:N	2.36	0.40
1:C:380:LYS:HE3	1:C:663:ILE:O	2.21	0.40
1:A:277:ILE:HG23	1:A:290:ILE:HG22	2.03	0.40
1:B:338:ASP:C	1:B:340:PHE:H	2.25	0.40
1:D:378:SER:N	1:D:403:ASN:HD21	2.02	0.40
1:C:427:LEU:HD13	1:C:470:ARG:NH2	2.37	0.40
1:C:290:ILE:N	1:C:298:MSE:O	2.49	0.40
1:C:320:GLU:HG3	1:C:329:ASN:C	2.42	0.40
1:C:237:THR:H	1:C:282:GLN:NE2	2.19	0.40
1:B:208:ASN:HD22	1:B:208:ASN:H	1.69	0.40
1:C:449:TYR:CD1	1:C:455:LYS:HB2	2.37	0.40
1:B:678:PRO:HB2	1:B:775:LEU:HD12	2.03	0.40
1:C:462:GLU:O	1:C:464:ASN:N	2.55	0.40
1:D:95:PRO:HG3	1:D:112:GLU:HG3	2.04	0.40
1:C:571:LEU:HB2	1:C:578:VAL:HB	2.03	0.40
1:A:243:ILE:HD12	1:A:252:PHE:HB2	2.02	0.40
1:B:446:ILE:HD13	1:B:469:VAL:HG21	2.03	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%)	8	41
1	B	724/781 (93%)	634 (88%)	71 (10%)	19 (3%)	7	36
1	C	724/781 (93%)	638 (88%)	69 (10%)	17 (2%)	8	39
1	D	724/781 (93%)	637 (88%)	69 (10%)	18 (2%)	7	37
All	All	2896/3124 (93%)	2541 (88%)	285 (10%)	70 (2%)	7	38

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
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

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	649/685 (95%)	570 (88%)	79 (12%)	6 26
1	B	649/685 (95%)	585 (90%)	64 (10%)	10 37
1	C	649/685 (95%)	579 (89%)	70 (11%)	8 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	649/685 (95%)	579 (89%)	70 (11%)	8 32
All	All	2596/2740 (95%)	2313 (89%)	283 (11%)	8 32

All (283) 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
1	A	124	GLU
1	A	125	ASP
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	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	276	TYR
1	A	290	ILE
1	A	298	MSE
1	A	322	ASP
1	A	323	ASN
1	A	345	ILE
1	A	348	TRP
1	A	371	GLN
1	A	375	SER
1	A	376	SER
1	A	377	LEU
1	A	380	LYS
1	A	383	SER

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Mol	Chain	Res	Type
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	459	ILE
1	A	464	ASN
1	A	471	VAL
1	A	491	ILE
1	A	493	LEU
1	A	497	LYS
1	A	498	VAL
1	A	507	SER
1	A	509	LEU
1	A	517	ILE
1	A	520	ASP
1	A	550	TYR
1	A	558	ILE
1	A	563	ARG
1	A	585	ASN
1	A	593	ARG
1	A	599	ASN
1	A	627	SER
1	A	629	LYS
1	A	647	SER
1	A	670	ASN
1	A	675	ILE
1	A	696	SER
1	A	697	ARG
1	A	699	LYS
1	A	712	GLU
1	A	715	HIS
1	A	716	GLU
1	A	722	LEU
1	A	724	PHE
1	A	733	ASN
1	A	734	GLN
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	46	GLN
1	B	49	LEU
1	B	72	GLU
1	B	130	ILE
1	B	133	ASP
1	B	142	GLN
1	B	167	THR
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	276	TYR
1	B	282	GLN
1	B	284	LYS
1	B	285	ASP
1	B	304	GLN
1	B	322	ASP
1	B	323	ASN
1	B	326	SER
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	461	LEU
1	B	464	ASN
1	B	470	ARG
1	B	471	VAL
1	B	476	LYS
1	B	484	THR
1	B	493	LEU
1	B	495	SER
1	B	498	VAL
1	B	507	SER
1	B	509	LEU
1	B	511	GLU

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Mol	Chain	Res	Type
1	B	556	ASN
1	B	558	ILE
1	B	563	ARG
1	B	585	ASN
1	B	595	GLU
1	B	599	ASN
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	717	GLN
1	B	746	ASN
1	B	752	ASN
1	B	755	ASN
1	B	758	THR
1	B	760	ARG
1	B	772	LYS
1	B	776	HIS
1	B	785	THR
1	C	29	ILE
1	C	49	LEU
1	C	117	SER
1	C	133	ASP
1	C	142	GLN
1	C	167	THR
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	276	TYR
1	C	282	GLN
1	C	283	LEU
1	C	285	ASP
1	C	294	LEU
1	C	299	ILE
1	C	305	ASN

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Mol	Chain	Res	Type
1	C	326	SER
1	C	338	ASP
1	C	347	THR
1	C	371	GLN
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	451	THR
1	C	455	LYS
1	C	457	GLN
1	C	459	ILE
1	C	464	ASN
1	C	471	VAL
1	C	480	ILE
1	C	491	ILE
1	C	495	SER
1	C	497	LYS
1	C	498	VAL
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	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	629	LYS
1	C	642	GLN
1	C	647	SER
1	C	673	ILE
1	C	687	LYS
1	C	696	SER

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Mol	Chain	Res	Type
1	C	697	ARG
1	C	713	LEU
1	C	717	GLN
1	C	746	ASN
1	C	755	ASN
1	C	758	THR
1	C	760	ARG
1	C	776	HIS
1	C	778	GLN
1	D	29	ILE
1	D	49	LEU
1	D	133	ASP
1	D	142	GLN
1	D	154	ARG
1	D	167	THR
1	D	172	SER
1	D	202	LEU
1	D	205	LEU
1	D	231	ARG
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	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	453	LEU
1	D	455	LYS
1	D	456	PHE
1	D	458	ILE
1	D	464	ASN
1	D	471	VAL
1	D	480	ILE
1	D	495	SER
1	D	498	VAL

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Mol	Chain	Res	Type
1	D	508	GLN
1	D	509	LEU
1	D	511	GLU
1	D	515	ARG
1	D	550	TYR
1	D	556	ASN
1	D	558	ILE
1	D	563	ARG
1	D	568	GLN
1	D	582	SER
1	D	593	ARG
1	D	594	LYS
1	D	595	GLU
1	D	599	ASN
1	D	600	THR
1	D	610	ASN
1	D	613	ILE
1	D	627	SER
1	D	629	LYS
1	D	640	ILE
1	D	646	ILE
1	D	647	SER
1	D	678	PRO
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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	58	ASN
1	A	94	GLN
1	A	132	ASN
1	A	142	GLN
1	A	170	ASN
1	A	197	HIS
1	A	208	ASN
1	A	253	ASN
1	A	282	GLN
1	A	323	ASN
1	A	341	ASN
1	A	353	ASN
1	A	357	ASN
1	A	379	ASN
1	A	403	ASN
1	A	450	ASN
1	A	464	ASN
1	A	556	ASN
1	A	599	ASN
1	A	601	HIS
1	A	664	ASN
1	A	715	HIS
1	A	721	ASN
1	A	725	ASN
1	A	733	ASN
1	A	734	GLN
1	A	752	ASN
1	A	754	GLN
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	282	GLN
1	B	304	GLN
1	B	323	ASN
1	B	341	ASN
1	B	353	ASN
1	B	357	ASN

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Mol	Chain	Res	Type
1	B	379	ASN
1	B	403	ASN
1	B	445	ASN
1	B	464	ASN
1	B	556	ASN
1	B	599	ASN
1	B	601	HIS
1	B	638	ASN
1	B	725	ASN
1	B	733	ASN
1	B	746	ASN
1	B	752	ASN
1	B	754	GLN
1	B	778	GLN
1	C	35	ASN
1	C	58	ASN
1	C	94	GLN
1	C	142	GLN
1	C	170	ASN
1	C	240	ASN
1	C	253	ASN
1	C	282	GLN
1	C	304	GLN
1	C	323	ASN
1	C	324	ASN
1	C	341	ASN
1	C	353	ASN
1	C	357	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	556	ASN
1	C	601	HIS
1	C	638	ASN
1	C	642	GLN
1	C	664	ASN
1	C	676	ASN
1	C	700	ASN
1	C	721	ASN

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Mol	Chain	Res	Type
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	94	GLN
1	D	132	ASN
1	D	142	GLN
1	D	170	ASN
1	D	197	HIS
1	D	240	ASN
1	D	253	ASN
1	D	282	GLN
1	D	304	GLN
1	D	323	ASN
1	D	341	ASN
1	D	353	ASN
1	D	357	ASN
1	D	403	ASN
1	D	445	ASN
1	D	457	GLN
1	D	542	GLN
1	D	556	ASN
1	D	568	GLN
1	D	599	ASN
1	D	601	HIS
1	D	638	ASN
1	D	642	GLN
1	D	721	ASN
1	D	725	ASN
1	D	733	ASN
1	D	734	GLN
1	D	746	ASN
1	D	752	ASN
1	D	755	ASN
1	D	792	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	731/781 (93%)	-0.05	3 (0%)	93 92	39, 71, 121, 177	0
1	B	731/781 (93%)	0.04	9 (1%)	81 76	44, 75, 135, 210	0
1	C	731/781 (93%)	0.07	15 (2%)	67 60	38, 80, 147, 221	0
1	D	731/781 (93%)	0.04	15 (2%)	67 60	43, 77, 149, 219	0
All	All	2924/3124 (93%)	0.02	42 (1%)	78 73	38, 76, 139, 221	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	699	LYS	5.8
1	D	700	ASN	5.5
1	D	697	ARG	5.1
1	C	697	ARG	4.4
1	D	460	GLU	4.3
1	D	698	GLU	4.3
1	C	676	ASN	3.9
1	B	467	LEU	3.6
1	C	700	ASN	3.6
1	B	466	LEU	3.5
1	C	126	PRO	3.2
1	C	677	SER	3.1
1	D	496	LYS	3.0
1	C	73	GLN	2.9
1	D	490	VAL	2.9
1	B	700	ASN	2.8
1	C	252	PHE	2.6
1	D	73	GLN	2.6
1	A	402	ILE	2.6
1	B	460	GLU	2.6
1	D	437	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	257	GLU	2.5
1	B	485	HIS	2.5
1	C	464	ASN	2.5
1	B	699	LYS	2.5
1	B	74	SER	2.5
1	C	675	ILE	2.4
1	A	696	SER	2.4
1	D	459	ILE	2.4
1	D	464	ASN	2.3
1	D	502	TYR	2.3
1	C	205	LEU	2.2
1	C	258	THR	2.2
1	B	464	ASN	2.2
1	B	496	LYS	2.1
1	D	72	GLU	2.1
1	A	424	ASN	2.1
1	D	252	PHE	2.1
1	C	81	THR	2.0
1	D	173	THR	2.0
1	C	169	TYR	2.0
1	C	305	ASN	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 carbohydrates 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.