



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

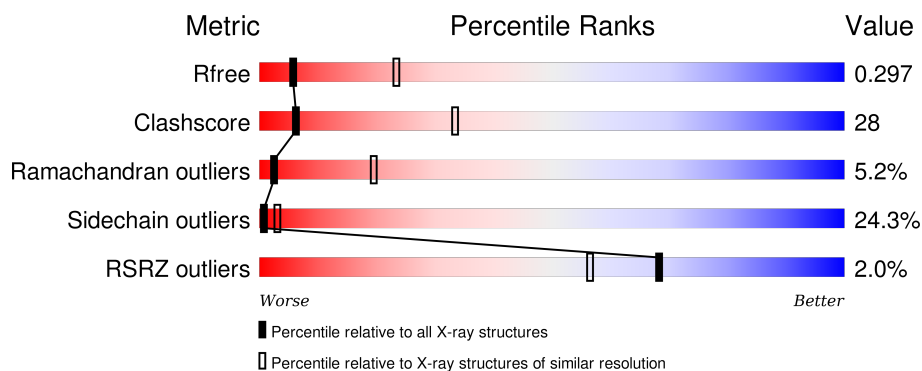
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	 3% 40% 36% 16% • 7%
1	B	585	 2% 40% 37% 15% • 7%
1	C	585	 0% 39% 37% 17% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

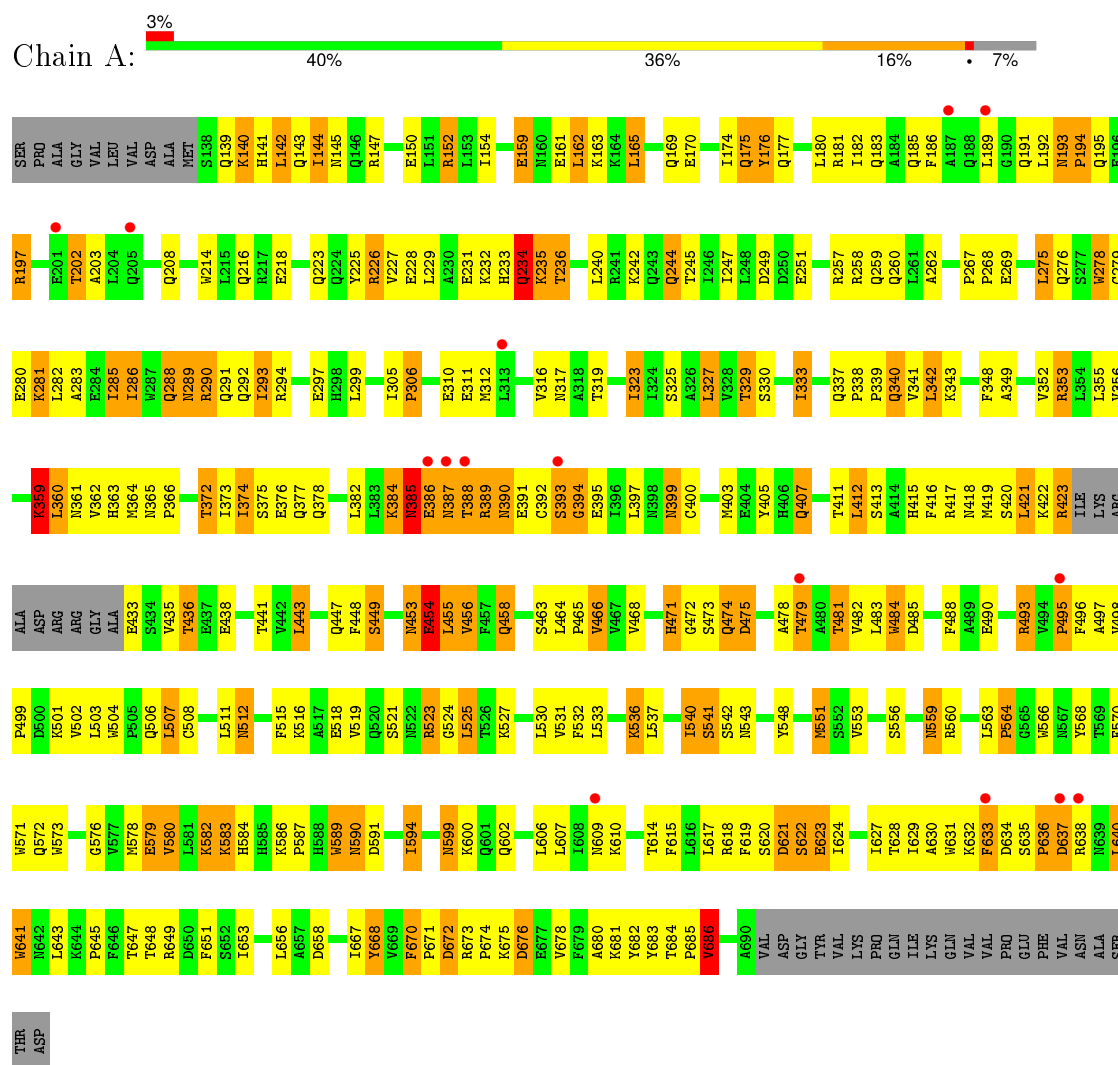
- Molecule 1 is a protein called Signal transducer and activator of transcription 5A.

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

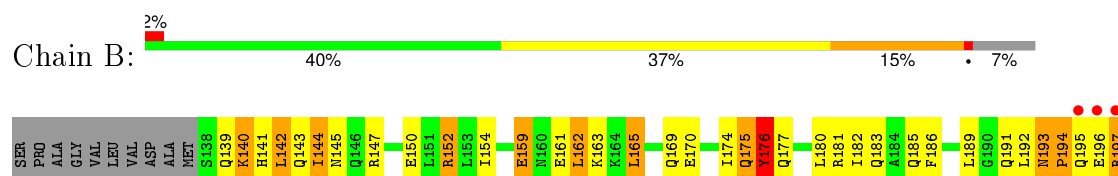
3 Residue-property plots

These plots are drawn for all protein, RNA 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: Signal transducer and activator of transcription 5A



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



VAL
VAL
PRO
GLU
PHE
VAL
ASN
ALA
SER
THR
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.02Å 235.43Å 111.42Å 90.00° 108.76° 90.00°	Depositor
Resolution (Å)	78.56 – 3.21 78.56 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (78.56-3.21) 98.6 (78.56-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.266 , 0.299 0.264 , 0.297	Depositor DCC
R_{free} test set	5010 reflections (9.81%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 56833 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13293	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.66	1/4527 (0.0%)	0.80	1/6134 (0.0%)
1	B	0.65	1/4527 (0.0%)	0.80	2/6134 (0.0%)
1	C	0.65	0/4527	0.80	2/6134 (0.0%)
All	All	0.66	2/13581 (0.0%)	0.80	5/18402 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
1	C	0	5
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	CYS	CB-SG	-7.35	1.69	1.82
1	B	579	GLU	CG-CD	5.12	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	GLY	N-CA-C	-6.00	98.10	113.10
1	C	472	GLY	N-CA-C	-5.58	99.14	113.10
1	B	176	TYR	CA-CB-CG	5.38	123.63	113.40
1	B	472	GLY	N-CA-C	-5.25	99.98	113.10
1	C	176	TYR	CA-CB-CG	5.15	123.18	113.40

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Peptide
1	A	360	LEU	Peptide
1	A	387	ASN	Peptide
1	A	471	HIS	Peptide
1	A	623	GLU	Peptide
1	B	197	ARG	Peptide
1	B	360	LEU	Peptide
1	B	387	ASN	Peptide
1	B	471	HIS	Peptide
1	B	565	GLY	Peptide
1	B	623	GLU	Peptide
1	C	197	ARG	Peptide
1	C	360	LEU	Peptide
1	C	387	ASN	Peptide
1	C	471	HIS	Peptide
1	C	623	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4415	258	0
1	B	4431	0	4415	253	0
1	C	4431	0	4415	247	0
All	All	13293	0	13245	744	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 28.

All (744) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:TYR:HB3	1:A:674:PRO:HA	1.21	1.14
1:C:668:TYR:HB3	1:C:674:PRO:HA	1.19	1.13
1:A:226:ARG:HH12	1:A:305:ILE:HG12	1.04	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:TYR:HB3	1:B:674:PRO:HA	1.21	1.13
1:C:226:ARG:HH12	1:C:305:ILE:HG12	0.96	1.12
1:B:226:ARG:HH12	1:B:305:ILE:HG12	1.04	1.08
1:C:186:PHE:HE1	1:C:208:GLN:HE22	1.04	1.01
1:A:361:ASN:HD22	1:B:361:ASN:HD22	1.00	0.99
1:B:399:ASN:O	1:B:400:CYS:SG	2.21	0.98
1:C:226:ARG:NH1	1:C:305:ILE:HG12	1.78	0.97
1:B:186:PHE:HE1	1:B:208:GLN:HE22	0.98	0.96
1:A:226:ARG:NH1	1:A:305:ILE:HG12	1.81	0.94
1:A:186:PHE:HE1	1:A:208:GLN:HE22	0.96	0.93
1:B:226:ARG:NH1	1:B:305:ILE:HG12	1.81	0.93
1:B:523:ARG:HB3	1:B:589:TRP:CZ3	2.03	0.92
1:C:668:TYR:HB3	1:C:674:PRO:CA	2.01	0.91
1:A:364:MET:HG3	1:B:361:ASN:ND2	1.85	0.90
1:A:361:ASN:ND2	1:B:364:MET:HG3	1.85	0.90
1:A:523:ARG:HB3	1:A:589:TRP:CZ3	2.06	0.90
1:C:523:ARG:HB3	1:C:589:TRP:CZ3	2.06	0.89
1:A:361:ASN:HD22	1:B:361:ASN:ND2	1.71	0.88
1:B:668:TYR:HB3	1:B:674:PRO:CA	2.04	0.87
1:A:385:ASN:N	1:A:385:ASN:HD22	1.72	0.87
1:B:378:GLN:HE22	1:B:393:SER:H	1.21	0.87
1:A:361:ASN:ND2	1:B:361:ASN:HD22	1.73	0.86
1:B:186:PHE:HE1	1:B:208:GLN:NE2	1.74	0.86
1:A:668:TYR:HB3	1:A:674:PRO:CA	2.04	0.85
1:B:523:ARG:HB3	1:B:589:TRP:HZ3	1.39	0.85
1:A:214:TRP:NE1	1:A:218:GLU:OE1	2.09	0.85
1:C:399:ASN:O	1:C:400:CYS:SG	2.35	0.84
1:C:385:ASN:HD22	1:C:385:ASN:N	1.75	0.84
1:A:385:ASN:H	1:A:385:ASN:ND2	1.72	0.84
1:B:281:LYS:O	1:B:285:ILE:HG22	1.76	0.84
1:A:378:GLN:HE22	1:A:393:SER:H	1.24	0.84
1:B:385:ASN:HD22	1:B:385:ASN:N	1.74	0.84
1:A:186:PHE:HE1	1:A:208:GLN:NE2	1.75	0.84
1:B:214:TRP:NE1	1:B:218:GLU:OE1	2.10	0.84
1:B:385:ASN:H	1:B:385:ASN:ND2	1.75	0.83
1:C:281:LYS:O	1:C:285:ILE:HG22	1.77	0.83
1:C:523:ARG:HB3	1:C:589:TRP:HZ3	1.42	0.83
1:B:670:PHE:HB3	1:B:671:PRO:HD3	1.60	0.83
1:A:186:PHE:CE1	1:A:208:GLN:NE2	2.47	0.83
1:A:523:ARG:HB3	1:A:589:TRP:HZ3	1.44	0.83
1:C:378:GLN:HE22	1:C:393:SER:H	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ASN:H	1:C:385:ASN:ND2	1.74	0.82
1:B:602:GLN:O	1:B:606:LEU:HG	1.80	0.82
1:A:399:ASN:HB3	1:A:419:MET:HG2	1.61	0.82
1:C:214:TRP:NE1	1:C:218:GLU:OE1	2.12	0.82
1:C:602:GLN:O	1:C:606:LEU:HG	1.80	0.81
1:A:670:PHE:HB3	1:A:671:PRO:HD3	1.60	0.80
1:B:186:PHE:CE1	1:B:208:GLN:NE2	2.48	0.80
1:B:599:ASN:ND2	1:B:602:GLN:H	1.79	0.80
1:A:281:LYS:O	1:A:285:ILE:HG22	1.82	0.80
1:B:620:SER:OG	1:B:628:THR:HG23	1.81	0.80
1:C:670:PHE:HB3	1:C:671:PRO:HD3	1.64	0.80
1:C:399:ASN:HB3	1:C:419:MET:HG2	1.64	0.80
1:C:503:LEU:O	1:C:506:GLN:HG2	1.83	0.79
1:C:186:PHE:HE1	1:C:208:GLN:NE2	1.79	0.79
1:C:634:ASP:O	1:C:636:PRO:HD3	1.82	0.78
1:B:378:GLN:NE2	1:B:393:SER:H	1.80	0.78
1:A:634:ASP:O	1:A:636:PRO:HD3	1.83	0.78
1:A:385:ASN:N	1:A:385:ASN:ND2	2.30	0.78
1:A:418:ASN:HD21	1:B:170:GLU:HG3	1.49	0.77
1:C:681:LYS:HD2	1:C:682:TYR:CZ	2.19	0.77
1:B:634:ASP:O	1:B:636:PRO:HD3	1.84	0.77
1:B:399:ASN:HB3	1:B:419:MET:HG2	1.65	0.77
1:C:385:ASN:N	1:C:385:ASN:ND2	2.32	0.77
1:C:378:GLN:NE2	1:C:393:SER:H	1.83	0.77
1:A:170:GLU:HG3	1:B:418:ASN:HD21	1.51	0.76
1:B:503:LEU:O	1:B:506:GLN:HG2	1.85	0.76
1:C:186:PHE:CE1	1:C:208:GLN:NE2	2.51	0.75
1:B:385:ASN:ND2	1:B:385:ASN:N	2.32	0.75
1:C:599:ASN:ND2	1:C:602:GLN:H	1.84	0.75
1:B:193:ASN:HB2	1:B:194:PRO:CD	2.16	0.75
1:A:193:ASN:HB2	1:A:194:PRO:CD	2.16	0.75
1:A:602:GLN:O	1:A:606:LEU:HG	1.87	0.75
1:A:378:GLN:NE2	1:A:393:SER:H	1.84	0.75
1:B:623:GLU:HB3	1:B:645:PRO:HG2	1.69	0.74
1:A:556:SER:HA	1:A:560:ARG:HB3	1.70	0.74
1:B:251:GLU:HA	1:B:251:GLU:OE2	1.87	0.74
1:C:587:PRO:O	1:C:591:ASP:HB2	1.88	0.74
1:C:620:SER:OG	1:C:628:THR:HG23	1.88	0.73
1:B:556:SER:HA	1:B:560:ARG:HB3	1.69	0.73
1:C:251:GLU:OE2	1:C:251:GLU:HA	1.87	0.73
1:B:193:ASN:HB2	1:B:194:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:TYR:HA	1:A:551:MET:HG3	1.70	0.73
1:C:392:CYS:O	1:C:394:GLY:N	2.22	0.73
1:B:490:GLU:O	1:B:493:ARG:HG3	1.88	0.73
1:A:503:LEU:O	1:A:506:GLN:HG2	1.88	0.73
1:A:620:SER:OG	1:A:628:THR:HG23	1.88	0.73
1:A:490:GLU:O	1:A:493:ARG:HG3	1.89	0.72
1:A:471:HIS:CD2	1:A:474:GLN:HB2	2.24	0.72
1:C:193:ASN:HB2	1:C:194:PRO:CD	2.19	0.72
1:A:599:ASN:ND2	1:A:602:GLN:H	1.88	0.72
1:A:386:GLU:O	1:A:386:GLU:HG2	1.89	0.72
1:A:193:ASN:HB2	1:A:194:PRO:HD3	1.71	0.72
1:B:392:CYS:O	1:B:394:GLY:N	2.23	0.72
1:C:548:TYR:HA	1:C:551:MET:HG3	1.72	0.71
1:B:386:GLU:O	1:B:386:GLU:HG2	1.90	0.71
1:C:471:HIS:CD2	1:C:474:GLN:HB2	2.26	0.71
1:C:386:GLU:HG2	1:C:386:GLU:O	1.90	0.71
1:A:392:CYS:O	1:A:394:GLY:N	2.25	0.70
1:C:680:ALA:HA	1:C:683:TYR:CD1	2.27	0.70
1:A:251:GLU:HA	1:A:251:GLU:OE2	1.90	0.70
1:A:587:PRO:O	1:A:591:ASP:HB2	1.92	0.70
1:B:582:LYS:HA	1:B:586:LYS:HG2	1.74	0.70
1:A:399:ASN:O	1:A:400:CYS:SG	2.47	0.69
1:C:490:GLU:O	1:C:493:ARG:HG3	1.91	0.69
1:A:175:GLN:HA	1:A:175:GLN:HE21	1.57	0.69
1:A:139:GLN:HG3	1:A:140:LYS:HD3	1.73	0.69
1:A:620:SER:HB3	1:A:622:SER:HB2	1.74	0.69
1:C:193:ASN:HB2	1:C:194:PRO:HD3	1.74	0.69
1:C:225:TYR:HA	1:C:228:GLU:HG3	1.74	0.69
1:A:523:ARG:HA	1:A:523:ARG:HH11	1.58	0.69
1:A:202:THR:CG2	1:A:203:ALA:N	2.56	0.69
1:B:471:HIS:CD2	1:B:474:GLN:HB2	2.28	0.69
1:A:559:ASN:OD1	1:A:571:TRP:HB3	1.91	0.68
1:C:556:SER:HA	1:C:560:ARG:HB3	1.73	0.68
1:B:139:GLN:HG3	1:B:140:LYS:HD3	1.74	0.68
1:B:620:SER:HB3	1:B:622:SER:HB2	1.76	0.68
1:C:139:GLN:HG3	1:C:140:LYS:HD3	1.75	0.68
1:B:548:TYR:HA	1:B:551:MET:HG3	1.75	0.68
1:B:286:ILE:HG13	1:B:323:ILE:HD11	1.76	0.67
1:C:374:ILE:HG22	1:C:441:THR:HG23	1.77	0.67
1:C:527:LYS:HD3	1:C:527:LYS:H	1.59	0.67
1:A:582:LYS:HA	1:A:586:LYS:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:LYS:O	1:C:632:LYS:HE2	1.95	0.67
1:A:623:GLU:HB3	1:A:645:PRO:HG2	1.77	0.67
1:C:623:GLU:HB3	1:C:645:PRO:HG2	1.77	0.67
1:B:681:LYS:HD2	1:B:682:TYR:CZ	2.31	0.66
1:B:395:GLU:CB	1:B:423:ARG:HD3	2.26	0.66
1:A:681:LYS:HD2	1:A:682:TYR:CZ	2.30	0.66
1:A:361:ASN:ND2	1:B:361:ASN:ND2	2.37	0.66
1:B:191:GLN:O	1:B:197:ARG:HD2	1.96	0.66
1:B:202:THR:CG2	1:B:203:ALA:N	2.59	0.66
1:A:680:ALA:HA	1:A:683:TYR:CD1	2.31	0.66
1:B:395:GLU:OE1	1:B:423:ARG:NH1	2.29	0.65
1:B:399:ASN:C	1:B:400:CYS:SG	2.74	0.65
1:C:537:LEU:HD23	1:C:570:PHE:CG	2.31	0.65
1:B:610:LYS:O	1:B:632:LYS:HE2	1.97	0.65
1:C:631:TRP:CE2	1:C:641:TRP:HB3	2.32	0.64
1:A:475:ASP:O	1:A:479:THR:HB	1.97	0.64
1:A:527:LYS:H	1:A:527:LYS:HD3	1.62	0.64
1:B:225:TYR:HA	1:B:228:GLU:HG3	1.78	0.64
1:C:582:LYS:HA	1:C:586:LYS:HG2	1.80	0.64
1:C:340:GLN:HG2	1:C:482:VAL:HG13	1.80	0.64
1:B:599:ASN:HD22	1:B:602:GLN:H	1.44	0.64
1:A:275:LEU:O	1:A:278:TRP:HB2	1.96	0.64
1:A:202:THR:HG22	1:A:203:ALA:H	1.62	0.64
1:B:275:LEU:O	1:B:278:TRP:HB2	1.97	0.64
1:B:523:ARG:HH11	1:B:523:ARG:HA	1.62	0.64
1:A:610:LYS:O	1:A:632:LYS:HE2	1.98	0.64
1:B:186:PHE:O	1:B:189:LEU:HG	1.97	0.64
1:A:225:TYR:HA	1:A:228:GLU:HG3	1.80	0.63
1:A:556:SER:CA	1:A:560:ARG:HB3	2.28	0.63
1:B:475:ASP:O	1:B:479:THR:HB	1.98	0.63
1:C:202:THR:CG2	1:C:203:ALA:N	2.60	0.63
1:C:186:PHE:O	1:C:189:LEU:HG	1.97	0.63
1:A:186:PHE:O	1:A:189:LEU:HG	1.99	0.63
1:A:140:LYS:HZ2	1:A:140:LYS:H	1.46	0.63
1:A:340:GLN:HG2	1:A:482:VAL:HG13	1.81	0.63
1:B:340:GLN:HG2	1:B:482:VAL:HG13	1.79	0.63
1:A:537:LEU:HD23	1:A:570:PHE:CG	2.34	0.63
1:B:587:PRO:O	1:B:591:ASP:HB2	1.98	0.63
1:C:512:ASN:HA	1:C:525:LEU:HD22	1.81	0.63
1:C:372:THR:HG23	1:C:443:LEU:HD23	1.79	0.63
1:C:325:SER:O	1:C:329:THR:OG1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LEU:HA	1:B:533:LEU:HD12	1.81	0.63
1:A:319:THR:O	1:A:323:ILE:HG23	1.99	0.63
1:C:620:SER:HB3	1:C:622:SER:HB2	1.80	0.63
1:C:395:GLU:CB	1:C:423:ARG:HD3	2.29	0.63
1:C:286:ILE:HG13	1:C:323:ILE:HD11	1.80	0.62
1:B:185:GLN:HE21	1:B:185:GLN:HA	1.65	0.62
1:B:374:ILE:HG22	1:B:441:THR:HG23	1.80	0.62
1:B:436:THR:O	1:B:481:THR:HG21	1.99	0.62
1:B:631:TRP:CE2	1:B:641:TRP:HB3	2.35	0.62
1:B:142:LEU:HD13	1:B:145:ASN:HD22	1.65	0.62
1:A:374:ILE:HG22	1:A:441:THR:HG23	1.81	0.62
1:C:668:TYR:CB	1:C:674:PRO:HA	2.14	0.62
1:B:385:ASN:HD22	1:B:385:ASN:H	1.39	0.62
1:B:413:SER:HB3	1:B:415:HIS:CE1	2.33	0.62
1:B:372:THR:HG23	1:B:443:LEU:HD23	1.81	0.62
1:B:521:SER:OG	1:B:590:ASN:HB3	1.98	0.62
1:B:537:LEU:HD23	1:B:570:PHE:CG	2.34	0.61
1:A:413:SER:HB3	1:A:415:HIS:CE1	2.35	0.61
1:A:395:GLU:CB	1:A:423:ARG:HD3	2.29	0.61
1:A:372:THR:HG23	1:A:443:LEU:HD23	1.81	0.61
1:C:305:ILE:O	1:C:306:PRO:C	2.39	0.61
1:C:530:LEU:HA	1:C:533:LEU:HD12	1.81	0.61
1:B:680:ALA:HA	1:B:683:TYR:CD1	2.36	0.61
1:C:223:GLN:O	1:C:227:VAL:HG23	2.00	0.61
1:C:436:THR:O	1:C:481:THR:HG21	2.01	0.61
1:B:556:SER:CA	1:B:560:ARG:HB3	2.30	0.61
1:C:556:SER:CA	1:C:560:ARG:HB3	2.29	0.61
1:B:175:GLN:HA	1:B:175:GLN:HE21	1.66	0.60
1:C:399:ASN:C	1:C:400:CYS:SG	2.76	0.60
1:A:631:TRP:CE2	1:A:641:TRP:HB3	2.36	0.60
1:B:325:SER:O	1:B:329:THR:OG1	2.18	0.60
1:A:276:GLN:HE21	1:A:355:LEU:HA	1.66	0.60
1:B:293:ILE:O	1:B:297:GLU:HG2	2.01	0.60
1:B:523:ARG:HB3	1:B:589:TRP:CE3	2.37	0.60
1:A:305:ILE:O	1:A:306:PRO:C	2.37	0.60
1:A:399:ASN:CB	1:A:419:MET:HG2	2.32	0.60
1:A:436:THR:O	1:A:481:THR:HG21	2.01	0.60
1:C:175:GLN:HE21	1:C:175:GLN:HA	1.67	0.60
1:C:599:ASN:HD22	1:C:602:GLN:H	1.50	0.60
1:C:559:ASN:OD1	1:C:571:TRP:HB3	2.02	0.60
1:A:339:PRO:HG2	1:A:348:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:THR:HG22	1:C:203:ALA:H	1.66	0.60
1:A:395:GLU:OE1	1:A:423:ARG:NH1	2.34	0.60
1:B:640:LEU:HD23	1:B:641:TRP:H	1.67	0.59
1:C:502:VAL:HG13	1:C:506:GLN:HG3	1.84	0.59
1:A:521:SER:OG	1:A:590:ASN:HB3	2.02	0.59
1:C:681:LYS:HD2	1:C:682:TYR:CE1	2.37	0.59
1:B:339:PRO:HG2	1:B:348:PHE:HB2	1.84	0.59
1:B:375:SER:HB3	1:B:393:SER:HB2	1.85	0.59
1:A:512:ASN:HA	1:A:525:LEU:HD22	1.83	0.59
1:C:413:SER:HB3	1:C:415:HIS:CE1	2.37	0.59
1:C:521:SER:OG	1:C:590:ASN:HB3	2.03	0.59
1:C:475:ASP:O	1:C:479:THR:HB	2.02	0.59
1:C:293:ILE:O	1:C:297:GLU:HG2	2.02	0.59
1:A:405:TYR:CE2	1:A:407:GLN:HA	2.38	0.59
1:A:502:VAL:HG13	1:A:506:GLN:HG3	1.85	0.58
1:B:305:ILE:O	1:B:306:PRO:C	2.42	0.58
1:A:530:LEU:HA	1:A:533:LEU:HD12	1.85	0.58
1:A:651:PHE:CE2	1:A:656:LEU:HB2	2.38	0.58
1:C:191:GLN:O	1:C:197:ARG:HD2	2.04	0.58
1:B:527:LYS:HD3	1:B:527:LYS:H	1.68	0.58
1:B:566:TRP:HB3	1:B:568:TYR:CE1	2.38	0.58
1:C:337:GLN:HE21	1:C:338:PRO:HD2	1.67	0.58
1:A:142:LEU:HD13	1:A:145:ASN:HD22	1.69	0.58
1:A:286:ILE:C	1:A:286:ILE:HD13	2.25	0.57
1:B:559:ASN:OD1	1:B:571:TRP:HB3	2.04	0.57
1:B:576:GLY:O	1:B:580:VAL:HG22	2.04	0.57
1:B:202:THR:HG22	1:B:203:ALA:H	1.69	0.57
1:A:640:LEU:HD23	1:A:641:TRP:H	1.68	0.57
1:B:502:VAL:HG13	1:B:506:GLN:HG3	1.87	0.57
1:A:576:GLY:O	1:A:580:VAL:HG22	2.04	0.57
1:A:584:HIS:HE1	1:A:648:THR:OG1	1.87	0.57
1:A:286:ILE:HG13	1:A:323:ILE:HD11	1.85	0.57
1:C:395:GLU:OE1	1:C:423:ARG:NH1	2.37	0.57
1:C:504:TRP:NE1	1:C:508:CYS:SG	2.77	0.57
1:B:259:GLN:HB2	1:B:269:GLU:HG2	1.87	0.57
1:C:319:THR:O	1:C:323:ILE:HG23	2.04	0.57
1:B:397:LEU:HA	1:B:420:SER:O	2.04	0.57
1:B:378:GLN:HE22	1:B:393:SER:N	1.99	0.57
1:C:527:LYS:H	1:C:527:LYS:CD	2.17	0.57
1:A:337:GLN:HE21	1:A:338:PRO:HD2	1.70	0.57
1:A:293:ILE:O	1:A:297:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:PRO:HG2	1:A:673:ARG:NH1	2.20	0.57
1:A:599:ASN:HD22	1:A:602:GLN:H	1.52	0.57
1:C:159:GLU:HA	1:C:162:LEU:HB2	1.87	0.57
1:A:566:TRP:HB3	1:A:568:TYR:CE1	2.40	0.56
1:A:240:LEU:HD22	1:A:285:ILE:CD1	2.35	0.56
1:C:640:LEU:HD23	1:C:641:TRP:H	1.70	0.56
1:C:584:HIS:HE1	1:C:648:THR:OG1	1.87	0.56
1:B:518:GLU:HG2	1:B:578:MET:HB3	1.86	0.56
1:A:174:ILE:HA	1:A:177:GLN:NE2	2.19	0.56
1:B:516:LYS:HD3	1:B:524:GLY:CA	2.35	0.56
1:B:405:TYR:CE2	1:B:407:GLN:HA	2.41	0.56
1:A:191:GLN:O	1:A:197:ARG:HD2	2.06	0.56
1:A:515:PHE:O	1:A:519:VAL:HG22	2.06	0.56
1:A:312:MET:O	1:A:316:VAL:HB	2.05	0.56
1:A:337:GLN:HE21	1:A:463:SER:HB2	1.71	0.56
1:A:685:PRO:O	1:A:686:VAL:HG22	2.06	0.56
1:C:523:ARG:HA	1:C:523:ARG:HH11	1.72	0.55
1:C:140:LYS:H	1:C:140:LYS:HZ2	1.54	0.55
1:B:340:GLN:HG2	1:B:482:VAL:CG1	2.36	0.55
1:A:594:ILE:O	1:A:594:ILE:HG13	2.05	0.55
1:A:202:THR:HG22	1:A:203:ALA:N	2.21	0.55
1:C:342:LEU:HD11	1:C:466:VAL:HG11	1.88	0.55
1:C:566:TRP:HB3	1:C:568:TYR:CE1	2.42	0.55
1:C:142:LEU:HD13	1:C:145:ASN:HD22	1.70	0.55
1:A:375:SER:HB3	1:A:393:SER:HB2	1.88	0.55
1:A:671:PRO:HG2	1:A:673:ARG:HH12	1.72	0.55
1:A:633:PHE:H	1:A:641:TRP:HD1	1.55	0.55
1:C:185:GLN:HE21	1:C:185:GLN:HA	1.71	0.55
1:C:516:LYS:HD3	1:C:524:GLY:CA	2.35	0.55
1:A:518:GLU:HG2	1:A:578:MET:HB3	1.89	0.55
1:B:319:THR:O	1:B:323:ILE:HG23	2.07	0.55
1:B:579:GLU:O	1:B:583:LYS:HB2	2.07	0.55
1:B:584:HIS:HE1	1:B:648:THR:OG1	1.90	0.55
1:B:312:MET:O	1:B:316:VAL:HB	2.07	0.55
1:A:282:LEU:O	1:A:286:ILE:HG22	2.07	0.55
1:A:681:LYS:HD2	1:A:682:TYR:CE1	2.42	0.55
1:A:340:GLN:HG2	1:A:482:VAL:CG1	2.36	0.55
1:A:579:GLU:O	1:A:583:LYS:HB2	2.07	0.55
1:A:185:GLN:HA	1:A:185:GLN:HE21	1.71	0.55
1:C:399:ASN:CB	1:C:419:MET:HG2	2.35	0.54
1:B:607:LEU:CD2	1:B:614:THR:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ARG:HB3	1:A:589:TRP:CE3	2.42	0.54
1:B:640:LEU:CD2	1:B:641:TRP:H	2.20	0.54
1:B:140:LYS:H	1:B:140:LYS:NZ	2.04	0.54
1:B:191:GLN:C	1:B:197:ARG:HH11	2.10	0.54
1:B:174:ILE:HA	1:B:177:GLN:NE2	2.23	0.54
1:A:337:GLN:NE2	1:A:463:SER:HB2	2.22	0.54
1:B:140:LYS:HZ2	1:B:140:LYS:H	1.55	0.54
1:C:286:ILE:HD13	1:C:286:ILE:C	2.28	0.54
1:B:259:GLN:HA	1:B:269:GLU:HG3	1.89	0.54
1:C:276:GLN:HE21	1:C:355:LEU:HA	1.72	0.54
1:C:576:GLY:O	1:C:580:VAL:HG22	2.07	0.54
1:C:668:TYR:HB2	1:C:673:ARG:O	2.08	0.54
1:B:395:GLU:HB3	1:B:423:ARG:HD3	1.90	0.54
1:A:636:PRO:HB2	1:A:640:LEU:HG	1.90	0.54
1:C:507:LEU:HD22	1:C:511:LEU:HG	1.89	0.54
1:B:276:GLN:HE21	1:B:355:LEU:HA	1.71	0.54
1:B:633:PHE:H	1:B:641:TRP:HD1	1.55	0.54
1:C:586:LYS:HB2	1:C:587:PRO:HD3	1.89	0.54
1:B:202:THR:HG22	1:B:203:ALA:N	2.23	0.54
1:C:174:ILE:HA	1:C:177:GLN:NE2	2.22	0.54
1:B:165:LEU:HD11	1:B:226:ARG:HD2	1.89	0.54
1:B:185:GLN:NE2	1:B:185:GLN:HA	2.22	0.54
1:A:527:LYS:H	1:A:527:LYS:CD	2.20	0.54
1:B:681:LYS:HD2	1:B:682:TYR:CE1	2.44	0.53
1:C:493:ARG:HB2	1:C:497:ALA:HB3	1.90	0.53
1:C:373:ILE:HD13	1:C:421:LEU:HD11	1.90	0.53
1:C:202:THR:HG22	1:C:203:ALA:N	2.23	0.53
1:C:508:CYS:SG	1:C:530:LEU:HD22	2.49	0.53
1:B:512:ASN:HA	1:B:525:LEU:HD22	1.90	0.53
1:A:165:LEU:HD11	1:A:226:ARG:HD2	1.90	0.53
1:B:286:ILE:HD13	1:B:286:ILE:C	2.28	0.53
1:A:516:LYS:HD3	1:A:524:GLY:CA	2.39	0.53
1:C:339:PRO:HG2	1:C:348:PHE:HB2	1.89	0.53
1:C:671:PRO:HG2	1:C:673:ARG:NH1	2.24	0.53
1:C:165:LEU:HD11	1:C:226:ARG:HD2	1.91	0.53
1:A:233:HIS:O	1:A:234:GLN:C	2.47	0.53
1:B:399:ASN:CB	1:B:419:MET:HG2	2.37	0.53
1:B:685:PRO:O	1:B:686:VAL:HG22	2.09	0.53
1:B:636:PRO:HB2	1:B:640:LEU:HG	1.91	0.52
1:C:340:GLN:HG3	1:C:465:PRO:O	2.10	0.52
1:C:312:MET:O	1:C:316:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:ARG:HH21	1:C:618:ARG:HG2	1.74	0.52
1:B:586:LYS:HB2	1:B:587:PRO:HD3	1.90	0.52
1:A:337:GLN:NE2	1:A:338:PRO:HD2	2.24	0.52
1:A:259:GLN:HB2	1:A:269:GLU:HG2	1.92	0.52
1:C:405:TYR:CE2	1:C:407:GLN:HA	2.44	0.52
1:B:515:PHE:O	1:B:519:VAL:HG22	2.09	0.52
1:C:515:PHE:O	1:C:519:VAL:HG22	2.08	0.52
1:A:403:MET:HB3	1:A:412:LEU:CD2	2.39	0.52
1:B:159:GLU:HA	1:B:162:LEU:HB2	1.92	0.52
1:C:337:GLN:NE2	1:C:338:PRO:HD2	2.25	0.52
1:C:337:GLN:HE21	1:C:463:SER:HB2	1.75	0.52
1:C:152:ARG:HH21	1:C:285:ILE:HB	1.75	0.52
1:C:375:SER:HB3	1:C:393:SER:HB2	1.92	0.52
1:A:512:ASN:C	1:A:512:ASN:HD22	2.13	0.52
1:B:337:GLN:HE21	1:B:338:PRO:HD2	1.75	0.52
1:C:340:GLN:HG2	1:C:482:VAL:CG1	2.40	0.52
1:A:607:LEU:CD2	1:A:614:THR:HG22	2.39	0.52
1:B:447:GLN:O	1:B:448:PHE:HB3	2.09	0.52
1:A:507:LEU:HD22	1:A:511:LEU:HG	1.92	0.52
1:A:599:ASN:C	1:A:599:ASN:HD22	2.13	0.51
1:A:504:TRP:NE1	1:A:508:CYS:SG	2.83	0.51
1:B:493:ARG:HB2	1:B:497:ALA:HB3	1.92	0.51
1:C:140:LYS:H	1:C:140:LYS:NZ	2.07	0.51
1:C:579:GLU:O	1:C:583:LYS:HB2	2.10	0.51
1:C:633:PHE:H	1:C:641:TRP:HD1	1.58	0.51
1:C:518:GLU:HG2	1:C:578:MET:HB3	1.92	0.51
1:C:337:GLN:NE2	1:C:463:SER:HB2	2.26	0.51
1:A:342:LEU:HD11	1:A:466:VAL:HG11	1.92	0.51
1:B:563:LEU:HD11	1:B:570:PHE:HA	1.93	0.51
1:C:685:PRO:O	1:C:686:VAL:HG22	2.11	0.51
1:B:259:GLN:CA	1:B:269:GLU:HG3	2.41	0.51
1:B:373:ILE:HD13	1:B:421:LEU:HD11	1.92	0.51
1:A:399:ASN:C	1:A:400:CYS:SG	2.90	0.51
1:A:573:TRP:HE1	1:A:621:ASP:HA	1.76	0.51
1:A:678:VAL:O	1:A:678:VAL:HG12	2.11	0.51
1:C:523:ARG:HB3	1:C:589:TRP:CE3	2.46	0.51
1:B:651:PHE:CE2	1:B:656:LEU:HB2	2.45	0.51
1:C:678:VAL:HG12	1:C:678:VAL:O	2.11	0.51
1:B:670:PHE:CB	1:B:671:PRO:HD3	2.36	0.50
1:B:537:LEU:HB2	1:B:570:PHE:CE2	2.46	0.50
1:B:527:LYS:H	1:B:527:LYS:CD	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ALA:HA	1:B:416:PHE:O	2.11	0.50
1:C:141:HIS:C	1:C:143:GLN:H	2.14	0.50
1:C:150:GLU:O	1:C:154:ILE:HG22	2.11	0.50
1:A:159:GLU:HA	1:A:162:LEU:HB2	1.93	0.50
1:C:668:TYR:CB	1:C:673:ARG:O	2.59	0.50
1:B:141:HIS:C	1:B:143:GLN:H	2.13	0.50
1:C:254:GLN:HG2	1:C:258:ARG:HH21	1.77	0.50
1:C:191:GLN:C	1:C:197:ARG:HH11	2.15	0.50
1:C:594:ILE:O	1:C:594:ILE:HG13	2.11	0.50
1:B:618:ARG:HH21	1:B:618:ARG:HG2	1.76	0.50
1:B:675:LYS:O	1:B:676:ASP:C	2.50	0.50
1:A:170:GLU:HG3	1:B:418:ASN:ND2	2.23	0.50
1:A:484:TRP:HZ3	1:A:499:PRO:O	1.95	0.50
1:A:465:PRO:HG2	1:A:485:ASP:OD1	2.12	0.50
1:C:449:SER:HA	1:C:456:VAL:HA	1.94	0.50
1:C:397:LEU:HA	1:C:420:SER:O	2.12	0.50
1:A:231:GLU:HA	1:A:234:GLN:HB2	1.94	0.50
1:A:244:GLN:HE22	1:A:327:LEU:HG	1.76	0.50
1:C:285:ILE:HD13	1:C:285:ILE:C	2.32	0.49
1:A:340:GLN:HG3	1:A:465:PRO:O	2.11	0.49
1:B:512:ASN:HD22	1:B:512:ASN:C	2.15	0.49
1:A:140:LYS:H	1:A:140:LYS:NZ	2.09	0.49
1:C:282:LEU:O	1:C:286:ILE:HG22	2.13	0.49
1:A:586:LYS:HB2	1:A:587:PRO:HD3	1.95	0.49
1:C:594:ILE:HD11	1:C:619:PHE:CE2	2.47	0.49
1:C:245:THR:HG23	1:C:249:ASP:OD2	2.12	0.49
1:C:523:ARG:N	1:C:523:ARG:HD2	2.26	0.49
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.26	0.49
1:A:327:LEU:HD22	1:A:356:VAL:HG11	1.93	0.49
1:B:658:ASP:OD1	1:B:684:THR:HG22	2.12	0.49
1:C:636:PRO:HB2	1:C:640:LEU:HG	1.94	0.49
1:A:259:GLN:CA	1:A:269:GLU:HG3	2.42	0.49
1:A:373:ILE:HD13	1:A:421:LEU:HD11	1.92	0.49
1:B:231:GLU:HA	1:B:234:GLN:HB2	1.94	0.49
1:B:150:GLU:O	1:B:154:ILE:HG22	2.12	0.49
1:C:185:GLN:NE2	1:C:185:GLN:HA	2.27	0.49
1:C:231:GLU:HA	1:C:234:GLN:HB2	1.95	0.49
1:C:259:GLN:HA	1:C:269:GLU:HG3	1.94	0.49
1:B:449:SER:HA	1:B:456:VAL:HA	1.94	0.49
1:B:599:ASN:HD22	1:B:599:ASN:C	2.16	0.49
1:A:260:GLN:HG3	1:A:464:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLN:HG3	1:B:464:LEU:HD22	1.95	0.49
1:C:403:MET:HB3	1:C:412:LEU:CD2	2.43	0.49
1:A:141:HIS:C	1:A:143:GLN:H	2.15	0.49
1:C:512:ASN:C	1:C:512:ASN:HD22	2.16	0.49
1:B:223:GLN:O	1:B:227:VAL:HG23	2.13	0.49
1:C:599:ASN:C	1:C:599:ASN:HD22	2.17	0.48
1:C:537:LEU:HB2	1:C:570:PHE:CE2	2.48	0.48
1:A:290:ARG:HH12	1:A:455:LEU:HD22	1.78	0.48
1:B:152:ARG:HH21	1:B:285:ILE:HB	1.78	0.48
1:C:527:LYS:HD3	1:C:527:LYS:N	2.27	0.48
1:B:342:LEU:HD11	1:B:466:VAL:HG11	1.95	0.48
1:A:259:GLN:HA	1:A:269:GLU:HG3	1.94	0.48
1:B:141:HIS:O	1:B:144:ILE:HG12	2.13	0.48
1:B:507:LEU:HD22	1:B:511:LEU:HG	1.94	0.48
1:C:241:ARG:NH1	1:C:244:GLN:HG2	2.28	0.48
1:A:397:LEU:HA	1:A:420:SER:O	2.13	0.48
1:A:670:PHE:CB	1:A:671:PRO:HD3	2.38	0.48
1:C:247:ILE:O	1:C:251:GLU:HB2	2.13	0.48
1:A:493:ARG:HB2	1:A:497:ALA:HB3	1.96	0.48
1:A:527:LYS:N	1:A:527:LYS:HD3	2.27	0.48
1:B:340:GLN:HG3	1:B:465:PRO:O	2.13	0.48
1:C:141:HIS:O	1:C:144:ILE:HG12	2.13	0.48
1:B:508:CYS:SG	1:B:530:LEU:HD22	2.54	0.48
1:B:259:GLN:O	1:B:262:ALA:HB3	2.14	0.48
1:B:327:LEU:HD22	1:B:356:VAL:HG11	1.95	0.48
1:B:671:PRO:HG2	1:B:673:ARG:NH1	2.29	0.48
1:B:233:HIS:HA	1:B:236:THR:HG23	1.96	0.48
1:A:285:ILE:HD13	1:A:285:ILE:C	2.34	0.48
1:C:395:GLU:HB3	1:C:423:ARG:HD3	1.94	0.48
1:B:162:LEU:HD23	1:B:229:LEU:HD11	1.95	0.48
1:C:365:ASN:HA	1:C:366:PRO:HD2	1.62	0.48
1:A:618:ARG:HH21	1:A:618:ARG:HG2	1.78	0.48
1:C:563:LEU:HD11	1:C:570:PHE:HA	1.95	0.48
1:B:247:ILE:HD12	1:B:278:TRP:HB3	1.95	0.48
1:C:372:THR:CG2	1:C:443:LEU:HD23	2.44	0.47
1:A:395:GLU:HB3	1:A:423:ARG:HD3	1.96	0.47
1:C:629:ILE:HB	1:C:643:LEU:CD2	2.44	0.47
1:A:675:LYS:O	1:A:676:ASP:C	2.52	0.47
1:A:378:GLN:HE22	1:A:393:SER:N	2.01	0.47
1:B:537:LEU:HD11	1:B:553:VAL:HG13	1.96	0.47
1:C:233:HIS:HA	1:C:236:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:NH1	1:B:244:GLN:HG2	2.30	0.47
1:A:516:LYS:HD3	1:A:524:GLY:HA3	1.96	0.47
1:C:378:GLN:HE22	1:C:393:SER:N	2.01	0.47
1:A:337:GLN:HG2	1:A:464:LEU:HD12	1.97	0.47
1:C:259:GLN:HB2	1:C:269:GLU:HG2	1.97	0.47
1:A:361:ASN:HD21	1:B:364:MET:HG3	1.74	0.47
1:B:337:GLN:HE21	1:B:463:SER:HB2	1.79	0.47
1:C:233:HIS:O	1:C:234:GLN:C	2.52	0.47
1:A:382:LEU:HD23	1:A:387:ASN:OD1	2.14	0.47
1:C:488:PHE:HB3	1:C:499:PRO:HG2	1.97	0.47
1:C:151:LEU:HD13	1:C:240:LEU:HD13	1.97	0.47
1:B:384:LYS:O	1:B:386:GLU:N	2.47	0.47
1:B:504:TRP:NE1	1:B:508:CYS:SG	2.87	0.47
1:C:669:VAL:HG22	1:C:673:ARG:HG3	1.96	0.47
1:A:152:ARG:HH21	1:A:285:ILE:HB	1.80	0.47
1:A:418:ASN:ND2	1:B:170:GLU:HG3	2.24	0.47
1:B:413:SER:CB	1:B:415:HIS:CE1	2.96	0.47
1:A:259:GLN:O	1:A:262:ALA:HB3	2.15	0.47
1:C:259:GLN:O	1:C:262:ALA:HB3	2.14	0.47
1:B:573:TRP:HE1	1:B:621:ASP:HA	1.80	0.47
1:C:275:LEU:O	1:C:278:TRP:HB2	2.15	0.47
1:C:340:GLN:O	1:C:466:VAL:HA	2.15	0.47
1:A:670:PHE:HB3	1:A:671:PRO:CD	2.39	0.46
1:B:282:LEU:O	1:B:286:ILE:HG22	2.15	0.46
1:A:191:GLN:C	1:A:197:ARG:HH11	2.17	0.46
1:A:678:VAL:CG1	1:A:678:VAL:O	2.63	0.46
1:A:349:ALA:HA	1:A:416:PHE:O	2.16	0.46
1:B:629:ILE:HB	1:B:643:LEU:CD2	2.44	0.46
1:A:540:ILE:HA	1:A:540:ILE:HD12	1.84	0.46
1:B:342:LEU:O	1:B:468:VAL:HA	2.15	0.46
1:A:413:SER:CB	1:A:415:HIS:CE1	2.98	0.46
1:A:617:LEU:HB3	1:A:627:ILE:HG21	1.98	0.46
1:A:594:ILE:HD11	1:A:619:PHE:CE2	2.51	0.46
1:C:516:LYS:HD3	1:C:524:GLY:HA3	1.96	0.46
1:B:254:GLN:HG2	1:B:258:ARG:HH21	1.81	0.46
1:A:523:ARG:N	1:A:523:ARG:HD2	2.29	0.46
1:A:247:ILE:HD12	1:A:278:TRP:HB3	1.97	0.46
1:B:533:LEU:O	1:B:536:LYS:N	2.48	0.46
1:A:294:ARG:NH1	1:A:454:GLU:OE2	2.49	0.46
1:B:365:ASN:HA	1:B:366:PRO:HD2	1.60	0.46
1:A:519:VAL:O	1:A:586:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:HIS:O	1:B:234:GLN:C	2.53	0.46
1:A:629:ILE:HB	1:A:643:LEU:CD2	2.45	0.46
1:A:640:LEU:CD2	1:A:641:TRP:H	2.29	0.46
1:C:465:PRO:HG2	1:C:485:ASP:OD1	2.15	0.46
1:B:363:HIS:N	1:B:363:HIS:CD2	2.84	0.46
1:C:573:TRP:HE1	1:C:621:ASP:HA	1.80	0.46
1:C:640:LEU:CD2	1:C:641:TRP:H	2.29	0.46
1:B:337:GLN:NE2	1:B:338:PRO:HD2	2.31	0.46
1:A:141:HIS:O	1:A:144:ILE:HG12	2.15	0.46
1:C:670:PHE:HB3	1:C:671:PRO:CD	2.42	0.46
1:A:364:MET:HG3	1:B:361:ASN:HD21	1.70	0.46
1:B:471:HIS:NE2	1:B:474:GLN:HB2	2.31	0.46
1:A:294:ARG:HA	1:A:297:GLU:HG2	1.98	0.46
1:A:259:GLN:HB2	1:A:269:GLU:CG	2.46	0.46
1:A:658:ASP:OD1	1:A:684:THR:HG22	2.16	0.45
1:C:651:PHE:CE2	1:C:656:LEU:HB2	2.51	0.45
1:C:382:LEU:HD23	1:C:387:ASN:OD1	2.16	0.45
1:B:632:LYS:HG3	1:B:640:LEU:HD11	1.99	0.45
1:C:453:ASN:O	1:C:454:GLU:C	2.54	0.45
1:A:223:GLN:O	1:A:227:VAL:HG23	2.16	0.45
1:C:349:ALA:HA	1:C:416:PHE:O	2.15	0.45
1:B:516:LYS:HD3	1:B:524:GLY:HA3	1.98	0.45
1:B:363:HIS:H	1:B:363:HIS:CD2	2.35	0.45
1:A:388:THR:O	1:A:390:ASN:N	2.50	0.45
1:C:181:ARG:C	1:C:183:GLN:H	2.20	0.45
1:B:523:ARG:HD2	1:B:523:ARG:N	2.32	0.45
1:B:340:GLN:O	1:B:466:VAL:HA	2.17	0.45
1:B:337:GLN:HE22	1:B:463:SER:HA	1.82	0.45
1:A:531:VAL:O	1:A:532:PHE:C	2.53	0.45
1:B:382:LEU:HD23	1:B:387:ASN:OD1	2.17	0.45
1:B:465:PRO:HG2	1:B:485:ASP:CG	2.37	0.45
1:B:527:LYS:N	1:B:527:LYS:HD3	2.31	0.45
1:A:183:GLN:C	1:A:185:GLN:H	2.18	0.45
1:A:471:HIS:NE2	1:A:474:GLN:HB2	2.31	0.45
1:C:384:LYS:O	1:C:386:GLU:N	2.49	0.45
1:B:474:GLN:HG2	1:B:477:ASN:HD22	1.82	0.45
1:A:537:LEU:HB2	1:A:570:PHE:CE2	2.51	0.45
1:B:537:LEU:HB2	1:B:570:PHE:CD2	2.51	0.45
1:A:216:GLN:HE22	1:C:686:VAL:HG13	1.82	0.45
1:C:259:GLN:CA	1:C:269:GLU:HG3	2.46	0.45
1:B:285:ILE:HD13	1:B:285:ILE:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HD22	1:C:356:VAL:HG11	1.97	0.45
1:C:288:GLN:O	1:C:290:ARG:N	2.50	0.45
1:B:668:TYR:HB2	1:B:673:ARG:O	2.16	0.45
1:C:363:HIS:O	1:C:366:PRO:HD3	2.17	0.45
1:B:403:MET:HB3	1:B:412:LEU:CD2	2.47	0.45
1:C:556:SER:HA	1:C:560:ARG:CB	2.44	0.45
1:A:289:ASN:O	1:A:293:ILE:HG23	2.17	0.45
1:A:449:SER:HA	1:A:456:VAL:HA	1.98	0.45
1:A:556:SER:HA	1:A:560:ARG:CB	2.44	0.44
1:A:563:LEU:HD11	1:A:570:PHE:HA	1.99	0.44
1:A:363:HIS:CD2	1:A:363:HIS:N	2.85	0.44
1:A:384:LYS:O	1:A:386:GLU:N	2.51	0.44
1:C:474:GLN:HG2	1:C:477:ASN:HD22	1.82	0.44
1:C:670:PHE:O	1:C:671:PRO:C	2.55	0.44
1:A:325:SER:O	1:A:329:THR:OG1	2.25	0.44
1:B:224:GLN:O	1:B:228:GLU:HG2	2.18	0.44
1:B:465:PRO:HG2	1:B:485:ASP:OD1	2.17	0.44
1:C:484:TRP:HZ3	1:C:499:PRO:O	2.00	0.44
1:B:594:ILE:O	1:B:594:ILE:HG13	2.16	0.44
1:B:290:ARG:HH12	1:B:455:LEU:HD22	1.82	0.44
1:A:286:ILE:HD13	1:A:286:ILE:O	2.16	0.44
1:C:658:ASP:OD1	1:C:684:THR:HG22	2.17	0.44
1:B:678:VAL:O	1:B:678:VAL:HG12	2.17	0.44
1:B:670:PHE:CB	1:B:671:PRO:CD	2.96	0.44
1:B:413:SER:CB	1:B:415:HIS:HE1	2.30	0.44
1:A:478:ALA:O	1:A:481:THR:HG23	2.18	0.44
1:C:260:GLN:HG3	1:C:464:LEU:HD22	1.98	0.44
1:C:618:ARG:HG2	1:C:618:ARG:NH2	2.32	0.44
1:B:240:LEU:HD22	1:B:285:ILE:CD1	2.47	0.44
1:B:175:GLN:C	1:B:177:GLN:N	2.71	0.44
1:C:175:GLN:C	1:C:177:GLN:N	2.70	0.44
1:C:678:VAL:O	1:C:678:VAL:CG1	2.65	0.44
1:A:615:PHE:HB2	1:A:630:ALA:O	2.17	0.44
1:B:193:ASN:CB	1:B:194:PRO:CD	2.94	0.44
1:A:193:ASN:CB	1:A:194:PRO:CD	2.94	0.44
1:C:251:GLU:CA	1:C:251:GLU:OE2	2.59	0.44
1:C:140:LYS:HD3	1:C:140:LYS:N	2.33	0.44
1:B:395:GLU:HB2	1:B:423:ARG:HB2	1.99	0.44
1:C:376:GLU:HG3	1:C:496:PHE:HD1	1.83	0.44
1:B:372:THR:CG2	1:B:443:LEU:HD23	2.48	0.44
1:B:363:HIS:O	1:B:366:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLN:O	1:C:448:PHE:HB3	2.18	0.44
1:A:465:PRO:HG2	1:A:485:ASP:CG	2.37	0.44
1:B:337:GLN:NE2	1:B:464:LEU:H	2.16	0.44
1:B:541:SER:O	1:B:542:SER:C	2.57	0.44
1:C:226:ARG:NH2	1:C:300:CYS:HA	2.33	0.43
1:A:471:HIS:HD2	1:A:474:GLN:N	2.16	0.43
1:C:162:LEU:HD23	1:C:229:LEU:HD11	2.00	0.43
1:A:247:ILE:O	1:A:251:GLU:HB2	2.17	0.43
1:A:283:ALA:HA	1:A:286:ILE:HG22	2.00	0.43
1:C:617:LEU:HB3	1:C:627:ILE:HG21	1.99	0.43
1:B:668:TYR:CB	1:B:673:ARG:O	2.66	0.43
1:C:471:HIS:NE2	1:C:474:GLN:HB2	2.32	0.43
1:B:283:ALA:HA	1:B:286:ILE:HG22	2.00	0.43
1:A:488:PHE:HB3	1:A:499:PRO:HG2	2.00	0.43
1:C:607:LEU:CD2	1:C:614:THR:HG22	2.47	0.43
1:B:256:LYS:O	1:B:259:GLN:HB3	2.18	0.43
1:B:671:PRO:HG2	1:B:673:ARG:HH12	1.83	0.43
1:A:175:GLN:C	1:A:177:GLN:N	2.69	0.43
1:C:399:ASN:HB2	1:C:419:MET:HA	2.01	0.43
1:A:223:GLN:HE21	1:C:685:PRO:HG3	1.84	0.43
1:B:618:ARG:HG2	1:B:618:ARG:NH2	2.33	0.43
1:A:294:ARG:CZ	1:A:454:GLU:OE2	2.66	0.43
1:A:670:PHE:O	1:A:671:PRO:C	2.56	0.43
1:B:518:GLU:HG3	1:B:582:LYS:HG2	2.01	0.43
1:C:537:LEU:HD11	1:C:553:VAL:HG13	2.01	0.43
1:B:480:ALA:HB2	1:B:571:TRP:CD1	2.54	0.43
1:A:162:LEU:HD23	1:A:229:LEU:HD11	2.01	0.43
1:A:629:ILE:HD12	1:A:643:LEU:HD21	2.01	0.43
1:B:647:THR:HG21	1:B:649:ARG:HH22	1.84	0.43
1:B:376:GLU:HG3	1:B:496:PHE:HD1	1.84	0.43
1:B:484:TRP:HZ3	1:B:499:PRO:O	2.01	0.43
1:B:195:GLN:HB2	1:B:196:GLU:OE2	2.19	0.43
1:B:447:GLN:HG3	1:B:458:GLN:HB3	2.01	0.43
1:C:397:LEU:HB2	1:C:420:SER:O	2.19	0.43
1:B:594:ILE:HD11	1:B:619:PHE:CE2	2.54	0.43
1:B:488:PHE:HB3	1:B:499:PRO:HG2	2.00	0.43
1:B:453:ASN:O	1:B:454:GLU:C	2.57	0.43
1:C:413:SER:CB	1:C:415:HIS:CE1	3.01	0.42
1:A:233:HIS:C	1:A:235:LYS:N	2.71	0.42
1:A:233:HIS:HA	1:A:236:THR:HG23	2.01	0.42
1:C:537:LEU:HB2	1:C:570:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:O	1:A:468:VAL:HA	2.19	0.42
1:C:283:ALA:HA	1:C:286:ILE:HG22	2.01	0.42
1:C:337:GLN:HG2	1:C:464:LEU:HD12	1.99	0.42
1:A:376:GLU:HG3	1:A:496:PHE:HD1	1.83	0.42
1:A:471:HIS:HD2	1:A:474:GLN:HB2	1.81	0.42
1:A:372:THR:CG2	1:A:443:LEU:HD23	2.47	0.42
1:A:338:PRO:HA	1:A:339:PRO:HD2	1.82	0.42
1:C:294:ARG:CZ	1:C:454:GLU:OE2	2.67	0.42
1:A:288:GLN:O	1:A:290:ARG:N	2.52	0.42
1:A:458:GLN:HE21	1:A:458:GLN:HB3	1.68	0.42
1:A:150:GLU:O	1:A:154:ILE:HG22	2.19	0.42
1:C:670:PHE:CB	1:C:671:PRO:HD3	2.42	0.42
1:B:183:GLN:C	1:B:185:GLN:H	2.22	0.42
1:C:632:LYS:HG3	1:C:640:LEU:HD11	2.01	0.42
1:C:465:PRO:HG2	1:C:485:ASP:CG	2.39	0.42
1:C:294:ARG:NH2	1:C:454:GLU:OE2	2.51	0.42
1:A:327:LEU:HD22	1:A:356:VAL:CG1	2.49	0.42
1:B:181:ARG:C	1:B:183:GLN:H	2.23	0.42
1:A:340:GLN:O	1:A:466:VAL:HA	2.20	0.42
1:A:537:LEU:HD11	1:A:553:VAL:HG13	2.01	0.42
1:B:162:LEU:HD23	1:B:229:LEU:CD1	2.49	0.42
1:B:507:LEU:HD21	1:B:558:PHE:CE1	2.55	0.42
1:A:447:GLN:O	1:A:448:PHE:HB3	2.19	0.42
1:B:388:THR:O	1:B:390:ASN:N	2.52	0.42
1:C:631:TRP:CZ2	1:C:641:TRP:HB3	2.54	0.42
1:C:289:ASN:O	1:C:293:ILE:HG23	2.20	0.42
1:B:259:GLN:HB2	1:B:269:GLU:CG	2.49	0.42
1:A:290:ARG:O	1:A:293:ILE:HD13	2.19	0.42
1:C:142:LEU:HD13	1:C:145:ASN:ND2	2.34	0.42
1:C:333:ILE:HD13	1:C:355:LEU:HD11	2.00	0.42
1:C:388:THR:O	1:C:390:ASN:N	2.53	0.42
1:C:193:ASN:CB	1:C:194:PRO:CD	2.96	0.42
1:A:202:THR:HG23	1:A:203:ALA:N	2.32	0.42
1:B:142:LEU:HD13	1:B:145:ASN:ND2	2.32	0.42
1:A:453:ASN:O	1:A:454:GLU:C	2.58	0.42
1:B:337:GLN:NE2	1:B:463:SER:HB2	2.35	0.42
1:A:363:HIS:O	1:A:366:PRO:HD3	2.20	0.42
1:B:453:ASN:C	1:B:453:ASN:ND2	2.73	0.42
1:A:447:GLN:HG3	1:A:458:GLN:HB3	2.00	0.42
1:A:541:SER:O	1:A:542:SER:C	2.57	0.42
1:B:267:PRO:HA	1:B:268:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:PRO:HA	1:C:268:PRO:HD3	1.93	0.42
1:B:670:PHE:O	1:B:671:PRO:C	2.58	0.42
1:C:518:GLU:HG3	1:C:582:LYS:HG2	2.02	0.42
1:A:183:GLN:C	1:A:185:GLN:N	2.72	0.42
1:B:327:LEU:HD22	1:B:356:VAL:CG1	2.50	0.42
1:C:247:ILE:HD12	1:C:278:TRP:HB3	2.01	0.42
1:C:294:ARG:HA	1:C:297:GLU:HG2	2.02	0.42
1:C:233:HIS:C	1:C:235:LYS:N	2.72	0.42
1:A:618:ARG:NH2	1:A:618:ARG:HG2	2.35	0.42
1:C:540:ILE:HD12	1:C:540:ILE:HA	1.90	0.42
1:B:286:ILE:HD13	1:B:286:ILE:O	2.20	0.41
1:A:376:GLU:OE1	1:A:496:PHE:HB2	2.20	0.41
1:C:600:LYS:HE2	1:C:600:LYS:O	2.20	0.41
1:C:240:LEU:HD22	1:C:285:ILE:CD1	2.49	0.41
1:C:636:PRO:HA	1:C:641:TRP:NE1	2.35	0.41
1:B:615:PHE:HB2	1:B:630:ALA:O	2.20	0.41
1:A:365:ASN:HA	1:A:366:PRO:HD2	1.60	0.41
1:A:337:GLN:HE22	1:A:463:SER:HA	1.85	0.41
1:A:280:GLU:HB2	1:A:359:LYS:HD3	2.02	0.41
1:C:675:LYS:O	1:C:676:ASP:C	2.59	0.41
1:C:680:ALA:HA	1:C:683:TYR:CE1	2.53	0.41
1:B:505:PRO:O	1:B:508:CYS:HB2	2.20	0.41
1:A:333:ILE:HD13	1:A:355:LEU:HD11	2.03	0.41
1:C:244:GLN:HE22	1:C:327:LEU:HG	1.85	0.41
1:C:363:HIS:N	1:C:363:HIS:CD2	2.88	0.41
1:C:195:GLN:HB2	1:C:196:GLU:OE2	2.20	0.41
1:C:601:GLN:O	1:C:604:HIS:HB3	2.21	0.41
1:B:531:VAL:O	1:B:532:PHE:C	2.59	0.41
1:C:274:VAL:O	1:C:277:SER:OG	2.39	0.41
1:C:615:PHE:HB3	1:C:631:TRP:CB	2.51	0.41
1:A:142:LEU:HD13	1:A:145:ASN:ND2	2.33	0.41
1:C:321:THR:HG22	1:C:455:LEU:HD21	2.03	0.41
1:A:140:LYS:HD3	1:A:140:LYS:N	2.35	0.41
1:A:435:VAL:HA	1:A:438:GLU:OE2	2.20	0.41
1:B:140:LYS:N	1:B:140:LYS:HD3	2.36	0.41
1:B:478:ALA:O	1:B:481:THR:HG23	2.21	0.41
1:C:554:SER:HB3	1:C:557:GLN:HG3	2.03	0.41
1:C:671:PRO:HG2	1:C:673:ARG:HH12	1.84	0.41
1:B:669:VAL:HG22	1:B:673:ARG:HG3	2.02	0.41
1:B:670:PHE:HB3	1:B:671:PRO:CD	2.38	0.41
1:A:240:LEU:HD22	1:A:285:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LYS:HG3	1:A:640:LEU:HD11	2.03	0.41
1:B:615:PHE:HB3	1:B:631:TRP:CB	2.51	0.41
1:A:502:VAL:HG13	1:A:506:GLN:CG	2.49	0.41
1:C:556:SER:CB	1:C:560:ARG:HB3	2.51	0.41
1:A:537:LEU:HB2	1:A:570:PHE:CD2	2.56	0.41
1:C:395:GLU:HB2	1:C:423:ARG:HB2	2.02	0.41
1:A:395:GLU:HB2	1:A:423:ARG:HB2	2.02	0.41
1:B:276:GLN:O	1:B:277:SER:C	2.60	0.41
1:A:397:LEU:HB2	1:A:420:SER:O	2.21	0.41
1:C:361:ASN:OD1	1:C:361:ASN:N	2.38	0.41
1:B:183:GLN:HE21	1:B:208:GLN:CD	2.24	0.41
1:B:244:GLN:HE22	1:B:327:LEU:HG	1.86	0.41
1:B:573:TRP:CZ3	1:B:577:VAL:HG21	2.56	0.41
1:A:292:GLN:HE21	1:A:292:GLN:HB3	1.70	0.41
1:A:353:ARG:NH1	1:A:411:THR:HG22	2.36	0.41
1:A:512:ASN:C	1:A:512:ASN:ND2	2.74	0.40
1:B:470:VAL:O	1:B:470:VAL:HG13	2.21	0.40
1:A:361:ASN:OD1	1:A:361:ASN:N	2.40	0.40
1:B:378:GLN:CD	1:B:393:SER:H	2.22	0.40
1:B:240:LEU:HD22	1:B:285:ILE:HD13	2.04	0.40
1:B:471:HIS:HD2	1:B:474:GLN:N	2.20	0.40
1:A:363:HIS:H	1:A:363:HIS:CD2	2.39	0.40
1:B:678:VAL:CG1	1:B:678:VAL:O	2.69	0.40
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.91	0.40
1:C:291:GLN:HE21	1:C:291:GLN:HB3	1.50	0.40
1:C:663:LEU:HB2	1:C:666:LEU:HD12	2.03	0.40
1:A:245:THR:HG23	1:A:249:ASP:OD2	2.21	0.40
1:C:342:LEU:O	1:C:468:VAL:HA	2.22	0.40
1:A:533:LEU:O	1:A:536:LYS:N	2.54	0.40
1:C:337:GLN:HE22	1:C:463:SER:HA	1.85	0.40
1:B:308:PRO:O	1:B:312:MET:HG3	2.21	0.40
1:A:162:LEU:HD23	1:A:229:LEU:CD1	2.51	0.40
1:C:256:LYS:O	1:C:259:GLN:HB3	2.22	0.40
1:B:523:ARG:CB	1:B:589:TRP:CE3	3.04	0.40
1:C:520:GLN:HE21	1:C:586:LYS:HE2	1.86	0.40
1:A:181:ARG:C	1:A:183:GLN:H	2.25	0.40
1:A:421:LEU:O	1:A:422:LYS:HG3	2.21	0.40
1:C:241:ARG:HH12	1:C:244:GLN:HG2	1.86	0.40
1:B:376:GLU:OE1	1:B:496:PHE:HB2	2.21	0.40
1:C:545:LEU:O	1:C:547:ASP:N	2.55	0.40
1:C:458:GLN:HE21	1:C:458:GLN:HB3	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:N	1:A:672:ASP:OD1	2.54	0.40
1:C:465:PRO:HG3	1:C:496:PHE:CD2	2.56	0.40
1:C:444:PHE:HB2	1:C:461:THR:CG2	2.51	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	540/585 (92%)	434 (80%)	78 (14%)	28 (5%)	2	19
1	B	540/585 (92%)	430 (80%)	84 (16%)	26 (5%)	3	22
1	C	540/585 (92%)	440 (82%)	69 (13%)	31 (6%)	2	18
All	All	1620/1755 (92%)	1304 (80%)	231 (14%)	85 (5%)	2	19

All (85) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	B	393	SER
1	B	495	PRO
1	B	636	PRO
1	B	670	PHE
1	C	193	ASN
1	C	194	PRO
1	C	359	LYS
1	C	385	ASN
1	C	389	ARG
1	C	393	SER
1	C	495	PRO
1	C	636	PRO
1	C	670	PHE
1	A	176	TYR
1	A	289	ASN
1	A	390	ASN
1	A	454	GLU
1	A	637	ASP
1	A	672	ASP
1	A	686	VAL
1	B	289	ASN
1	B	390	ASN
1	B	454	GLU
1	B	635	SER
1	B	637	ASP
1	B	672	ASP
1	C	176	TYR
1	C	289	ASN
1	C	390	ASN
1	C	454	GLU
1	C	637	ASP
1	C	672	ASP
1	C	686	VAL
1	A	182	ILE
1	A	306	PRO
1	A	453	ASN
1	A	635	SER
1	B	142	LEU
1	B	176	TYR
1	B	182	ILE
1	B	306	PRO
1	B	453	ASN

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Mol	Chain	Res	Type
1	B	686	VAL
1	C	142	LEU
1	C	182	ILE
1	C	306	PRO
1	C	453	ASN
1	A	142	LEU
1	A	234	GLN
1	A	622	SER
1	A	641	TRP
1	A	649	ARG
1	B	641	TRP
1	C	363	HIS
1	C	622	SER
1	C	635	SER
1	C	641	TRP
1	C	649	ARG
1	A	288	GLN
1	C	409	THR
1	B	409	THR
1	B	542	SER
1	C	234	GLN
1	C	398	ASN
1	C	542	SER
1	B	564	PRO
1	A	564	PRO
1	B	394	GLY
1	C	394	GLY
1	C	564	PRO
1	A	394	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	490/523 (94%)	370 (76%)	120 (24%)	1 3
1	B	490/523 (94%)	373 (76%)	117 (24%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	490/523 (94%)	370 (76%)	120 (24%)	1	3
All	All	1470/1569 (94%)	1113 (76%)	357 (24%)	1	3

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	144	ILE
1	A	147	ARG
1	A	152	ARG
1	A	159	GLU
1	A	161	GLU
1	A	162	LEU
1	A	163	LYS
1	A	165	LEU
1	A	169	GLN
1	A	175	GLN
1	A	176	TYR
1	A	180	LEU
1	A	192	LEU
1	A	195	GLN
1	A	202	THR
1	A	226	ARG
1	A	232	LYS
1	A	234	GLN
1	A	235	LYS
1	A	236	THR
1	A	242	LYS
1	A	244	GLN
1	A	257	ARG
1	A	258	ARG
1	A	275	LEU
1	A	278	TRP
1	A	281	LYS
1	A	285	ILE
1	A	286	ILE
1	A	290	ARG
1	A	291	GLN
1	A	293	ILE
1	A	299	LEU
1	A	310	GLU
1	A	311	GLU

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Mol	Chain	Res	Type
1	A	317	ASN
1	A	323	ILE
1	A	327	LEU
1	A	329	THR
1	A	330	SER
1	A	333	ILE
1	A	340	GLN
1	A	341	VAL
1	A	342	LEU
1	A	343	LYS
1	A	352	VAL
1	A	353	ARG
1	A	359	LYS
1	A	360	LEU
1	A	362	VAL
1	A	372	THR
1	A	374	ILE
1	A	377	GLN
1	A	384	LYS
1	A	385	ASN
1	A	386	GLU
1	A	388	THR
1	A	389	ARG
1	A	391	GLU
1	A	399	ASN
1	A	407	GLN
1	A	412	LEU
1	A	417	ARG
1	A	421	LEU
1	A	423	ARG
1	A	433	GLU
1	A	436	THR
1	A	443	LEU
1	A	449	SER
1	A	454	GLU
1	A	455	LEU
1	A	456	VAL
1	A	458	GLN
1	A	466	VAL
1	A	473	SER
1	A	474	GLN
1	A	475	ASP

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Mol	Chain	Res	Type
1	A	479	THR
1	A	481	THR
1	A	483	LEU
1	A	484	TRP
1	A	493	ARG
1	A	495	PRO
1	A	498	VAL
1	A	501	LYS
1	A	507	LEU
1	A	512	ASN
1	A	523	ARG
1	A	525	LEU
1	A	536	LYS
1	A	540	ILE
1	A	541	SER
1	A	543	ASN
1	A	551	MET
1	A	559	ASN
1	A	564	PRO
1	A	572	GLN
1	A	579	GLU
1	A	580	VAL
1	A	582	LYS
1	A	583	LYS
1	A	589	TRP
1	A	590	ASN
1	A	594	ILE
1	A	599	ASN
1	A	600	LYS
1	A	609	ASN
1	A	621	ASP
1	A	624	ILE
1	A	633	PHE
1	A	637	ASP
1	A	638	ARG
1	A	640	LEU
1	A	647	THR
1	A	653	ILE
1	A	667	ILE
1	A	668	TYR
1	A	676	ASP
1	A	686	VAL

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Mol	Chain	Res	Type
1	B	140	LYS
1	B	144	ILE
1	B	147	ARG
1	B	152	ARG
1	B	159	GLU
1	B	161	GLU
1	B	162	LEU
1	B	163	LYS
1	B	165	LEU
1	B	169	GLN
1	B	175	GLN
1	B	176	TYR
1	B	180	LEU
1	B	192	LEU
1	B	202	THR
1	B	226	ARG
1	B	232	LYS
1	B	234	GLN
1	B	235	LYS
1	B	236	THR
1	B	242	LYS
1	B	244	GLN
1	B	257	ARG
1	B	258	ARG
1	B	278	TRP
1	B	281	LYS
1	B	285	ILE
1	B	286	ILE
1	B	290	ARG
1	B	291	GLN
1	B	293	ILE
1	B	299	LEU
1	B	310	GLU
1	B	317	ASN
1	B	321	THR
1	B	323	ILE
1	B	325	SER
1	B	327	LEU
1	B	329	THR
1	B	330	SER
1	B	333	ILE
1	B	340	GLN

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Mol	Chain	Res	Type
1	B	341	VAL
1	B	342	LEU
1	B	343	LYS
1	B	352	VAL
1	B	353	ARG
1	B	359	LYS
1	B	360	LEU
1	B	362	VAL
1	B	372	THR
1	B	374	ILE
1	B	377	GLN
1	B	384	LYS
1	B	385	ASN
1	B	386	GLU
1	B	388	THR
1	B	389	ARG
1	B	391	GLU
1	B	399	ASN
1	B	407	GLN
1	B	412	LEU
1	B	421	LEU
1	B	423	ARG
1	B	433	GLU
1	B	449	SER
1	B	454	GLU
1	B	455	LEU
1	B	456	VAL
1	B	458	GLN
1	B	466	VAL
1	B	473	SER
1	B	474	GLN
1	B	475	ASP
1	B	479	THR
1	B	481	THR
1	B	483	LEU
1	B	484	TRP
1	B	493	ARG
1	B	495	PRO
1	B	498	VAL
1	B	501	LYS
1	B	507	LEU
1	B	512	ASN

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Mol	Chain	Res	Type
1	B	523	ARG
1	B	525	LEU
1	B	536	LYS
1	B	540	ILE
1	B	541	SER
1	B	543	ASN
1	B	551	MET
1	B	559	ASN
1	B	564	PRO
1	B	572	GLN
1	B	579	GLU
1	B	580	VAL
1	B	582	LYS
1	B	583	LYS
1	B	589	TRP
1	B	590	ASN
1	B	594	ILE
1	B	599	ASN
1	B	600	LYS
1	B	609	ASN
1	B	621	ASP
1	B	624	ILE
1	B	633	PHE
1	B	637	ASP
1	B	638	ARG
1	B	640	LEU
1	B	647	THR
1	B	653	ILE
1	B	667	ILE
1	B	668	TYR
1	B	669	VAL
1	B	676	ASP
1	B	686	VAL
1	C	140	LYS
1	C	144	ILE
1	C	147	ARG
1	C	152	ARG
1	C	159	GLU
1	C	161	GLU
1	C	162	LEU
1	C	163	LYS
1	C	165	LEU

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Mol	Chain	Res	Type
1	C	169	GLN
1	C	175	GLN
1	C	176	TYR
1	C	180	LEU
1	C	192	LEU
1	C	195	GLN
1	C	202	THR
1	C	223	GLN
1	C	226	ARG
1	C	232	LYS
1	C	234	GLN
1	C	235	LYS
1	C	236	THR
1	C	242	LYS
1	C	244	GLN
1	C	257	ARG
1	C	258	ARG
1	C	278	TRP
1	C	281	LYS
1	C	285	ILE
1	C	286	ILE
1	C	290	ARG
1	C	291	GLN
1	C	293	ILE
1	C	299	LEU
1	C	310	GLU
1	C	311	GLU
1	C	317	ASN
1	C	323	ILE
1	C	325	SER
1	C	327	LEU
1	C	329	THR
1	C	330	SER
1	C	333	ILE
1	C	340	GLN
1	C	341	VAL
1	C	342	LEU
1	C	343	LYS
1	C	352	VAL
1	C	353	ARG
1	C	359	LYS
1	C	360	LEU

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Mol	Chain	Res	Type
1	C	362	VAL
1	C	372	THR
1	C	374	ILE
1	C	377	GLN
1	C	384	LYS
1	C	385	ASN
1	C	386	GLU
1	C	388	THR
1	C	389	ARG
1	C	391	GLU
1	C	399	ASN
1	C	407	GLN
1	C	412	LEU
1	C	417	ARG
1	C	421	LEU
1	C	423	ARG
1	C	433	GLU
1	C	436	THR
1	C	449	SER
1	C	454	GLU
1	C	455	LEU
1	C	456	VAL
1	C	458	GLN
1	C	466	VAL
1	C	474	GLN
1	C	475	ASP
1	C	479	THR
1	C	481	THR
1	C	483	LEU
1	C	484	TRP
1	C	493	ARG
1	C	495	PRO
1	C	498	VAL
1	C	501	LYS
1	C	507	LEU
1	C	512	ASN
1	C	523	ARG
1	C	525	LEU
1	C	527	LYS
1	C	536	LYS
1	C	540	ILE
1	C	543	ASN

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Mol	Chain	Res	Type
1	C	551	MET
1	C	559	ASN
1	C	564	PRO
1	C	572	GLN
1	C	579	GLU
1	C	580	VAL
1	C	582	LYS
1	C	583	LYS
1	C	589	TRP
1	C	590	ASN
1	C	594	ILE
1	C	599	ASN
1	C	600	LYS
1	C	609	ASN
1	C	621	ASP
1	C	624	ILE
1	C	632	LYS
1	C	633	PHE
1	C	637	ASP
1	C	638	ARG
1	C	640	LEU
1	C	647	THR
1	C	653	ILE
1	C	667	ILE
1	C	668	TYR
1	C	676	ASP
1	C	686	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	167	GLN
1	A	175	GLN
1	A	177	GLN
1	A	183	GLN
1	A	185	GLN
1	A	216	GLN
1	A	223	GLN
1	A	234	GLN
1	A	244	GLN
1	A	276	GLN

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	292	GLN
1	A	317	ASN
1	A	337	GLN
1	A	340	GLN
1	A	361	ASN
1	A	363	HIS
1	A	368	GLN
1	A	385	ASN
1	A	399	ASN
1	A	415	HIS
1	A	418	ASN
1	A	458	GLN
1	A	474	GLN
1	A	477	ASN
1	A	486	ASN
1	A	512	ASN
1	A	520	GLN
1	A	529	ASN
1	A	584	HIS
1	A	599	ASN
1	A	602	GLN
1	A	609	ASN
1	B	145	ASN
1	B	167	GLN
1	B	175	GLN
1	B	177	GLN
1	B	183	GLN
1	B	185	GLN
1	B	234	GLN
1	B	244	GLN
1	B	276	GLN
1	B	291	GLN
1	B	292	GLN
1	B	298	HIS
1	B	317	ASN
1	B	337	GLN
1	B	340	GLN
1	B	363	HIS
1	B	368	GLN
1	B	385	ASN
1	B	399	ASN

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Mol	Chain	Res	Type
1	B	407	GLN
1	B	415	HIS
1	B	418	ASN
1	B	458	GLN
1	B	474	GLN
1	B	477	ASN
1	B	486	ASN
1	B	512	ASN
1	B	520	GLN
1	B	584	HIS
1	B	599	ASN
1	B	602	GLN
1	B	609	ASN
1	C	145	ASN
1	C	167	GLN
1	C	175	GLN
1	C	177	GLN
1	C	183	GLN
1	C	185	GLN
1	C	234	GLN
1	C	244	GLN
1	C	276	GLN
1	C	291	GLN
1	C	292	GLN
1	C	317	ASN
1	C	337	GLN
1	C	340	GLN
1	C	363	HIS
1	C	368	GLN
1	C	385	ASN
1	C	399	ASN
1	C	407	GLN
1	C	415	HIS
1	C	453	ASN
1	C	458	GLN
1	C	474	GLN
1	C	477	ASN
1	C	486	ASN
1	C	512	ASN
1	C	520	GLN
1	C	544	HIS
1	C	584	HIS

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Mol	Chain	Res	Type
1	C	599	ASN
1	C	602	GLN
1	C	609	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	544/585 (92%)	0.42	15 (2%) 56 44	31, 53, 77, 94	0
1	B	544/585 (92%)	0.37	9 (1%) 73 62	31, 53, 77, 94	0
1	C	544/585 (92%)	0.36	8 (1%) 76 65	31, 53, 77, 94	0
All	All	1632/1755 (92%)	0.38	32 (1%) 68 56	31, 53, 77, 94	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	GLU	4.0
1	A	393	SER	3.8
1	C	386	GLU	3.1
1	A	388	THR	2.9
1	A	187	ALA	2.8
1	A	386	GLU	2.8
1	A	189	LEU	2.8
1	C	393	SER	2.7
1	B	195	GLN	2.7
1	C	495	PRO	2.6
1	A	609	ASN	2.6
1	A	637	ASP	2.5
1	B	393	SER	2.5
1	B	197	ARG	2.5
1	C	637	ASP	2.4
1	A	387	ASN	2.4
1	C	387	ASN	2.3
1	C	667	ILE	2.3
1	A	638	ARG	2.3
1	B	637	ASP	2.3
1	B	633	PHE	2.2
1	A	495	PRO	2.2
1	A	633	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	LEU	2.1
1	B	495	PRO	2.1
1	B	386	GLU	2.1
1	A	205	GLN	2.1
1	C	196	GLU	2.1
1	A	201	GLU	2.0
1	B	639	ASN	2.0
1	C	195	GLN	2.0
1	A	479	THR	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.