



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YVL
Title : Structure of Unphosphorylated STAT1
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Deposited on : 2005-02-16
Resolution : 3.00 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

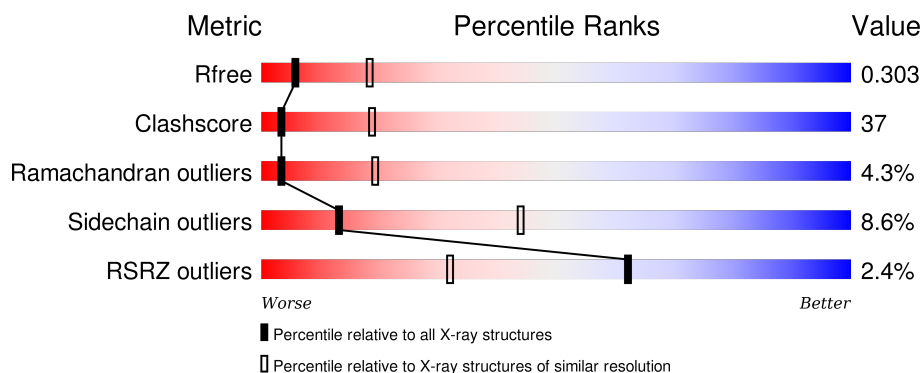
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	683	<div> <div>2%</div> <div>39% 49% 7% 5%</div> </div>
1	B	683	<div> <div>3%</div> <div>38% 49% 8% . .</div> </div>
2	C	5	<div> <div>60% 40%</div> </div>
2	D	5	<div> <div>80% 20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10863 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 1-alpha/beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	0	0
			5372	3435	922	991	24			
1	B	653	Total	C	N	O	S	0	0	0
			5387	3442	924	997	24			

- Molecule 2 is a protein called 5-residue peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			51	30	8	12	1			
2	D	5	Total	C	N	O	P	0	0	0
			51	30	8	12	1			

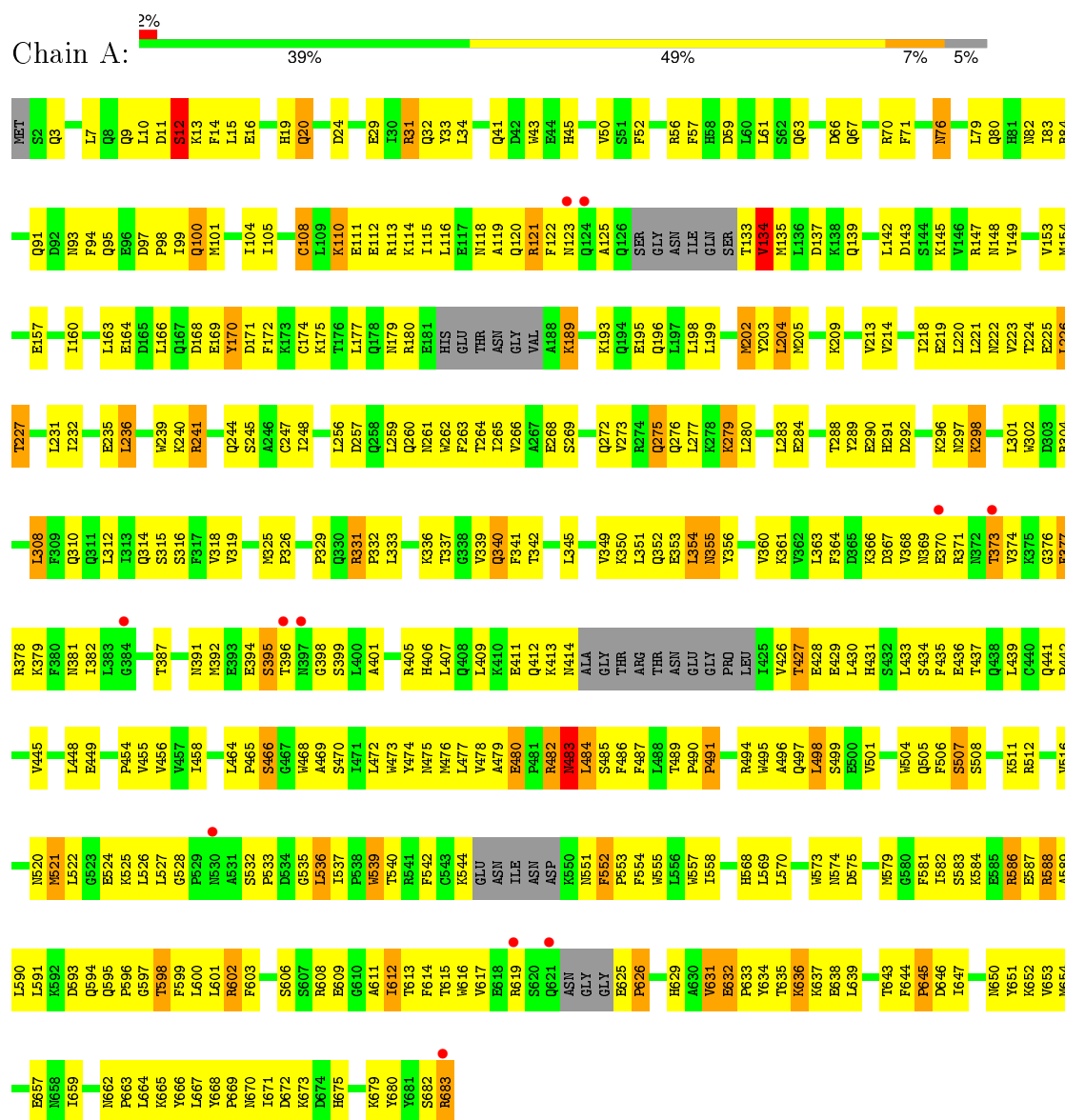
- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Au	0	0
			1	1		
3	A	1	Total	Au	0	0
			1	1		

3 Residue-property plots

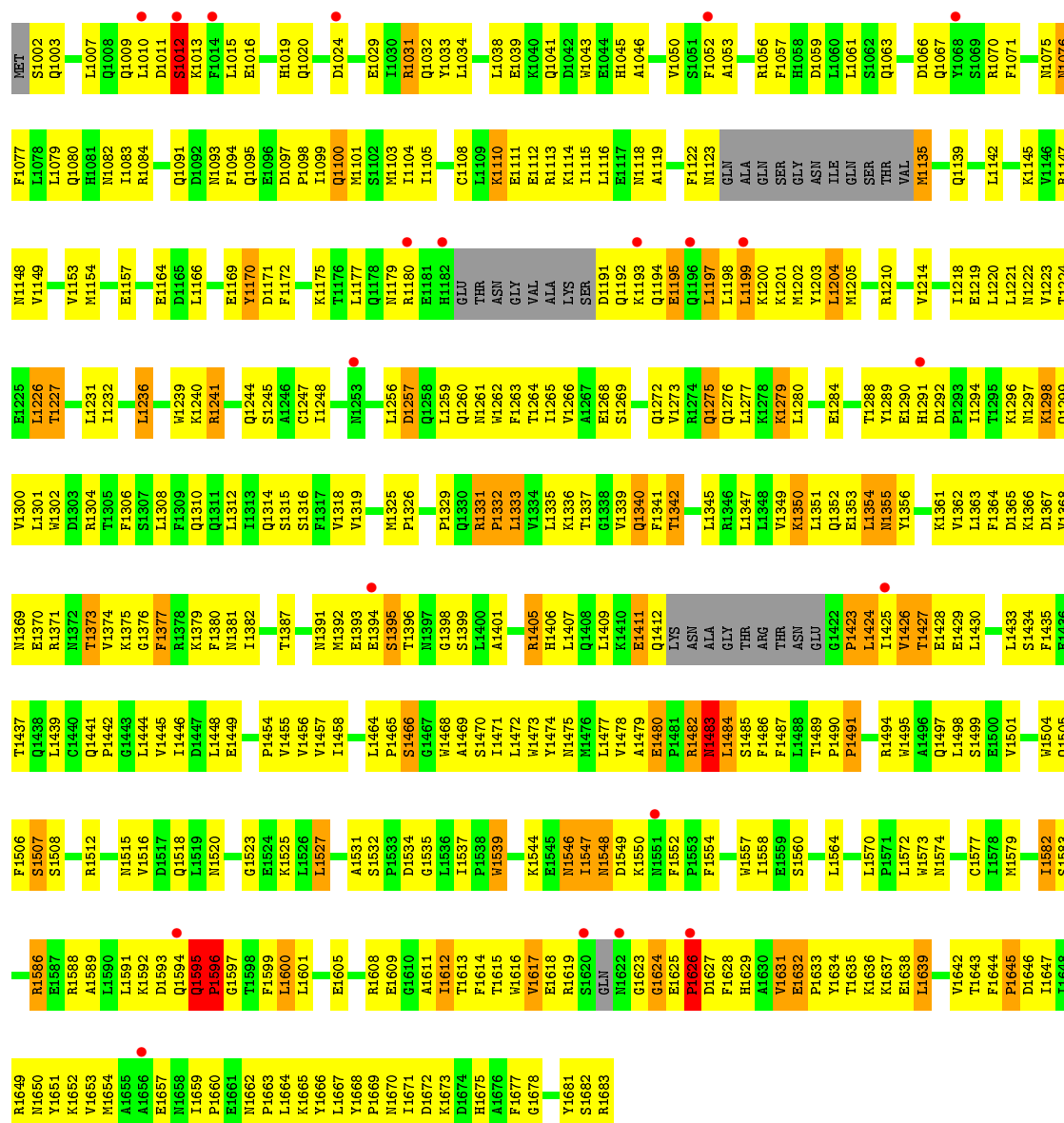
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 1-alpha/beta



- Molecule 1: Signal transducer and activator of transcription 1-alpha/beta





- Molecule 2: 5-residue peptide

Chain C: 60% 40%



- Molecule 2: 5-residue peptide

Chain D: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.55Å 102.55Å 646.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 95.0 (29.79-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.281 0.264 , 0.303	Depositor DCC
R_{free} test set	983 reflections (2.42%)	DCC
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92679 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10863	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AU, PTR

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	0.42	0/5486	0.67	2/7413 (0.0%)
1	B	0.45	1/5503 (0.0%)	0.69	4/7437 (0.1%)
2	C	0.42	0/36	1.10	1/46 (2.2%)
2	D	0.45	0/36	1.23	1/46 (2.2%)
All	All	0.44	1/11061 (0.0%)	0.68	8/14942 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1577	CYS	CB-SG	5.97	1.92	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1441	ASP	N-CA-CB	7.17	123.50	110.60
1	B	1405	ARG	N-CA-C	-7.12	91.77	111.00
1	A	405	ARG	N-CA-C	-6.20	94.25	111.00
2	C	441	ASP	N-CA-CB	6.14	121.66	110.60
1	B	1595	GLN	N-CA-C	-5.85	95.22	111.00
1	B	1395	SER	N-CA-C	-5.75	95.48	111.00
1	A	395	SER	N-CA-C	-5.71	95.57	111.00
1	B	1595	GLN	C-N-CD	-5.37	108.78	120.60

There are no chirality outliers.

There are no planarity outliers.

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	5372	0	5335	398	0
1	B	5387	0	5349	407	0
2	C	51	0	39	2	0
2	D	51	0	39	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
All	All	10863	0	10762	798	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 37.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1194:GLN:O	1:B:1195:GLU:HG3	1.47	1.12
1:B:1612:ILE:H	1:B:1612:ILE:HD13	1.08	1.11
1:A:551:ASN:HB3	1:A:608:ARG:HD3	1.23	1.11
1:B:1441:GLN:HB3	1:B:1442:PRO:HD2	1.34	1.07
1:A:441:GLN:HB3	1:A:442:PRO:HD2	1.34	1.03
1:B:1033:TYR:HB3	1:B:1067:GLN:HE21	1.23	1.03
1:A:3:GLN:HE22	1:A:113:ARG:HG3	1.22	1.00
1:A:33:TYR:HB3	1:A:67:GLN:HE21	1.26	0.99
1:A:597:GLY:HA3	1:A:665:LYS:HB2	1.42	0.99
1:B:1651:TYR:O	1:B:1662:ASN:HB3	1.64	0.98
1:A:595:GLN:O	1:A:598:THR:HG22	1.64	0.97
1:B:1608:ARG:HH11	1:B:1609:GLU:HG2	1.30	0.96
1:A:426:VAL:HG12	1:A:427:THR:H	1.28	0.96
1:A:651:TYR:O	1:A:662:ASN:HB3	1.65	0.95
1:B:1527:LEU:HD12	1:B:1531:ALA:HB1	1.49	0.95
1:B:1194:GLN:O	1:B:1195:GLU:CG	2.14	0.95
1:A:288:THR:HG22	1:A:289:TYR:H	1.33	0.94
1:B:1424:LEU:H	1:B:1424:LEU:HD12	1.34	0.93
1:A:612:ILE:HD13	1:A:612:ILE:H	1.30	0.93
1:B:1426:VAL:HG12	1:B:1427:THR:H	1.30	0.92
1:B:1668:TYR:HB3	1:B:1669:PRO:HD3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:TYR:HB3	1:A:669:PRO:HD3	1.51	0.91
1:B:1547:ILE:HG23	1:B:1550:LYS:HD3	1.53	0.91
1:B:1288:THR:HG22	1:B:1289:TYR:H	1.35	0.90
1:B:1612:ILE:HD13	1:B:1612:ILE:N	1.87	0.89
1:A:279:LYS:HE3	1:A:279:LYS:HA	1.54	0.89
1:A:482:ARG:HH11	1:A:482:ARG:HB3	1.38	0.88
1:B:1279:LYS:HE3	1:B:1279:LYS:HA	1.54	0.88
1:A:169:GLU:HG2	1:B:1406:HIS:HE1	1.39	0.88
1:B:1643:THR:HG23	1:B:1645:PRO:HD2	1.56	0.87
1:B:1482:ARG:HB3	1:B:1482:ARG:HH11	1.40	0.86
1:B:1672:ASP:HB2	1:B:1675:HIS:HB2	1.57	0.85
1:A:672:ASP:HB2	1:A:675:HIS:HB2	1.57	0.84
1:A:625:GLU:HB3	1:A:626:PRO:HD2	1.59	0.84
1:A:643:THR:HG23	1:A:645:PRO:HD2	1.57	0.84
1:A:272:GLN:O	1:A:276:GLN:HG2	1.78	0.84
1:B:1437:THR:HG22	1:B:1448:LEU:HB2	1.58	0.84
1:A:437:THR:HG22	1:A:448:LEU:HB2	1.59	0.83
1:B:1381:ASN:ND2	1:B:1412:GLN:HB2	1.93	0.82
1:B:1381:ASN:HD21	1:B:1412:GLN:HB2	1.44	0.82
1:B:1649:ARG:HB2	1:B:1681:TYR:CE1	2.13	0.82
1:B:1272:GLN:O	1:B:1276:GLN:HG2	1.78	0.82
1:B:1608:ARG:NH1	1:B:1609:GLU:HG2	1.94	0.81
1:B:1612:ILE:H	1:B:1612:ILE:CD1	1.91	0.81
1:B:1247:CYS:SG	3:B:2002:AU:AU	2.08	0.81
1:B:1597:GLY:CA	1:B:1665:LYS:HB2	2.10	0.81
1:A:247:CYS:SG	3:A:2001:AU:AU	2.09	0.81
1:A:288:THR:HG22	1:A:289:TYR:N	1.96	0.80
1:A:169:GLU:HG2	1:B:1406:HIS:CE1	2.18	0.79
1:B:1643:THR:CG2	1:B:1645:PRO:HD2	2.11	0.79
1:B:1033:TYR:HB3	1:B:1067:GLN:NE2	1.98	0.79
1:B:1594:GLN:HG2	1:B:1619:ARG:NE	1.97	0.79
1:A:625:GLU:HB3	1:A:626:PRO:CD	2.13	0.79
1:A:643:THR:CG2	1:A:645:PRO:HD2	2.13	0.78
1:B:1248:ILE:HG13	1:B:1472:LEU:HD23	1.66	0.78
1:B:1195:GLU:OE1	1:B:1197:LEU:HD11	1.85	0.77
1:B:1527:LEU:CD1	1:B:1531:ALA:HB1	2.14	0.77
1:B:1288:THR:HG22	1:B:1289:TYR:N	1.98	0.77
1:B:1349:VAL:O	1:B:1350:LYS:HB3	1.83	0.77
1:B:1310:GLN:O	1:B:1314:GLN:HG3	1.84	0.76
1:A:33:TYR:HB3	1:A:67:GLN:NE2	2.00	0.76
1:A:378:ARG:HD2	1:A:413:LYS:HZ1	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1646:ASP:OD2	1:B:1682:SER:HB2	1.85	0.76
1:B:1549:ASP:C	1:B:1550:LYS:HD2	2.06	0.76
1:A:411:GLU:HG3	1:A:413:LYS:HE3	1.67	0.76
1:B:1601:LEU:HD23	1:B:1614:PHE:HB3	1.69	0.76
1:A:3:GLN:NE2	1:A:113:ARG:HG3	2.01	0.75
1:A:441:GLN:HB3	1:A:442:PRO:CD	2.14	0.75
1:B:1594:GLN:HG2	1:B:1619:ARG:HE	1.51	0.75
1:A:310:GLN:O	1:A:314:GLN:HG3	1.87	0.74
1:A:153:VAL:HG22	1:A:220:LEU:HD11	1.70	0.73
1:A:406:HIS:CE1	1:B:1169:GLU:HG2	2.23	0.73
1:B:1066:ASP:O	1:B:1070:ARG:HG3	1.88	0.73
1:A:552:PHE:HB2	1:A:553:PRO:HD2	1.69	0.73
1:A:619:ARG:NH1	1:A:626:PRO:HG3	2.03	0.73
1:A:355:ASN:HD21	1:A:392:MET:CG	2.02	0.73
1:A:349:VAL:O	1:A:350:LYS:HB3	1.86	0.73
1:A:273:VAL:HA	1:A:276:GLN:HG3	1.71	0.73
1:B:1264:THR:O	1:B:1268:GLU:HG3	1.89	0.72
1:B:1441:GLN:HB3	1:B:1442:PRO:CD	2.14	0.72
1:B:1355:ASN:HD21	1:B:1392:MET:CG	2.02	0.72
1:B:1424:LEU:N	1:B:1424:LEU:HD12	2.05	0.72
1:B:1564:LEU:HD21	1:B:1612:ILE:HD12	1.72	0.72
1:B:1594:GLN:HG2	1:B:1619:ARG:NH2	2.03	0.72
1:A:264:THR:O	1:A:268:GLU:HG3	1.89	0.72
1:B:1426:VAL:HG12	1:B:1427:THR:N	2.05	0.71
1:A:66:ASP:O	1:A:70:ARG:HG3	1.90	0.71
1:B:1364:PHE:HB2	1:B:1382:ILE:HD11	1.70	0.71
1:B:1100:GLN:O	1:B:1104:ILE:HG12	1.89	0.71
1:B:1597:GLY:HA3	1:B:1665:LYS:HB2	1.72	0.71
1:A:644:PHE:HB3	1:A:645:PRO:HD3	1.71	0.71
1:B:1594:GLN:CD	1:B:1625:GLU:HG3	2.11	0.71
1:A:370:GLU:HA	1:A:374:VAL:H	1.55	0.71
1:A:100:GLN:O	1:A:104:ILE:HG12	1.90	0.71
1:B:1594:GLN:HG2	1:B:1619:ARG:CZ	2.20	0.71
1:A:164:GLU:HG3	1:A:283:LEU:HD21	1.72	0.71
1:B:1644:PHE:HB3	1:B:1645:PRO:HD3	1.72	0.71
1:A:364:PHE:HB2	1:A:382:ILE:HD11	1.71	0.71
1:B:1261:ASN:O	1:B:1265:ILE:HG12	1.90	0.71
1:A:540:THR:HA	1:A:544:LYS:HB3	1.74	0.70
1:A:597:GLY:CA	1:A:665:LYS:HB2	2.20	0.70
1:A:598:THR:HA	1:A:666:TYR:O	1.92	0.70
1:B:1153:VAL:HG21	1:B:1269:SER:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1370:GLU:HA	1:B:1374:VAL:H	1.57	0.70
1:A:220:LEU:HD23	1:A:220:LEU:C	2.13	0.70
1:A:345:LEU:O	1:A:401:ALA:HB1	1.92	0.70
1:B:1273:VAL:HA	1:B:1276:GLN:HG3	1.72	0.69
1:A:261:ASN:O	1:A:265:ILE:HG12	1.93	0.69
1:B:1153:VAL:HG22	1:B:1220:LEU:HD11	1.73	0.69
1:B:1197:LEU:O	1:B:1201:LYS:HB2	1.92	0.69
1:A:248:ILE:HD12	1:A:468:TRP:CH2	2.28	0.69
1:A:595:GLN:HG2	1:A:666:TYR:CD1	2.27	0.69
1:B:1052:PHE:HE2	1:B:1056:ARG:CZ	2.05	0.69
1:A:411:GLU:OE1	1:A:413:LYS:HD2	1.93	0.68
1:B:1220:LEU:HD23	1:B:1220:LEU:C	2.12	0.68
1:A:437:THR:CG2	1:A:448:LEU:HB2	2.24	0.68
1:B:1595:GLN:O	1:B:1597:GLY:N	2.27	0.68
1:B:1355:ASN:ND2	1:B:1392:MET:HG2	2.08	0.68
1:B:1381:ASN:HD21	1:B:1412:GLN:CB	2.07	0.68
1:B:1325:MET:HE3	1:B:1339:VAL:HB	1.76	0.67
1:A:355:ASN:HD21	1:A:392:MET:HG2	1.60	0.67
1:A:426:VAL:O	1:A:428:GLU:N	2.28	0.67
1:B:1437:THR:CG2	1:B:1448:LEU:HB2	2.22	0.67
1:A:427:THR:O	1:A:427:THR:HG22	1.94	0.67
1:A:288:THR:CG2	1:A:289:TYR:H	2.08	0.67
1:B:1108:CYS:O	1:B:1112:GLU:HG3	1.95	0.67
1:B:1657:GLU:N	1:B:1657:GLU:OE1	2.28	0.67
1:A:134:VAL:HG23	1:A:135:MET:H	1.58	0.67
1:B:1381:ASN:HD21	1:B:1412:GLN:HG3	1.60	0.66
1:A:489:THR:N	1:A:490:PRO:HD3	2.10	0.66
1:A:586:ARG:O	1:A:589:ALA:HB3	1.96	0.66
1:A:612:ILE:N	1:A:612:ILE:HD13	2.07	0.66
1:A:378:ARG:HD2	1:A:413:LYS:NZ	2.09	0.66
1:B:1355:ASN:HD21	1:B:1392:MET:HG2	1.58	0.66
1:A:355:ASN:ND2	1:A:392:MET:HG2	2.10	0.66
1:B:1364:PHE:HD1	1:B:1433:LEU:HD23	1.60	0.66
1:A:468:TRP:HE1	1:A:505:GLN:NE2	1.94	0.66
1:A:52:PHE:HE2	1:A:56:ARG:CZ	2.09	0.66
1:B:1244:GLN:HG2	1:B:1475:ASN:OD1	1.96	0.65
1:A:657:GLU:OE1	1:A:657:GLU:N	2.28	0.65
1:A:325:MET:HE3	1:A:339:VAL:HB	1.77	0.65
1:B:1594:GLN:HG2	1:B:1619:ARG:HH21	1.60	0.65
1:A:108:CYS:O	1:A:112:GLU:HG3	1.97	0.65
1:B:1218:ILE:HG22	1:B:1222:ASN:HD21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:PHE:CE2	1:B:1411:GLU:HG2	2.32	0.65
1:B:1468:TRP:HE1	1:B:1505:GLN:NE2	1.95	0.64
1:A:552:PHE:H	1:A:608:ARG:HH11	1.46	0.64
1:B:1592:LYS:HA	1:B:1625:GLU:OE1	1.97	0.64
1:A:218:ILE:HG22	1:A:222:ASN:HD21	1.63	0.64
1:B:1678:GLY:HA2	1:B:1681:TYR:CD2	2.33	0.64
1:B:1427:THR:O	1:B:1427:THR:HG23	1.96	0.64
1:A:381:ASN:HD21	1:A:412:GLN:HB2	1.61	0.64
1:B:1489:THR:N	1:B:1490:PRO:HD3	2.12	0.64
1:B:1424:LEU:CD1	1:B:1424:LEU:H	2.08	0.64
1:A:170:TYR:OH	1:A:203:TYR:CG	2.52	0.64
1:B:1430:LEU:HB2	1:B:1484:LEU:HA	1.81	0.63
1:A:20:GLN:NE2	1:A:511:LYS:HD2	2.13	0.63
1:A:33:TYR:C	1:A:34:LEU:HD12	2.18	0.63
1:A:153:VAL:HG21	1:A:269:SER:HB3	1.80	0.63
1:A:236:LEU:O	1:A:240:LYS:HG2	1.98	0.63
1:B:1236:LEU:O	1:B:1240:LYS:HG2	1.99	0.63
1:A:174:CYS:SG	1:A:199:LEU:HD22	2.38	0.63
1:A:340:GLN:HB2	1:B:1172:PHE:CZ	2.34	0.63
1:B:1288:THR:CG2	1:B:1289:TYR:H	2.08	0.63
1:B:1205:MET:CE	1:B:1205:MET:HA	2.29	0.63
1:A:195:GLU:HA	1:A:198:LEU:HD13	1.79	0.62
1:A:646:ASP:OD2	1:A:682:SER:HB2	1.98	0.62
1:B:1198:LEU:C	1:B:1200:LYS:H	2.02	0.62
1:A:381:ASN:ND2	1:A:412:GLN:HB2	2.14	0.62
1:B:1033:TYR:O	1:B:1034:LEU:HD12	1.99	0.62
1:A:683:ARG:HA	1:A:683:ARG:NE	2.14	0.62
1:B:1332:PRO:HD2	1:B:1468:TRP:CZ3	2.34	0.62
1:B:1033:TYR:C	1:B:1034:LEU:HD12	2.19	0.61
1:B:1635:THR:HG22	1:B:1638:GLU:OE1	2.00	0.61
1:B:1245:SER:O	1:B:1248:ILE:HG22	2.00	0.61
1:A:170:TYR:OH	1:A:203:TYR:CD1	2.53	0.61
1:A:360:VAL:HG22	1:A:437:THR:HB	1.83	0.61
1:B:1381:ASN:HD21	1:B:1412:GLN:CG	2.13	0.61
1:B:1170:TYR:C	1:B:1170:TYR:HD2	2.04	0.61
1:A:170:TYR:C	1:A:170:TYR:HD2	2.04	0.61
1:A:430:LEU:HB2	1:A:484:LEU:HA	1.82	0.61
1:B:1611:ALA:HB1	1:B:1634:TYR:O	2.00	0.60
1:A:33:TYR:O	1:A:34:LEU:HD12	2.00	0.60
1:A:142:LEU:HD23	1:A:262:TRP:CE3	2.37	0.60
1:A:205:MET:HA	1:A:205:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:HA	1:A:683:ARG:CZ	2.31	0.60
1:A:487:PHE:HA	1:A:490:PRO:HG3	1.84	0.60
1:A:635:THR:HG22	1:A:638:GLU:OE1	2.01	0.60
1:A:554:PHE:O	1:A:557:TRP:HB3	2.00	0.60
1:A:654:MET:HE2	1:A:654:MET:HA	1.84	0.60
1:B:1195:GLU:HB3	1:B:1197:LEU:HG	1.83	0.60
1:B:1454:PRO:HG3	1:B:1474:TYR:CZ	2.37	0.60
1:B:1512:ARG:HD3	1:B:1573:TRP:O	2.02	0.60
1:B:1570:LEU:CD2	1:B:1574:ASN:HD21	2.15	0.60
1:A:245:SER:O	1:A:248:ILE:HG22	2.02	0.59
1:A:111:GLU:OE2	1:A:114:LYS:HD2	2.02	0.59
1:A:454:PRO:HG3	1:A:474:TYR:CZ	2.38	0.59
1:B:1262:TRP:O	1:B:1266:VAL:HG12	2.01	0.59
1:A:426:VAL:HG12	1:A:427:THR:N	2.09	0.59
1:A:262:TRP:O	1:A:266:VAL:HG12	2.03	0.59
1:A:170:TYR:C	1:A:170:TYR:CD2	2.76	0.59
1:B:1672:ASP:HB2	1:B:1675:HIS:CB	2.32	0.59
1:B:1464:LEU:N	1:B:1465:PRO:HD2	2.18	0.59
1:B:1649:ARG:NH1	1:B:1681:TYR:HB3	2.18	0.59
1:A:464:LEU:N	1:A:465:PRO:HD2	2.17	0.59
1:A:672:ASP:HB2	1:A:675:HIS:CB	2.31	0.59
1:B:1170:TYR:C	1:B:1170:TYR:CD2	2.76	0.59
1:A:266:VAL:HG13	1:A:312:LEU:HD21	1.85	0.59
1:B:1350:LYS:O	1:B:1351:LEU:HD23	2.03	0.58
1:B:1612:ILE:HD11	1:B:1639:LEU:HD21	1.85	0.58
1:B:1220:LEU:O	1:B:1220:LEU:HD23	2.04	0.58
1:A:524:GLU:C	1:A:526:LEU:H	2.07	0.58
1:A:498:LEU:HD21	1:A:542:PHE:CE1	2.39	0.58
1:A:220:LEU:HD23	1:A:220:LEU:O	2.03	0.58
1:A:142:LEU:HD23	1:A:262:TRP:CZ3	2.37	0.58
1:A:552:PHE:O	1:A:552:PHE:HD1	1.86	0.58
1:B:1612:ILE:N	1:B:1612:ILE:CD1	2.55	0.58
1:B:1314:GLN:HA	1:B:1448:LEU:HD22	1.84	0.58
1:B:1031:ARG:NH1	1:B:1112:GLU:OE1	2.36	0.58
1:B:1111:GLU:OE2	1:B:1114:LYS:HD2	2.04	0.57
1:B:1651:TYR:O	1:B:1652:LYS:HG2	2.05	0.57
1:B:1423:PRO:HG2	1:B:1425:ILE:O	2.03	0.57
1:A:579:MET:SD	1:A:600:LEU:HD11	2.45	0.57
1:B:1650:ASN:O	1:B:1652:LYS:HG3	2.05	0.57
1:B:1601:LEU:CD2	1:B:1614:PHE:HB3	2.33	0.57
1:B:1597:GLY:HA2	1:B:1665:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH1	1:A:112:GLU:OE1	2.38	0.57
1:B:1266:VAL:HG13	1:B:1312:LEU:HD21	1.86	0.57
1:A:363:LEU:HD22	1:A:366:LYS:HD3	1.87	0.57
1:B:1527:LEU:HD21	1:B:1535:GLY:O	2.03	0.57
1:B:1482:ARG:NH1	1:B:1482:ARG:HB3	2.17	0.57
1:B:1012:SER:HA	1:B:1015:LEU:HD11	1.87	0.57
1:B:1363:LEU:HD22	1:B:1366:LYS:HD3	1.86	0.57
1:B:1591:LEU:C	1:B:1593:ASP:H	2.08	0.57
1:A:591:LEU:O	1:A:617:VAL:HG21	2.05	0.57
1:B:1153:VAL:CG2	1:B:1220:LEU:HD11	2.35	0.57
1:B:1651:TYR:O	1:B:1662:ASN:CB	2.47	0.57
1:A:551:ASN:CB	1:A:608:ARG:HD3	2.16	0.56
1:B:1619:ARG:NH1	1:B:1625:GLU:HA	2.19	0.56
1:A:370:GLU:HA	1:A:373:THR:HB	1.88	0.56
1:B:1546:ASN:HD22	1:B:1546:ASN:C	2.08	0.56
1:A:170:TYR:OH	1:A:203:TYR:CD2	2.59	0.56
1:B:1478:VAL:HG12	1:B:1479:ALA:N	2.20	0.56
1:B:1668:TYR:CB	1:B:1669:PRO:HD3	2.32	0.56
1:B:1487:PHE:HA	1:B:1490:PRO:HG3	1.87	0.56
1:A:378:ARG:HB2	1:A:429:GLU:OE2	2.06	0.56
1:B:1579:MET:HG2	1:B:1582:ILE:HG12	1.86	0.56
1:A:153:VAL:CG2	1:A:220:LEU:HD11	2.36	0.56
1:A:177:LEU:HD23	1:A:180:ARG:NH2	2.20	0.56
1:A:664:LEU:O	1:A:673:LYS:HD3	2.06	0.56
1:B:1664:LEU:O	1:B:1673:LYS:HD3	2.05	0.56
1:A:12:SER:HA	1:A:15:LEU:HD11	1.88	0.56
1:B:1482:ARG:C	1:B:1483:ASN:OD1	2.44	0.56
1:B:1586:ARG:O	1:B:1589:ALA:HB3	2.05	0.56
1:A:350:LYS:O	1:A:351:LEU:HD23	2.06	0.55
1:B:1579:MET:SD	1:B:1600:LEU:HD12	2.46	0.55
1:B:1546:ASN:HD21	1:B:1550:LYS:C	2.10	0.55
1:A:59:ASP:O	1:A:63:GLN:HG2	2.07	0.55
1:A:570:LEU:CD2	1:A:574:ASN:HD21	2.18	0.55
1:B:1135:MET:O	1:B:1139:GLN:HG2	2.07	0.55
1:A:651:TYR:O	1:A:652:LYS:HG2	2.06	0.55
1:B:1002:SER:HB2	1:B:1039:GLU:OE2	2.06	0.55
1:B:1370:GLU:HG3	1:B:1374:VAL:HG23	1.89	0.55
1:B:1583:SER:HB3	1:B:1586:ARG:HB2	1.89	0.55
1:B:1248:ILE:HD11	1:B:1472:LEU:HA	1.89	0.55
1:A:654:MET:CE	1:A:654:MET:HA	2.36	0.55
1:B:1654:MET:HA	1:B:1654:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:VAL:HG12	1:A:479:ALA:N	2.22	0.55
1:A:617:VAL:CG1	1:A:626:PRO:HB3	2.37	0.55
1:A:351:LEU:O	1:A:354:LEU:HB2	2.07	0.55
1:B:1029:GLU:OE2	1:B:1082:ASN:HB3	2.07	0.55
1:A:29:GLU:OE2	1:A:82:ASN:HB3	2.07	0.55
1:A:651:TYR:O	1:A:662:ASN:CB	2.47	0.54
1:A:172:PHE:CZ	1:B:1340:GLN:HB2	2.42	0.54
1:B:1351:LEU:O	1:B:1354:LEU:HB2	2.07	0.54
1:B:1591:LEU:HD11	1:B:1600:LEU:HD22	1.88	0.54
1:A:355:ASN:ND2	1:A:392:MET:CG	2.67	0.54
1:A:579:MET:HB3	1:A:582:ILE:HD11	1.89	0.54
1:A:668:TYR:CB	1:A:669:PRO:HD3	2.31	0.54
1:B:1355:ASN:ND2	1:B:1392:MET:CG	2.67	0.54
1:A:120:GLN:C	1:A:122:PHE:H	2.09	0.54
1:A:595:GLN:O	1:A:598:THR:CG2	2.49	0.54
1:A:261:ASN:O	1:A:264:THR:HG22	2.07	0.54
1:B:1594:GLN:HB2	1:B:1625:GLU:OE1	2.07	0.54
1:A:175:LYS:O	1:A:179:ASN:HB2	2.07	0.54
1:B:1370:GLU:HA	1:B:1373:THR:HB	1.89	0.54
1:A:376:GLY:O	1:A:377:PHE:C	2.46	0.54
1:B:1059:ASP:O	1:B:1063:GLN:HG2	2.08	0.54
1:A:540:THR:CA	1:A:544:LYS:HB3	2.38	0.54
1:B:1454:PRO:HG3	1:B:1474:TYR:CE1	2.43	0.54
1:B:1177:LEU:HD23	1:B:1180:ARG:NH2	2.22	0.54
1:A:435:PHE:O	1:A:449:GLU:HA	2.08	0.54
1:A:650:ASN:O	1:A:652:LYS:HG3	2.07	0.54
1:B:1649:ARG:HD2	1:B:1681:TYR:CD1	2.43	0.54
1:A:586:ARG:HD2	1:A:590:LEU:CD1	2.38	0.54
1:B:1218:ILE:HG22	1:B:1222:ASN:ND2	2.23	0.54
1:B:1175:LYS:O	1:B:1179:ASN:HB2	2.08	0.54
1:A:364:PHE:HD1	1:A:433:LEU:HD23	1.73	0.54
1:A:370:GLU:HG3	1:A:374:VAL:HG23	1.89	0.54
1:A:326:PRO:O	1:A:329:PRO:HD3	2.08	0.54
1:A:168:ASP:HB3	1:B:1406:HIS:CD2	2.43	0.53
1:B:1110:LYS:HA	1:B:1113:ARG:HH21	1.73	0.53
1:A:318:VAL:HG22	1:A:319:VAL:N	2.21	0.53
1:A:170:TYR:CE1	1:A:202:MET:HB3	2.43	0.53
1:A:489:THR:N	1:A:490:PRO:CD	2.71	0.53
1:B:1011:ASP:O	1:B:1013:LYS:N	2.41	0.53
1:B:1425:ILE:HD13	1:B:1429:GLU:HB3	1.90	0.53
1:B:1336:LYS:HA	1:B:1458:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:CG2	1:A:319:VAL:N	2.72	0.53
1:A:595:GLN:HE21	1:A:596:PRO:HD2	1.73	0.53
1:A:612:ILE:H	1:A:612:ILE:CD1	2.14	0.53
1:B:1318:VAL:HG22	1:B:1319:VAL:N	2.22	0.53
1:A:11:ASP:O	1:A:13:LYS:N	2.42	0.53
1:A:570:LEU:O	1:A:574:ASN:ND2	2.42	0.53
1:A:611:ALA:HB1	1:A:634:TYR:O	2.08	0.53
1:B:1376:GLY:O	1:B:1377:PHE:C	2.46	0.53
1:A:91:GLN:O	1:A:95:GLN:HB2	2.09	0.53
1:A:406:HIS:O	1:A:407:LEU:HD23	2.08	0.53
1:A:218:ILE:HG22	1:A:222:ASN:ND2	2.24	0.53
1:B:1157:GLU:HB2	1:B:1272:GLN:NE2	2.23	0.53
1:A:595:GLN:HG2	1:A:666:TYR:CE1	2.44	0.52
1:A:594:GLN:HG3	1:A:598:THR:HG21	1.90	0.52
1:A:643:THR:HG22	1:A:646:ASP:H	1.73	0.52
1:B:1195:GLU:OE1	1:B:1197:LEU:CD1	2.56	0.52
1:B:1483:ASN:C	1:B:1485:SER:H	2.12	0.52
1:B:1380:PHE:HE2	1:B:1411:GLU:HG2	1.73	0.52
1:A:368:VAL:O	1:A:371:ARG:HG3	2.10	0.52
1:B:1435:PHE:O	1:B:1449:GLU:HA	2.10	0.52
1:B:1199:LEU:HD12	1:B:1199:LEU:H	1.75	0.52
1:A:361:LYS:HB3	1:A:387:THR:HG22	1.90	0.52
1:A:284:GLU:OE2	1:A:298:LYS:HE2	2.10	0.52
1:A:632:GLU:OE1	1:A:633:PRO:HD2	2.10	0.52
1:B:1091:GLN:O	1:B:1095:GLN:HB2	2.10	0.52
1:B:1361:LYS:HB3	1:B:1387:THR:HG22	1.91	0.52
1:B:1368:VAL:O	1:B:1371:ARG:HG3	2.09	0.52
1:A:615:THR:HG23	1:A:629:HIS:O	2.09	0.52
1:A:552:PHE:CD1	1:A:552:PHE:C	2.83	0.52
1:B:1284:GLU:OE2	1:B:1298:LYS:HE2	2.10	0.52
1:A:482:ARG:C	1:A:483:ASN:OD1	2.48	0.52
1:A:454:PRO:HG3	1:A:474:TYR:CE1	2.45	0.52
1:B:1570:LEU:O	1:B:1574:ASN:ND2	2.43	0.52
1:A:279:LYS:HE3	1:A:279:LYS:CA	2.36	0.52
1:B:1241:ARG:O	1:B:1244:GLN:HB2	2.10	0.52
1:B:1318:VAL:CG2	1:B:1319:VAL:N	2.72	0.52
1:A:552:PHE:CB	1:A:553:PRO:HD2	2.40	0.52
1:B:1550:LYS:HG2	1:B:1552:PHE:CZ	2.45	0.52
1:B:1643:THR:HG22	1:B:1646:ASP:H	1.74	0.52
1:B:1594:GLN:HB2	1:B:1625:GLU:CD	2.31	0.52
1:B:1593:ASP:OD2	1:B:1593:ASP:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LEU:CD1	1:A:535:GLY:HA3	2.40	0.52
1:A:552:PHE:CZ	1:A:608:ARG:HA	2.45	0.51
1:A:603:PHE:CD1	1:A:612:ILE:HG22	2.46	0.51
1:B:1599:PHE:HB2	1:B:1615:THR:O	2.11	0.51
1:A:291:HIS:HA	1:A:296:LYS:NZ	2.25	0.51
1:A:496:ALA:HB2	1:A:533:PRO:O	2.10	0.51
1:A:482:ARG:HB3	1:A:482:ARG:NH1	2.15	0.51
1:A:682:SER:O	1:A:683:ARG:HG2	2.10	0.51
1:B:1624:GLY:C	1:B:1626:PRO:HD2	2.31	0.51
1:A:241:ARG:O	1:A:244:GLN:HB2	2.11	0.51
1:B:1341:PHE:HE2	1:B:1433:LEU:HD11	1.76	0.51
1:A:171:ASP:OD1	1:A:175:LYS:HE3	2.11	0.51
1:A:290:GLU:O	1:A:291:HIS:HB2	2.11	0.51
1:B:1147:ARG:HG3	1:B:1147:ARG:NH1	2.26	0.51
1:B:1326:PRO:O	1:B:1329:PRO:HD3	2.10	0.51
1:B:1544:LYS:NZ	1:B:1544:LYS:HB2	2.25	0.51
1:A:355:ASN:HD21	1:A:392:MET:HG3	1.76	0.51
1:B:1368:VAL:HB	1:B:1371:ARG:CG	2.41	0.51
1:B:1291:HIS:HA	1:B:1296:LYS:NZ	2.26	0.51
1:B:1145:LYS:O	1:B:1148:ASN:HB3	2.11	0.51
1:A:110:LYS:HA	1:A:113:ARG:HH21	1.74	0.51
1:B:1340:GLN:HA	1:B:1407:LEU:O	2.11	0.51
1:B:1147:ARG:HG3	1:B:1147:ARG:HH11	1.74	0.51
1:A:426:VAL:C	1:A:428:GLU:H	2.14	0.51
1:B:1289:TYR:CE1	1:B:1292:ASP:HA	2.46	0.51
1:A:341:PHE:HE2	1:A:433:LEU:HD11	1.76	0.51
1:B:1632:GLU:OE1	1:B:1633:PRO:HD2	2.11	0.51
1:A:121:ARG:C	1:A:123:ASN:H	2.14	0.51
1:B:1588:ARG:HG3	1:B:1628:PHE:CD2	2.45	0.51
1:B:1666:TYR:HA	1:B:1671:ILE:O	2.11	0.51
1:A:231:LEU:HD21	1:A:263:PHE:CD1	2.46	0.51
1:A:617:VAL:HG11	1:A:626:PRO:HB3	1.93	0.50
1:B:1316:SER:CB	1:B:1349:VAL:HG23	2.41	0.50
1:B:1352:GLN:C	1:B:1354:LEU:H	2.14	0.50
1:A:594:GLN:HE21	1:A:670:ASN:HD21	1.59	0.50
1:A:483:ASN:C	1:A:485:SER:H	2.14	0.50
1:A:352:GLN:C	1:A:354:LEU:H	2.14	0.50
1:B:1261:ASN:O	1:B:1264:THR:HG22	2.11	0.50
1:B:1489:THR:N	1:B:1490:PRO:CD	2.73	0.50
1:A:600:LEU:HD12	1:A:601:LEU:H	1.76	0.50
1:B:1171:ASP:OD1	1:B:1175:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:O	1:A:469:ALA:HB3	2.11	0.50
1:A:537:ILE:HD12	1:A:537:ILE:N	2.27	0.50
1:B:1197:LEU:HD23	1:B:1197:LEU:N	2.27	0.50
1:B:1613:THR:OG1	1:B:1631:VAL:HG23	2.11	0.50
1:B:1483:ASN:N	1:B:1483:ASN:OD1	2.44	0.50
1:B:1157:GLU:HB2	1:B:1272:GLN:HE21	1.76	0.50
1:A:602:ARG:NH2	2:C:440:PTR:OH	2.44	0.50
1:A:596:PRO:O	1:A:617:VAL:O	2.30	0.50
1:A:666:TYR:HA	1:A:671:ILE:O	2.12	0.50
1:B:1594:GLN:CG	1:B:1619:ARG:HE	2.21	0.50
1:A:325:MET:HE2	1:A:339:VAL:HG11	1.93	0.50
1:B:1362:VAL:HG22	1:B:1435:PHE:CE1	2.47	0.50
1:B:1260:GLN:HE22	1:B:1399:SER:HA	1.76	0.50
1:B:1395:SER:H	1:B:1398:GLY:HA2	1.76	0.50
1:A:145:LYS:O	1:A:148:ASN:HB3	2.11	0.50
1:A:219:GLU:HA	1:A:222:ASN:HD22	1.77	0.50
1:B:1470:SER:HB3	1:B:1487:PHE:CE2	2.47	0.50
1:A:512:ARG:NH1	1:A:574:ASN:O	2.35	0.50
1:B:1345:LEU:O	1:B:1401:ALA:HB1	2.12	0.50
1:B:1071:PHE:CE1	1:B:1079:LEU:HB3	2.46	0.50
1:B:1466:SER:O	1:B:1469:ALA:HB3	2.10	0.50
1:B:1232:ILE:HD13	1:B:1315:SER:OG	2.11	0.50
1:B:1483:ASN:O	1:B:1485:SER:N	2.45	0.50
1:A:350:LYS:O	1:A:350:LYS:HG2	2.12	0.50
1:A:586:ARG:HD2	1:A:590:LEU:HD11	1.94	0.50
1:B:1501:VAL:O	1:B:1504:TRP:HB2	2.11	0.50
1:A:583:SER:O	1:A:587:GLU:HB2	2.12	0.50
1:B:1057:PHE:HE2	1:B:1095:GLN:HG3	1.77	0.50
1:B:1653:VAL:HG22	1:B:1663:PRO:HD3	1.94	0.50
1:B:1273:VAL:HA	1:B:1276:GLN:CG	2.42	0.49
1:B:1010:LEU:HD11	1:B:1116:LEU:HD23	1.94	0.49
1:B:1290:GLU:O	1:B:1291:HIS:HB2	2.12	0.49
1:A:57:PHE:CE2	1:A:61:LEU:HD11	2.48	0.49
1:A:535:GLY:O	1:A:536:LEU:HG	2.11	0.49
1:A:226:LEU:HD23	1:A:227:THR:N	2.26	0.49
1:B:1003:GLN:OE1	1:B:1112:GLU:OE1	2.29	0.49
1:B:1219:GLU:HA	1:B:1222:ASN:HD22	1.76	0.49
1:A:195:GLU:CA	1:A:198:LEU:HD13	2.42	0.49
1:A:368:VAL:HB	1:A:371:ARG:CG	2.41	0.49
1:B:1239:TRP:CZ2	1:B:1256:LEU:HD21	2.46	0.49
1:B:1425:ILE:CD1	1:B:1429:GLU:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HA	1:B:1406:HIS:CE1	2.47	0.49
1:B:1057:PHE:CE2	1:B:1095:GLN:HG3	2.47	0.49
1:A:486:PHE:CZ	1:A:491:PRO:HD2	2.47	0.49
1:A:220:LEU:C	1:A:220:LEU:CD2	2.81	0.49
1:A:395:SER:H	1:A:398:GLY:HA2	1.77	0.49
1:B:1003:GLN:HB3	1:B:1039:GLU:OE1	2.13	0.49
1:A:218:ILE:HG12	1:A:301:LEU:HD21	1.95	0.49
1:A:170:TYR:OH	1:A:203:TYR:CE1	2.65	0.49
1:A:57:PHE:HE2	1:A:95:GLN:HG3	1.77	0.49
1:A:289:TYR:CE1	1:A:292:ASP:HA	2.48	0.49
1:A:584:LYS:HE2	1:A:602:ARG:NH2	2.28	0.49
1:B:1455:VAL:HG12	1:B:1456:VAL:N	2.27	0.49
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.77	0.49
1:B:1284:GLU:HG2	1:B:1288:THR:OG1	2.13	0.49
1:B:1594:GLN:NE2	1:B:1618:GLU:O	2.46	0.49
1:B:1220:LEU:C	1:B:1220:LEU:CD2	2.81	0.49
1:A:600:LEU:O	1:A:614:PHE:HA	2.13	0.49
1:A:643:THR:HB	1:A:646:ASP:OD2	2.13	0.48
1:B:1170:TYR:OH	1:B:1203:TYR:CE2	2.66	0.48
1:B:1226:LEU:HD23	1:B:1227:THR:N	2.28	0.48
1:A:147:ARG:NH1	1:A:147:ARG:HG3	2.28	0.48
1:B:1204:LEU:O	1:B:1204:LEU:HD13	2.12	0.48
1:B:1495:TRP:HB2	1:B:1537:ILE:HD11	1.93	0.48
1:A:239:TRP:CZ2	1:A:256:LEU:HD21	2.48	0.48
1:A:470:SER:HB3	1:A:487:PHE:CE2	2.48	0.48
1:A:483:ASN:N	1:A:483:ASN:OD1	2.45	0.48
1:B:1494:ARG:O	1:B:1497:GLN:N	2.39	0.48
1:A:232:ILE:HD13	1:A:315:SER:OG	2.13	0.48
1:B:1560:SER:HB2	1:B:1609:GLU:O	2.13	0.48
1:A:426:VAL:CG1	1:A:427:THR:H	2.11	0.48
1:B:1355:ASN:HD21	1:B:1392:MET:HG3	1.78	0.48
1:B:1325:MET:HE2	1:B:1339:VAL:HG11	1.96	0.48
1:B:1570:LEU:HD22	1:B:1574:ASN:HD21	1.76	0.48
1:A:10:LEU:HD11	1:A:116:LEU:HD23	1.94	0.48
1:B:1668:TYR:HB3	1:B:1669:PRO:CD	2.35	0.48
1:A:411:GLU:HG3	1:A:413:LYS:CE	2.41	0.48
1:B:1007:LEU:HD11	1:B:1112:GLU:HB3	1.96	0.48
1:A:170:TYR:CG	1:A:202:MET:SD	3.07	0.48
1:A:366:LYS:HE3	1:A:367:ASP:OD2	2.14	0.48
1:A:57:PHE:CE2	1:A:95:GLN:HG3	2.48	0.48
1:A:284:GLU:HG2	1:A:288:THR:OG1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1657:GLU:HB2	1:B:1659:ILE:HG22	1.96	0.48
1:B:1616:TRP:CE2	1:B:1629:HIS:HB2	2.49	0.48
1:A:316:SER:CB	1:A:349:VAL:HG23	2.43	0.48
1:A:586:ARG:O	1:A:590:LEU:HD13	2.14	0.48
1:B:1486:PHE:CZ	1:B:1491:PRO:HD2	2.49	0.48
1:B:1050:VAL:HG22	1:B:1099:ILE:HD11	1.95	0.48
1:B:1594:GLN:HG3	1:B:1596:PRO:HD3	1.95	0.48
1:B:1221:LEU:HD13	1:B:1304:ARG:HB3	1.95	0.48
1:B:1333:LEU:HB2	1:B:1471:ILE:HD12	1.95	0.48
1:B:1425:ILE:O	1:B:1425:ILE:HD12	2.13	0.48
1:B:1646:ASP:CG	1:B:1682:SER:HB2	2.34	0.48
1:B:1218:ILE:HG12	1:B:1301:LEU:HD21	1.96	0.48
1:B:1057:PHE:CE2	1:B:1061:LEU:HD11	2.49	0.48
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.67	0.48
1:A:71:PHE:CE1	1:A:79:LEU:HB3	2.49	0.48
1:A:7:LEU:HD11	1:A:112:GLU:HB3	1.96	0.47
1:A:483:ASN:O	1:A:485:SER:N	2.47	0.47
1:B:1331:ARG:HG3	1:B:1464:LEU:HD22	1.96	0.47
1:A:527:LEU:HD11	1:A:535:GLY:HA3	1.96	0.47
1:B:1288:THR:CG2	1:B:1289:TYR:N	2.68	0.47
1:A:260:GLN:HE22	1:A:399:SER:HA	1.79	0.47
1:B:1170:TYR:OH	1:B:1203:TYR:CZ	2.65	0.47
1:A:653:VAL:HG22	1:A:663:PRO:HD3	1.94	0.47
1:B:1668:TYR:O	1:B:1670:ASN:N	2.47	0.47
1:A:570:LEU:HD22	1:A:574:ASN:HD21	1.78	0.47
1:B:1191:ASP:C	1:B:1193:LYS:H	2.18	0.47
1:A:516:VAL:HG12	1:A:520:ASN:HD21	1.79	0.47
1:B:1643:THR:HB	1:B:1646:ASP:OD2	2.13	0.47
1:B:1474:TYR:CD2	1:B:1474:TYR:C	2.88	0.47
1:B:1516:VAL:HG12	1:B:1520:ASN:HD21	1.79	0.47
1:A:204:LEU:HD13	1:A:204:LEU:O	2.14	0.47
1:A:133:THR:HG23	1:A:137:ASP:OD2	2.14	0.47
1:B:1426:VAL:CG1	1:B:1427:THR:N	2.77	0.47
1:B:1572:LEU:HD21	1:B:1645:PRO:HG3	1.96	0.47
1:A:273:VAL:HA	1:A:276:GLN:CG	2.42	0.47
1:A:588:ARG:O	1:A:589:ALA:C	2.53	0.47
1:B:1094:PHE:CG	1:B:1101:MET:HB2	2.49	0.47
1:A:163:LEU:HD13	1:A:209:LYS:HB3	1.96	0.47
1:A:32:GLN:HE21	1:A:33:TYR:HE2	1.62	0.47
1:B:1279:LYS:HE3	1:B:1279:LYS:CA	2.35	0.47
1:A:157:GLU:HB2	1:A:272:GLN:HE21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1594:GLN:OE1	1:B:1617:VAL:HB	2.14	0.47
1:B:1617:VAL:HG12	1:B:1628:PHE:CD1	2.50	0.47
1:B:1350:LYS:HG2	1:B:1350:LYS:O	2.14	0.47
1:B:1591:LEU:C	1:B:1593:ASP:N	2.68	0.47
1:A:557:TRP:CE3	1:A:558:ILE:HG12	2.49	0.47
1:A:524:GLU:O	1:A:526:LEU:N	2.48	0.47
1:B:1455:VAL:CG1	1:B:1456:VAL:N	2.78	0.47
1:B:1554:PHE:O	1:B:1557:TRP:HB3	2.15	0.47
1:A:94:PHE:CG	1:A:101:MET:HB2	2.50	0.47
1:B:1557:TRP:CE3	1:B:1558:ILE:HG12	2.49	0.47
1:A:101:MET:O	1:A:105:ILE:HG13	2.14	0.47
1:A:356:TYR:CE2	1:A:391:ASN:OD1	2.67	0.47
1:B:1589:ALA:O	1:B:1592:LYS:HB2	2.15	0.47
1:B:1594:GLN:CG	1:B:1625:GLU:HG3	2.44	0.47
1:A:657:GLU:HB2	1:A:659:ILE:HG22	1.96	0.47
1:B:1570:LEU:HD23	1:B:1574:ASN:HD21	1.80	0.47
1:B:1356:TYR:CE2	1:B:1391:ASN:OD1	2.67	0.47
1:A:170:TYR:CB	1:A:202:MET:SD	3.03	0.47
1:A:540:THR:O	1:A:544:LYS:HB3	2.15	0.46
1:B:1041:GLN:HB2	1:B:1043:TRP:CE2	2.50	0.46
1:A:524:GLU:C	1:A:526:LEU:N	2.67	0.46
1:A:455:VAL:HG12	1:A:456:VAL:N	2.28	0.46
1:B:1368:VAL:HB	1:B:1371:ARG:HD2	1.97	0.46
1:B:1224:THR:HA	1:B:1227:THR:HG23	1.96	0.46
1:A:248:ILE:HD12	1:A:248:ILE:HA	1.74	0.46
1:A:50:VAL:HG22	1:A:99:ILE:HD11	1.97	0.46
1:A:110:LYS:HG2	1:A:113:ARG:NH2	2.30	0.46
1:B:1045:HIS:ND1	1:B:1052:PHE:HD1	2.14	0.46
1:A:45:HIS:ND1	1:A:52:PHE:HD1	2.13	0.46
1:B:1654:MET:HA	1:B:1654:MET:HE2	1.95	0.46
1:B:1439:LEU:O	1:B:1445:VAL:HA	2.15	0.46
1:B:1342:THR:HB	1:B:1405:ARG:HA	1.98	0.46
1:A:476:MET:SD	1:A:501:VAL:HG21	2.56	0.46
1:B:1248:ILE:HD12	1:B:1248:ILE:HA	1.77	0.46
1:A:368:VAL:HB	1:A:371:ARG:HG3	1.97	0.46
1:A:224:THR:HA	1:A:227:THR:HG23	1.97	0.46
1:B:1659:ILE:HG23	1:B:1659:ILE:O	2.16	0.46
1:A:590:LEU:N	1:A:590:LEU:HD12	2.30	0.46
1:B:1332:PRO:HD2	1:B:1468:TRP:CH2	2.50	0.46
1:B:1110:LYS:HG2	1:B:1113:ARG:NH2	2.31	0.46
1:A:615:THR:HA	1:A:629:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:GLN:O	1:B:1084:ARG:HB2	2.16	0.46
1:B:1667:LEU:HD13	1:B:1677:PHE:CE1	2.51	0.46
1:A:325:MET:HE3	1:A:336:LYS:HB3	1.97	0.46
1:B:1198:LEU:O	1:B:1200:LYS:N	2.49	0.46
1:A:474:TYR:CD2	1:A:474:TYR:C	2.89	0.46
1:A:613:THR:OG1	1:A:631:VAL:HG23	2.16	0.46
1:A:336:LYS:HD3	1:A:339:VAL:HG21	1.98	0.45
1:B:1615:THR:HG23	1:B:1629:HIS:O	2.16	0.45
1:A:368:VAL:HB	1:A:371:ARG:HD2	1.97	0.45
1:B:1214:VAL:HG11	1:B:1297:ASN:ND2	2.31	0.45
1:A:597:GLY:HA3	1:A:665:LYS:CB	2.31	0.45
1:B:1669:PRO:O	1:B:1670:ASN:HB2	2.16	0.45
1:B:1325:MET:HE3	1:B:1336:LYS:HB3	1.99	0.45
1:A:455:VAL:CG1	1:A:456:VAL:N	2.79	0.45
1:A:41:GLN:HB2	1:A:43:TRP:CE2	2.51	0.45
1:B:1310:GLN:HE21	1:B:1446:ILE:HG12	1.81	0.45
1:B:1592:LYS:CA	1:B:1625:GLU:OE1	2.65	0.45
1:A:142:LEU:HD23	1:A:262:TRP:CD2	2.51	0.45
1:B:1336:LYS:HD3	1:B:1339:VAL:HG21	1.97	0.45
1:A:587:GLU:OE1	1:A:588:ARG:NH1	2.49	0.45
1:B:1368:VAL:HB	1:B:1371:ARG:HG3	1.97	0.45
1:B:1532:SER:C	1:B:1534:ASP:H	2.19	0.45
1:A:612:ILE:N	1:A:612:ILE:CD1	2.77	0.45
1:A:679:LYS:HG3	1:A:680:TYR:N	2.31	0.45
1:A:83:ILE:HA	1:A:83:ILE:HD13	1.80	0.45
1:A:221:LEU:HD13	1:A:304:ARG:HB3	1.98	0.45
1:A:288:THR:CG2	1:A:289:TYR:N	2.67	0.45
1:A:524:GLU:HA	1:A:528:GLY:O	2.16	0.45
1:A:157:GLU:HB2	1:A:272:GLN:NE2	2.32	0.45
1:B:1625:GLU:N	1:B:1626:PRO:CD	2.79	0.45
1:A:170:TYR:OH	1:A:203:TYR:CE2	2.69	0.45
1:B:1335:LEU:O	1:B:1457:VAL:HA	2.16	0.45
1:A:599:PHE:CE1	1:A:667:LEU:HD13	2.51	0.45
1:A:439:LEU:O	1:A:445:VAL:HA	2.17	0.45
1:B:1523:GLY:O	1:B:1527:LEU:N	2.46	0.45
1:B:1547:ILE:HG12	1:B:1548:ASN:N	2.31	0.45
1:A:244:GLN:HG2	1:A:475:ASN:OD1	2.17	0.45
1:B:1099:ILE:HD12	1:B:1099:ILE:H	1.82	0.45
1:B:1097:ASP:N	1:B:1098:PRO:HD3	2.32	0.45
1:B:1349:VAL:HG12	1:B:1351:LEU:HG	2.00	0.44
1:A:398:GLY:O	1:A:399:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1635:THR:HG23	1:B:1637:LYS:H	1.82	0.44
1:B:1600:LEU:O	1:B:1614:PHE:HA	2.17	0.44
1:A:170:TYR:HB2	1:A:202:MET:SD	2.57	0.44
1:A:177:LEU:HD23	1:A:180:ARG:HH21	1.82	0.44
1:B:1477:LEU:HD13	1:B:1491:PRO:HB2	1.98	0.44
1:B:1532:SER:C	1:B:1534:ASP:N	2.70	0.44
1:A:669:PRO:O	1:A:670:ASN:HB2	2.18	0.44
1:A:80:GLN:O	1:A:84:ARG:HB2	2.17	0.44
1:A:214:VAL:HG11	1:A:297:ASN:ND2	2.32	0.44
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.74	0.44
1:B:1512:ARG:CD	1:B:1573:TRP:O	2.66	0.44
1:B:1366:LYS:HE3	1:B:1367:ASP:OD2	2.16	0.44
1:A:427:THR:CG2	1:A:427:THR:O	2.65	0.44
1:B:1625:GLU:N	1:B:1626:PRO:HD2	2.32	0.44
1:A:248:ILE:HG13	1:A:472:LEU:HD23	2.00	0.44
1:B:1495:TRP:CE2	1:B:1499:SER:HB3	2.53	0.44
1:A:609:GLU:HB3	1:A:636:LYS:NZ	2.33	0.44
1:A:325:MET:HE3	1:A:339:VAL:CB	2.47	0.44
1:B:1142:LEU:HD23	1:B:1262:TRP:CZ3	2.53	0.44
1:A:331:ARG:HG3	1:A:464:LEU:HD22	1.99	0.44
1:A:478:VAL:HG12	1:A:479:ALA:H	1.83	0.44
1:B:1667:LEU:HD12	1:B:1667:LEU:HA	1.72	0.44
1:A:275:GLN:HE21	1:A:275:GLN:CA	2.31	0.44
1:A:668:TYR:O	1:A:670:ASN:N	2.49	0.44
1:B:1643:THR:O	1:B:1647:ILE:HG13	2.18	0.44
1:B:1003:GLN:N	1:B:1039:GLU:OE1	2.39	0.44
1:B:1198:LEU:C	1:B:1200:LYS:N	2.71	0.44
1:A:635:THR:HG23	1:A:637:LYS:H	1.83	0.44
1:B:1032:GLN:HE21	1:B:1033:TYR:HE2	1.62	0.44
1:B:1525:LYS:HG2	1:B:1547:ILE:HD11	2.00	0.44
1:A:606:SER:HG	2:C:440:PTR:P	2.40	0.44
1:A:552:PHE:HD1	1:A:552:PHE:C	2.21	0.44
1:A:668:TYR:HB3	1:A:669:PRO:CD	2.35	0.44
1:B:1364:PHE:O	1:B:1365:ASP:HB2	2.18	0.44
1:B:1654:MET:HE1	1:B:1660:PRO:HD3	1.99	0.44
1:A:575:ASP:OD2	1:A:680:TYR:OH	2.33	0.44
1:B:1194:GLN:O	1:B:1195:GLU:CB	2.66	0.43
1:A:169:GLU:O	1:A:172:PHE:HB3	2.18	0.43
1:A:643:THR:O	1:A:647:ILE:HG13	2.18	0.43
1:B:1599:PHE:CD1	1:B:1666:TYR:O	2.71	0.43
1:B:1512:ARG:HD2	1:B:1574:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1145:LYS:HB3	1:B:1227:THR:HB	1.99	0.43
1:A:469:ALA:HB2	1:A:555:TRP:CD1	2.53	0.43
1:B:1552:PHE:HZ	1:B:1605:GLU:O	2.02	0.43
1:B:1169:GLU:O	1:B:1172:PHE:HB3	2.19	0.43
1:A:12:SER:HA	1:A:15:LEU:CG	2.48	0.43
1:A:76:ASN:O	1:A:80:GLN:HG3	2.18	0.43
1:A:160:ILE:CD1	1:A:213:VAL:HG11	2.48	0.43
1:A:532:SER:OG	1:A:533:PRO:HD2	2.18	0.43
1:B:1596:PRO:HG3	1:B:1619:ARG:HG2	2.00	0.43
1:A:97:ASP:N	1:A:98:PRO:HD3	2.33	0.43
1:A:349:VAL:HG12	1:A:351:LEU:HG	2.00	0.43
1:A:501:VAL:O	1:A:504:TRP:HB2	2.18	0.43
1:B:1012:SER:HA	1:B:1015:LEU:CG	2.48	0.43
1:B:1291:HIS:HA	1:B:1296:LYS:HZ3	1.83	0.43
1:A:369:ASN:HB3	1:A:373:THR:OG1	2.18	0.43
1:A:189:LYS:O	1:A:193:LYS:HG2	2.18	0.43
1:A:570:LEU:HD23	1:A:574:ASN:HD21	1.84	0.43
1:A:99:ILE:HD12	1:A:99:ILE:H	1.82	0.43
1:A:506:PHE:C	1:A:508:SER:H	2.21	0.43
1:B:1643:THR:CG2	1:B:1645:PRO:CD	2.90	0.43
1:B:1204:LEU:HD22	1:B:1204:LEU:HA	1.90	0.43
1:B:1046:ALA:O	1:B:1053:ALA:HB2	2.19	0.43
1:A:413:LYS:O	1:A:414:ASN:ND2	2.50	0.43
1:A:148:ASN:O	1:A:149:VAL:C	2.57	0.43
1:B:1231:LEU:HD21	1:B:1263:PHE:CD1	2.53	0.43
1:A:225:GLU:HB2	1:A:308:LEU:HD21	2.00	0.43
1:B:1364:PHE:CD1	1:B:1433:LEU:HD23	2.46	0.43
1:A:196:GLN:O	1:A:199:LEU:HB2	2.19	0.43
1:B:1478:VAL:HG12	1:B:1479:ALA:H	1.82	0.43
1:A:634:TYR:HB3	1:A:639:LEU:CD1	2.49	0.43
1:A:477:LEU:HD13	1:A:491:PRO:HB2	2.00	0.43
1:B:1101:MET:O	1:B:1105:ILE:HG13	2.18	0.43
1:B:1473:TRP:CE2	1:B:1539:TRP:HB2	2.54	0.43
1:A:361:LYS:HG3	1:A:436:GLU:HB2	2.01	0.43
1:A:512:ARG:HD3	1:A:573:TRP:O	2.19	0.42
1:A:123:ASN:C	1:A:125:ALA:H	2.23	0.42
1:B:1369:ASN:HB3	1:B:1373:THR:OG1	2.19	0.42
1:B:1011:ASP:C	1:B:1013:LYS:H	2.22	0.42
1:A:473:TRP:NE1	1:A:539:TRP:HB2	2.35	0.42
1:A:522:LEU:HD21	1:A:581:PHE:CD2	2.54	0.42
1:B:1441:GLN:CB	1:B:1442:PRO:CD	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:HA	1:A:436:GLU:O	2.20	0.42
1:A:260:GLN:O	1:A:264:THR:HB	2.19	0.42
1:B:1012:SER:HA	1:B:1015:LEU:CD1	2.48	0.42
1:B:1480:GLU:HG3	1:B:1480:GLU:H	1.70	0.42
1:A:16:GLU:O	1:A:19:HIS:HB2	2.20	0.42
1:A:478:VAL:HG12	1:A:480:GLU:H	1.83	0.42
1:A:120:GLN:C	1:A:122:PHE:N	2.72	0.42
1:A:256:LEU:O	1:A:259:LEU:N	2.52	0.42
1:B:1122:PHE:O	1:B:1123:ASN:HB2	2.20	0.42
1:A:594:GLN:NE2	1:A:670:ASN:ND2	2.67	0.42
1:B:1592:LYS:HA	1:B:1625:GLU:CD	2.39	0.42
1:B:1325:MET:HE3	1:B:1339:VAL:CB	2.46	0.42
1:A:163:LEU:HD13	1:A:209:LYS:CB	2.48	0.42
1:B:1231:LEU:HD11	1:B:1263:PHE:CE1	2.54	0.42
1:B:1625:GLU:HB3	1:B:1626:PRO:HD3	2.01	0.42
1:B:1325:MET:CE	1:B:1336:LYS:HB3	2.49	0.42
1:A:11:ASP:C	1:A:13:LYS:H	2.22	0.42
1:B:1224:THR:CA	1:B:1227:THR:HG23	2.50	0.42
1:A:115:ILE:O	1:A:119:ALA:HB2	2.20	0.42
1:B:1115:ILE:O	1:B:1119:ALA:HB2	2.20	0.42
1:B:1506:PHE:C	1:B:1508:SER:H	2.23	0.42
1:B:1515:ASN:OD1	1:B:1518:GLN:HG3	2.19	0.42
1:A:668:TYR:C	1:A:670:ASN:H	2.23	0.42
1:B:1483:ASN:C	1:B:1485:SER:N	2.73	0.42
1:A:218:ILE:O	1:A:219:GLU:C	2.58	0.42
1:B:1478:VAL:HG12	1:B:1480:GLU:H	1.84	0.42
1:A:616:TRP:CZ2	1:A:663:PRO:HG3	2.55	0.42
1:A:521:MET:SD	1:A:581:PHE:HB3	2.60	0.42
1:B:1277:LEU:HA	1:B:1277:LEU:HD23	1.77	0.42
1:A:139:GLN:O	1:A:143:ASP:OD2	2.38	0.42
1:A:591:LEU:HB3	1:A:617:VAL:CG2	2.49	0.42
1:A:643:THR:CG2	1:A:645:PRO:CD	2.92	0.42
1:B:1616:TRP:HE1	1:B:1618:GLU:CD	2.23	0.42
1:B:1007:LEU:C	1:B:1009:GLN:H	2.23	0.42
1:A:659:ILE:HG23	1:A:659:ILE:O	2.19	0.42
1:A:594:GLN:HE21	1:A:670:ASN:ND2	2.17	0.42
1:B:1316:SER:OG	1:B:1347:LEU:HG	2.20	0.42
1:B:1007:LEU:HD23	1:B:1116:LEU:HD21	2.02	0.42
1:A:142:LEU:HD23	1:A:262:TRP:CH2	2.55	0.42
1:B:1076:ASN:OD1	1:B:1079:LEU:HG	2.20	0.42
1:A:76:ASN:OD1	1:A:79:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HA	1:A:280:LEU:HD23	1.88	0.42
1:B:1164:GLU:OE1	1:B:1279:LYS:HD3	2.19	0.42
1:A:12:SER:HA	1:A:15:LEU:CD1	2.49	0.42
1:B:1682:SER:O	1:B:1683:ARG:OXT	2.37	0.41
1:B:1593:ASP:OD2	1:B:1593:ASP:C	2.58	0.41
1:B:1031:ARG:HA	1:B:1038:LEU:CD1	2.50	0.41
1:B:1299:GLN:O	1:B:1300:VAL:C	2.58	0.41
1:A:552:PHE:H	1:A:608:ARG:CD	2.34	0.41
1:A:7:LEU:C	1:A:9:GLN:H	2.22	0.41
1:B:1331:ARG:HD3	1:B:1468:TRP:HB2	2.02	0.41
1:B:1366:LYS:O	1:B:1368:VAL:HG23	2.20	0.41
1:B:1634:TYR:HB3	1:B:1639:LEU:CD1	2.50	0.41
1:B:1041:GLN:HE21	1:B:1056:ARG:HE	1.69	0.41
1:B:1314:GLN:HG2	1:B:1448:LEU:HD23	2.02	0.41
1:B:1430:LEU:HD13	1:B:1454:PRO:HB2	2.02	0.41
1:A:600:LEU:HD12	1:A:601:LEU:N	2.36	0.41
1:A:226:LEU:C	1:A:226:LEU:HD23	2.41	0.41
1:A:235:GLU:HB3	1:A:259:LEU:HD21	2.02	0.41
1:A:495:TRP:CE2	1:A:499:SER:HB3	2.54	0.41
1:B:1280:LEU:HD23	1:B:1280:LEU:HA	1.83	0.41
1:B:1016:GLU:O	1:B:1019:HIS:HB2	2.20	0.41
1:A:378:ARG:CD	1:A:413:LYS:NZ	2.82	0.41
1:A:364:PHE:HB2	1:A:382:ILE:CD1	2.47	0.41
1:A:512:ARG:HD2	1:A:574:ASN:O	2.20	0.41
1:A:231:LEU:HD11	1:A:263:PHE:CE1	2.56	0.41
1:B:1393:GLU:O	1:B:1398:GLY:HA2	2.21	0.41
1:B:1275:GLN:CA	1:B:1275:GLN:HE21	2.31	0.41
1:B:1599:PHE:HB3	1:B:1616:TRP:HB3	2.02	0.41
1:B:1625:GLU:O	1:B:1626:PRO:C	2.58	0.41
1:A:336:LYS:HA	1:A:458:ILE:HG13	2.01	0.41
1:A:193:LYS:C	1:A:195:GLU:H	2.23	0.41
1:B:1256:LEU:O	1:B:1257:ASP:C	2.59	0.41
1:B:1306:PHE:HE1	1:B:1444:LEU:CD1	2.33	0.41
1:A:325:MET:CE	1:A:339:VAL:HG11	2.50	0.41
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.79	0.41
1:B:1083:ILE:HD13	1:B:1083:ILE:HA	1.81	0.41
1:B:1572:LEU:N	1:B:1572:LEU:HD12	2.36	0.41
1:B:1437:THR:CG2	1:B:1448:LEU:HD12	2.50	0.41
1:A:314:GLN:HA	1:A:448:LEU:HD22	2.02	0.41
1:A:45:HIS:CG	1:A:52:PHE:HD1	2.38	0.41
1:B:1148:ASN:O	1:B:1149:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1398:GLY:O	1:B:1399:SER:HB3	2.21	0.41
1:A:204:LEU:HD22	1:A:204:LEU:HA	1.90	0.41
1:B:1075:ASN:O	1:B:1077:PHE:N	2.53	0.41
1:B:1668:TYR:C	1:B:1670:ASN:H	2.22	0.41
1:B:1045:HIS:CG	1:B:1052:PHE:HD1	2.39	0.41
1:A:231:LEU:HD11	1:A:263:PHE:CD1	2.56	0.41
1:B:1495:TRP:CZ2	1:B:1499:SER:HB3	2.56	0.41
1:B:1547:ILE:CG2	1:B:1550:LYS:HD3	2.39	0.41
1:A:341:PHE:CE1	1:A:407:LEU:HB3	2.55	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.86	0.41
1:B:1166:LEU:HD23	1:B:1166:LEU:HA	1.73	0.41
1:B:1425:ILE:O	1:B:1426:VAL:O	2.39	0.40
1:A:579:MET:HG2	1:A:582:ILE:HG13	2.03	0.40
1:B:1210:ARG:HD3	1:B:1294:ILE:HG13	2.04	0.40
1:A:164:GLU:OE1	1:A:279:LYS:HD3	2.21	0.40
1:A:472:LEU:HD22	1:A:501:VAL:CG1	2.50	0.40
1:A:430:LEU:C	1:A:431:HIS:HD2	2.24	0.40
1:A:554:PHE:O	1:A:557:TRP:N	2.54	0.40
1:A:634:TYR:HB3	1:A:639:LEU:HD11	2.02	0.40
1:B:1231:LEU:HD11	1:B:1263:PHE:CD1	2.57	0.40
1:A:568:HIS:O	1:A:569:LEU:HD23	2.21	0.40
1:A:494:ARG:O	1:A:497:GLN:N	2.41	0.40
1:B:1642:VAL:HG12	1:B:1647:ILE:HG13	2.02	0.40
1:B:1579:MET:HB3	1:B:1582:ILE:HD11	2.03	0.40
1:A:579:MET:HG2	1:A:582:ILE:CG1	2.52	0.40
1:A:11:ASP:HB2	1:A:14:PHE:CE1	2.56	0.40
1:B:1544:LYS:HB2	1:B:1544:LYS:HZ2	1.85	0.40
1:A:121:ARG:C	1:A:123:ASN:N	2.74	0.40
1:B:1099:ILE:O	1:B:1103:MET:HG3	2.21	0.40
1:A:616:TRP:CD1	1:A:663:PRO:HB2	2.56	0.40
1:A:594:GLN:NE2	1:A:670:ASN:HD21	2.19	0.40
1:B:1617:VAL:CG1	1:B:1628:PHE:HD1	2.35	0.40
1:B:1325:MET:CE	1:B:1339:VAL:HG11	2.51	0.40
1:A:430:LEU:HD13	1:A:454:PRO:HB2	2.03	0.40
1:B:1375:LYS:C	1:B:1377:PHE:H	2.25	0.40
1:B:1341:PHE:CE1	1:B:1407:LEU:HB3	2.57	0.40
1:A:325:MET:CE	1:A:336:LYS:HB3	2.51	0.40
1:A:11:ASP:HB2	1:A:14:PHE:HE1	1.87	0.40
1:B:1256:LEU:O	1:B:1259:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/683 (94%)	525 (82%)	92 (14%)	23 (4%)	4	24
1	B	643/683 (94%)	520 (81%)	91 (14%)	32 (5%)	3	15
2	C	3/5 (60%)	3 (100%)	0	0	100	100
2	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1289/1376 (94%)	1051 (82%)	183 (14%)	55 (4%)	3	19

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	THR
1	B	1426	VAL
1	B	1547	ILE
1	B	1548	ASN
1	B	1595	GLN
1	B	1596	PRO
1	B	1627	ASP
1	A	12	SER
1	A	134	VAL
1	A	483	ASN
1	A	484	LEU
1	B	1012	SER
1	B	1195	GLU
1	B	1298	LYS
1	B	1483	ASN
1	B	1484	LEU
1	B	1623	GLY
1	A	257	ASP
1	A	298	LYS
1	A	332	PRO
1	A	333	LEU
1	A	353	GLU

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Mol	Chain	Res	Type
1	A	373	THR
1	A	377	PHE
1	A	394	GLU
1	A	507	SER
1	A	593	ASP
1	A	598	THR
1	B	1192	GLN
1	B	1199	LEU
1	B	1257	ASP
1	B	1332	PRO
1	B	1353	GLU
1	B	1373	THR
1	B	1377	PHE
1	B	1394	GLU
1	B	1507	SER
1	B	1527	LEU
1	A	20	GLN
1	A	525	LYS
1	B	1020	GLN
1	B	1333	LEU
1	B	1626	PRO
1	B	1639	LEU
1	A	491	PRO
1	B	1491	PRO
1	A	76	ASN
1	A	189	LYS
1	B	1076	ASN
1	B	1350	LYS
1	A	223	VAL
1	B	1223	VAL
1	B	1423	PRO
1	A	626	PRO
1	B	1624	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	599/634 (94%)	549 (92%)	50 (8%)	14	46
1	B	603/634 (95%)	549 (91%)	54 (9%)	12	41
2	C	4/4 (100%)	4 (100%)	0	100	100
2	D	4/4 (100%)	4 (100%)	0	100	100
All	All	1210/1276 (95%)	1106 (91%)	104 (9%)	13	44

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	24	ASP
1	A	31	ARG
1	A	93	ASN
1	A	100	GLN
1	A	108	CYS
1	A	110	LYS
1	A	118	ASN
1	A	121	ARG
1	A	134	VAL
1	A	154	MET
1	A	170	TYR
1	A	202	MET
1	A	204	LEU
1	A	226	LEU
1	A	227	THR
1	A	236	LEU
1	A	241	ARG
1	A	275	GLN
1	A	279	LYS
1	A	302	TRP
1	A	308	LEU
1	A	331	ARG
1	A	337	THR
1	A	340	GLN
1	A	342	THR
1	A	354	LEU
1	A	355	ASN
1	A	379	LYS
1	A	396	THR
1	A	434	SER
1	A	466	SER
1	A	480	GLU

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Mol	Chain	Res	Type
1	A	482	ARG
1	A	483	ASN
1	A	498	LEU
1	A	507	SER
1	A	521	MET
1	A	536	LEU
1	A	539	TRP
1	A	552	PHE
1	A	586	ARG
1	A	588	ARG
1	A	602	ARG
1	A	612	ILE
1	A	631	VAL
1	A	632	GLU
1	A	636	LYS
1	A	645	PRO
1	A	683	ARG
1	B	1012	SER
1	B	1024	ASP
1	B	1031	ARG
1	B	1093	ASN
1	B	1100	GLN
1	B	1110	LYS
1	B	1118	ASN
1	B	1135	MET
1	B	1154	MET
1	B	1170	TYR
1	B	1197	LEU
1	B	1202	MET
1	B	1204	LEU
1	B	1226	LEU
1	B	1227	THR
1	B	1236	LEU
1	B	1241	ARG
1	B	1275	GLN
1	B	1279	LYS
1	B	1302	TRP
1	B	1308	LEU
1	B	1331	ARG
1	B	1337	THR
1	B	1340	GLN
1	B	1342	THR

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Mol	Chain	Res	Type
1	B	1354	LEU
1	B	1355	ASN
1	B	1379	LYS
1	B	1396	THR
1	B	1409	LEU
1	B	1411	GLU
1	B	1424	LEU
1	B	1427	THR
1	B	1428	GLU
1	B	1434	SER
1	B	1466	SER
1	B	1480	GLU
1	B	1482	ARG
1	B	1483	ASN
1	B	1498	LEU
1	B	1507	SER
1	B	1539	TRP
1	B	1546	ASN
1	B	1582	ILE
1	B	1586	ARG
1	B	1596	PRO
1	B	1600	LEU
1	B	1612	ILE
1	B	1617	VAL
1	B	1626	PRO
1	B	1631	VAL
1	B	1632	GLU
1	B	1636	LYS
1	B	1645	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	GLN
1	A	41	GLN
1	A	67	GLN
1	A	82	ASN
1	A	93	ASN
1	A	118	ASN
1	A	222	ASN
1	A	228	GLN

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	243	GLN
1	A	260	GLN
1	A	271	GLN
1	A	272	GLN
1	A	276	GLN
1	A	297	ASN
1	A	340	GLN
1	A	355	ASN
1	A	381	ASN
1	A	397	ASN
1	A	406	HIS
1	A	408	GLN
1	A	412	GLN
1	A	414	ASN
1	A	438	GLN
1	A	505	GLN
1	A	520	ASN
1	A	574	ASN
1	A	594	GLN
1	A	595	GLN
1	A	621	GLN
1	A	662	ASN
1	B	1041	GLN
1	B	1067	GLN
1	B	1082	ASN
1	B	1093	ASN
1	B	1118	ASN
1	B	1208	ASN
1	B	1222	ASN
1	B	1228	GLN
1	B	1229	ASN
1	B	1243	GLN
1	B	1260	GLN
1	B	1271	GLN
1	B	1272	GLN
1	B	1275	GLN
1	B	1276	GLN
1	B	1310	GLN
1	B	1340	GLN
1	B	1355	ASN
1	B	1381	ASN

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Mol	Chain	Res	Type
1	B	1397	ASN
1	B	1406	HIS
1	B	1438	GLN
1	B	1505	GLN
1	B	1520	ASN
1	B	1546	ASN
1	B	1629	HIS
1	B	1662	ASN
1	B	1670	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PTR	C	440	2	14,16,17	1.10	0	18,22,24	1.15	1 (5%)
2	PTR	D	1440	2	14,16,17	1.14	1 (7%)	18,22,24	1.87	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	C	440	2	-	0/9/11/13	0/1/1/1
2	PTR	D	1440	2	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1440	PTR	CE1-CZ	2.09	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1440	PTR	O-C-CA	-6.16	109.44	125.49
2	D	1440	PTR	CD2-CE2-CZ	-2.46	116.65	119.74
2	C	440	PTR	CD2-CE2-CZ	-2.43	116.69	119.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	440	PTR	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	652/683 (95%)	-0.24	11 (1%) 73 45	41, 70, 112, 144	0
1	B	653/683 (95%)	-0.23	21 (3%) 51 23	29, 68, 131, 150	0
2	C	4/5 (80%)	-0.60	0 100 100	53, 58, 59, 60	0
2	D	4/5 (80%)	-0.25	0 100 100	87, 89, 89, 90	0
All	All	1313/1376 (95%)	-0.23	32 (2%) 62 32	29, 69, 122, 150	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1594	GLN	4.8
1	B	1182	HIS	4.4
1	A	621	GLN	3.1
1	A	396	THR	3.0
1	B	1394	GLU	3.0
1	A	124	GLN	2.9
1	B	1253	ASN	2.7
1	B	1425	ILE	2.6
1	B	1626	PRO	2.6
1	A	619	ARG	2.6
1	A	370	GLU	2.6
1	B	1622	ASN	2.6
1	B	1180	ARG	2.5
1	B	1024	ASP	2.5
1	B	1196	GLN	2.4
1	A	384	GLY	2.4
1	B	1551	ASN	2.4
1	B	1656	ALA	2.3
1	B	1068	TYR	2.3
1	B	1199	LEU	2.3
1	A	397	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1014	PHE	2.3
1	B	1012	SER	2.2
1	B	1052	PHE	2.1
1	A	530	ASN	2.1
1	B	1010	LEU	2.1
1	A	683	ARG	2.1
1	A	373	THR	2.1
1	A	123	ASN	2.0
1	B	1193	LYS	2.0
1	B	1291	HIS	2.0
1	B	1620	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PTR	C	440	16/17	0.93	0.20	-	36,47,59,61	0
2	PTR	D	1440	16/17	0.94	0.13	-	48,52,55,62	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	AU	A	2001	1/1	0.98	0.25	-	24,24,24,24	1
3	AU	B	2002	1/1	0.95	0.27	-	6,6,6,6	1

6.5 Other polymers [i](#)

There are no such residues in this entry.