



Full wwPDB X-ray Structure Validation Report i

Sep 13, 2020 – 10:05 AM BST

PDB ID : 1XYZ
Title : Structures of Yeast Ribonucleotide Reductase I
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Deposited on : 2005-06-13
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

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

MolProbit	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

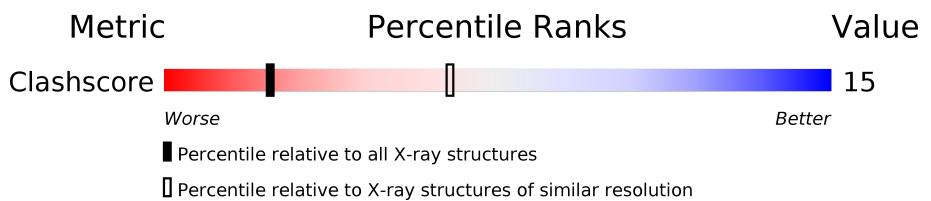
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	888	 64% 23% • 13%
1	B	888	 64% 22% • 13%

2 Entry composition [\(i\)](#)

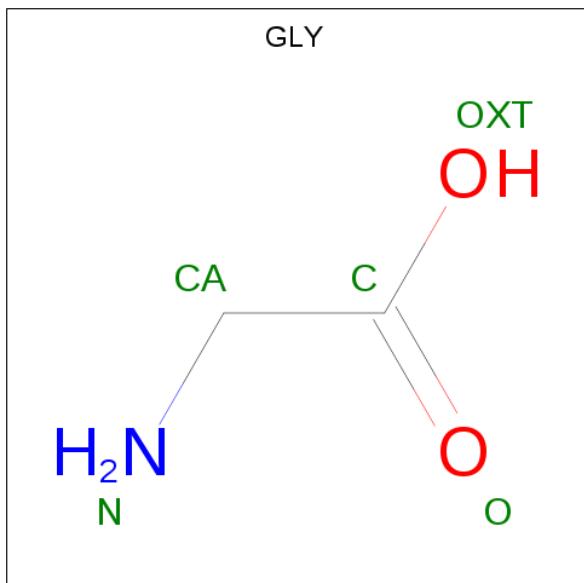
There are 2 unique types of molecules in this entry. The entry contains 12275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C 6159	N 3913	O 1049	S 1162	35	0	0
1	B	769	Total	C 6108	N 3882	O 1040	S 1151	35	0	0

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



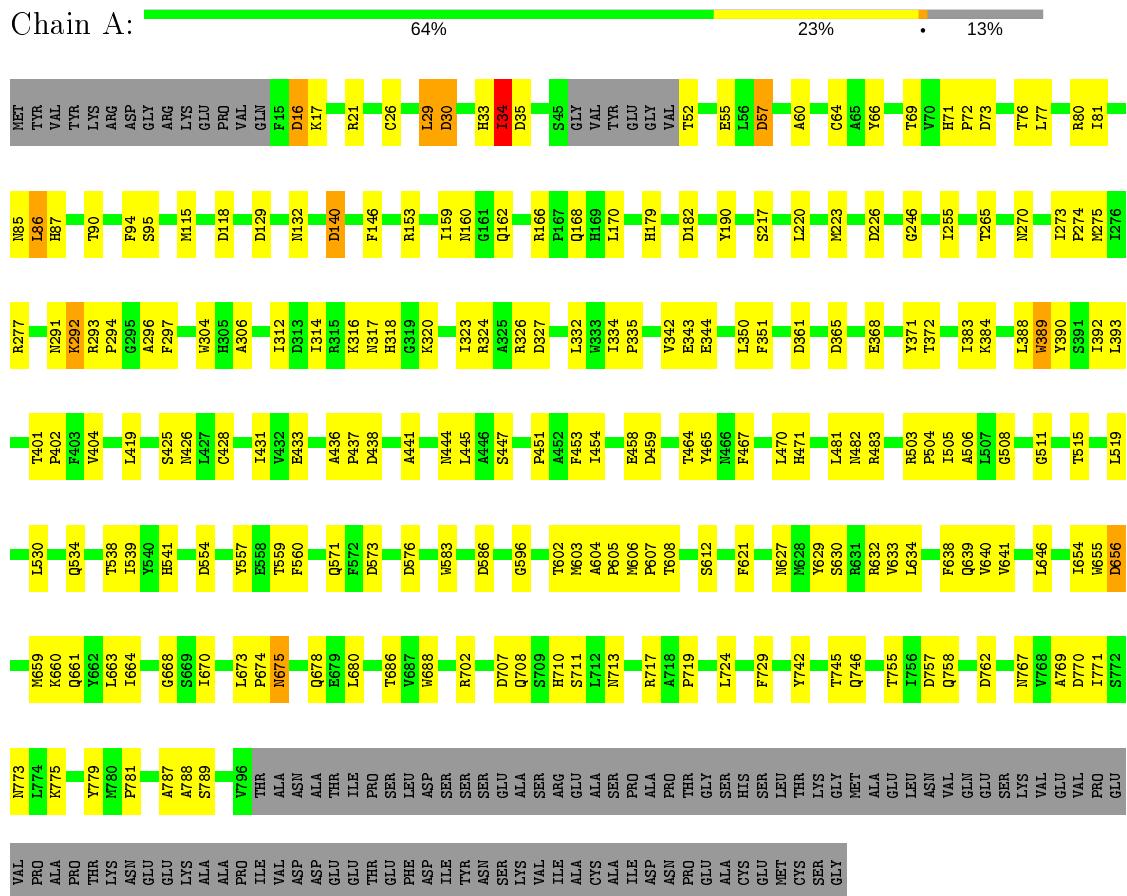
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C 4	N 2	O 1	1	0
2	A	1	Total	C 4	N 2	O 1	1	0

3 Residue-property plots [\(i\)](#)

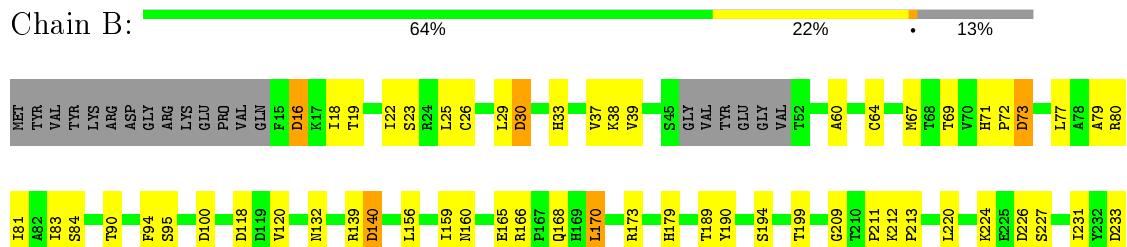
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

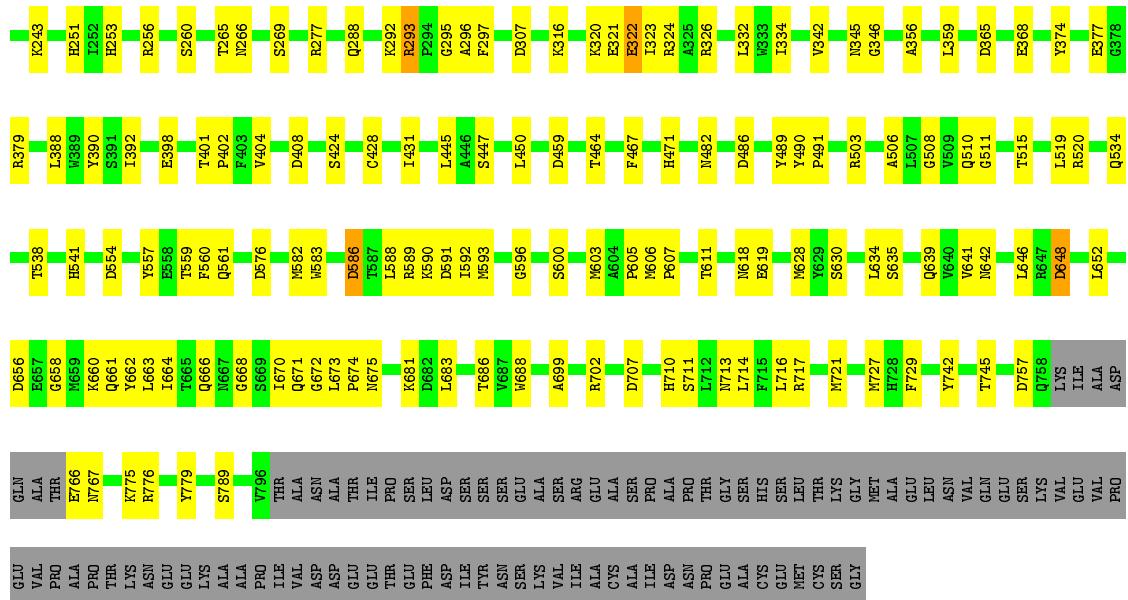
Note EDS failed to run properly.

- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1





4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	433.70 Å 433.70 Å 433.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.4 (50.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ ¹	7.21 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.217 , 0.257	Depositor
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning ²	$< L > = 0.53, < L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12275	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.64	1/6296 (0.0%)	0.91	27/8531 (0.3%)
1	B	0.62	0/6244	0.86	19/8459 (0.2%)
All	All	0.63	1/12540 (0.0%)	0.88	46/16990 (0.3%)

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	7
1	B	0	5
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	TRP	C-N	5.91	1.47	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ILE	O-C-N	-8.58	108.97	122.70
1	B	16	ASP	CB-CG-OD2	7.38	124.94	118.30
1	B	586	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	118	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	226	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	675	ASN	CB-CG-ND2	-6.72	100.57	116.70
1	A	140	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	170	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	182	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	530	LEU	CA-CB-CG	6.57	130.42	115.30
1	B	554	ASP	CB-CG-OD2	6.50	124.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	140	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	438	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	390	TYR	N-CA-CB	5.92	121.25	110.60
1	A	30	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	226	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	86	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	57	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	762	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	100	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	573	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	389	TRP	CA-C-N	-5.62	104.83	117.20
1	A	675	ASN	OD1-CG-ND2	-5.58	109.06	121.90
1	B	576	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	757	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	118	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	170	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	307	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	428	CYS	C-N-CA	-5.33	108.37	121.70
1	B	459	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	576	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	586	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	16	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	29	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	129	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	408	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	30	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	428	CYS	C-N-CA	-5.10	108.94	121.70
1	A	327	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	554	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	361	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	73	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	648	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	365	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	591	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASP	Peptide
1	A	265	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	292	LYS	Peptide
1	A	34	ILE	Mainchain
1	A	656	ASP	Peptide
1	A	674	PRO	Peptide
1	A	675	ASN	Sidechain
1	B	265	THR	Peptide
1	B	266	ASN	Peptide
1	B	293	ARG	Peptide
1	B	321	GLU	Peptide
1	B	322	GLU	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6159	0	6095	189	0
1	B	6108	0	6041	167	0
2	A	8	0	4	2	0
All	All	12275	0	12140	356	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 15.

All (356) 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:220:LEU:CD2	1:A:431:ILE:HD11	1.79	1.13
1:A:220:LEU:HD21	1:A:431:ILE:CD1	1.84	1.07
1:B:464:THR:HG21	1:B:789:SER:HB3	1.43	0.99
1:A:179:HIS:HD2	1:A:483:ARG:HH11	1.06	0.98
1:A:220:LEU:HD21	1:A:431:ILE:HD11	0.98	0.97
1:B:464:THR:CG2	1:B:789:SER:HB3	1.96	0.96
1:A:447:SER:HB3	1:A:606:MET:CE	1.97	0.95
1:A:179:HIS:CD2	1:A:483:ARG:HH11	1.86	0.94
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.50	0.91
1:A:153:ARG:HH22	1:A:632:ARG:HH11	1.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:HB3	1:A:85:ASN:HD21	1.37	0.90
1:B:277:ARG:HB2	1:B:277:ARG:HH11	1.36	0.89
1:B:316:LYS:O	1:B:324:ARG:HD3	1.73	0.88
1:B:95:SER:H	1:B:132:ASN:HD21	1.22	0.86
1:A:717:ARG:O	1:A:719:PRO:HD3	1.75	0.86
1:A:179:HIS:HD2	1:A:483:ARG:NH1	1.73	0.85
1:B:377:GLU:HG3	1:B:379:ARG:HD3	1.61	0.82
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.62	0.81
1:A:538:THR:HB	1:A:583:TRP:NE1	1.96	0.81
1:A:505:ILE:HG22	1:A:602:THR:HA	1.61	0.81
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.63	0.80
1:A:57:ASP:HB3	1:A:85:ASN:ND2	1.97	0.80
1:B:557:TYR:HE1	1:B:559:THR:HG22	1.46	0.79
1:A:90:THR:CG2	1:A:166:ARG:HE	1.96	0.79
1:B:277:ARG:HD2	1:B:322:GLU:CD	2.03	0.79
1:A:787:ALA:O	1:A:788:ALA:HB2	1.84	0.77
1:A:368:GLU:O	1:A:372:THR:HB	1.84	0.77
1:A:538:THR:HB	1:A:583:TRP:HE1	1.48	0.77
1:B:277:ARG:HB2	1:B:277:ARG:NH1	1.98	0.77
1:B:332:LEU:HD11	1:B:392:ILE:HD12	1.65	0.77
1:B:277:ARG:HD2	1:B:322:GLU:OE2	1.87	0.74
1:A:71:HIS:HD2	1:A:73:ASP:HB2	1.52	0.74
1:B:776:ARG:HH11	1:B:776:ARG:HG3	1.53	0.74
1:B:520:ARG:HH11	1:B:520:ARG:HG3	1.51	0.74
1:A:153:ARG:HH22	1:A:632:ARG:NH1	1.84	0.73
1:A:57:ASP:CB	1:A:85:ASN:HD21	2.01	0.73
1:A:317:ASN:HA	1:A:326:ARG:HH21	1.54	0.72
1:A:426:ASN:HB3	1:A:431:ILE:CD1	2.21	0.71
1:B:538:THR:HB	1:B:583:TRP:NE1	2.06	0.71
1:A:320:LYS:H	1:A:320:LYS:HD2	1.56	0.70
1:B:320:LYS:HG3	1:B:323:ILE:HD13	1.74	0.70
1:A:95:SER:H	1:A:132:ASN:HD21	1.39	0.70
1:A:447:SER:HB3	1:A:606:MET:HE1	1.74	0.70
1:A:179:HIS:CD2	1:A:483:ARG:NH1	2.54	0.69
1:A:447:SER:HB3	1:A:606:MET:HE3	1.72	0.69
1:A:481:LEU:HB3	1:A:505:ILE:HG12	1.75	0.69
1:A:81:ILE:O	1:A:85:ASN:HB2	1.94	0.67
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.60	0.67
1:B:260:SER:H	1:B:269:SER:HB3	1.59	0.67
1:A:534:GLN:O	1:A:538:THR:HG22	1.95	0.67
1:A:26:CYS:HB2	1:A:29:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ASN:O	1:B:619:GLU:O	2.12	0.67
1:B:675:ASN:ND2	1:B:675:ASN:H	1.93	0.67
1:A:571:GLN:HE21	1:A:571:GLN:HA	1.60	0.66
1:B:365:ASP:HA	1:B:368:GLU:HB2	1.78	0.66
1:A:153:ARG:NH2	1:A:632:ARG:HH11	1.85	0.66
1:B:94:PHE:HB3	1:B:132:ASN:HD22	1.61	0.66
1:A:770:ASP:O	1:A:771:ILE:HB	1.96	0.65
1:B:538:THR:HB	1:B:583:TRP:HE1	1.60	0.65
1:A:454:ILE:HD12	1:A:519:LEU:CD1	2.27	0.65
1:B:170:LEU:HD22	1:B:173:ARG:NH2	2.12	0.65
1:B:211:PRO:O	1:B:213:PRO:HD3	1.96	0.65
1:A:66:TYR:HA	1:A:638:PHE:CZ	2.32	0.65
1:B:586:ASP:O	1:B:590:LYS:HG2	1.97	0.65
1:A:717:ARG:NH1	1:A:746:GLN:OE1	2.30	0.64
1:A:393:LEU:HD22	1:A:724:LEU:CD1	2.26	0.64
1:A:632:ARG:HG2	1:A:633:VAL:N	2.12	0.64
1:A:602:THR:N	1:A:707:ASP:OD2	2.26	0.64
1:B:776:ARG:NH1	1:B:776:ARG:HG3	2.11	0.64
1:B:316:LYS:HE2	1:B:398:GLU:OE2	1.98	0.64
1:A:454:ILE:HD12	1:A:519:LEU:HD11	1.80	0.64
1:A:787:ALA:O	1:A:788:ALA:CB	2.46	0.64
1:A:389:TRP:CE3	1:A:389:TRP:HA	2.31	0.64
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.80	0.63
1:B:220:LEU:HD11	1:B:431:ILE:HD11	1.80	0.63
1:A:312:ILE:CD1	1:A:332:LEU:HD21	2.29	0.63
1:A:458:GLU:OE2	1:A:458:GLU:HA	1.99	0.62
1:B:447:SER:HB3	1:B:606:MET:CE	2.29	0.62
1:A:87:HIS:HE1	1:A:140:ASP:OD1	1.82	0.62
1:B:18:ILE:O	1:B:22:ILE:HD13	1.99	0.62
1:A:293:ARG:O	1:A:294:PRO:C	2.39	0.61
1:A:534:GLN:O	1:A:538:THR:CG2	2.48	0.61
1:B:467:PHE:HB3	1:B:582:MET:HE1	1.81	0.61
1:A:654:ILE:HD11	1:A:769:ALA:HB2	1.83	0.61
1:A:444:ASN:C	1:A:445:LEU:HD23	2.21	0.60
1:B:94:PHE:HB3	1:B:132:ASN:ND2	2.16	0.60
1:B:16:ASP:HB3	1:B:18:ILE:HG23	1.83	0.60
1:A:389:TRP:O	1:A:392:ILE:HB	2.02	0.60
1:B:520:ARG:HH11	1:B:520:ARG:CG	2.14	0.60
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.14	0.60
2:A:890:GLY:N	1:B:745:THR:HG1	1.99	0.60
1:B:288:GLN:HE22	1:B:293:ARG:NH1	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:CG2	1:B:166:ARG:HE	2.15	0.60
1:B:159:ILE:HG23	1:B:160:ASN:H	1.68	0.59
1:B:401:THR:HB	1:B:402:PRO:HA	1.84	0.59
1:B:663:LEU:HD22	1:B:668:GLY:HA2	1.83	0.59
1:A:447:SER:HA	1:A:508:GLY:O	2.01	0.59
1:A:69:THR:O	1:A:655:TRP:CZ3	2.55	0.59
1:A:255:ILE:HD13	1:A:275:MET:SD	2.43	0.59
1:A:153:ARG:NH2	1:A:632:ARG:HD3	2.17	0.58
1:B:464:THR:HG23	1:B:789:SER:HB3	1.84	0.58
1:A:771:ILE:C	1:A:773:ASN:H	2.07	0.58
1:A:779:TYR:O	1:A:781:PRO:HD3	2.04	0.58
1:A:770:ASP:O	1:A:771:ILE:CB	2.51	0.58
1:A:94:PHE:HB3	1:A:132:ASN:ND2	2.19	0.57
1:B:520:ARG:NH2	1:B:648:ASP:OD2	2.36	0.57
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.03	0.57
1:A:481:LEU:C	1:A:505:ILE:HD11	2.24	0.57
1:B:179:HIS:HE1	1:B:189:THR:HG21	1.70	0.57
1:B:30:ASP:HB3	1:B:33:HIS:CE1	2.40	0.57
1:B:557:TYR:CE1	1:B:559:THR:HG22	2.34	0.57
1:B:671:GLN:O	1:B:672:GLY:C	2.43	0.56
1:B:467:PHE:CB	1:B:582:MET:HE1	2.35	0.56
1:B:467:PHE:CB	1:B:582:MET:CE	2.83	0.56
1:B:588:LEU:O	1:B:592:ILE:HG12	2.05	0.56
1:B:471:HIS:HE1	1:B:541:HIS:ND1	2.03	0.56
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.40	0.56
1:A:467:PHE:HD2	1:A:538:THR:HG21	1.70	0.56
1:B:26:CYS:O	1:B:29:LEU:HG	2.05	0.56
1:A:69:THR:HG23	1:A:655:TRP:HH2	1.70	0.56
1:B:288:GLN:HE22	1:B:293:ARG:CZ	2.19	0.56
1:A:223:MET:HG2	1:A:255:ILE:CD1	2.36	0.56
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.41	0.56
1:B:388:LEU:O	1:B:392:ILE:HG12	2.04	0.56
1:B:179:HIS:CE1	1:B:189:THR:HG21	2.41	0.56
1:B:431:ILE:C	1:B:431:ILE:HD12	2.26	0.56
1:A:419:LEU:HD21	1:A:559:THR:HG21	1.88	0.55
1:B:686:THR:HG22	1:B:688:TRP:H	1.71	0.55
1:B:220:LEU:N	1:B:220:LEU:HD23	2.21	0.55
1:B:447:SER:HB3	1:B:606:MET:HE2	1.88	0.55
1:A:71:HIS:CD2	1:A:73:ASP:HB2	2.38	0.55
1:B:80:ARG:O	1:B:84:SER:HB2	2.07	0.55
1:B:467:PHE:CG	1:B:582:MET:HE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ASN:OD1	1:B:503:ARG:NH1	2.39	0.55
1:A:76:THR:O	1:A:80:ARG:HG2	2.07	0.54
1:B:342:VAL:HG22	1:B:729:PHE:HZ	1.71	0.54
1:B:293:ARG:HB3	1:B:295:GLY:N	2.23	0.54
1:A:445:LEU:CD2	1:A:506:ALA:HB3	2.37	0.54
1:A:557:TYR:HE1	1:A:559:THR:HG22	1.73	0.54
1:A:656:ASP:HB2	1:A:659:MET:H	1.73	0.54
1:A:571:GLN:NE2	1:A:571:GLN:HA	2.23	0.54
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.41	0.53
1:A:511:GLY:O	1:A:515:THR:HG23	2.09	0.53
1:A:66:TYR:HA	1:A:638:PHE:CE2	2.43	0.53
1:B:607:PRO:HD3	1:B:711:SER:OG	2.09	0.53
1:A:633:VAL:O	1:A:634:LEU:HB2	2.08	0.53
1:B:658:GLY:HA2	1:B:661:GLN:HB2	1.91	0.53
1:B:675:ASN:HD22	1:B:675:ASN:H	1.55	0.53
1:A:34:ILE:HG23	1:A:35:ASP:N	2.25	0.52
1:A:629:TYR:CE1	1:A:640:VAL:HG12	2.44	0.52
1:A:71:HIS:CD2	1:A:73:ASP:H	2.28	0.52
1:A:159:ILE:HG22	1:A:160:ASN:N	2.23	0.52
1:A:686:THR:HG22	1:A:688:TRP:H	1.74	0.52
1:A:661:GLN:HE22	1:A:757:ASP:H	1.57	0.52
1:B:292:LYS:HB2	1:B:293:ARG:HH21	1.74	0.52
1:B:714:LEU:HB3	1:B:727:MET:HE1	1.92	0.52
1:A:426:ASN:HB3	1:A:431:ILE:HD12	1.91	0.52
1:A:318:HIS:O	1:A:324:ARG:NH1	2.40	0.52
1:B:467:PHE:HB3	1:B:582:MET:CE	2.39	0.52
1:B:673:LEU:HD23	1:B:674:PRO:HD2	1.91	0.52
1:B:686:THR:HG21	1:B:688:TRP:HD1	1.74	0.52
1:A:388:LEU:O	1:A:389:TRP:C	2.45	0.51
1:A:60:ALA:O	1:A:64:CYS:HB2	2.09	0.51
1:B:628:MET:CE	1:B:639:GLN:HG2	2.41	0.51
1:A:293:ARG:HG3	1:A:293:ARG:O	2.10	0.51
1:B:159:ILE:HG23	1:B:160:ASN:N	2.25	0.51
1:B:334:ILE:HD12	1:B:404:VAL:HG13	1.92	0.51
1:B:67:MET:C	1:B:69:THR:H	2.13	0.51
1:B:662:TYR:CE2	1:B:673:LEU:HG	2.45	0.51
1:A:34:ILE:O	1:A:35:ASP:CB	2.58	0.51
1:A:639:GLN:HE21	1:A:639:GLN:HA	1.75	0.51
1:A:482:ASN:N	1:A:505:ILE:HD11	2.26	0.50
1:B:486:ASP:OD2	1:B:503:ARG:NH2	2.44	0.50
1:B:511:GLY:O	1:B:515:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:HB3	1:A:132:ASN:HD22	1.76	0.50
1:B:630:SER:HA	1:B:639:GLN:HB2	1.92	0.50
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.30	0.50
1:B:606:MET:HB2	1:B:607:PRO:HD2	1.93	0.50
1:A:471:HIS:HE1	1:A:541:HIS:ND1	2.09	0.50
1:A:64:CYS:SG	1:A:77:LEU:HB3	2.51	0.50
1:A:433:GLU:OE1	1:A:441:ALA:HB1	2.12	0.49
1:A:220:LEU:N	1:A:220:LEU:HD23	2.27	0.49
1:A:312:ILE:HD11	1:A:332:LEU:HD21	1.94	0.49
1:A:661:GLN:HA	1:A:664:ILE:CG2	2.42	0.49
1:A:17:LYS:HA	1:A:17:LYS:HE3	1.92	0.49
1:B:190:TYR:O	1:B:194:SER:HB2	2.12	0.49
1:A:660:LYS:O	1:A:664:ILE:HG22	2.13	0.49
1:A:342:VAL:HG22	1:A:729:PHE:HZ	1.78	0.49
1:B:224:LYS:HD3	1:B:233:ASP:HB3	1.95	0.49
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.95	0.49
1:A:383:ILE:HG12	1:A:384:LYS:N	2.27	0.49
1:A:511:GLY:O	1:A:515:THR:CG2	2.61	0.49
1:B:345:ASN:O	1:B:346:GLY:O	2.31	0.49
1:B:447:SER:HB3	1:B:606:MET:HE1	1.92	0.49
1:B:79:ALA:O	1:B:83:ILE:HG12	2.13	0.49
1:A:661:GLN:HA	1:A:664:ILE:HG22	1.95	0.48
1:A:316:LYS:O	1:A:324:ARG:HD3	2.14	0.48
1:B:561:GLN:CD	1:B:561:GLN:H	2.16	0.48
1:A:663:LEU:HD21	1:A:670:ILE:CD1	2.44	0.48
1:B:293:ARG:H	1:B:293:ARG:HE	1.62	0.48
1:B:766:GLU:HA	1:B:766:GLU:OE2	2.13	0.48
1:A:608:THR:OG1	1:A:612:SER:HB3	2.14	0.48
1:B:37:VAL:HG23	1:B:38:LYS:H	1.77	0.48
1:B:288:GLN:NE2	1:B:293:ARG:NH1	2.62	0.48
1:B:538:THR:CB	1:B:583:TRP:HE1	2.26	0.48
1:A:146:PHE:HD1	1:A:632:ARG:NH2	2.12	0.48
1:B:450:LEU:CB	1:B:515:THR:HG21	2.43	0.48
1:B:520:ARG:NH1	1:B:520:ARG:HG3	2.25	0.48
1:B:589:ARG:O	1:B:593:MET:HG3	2.12	0.48
1:B:190:TYR:O	1:B:194:SER:CB	2.62	0.48
1:B:662:TYR:O	1:B:666:GLN:HB2	2.14	0.48
1:A:745:THR:H	2:A:889:GLY:N	2.12	0.47
1:B:450:LEU:HB2	1:B:515:THR:HG21	1.94	0.47
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.97	0.47
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HB3	1:A:724:LEU:HD12	1.96	0.47
1:A:656:ASP:OD2	1:A:767:ASN:OD1	2.32	0.47
1:B:688:TRP:HB3	1:B:717:ARG:HG3	1.95	0.47
1:A:771:ILE:C	1:A:773:ASN:N	2.68	0.47
1:B:39:VAL:HG22	1:B:67:MET:SD	2.55	0.47
1:A:312:ILE:CD1	1:A:402:PRO:HG3	2.45	0.47
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.95	0.47
1:B:775:LYS:HD3	1:B:775:LYS:HA	1.69	0.47
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.80	0.47
1:A:503:ARG:N	1:A:504:PRO:HD3	2.30	0.47
1:B:766:GLU:HG3	1:B:767:ASN:H	1.80	0.47
1:A:632:ARG:HG2	1:A:633:VAL:H	1.78	0.46
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.51	0.46
1:A:627:ASN:HB2	1:A:668:GLY:O	2.14	0.46
1:A:656:ASP:CB	1:A:659:MET:H	2.29	0.46
1:A:605:PRO:HD2	1:A:710:HIS:HB3	1.97	0.46
1:B:60:ALA:O	1:B:64:CYS:HB2	2.13	0.46
1:B:511:GLY:O	1:B:515:THR:CG2	2.63	0.46
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.97	0.46
1:A:606:MET:HB2	1:A:607:PRO:HD2	1.97	0.46
1:B:356:ALA:HB1	1:B:374:TYR:CD1	2.51	0.46
1:B:560:PHE:CZ	1:B:596:GLY:HA2	2.50	0.46
1:A:454:ILE:HD13	1:A:465:TYR:HD1	1.79	0.46
1:B:64:CYS:SG	1:B:77:LEU:HD12	2.56	0.46
1:A:190:TYR:CD2	1:A:190:TYR:C	2.87	0.46
1:A:419:LEU:HD21	1:A:559:THR:CG2	2.46	0.46
1:B:534:GLN:O	1:B:538:THR:HG23	2.16	0.46
1:B:660:LYS:HD3	1:B:664:ILE:HD11	1.98	0.46
1:B:464:THR:HG21	1:B:789:SER:CB	2.32	0.46
1:B:77:LEU:HD13	1:B:81:ILE:HD11	1.98	0.46
1:B:212:LYS:H	1:B:212:LYS:HG3	1.58	0.46
1:B:213:PRO:HD2	1:B:489:TYR:HB2	1.97	0.46
1:A:217:SER:O	1:A:246:GLY:HA2	2.16	0.45
1:A:454:ILE:HD13	1:A:465:TYR:CD1	2.51	0.45
1:A:464:THR:HG23	1:A:789:SER:OG	2.16	0.45
1:B:293:ARG:HB3	1:B:295:GLY:H	1.81	0.45
1:B:332:LEU:CD1	1:B:392:ILE:HD12	2.39	0.45
1:A:273:ILE:HG21	1:A:323:ILE:HG13	1.97	0.45
1:A:458:GLU:O	1:A:459:ASP:HB3	2.15	0.45
1:A:654:ILE:CD1	1:A:769:ALA:HB2	2.45	0.45
1:B:634:LEU:O	1:B:635:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:PRO:HD2	1:B:710:HIS:HB3	1.98	0.45
1:A:678:GLN:OE1	1:A:678:GLN:HA	2.15	0.45
1:A:297:PHE:N	1:A:297:PHE:CD2	2.83	0.45
1:B:139:ARG:HD3	1:B:194:SER:OG	2.16	0.45
1:A:95:SER:N	1:A:132:ASN:HD21	2.11	0.45
1:B:64:CYS:SG	1:B:77:LEU:CD1	3.04	0.45
1:A:304:TRP:O	1:A:350:LEU:HA	2.16	0.45
1:A:401:THR:HB	1:A:402:PRO:HA	1.99	0.45
1:A:758:GLN:NE2	1:A:758:GLN:O	2.50	0.45
1:B:445:LEU:HD22	1:B:506:ALA:HB3	1.98	0.45
1:B:686:THR:CG2	1:B:688:TRP:CD1	2.99	0.45
1:A:453:PHE:CE2	1:A:470:LEU:HA	2.51	0.45
1:A:458:GLU:CA	1:A:458:GLU:OE2	2.63	0.45
1:B:120:VAL:HG21	1:B:209:GLY:HA2	1.97	0.45
1:B:652:LEU:HD23	1:B:652:LEU:HA	1.89	0.45
1:B:716:LEU:O	1:B:745:THR:HA	2.16	0.45
1:B:19:THR:HG22	1:B:23:SER:HB3	1.98	0.45
1:B:670:ILE:HA	1:B:670:ILE:HD13	1.58	0.44
1:A:467:PHE:CD2	1:A:538:THR:HG21	2.51	0.44
1:B:25:LEU:O	1:B:80:ARG:HD3	2.17	0.44
1:B:251:HIS:HB3	1:B:424:SER:HB3	1.99	0.44
1:A:717:ARG:O	1:A:746:GLN:O	2.36	0.44
1:B:603:MET:HB2	1:B:707:ASP:HB2	1.98	0.44
1:B:95:SER:N	1:B:132:ASN:HD21	2.02	0.44
1:B:227:SER:O	1:B:231:ILE:HG13	2.17	0.44
1:B:359:LEU:HA	1:B:359:LEU:HD12	1.84	0.44
1:B:766:GLU:CG	1:B:767:ASN:H	2.31	0.44
1:A:296:ALA:C	1:A:297:PHE:HD2	2.21	0.44
1:A:454:ILE:HD12	1:A:519:LEU:HD13	2.00	0.44
1:A:702:ARG:HD2	1:A:710:HIS:CE1	2.52	0.44
1:A:291:ASN:O	1:A:292:LYS:CG	2.67	0.43
1:A:481:LEU:CB	1:A:505:ILE:HG12	2.47	0.43
1:B:519:LEU:HG	1:B:779:TYR:CD1	2.53	0.43
1:A:34:ILE:HG23	1:A:35:ASP:H	1.83	0.43
1:B:713:ASN:ND2	1:B:742:TYR:H	2.15	0.43
1:B:156:LEU:HG	1:B:165:GLU:O	2.19	0.43
1:B:714:LEU:HG	1:B:727:MET:HE3	2.01	0.43
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.82	0.43
1:B:490:TYR:HA	1:B:491:PRO:HD3	1.92	0.43
1:B:641:VAL:HG13	1:B:646:LEU:HD22	2.00	0.43
1:A:425:SER:OG	1:A:426:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:SER:OG	1:B:510:GLN:NE2	2.51	0.43
1:A:343:GLU:C	1:A:344:GLU:O	2.57	0.43
1:A:334:ILE:HA	1:A:335:PRO:HD3	1.84	0.42
1:A:680:LEU:HA	1:A:680:LEU:HD22	1.87	0.42
1:B:673:LEU:H	1:B:681:LYS:NZ	2.17	0.42
1:A:607:PRO:HD3	1:A:711:SER:OG	2.19	0.42
1:B:713:ASN:ND2	1:B:742:TYR:HB2	2.35	0.42
1:B:199:THR:HG21	1:B:611:THR:HB	2.00	0.42
1:A:630:SER:HA	1:A:638:PHE:O	2.19	0.42
1:B:447:SER:HA	1:B:508:GLY:O	2.19	0.42
1:B:603:MET:H	1:B:707:ASP:HB2	1.84	0.42
1:B:390:TYR:HD2	1:B:721:MET:CE	2.32	0.42
1:A:160:ASN:C	1:A:162:GLN:H	2.22	0.42
1:A:297:PHE:N	1:A:297:PHE:HD2	2.17	0.42
1:A:539:ILE:HG22	1:A:603:MET:SD	2.60	0.42
1:B:220:LEU:HD21	1:B:431:ILE:CG1	2.49	0.42
1:B:467:PHE:CG	1:B:582:MET:CE	3.02	0.42
1:A:458:GLU:O	1:A:459:ASP:CB	2.67	0.42
1:A:654:ILE:CG2	1:A:654:ILE:O	2.67	0.42
1:A:670:ILE:HG13	1:A:673:LEU:HD12	2.02	0.42
1:A:686:THR:CG2	1:A:688:TRP:CD1	3.03	0.42
1:B:277:ARG:CB	1:B:277:ARG:HH11	2.19	0.42
1:B:326:ARG:HB2	1:B:326:ARG:NH1	2.35	0.42
1:A:451:PRO:HG3	1:A:515:THR:HG22	2.02	0.42
1:A:115:MET:HE3	1:A:115:MET:HB2	1.96	0.42
1:A:312:ILE:HD11	1:A:402:PRO:HG3	2.01	0.42
1:A:312:ILE:HD13	1:A:332:LEU:HD21	2.00	0.42
1:B:296:ALA:C	1:B:297:PHE:HD1	2.23	0.42
1:A:641:VAL:HG13	1:A:646:LEU:HD22	2.01	0.42
1:B:251:HIS:HB2	1:B:253:HIS:NE2	2.35	0.42
1:B:713:ASN:HD22	1:B:742:TYR:H	1.68	0.42
1:A:86:LEU:O	1:A:90:THR:HB	2.20	0.42
1:B:211:PRO:C	1:B:213:PRO:HD3	2.39	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.83	0.41
1:B:256:ARG:HG3	1:B:269:SER:OG	2.20	0.41
1:B:71:HIS:ND1	1:B:72:PRO:HD2	2.34	0.41
1:A:621:PHE:CD2	1:A:621:PHE:N	2.87	0.41
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.20	0.41
1:B:699:ALA:HA	1:B:702:ARG:NH1	2.36	0.41
1:A:713:ASN:HD22	1:A:742:TYR:H	1.67	0.41
1:B:243:LYS:HD2	1:B:293:ARG:HH12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HA	1:A:314:ILE:HD13	1.67	0.41
1:B:220:LEU:CD1	1:B:431:ILE:HD11	2.49	0.41
1:B:179:HIS:CE1	1:B:189:THR:CG2	3.04	0.41
1:B:71:HIS:HD2	1:B:73:ASP:HB2	1.86	0.41
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.39	0.41
1:A:604:ALA:HB2	1:A:708:GLN:HB2	2.03	0.41
1:B:642:ASN:C	1:B:642:ASN:OD1	2.59	0.41
1:B:714:LEU:HA	1:B:714:LEU:HD12	1.90	0.41
1:A:30:ASP:HB3	1:A:33:HIS:HB2	2.03	0.40
1:A:459:ASP:C	1:A:459:ASP:OD1	2.60	0.40
1:A:661:GLN:HE21	1:A:755:THR:CG2	2.34	0.40
1:B:559:THR:CG2	1:B:559:THR:O	2.69	0.40
1:A:775:LYS:HD2	1:A:775:LYS:HA	1.87	0.40
1:B:220:LEU:HD11	1:B:431:ILE:CD1	2.48	0.40
1:A:52:THR:N	1:A:55:GLU:HG2	2.36	0.40
1:A:21:ARG:NH2	1:A:57:ASP:OD2	2.55	0.40
1:B:557:TYR:CZ	1:B:600:SER:HB3	2.57	0.40
1:B:683:LEU:HD12	1:B:683:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [\(i\)](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

2 ligands 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	GLY	A	890	-	3,3,4	0.76	0	0,2,4	0.00	-
2	GLY	A	889	-	3,3,4	0.78	0	0,2,4	0.00	-

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	GLY	A	890	-	-	0/0/1/2	-
2	GLY	A	889	-	-	0/0/1/2	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	890	GLY	1	0
2	A	889	GLY	1	0

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 [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section is therefore empty.