



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:10 AM GMT

PDB ID : 1ZZY
Title : Structures of Yeast Ribonucleotide Reductase I
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.
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
<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

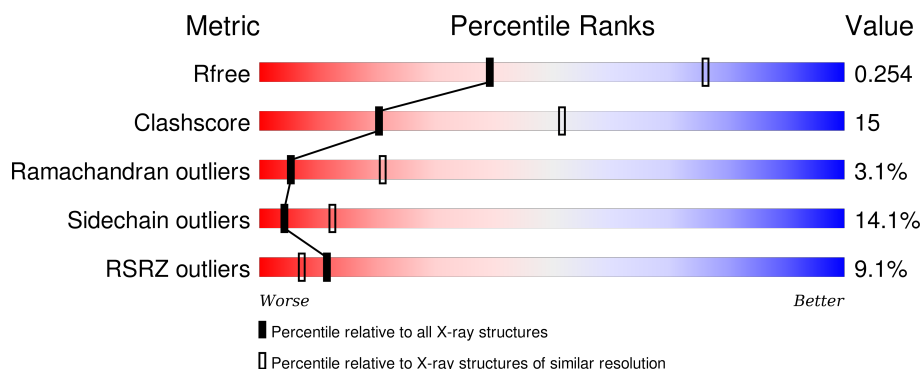
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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	888	 7% 58% 21% 7% • 13%
1	B	888	 9% 57% 22% 7% • 13%

2 Entry composition [i](#)

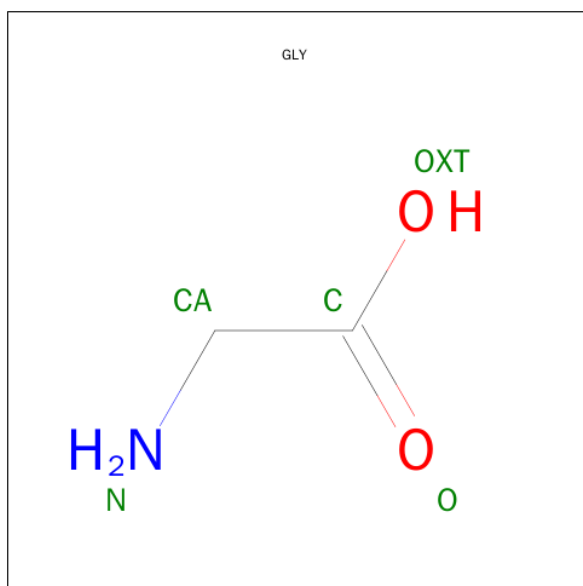
There are 2 unique types of molecules in this entry. The entry contains 12275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	N	O	S	0	0	0
			6159	3913	1049	1162	35			
1	B	769	Total	C	N	O	S	0	0	0
			6108	3882	1040	1151	35			

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

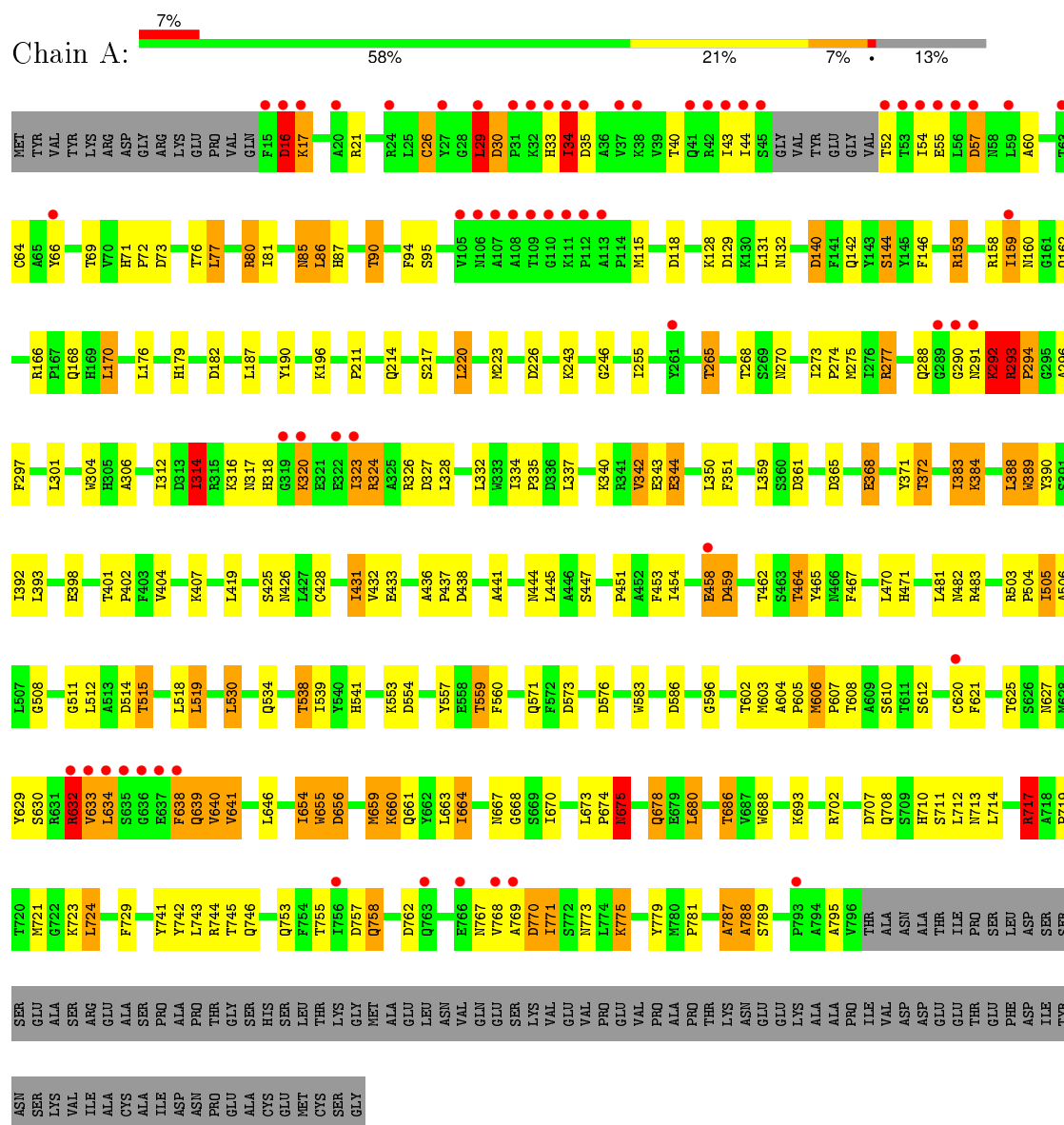


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			8	4	2	2		

3 Residue-property plots [i](#)

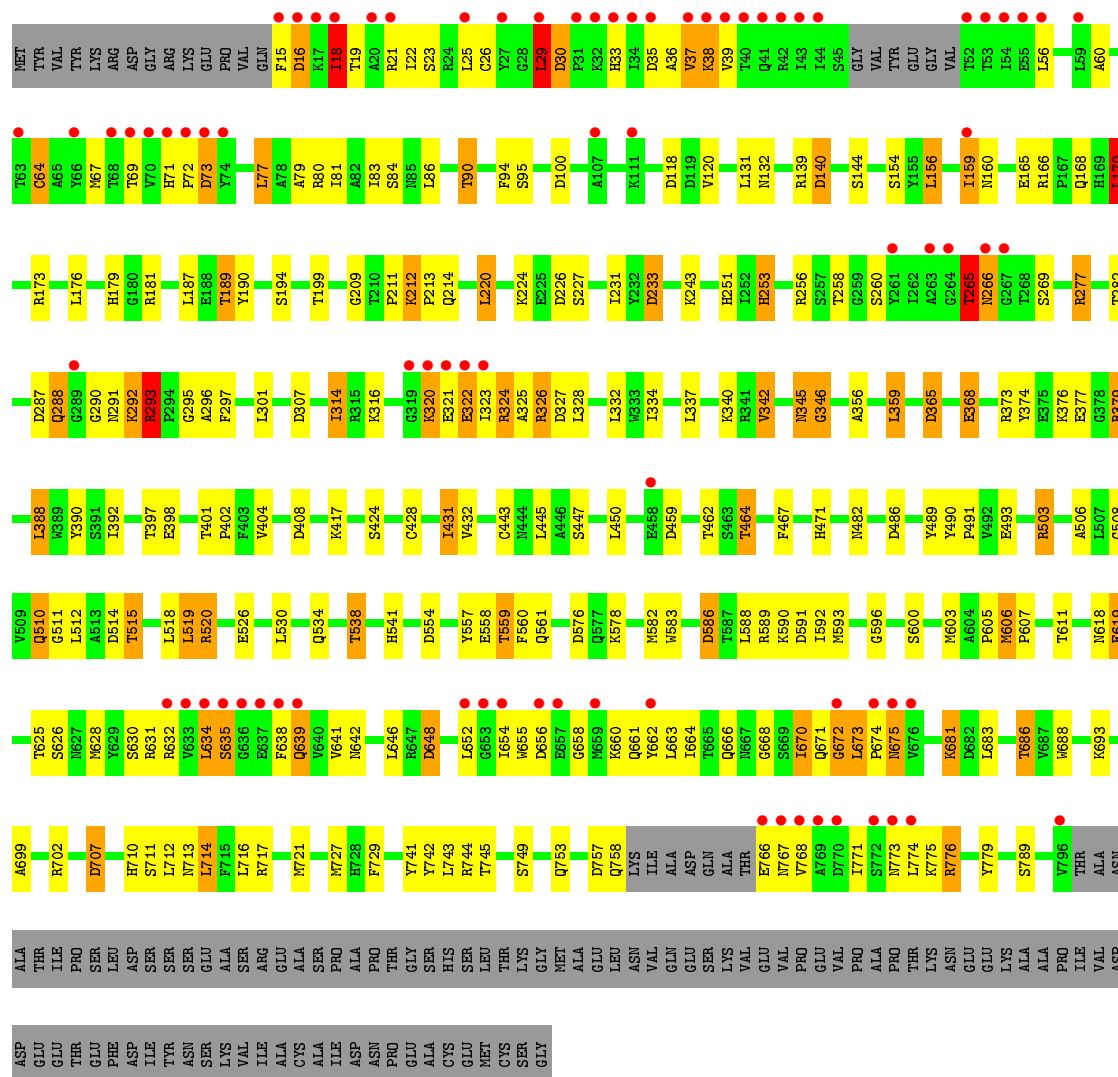
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1





4 Data and refinement statistics

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 49.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.90) 95.7 (49.75-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.21 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.217 , 0.257 0.215 , 0.254	Depositor DCC
R_{free} test set	3825 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 90679 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [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 ⓘ

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:B:277:ARG:HB2	1:B:277:ARG:NH1	1.98	0.77
1:A:538:THR:HB	1:A:583:TRP:HE1	1.48	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:675:ASN:H	1:B:675:ASN:ND2	1.93	0.67
1:B:618:ASN:O	1:B:619:GLU:O	2.12	0.67
1:B:365:ASP:HA	1:B:368:GLU:HB2	1.78	0.66
1:A:571:GLN:HE21	1:A:571:GLN:HA	1.60	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:B:211:PRO:O	1:B:213:PRO:HD3	1.96	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:586:ASP:O	1:B:590:LYS:HG2	1.97	0.65
1:A:66:TYR:HA	1:A:638:PHE:CZ	2.32	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:787:ALA:O	1:A:788:ALA:CB	2.46	0.64
1:A:454:ILE:HD12	1:A:519:LEU:HD11	1.80	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:534:GLN:O	1:A:538:THR:CG2	2.48	0.61
1:A:293:ARG:O	1:A:294:PRO:C	2.39	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:B:94:PHE:HB3	1:B:132:ASN:ND2	2.16	0.60
1:A:444:ASN:C	1:A:445:LEU:HD23	2.21	0.60
1:B:16:ASP:HB3	1:B:18:ILE:HG23	1.83	0.60
1:B:520:ARG:HH11	1:B:520:ARG:CG	2.14	0.60
1:A:389:TRP:O	1:A:392:ILE:HB	2.02	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:557:TYR:CE1	1:B:559:THR:HG22	2.34	0.57
1:B:30:ASP:HB3	1:B:33:HIS:CE1	2.40	0.57
1:B:179:HIS:HE1	1:B:189:THR:HG21	1.70	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:CE	2.83	0.56
1:B:467:PHE:CB	1:B:582:MET:HE1	2.35	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:B:388:LEU:O	1:B:392:ILE:HG12	2.04	0.56
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.41	0.56
1:A:223:MET:HG2	1:A:255:ILE:CD1	2.36	0.56
1:B:431:ILE:C	1:B:431:ILE:HD12	2.26	0.56
1:B:179:HIS:CE1	1:B:189:THR:HG21	2.41	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:H	1:B:675:ASN:HD22	1.55	0.53
1:A:71:HIS:CD2	1:A:73:ASP:H	2.28	0.52
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:B:292:LYS:HB2	1:B:293:ARG:HH21	1.74	0.52
1:A:686:THR:HG22	1:A:688:TRP:H	1.74	0.52
1:B:714:LEU:HB3	1:B:727:MET:HE1	1.92	0.52
1:A:661:GLN:HE22	1:A:757:ASP:H	1.57	0.52
1:A:159:ILE:HG22	1:A:160:ASN:N	2.23	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:B:628:MET:CE	1:B:639:GLN:HG2	2.41	0.51
1:A:60:ALA:O	1:A:64:CYS:HB2	2.09	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:B:606:MET:HB2	1:B:607:PRO:HD2	1.93	0.50
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.30	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:B:190:TYR:O	1:B:194:SER:HB2	2.12	0.49
1:A:17:LYS:HA	1:A:17:LYS:HE3	1.92	0.49
1:A:660:LYS:O	1:A:664:ILE:HG22	2.13	0.49
1:B:224:LYS:HD3	1:B:233:ASP:HB3	1.95	0.49
1:A:342:VAL:HG22	1:A:729:PHE:HZ	1.78	0.49
1:A:511:GLY:O	1:A:515:THR:CG2	2.61	0.49
1:A:383:ILE:HG12	1:A:384:LYS:N	2.27	0.49
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.95	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:B:345:ASN:O	1:B:346:GLY:O	2.31	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:B:293:ARG:H	1:B:293:ARG:HE	1.62	0.48
1:A:663:LEU:HD21	1:A:670:ILE:CD1	2.44	0.48
1:B:766:GLU:HA	1:B:766:GLU:OE2	2.13	0.48
1:B:37:VAL:HG23	1:B:38:LYS:H	1.77	0.48
1:A:608:THR:OG1	1:A:612:SER:HB3	2.14	0.48
1:B:538:THR:CB	1:B:583:TRP:HE1	2.26	0.48
1:B:288:GLN:NE2	1:B:293:ARG:NH1	2.62	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:HG3	1:B:520:ARG:NH1	2.25	0.48
1:B:589:ARG:O	1:B:593:MET:HG3	2.12	0.48
1:B:662:TYR:O	1:B:666:GLN:HB2	2.14	0.48
1:B:190:TYR:O	1:B:194:SER:CB	2.62	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:393:LEU:HB3	1:A:724:LEU:HD12	1.96	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:656:ASP:OD2	1:A:767:ASN:OD1	2.32	0.47
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.97	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:B:775:LYS:HD3	1:B:775:LYS:HA	1.69	0.47
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.95	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:656:ASP:CB	1:A:659:MET:H	2.29	0.46
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.51	0.46
1:B:60:ALA:O	1:B:64:CYS:HB2	2.13	0.46
1:A:605:PRO:HD2	1:A:710:HIS:HB3	1.97	0.46
1:A:627:ASN:HB2	1:A:668:GLY:O	2.14	0.46
1:B:511:GLY:O	1:B:515:THR:CG2	2.63	0.46
1:A:606:MET:HB2	1:A:607:PRO:HD2	1.97	0.46
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.97	0.46
1:B:560:PHE:CZ	1:B:596:GLY:HA2	2.50	0.46
1:B:356:ALA:HB1	1:B:374:TYR:CD1	2.51	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:B:534:GLN:O	1:B:538:THR:HG23	2.16	0.46
1:A:419:LEU:HD21	1:A:559:THR:CG2	2.46	0.46
1:A:190:TYR:CD2	1:A:190:TYR:C	2.87	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:213:PRO:HD2	1:B:489:TYR:HB2	1.97	0.46
1:B:212:LYS:H	1:B:212:LYS:HG3	1.58	0.46
1:B:332:LEU:CD1	1:B:392:ILE:HD12	2.39	0.45
1:A:454:ILE:HD13	1:A:465:TYR:CD1	2.51	0.45
1:B:293:ARG:HB3	1:B:295:GLY:H	1.81	0.45
1:A:464:THR:HG23	1:A:789:SER:OG	2.16	0.45
1:A:217:SER:O	1:A:246:GLY:HA2	2.16	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:A:273:ILE:HG21	1:A:323:ILE:HG13	1.97	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:B:139:ARG:HD3	1:B:194:SER:OG	2.16	0.45
1:A:297:PHE:N	1:A:297:PHE:CD2	2.83	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:401:THR:HB	1:A:402:PRO:HA	1.99	0.45
1:A:304:TRP:O	1:A:350:LEU:HA	2.16	0.45
1:B:686:THR:CG2	1:B:688:TRP:CD1	2.99	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:A:458:GLU:CA	1:A:458:GLU:OE2	2.63	0.45
1:B:716:LEU:O	1:B:745:THR:HA	2.16	0.45
1:B:652:LEU:HD23	1:B:652:LEU:HA	1.89	0.45
1:B:120:VAL:HG21	1:B:209:GLY:HA2	1.97	0.45
1:A:453:PHE:CE2	1:A:470:LEU:HA	2.51	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:766:GLU:CG	1:B:767:ASN:H	2.31	0.44
1:B:359:LEU:HA	1:B:359:LEU:HD12	1.84	0.44
1:B:227:SER:O	1:B:231:ILE:HG13	2.17	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:481:LEU:CB	1:A:505:ILE:HG12	2.47	0.43
1:A:291:ASN:O	1:A:292:LYS:CG	2.67	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:714:LEU:HG	1:B:727:MET:HE3	2.01	0.43
1:B:156:LEU:HG	1:B:165:GLU:O	2.19	0.43
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.82	0.43
1:B:641:VAL:HG13	1:B:646:LEU:HD22	2.00	0.43
1:B:490:TYR:HA	1:B:491:PRO:HD3	1.92	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:B:673:LEU:H	1:B:681:LYS:NZ	2.17	0.42
1:A:680:LEU:HA	1:A:680:LEU:HD22	1.87	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: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: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:277:ARG:CB	1:B:277:ARG:HH11	2.19	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:686:THR:CG2	1:A:688:TRP:CD1	3.03	0.42
1:A:670:ILE:HG13	1:A:673:LEU:HD12	2.02	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: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:115:MET:HE3	1:A:115:MET:HB2	1.96	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:641:VAL:HG13	1:A:646:LEU:HD22	2.01	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: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:663:LEU:HD23	1:A:663:LEU:HA	1.83	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:B:243:LYS:HD2	1:B:293:ARG:HH12	1.84	0.41
1:A:713:ASN:HD22	1:A:742:TYR:H	1.67	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:B:642:ASN:C	1:B:642:ASN:OD1	2.59	0.41
1:A:604:ALA:HB2	1:A:708:GLN:HB2	2.03	0.41
1:B:714:LEU:HA	1:B:714:LEU:HD12	1.90	0.41
1:A:459:ASP:C	1:A:459:ASP:OD1	2.60	0.40
1:A:30:ASP:HB3	1:A:33:HIS:HB2	2.03	0.40
1:B:559:THR:CG2	1:B:559:THR:O	2.69	0.40
1:A:661:GLN:HE21	1:A:755:THR:CG2	2.34	0.40
1:B:220:LEU:HD11	1:B:431:ILE:CD1	2.48	0.40
1:A:775:LYS:HD2	1:A:775:LYS:HA	1.87	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:A:52:THR:N	1:A:55:GLU:HG2	2.36	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](#)

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	772/888 (87%)	694 (90%)	54 (7%)	24 (3%)	5	21
1	B	763/888 (86%)	685 (90%)	55 (7%)	23 (3%)	5	22
All	All	1535/1776 (86%)	1379 (90%)	109 (7%)	47 (3%)	5	21

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO
1	A	314	ILE
1	A	633	VAL
1	A	654	ILE
1	A	675	ASN
1	A	770	ASP
1	A	771	ILE
1	A	787	ALA
1	B	37	VAL
1	B	265	THR
1	B	346	GLY
1	B	417	LYS
1	B	619	GLU
1	B	634	LEU
1	B	635	SER
1	A	290	GLY
1	A	459	ASP
1	A	632	ARG
1	A	788	ALA
1	B	36	ALA
1	B	290	GLY
1	B	314	ILE
1	B	672	GLY
1	B	741	TYR
1	B	773	ASN
1	B	774	LEU
1	A	620	CYS
1	A	634	LEU
1	A	741	TYR
1	B	35	ASP
1	B	287	ASP
1	A	144	SER
1	A	159	ILE
1	A	292	LYS
1	A	344	GLU
1	B	325	ALA
1	B	768	VAL
1	A	29	LEU
1	A	717	ARG
1	A	795	ALA
1	B	29	LEU
1	B	266	ASN
1	B	753	GLN

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Mol	Chain	Res	Type
1	B	253	HIS
1	A	293	ARG
1	A	43	ILE
1	B	18	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/761 (88%)	574 (86%)	93 (14%)	4	12
1	B	662/761 (87%)	567 (86%)	95 (14%)	4	12
All	All	1329/1522 (87%)	1141 (86%)	188 (14%)	4	12

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	LYS
1	A	26	CYS
1	A	29	LEU
1	A	34	ILE
1	A	40	THR
1	A	44	ILE
1	A	54	ILE
1	A	77	LEU
1	A	80	ARG
1	A	85	ASN
1	A	90	THR
1	A	128	LYS
1	A	131	LEU
1	A	142	GLN
1	A	144	SER
1	A	153	ARG
1	A	158	ARG
1	A	170	LEU

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Mol	Chain	Res	Type
1	A	176	LEU
1	A	187	LEU
1	A	196	LYS
1	A	211	PRO
1	A	214	GLN
1	A	220	LEU
1	A	243	LYS
1	A	265	THR
1	A	268	THR
1	A	277	ARG
1	A	288	GLN
1	A	293	ARG
1	A	301	LEU
1	A	314	ILE
1	A	320	LYS
1	A	323	ILE
1	A	324	ARG
1	A	328	LEU
1	A	337	LEU
1	A	340	LYS
1	A	342	VAL
1	A	359	LEU
1	A	368	GLU
1	A	372	THR
1	A	383	ILE
1	A	384	LYS
1	A	388	LEU
1	A	398	GLU
1	A	407	LYS
1	A	431	ILE
1	A	432	VAL
1	A	458	GLU
1	A	462	THR
1	A	464	THR
1	A	505	ILE
1	A	512	LEU
1	A	514	ASP
1	A	515	THR
1	A	518	LEU
1	A	519	LEU
1	A	530	LEU
1	A	538	THR

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Mol	Chain	Res	Type
1	A	553	LYS
1	A	559	THR
1	A	606	MET
1	A	610	SER
1	A	625	THR
1	A	632	ARG
1	A	638	PHE
1	A	639	GLN
1	A	640	VAL
1	A	641	VAL
1	A	655	TRP
1	A	659	MET
1	A	660	LYS
1	A	664	ILE
1	A	667	ASN
1	A	675	ASN
1	A	678	GLN
1	A	680	LEU
1	A	686	THR
1	A	693	LYS
1	A	712	LEU
1	A	714	LEU
1	A	717	ARG
1	A	721	MET
1	A	723	LYS
1	A	724	LEU
1	A	743	LEU
1	A	744	ARG
1	A	753	GLN
1	A	758	GLN
1	A	768	VAL
1	A	775	LYS
1	B	15	PHE
1	B	18	ILE
1	B	21	ARG
1	B	29	LEU
1	B	38	LYS
1	B	56	LEU
1	B	64	CYS
1	B	77	LEU
1	B	86	LEU
1	B	90	THR

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Mol	Chain	Res	Type
1	B	131	LEU
1	B	144	SER
1	B	154	SER
1	B	156	LEU
1	B	159	ILE
1	B	170	LEU
1	B	176	LEU
1	B	181	ARG
1	B	187	LEU
1	B	189	THR
1	B	212	LYS
1	B	214	GLN
1	B	220	LEU
1	B	233	ASP
1	B	258	THR
1	B	265	THR
1	B	277	ARG
1	B	282	THR
1	B	288	GLN
1	B	291	ASN
1	B	292	LYS
1	B	293	ARG
1	B	301	LEU
1	B	314	ILE
1	B	320	LYS
1	B	324	ARG
1	B	326	ARG
1	B	327	ASP
1	B	328	LEU
1	B	337	LEU
1	B	340	LYS
1	B	342	VAL
1	B	345	ASN
1	B	359	LEU
1	B	365	ASP
1	B	368	GLU
1	B	373	ARG
1	B	376	LYS
1	B	379	ARG
1	B	388	LEU
1	B	397	THR
1	B	431	ILE

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Mol	Chain	Res	Type
1	B	432	VAL
1	B	443	CYS
1	B	462	THR
1	B	464	THR
1	B	493	GLU
1	B	503	ARG
1	B	510	GLN
1	B	512	LEU
1	B	514	ASP
1	B	515	THR
1	B	518	LEU
1	B	519	LEU
1	B	520	ARG
1	B	526	GLU
1	B	530	LEU
1	B	538	THR
1	B	558	GLU
1	B	559	THR
1	B	578	LYS
1	B	606	MET
1	B	625	THR
1	B	626	SER
1	B	631	ARG
1	B	632	ARG
1	B	638	PHE
1	B	639	GLN
1	B	654	ILE
1	B	655	TRP
1	B	670	ILE
1	B	673	LEU
1	B	675	ASN
1	B	681	LYS
1	B	686	THR
1	B	693	LYS
1	B	707	ASP
1	B	712	LEU
1	B	714	LEU
1	B	743	LEU
1	B	744	ARG
1	B	749	SER
1	B	758	GLN
1	B	771	ILE

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Mol	Chain	Res	Type
1	B	776	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	85	ASN
1	A	87	HIS
1	A	132	ASN
1	A	142	GLN
1	A	179	HIS
1	A	207	ASN
1	A	251	HIS
1	A	266	ASN
1	A	444	ASN
1	A	471	HIS
1	A	567	GLN
1	A	595	HIS
1	A	639	GLN
1	A	661	GLN
1	A	667	ASN
1	A	675	ASN
1	A	710	HIS
1	A	713	ASN
1	A	758	GLN
1	A	767	ASN
1	B	71	HIS
1	B	87	HIS
1	B	132	ASN
1	B	179	HIS
1	B	207	ASN
1	B	251	HIS
1	B	266	ASN
1	B	288	GLN
1	B	444	ASN
1	B	471	HIS
1	B	510	GLN
1	B	618	ASN
1	B	639	GLN
1	B	675	ASN
1	B	710	HIS
1	B	713	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	889	-	3,3,4	0.89	0	0,2,4	0.00	-
2	GLY	A	890	-	3,3,4	0.87	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	889	-	-	0/0/1/2	0/0/0/0
2	GLY	A	890	-	-	0/0/1/2	0/0/0/0

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	889	GLY	1	0
2	A	890	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

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	776/888 (87%)	0.30	61 (7%) 15 10	27, 43, 101, 130	0
1	B	769/888 (86%)	0.36	80 (10%) 8 5	25, 42, 115, 135	0
All	All	1545/1776 (86%)	0.33	141 (9%) 11 7	25, 43, 113, 135	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	633	VAL	7.9
1	B	634	LEU	7.6
1	B	52	THR	6.9
1	A	52	THR	6.6
1	A	107	ALA	6.5
1	B	32	LYS	6.1
1	B	15	PHE	6.0
1	B	18	ILE	6.0
1	B	635	SER	5.8
1	B	767	ASN	5.7
1	B	769	ALA	5.6
1	B	54	ILE	5.5
1	A	16	ASP	5.3
1	B	53	THR	5.3
1	B	636	GLY	5.2
1	A	106	ASN	5.2
1	A	108	ALA	5.2
1	A	638	PHE	5.2
1	B	33	HIS	4.8
1	B	69	THR	4.8
1	A	54	ILE	4.6
1	A	632	ARG	4.6
1	B	31	PRO	4.6
1	A	32	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	768	VAL	4.4
1	B	68	THR	4.3
1	A	637	GLU	4.2
1	B	70	VAL	4.2
1	B	796	VAL	4.2
1	A	112	PRO	4.2
1	B	34	ILE	4.2
1	B	44	ILE	4.1
1	B	638	PHE	4.1
1	A	636	GLY	3.9
1	A	34	ILE	3.9
1	B	320	LYS	3.9
1	B	322	GLU	3.8
1	A	634	LEU	3.8
1	A	45	SER	3.8
1	B	637	GLU	3.8
1	B	766	GLU	3.7
1	B	656	ASP	3.7
1	A	37	VAL	3.7
1	A	41	GLN	3.7
1	A	635	SER	3.7
1	B	674	PRO	3.6
1	A	33	HIS	3.6
1	A	57	ASP	3.6
1	A	320	LYS	3.6
1	B	770	ASP	3.6
1	B	55	GLU	3.5
1	A	319	GLY	3.5
1	A	105	VAL	3.5
1	B	37	VAL	3.5
1	A	15	PHE	3.5
1	B	59	LEU	3.5
1	B	20	ALA	3.5
1	B	319	GLY	3.5
1	B	41	GLN	3.5
1	B	639	GLN	3.5
1	A	56	LEU	3.5
1	B	39	VAL	3.4
1	B	659	MET	3.4
1	A	17	LYS	3.4
1	A	66	TYR	3.4
1	B	27	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	42	ARG	3.3
1	B	17	LYS	3.2
1	A	322	GLU	3.2
1	A	42	ARG	3.2
1	A	38	LYS	3.2
1	B	264	GLY	3.2
1	B	267	GLY	3.2
1	B	657	GLU	3.2
1	B	16	ASP	3.2
1	A	110	GLY	3.1
1	B	633	VAL	3.1
1	A	53	THR	3.1
1	B	773	ASN	3.1
1	B	72	PRO	3.1
1	A	111	LYS	3.1
1	B	654	ILE	3.1
1	B	159	ILE	3.0
1	B	675	ASN	3.0
1	B	43	ILE	3.0
1	B	662	TYR	2.9
1	B	74	TYR	2.9
1	A	769	ALA	2.9
1	A	31	PRO	2.9
1	B	56	LEU	2.8
1	B	66	TYR	2.8
1	B	263	ALA	2.8
1	B	321	GLU	2.8
1	B	632	ARG	2.8
1	B	652	LEU	2.8
1	B	38	LYS	2.8
1	A	44	ILE	2.7
1	B	323	ILE	2.7
1	A	763	GLN	2.7
1	B	261	TYR	2.7
1	B	772	SER	2.7
1	B	676	VAL	2.6
1	B	21	ARG	2.6
1	A	289	GLY	2.6
1	A	113	ALA	2.6
1	B	111	LYS	2.5
1	A	29	LEU	2.5
1	B	107	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	63	THR	2.5
1	B	73	ASP	2.5
1	A	458	GLU	2.4
1	A	261	TYR	2.4
1	B	29	LEU	2.4
1	A	109	THR	2.4
1	A	55	GLU	2.4
1	B	289	GLY	2.4
1	A	766	GLU	2.4
1	A	290	GLY	2.3
1	A	768	VAL	2.3
1	A	24	ARG	2.3
1	A	323	ILE	2.3
1	A	291	ASN	2.3
1	A	793	PRO	2.3
1	B	672	GLY	2.3
1	A	35	ASP	2.3
1	A	27	TYR	2.3
1	B	653	GLY	2.3
1	A	59	LEU	2.3
1	A	159	ILE	2.2
1	A	20	ALA	2.2
1	A	756	ILE	2.2
1	A	43	ILE	2.2
1	B	25	LEU	2.2
1	B	35	ASP	2.2
1	B	40	THR	2.1
1	B	458	GLU	2.1
1	A	63	THR	2.1
1	B	774	LEU	2.1
1	B	71	HIS	2.1
1	A	620	CYS	2.1
1	B	266	ASN	2.1

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

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

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
2	GLY	A	890	4/5	0.68	0.32	-	61,61,61,61	0
2	GLY	A	889	4/5	0.53	0.36	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.