



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:33 pm BST

PDB ID : 4RBN
Title : The crystal structure of Nitrosomonas europaea sucrose synthase: Insights into the evolutionary origin of sucrose metabolism in prokaryotes
Authors : Wu, R.; Asencion Diez, M.D.; Figueroa, C.M.; Machtey, M.; Iglesias, A.A.; Ballicora, M.A.; Liu, D.
Deposited on : 2014-09-12
Resolution : 3.05 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

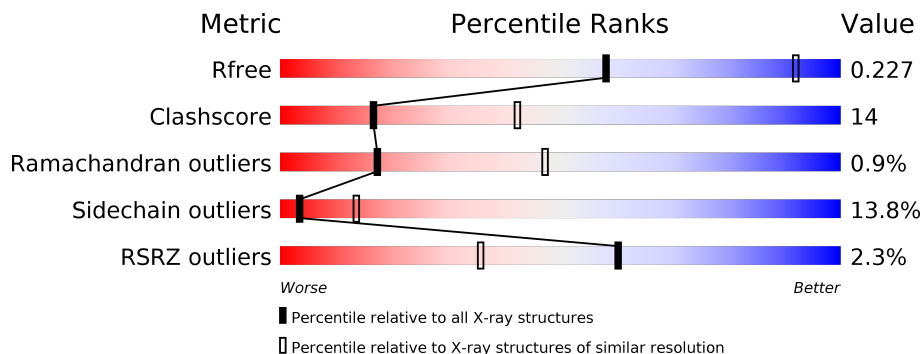
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 $\leq 5\%$. 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	794	
1	B	794	
1	C	794	
1	D	794	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25595 atoms, of which 0 are hydrogens and 0 are deuteriums.

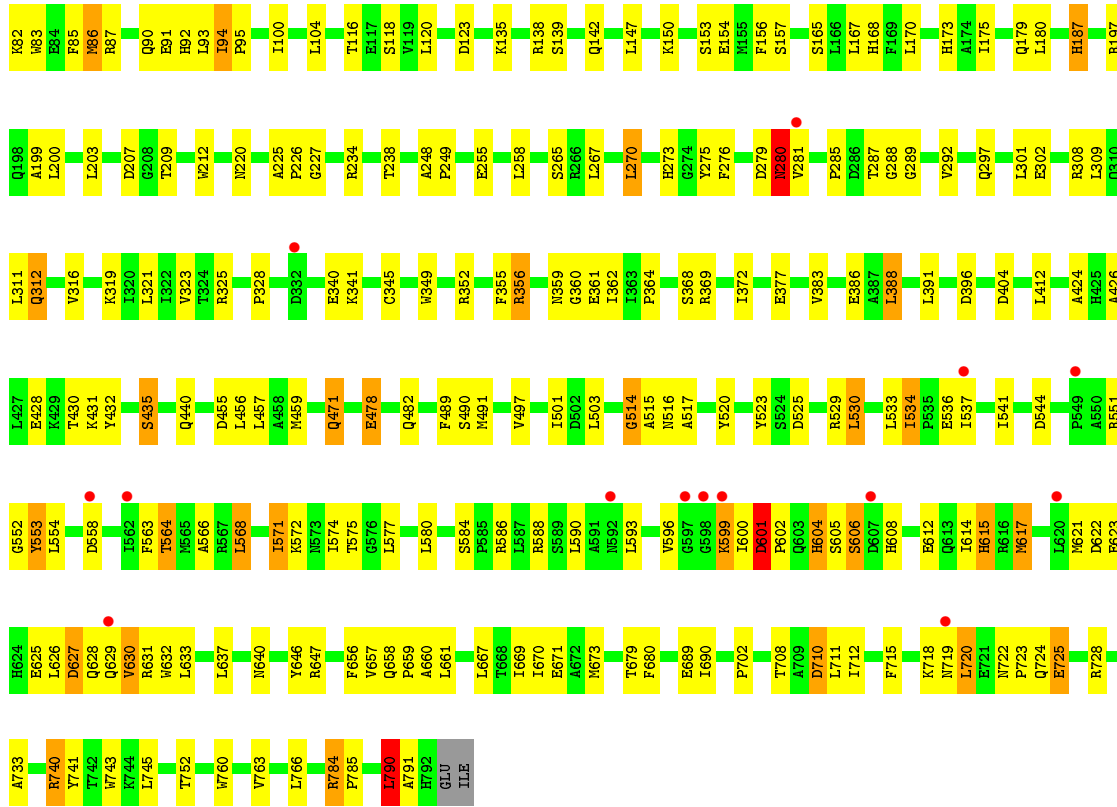
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sucrose synthase:Glycosyl transferases group 1.

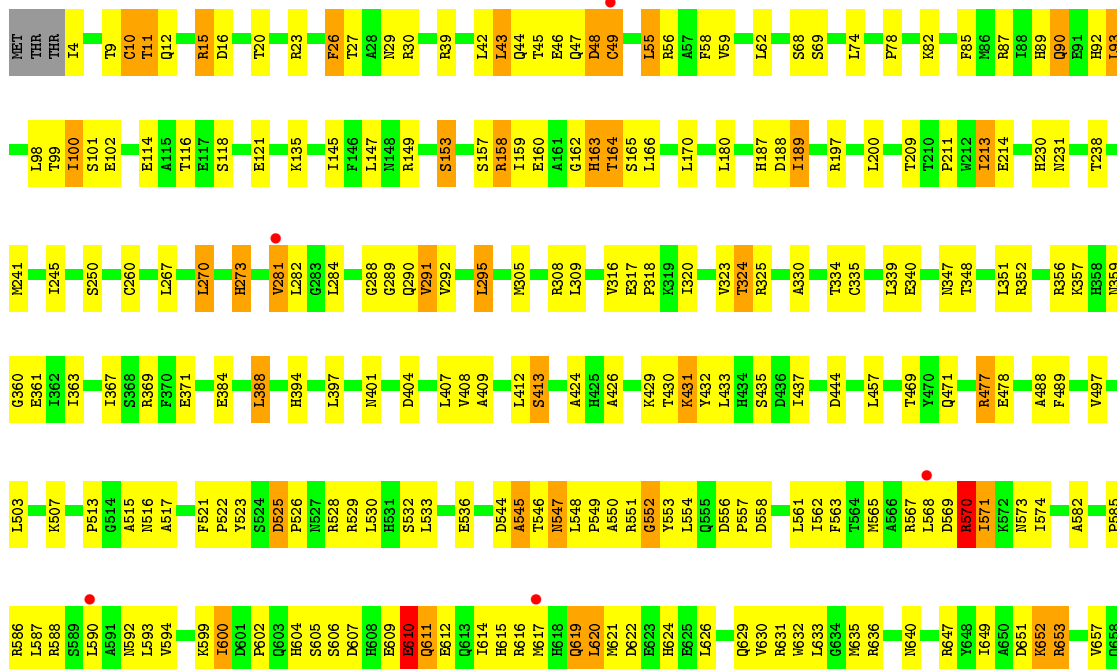
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	789	6332	4033	1106	1165	28	0	0	0
1	C	789	6360	4047	1112	1173	28	0	0	0
1	B	789	6346	4040	1106	1172	28	0	0	0
1	D	789	6352	4039	1111	1174	28	0	0	0

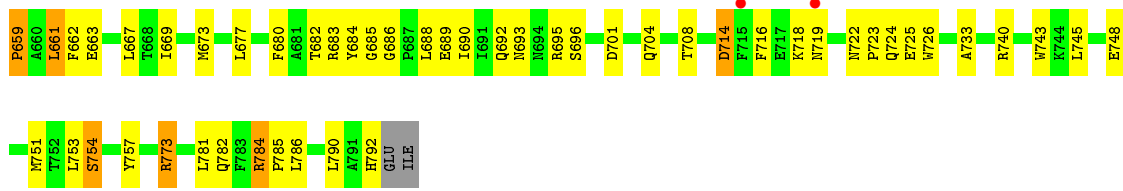
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total	O	0	0
			52	52		
2	C	50	Total	O	0	0
			50	50		
2	B	66	Total	O	0	0
			66	66		
2	D	37	Total	O	0	0
			37	37		

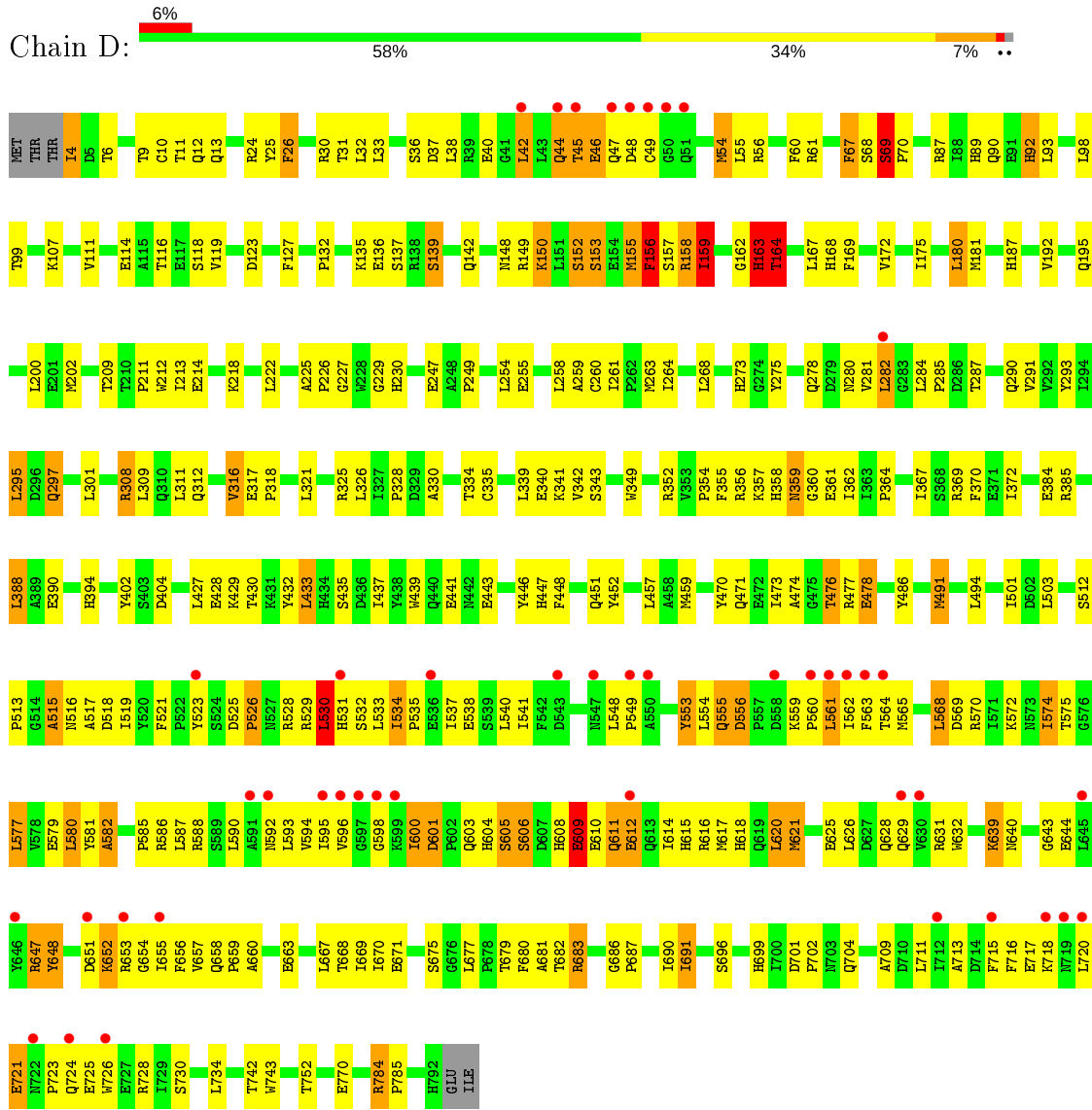


• Molecule 1: Sucrose synthase:Glycosyl transferases group 1





• Molecule 1: Sucrose synthase:Glycosyl transferases group 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.90Å 236.90Å 213.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.39 – 3.05 72.88 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (68.39-3.05) 93.5 (72.88-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.176 , 0.228 0.177 , 0.227	Depositor DCC
R_{free} test set	6337 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtrriage
Anisotropy	0.076	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25595	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, 0.333 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	0.51	1/6481 (0.0%)	0.74	5/8786 (0.1%)
1	B	0.48	0/6496	0.73	0/8806
1	C	0.47	0/6511	0.70	1/8825 (0.0%)
1	D	0.46	0/6501	0.72	7/8812 (0.1%)
All	All	0.48	1/25989 (0.0%)	0.72	13/35229 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	6
1	D	0	12
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	CYS	CB-SG	-7.03	1.70	1.82

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	530	LEU	CA-CB-CG	6.82	130.98	115.30
1	D	163	HIS	N-CA-C	-6.72	92.86	111.00
1	D	611	GLN	N-CA-C	-6.63	93.10	111.00
1	A	790	LEU	N-CA-C	6.37	128.19	111.00
1	A	569	ASP	C-N-CA	6.26	137.35	121.70
1	A	528	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	161	ALA	N-CA-C	-5.60	95.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	PHE	C-N-CA	5.58	135.65	121.70
1	A	164	THR	N-CA-C	-5.54	96.06	111.00
1	D	282	LEU	CA-CB-CG	5.46	127.87	115.30
1	D	164	THR	N-CA-C	-5.44	96.30	111.00
1	D	362	ILE	N-CA-C	5.27	125.24	111.00
1	C	790	LEU	N-CA-C	5.24	125.14	111.00

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLN	Peptide
1	A	13	GLN	Peptide
1	A	27	THR	Peptide
1	A	359	ASN	Peptide
1	A	551	ARG	Peptide
1	A	569	ASP	Peptide
1	B	163	HIS	Peptide
1	B	359	ASN	Peptide
1	B	545	ALA	Peptide
1	B	552	GLY	Peptide
1	B	570	ARG	Peptide
1	C	13	GLN	Peptide
1	C	359	ASN	Peptide
1	C	514	GLY	Peptide
1	C	599	LYS	Peptide
1	C	720	LEU	Peptide
1	C	790	LEU	Peptide
1	D	13	GLN	Peptide
1	D	155	MET	Peptide
1	D	159	ILE	Peptide
1	D	359	ASN	Peptide
1	D	526	PRO	Peptide
1	D	548	LEU	Peptide
1	D	549	PRO	Peptide
1	D	563	PHE	Peptide
1	D	582	ALA	Peptide
1	D	606	SER	Peptide
1	D	609	GLU	Peptide
1	D	702	PRO	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	6332	0	6210	169	0
1	B	6346	0	6220	177	0
1	C	6360	0	6240	167	0
1	D	6352	0	6235	218	0
2	A	52	0	0	1	0
2	B	66	0	0	4	0
2	C	50	0	0	0	0
2	D	37	0	0	0	0
All	All	25595	0	24905	716	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 14.

All (716) 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:D:516:ASN:HB3	1:D:518:ASP:H	1.25	1.01
1:D:654:GLY:O	1:D:655:ILE:HD13	1.66	0.94
1:D:360:GLY:HA2	1:D:361:GLU:HB3	1.52	0.91
1:D:654:GLY:O	1:D:655:ILE:CD1	2.22	0.86
1:D:369:ARG:NH2	1:D:428:GLU:OE2	2.08	0.86
1:B:604:HIS:HB2	1:B:605:SER:HB3	1.58	0.86
1:A:515:ALA:HB3	1:A:743:TRP:HD1	1.42	0.83
1:D:157:SER:O	1:D:159:ILE:N	2.11	0.82
1:B:515:ALA:HB3	1:B:743:TRP:HD1	1.43	0.81
1:D:716:PHE:HA	1:D:721:GLU:HG3	1.62	0.80
1:A:162:GLY:HA2	1:A:164:THR:H	1.45	0.80
1:D:579:GLU:HG2	1:D:580:LEU:HD22	1.65	0.79
1:A:657:VAL:HG22	1:A:680:PHE:HB2	1.64	0.78
1:D:611:GLN:O	1:D:614:ILE:N	2.15	0.78
1:B:288:GLY:H	1:B:290:GLN:HG3	1.48	0.78
1:A:136:GLU:OE2	1:C:197:ARG:NH1	2.16	0.78
1:D:340:GLU:OE1	1:D:352:ARG:NH2	2.16	0.77
1:C:12:GLN:HA	1:C:15:ARG:HB3	1.65	0.77
1:B:340:GLU:OE1	1:B:352:ARG:NH2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLY:HA2	1:D:164:THR:H	1.50	0.76
1:C:340:GLU:OE1	1:C:352:ARG:NH2	2.18	0.76
1:D:4:ILE:HG21	1:D:61:ARG:HG3	1.69	0.75
1:B:586:ARG:NH2	1:B:714:ASP:OD2	2.19	0.75
1:C:718:LYS:O	1:C:722:ASN:N	2.19	0.75
1:D:281:VAL:HG13	1:D:284:LEU:HD12	1.69	0.74
1:A:43:LEU:HA	1:A:46:GLU:HB2	1.69	0.74
1:D:54:MET:HG2	1:D:55:LEU:HD23	1.68	0.74
1:D:644:GLU:HA	1:D:648:TYR:HE1	1.51	0.74
1:B:360:GLY:HA2	1:B:361:GLU:HB2	1.69	0.73
1:C:123:ASP:OD2	1:B:773:ARG:NH1	2.21	0.73
1:B:515:ALA:HB3	1:B:743:TRP:CD1	2.24	0.72
1:B:356:ARG:HB3	1:B:360:GLY:HA3	1.70	0.72
1:C:69:SER:HB2	1:C:70:PRO:HD2	1.72	0.71
1:D:577:LEU:HB2	1:D:659:PRO:HG3	1.70	0.71
1:D:616:ARG:HH11	1:D:620:LEU:HD21	1.55	0.71
1:A:706:ALA:HA	1:A:709:ALA:HB3	1.73	0.70
1:B:549:PRO:HB3	1:B:600:ILE:HB	1.73	0.70
1:C:715:PHE:O	1:C:722:ASN:ND2	2.23	0.70
1:C:287:THR:HG22	1:C:288:GLY:H	1.56	0.70
1:B:682:THR:HG22	1:B:684:TYR:H	1.54	0.70
1:D:521:PHE:HB2	1:D:647:ARG:HH11	1.57	0.70
1:C:571:ILE:HA	1:C:661:LEU:HD12	1.74	0.70
1:C:33:LEU:HB2	1:C:67:PHE:HE2	1.57	0.70
1:A:360:GLY:HA2	1:A:361:GLU:HB3	1.73	0.69
1:D:357:LYS:O	1:D:359:ASN:N	2.25	0.68
1:D:530:LEU:HB2	1:D:648:TYR:CE2	2.28	0.68
1:D:562:ILE:HG22	1:D:564:THR:HG23	1.73	0.68
1:B:4:ILE:HD11	1:B:58:PHE:HA	1.75	0.68
1:D:604:HIS:HA	1:D:606:SER:N	2.09	0.68
1:A:162:GLY:HA2	1:A:164:THR:N	2.09	0.68
1:C:369:ARG:NH2	1:C:428:GLU:OE2	2.28	0.67
1:D:155:MET:HA	1:D:157:SER:HB2	1.76	0.67
1:B:43:LEU:HA	1:B:46:GLU:HB2	1.75	0.67
1:C:360:GLY:HA2	1:C:361:GLU:HB2	1.77	0.67
1:C:588:ARG:HH11	1:C:629:GLN:HG3	1.60	0.67
1:C:622:ASP:OD2	1:C:623:GLU:N	2.27	0.66
1:B:528:ARG:HG3	1:B:528:ARG:HH11	1.60	0.66
1:C:719:ASN:ND2	1:C:724:GLN:OE1	2.29	0.66
1:D:515:ALA:HB1	1:D:516:ASN:HA	1.75	0.66
1:A:582:ALA:HA	1:A:588:ARG:HE	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:GLY:O	1:D:655:ILE:CG1	2.43	0.66
1:D:515:ALA:HB3	1:D:743:TRP:HD1	1.60	0.66
1:B:250:SER:HB3	1:D:149:ARG:HD3	1.78	0.66
1:B:163:HIS:N	1:B:164:THR:O	2.29	0.66
1:A:118:SER:O	1:D:784:ARG:NH2	2.27	0.66
1:B:701:ASP:HB3	1:B:704:GLN:HB2	1.76	0.66
1:D:644:GLU:HA	1:D:648:TYR:CE1	2.31	0.65
1:C:275:TYR:HE1	1:C:285:PRO:HG2	1.62	0.65
1:D:574:ILE:HD12	1:D:574:ILE:H	1.61	0.65
1:A:784:ARG:NH2	1:D:118:SER:O	2.25	0.65
1:D:643:GLY:O	1:D:647:ARG:NH2	2.27	0.65
1:A:569:ASP:HB2	1:A:570:ARG:HB3	1.79	0.64
1:A:673:MET:HG2	1:A:733:ALA:HB1	1.80	0.64
1:D:281:VAL:HG11	1:D:287:THR:HG21	1.79	0.64
1:D:24:ARG:HH21	1:D:44:GLN:HB3	1.61	0.64
1:D:516:ASN:HA	1:D:517:ALA:HB3	1.79	0.64
1:D:651:ASP:N	1:D:652:LYS:O	2.31	0.64
1:D:162:GLY:HA2	1:D:164:THR:N	2.12	0.64
1:C:29:ASN:OD1	1:C:29:ASN:N	2.29	0.63
1:D:554:LEU:O	1:D:559:LYS:NZ	2.28	0.63
1:D:626:LEU:HB3	1:D:628:GLN:H	1.64	0.63
1:A:580:LEU:HD12	1:A:709:ALA:HB2	1.79	0.63
1:B:621:MET:HA	1:B:626:LEU:HD12	1.81	0.63
1:A:469:THR:OG1	1:A:472:GLU:HG3	1.98	0.63
1:A:48:ASP:OD1	1:A:48:ASP:N	2.32	0.63
1:D:157:SER:C	1:D:159:ILE:H	2.00	0.63
1:A:649:ILE:HG22	1:A:654:GLY:HA3	1.80	0.62
1:C:523:TYR:HA	1:C:647:ARG:HG2	1.80	0.62
1:C:11:THR:C	1:C:13:GLN:H	2.03	0.62
1:D:155:MET:HB2	1:D:249:PRO:HG3	1.82	0.62
1:B:673:MET:HG2	1:B:733:ALA:HB1	1.81	0.62
1:D:404:ASP:N	1:D:404:ASP:OD1	2.31	0.62
1:D:587:LEU:HG	1:D:709:ALA:HB2	1.81	0.61
1:D:717:GLU:HG3	1:D:718:LYS:H	1.64	0.61
1:B:158:ARG:NH2	1:B:159:ILE:HG12	2.15	0.61
1:C:600:ILE:HG23	1:C:601:ASP:O	2.01	0.61
1:D:553:TYR:N	1:D:628:GLN:O	2.30	0.61
1:B:16:ASP:O	1:B:20:THR:OG1	2.12	0.61
1:B:48:ASP:OD1	1:B:48:ASP:N	2.31	0.61
1:B:610:GLU:C	1:B:612:GLU:H	2.04	0.60
1:B:26:PHE:CE2	1:B:90:GLN:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ALA:HB1	1:A:517:ALA:N	2.17	0.60
1:C:600:ILE:HG21	1:C:614:ILE:HG23	1.84	0.60
1:A:162:GLY:H	1:A:164:THR:HG23	1.66	0.60
1:A:515:ALA:HB3	1:A:743:TRP:CD1	2.31	0.60
1:A:61:ARG:HD3	1:A:78:PRO:HA	1.83	0.60
1:B:135:LYS:HB2	1:D:247:GLU:HG3	1.83	0.60
1:B:521:PHE:HB2	1:B:522:PRO:HD2	1.83	0.60
1:D:720:LEU:HD13	1:D:723:PRO:HG2	1.84	0.60
1:D:654:GLY:O	1:D:655:ILE:HG12	2.02	0.60
1:D:175:ILE:HG12	1:D:180:LEU:HD22	1.84	0.59
1:D:515:ALA:HB3	1:D:743:TRP:CD1	2.37	0.59
1:B:360:GLY:HA2	1:B:361:GLU:CB	2.30	0.59
1:C:784:ARG:NH2	1:B:118:SER:O	2.33	0.59
1:C:723:PRO:HD2	1:C:724:GLN:HB2	1.83	0.59
1:A:382:ASP:OD1	1:A:385:ARG:NH1	2.31	0.59
1:A:163:HIS:ND1	1:A:165:SER:HB2	2.17	0.59
1:B:568:LEU:HD12	1:B:574:ILE:HD13	1.85	0.59
1:B:523:TYR:O	1:B:529:ARG:HD2	2.03	0.59
1:B:26:PHE:HE2	1:B:90:GLN:HB2	1.68	0.58
1:C:428:GLU:HG2	1:C:431:LYS:HD3	1.85	0.58
1:A:269:ILE:HD12	1:A:399:ILE:HD12	1.85	0.58
1:D:167:LEU:HD13	1:D:192:VAL:HG21	1.86	0.58
1:B:431:LYS:HE2	1:B:432:TYR:CZ	2.37	0.58
1:B:477:ARG:HH11	1:B:477:ARG:HB3	1.69	0.58
1:C:584:SER:O	1:C:588:ARG:HG3	2.03	0.58
1:B:85:PHE:CE2	1:B:100:ILE:HG12	2.38	0.58
1:D:562:ILE:HG22	1:D:564:THR:CG2	2.32	0.58
1:A:9:THR:O	1:A:12:GLN:HG3	2.03	0.58
1:A:693:ASN:HB2	1:A:699:HIS:ND1	2.19	0.57
1:D:656:PHE:HB2	1:D:677:LEU:HD23	1.86	0.57
1:B:324:THR:OG1	1:B:325:ARG:N	2.35	0.57
1:B:547:ASN:OD1	1:B:547:ASN:N	2.32	0.57
1:B:599:LYS:HB2	1:B:614:ILE:HD11	1.86	0.57
1:B:652:LYS:HG2	1:B:653:ARG:HG2	1.86	0.57
1:C:227:GLY:O	1:C:312:GLN:HG3	2.04	0.57
1:D:570:ARG:HD3	1:D:610:GLU:HG2	1.85	0.57
1:D:621:MET:HB2	1:D:632:TRP:CH2	2.39	0.57
1:B:550:ALA:HB1	1:B:551:ARG:HA	1.87	0.57
1:C:669:ILE:HG23	1:C:679:THR:HG21	1.86	0.57
1:C:670:ILE:HD11	1:C:690:ILE:HD13	1.87	0.57
1:C:360:GLY:HA2	1:C:361:GLU:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:PRO:HG2	1:C:364:PRO:HA	1.85	0.57
1:A:270:LEU:HD21	1:A:412:LEU:HD12	1.87	0.57
1:B:44:GLN:N	1:B:46:GLU:H	2.03	0.57
1:C:627:ASP:N	1:C:627:ASP:OD1	2.29	0.57
1:A:572:LYS:NZ	1:A:663:GLU:OE1	2.36	0.56
1:C:632:TRP:HD1	1:C:633:LEU:N	2.03	0.56
1:A:441:GLU:OE1	1:A:441:GLU:N	2.38	0.56
1:C:356:ARG:HB3	1:C:360:GLY:HA3	1.86	0.56
1:A:569:ASP:HB2	1:A:570:ARG:HD2	1.85	0.56
1:D:357:LYS:C	1:D:359:ASN:H	2.06	0.56
1:D:341:LYS:HB2	1:D:349:TRP:CZ3	2.41	0.56
1:A:355:PHE:HB3	1:A:363:ILE:HD12	1.87	0.56
1:B:15:ARG:HB3	1:B:15:ARG:HH11	1.69	0.56
1:D:92:HIS:H	1:D:92:HIS:CD2	2.22	0.56
1:A:577:LEU:HA	1:A:580:LEU:HD23	1.88	0.56
1:B:320:ILE:HB	1:B:348:THR:HG23	1.86	0.56
1:B:288:GLY:N	1:B:290:GLN:HG3	2.19	0.56
1:B:657:VAL:HG22	1:B:680:PHE:HB2	1.88	0.56
1:A:562:ILE:HD11	1:A:716:PHE:HE2	1.71	0.56
1:B:609:GLU:O	1:B:611:GLN:NE2	2.38	0.55
1:C:459:MET:CE	1:C:501:ILE:HB	2.36	0.55
1:A:773:ARG:NH1	1:D:123:ASP:OD2	2.39	0.55
1:A:87:ARG:HB3	1:A:98:LEU:HD11	1.87	0.55
1:C:600:ILE:HG12	1:C:614:ILE:HG13	1.87	0.55
1:A:111:VAL:HG12	1:A:112:LYS:HG2	1.88	0.55
1:A:369:ARG:NH2	1:A:428:GLU:OE1	2.39	0.55
1:A:79:GLU:OE2	1:A:477:ARG:NH2	2.39	0.55
1:A:566:ALA:HB3	1:A:574:ILE:HD11	1.89	0.55
1:D:582:ALA:HA	1:D:585:PRO:HG3	1.88	0.55
1:D:660:ALA:HB3	1:D:663:GLU:HB2	1.87	0.55
1:D:211:PRO:HB2	1:D:213:ILE:HG22	1.87	0.55
1:D:325:ARG:HH12	1:D:367:ILE:HG13	1.71	0.55
1:B:544:ASP:HB3	1:B:553:TYR:CD1	2.41	0.55
1:B:723:PRO:HG2	1:B:724:GLN:NE2	2.22	0.55
1:A:230:HIS:CG	1:A:231:ASN:H	2.24	0.55
1:C:42:LEU:HD11	1:C:55:LEU:HD12	1.89	0.55
1:C:43:LEU:HA	1:C:46:GLU:HB2	1.89	0.55
1:C:24:ARG:HG3	1:C:45:THR:HG23	1.89	0.55
1:D:601:ASP:OD2	1:D:605:SER:OG	2.25	0.55
1:D:668:THR:HA	1:D:671:GLU:OE2	2.07	0.55
1:A:368:SER:HB3	1:A:371:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:H	1:D:433:LEU:HD22	1.72	0.54
1:A:238:THR:HG21	1:A:312:GLN:HE22	1.72	0.54
1:A:297:GLN:HG3	1:A:301:LEU:HD22	1.90	0.54
1:B:289:GLY:O	1:B:292:VAL:HG12	2.08	0.54
1:B:357:LYS:HG3	1:B:363:ILE:HD11	1.89	0.54
1:C:725:GLU:OE2	1:C:728:ARG:NH1	2.39	0.54
1:D:326:LEU:HD13	1:D:354:PRO:HG3	1.89	0.54
1:A:149:ARG:O	1:A:153:SER:HB3	2.08	0.54
1:B:669:ILE:HG22	1:B:673:MET:HE2	1.88	0.54
1:D:593:LEU:HD22	1:D:595:ILE:HD11	1.90	0.54
1:A:593:LEU:HD13	1:A:595:ILE:HD11	1.89	0.54
1:B:197:ARG:NH1	1:D:136:GLU:OE2	2.41	0.54
1:B:305:MET:HG2	1:B:751:MET:SD	2.48	0.54
1:D:175:ILE:HG21	1:D:316:VAL:HG21	1.89	0.54
1:A:23:ARG:O	1:A:27:THR:HG23	2.07	0.53
1:D:11:THR:OG1	1:D:55:LEU:HD21	2.08	0.53
1:D:360:GLY:HA2	1:D:361:GLU:CB	2.23	0.53
1:B:397:LEU:HD22	1:B:754:SER:HB3	1.90	0.53
1:C:723:PRO:CD	1:C:724:GLN:HB2	2.37	0.53
1:A:164:THR:HB	1:A:187:HIS:CD2	2.44	0.53
1:A:547:ASN:N	1:A:547:ASN:OD1	2.41	0.53
1:B:574:ILE:H	1:B:574:ILE:HD12	1.73	0.53
1:C:604:HIS:HA	1:C:605:SER:C	2.28	0.53
1:A:513:PRO:HB3	1:A:743:TRP:CZ2	2.43	0.53
1:C:150:LYS:NZ	1:C:154:GLU:OE1	2.37	0.53
1:C:784:ARG:HB3	1:C:785:PRO:HD3	1.90	0.53
1:D:111:VAL:HG21	1:D:437:ILE:HG12	1.91	0.53
1:D:617:MET:HG2	1:D:632:TRP:HZ2	1.73	0.53
1:A:540:LEU:HB3	1:A:633:LEU:HD21	1.89	0.53
1:B:211:PRO:HG2	1:B:214:GLU:HG2	1.91	0.53
1:D:568:LEU:HD22	1:D:598:GLY:HA3	1.90	0.53
1:D:569:ASP:HB3	1:D:572:LYS:HB2	1.90	0.53
1:D:565:MET:HG3	1:D:596:VAL:HB	1.90	0.53
1:D:297:GLN:HB2	1:D:743:TRP:CZ3	2.43	0.53
1:A:163:HIS:CG	1:A:165:SER:HB2	2.44	0.53
1:B:42:LEU:HD13	1:B:59:VAL:HG21	1.90	0.53
1:B:611:GLN:N	2:B:846:HOH:O	2.42	0.53
1:B:602:PRO:HD3	1:B:614:ILE:HG21	1.91	0.53
1:B:790:LEU:C	1:B:792:HIS:H	2.10	0.53
1:D:6:THR:O	1:D:9:THR:HG22	2.09	0.52
1:B:554:LEU:H	1:B:554:LEU:HD12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:MET:SD	1:D:632:TRP:NE1	2.82	0.52
1:B:291:VAL:HG13	1:B:295:LEU:HD23	1.90	0.52
1:D:604:HIS:NE2	1:D:612:GLU:HG3	2.25	0.52
1:C:6:THR:HG23	1:C:7:LEU:HD12	1.90	0.52
1:B:273:HIS:CD2	1:B:273:HIS:C	2.83	0.52
1:A:324:THR:OG1	1:A:325:ARG:N	2.42	0.52
1:D:669:ILE:HG23	1:D:679:THR:HG21	1.91	0.52
1:A:299:ARG:HG2	1:A:345:CYS:SG	2.49	0.52
1:A:582:ALA:HB1	1:A:624:HIS:ND1	2.25	0.52
1:C:566:ALA:HB1	1:C:572:LYS:HD2	1.91	0.52
1:A:556:ASP:N	1:A:556:ASP:OD2	2.43	0.52
1:C:156:PHE:CD2	1:C:249:PRO:HD2	2.45	0.52
1:D:139:SER:O	1:D:142:GLN:HB2	2.10	0.52
1:D:291:VAL:O	1:D:295:LEU:HB2	2.10	0.52
1:C:20:THR:HG23	1:C:23:ARG:HH21	1.75	0.51
1:C:599:LYS:O	1:C:601:ASP:HB2	2.09	0.51
1:C:552:GLY:HA3	1:C:631:ARG:HA	1.92	0.51
1:D:691:ILE:HG22	1:D:699:HIS:NE2	2.25	0.51
1:A:569:ASP:HB2	1:A:570:ARG:CD	2.40	0.51
1:B:42:LEU:HD21	1:B:56:ARG:HG2	1.93	0.51
1:D:603:GLN:H	1:D:603:GLN:NE2	2.09	0.51
1:A:600:ILE:H	1:A:634:GLY:HA3	1.75	0.51
1:B:571:ILE:HD11	1:B:662:PHE:H	1.76	0.51
1:D:679:THR:HG22	1:D:681:ALA:H	1.76	0.51
1:A:150:LYS:NZ	1:A:154:GLU:OE1	2.37	0.51
1:C:459:MET:HE1	1:C:501:ILE:HB	1.93	0.51
1:C:516:ASN:HA	1:C:517:ALA:HB3	1.92	0.51
1:D:132:PRO:HG3	1:D:150:LYS:HD2	1.91	0.51
1:D:608:HIS:ND1	1:D:611:GLN:HG2	2.25	0.51
1:C:514:GLY:O	1:C:743:TRP:NE1	2.44	0.51
1:D:473:ILE:HG22	1:D:503:LEU:HD12	1.93	0.51
1:D:92:HIS:HD2	1:D:92:HIS:H	1.58	0.51
1:A:155:MET:HG3	1:A:163:HIS:HB2	1.93	0.50
1:A:288:GLY:H	1:A:290:GLN:HG3	1.74	0.50
1:A:338:ARG:HH21	1:A:386:GLU:HG2	1.76	0.50
1:B:647:ARG:NH1	2:B:839:HOH:O	2.43	0.50
1:D:541:ILE:O	1:D:631:ARG:NH1	2.25	0.50
1:C:612:GLU:O	1:C:615:HIS:HB2	2.12	0.50
1:D:87:ARG:HB3	1:D:98:LEU:HD11	1.93	0.50
1:A:528:ARG:CG	1:A:528:ARG:HH11	2.23	0.50
1:A:31:THR:HB	1:A:67:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:VAL:HG22	1:C:680:PHE:HB2	1.93	0.50
1:A:593:LEU:HD22	1:A:595:ILE:HD11	1.93	0.50
1:D:521:PHE:O	1:D:675:SER:HA	2.10	0.50
1:A:569:ASP:CA	1:A:570:ARG:HB3	2.41	0.50
1:A:85:PHE:CZ	1:A:100:ILE:HD13	2.46	0.50
1:B:424:ALA:C	1:B:426:ALA:H	2.15	0.50
1:D:568:LEU:HD13	1:D:598:GLY:HA3	1.92	0.50
1:D:784:ARG:HB3	1:D:785:PRO:HD3	1.93	0.50
1:B:89:HIS:HB3	1:B:92:HIS:O	2.12	0.50
1:C:377:GLU:OE1	1:C:784:ARG:NH1	2.44	0.50
1:D:355:PHE:O	1:D:356:ARG:HG3	2.12	0.50
1:D:370:PHE:CE1	1:D:446:TYR:HD1	2.30	0.50
1:D:526:PRO:HA	1:D:529:ARG:HB2	1.93	0.50
1:B:563:PHE:CZ	1:B:565:MET:HE2	2.47	0.50
1:B:600:ILE:HG12	1:B:632:TRP:CH2	2.47	0.50
1:D:157:SER:O	1:D:159:ILE:HG13	2.11	0.50
1:C:270:LEU:HD21	1:C:412:LEU:HD12	1.94	0.50
1:D:227:GLY:O	1:D:312:GLN:HB3	2.11	0.50
1:D:586:ARG:HH11	1:D:713:ALA:HB2	1.76	0.50
1:A:527:ASN:OD1	1:A:527:ASN:N	2.45	0.50
1:A:587:LEU:HD22	1:A:709:ALA:HB1	1.94	0.50
1:A:384:GLU:O	1:A:388:LEU:HB2	2.12	0.49
1:B:158:ARG:HB2	1:B:162:GLY:HA3	1.94	0.49
1:D:156:PHE:H	1:D:158:ARG:HB3	1.76	0.49
1:A:633:LEU:HD23	1:A:635:MET:SD	2.52	0.49
1:A:288:GLY:C	1:A:290:GLN:H	2.14	0.49
1:B:563:PHE:HZ	1:B:565:MET:HE2	1.77	0.49
1:D:470:TYR:CE1	1:D:474:ALA:HB3	2.47	0.49
1:D:562:ILE:CG2	1:D:564:THR:CG2	2.90	0.49
1:B:429:LYS:HE2	1:B:489:PHE:CG	2.47	0.49
1:B:582:ALA:HB1	1:B:624:HIS:CE1	2.48	0.49
1:B:92:HIS:H	1:B:92:HIS:CD2	2.30	0.49
1:C:621:MET:HG3	1:C:626:LEU:HD12	1.94	0.49
1:A:442:ASN:HB3	1:A:446:TYR:HD2	1.76	0.49
1:B:515:ALA:HB1	1:B:516:ASN:HA	1.94	0.49
1:C:673:MET:HB3	1:C:733:ALA:HB1	1.94	0.49
1:C:77:ARG:HD2	1:C:83:TRP:CZ2	2.48	0.49
1:D:30:ARG:NH2	1:D:37:ASP:OD2	2.45	0.49
1:C:33:LEU:HD22	1:C:37:ASP:HB2	1.95	0.49
1:C:596:VAL:HG11	1:C:637:LEU:HG	1.95	0.49
1:D:600:ILE:HG13	1:D:618:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:PRO:HD2	1:C:364:PRO:O	2.13	0.49
1:D:212:TRP:CZ2	1:D:226:PRO:HA	2.48	0.49
1:D:491:MET:O	1:D:494:LEU:HB2	2.13	0.49
1:A:209:THR:HA	1:A:231:ASN:HB2	1.93	0.49
1:A:621:MET:HA	1:A:626:LEU:CG	2.43	0.49
1:B:588:ARG:HH11	1:B:629:GLN:HE21	1.60	0.49
1:B:784:ARG:HB3	1:B:785:PRO:HD3	1.95	0.49
1:C:118:SER:O	1:B:784:ARG:NH2	2.29	0.49
1:B:153:SER:HA	1:D:153:SER:HB2	1.95	0.49
1:B:568:LEU:HA	1:B:574:ILE:HD13	1.95	0.49
1:A:28:ALA:C	1:A:30:ARG:H	2.15	0.48
1:A:569:ASP:HA	1:A:570:ARG:HB3	1.95	0.48
1:C:33:LEU:HB2	1:C:67:PHE:CE2	2.44	0.48
1:D:42:LEU:HD11	1:D:56:ARG:HH11	1.77	0.48
1:D:617:MET:HG2	1:D:632:TRP:CZ2	2.48	0.48
1:A:569:ASP:CB	1:A:570:ARG:HB3	2.42	0.48
1:C:614:ILE:HA	1:C:617:MET:HB2	1.95	0.48
1:D:581:TYR:CE1	1:D:587:LEU:HB3	2.48	0.48
1:B:163:HIS:O	1:B:166:LEU:HB3	2.13	0.48
1:B:570:ARG:HA	2:B:851:HOH:O	2.13	0.48
1:D:476:THR:HB	1:D:478:GLU:OE2	2.13	0.48
1:D:701:ASP:O	1:D:704:GLN:HB2	2.13	0.48
1:A:4:ILE:HG23	1:A:8:ALA:HB2	1.94	0.48
1:B:325:ARG:HH12	1:B:367:ILE:HG13	1.77	0.48
1:C:369:ARG:HH22	1:C:428:GLU:CD	2.15	0.48
1:D:428:GLU:HG3	1:D:451:GLN:OE1	2.14	0.48
1:C:9:THR:C	1:C:11:THR:H	2.17	0.48
1:C:577:LEU:HD12	1:C:580:LEU:HD11	1.96	0.48
1:D:609:GLU:HG3	1:D:609:GLU:O	2.13	0.48
1:D:670:ILE:HD11	1:D:690:ILE:HD13	1.96	0.48
1:B:611:GLN:O	1:B:615:HIS:ND1	2.46	0.48
1:B:59:VAL:HA	1:B:62:LEU:HD12	1.95	0.48
1:D:321:LEU:HD11	1:D:390:GLU:HB3	1.95	0.48
1:D:330:ALA:HB2	1:D:335:CYS:HB2	1.94	0.48
1:A:578:VAL:O	1:A:581:TYR:HB3	2.14	0.48
1:A:626:LEU:O	1:A:630:VAL:HB	2.14	0.48
1:D:156:PHE:H	1:D:158:ARG:CB	2.27	0.47
1:D:429:LYS:HG3	1:D:452:TYR:CE2	2.48	0.47
1:D:308:ARG:NH2	1:D:752:THR:OG1	2.46	0.47
1:A:89:HIS:CE1	1:A:91:GLU:H	2.32	0.47
1:D:555:GLN:O	1:D:559:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:HA	1:A:698:PHE:CE1	2.50	0.47
1:C:529:ARG:HE	1:C:529:ARG:HB3	1.52	0.47
1:A:8:ALA:O	1:A:11:THR:OG1	2.31	0.47
1:A:212:TRP:N	1:A:230:HIS:O	2.47	0.47
1:A:328:PRO:HG3	1:A:362:ILE:HD11	1.95	0.47
1:A:722:ASN:HD21	1:A:725:GLU:HG2	1.79	0.47
1:D:647:ARG:H	1:D:647:ARG:HG2	1.34	0.47
1:A:539:SER:O	1:A:543:ASP:HB2	2.13	0.47
1:D:275:TYR:HD1	1:D:335:CYS:SG	2.38	0.47
1:B:10:CYS:C	1:B:12:GLN:H	2.17	0.47
1:A:558:ASP:N	1:A:558:ASP:OD2	2.47	0.47
1:B:515:ALA:HB1	1:B:517:ALA:N	2.29	0.47
1:B:471:GLN:HG3	1:B:689:GLU:OE1	2.14	0.47
1:D:264:ILE:O	1:D:309:LEU:HD21	2.15	0.47
1:D:639:LYS:HD2	1:D:639:LYS:H	1.79	0.47
1:A:680:PHE:CD2	1:A:698:PHE:HB2	2.49	0.47
1:C:276:PHE:O	1:C:281:VAL:HG11	2.14	0.47
1:D:428:GLU:HB3	1:D:432:TYR:CE2	2.50	0.47
1:D:259:ALA:HB2	1:D:752:THR:HG23	1.97	0.47
1:A:320:ILE:HB	1:A:348:THR:HG23	1.97	0.47
1:C:533:LEU:O	1:C:537:ILE:HG13	2.14	0.47
1:D:155:MET:HB3	1:D:158:ARG:NH1	2.30	0.47
1:D:592:ASN:O	1:D:593:LEU:HG	2.15	0.47
1:C:234:ARG:O	1:C:238:THR:HG23	2.15	0.47
1:D:195:GLN:NE2	1:D:222:LEU:O	2.34	0.47
1:D:293:TYR:O	1:D:297:GLN:HB3	2.15	0.47
1:D:427:LEU:HD13	1:D:486:TYR:CE1	2.50	0.47
1:C:302:GLU:OE1	1:C:345:CYS:HB3	2.15	0.47
1:C:85:PHE:CZ	1:C:100:ILE:HD13	2.50	0.47
1:D:169:PHE:O	1:D:172:VAL:HG22	2.15	0.47
1:D:586:ARG:HH11	1:D:713:ALA:CB	2.28	0.47
1:B:318:PRO:O	1:B:347:ASN:HB3	2.16	0.46
1:B:325:ARG:NH1	1:B:367:ILE:HG13	2.31	0.46
1:C:515:ALA:HB1	1:C:517:ALA:HB2	1.97	0.46
1:D:568:LEU:HA	1:D:574:ILE:HD13	1.96	0.46
1:D:691:ILE:HG22	1:D:699:HIS:HE2	1.80	0.46
1:D:284:LEU:HB3	1:D:285:PRO:HD2	1.98	0.46
1:D:428:GLU:HB3	1:D:432:TYR:HE2	1.81	0.46
1:A:568:LEU:HD12	1:A:574:ILE:HD13	1.98	0.46
1:D:148:ASN:O	1:D:152:SER:HB3	2.14	0.46
1:A:562:ILE:HG12	1:A:655:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD11	1:A:107:LYS:HD2	1.96	0.46
1:B:270:LEU:O	1:B:401:ASN:HB2	2.16	0.46
1:B:550:ALA:O	1:B:600:ILE:HG21	2.16	0.46
1:B:653:ARG:HA	1:B:726:TRP:CE2	2.51	0.46
1:C:790:LEU:H	1:C:791:ALA:HB3	1.79	0.46
1:B:15:ARG:NH1	1:B:15:ARG:HB3	2.31	0.46
1:B:561:LEU:HD11	1:B:594:VAL:HG23	1.97	0.46
1:C:120:LEU:HD22	1:B:781:LEU:HD21	1.97	0.46
1:C:424:ALA:C	1:C:426:ALA:H	2.18	0.46
1:B:669:ILE:HG22	1:B:673:MET:CE	2.46	0.46
1:C:74:LEU:HB2	1:C:86:MET:HG2	1.97	0.46
1:A:230:HIS:CG	1:A:231:ASN:N	2.84	0.46
1:C:355:PHE:HZ	1:C:372:ILE:HD11	1.80	0.46
1:C:719:ASN:HB3	1:C:723:PRO:HD2	1.97	0.46
1:D:432:TYR:HB2	1:D:435:SER:OG	2.16	0.46
1:B:593:LEU:HB3	1:B:630:VAL:HG12	1.97	0.46
1:B:692:GLN:H	1:B:696:SER:HB2	1.81	0.46
1:C:459:MET:HB2	1:C:459:MET:HE2	1.75	0.46
1:A:770:GLU:HG2	1:D:127:PHE:CD2	2.51	0.46
1:A:585:PRO:HG2	2:A:843:HOH:O	2.15	0.46
1:B:101:SER:OG	1:B:121:GLU:OE2	2.31	0.46
1:B:78:PRO:HD2	1:B:82:LYS:O	2.15	0.46
1:C:601:ASP:HB3	1:C:602:PRO:HD2	1.98	0.46
1:D:158:ARG:HH11	1:D:163:HIS:HB2	1.80	0.46
1:D:211:PRO:HG2	1:D:214:GLU:HG3	1.97	0.46
1:D:290:GLN:HB2	1:D:402:TYR:OH	2.16	0.46
1:D:107:LYS:HG2	1:D:437:ILE:HD13	1.98	0.46
1:D:604:HIS:CD2	1:D:606:SER:HB2	2.50	0.46
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.63	0.46
1:A:540:LEU:HB3	1:A:633:LEU:CD2	2.45	0.46
1:B:330:ALA:HB2	1:B:335:CYS:HB2	1.97	0.46
1:B:44:GLN:N	1:B:46:GLU:N	2.64	0.46
1:C:690:ILE:HA	1:C:741:TYR:OH	2.15	0.46
1:A:618:HIS:O	1:A:621:MET:HB3	2.16	0.45
1:D:512:SER:HA	1:D:513:PRO:HD3	1.61	0.45
1:B:515:ALA:HB1	1:B:516:ASN:CA	2.46	0.45
1:D:683:ARG:HB2	1:D:683:ARG:CZ	2.46	0.45
1:A:247:GLU:HG3	1:C:135:LYS:HB2	1.98	0.45
1:A:528:ARG:HH11	1:A:528:ARG:HB2	1.82	0.45
1:B:282:LEU:HD22	1:B:636:ARG:NH2	2.30	0.45
1:B:87:ARG:HB3	1:B:98:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:THR:OG1	1:B:102:GLU:HG3	2.16	0.45
1:D:258:LEU:HD23	1:D:261:ILE:HD11	1.98	0.45
1:A:43:LEU:H	1:A:43:LEU:HD23	1.82	0.45
1:B:388:LEU:HA	1:B:388:LEU:HD12	1.68	0.45
1:B:409:ALA:O	1:B:413:SER:HB3	2.16	0.45
1:B:615:HIS:O	1:B:619:GLN:HB2	2.16	0.45
1:B:616:ARG:O	1:B:620:LEU:HB2	2.17	0.45
1:D:680:PHE:CE2	1:D:711:LEU:HD21	2.50	0.45
1:B:323:VAL:HA	1:B:351:LEU:O	2.17	0.45
1:B:48:ASP:HA	1:B:49:CYS:HA	1.50	0.45
1:B:626:LEU:O	1:B:629:GLN:HB2	2.16	0.45
1:C:724:GLN:O	1:C:725:GLU:HB3	2.16	0.45
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.71	0.45
1:A:69:SER:HB3	1:A:70:PRO:HD2	1.99	0.45
1:C:520:TYR:CD2	1:C:671:GLU:HG2	2.52	0.45
1:A:193:ARG:O	1:A:197:ARG:HG3	2.17	0.45
1:A:72:ALA:HB3	1:A:88:ILE:HG22	1.98	0.45
1:C:566:ALA:HB3	1:C:574:ILE:HD11	1.97	0.45
1:C:605:SER:HA	1:C:606:SER:HA	1.36	0.45
1:A:261:ILE:HG22	1:A:263:MET:HG2	1.99	0.45
1:B:288:GLY:C	1:B:290:GLN:H	2.20	0.45
1:C:626:LEU:HB3	1:C:630:VAL:HG13	1.98	0.45
1:D:533:LEU:HB2	1:D:537:ILE:HG12	1.99	0.45
1:A:203:LEU:HD22	1:A:232:ALA:HB1	1.99	0.45
1:A:230:HIS:CD2	1:A:231:ASN:H	2.35	0.45
1:A:621:MET:HA	1:A:626:LEU:HG	1.99	0.45
1:B:651:ASP:HA	1:B:652:LYS:HA	1.57	0.45
1:C:78:PRO:HD2	1:C:82:LYS:O	2.16	0.45
1:D:168:HIS:HB2	1:D:187:HIS:CE1	2.51	0.45
1:D:441:GLU:OE1	1:D:441:GLU:N	2.42	0.45
1:B:11:THR:HG21	1:B:55:LEU:HD23	1.98	0.45
1:A:449:SER:HA	1:A:491:MET:CE	2.47	0.44
1:A:651:ASP:HA	1:A:652:LYS:HA	1.70	0.44
1:C:568:LEU:HA	1:C:568:LEU:HD22	1.85	0.44
1:C:577:LEU:HB2	1:C:659:PRO:HG3	1.99	0.44
1:D:439:TRP:CD1	1:D:491:MET:HG3	2.52	0.44
1:D:585:PRO:HB2	1:D:588:ARG:H	1.82	0.44
1:A:153:SER:HB2	1:C:153:SER:HA	2.00	0.44
1:A:293:TYR:O	1:A:297:GLN:HB3	2.17	0.44
1:A:537:ILE:HG22	1:A:648:TYR:HD2	1.82	0.44
1:A:722:ASN:CG	1:A:726:TRP:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:ARG:HD3	1:B:773:ARG:HA	1.86	0.44
1:C:601:ASP:N	1:C:601:ASP:OD1	2.51	0.44
1:A:257:PHE:O	1:A:260:CYS:HB2	2.17	0.44
1:B:571:ILE:HD12	1:B:661:LEU:HB2	1.97	0.44
1:C:33:LEU:HD23	1:C:33:LEU:HA	1.67	0.44
1:C:432:TYR:O	1:C:435:SER:OG	2.26	0.44
1:C:478:GLU:H	1:C:478:GLU:HG2	1.60	0.44
1:D:384:GLU:O	1:D:388:LEU:HB2	2.17	0.44
1:D:686:GLY:O	1:D:690:ILE:HG13	2.17	0.44
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.82	0.44
1:B:633:LEU:HD22	1:B:635:MET:HE1	1.99	0.44
1:B:683:ARG:HE	1:B:684:TYR:HE1	1.65	0.44
1:C:279:ASP:OD2	1:C:280:ASN:N	2.50	0.44
1:D:26:PHE:CE1	1:D:67:PHE:HB3	2.52	0.44
1:B:10:CYS:C	1:B:12:GLN:N	2.71	0.44
1:B:291:VAL:HG13	1:B:295:LEU:CD2	2.48	0.44
1:B:605:SER:HA	1:B:606:SER:HA	1.71	0.44
1:A:569:ASP:HB2	1:A:570:ARG:CB	2.46	0.44
1:D:155:MET:O	1:D:156:PHE:HB2	2.18	0.44
1:D:523:TYR:O	1:D:526:PRO:HD3	2.17	0.44
1:B:12:GLN:O	1:B:15:ARG:HG3	2.18	0.44
1:D:328:PRO:HD2	1:D:364:PRO:HA	1.98	0.44
1:A:429:LYS:HE2	1:A:485:SER:OG	2.17	0.44
1:B:241:MET:O	1:B:245:ILE:HD12	2.17	0.44
1:B:281:VAL:HG11	1:B:291:VAL:HG11	1.99	0.44
1:B:39:ARG:NH2	1:B:478:GLU:OE1	2.50	0.44
1:C:456:LEU:HD21	1:C:497:VAL:HG11	2.00	0.44
1:D:275:TYR:H	1:D:287:THR:HG1	1.63	0.44
1:D:46:GLU:HG3	1:D:47:GLN:HG3	2.00	0.44
1:D:570:ARG:HG2	1:D:570:ARG:H	1.63	0.44
1:B:267:LEU:HB2	1:B:320:ILE:HG12	2.00	0.44
1:B:562:ILE:HD11	1:B:716:PHE:HE2	1.83	0.44
1:C:199:ALA:O	1:C:203:LEU:HG	2.17	0.44
1:D:158:ARG:HG3	1:D:158:ARG:O	2.18	0.44
1:D:268:LEU:HD12	1:D:321:LEU:HB2	1.99	0.44
1:B:551:ARG:HB2	1:B:552:GLY:H	1.65	0.43
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.74	0.43
1:A:273:HIS:HD2	1:A:404:ASP:OD1	2.01	0.43
1:C:147:LEU:HD21	1:C:760:TRP:HB2	1.99	0.43
1:C:471:GLN:HG2	1:C:689:GLU:OE1	2.18	0.43
1:C:48:ASP:N	1:C:48:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:PHE:CD2	1:D:726:TRP:HB2	2.53	0.43
1:A:44:GLN:HA	1:A:45:THR:HA	1.80	0.43
1:B:27:THR:O	1:B:27:THR:OG1	2.35	0.43
1:B:513:PRO:HB3	1:B:743:TRP:CH2	2.53	0.43
1:B:513:PRO:HB3	1:B:743:TRP:CZ2	2.53	0.43
1:A:305:MET:HG2	1:A:751:MET:SD	2.57	0.43
1:B:188:ASP:O	1:B:189:ILE:HB	2.18	0.43
1:C:147:LEU:HD11	1:C:760:TRP:CD2	2.54	0.43
1:A:669:ILE:HG22	1:A:673:MET:CE	2.47	0.43
1:B:281:VAL:HA	1:B:284:LEU:HD12	2.00	0.43
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.70	0.43
1:C:323:VAL:HG11	1:C:383:VAL:HG13	2.00	0.43
1:C:404:ASP:N	1:C:404:ASP:OD1	2.48	0.43
1:C:455:ASP:O	1:C:459:MET:HG3	2.17	0.43
1:A:360:GLY:HA2	1:A:361:GLU:CB	2.40	0.43
1:C:31:THR:HG22	1:C:67:PHE:O	2.19	0.43
1:C:544:ASP:N	1:C:544:ASP:OD1	2.51	0.43
1:D:582:ALA:HA	1:D:585:PRO:CG	2.49	0.43
1:D:680:PHE:CZ	1:D:711:LEU:HD21	2.53	0.43
1:A:175:ILE:HG22	1:A:176:GLU:HG2	2.00	0.43
1:A:528:ARG:HH11	1:A:528:ARG:CB	2.32	0.43
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.75	0.43
1:C:297:GLN:HB2	1:C:743:TRP:CZ3	2.53	0.43
1:C:71:TRP:CZ3	1:C:87:ARG:HD2	2.53	0.43
1:D:604:HIS:HA	1:D:606:SER:H	1.84	0.43
1:D:654:GLY:C	1:D:655:ILE:HG12	2.38	0.43
1:A:12:GLN:HB3	1:A:18:VAL:HG21	1.99	0.43
1:A:215:LEU:H	1:A:215:LEU:HG	1.69	0.43
1:C:26:PHE:CE2	1:C:90:GLN:HB2	2.54	0.43
1:D:212:TRP:N	1:D:230:HIS:O	2.50	0.43
1:D:669:ILE:HD13	1:D:687:PRO:HB3	2.00	0.43
1:B:610:GLU:O	1:B:612:GLU:N	2.52	0.43
1:C:281:VAL:HB	1:C:287:THR:HG21	2.00	0.43
1:C:600:ILE:HA	1:C:601:ASP:HB2	2.00	0.43
1:D:588:ARG:NH2	1:D:629:GLN:HG3	2.33	0.43
1:C:623:GLU:C	1:C:625:GLU:H	2.21	0.43
1:C:646:TYR:HE1	1:C:656:PHE:CE2	2.37	0.43
1:D:155:MET:HE1	1:D:254:LEU:HD11	2.00	0.43
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.86	0.42
1:A:789:ARG:HD3	1:A:789:ARG:HA	1.86	0.42
1:B:384:GLU:O	1:B:388:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:THR:HG23	1:C:23:ARG:NH2	2.34	0.42
1:C:355:PHE:C	1:C:356:ARG:HG2	2.39	0.42
1:C:564:THR:OG1	1:C:657:VAL:O	2.35	0.42
1:C:308:ARG:NH2	1:C:752:THR:OG1	2.52	0.42
1:C:94:ILE:HA	1:C:95:PRO:HD3	1.85	0.42
1:D:309:LEU:HA	1:D:309:LEU:HD13	1.83	0.42
1:D:44:GLN:HA	1:D:45:THR:HA	1.55	0.42
1:D:429:LYS:HG3	1:D:452:TYR:CZ	2.53	0.42
1:D:429:LYS:HA	1:D:452:TYR:OH	2.19	0.42
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.77	0.42
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.65	0.42
1:A:540:LEU:HD23	1:A:548:LEU:HD22	2.01	0.42
1:A:605:SER:N	1:A:606:SER:HA	2.34	0.42
1:B:620:LEU:HA	1:B:620:LEU:HD22	1.92	0.42
1:A:544:ASP:HB3	1:A:553:TYR:CD2	2.55	0.42
1:B:573:ASN:HB3	1:B:659:PRO:O	2.19	0.42
1:C:11:THR:C	1:C:13:GLN:N	2.71	0.42
1:C:362:ILE:HD12	1:C:362:ILE:H	1.84	0.42
1:C:740:ARG:HB3	1:C:741:TYR:CD2	2.55	0.42
1:D:711:LEU:H	1:D:711:LEU:HD23	1.84	0.42
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.81	0.42
1:B:55:LEU:O	1:B:59:VAL:HG23	2.19	0.42
1:B:633:LEU:CD2	1:B:635:MET:HE1	2.49	0.42
1:D:585:PRO:HB3	1:D:587:LEU:HB2	2.01	0.42
1:C:552:GLY:H	1:C:631:ARG:HH11	1.67	0.42
1:A:299:ARG:HA	1:A:345:CYS:SG	2.60	0.42
1:A:503:LEU:HA	1:A:503:LEU:HD12	1.84	0.42
1:B:610:GLU:C	1:B:612:GLU:N	2.73	0.42
1:B:611:GLN:HG3	2:B:846:HOH:O	2.20	0.42
1:B:600:ILE:HG12	1:B:632:TRP:CZ2	2.54	0.42
1:B:683:ARG:O	1:B:688:LEU:HD22	2.19	0.42
1:C:173:HIS:O	1:C:180:LEU:HB2	2.20	0.42
1:C:289:GLY:HA2	1:C:292:VAL:HG23	2.02	0.42
1:D:61:ARG:NH2	1:D:477:ARG:HH12	2.18	0.42
1:B:145:ILE:O	1:B:149:ARG:HG3	2.20	0.42
1:B:488:ALA:HA	1:B:497:VAL:O	2.19	0.42
1:B:89:HIS:O	1:B:93:LEU:HD23	2.19	0.42
1:C:68:SER:O	1:C:69:SER:OG	2.29	0.42
1:D:388:LEU:HD12	1:D:388:LEU:HA	1.77	0.42
1:B:164:THR:HB	1:B:165:SER:H	1.52	0.42
1:B:43:LEU:H	1:B:43:LEU:HG	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLN:O	1:C:39:ARG:HG3	2.20	0.42
1:C:388:LEU:HA	1:C:388:LEU:HD12	1.81	0.42
1:C:725:GLU:O	1:C:725:GLU:HG3	2.18	0.42
1:D:459:MET:CE	1:D:501:ILE:HB	2.50	0.42
1:B:585:PRO:HA	1:B:588:ARG:HB2	2.01	0.42
1:A:626:LEU:HD13	1:A:630:VAL:HG11	2.02	0.42
1:B:189:ILE:HG21	1:B:189:ILE:HD13	1.83	0.42
1:B:525:ASP:HA	1:B:526:PRO:HD3	1.86	0.42
1:A:580:LEU:HD12	1:A:706:ALA:H	1.85	0.41
1:A:494:LEU:HD21	1:A:786:LEU:HD21	2.01	0.41
1:B:663:GLU:O	1:B:685:GLY:HA3	2.19	0.41
1:D:534:ILE:HG12	1:D:535:PRO:HD3	2.01	0.41
1:A:447:HIS:CG	1:A:790:LEU:HD21	2.55	0.41
1:A:5:ASP:HB2	1:A:84:GLU:OE1	2.20	0.41
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.84	0.41
1:B:563:PHE:CD2	1:B:649:ILE:HG13	2.55	0.41
1:B:753:LEU:HD22	1:B:757:TYR:HE2	1.85	0.41
1:C:321:LEU:HG	1:C:391:LEU:HD21	2.02	0.41
1:C:617:MET:HB3	1:C:632:TRP:CH2	2.55	0.41
1:D:590:LEU:HA	1:D:590:LEU:HD23	1.85	0.41
1:A:790:LEU:H	1:A:791:ALA:HB3	1.84	0.41
1:A:89:HIS:HE1	1:A:91:GLU:HB2	1.85	0.41
1:B:213:ILE:HA	1:B:213:ILE:HD12	1.88	0.41
1:D:301:LEU:HA	1:D:301:LEU:HD12	1.93	0.41
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.89	0.41
1:D:518:ASP:O	1:D:519:ILE:HD13	2.20	0.41
1:D:581:TYR:OH	1:D:592:ASN:HA	2.21	0.41
1:D:89:HIS:O	1:D:93:LEU:HD23	2.20	0.41
1:A:75:ALA:HB2	1:A:103:PHE:CZ	2.56	0.41
1:A:521:PHE:CZ	1:A:528:ARG:HB3	2.56	0.41
1:B:718:LYS:O	1:B:722:ASN:HA	2.19	0.41
1:C:156:PHE:HE2	1:C:248:ALA:HB1	1.85	0.41
1:C:489:PHE:CZ	1:C:497:VAL:HG21	2.56	0.41
1:A:213:ILE:HD12	1:A:213:ILE:HA	1.89	0.41
1:B:554:LEU:HD23	1:B:592:ASN:CG	2.40	0.41
1:C:212:TRP:NE1	1:C:226:PRO:HB3	2.35	0.41
1:C:426:ALA:HA	1:C:482:GLN:OE1	2.19	0.41
1:C:720:LEU:HB2	1:C:723:PRO:HG3	2.03	0.41
1:D:10:CYS:SG	1:D:10:CYS:O	2.78	0.41
1:D:435:SER:HB3	1:D:448:PHE:CD2	2.56	0.41
1:D:561:LEU:HD22	1:D:594:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:O	1:A:149:ARG:HG3	2.21	0.41
1:A:288:GLY:C	1:A:290:GLN:N	2.73	0.41
1:B:567:ARG:HD2	1:B:567:ARG:HA	1.82	0.41
1:C:21:LEU:HG	1:C:25:TYR:CE2	2.56	0.41
1:C:325:ARG:HD2	1:C:355:PHE:CZ	2.54	0.41
1:C:586:ARG:O	1:C:590:LEU:HD12	2.20	0.41
1:C:632:TRP:CD1	1:C:633:LEU:N	2.85	0.41
1:C:586:ARG:NH1	1:C:710:ASP:OD1	2.54	0.41
1:D:181:MET:N	1:D:225:ALA:HB3	2.35	0.41
1:D:229:GLY:HA2	1:D:312:GLN:HA	2.02	0.41
1:D:603:GLN:HG3	1:D:614:ILE:CG2	2.50	0.41
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.82	0.41
1:C:168:HIS:HB2	1:C:187:HIS:NE2	2.35	0.41
1:C:553:TYR:O	1:C:628:GLN:HA	2.20	0.41
1:D:48:ASP:HA	1:D:49:CYS:HA	1.55	0.41
1:D:531:HIS:HB3	1:D:532:SER:H	1.71	0.41
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.83	0.41
1:A:89:HIS:O	1:A:93:LEU:HD23	2.21	0.41
1:B:44:GLN:H	1:B:46:GLU:N	2.19	0.41
1:C:341:LYS:HB2	1:C:349:TRP:CZ3	2.55	0.41
1:D:339:LEU:HD23	1:D:339:LEU:HA	1.71	0.41
1:D:278:GLN:NE2	1:D:342:VAL:HA	2.35	0.41
1:D:559:LYS:HA	1:D:560:PRO:HD3	1.78	0.41
1:D:585:PRO:HG2	1:D:588:ARG:HG2	2.02	0.41
1:A:215:LEU:CD2	1:A:232:ALA:HB2	2.50	0.41
1:B:550:ALA:HB1	1:B:631:ARG:HH12	1.85	0.41
1:B:582:ALA:HB1	1:B:624:HIS:ND1	2.36	0.41
1:B:633:LEU:HB3	1:B:635:MET:CE	2.50	0.41
1:A:162:GLY:HA2	1:A:163:HIS:HA	1.75	0.41
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.84	0.41
1:B:624:HIS:HB2	1:B:626:LEU:HG	2.03	0.41
1:C:328:PRO:CG	1:C:364:PRO:HA	2.49	0.41
1:C:459:MET:HE3	1:C:501:ILE:HB	2.02	0.41
1:C:534:ILE:HA	1:C:537:ILE:HD12	2.03	0.41
1:C:554:LEU:HA	1:C:628:GLN:HA	2.03	0.41
1:C:708:THR:O	1:C:712:ILE:HG13	2.21	0.41
1:A:45:THR:HB	1:A:48:ASP:O	2.20	0.41
1:B:561:LEU:HA	1:B:561:LEU:HD12	1.82	0.41
1:C:593:LEU:HB3	1:C:630:VAL:HB	2.03	0.41
1:A:28:ALA:HB1	1:A:30:ARG:O	2.20	0.40
1:A:563:PHE:CZ	1:A:565:MET:HE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:GLY:O	1:B:690:ILE:HG13	2.21	0.40
1:C:13:GLN:O	1:C:14:ASN:HB2	2.21	0.40
1:C:53:ASP:N	1:C:53:ASP:OD1	2.36	0.40
1:D:282:LEU:HB2	1:D:284:LEU:HG	2.03	0.40
1:D:657:VAL:HG22	1:D:680:PHE:HB2	2.03	0.40
1:A:281:VAL:HG11	1:A:291:VAL:HB	2.02	0.40
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.40
1:A:469:THR:HG1	1:A:472:GLU:HG3	1.83	0.40
1:A:742:THR:OG1	1:A:745:LEU:HB2	2.20	0.40
1:B:238:THR:O	1:B:241:MET:HB2	2.20	0.40
1:B:782:GLN:O	1:B:786:LEU:HG	2.21	0.40
1:C:554:LEU:HG	1:C:631:ARG:HB2	2.04	0.40
1:C:563:PHE:CD1	1:C:564:THR:N	2.89	0.40
1:C:660:ALA:O	1:C:702:PRO:HG3	2.21	0.40
1:D:317:GLU:HA	1:D:318:PRO:HD2	1.90	0.40
1:D:555:GLN:CD	1:D:556:ASP:H	2.23	0.40
1:A:34:LEU:HD22	1:A:433:LEU:HD13	2.02	0.40
1:A:437:ILE:HD12	1:A:437:ILE:HA	1.88	0.40
1:A:669:ILE:HG22	1:A:673:MET:HE2	2.01	0.40
1:A:69:SER:HB2	1:A:71:TRP:HB2	2.04	0.40
1:A:715:PHE:HZ	1:A:726:TRP:CD1	2.38	0.40
1:B:408:VAL:HG12	1:B:412:LEU:HD12	2.02	0.40
1:C:225:ALA:HB1	1:C:226:PRO:HD2	2.03	0.40
1:C:265:SER:N	1:C:396:ASP:OD2	2.44	0.40
1:C:530:LEU:HD23	1:C:533:LEU:HD22	2.02	0.40
1:D:25:TYR:CZ	1:D:38:LEU:HD23	2.57	0.40
1:D:443:GLU:O	1:D:447:HIS:ND1	2.54	0.40
1:D:612:GLU:O	1:D:615:HIS:HB2	2.21	0.40
1:D:718:LYS:HB2	1:D:725:GLU:HB2	2.03	0.40
1:A:241:MET:O	1:A:245:ILE:HG13	2.21	0.40
1:A:604:HIS:CB	1:A:605:SER:HB3	2.51	0.40
1:A:661:LEU:HD12	1:A:661:LEU:HA	1.84	0.40
1:B:587:LEU:HA	1:B:590:LEU:HB2	2.03	0.40
1:B:753:LEU:HD22	1:B:757:TYR:CE2	2.56	0.40
1:C:139:SER:O	1:C:142:GLN:HB2	2.20	0.40
1:C:632:TRP:C	1:C:632:TRP:CD1	2.93	0.40
1:A:521:PHE:HB2	1:A:522:PRO:CD	2.51	0.40
1:B:230:HIS:CG	1:B:231:ASN:N	2.90	0.40
1:D:282:LEU:HD13	1:D:284:LEU:HD11	2.04	0.40
1:D:428:GLU:HG2	1:D:428:GLU:H	1.72	0.40
1:D:69:SER:OG	1:D:70:PRO:HD2	2.21	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	787/794 (99%)	707 (90%)	78 (10%)	2 (0%)	41	70
1	B	787/794 (99%)	699 (89%)	76 (10%)	12 (2%)	10	35
1	C	787/794 (99%)	713 (91%)	68 (9%)	6 (1%)	19	50
1	D	787/794 (99%)	692 (88%)	88 (11%)	7 (1%)	17	47
All	All	3148/3176 (99%)	2811 (89%)	310 (10%)	27 (1%)	17	47

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	B	160	GLU
1	B	189	ILE
1	C	11	THR
1	B	11	THR
1	B	69	SER
1	B	164	THR
1	D	158	ARG
1	D	358	HIS
1	A	69	SER
1	C	12	GLN
1	D	69	SER
1	D	515	ALA
1	D	612	GLU
1	A	570	ARG
1	C	280	ASN
1	B	545	ALA
1	B	610	GLU
1	C	69	SER
1	B	281	VAL

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Mol	Chain	Res	Type
1	B	611	GLN
1	D	156	PHE
1	B	600	ILE
1	D	609	GLU
1	B	557	PRO
1	C	601	ASP
1	B	659	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	673/687 (98%)	576 (86%)	97 (14%)	3 12
1	B	677/687 (98%)	583 (86%)	94 (14%)	3 13
1	C	680/687 (99%)	598 (88%)	82 (12%)	5 17
1	D	679/687 (99%)	579 (85%)	100 (15%)	3 11
All	All	2709/2748 (99%)	2336 (86%)	373 (14%)	3 13

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	11	THR
1	A	12	GLN
1	A	16	ASP
1	A	20	THR
1	A	29	ASN
1	A	43	LEU
1	A	47	GLN
1	A	48	ASP
1	A	55	LEU
1	A	68	SER
1	A	74	LEU
1	A	84	GLU
1	A	92	HIS

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Mol	Chain	Res	Type
1	A	105	LYS
1	A	114	GLU
1	A	135	LYS
1	A	138	ARG
1	A	153	SER
1	A	156	PHE
1	A	163	HIS
1	A	165	SER
1	A	176	GLU
1	A	179	GLN
1	A	185	ASN
1	A	186	SER
1	A	194	ASN
1	A	200	LEU
1	A	201	GLU
1	A	215	LEU
1	A	218	LYS
1	A	243	MET
1	A	256	GLU
1	A	263	MET
1	A	266	ARG
1	A	270	LEU
1	A	273	HIS
1	A	278	GLN
1	A	281	VAL
1	A	297	GLN
1	A	301	LEU
1	A	305	MET
1	A	308	ARG
1	A	309	LEU
1	A	311	LEU
1	A	332	ASP
1	A	334	THR
1	A	341	LYS
1	A	362	ILE
1	A	369	ARG
1	A	371	GLU
1	A	388	LEU
1	A	391	LEU
1	A	404	ASP
1	A	413	SER
1	A	429	LYS

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Mol	Chain	Res	Type
1	A	430	THR
1	A	441	GLU
1	A	457	LEU
1	A	464	PHE
1	A	471	GLN
1	A	501	ILE
1	A	503	LEU
1	A	525	ASP
1	A	527	ASN
1	A	528	ARG
1	A	530	LEU
1	A	547	ASN
1	A	548	LEU
1	A	553	TYR
1	A	554	LEU
1	A	556	ASP
1	A	561	LEU
1	A	570	ARG
1	A	579	GLU
1	A	580	LEU
1	A	584	SER
1	A	589	SER
1	A	614	ILE
1	A	620	LEU
1	A	628	GLN
1	A	629	GLN
1	A	636	ARG
1	A	637	LEU
1	A	638	ASP
1	A	658	GLN
1	A	661	LEU
1	A	662	PHE
1	A	667	LEU
1	A	682	THR
1	A	696	SER
1	A	736	ARG
1	A	745	LEU
1	A	772	ASP
1	A	773	ARG
1	A	784	ARG
1	A	790	LEU
1	C	4	ILE

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Mol	Chain	Res	Type
1	C	5	ASP
1	C	9	THR
1	C	12	GLN
1	C	29	ASN
1	C	31	THR
1	C	32	LEU
1	C	34	LEU
1	C	53	ASP
1	C	55	LEU
1	C	74	LEU
1	C	86	MET
1	C	91	GLU
1	C	92	HIS
1	C	93	LEU
1	C	94	ILE
1	C	116	THR
1	C	138	ARG
1	C	157	SER
1	C	165	SER
1	C	175	ILE
1	C	179	GLN
1	C	187	HIS
1	C	200	LEU
1	C	207	ASP
1	C	209	THR
1	C	220	ASN
1	C	255	GLU
1	C	267	LEU
1	C	270	LEU
1	C	273	HIS
1	C	280	ASN
1	C	301	LEU
1	C	309	LEU
1	C	311	LEU
1	C	312	GLN
1	C	316	VAL
1	C	319	LYS
1	C	356	ARG
1	C	368	SER
1	C	386	GLU
1	C	388	LEU
1	C	430	THR

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Mol	Chain	Res	Type
1	C	435	SER
1	C	440	GLN
1	C	457	LEU
1	C	471	GLN
1	C	478	GLU
1	C	490	SER
1	C	491	MET
1	C	503	LEU
1	C	525	ASP
1	C	530	LEU
1	C	534	ILE
1	C	536	GLU
1	C	541	ILE
1	C	551	ARG
1	C	553	TYR
1	C	558	ASP
1	C	564	THR
1	C	568	LEU
1	C	571	ILE
1	C	575	THR
1	C	601	ASP
1	C	604	HIS
1	C	606	SER
1	C	608	HIS
1	C	615	HIS
1	C	617	MET
1	C	627	ASP
1	C	630	VAL
1	C	640	ASN
1	C	658	GLN
1	C	667	LEU
1	C	710	ASP
1	C	711	LEU
1	C	725	GLU
1	C	740	ARG
1	C	745	LEU
1	C	763	VAL
1	C	766	LEU
1	C	784	ARG
1	B	9	THR
1	B	10	CYS
1	B	15	ARG

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Mol	Chain	Res	Type
1	B	23	ARG
1	B	26	PHE
1	B	29	ASN
1	B	30	ARG
1	B	43	LEU
1	B	45	THR
1	B	47	GLN
1	B	48	ASP
1	B	49	CYS
1	B	55	LEU
1	B	68	SER
1	B	74	LEU
1	B	90	GLN
1	B	93	LEU
1	B	100	ILE
1	B	114	GLU
1	B	116	THR
1	B	153	SER
1	B	157	SER
1	B	158	ARG
1	B	187	HIS
1	B	200	LEU
1	B	209	THR
1	B	213	ILE
1	B	260	CYS
1	B	270	LEU
1	B	273	HIS
1	B	291	VAL
1	B	295	LEU
1	B	308	ARG
1	B	309	LEU
1	B	316	VAL
1	B	317	GLU
1	B	324	THR
1	B	334	THR
1	B	339	LEU
1	B	369	ARG
1	B	371	GLU
1	B	388	LEU
1	B	394	HIS
1	B	404	ASP
1	B	407	LEU

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Mol	Chain	Res	Type
1	B	413	SER
1	B	430	THR
1	B	431	LYS
1	B	433	LEU
1	B	435	SER
1	B	437	ILE
1	B	444	ASP
1	B	457	LEU
1	B	469	THR
1	B	477	ARG
1	B	503	LEU
1	B	507	LYS
1	B	525	ASP
1	B	530	LEU
1	B	532	SER
1	B	533	LEU
1	B	536	GLU
1	B	546	THR
1	B	547	ASN
1	B	548	LEU
1	B	556	ASP
1	B	558	ASP
1	B	569	ASP
1	B	570	ARG
1	B	571	ILE
1	B	607	ASP
1	B	610	GLU
1	B	617	MET
1	B	619	GLN
1	B	620	LEU
1	B	622	ASP
1	B	640	ASN
1	B	652	LYS
1	B	653	ARG
1	B	661	LEU
1	B	667	LEU
1	B	677	LEU
1	B	693	ASN
1	B	695	ARG
1	B	708	THR
1	B	714	ASP
1	B	719	ASN

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Mol	Chain	Res	Type
1	B	725	GLU
1	B	740	ARG
1	B	745	LEU
1	B	748	GLU
1	B	754	SER
1	B	773	ARG
1	B	784	ARG
1	D	4	ILE
1	D	12	GLN
1	D	26	PHE
1	D	31	THR
1	D	32	LEU
1	D	36	SER
1	D	40	GLU
1	D	42	LEU
1	D	44	GLN
1	D	45	THR
1	D	46	GLU
1	D	54	MET
1	D	60	PHE
1	D	67	PHE
1	D	68	SER
1	D	69	SER
1	D	90	GLN
1	D	92	HIS
1	D	99	THR
1	D	114	GLU
1	D	116	THR
1	D	119	VAL
1	D	135	LYS
1	D	137	SER
1	D	139	SER
1	D	150	LYS
1	D	152	SER
1	D	153	SER
1	D	159	ILE
1	D	163	HIS
1	D	164	THR
1	D	180	LEU
1	D	200	LEU
1	D	202	MET
1	D	209	THR

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Mol	Chain	Res	Type
1	D	218	LYS
1	D	255	GLU
1	D	260	CYS
1	D	263	MET
1	D	273	HIS
1	D	280	ASN
1	D	295	LEU
1	D	297	GLN
1	D	308	ARG
1	D	311	LEU
1	D	316	VAL
1	D	334	THR
1	D	343	SER
1	D	372	ILE
1	D	385	ARG
1	D	388	LEU
1	D	394	HIS
1	D	430	THR
1	D	433	LEU
1	D	457	LEU
1	D	471	GLN
1	D	476	THR
1	D	478	GLU
1	D	491	MET
1	D	525	ASP
1	D	528	ARG
1	D	530	LEU
1	D	534	ILE
1	D	538	GLU
1	D	540	LEU
1	D	553	TYR
1	D	555	GLN
1	D	556	ASP
1	D	561	LEU
1	D	568	LEU
1	D	574	ILE
1	D	575	THR
1	D	577	LEU
1	D	580	LEU
1	D	600	ILE
1	D	601	ASP
1	D	605	SER

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Mol	Chain	Res	Type
1	D	620	LEU
1	D	621	MET
1	D	625	GLU
1	D	639	LYS
1	D	640	ASN
1	D	647	ARG
1	D	648	TYR
1	D	652	LYS
1	D	653	ARG
1	D	658	GLN
1	D	667	LEU
1	D	682	THR
1	D	683	ARG
1	D	691	ILE
1	D	696	SER
1	D	721	GLU
1	D	724	GLN
1	D	728	ARG
1	D	730	SER
1	D	734	LEU
1	D	742	THR
1	D	770	GLU
1	D	784	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	185	ASN
1	A	273	HIS
1	A	401	ASN
1	C	290	GLN
1	C	719	ASN
1	B	629	GLN
1	B	719	ASN
1	D	92	HIS
1	D	603	GLN
1	D	618	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	789/794 (99%)	-0.36	4 (0%) 91 79	8, 37, 104, 170	0
1	B	789/794 (99%)	-0.34	7 (0%) 84 66	9, 38, 103, 152	0
1	C	789/794 (99%)	-0.16	18 (2%) 60 36	10, 46, 111, 167	0
1	D	789/794 (99%)	0.01	45 (5%) 23 10	11, 60, 140, 180	0
All	All	3156/3176 (99%)	-0.21	74 (2%) 60 36	8, 44, 116, 180	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	562	ILE	5.8
1	A	282	LEU	5.5
1	A	281	VAL	5.4
1	D	49	CYS	4.8
1	C	719	ASN	4.5
1	D	595	ILE	4.3
1	D	47	GLN	4.3
1	D	724	GLN	4.2
1	D	50	GLY	4.2
1	D	630	VAL	4.2
1	C	599	LYS	4.2
1	C	281	VAL	3.9
1	D	560	PRO	3.8
1	D	282	LEU	3.8
1	D	45	THR	3.7
1	D	549	PRO	3.6
1	D	653	ARG	3.4
1	D	558	ASP	3.4
1	D	42	LEU	3.3
1	D	564	THR	3.2
1	C	332	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	719	ASN	3.1
1	D	645	LEU	3.1
1	D	543	ASP	3.1
1	D	51	GLN	3.0
1	D	722	ASN	3.0
1	D	599	LYS	3.0
1	D	597	GLY	2.9
1	D	44	GLN	2.9
1	C	558	ASP	2.9
1	D	536	GLU	2.9
1	D	48	ASP	2.8
1	C	620	LEU	2.7
1	D	547	ASN	2.7
1	C	49	CYS	2.7
1	D	612	GLU	2.7
1	D	720	LEU	2.6
1	D	726	TRP	2.6
1	D	715	PHE	2.6
1	D	591	ALA	2.6
1	D	550	ALA	2.6
1	A	719	ASN	2.5
1	D	531	HIS	2.5
1	C	597	GLY	2.5
1	D	655	ILE	2.5
1	C	537	ILE	2.5
1	D	718	LYS	2.4
1	B	281	VAL	2.4
1	A	715	PHE	2.4
1	D	561	LEU	2.3
1	D	563	PHE	2.3
1	B	568	LEU	2.3
1	D	598	GLY	2.3
1	B	49	CYS	2.3
1	D	523	TYR	2.2
1	C	629	GLN	2.2
1	C	607	ASP	2.2
1	C	549	PRO	2.2
1	D	592	ASN	2.2
1	C	592	ASN	2.2
1	B	719	ASN	2.2
1	C	43	LEU	2.1
1	C	48	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	646	TYR	2.1
1	B	590	LEU	2.1
1	D	596	VAL	2.1
1	C	47	GLN	2.1
1	B	617	MET	2.1
1	C	598	GLY	2.1
1	D	651	ASP	2.1
1	D	712	ILE	2.1
1	D	629	GLN	2.0
1	C	562	ILE	2.0
1	B	715	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.