



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 1PWV / pdb_00001pwv
Title : Crystal structure of Anthrax Lethal Factor wild-type protein complexed with an optimised peptide substrate.
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 2.85 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

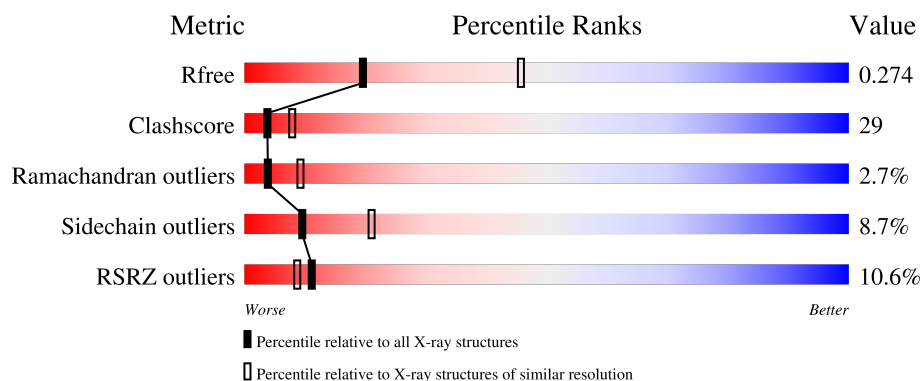
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of 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	776	10% 44% 42% 7% 6%
1	B	776	8% 46% 41% 7% 5%
2	C	20	40% 10% 20% 15% 55%
2	D	20	40% 15% 20% 10% 55%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12230 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			6028	3833	1015	1173	7			
1	B	736	Total	C	N	O	S	0	0	0
			6050	3848	1014	1181	7			

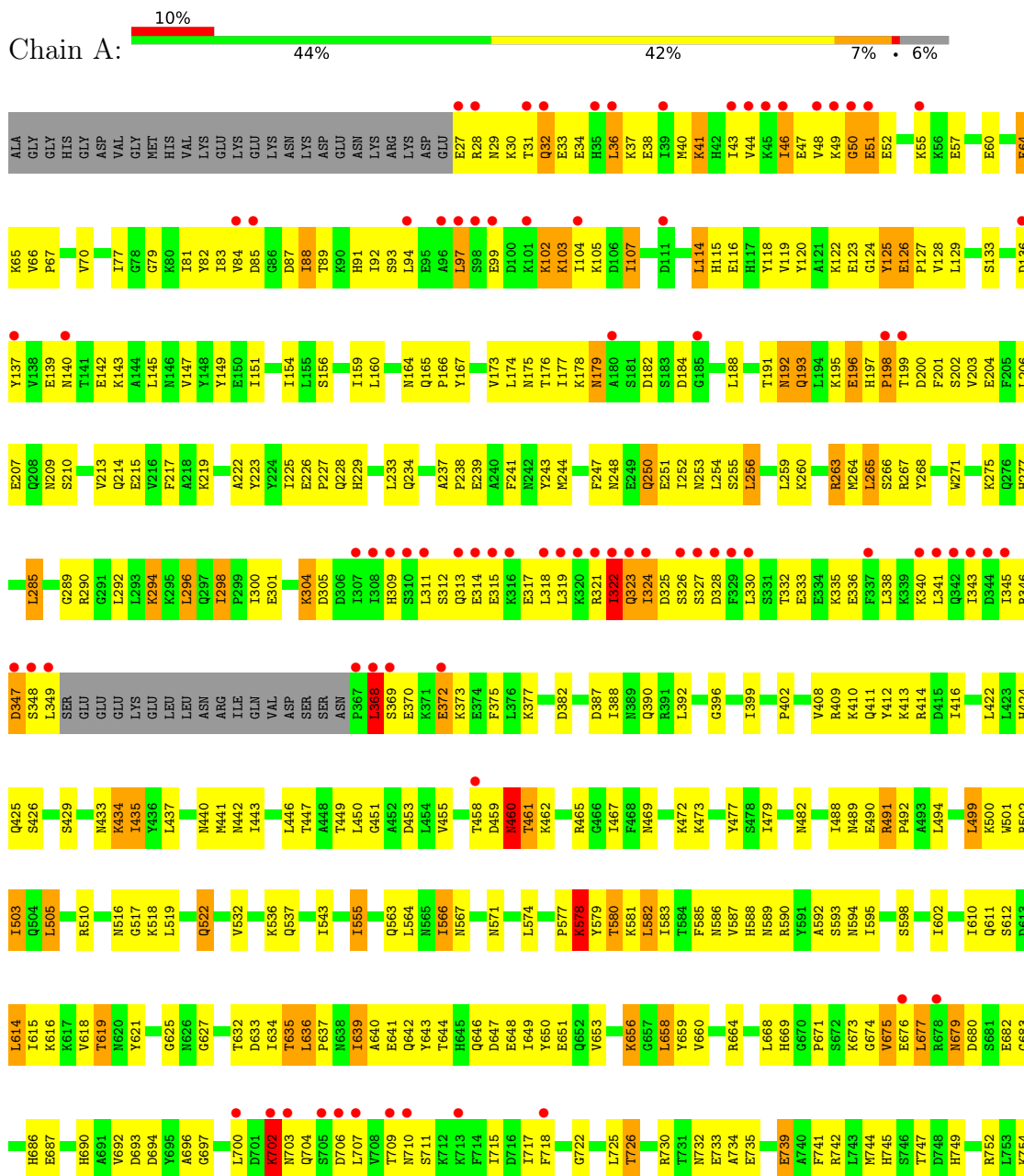
- Molecule 2 is a protein called LF20.

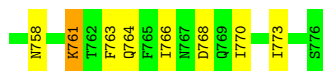
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	S	0	0	0
			76	52	9	14	1			
2	D	9	Total	C	N	O	S	0	0	0
			76	52	9	14	1			

3 Residue-property plots

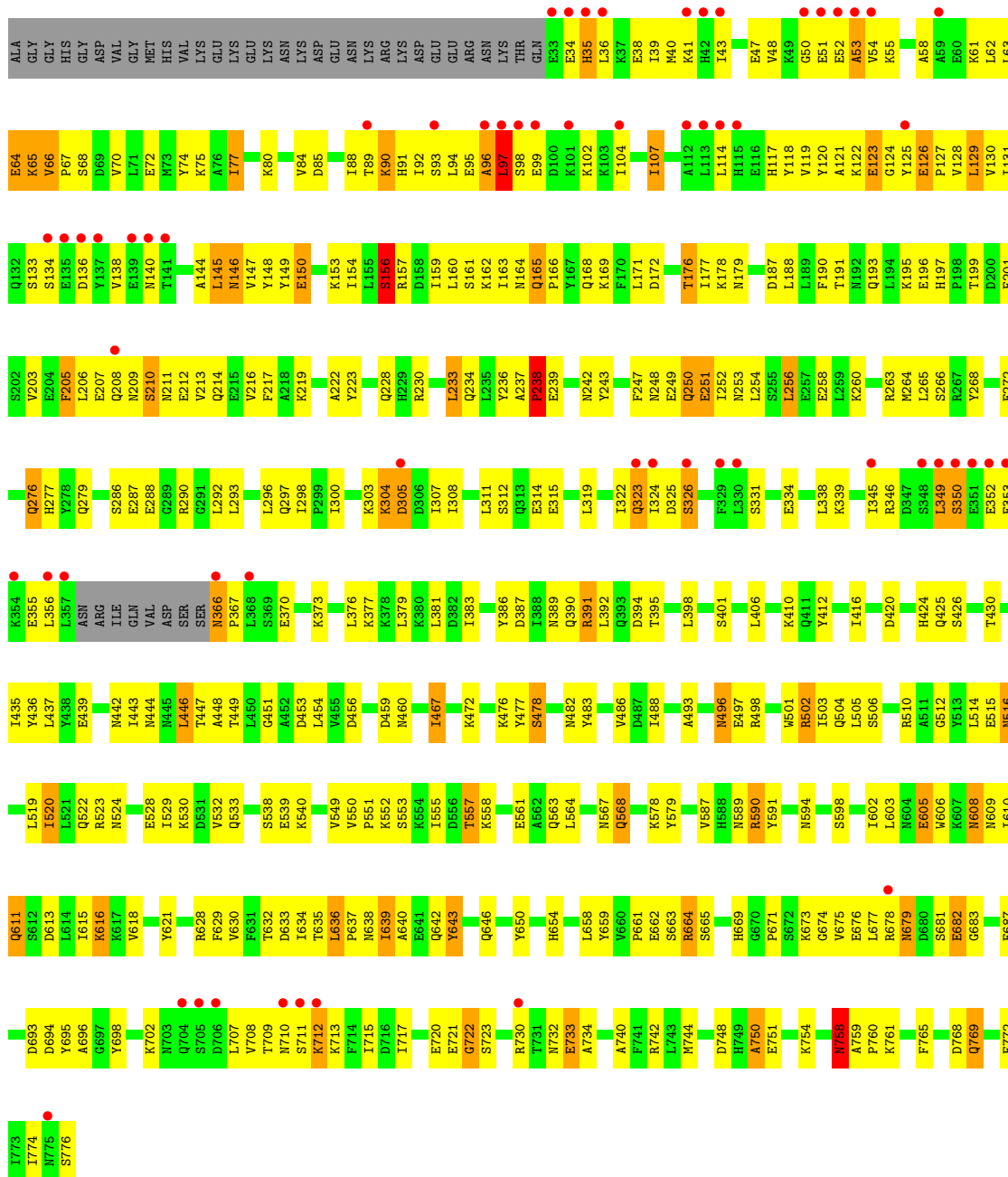
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

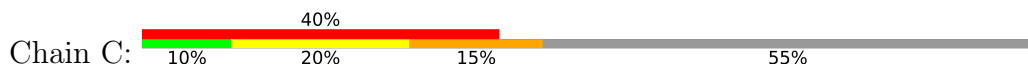




• Molecule 1: Lethal factor

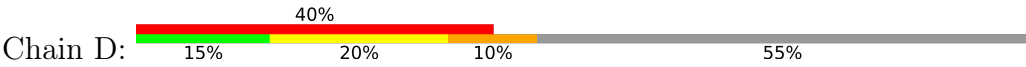


• Molecule 2: LF20





● Molecule 2: LF20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.85 46.06 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.8 (46.06-2.85) 85.8 (46.06-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.279 0.229 , 0.274	Depositor DCC
R_{free} test set	2578 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12230	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/6136	1.00	31/8263 (0.4%)
1	B	0.51	0/6158	1.02	32/8294 (0.4%)
2	C	0.64	0/80	1.49	3/111 (2.7%)
2	D	0.47	0/80	1.32	2/111 (1.8%)
All	All	0.50	0/12454	1.02	68/16779 (0.4%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	GLN	OE1-CD-NE2	-10.74	111.86	122.60
1	B	276	GLN	OE1-CD-NE2	-10.69	111.91	122.60
1	B	279	GLN	OE1-CD-NE2	-10.36	112.24	122.60
1	B	568	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	A	32	GLN	OE1-CD-NE2	-9.28	113.32	122.60
1	A	590	ARG	N-CA-C	8.59	123.51	112.34
1	B	506	SER	N-CA-C	-8.44	99.42	110.39
1	B	156	SER	N-CA-C	8.17	120.18	111.28
1	A	126	GLU	CA-C-N	7.88	127.93	119.90
1	A	126	GLU	C-N-CA	7.88	127.93	119.90
1	B	238	PRO	CA-N-CD	-7.33	101.74	112.00
1	A	137	TYR	N-CA-C	-7.03	104.19	114.39
1	B	276	GLN	CG-CD-NE2	7.02	126.93	116.40
1	A	97	LEU	CA-C-N	6.92	130.58	120.82
1	A	97	LEU	C-N-CA	6.92	130.58	120.82
1	B	568	GLN	CG-CD-NE2	6.87	126.70	116.40
1	A	704	GLN	CG-CD-NE2	6.78	126.58	116.40
1	B	589	ASN	N-CA-C	6.75	120.17	109.65
1	A	32	GLN	CG-CD-NE2	6.72	126.48	116.40
1	B	279	GLN	CG-CD-NE2	6.66	126.40	116.40
1	B	502	ARG	N-CA-C	-6.58	97.69	108.41
1	A	323	GLN	N-CA-C	-6.52	102.43	110.65
1	B	643	TYR	N-CA-C	6.49	119.17	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	PRO	CA-N-CD	-6.43	103.00	112.00
1	B	126	GLU	CA-C-N	6.42	126.39	119.78
1	B	126	GLU	C-N-CA	6.42	126.39	119.78
1	B	213	VAL	N-CA-C	-6.34	104.57	110.53
1	B	254	LEU	N-CA-C	-6.33	103.90	111.69
2	D	11	TYR	CA-C-N	6.32	127.74	119.84
2	D	11	TYR	C-N-CA	6.32	127.74	119.84
1	B	590	ARG	N-CA-C	6.31	124.23	110.80
2	C	11	TYR	CA-C-N	6.29	127.71	119.84
2	C	11	TYR	C-N-CA	6.29	127.71	119.84
1	A	503	ILE	N-CA-C	6.23	117.28	108.36
1	A	589	ASN	N-CA-C	6.16	119.90	110.36
1	A	461	THR	N-CA-C	-6.15	105.73	113.72
1	B	205	PHE	N-CA-C	-6.07	104.57	111.07
1	B	298	ILE	N-CA-C	6.06	114.08	107.60
1	A	151	ILE	N-CA-C	-6.04	104.42	111.00
1	B	558	LYS	N-CA-C	-6.03	104.62	111.07
1	A	298	ILE	CA-C-N	5.85	125.81	119.78
1	A	298	ILE	C-N-CA	5.85	125.81	119.78
1	B	150	GLU	N-CA-C	-5.85	104.49	111.69
1	A	587	VAL	N-CA-C	5.84	116.51	107.99
1	B	61	LYS	N-CA-C	-5.83	106.71	113.88
1	B	750	ALA	N-CA-C	-5.78	104.90	111.14
1	A	322	ILE	N-CA-C	5.62	116.40	108.36
1	B	126	GLU	N-CA-C	-5.60	97.44	109.81
1	B	176	THR	N-CA-C	-5.59	105.09	111.07
1	B	629	PHE	N-CA-C	-5.54	98.18	107.99
1	A	97	LEU	CA-C-O	5.53	126.91	120.49
1	A	191	THR	N-CA-C	-5.52	101.80	110.36
1	A	677	LEU	N-CA-C	-5.48	100.25	109.07
1	B	605	GLU	N-CA-C	-5.48	105.00	110.97
1	A	388	ILE	N-CA-C	5.34	115.79	110.23
1	A	747	THR	N-CA-C	-5.22	106.86	113.18
1	A	458	THR	N-CA-C	-5.19	106.64	113.12
1	A	768	ASP	N-CA-C	-5.18	105.28	111.03
1	B	96	ALA	N-CA-C	-5.18	107.25	113.21
1	A	368	LEU	N-CA-C	5.17	117.53	109.52
1	B	104	ILE	N-CA-C	5.12	116.84	109.51
1	B	191	THR	N-CA-C	-5.12	102.43	110.36
1	B	35	HIS	N-CA-C	-5.04	106.82	113.12
1	A	28	ARG	N-CA-C	-5.03	107.69	113.88
1	B	720	GLU	N-CA-C	5.03	117.87	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ASP	N-CA-C	5.00	117.47	111.71
1	A	164	ASN	N-CA-C	5.00	118.22	111.17
1	A	614	LEU	N-CA-C	-5.00	105.53	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6028	0	6018	375	0
1	B	6050	0	6034	330	0
2	C	76	0	69	12	0
2	D	76	0	69	8	0
All	All	12230	0	12190	701	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 29.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLU:O	1:B:356:LEU:HG	1.40	1.18
1:B:304:LYS:HD3	1:B:304:LYS:H	0.99	1.15
1:A:434:LYS:HB3	1:A:434:LYS:HZ2	1.11	1.14
1:A:319:LEU:HA	1:A:322:ILE:HD11	1.20	1.12
1:A:516:ASN:HD21	1:A:518:LYS:HD2	1.20	1.05
1:B:675:VAL:HG22	2:D:14:GLU:HG2	1.39	1.04
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.41	1.02
1:A:268:TYR:HB3	1:B:125:TYR:CE2	1.96	1.01
1:B:483:TYR:HB3	1:B:520:ILE:HD11	1.40	1.00
1:A:304:LYS:H	1:A:304:LYS:HD3	1.27	0.97
1:A:49:LYS:HG3	1:A:50:GLY:H	1.28	0.96
1:A:577:PRO:O	1:A:580:THR:HG22	1.65	0.95
1:B:712:LYS:H	1:B:712:LYS:HD2	1.27	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ARG:H	1:B:522:GLN:HE21	1.11	0.94
1:B:304:LYS:HD3	1:B:304:LYS:N	1.81	0.94
1:B:708:VAL:HG21	1:B:769:GLN:HE21	1.36	0.91
1:A:104:ILE:HG22	1:A:105:LYS:H	1.36	0.90
1:A:92:ILE:HD12	1:A:92:ILE:H	1.37	0.89
1:A:516:ASN:ND2	1:A:518:LYS:HD2	1.86	0.89
1:B:304:LYS:H	1:B:304:LYS:CD	1.86	0.89
1:B:498:ARG:HH21	1:B:540:LYS:HE3	1.39	0.88
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.56	0.88
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.56	0.87
1:A:563:GLN:NE2	1:A:585:PHE:H	1.72	0.86
1:B:711:SER:O	1:B:715:ILE:HG13	1.76	0.86
1:A:87:ASP:OD1	1:A:115:HIS:HB2	1.76	0.86
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.37	0.85
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.57	0.85
1:A:434:LYS:HB3	1:A:434:LYS:NZ	1.92	0.85
1:B:43:ILE:HD11	1:B:75:LYS:HB2	1.58	0.84
1:A:264:MET:HE3	1:A:265:LEU:HD13	1.58	0.83
1:A:675:VAL:HA	2:C:14:GLU:HG3	1.59	0.83
1:A:322:ILE:HG23	1:A:372:GLU:OE1	1.76	0.83
1:B:90:LYS:HE3	1:B:90:LYS:HA	1.61	0.83
1:B:324:ILE:HD12	1:B:324:ILE:H	1.41	0.83
1:A:244:MET:HE3	1:A:244:MET:HA	1.62	0.82
1:A:46:ILE:HD12	1:A:46:ILE:H	1.44	0.82
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.62	0.81
1:A:368:LEU:HD23	1:A:369:SER:N	1.95	0.81
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.62	0.81
1:B:77:ILE:HD11	1:B:162:LYS:HG3	1.61	0.80
1:A:104:ILE:HD11	1:A:114:LEU:HG	1.63	0.80
1:B:97:LEU:HB2	1:B:102:LYS:NZ	1.96	0.80
1:A:766:ILE:O	1:A:770:ILE:HG12	1.82	0.80
1:B:496:ASN:HD22	1:B:496:ASN:H	1.26	0.80
1:B:349:LEU:HG	1:B:350:SER:H	1.47	0.79
1:A:304:LYS:H	1:A:304:LYS:CD	1.95	0.79
1:A:368:LEU:HD23	1:A:369:SER:H	1.49	0.78
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.13	0.78
1:A:263:ARG:HD3	1:B:264:MET:HE2	1.66	0.78
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.65	0.78
1:B:516:ASN:H	1:B:516:ASN:HD22	1.32	0.77
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.66	0.77
1:A:263:ARG:HH11	1:A:263:ARG:HB3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:LYS:O	1:A:758:ASN:HB2	1.85	0.77
1:A:426:SER:HA	1:A:510:ARG:HA	1.67	0.77
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.01	0.76
1:B:89:THR:HG22	1:B:90:LYS:HZ2	1.48	0.76
1:B:712:LYS:H	1:B:712:LYS:CD	1.98	0.76
1:B:34:GLU:O	1:B:38:GLU:HB2	1.85	0.76
1:B:483:TYR:CB	1:B:520:ILE:HD11	2.17	0.75
1:A:318:LEU:HG	1:A:372:GLU:CD	2.12	0.75
1:B:628:ARG:H	1:B:665:SER:HB3	1.51	0.75
1:A:312:SER:HB3	1:A:315:GLU:HG3	1.68	0.74
1:B:454:LEU:HA	1:B:467:ILE:HG21	1.70	0.74
1:B:510:ARG:H	1:B:522:GLN:NE2	1.86	0.74
1:A:66:VAL:HG12	1:A:70:VAL:HG21	1.70	0.74
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.68	0.73
1:A:510:ARG:HB2	1:A:522:GLN:HG2	1.70	0.73
1:B:564:LEU:O	1:B:568:GLN:HG3	1.88	0.73
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.23	0.73
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.69	0.73
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.71	0.73
1:B:366:ASN:CB	1:B:367:PRO:HD3	2.18	0.72
1:B:165:GLN:HE21	1:B:166:PRO:HA	1.54	0.72
1:A:319:LEU:HA	1:A:322:ILE:CD1	2.11	0.72
1:B:677:LEU:HD11	2:D:11:TYR:CE1	2.25	0.72
1:B:516:ASN:HD22	1:B:516:ASN:N	1.86	0.72
1:A:49:LYS:HG3	1:A:50:GLY:N	2.02	0.71
1:A:79:GLY:HA2	1:A:127:PRO:HG2	1.72	0.71
1:A:598:SER:O	1:A:602:ILE:HG13	1.90	0.71
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.55	0.71
1:B:366:ASN:HB2	1:B:367:PRO:CD	2.19	0.70
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.56	0.70
1:A:296:LEU:HD22	1:A:296:LEU:O	1.90	0.70
1:A:676:GLU:HG2	2:C:14:GLU:OE2	1.91	0.70
1:B:406:LEU:O	1:B:406:LEU:HD12	1.91	0.70
1:B:258:GLU:HG3	1:B:502:ARG:NH1	2.07	0.70
1:B:679:ASN:C	1:B:679:ASN:HD22	1.99	0.70
1:B:258:GLU:HG3	1:B:502:ARG:HH12	1.56	0.70
1:A:333:GLU:H	1:A:333:GLU:CD	1.99	0.69
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.74	0.69
1:B:346:ARG:HE	1:B:356:LEU:HD13	1.56	0.69
1:B:496:ASN:HD22	1:B:496:ASN:N	1.89	0.69
1:A:412:TYR:O	1:A:416:ILE:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:PHE:O	1:A:745:HIS:HD2	1.74	0.69
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.22	0.69
1:A:123:GLU:HG2	1:A:124:GLY:H	1.58	0.68
1:B:352:GLU:O	1:B:356:LEU:CG	2.31	0.68
1:A:118:TYR:CD2	1:A:143:LYS:HD3	2.28	0.68
1:A:410:LYS:HE2	1:A:414:ARG:HH21	1.59	0.68
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.29	0.68
1:B:331:SER:OG	1:B:334:GLU:HG3	1.94	0.68
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.29	0.67
1:A:346:ARG:O	1:A:348:SER:N	2.23	0.67
1:A:370:GLU:HG3	1:A:373:LYS:HD3	1.77	0.67
1:A:679:ASN:HD22	1:A:679:ASN:C	2.03	0.67
1:A:449:THR:HA	1:A:673:LYS:HD3	1.76	0.67
1:A:658:LEU:HD21	2:C:8:VAL:HB	1.75	0.67
1:B:107:ILE:HB	1:B:146:ASN:ND2	2.10	0.67
1:A:156:SER:HB3	1:A:217:PHE:CD2	2.29	0.66
1:A:173:VAL:O	1:A:177:ILE:HG12	1.96	0.66
1:A:675:VAL:HG13	1:A:675:VAL:O	1.94	0.66
1:B:401:SER:CB	1:B:638:ASN:HD22	2.07	0.66
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.30	0.66
1:A:410:LYS:HE2	1:A:414:ARG:NH2	2.11	0.66
1:B:553:SER:O	1:B:557:THR:HG23	1.95	0.66
1:A:567:ASN:HD21	1:A:583:ILE:H	1.43	0.66
1:B:516:ASN:H	1:B:516:ASN:ND2	1.93	0.66
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.78	0.65
1:B:392:LEU:HD21	1:B:416:ILE:HD12	1.77	0.65
1:A:338:LEU:HA	1:A:341:LEU:HD12	1.77	0.65
1:B:134:SER:HB3	1:B:136:ASP:OD1	1.96	0.65
1:B:312:SER:OG	1:B:315:GLU:HG3	1.95	0.65
1:B:483:TYR:HB3	1:B:520:ILE:CD1	2.23	0.65
1:B:754:LYS:O	1:B:758:ASN:HB2	1.95	0.65
1:A:491:ARG:HH21	1:B:539:GLU:HG3	1.62	0.65
1:A:94:LEU:HD22	1:A:97:LEU:CD1	2.26	0.65
1:A:340:LYS:HG3	1:A:343:ILE:HD12	1.78	0.65
1:B:165:GLN:NE2	1:B:166:PRO:HA	2.11	0.65
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.11	0.65
1:A:732:ASN:ND2	1:A:735:GLU:HG2	2.12	0.64
1:A:595:ILE:HD11	1:A:633:ASP:HB3	1.79	0.64
1:B:237:ALA:N	1:B:238:PRO:CD	2.60	0.64
1:B:712:LYS:HD2	1:B:712:LYS:N	2.09	0.64
1:A:250:GLN:HG3	1:A:251:GLU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:N	1:A:460:ASN:HD22	1.96	0.64
1:B:733:GLU:CD	1:B:733:GLU:H	2.05	0.64
1:A:66:VAL:CG1	1:A:70:VAL:HG21	2.27	0.64
1:A:711:SER:O	1:A:715:ILE:HG13	1.98	0.64
1:B:207:GLU:HB3	1:B:208:GLN:HE21	1.63	0.64
1:A:94:LEU:HD22	1:A:97:LEU:HD12	1.79	0.64
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.62	0.64
1:B:721:GLU:OE1	1:B:761:LYS:HB2	1.98	0.63
1:A:99:GLU:O	1:A:103:LYS:HD3	1.97	0.63
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.14	0.63
1:A:319:LEU:CA	1:A:322:ILE:HD11	2.12	0.63
1:B:84:VAL:HG22	1:B:85:ASP:N	2.12	0.63
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.79	0.63
1:B:324:ILE:HD13	1:B:339:LYS:HG2	1.80	0.63
1:A:179:ASN:ND2	1:A:200:ASP:OD1	2.29	0.63
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.34	0.63
1:B:97:LEU:HB2	1:B:102:LYS:HZ1	1.62	0.62
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.80	0.62
1:A:625:GLY:HA3	1:A:664:ARG:HD2	1.81	0.62
1:B:759:ALA:N	1:B:760:PRO:HD3	2.14	0.62
1:A:332:THR:HG22	1:A:336:GLU:OE2	2.00	0.62
1:A:67:PRO:O	1:A:70:VAL:HG22	1.99	0.62
1:A:206:LEU:HD13	1:A:213:VAL:HG21	1.82	0.62
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.15	0.62
1:A:343:ILE:O	1:A:346:ARG:HG3	2.00	0.62
1:A:37:LYS:O	1:A:41:LYS:HG3	2.00	0.61
1:A:107:ILE:O	1:A:107:ILE:HD13	1.99	0.61
1:B:442:ASN:ND2	1:B:496:ASN:HB2	2.15	0.61
1:A:702:LYS:H	1:A:702:LYS:HD2	1.65	0.61
1:A:140:ASN:OD1	1:A:143:LYS:HG3	2.01	0.61
1:A:107:ILE:HD11	1:A:219:LYS:HG3	1.81	0.61
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.36	0.61
1:B:496:ASN:H	1:B:496:ASN:ND2	1.98	0.61
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.33	0.61
1:B:47:GLU:O	1:B:84:VAL:HG23	2.01	0.61
1:A:57:GLU:HA	1:A:60:GLU:OE2	2.00	0.61
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.36	0.60
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.36	0.60
1:B:256:LEU:HD22	1:B:260:LYS:HE2	1.82	0.60
1:A:392:LEU:HD21	1:A:416:ILE:HD13	1.83	0.60
1:B:555:ILE:HD12	1:B:555:ILE:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HE2	1:A:85:ASP:OD2	2.01	0.60
1:A:373:LYS:HE2	1:A:377:LYS:HE3	1.83	0.60
1:B:169:LYS:O	1:B:172:ASP:HB2	2.02	0.60
1:A:300:ILE:N	1:A:300:ILE:HD12	2.17	0.60
1:A:323:GLN:O	1:A:326:SER:N	2.33	0.60
1:A:578:LYS:HG2	1:A:579:TYR:CD2	2.37	0.60
1:B:304:LYS:O	1:B:308:ILE:HG13	2.01	0.60
1:A:710:ASN:O	1:A:715:ILE:HD11	2.02	0.59
1:A:315:GLU:HB3	1:A:375:PHE:HE1	1.67	0.59
1:B:107:ILE:H	1:B:146:ASN:HD21	1.50	0.59
1:B:304:LYS:HE2	1:B:305:ASP:OD2	2.02	0.59
1:A:491:ARG:HH21	1:B:539:GLU:CG	2.16	0.59
1:A:136:ASP:OD1	1:A:139:GLU:N	2.35	0.59
1:B:476:LYS:C	1:B:529:ILE:HD13	2.27	0.59
1:B:740:ALA:O	1:B:744:MET:HG3	2.02	0.59
1:A:102:LYS:O	1:A:114:LEU:HB2	2.01	0.59
1:A:578:LYS:HG2	1:A:579:TYR:CE2	2.38	0.59
1:A:679:ASN:ND2	1:A:682:GLU:HG3	2.18	0.59
1:B:85:ASP:OD1	1:B:133:SER:HB3	2.03	0.59
1:A:677:LEU:HD21	2:C:11:TYR:CE1	2.37	0.58
1:B:65:LYS:HB3	1:B:65:LYS:HZ2	1.68	0.58
1:B:478:SER:HB2	1:B:590:ARG:O	2.03	0.58
1:B:587:VAL:HA	1:B:633:ASP:OD1	2.04	0.58
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.11	0.58
1:A:615:ILE:O	1:A:619:THR:HB	2.04	0.58
1:B:679:ASN:ND2	1:B:682:GLU:H	2.01	0.58
1:A:656:LYS:O	1:A:668:LEU:HD12	2.03	0.58
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.19	0.58
1:B:628:ARG:O	1:B:665:SER:HB2	2.03	0.58
1:B:36:LEU:O	1:B:40:MET:HE3	2.03	0.58
1:B:187:ASP:HA	1:B:195:LYS:HE2	1.84	0.58
1:A:156:SER:HA	1:A:160:LEU:HD12	1.86	0.58
1:A:178:LYS:HG3	1:A:179:ASN:N	2.18	0.58
1:B:95:GLU:C	1:B:97:LEU:H	2.11	0.58
1:B:557:THR:O	1:B:561:GLU:HG3	2.04	0.58
1:A:411:GLN:HA	1:A:411:GLN:NE2	2.18	0.58
1:B:122:LYS:HB3	1:B:128:VAL:HG22	1.86	0.57
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.68	0.57
1:A:611:GLN:OE1	1:A:770:ILE:HG21	2.04	0.57
1:B:529:ILE:N	1:B:529:ILE:HD12	2.20	0.57
1:B:555:ILE:HD12	1:B:555:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:THR:OG1	1:A:637:PRO:HD2	2.04	0.57
1:B:123:GLU:HG2	1:B:124:GLY:H	1.70	0.57
1:B:510:ARG:N	1:B:522:GLN:HE21	1.91	0.57
1:B:658:LEU:HD12	1:B:659:TYR:H	1.70	0.57
1:A:574:LEU:HD23	1:A:619:THR:HG21	1.86	0.57
1:B:636:LEU:O	1:B:642:GLN:NE2	2.38	0.57
1:A:198:PRO:HG2	1:A:199:THR:H	1.69	0.57
1:A:435:ILE:HD12	1:A:435:ILE:N	2.19	0.56
1:B:683:GLY:O	1:B:687:GLU:HG2	2.05	0.56
1:A:196:GLU:O	1:A:197:HIS:C	2.49	0.56
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.41	0.56
1:B:65:LYS:HB3	1:B:65:LYS:NZ	2.19	0.56
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.41	0.56
1:A:717:ILE:HG23	1:A:761:LYS:HB3	1.88	0.56
1:A:675:VAL:HA	2:C:14:GLU:CG	2.34	0.56
1:B:401:SER:HB3	1:B:638:ASN:HD22	1.70	0.56
1:A:455:VAL:CG1	1:A:460:ASN:HA	2.35	0.56
1:A:165:GLN:HA	1:A:166:PRO:C	2.31	0.56
1:B:126:GLU:N	1:B:127:PRO:HD3	2.19	0.56
1:B:319:LEU:O	1:B:322:ILE:HG22	2.06	0.56
1:A:732:ASN:HD21	1:A:735:GLU:HG2	1.70	0.56
1:B:524:ASN:HD22	1:B:552:LYS:HE3	1.70	0.56
1:A:304:LYS:HD3	1:A:304:LYS:N	2.09	0.56
1:A:99:GLU:HA	1:A:99:GLU:OE1	2.06	0.55
1:A:234:GLN:HB2	1:A:241:PHE:CD2	2.41	0.55
1:A:455:VAL:HG12	1:A:460:ASN:HA	1.88	0.55
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.87	0.55
1:B:63:LEU:O	1:B:65:LYS:N	2.39	0.55
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.41	0.55
1:A:677:LEU:HD22	1:A:682:GLU:HB2	1.88	0.55
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.88	0.55
1:B:346:ARG:NE	1:B:356:LEU:HD13	2.21	0.55
1:B:677:LEU:HD22	1:B:682:GLU:HB3	1.89	0.55
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.36	0.55
1:A:83:ILE:HD12	1:A:83:ILE:N	2.21	0.55
1:B:107:ILE:HD13	1:B:219:LYS:HG2	1.89	0.54
1:A:396:GLY:HA3	1:A:588:HIS:HD2	1.71	0.54
1:A:66:VAL:HG12	1:A:70:VAL:CG2	2.37	0.54
1:A:79:GLY:CA	1:A:127:PRO:HG2	2.37	0.54
1:A:653:VAL:HG21	1:A:658:LEU:HG	1.90	0.54
1:A:67:PRO:HD3	1:A:225:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.88	0.54
1:B:90:LYS:HE3	1:B:90:LYS:CA	2.35	0.54
1:A:656:LYS:CE	1:A:680:ASP:OD2	2.55	0.54
1:B:460:ASN:O	1:B:498:ARG:NH2	2.37	0.54
1:A:140:ASN:HD21	1:A:142:GLU:HB2	1.73	0.54
1:A:247:PHE:HA	1:A:251:GLU:HB2	1.89	0.54
1:A:370:GLU:HA	1:A:373:LYS:HB3	1.88	0.54
1:A:252:ILE:O	1:A:255:SER:HB2	2.08	0.54
1:A:182:ASP:OD1	1:A:184:ASP:HB2	2.08	0.54
1:A:289:GLY:HA2	1:A:422:LEU:HD11	1.90	0.53
1:A:586:ASN:HB3	1:A:632:THR:HB	1.88	0.53
1:A:677:LEU:HD11	2:C:11:TYR:CE1	2.43	0.53
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.07	0.53
1:B:693:ASP:OD2	1:B:708:VAL:HG12	2.08	0.53
1:B:64:GLU:O	1:B:64:GLU:HG2	2.08	0.53
1:A:319:LEU:HD12	1:A:322:ILE:CD1	2.39	0.53
1:A:566:ILE:HG23	1:A:583:ILE:HD12	1.90	0.53
1:B:36:LEU:HG	1:B:40:MET:CE	2.38	0.53
1:A:346:ARG:C	1:A:348:SER:N	2.66	0.53
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.91	0.53
1:A:730:ARG:O	1:A:730:ARG:HG2	2.08	0.53
1:A:277:HIS:CE1	1:A:425:GLN:HE21	2.27	0.53
1:B:77:ILE:HG13	1:B:162:LYS:HE2	1.90	0.53
1:B:349:LEU:HG	1:B:350:SER:N	2.22	0.53
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.44	0.53
1:A:648:GLU:HB3	1:A:650:TYR:CE1	2.43	0.53
1:A:332:THR:O	1:A:336:GLU:HG3	2.09	0.53
1:A:674:GLY:O	1:A:676:GLU:N	2.42	0.53
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.90	0.53
1:B:618:VAL:O	1:B:621:TYR:HB3	2.09	0.53
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.73	0.53
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.91	0.52
1:B:456:ASP:HB3	1:B:459:ASP:O	2.09	0.52
1:A:103:LYS:HD2	1:A:103:LYS:N	2.23	0.52
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.07	0.52
1:B:97:LEU:CD1	1:B:102:LYS:HZ2	2.21	0.52
1:A:104:ILE:CG2	1:A:105:LYS:H	2.16	0.52
1:A:744:MET:HE3	1:A:763:PHE:CE1	2.45	0.52
1:A:346:ARG:C	1:A:348:SER:H	2.16	0.52
1:A:563:GLN:HE21	1:A:585:PHE:H	1.54	0.52
1:B:693:ASP:OD2	1:B:709:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HG2	1:B:248:ASN:OD1	2.10	0.52
1:A:387:ASP:CG	1:A:390:GLN:HB2	2.35	0.52
1:A:640:ALA:O	1:A:642:GLN:N	2.42	0.52
1:A:658:LEU:HD22	1:A:659:TYR:N	2.25	0.52
1:A:254:LEU:HD13	1:A:502:ARG:NH2	2.25	0.52
1:B:276:GLN:O	1:B:277:HIS:C	2.51	0.52
1:B:605:GLU:HG3	1:B:681:SER:OG	2.10	0.52
1:B:50:GLY:C	1:B:51:GLU:HG2	2.34	0.52
1:B:95:GLU:O	1:B:97:LEU:HD23	2.10	0.52
1:B:36:LEU:HG	1:B:40:MET:HE1	1.93	0.51
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.45	0.51
1:A:437:LEU:HD11	1:A:519:LEU:HD12	1.92	0.51
1:B:630:VAL:HG11	1:B:639:ILE:HD13	1.91	0.51
1:A:203:VAL:HG21	1:A:465:ARG:NH2	2.24	0.51
1:A:318:LEU:HD21	1:A:372:GLU:HG2	1.91	0.51
1:A:319:LEU:HD12	1:A:322:ILE:HD11	1.92	0.51
1:B:477:TYR:CD1	1:B:555:ILE:HG23	2.45	0.51
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.92	0.51
1:A:373:LYS:HE2	1:A:377:LYS:CE	2.39	0.51
1:A:399:ILE:CD1	1:A:413:LYS:HG3	2.40	0.51
1:A:435:ILE:HD12	1:A:435:ILE:H	1.76	0.51
1:A:656:LYS:HE2	1:A:680:ASP:OD2	2.11	0.51
1:B:287:GLU:CA	1:B:290:ARG:HH21	2.23	0.51
1:A:285:LEU:HD22	1:A:290:ARG:HD3	1.93	0.51
1:A:313:GLN:O	1:A:317:GLU:HG2	2.10	0.51
1:B:598:SER:O	1:B:602:ILE:HG13	2.11	0.51
1:A:243:TYR:CD1	1:A:243:TYR:C	2.88	0.51
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.11	0.51
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.11	0.51
1:B:84:VAL:CG2	1:B:85:ASP:N	2.73	0.51
1:B:426:SER:HA	1:B:510:ARG:HA	1.93	0.51
1:A:319:LEU:HD23	1:A:345:ILE:CD1	2.41	0.51
1:B:149:TYR:HA	1:B:222:ALA:HB2	1.92	0.51
1:A:697:GLY:HA3	1:A:706:ASP:O	2.11	0.50
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.40	0.50
1:B:637:PRO:HA	1:B:642:GLN:NE2	2.26	0.50
1:B:677:LEU:HD11	2:D:11:TYR:CZ	2.47	0.50
1:A:669:HIS:CD2	1:A:671:PRO:HD2	2.47	0.50
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.12	0.50
1:A:595:ILE:CD1	1:A:633:ASP:HB3	2.40	0.50
1:A:690:HIS:HB3	2:C:9:TYR:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:CD1	1:A:241:PHE:C	2.88	0.50
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.42	0.50
1:A:491:ARG:HB3	1:A:492:PRO:HD2	1.94	0.50
1:A:324:ILE:C	1:A:326:SER:H	2.19	0.50
1:B:63:LEU:C	1:B:65:LYS:H	2.20	0.50
1:B:287:GLU:HA	1:B:290:ARG:HH21	1.76	0.50
1:A:65:LYS:CE	1:A:227:PRO:HG3	2.41	0.50
1:A:675:VAL:HG12	2:C:11:TYR:HE2	1.76	0.50
1:B:150:GLU:O	1:B:153:LYS:HB2	2.11	0.50
1:B:197:HIS:HD2	1:B:199:THR:O	1.95	0.50
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.12	0.50
1:A:124:GLY:C	1:A:126:GLU:H	2.19	0.49
1:B:206:LEU:HD13	1:B:206:LEU:O	2.11	0.49
1:B:107:ILE:HG21	1:B:145:LEU:HD11	1.92	0.49
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.93	0.49
1:B:453:ASP:HB2	1:B:467:ILE:HG12	1.94	0.49
1:A:102:LYS:C	1:A:103:LYS:HD2	2.36	0.49
1:A:460:ASN:N	1:A:460:ASN:ND2	2.58	0.49
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.12	0.49
1:A:653:VAL:CG2	1:A:658:LEU:HG	2.43	0.49
1:B:93:SER:HB2	1:B:128:VAL:HG11	1.93	0.49
1:A:31:THR:HA	1:A:34:GLU:HB2	1.94	0.49
1:B:472:LYS:HG3	1:B:532:VAL:HB	1.94	0.49
1:B:478:SER:HB2	1:B:590:ARG:C	2.38	0.49
1:B:107:ILE:CD1	1:B:219:LYS:HG2	2.43	0.49
1:B:437:LEU:HD11	1:B:519:LEU:HD12	1.94	0.49
1:B:563:GLN:O	1:B:567:ASN:ND2	2.37	0.49
1:A:104:ILE:HG22	1:A:105:LYS:N	2.15	0.49
1:B:63:LEU:C	1:B:65:LYS:N	2.70	0.49
1:A:49:LYS:CG	1:A:50:GLY:H	2.13	0.49
1:A:165:GLN:HA	1:A:166:PRO:O	2.13	0.49
1:B:308:ILE:O	1:B:311:LEU:HB2	2.13	0.49
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.94	0.49
1:A:178:LYS:HG3	1:A:179:ASN:H	1.78	0.49
1:A:399:ILE:HD12	1:A:413:LYS:HG3	1.94	0.49
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.93	0.49
1:B:682:GLU:HG2	1:B:742:ARG:HH11	1.77	0.49
1:A:676:GLU:OE1	1:A:676:GLU:HA	2.12	0.49
1:A:472:LYS:HG3	1:A:532:VAL:HB	1.95	0.48
1:A:612:SER:O	1:A:616:LYS:HG3	2.13	0.48
1:A:300:ILE:HD12	1:A:300:ILE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:HIS:HD2	1:B:93:SER:OG	1.96	0.48
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.96	0.48
2:C:8:VAL:HG23	2:C:8:VAL:O	2.13	0.48
1:A:122:LYS:HE2	1:A:128:VAL:HG23	1.95	0.48
1:A:210:SER:O	1:A:214:GLN:HG3	2.13	0.48
1:A:571:ASN:OD1	1:A:580:THR:HG23	2.13	0.48
1:B:678:ARG:HH11	1:B:678:ARG:HB3	1.78	0.48
1:A:264:MET:HE3	1:A:265:LEU:CD1	2.36	0.48
1:A:442:ASN:C	1:A:442:ASN:OD1	2.56	0.48
1:A:627:GLY:HA3	1:A:664:ARG:O	2.14	0.48
1:B:129:LEU:HD13	1:B:131:ILE:HD11	1.94	0.48
1:A:424:HIS:O	1:A:510:ARG:HD2	2.14	0.48
1:A:643:TYR:HA	1:A:646:GLN:CG	2.38	0.48
1:B:578:LYS:O	1:B:579:TYR:HB2	2.14	0.48
1:B:323:GLN:NE2	1:B:325:ASP:HB2	2.28	0.48
1:B:250:GLN:O	1:B:252:ILE:N	2.47	0.48
1:A:49:LYS:O	1:A:51:GLU:N	2.46	0.48
1:A:321:ARG:HG3	1:A:321:ARG:O	2.13	0.48
1:A:328:ASP:C	1:A:330:LEU:H	2.22	0.48
1:A:453:ASP:HB2	1:A:467:ILE:HG12	1.95	0.48
1:B:608:ASN:N	1:B:608:ASN:HD22	2.10	0.48
1:A:277:HIS:CD2	1:A:429:SER:CB	2.96	0.48
1:B:233:LEU:CD2	1:B:237:ALA:HB3	2.40	0.48
1:B:325:ASP:O	1:B:326:SER:HB2	2.14	0.48
1:A:67:PRO:HD3	1:A:225:ILE:CD1	2.43	0.47
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.96	0.47
1:A:107:ILE:CD1	1:A:219:LYS:HG3	2.44	0.47
1:A:256:LEU:HD21	1:A:260:LYS:HE3	1.96	0.47
1:A:298:ILE:O	1:A:298:ILE:HG13	2.14	0.47
1:A:396:GLY:HA3	1:A:588:HIS:CD2	2.49	0.47
1:A:114:LEU:C	1:A:116:GLU:H	2.21	0.47
1:B:212:GLU:O	1:B:216:VAL:HG23	2.14	0.47
1:A:323:GLN:O	1:A:325:ASP:N	2.47	0.47
1:B:177:ILE:C	1:B:179:ASN:H	2.23	0.47
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.49	0.47
1:B:721:GLU:OE2	1:B:759:ALA:HA	2.13	0.47
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.30	0.47
1:A:87:ASP:CG	1:A:115:HIS:HB2	2.40	0.47
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.50	0.47
1:B:748:ASP:OD2	1:B:751:GLU:HG2	2.14	0.47
1:B:117:HIS:ND1	1:B:118:TYR:N	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD2	1:A:87:ASP:C	2.58	0.47
1:A:94:LEU:HD22	1:A:97:LEU:HD11	1.97	0.47
1:A:119:VAL:HG12	1:A:120:TYR:N	2.29	0.47
1:A:318:LEU:HG	1:A:372:GLU:OE2	2.14	0.47
1:A:660:VAL:HG22	2:C:8:VAL:HG12	1.96	0.47
1:B:236:TYR:C	1:B:238:PRO:HD2	2.39	0.47
1:B:381:LEU:HD11	1:B:650:TYR:HA	1.96	0.47
1:A:92:ILE:H	1:A:92:ILE:CD1	2.14	0.47
1:A:264:MET:O	1:A:268:TYR:HD2	1.96	0.47
1:B:121:ALA:HB1	1:B:154:ILE:CD1	2.42	0.47
1:A:136:ASP:CG	1:A:139:GLU:H	2.23	0.47
1:A:392:LEU:HD13	1:A:482:ASN:HA	1.96	0.47
1:A:567:ASN:O	1:A:571:ASN:HB2	2.15	0.47
1:A:732:ASN:OD1	1:A:734:ALA:N	2.48	0.47
1:A:244:MET:HE3	1:A:244:MET:CA	2.36	0.47
1:A:268:TYR:CB	1:B:125:TYR:CE2	2.83	0.47
1:A:319:LEU:HD23	1:A:345:ILE:HD12	1.96	0.47
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.37	0.47
1:B:370:GLU:OE1	1:B:373:LYS:HD3	2.15	0.46
1:B:662:GLU:CD	1:B:662:GLU:H	2.23	0.46
1:A:346:ARG:C	1:A:346:ARG:HD2	2.39	0.46
1:A:488:ILE:HG13	1:A:517:GLY:O	2.15	0.46
1:B:550:VAL:HB	1:B:551:PRO:CD	2.46	0.46
2:D:8:VAL:O	2:D:8:VAL:HG23	2.13	0.46
1:A:373:LYS:HE2	1:A:377:LYS:NZ	2.31	0.46
1:A:725:LEU:O	1:A:726:THR:O	2.33	0.46
1:B:723:SER:HB3	1:B:730:ARG:HD3	1.96	0.46
1:B:95:GLU:C	1:B:97:LEU:HD23	2.40	0.46
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.15	0.46
1:B:608:ASN:N	1:B:608:ASN:ND2	2.63	0.46
1:B:606:TRP:CZ2	1:B:615:ILE:HG23	2.51	0.46
1:A:725:LEU:O	1:A:726:THR:C	2.59	0.46
1:B:47:GLU:OE1	1:B:91:HIS:HE1	1.97	0.46
1:B:437:LEU:CD2	1:B:488:ILE:HA	2.45	0.46
1:B:658:LEU:HD12	1:B:659:TYR:N	2.30	0.46
1:B:693:ASP:CG	1:B:709:THR:HG23	2.40	0.46
1:A:125:TYR:O	1:A:126:GLU:HG3	2.16	0.46
1:A:610:ILE:CG2	1:A:614:LEU:HD23	2.45	0.46
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.98	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.16	0.46
1:B:524:ASN:HB3	1:B:552:LYS:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ARG:HG2	1:B:682:GLU:OE1	2.15	0.46
1:A:77:ILE:C	1:B:265:LEU:HD21	2.41	0.46
1:B:62:LEU:O	1:B:148:TYR:OH	2.29	0.46
1:B:80:LYS:O	1:B:128:VAL:HA	2.16	0.46
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.97	0.46
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.96	0.46
1:A:43:ILE:HG13	1:A:44:VAL:N	2.31	0.46
1:A:294:LYS:HA	1:A:294:LYS:HD3	1.77	0.46
1:A:347:ASP:O	1:A:347:ASP:CG	2.58	0.46
1:A:739:GLU:CD	1:A:742:ARG:HH21	2.24	0.46
1:B:114:LEU:HD11	1:B:120:TYR:HB2	1.98	0.46
1:B:449:THR:HA	1:B:673:LYS:HD3	1.97	0.46
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.42	0.45
1:A:33:GLU:O	1:A:37:LYS:HG3	2.16	0.45
1:A:402:PRO:HA	1:A:409:ARG:CZ	2.46	0.45
1:B:196:GLU:O	1:B:197:HIS:C	2.58	0.45
1:B:713:LYS:O	1:B:717:ILE:HG12	2.16	0.45
1:A:51:GLU:O	1:A:52:GLU:C	2.59	0.45
1:B:210:SER:O	1:B:214:GLN:HG3	2.17	0.45
1:A:373:LYS:O	1:A:377:LYS:HG3	2.15	0.45
1:A:477:TYR:H	1:A:593:SER:HB3	1.81	0.45
1:B:654:HIS:O	2:D:13:MET:HE2	2.15	0.45
1:B:748:ASP:OD2	1:B:750:ALA:HB3	2.16	0.45
1:A:123:GLU:HG2	1:A:124:GLY:N	2.27	0.45
1:A:348:SER:O	1:A:349:LEU:C	2.59	0.45
1:B:412:TYR:O	1:B:416:ILE:HG12	2.17	0.45
1:A:465:ARG:O	1:A:469:ASN:ND2	2.49	0.45
1:B:323:GLN:HE22	1:B:325:ASP:HB2	1.81	0.45
1:A:55:LYS:HD3	1:A:133:SER:HB2	1.99	0.45
1:A:65:LYS:HE2	1:A:227:PRO:CG	2.44	0.45
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.46	0.45
1:A:674:GLY:HA3	1:A:677:LEU:HD12	1.98	0.45
1:B:636:LEU:HD13	1:B:669:HIS:HB2	1.99	0.45
1:A:252:ILE:HG23	1:A:253:ASN:N	2.32	0.45
1:A:323:GLN:O	1:A:324:ILE:C	2.59	0.45
1:B:119:VAL:HG21	1:B:147:VAL:HG13	1.99	0.45
1:B:237:ALA:N	1:B:238:PRO:HD2	2.32	0.45
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.99	0.45
1:A:441:MET:HG2	1:A:442:ASN:N	2.32	0.45
1:A:749:HIS:CE1	1:A:752:ARG:HH11	2.34	0.45
1:B:126:GLU:N	1:B:127:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:O	1:A:37:LYS:C	2.60	0.44
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.82	0.44
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.78	0.44
1:A:346:ARG:NH1	1:A:347:ASP:HB3	2.32	0.44
1:A:567:ASN:ND2	1:A:582:LEU:H	2.14	0.44
1:B:48:VAL:CG2	1:B:52:GLU:HG2	2.46	0.44
1:A:40:MET:HE1	1:A:60:GLU:HA	1.98	0.44
1:A:64:GLU:O	1:A:64:GLU:HG2	2.16	0.44
1:A:330:LEU:HD13	1:A:338:LEU:CD1	2.47	0.44
1:A:479:ILE:HD11	1:A:555:ILE:CG2	2.48	0.44
1:B:168:GLN:HA	1:B:171:LEU:HD12	1.99	0.44
1:B:177:ILE:C	1:B:179:ASN:N	2.73	0.44
1:B:247:PHE:HA	1:B:251:GLU:HB2	1.99	0.44
1:B:594:ASN:O	1:B:598:SER:HB3	2.17	0.44
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.90	0.44
1:A:656:LYS:HE3	1:A:680:ASP:OD2	2.17	0.44
1:B:234:GLN:O	1:B:238:PRO:HG3	2.17	0.44
1:A:459:ASP:OD2	1:A:461:THR:HG23	2.18	0.44
1:B:379:LEU:O	1:B:383:ILE:HG23	2.17	0.44
1:B:765:PHE:O	1:B:768:ASP:HB2	2.17	0.44
1:B:324:ILE:HD12	1:B:324:ILE:N	2.23	0.44
1:B:401:SER:CB	1:B:638:ASN:ND2	2.79	0.44
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.98	0.44
1:B:398:LEU:HD22	1:B:398:LEU:H	1.83	0.44
1:A:649:ILE:C	1:A:651:GLU:H	2.25	0.44
1:A:675:VAL:O	1:A:675:VAL:CG1	2.64	0.44
1:B:51:GLU:HG3	1:B:55:LYS:HE3	2.00	0.44
1:B:249:GLU:C	1:B:250:GLN:HG3	2.43	0.44
2:D:13:MET:H	2:D:13:MET:HG3	1.48	0.44
1:A:46:ILE:O	1:A:47:GLU:HG3	2.17	0.44
1:A:693:ASP:CG	1:A:709:THR:HB	2.42	0.44
1:B:387:ASP:HB3	1:B:390:GLN:HB3	2.00	0.44
1:A:82:TYR:HE1	1:A:93:SER:HG	1.65	0.44
1:A:204:GLU:OE2	1:A:204:GLU:N	2.39	0.44
1:A:267:ARG:CZ	1:A:489:ASN:HB3	2.48	0.44
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.17	0.43
1:B:635:THR:HA	1:B:654:HIS:CE1	2.53	0.43
1:A:290:ARG:O	1:A:294:LYS:HB2	2.18	0.43
1:B:149:TYR:CA	1:B:222:ALA:HB2	2.49	0.43
1:B:161:SER:C	1:B:163:ILE:H	2.26	0.43
1:B:178:LYS:HD2	1:B:201:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASP:OD2	1:B:339:LYS:HD3	2.18	0.43
1:A:173:VAL:HG21	1:A:243:TYR:CD2	2.53	0.43
1:A:324:ILE:C	1:A:326:SER:N	2.76	0.43
1:A:707:LEU:CB	1:A:709:THR:HG22	2.48	0.43
1:B:524:ASN:HB3	1:B:552:LYS:HD2	2.00	0.43
1:B:603:LEU:O	1:B:606:TRP:HB3	2.19	0.43
1:B:669:HIS:HE1	1:B:671:PRO:HB2	1.84	0.43
1:B:35:HIS:NE2	1:B:72:GLU:OE2	2.48	0.43
1:B:50:GLY:O	1:B:51:GLU:HG2	2.19	0.43
1:B:444:ASN:ND2	1:B:451:GLY:HA3	2.34	0.43
1:B:698:TYR:CD1	1:B:698:TYR:C	2.97	0.43
1:A:159:ILE:HD12	1:A:159:ILE:N	2.32	0.43
1:A:91:HIS:CE1	1:A:93:SER:H	2.37	0.43
1:A:499:LEU:HD12	1:A:543:ILE:HB	2.00	0.43
1:A:749:HIS:CE1	1:A:752:ARG:NH1	2.85	0.43
1:B:164:ASN:N	1:B:164:ASN:HD22	2.15	0.43
1:B:443:ILE:CD1	1:B:454:LEU:HD22	2.49	0.43
1:A:330:LEU:HB2	1:A:335:LYS:HE3	1.99	0.43
1:A:443:ILE:HG21	1:A:451:GLY:HA2	2.01	0.43
1:B:223:TYR:O	1:B:230:ARG:HA	2.19	0.43
1:B:268:TYR:O	1:B:272:GLU:HG2	2.19	0.43
1:B:447:THR:HG23	1:B:447:THR:O	2.19	0.43
1:B:694:ASP:C	1:B:694:ASP:OD1	2.61	0.43
1:A:621:TYR:HE2	1:A:694:ASP:OD2	2.02	0.43
1:B:88:ILE:HG22	1:B:130:VAL:HG12	2.01	0.43
2:C:13:MET:H	2:C:13:MET:HG3	1.48	0.43
1:A:122:LYS:HB3	1:A:128:VAL:HB	2.01	0.43
1:A:237:ALA:N	1:A:238:PRO:HD3	2.33	0.43
1:A:243:TYR:HD1	1:A:244:MET:N	2.17	0.43
1:A:330:LEU:O	1:A:335:LYS:HE3	2.19	0.43
1:B:628:ARG:H	1:B:665:SER:CB	2.24	0.43
1:A:450:LEU:HB3	1:A:467:ILE:HG23	2.01	0.43
1:A:503:ILE:HD13	1:A:503:ILE:N	2.34	0.43
1:B:96:ALA:O	1:B:98:SER:N	2.52	0.43
1:A:305:ASP:O	1:A:309:HIS:HB2	2.19	0.42
1:A:330:LEU:HD13	1:A:338:LEU:HD12	2.01	0.42
1:B:123:GLU:OE1	1:B:157:ARG:HD2	2.19	0.42
1:B:311:LEU:HD22	1:B:315:GLU:CB	2.49	0.42
1:B:406:LEU:O	1:B:410:LYS:HG2	2.19	0.42
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.19	0.42
1:A:710:ASN:O	1:A:710:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:C	1:B:211:ASN:N	2.76	0.42
1:A:370:GLU:HA	1:A:373:LYS:CB	2.48	0.42
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.19	0.42
1:B:119:VAL:HA	1:B:130:VAL:O	2.20	0.42
1:B:164:ASN:N	1:B:164:ASN:ND2	2.65	0.42
1:A:149:TYR:HA	1:A:222:ALA:HB2	2.00	0.42
1:A:193:GLN:CA	1:A:193:GLN:HE21	2.32	0.42
1:A:460:ASN:ND2	1:A:460:ASN:H	2.17	0.42
1:A:522:GLN:HE21	1:A:522:GLN:HB2	1.60	0.42
1:A:574:LEU:N	1:A:574:LEU:HD12	2.34	0.42
1:A:636:LEU:HD12	1:A:636:LEU:HA	1.86	0.42
1:B:84:VAL:CG2	1:B:85:ASP:H	2.32	0.42
1:B:643:TYR:HA	1:B:646:GLN:HG3	2.02	0.42
1:B:707:LEU:HD11	2:D:9:TYR:CZ	2.54	0.42
1:A:29:ASN:O	1:A:32:GLN:HB2	2.20	0.42
1:B:145:LEU:O	1:B:145:LEU:HD22	2.19	0.42
1:B:193:GLN:NE2	1:B:212:GLU:HG3	2.35	0.42
1:A:693:ASP:OD1	1:A:709:THR:CG2	2.68	0.42
1:B:90:LYS:HA	1:B:90:LYS:CE	2.41	0.42
1:B:122:LYS:HE2	1:B:128:VAL:HG22	2.01	0.42
1:A:140:ASN:C	1:A:140:ASN:HD22	2.27	0.42
1:A:693:ASP:OD1	1:A:709:THR:HB	2.20	0.42
1:A:741:PHE:CD2	1:A:741:PHE:C	2.98	0.42
1:B:94:LEU:O	1:B:97:LEU:N	2.53	0.42
1:B:97:LEU:HD13	1:B:102:LYS:HZ2	1.84	0.42
1:B:286:SER:C	1:B:288:GLU:N	2.73	0.42
1:B:401:SER:HB3	1:B:638:ASN:ND2	2.33	0.42
1:B:528:GLU:CD	1:B:530:LYS:HE2	2.44	0.42
1:B:136:ASP:O	1:B:140:ASN:HB3	2.20	0.42
1:B:144:ALA:C	1:B:146:ASN:N	2.73	0.42
1:B:303:LYS:O	1:B:307:ILE:HG12	2.19	0.42
1:B:376:LEU:O	1:B:377:LYS:C	2.62	0.42
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.54	0.42
1:A:263:ARG:HH11	1:A:263:ARG:CB	2.27	0.42
1:A:338:LEU:O	1:A:341:LEU:HB2	2.19	0.42
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.42
1:A:38:GLU:O	1:A:41:LYS:HB2	2.19	0.42
1:A:333:GLU:CD	1:A:333:GLU:N	2.70	0.42
1:A:433:ASN:O	1:A:435:ILE:HD11	2.19	0.41
1:A:500:LYS:HZ2	1:A:500:LYS:HG2	1.72	0.41
1:A:594:ASN:O	1:A:595:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LYS:NZ	1:B:251:GLU:OE2	2.53	0.41
1:B:293:LEU:O	1:B:296:LEU:HB3	2.20	0.41
1:A:435:ILE:N	1:A:435:ILE:CD1	2.82	0.41
1:B:366:ASN:CB	1:B:367:PRO:CD	2.91	0.41
1:B:674:GLY:HA3	1:B:677:LEU:HD12	2.02	0.41
1:A:83:ILE:O	1:A:83:ILE:HG22	2.20	0.41
1:A:271:TRP:HD1	1:A:271:TRP:O	2.03	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:A:744:MET:HE3	1:A:763:PHE:CD1	2.55	0.41
1:B:338:LEU:HD22	1:B:379:LEU:HD13	2.02	0.41
1:B:632:THR:HG21	1:B:639:ILE:HD11	2.02	0.41
1:A:311:LEU:HD11	1:A:319:LEU:HD22	2.02	0.41
1:A:459:ASP:C	1:A:461:THR:H	2.27	0.41
1:A:696:ALA:HB2	1:A:773:ILE:HD11	2.01	0.41
1:B:659:TYR:O	1:B:661:PRO:HD3	2.21	0.41
1:B:675:VAL:CG2	2:D:14:GLU:HG2	2.28	0.41
1:A:88:ILE:H	1:A:88:ILE:HG12	1.69	0.41
1:A:89:THR:HG22	1:A:114:LEU:HD13	2.01	0.41
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.80	0.41
1:B:125:TYR:C	1:B:127:PRO:HD3	2.45	0.41
1:B:190:PHE:O	1:B:195:LYS:HE3	2.21	0.41
1:B:394:ASP:O	1:B:634:ILE:HB	2.21	0.41
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.55	0.41
1:B:439:GLU:HB2	1:B:486:VAL:HG12	2.01	0.41
1:A:118:TYR:CD1	1:A:118:TYR:N	2.88	0.41
1:A:165:GLN:HB3	1:A:166:PRO:HA	2.01	0.41
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.02	0.41
1:A:226:GLU:HA	1:A:227:PRO:HD2	1.77	0.41
1:A:640:ALA:C	1:A:642:GLN:N	2.78	0.41
1:B:123:GLU:HG2	1:B:124:GLY:N	2.35	0.41
1:B:772:PHE:O	1:B:776:SER:HB3	2.20	0.41
1:A:82:TYR:C	1:A:83:ILE:HD12	2.46	0.41
1:A:324:ILE:HG22	1:A:335:LYS:HD3	2.02	0.41
1:B:95:GLU:C	1:B:97:LEU:N	2.78	0.41
1:B:252:ILE:HG23	1:B:253:ASN:N	2.35	0.41
1:B:353:GLU:HA	1:B:356:LEU:HD12	2.03	0.41
1:A:263:ARG:HB2	1:A:266:SER:HB2	2.03	0.41
1:A:322:ILE:HD12	1:A:324:ILE:HD11	2.03	0.41
1:B:242:ASN:O	1:B:243:TYR:C	2.62	0.41
1:B:263:ARG:HB2	1:B:266:SER:HB2	2.02	0.41
1:A:440:ASN:ND2	1:A:500:LYS:HZ2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASN:ND2	1:A:500:LYS:NZ	2.68	0.41
1:A:676:GLU:CG	2:C:14:GLU:OE2	2.66	0.41
1:A:718:PHE:O	1:A:722:GLY:HA3	2.21	0.41
1:B:52:GLU:O	1:B:53:ALA:C	2.63	0.41
1:B:205:PHE:CD1	1:B:205:PHE:C	2.99	0.41
1:B:512:GLY:O	1:B:520:ILE:HG22	2.20	0.41
1:B:639:ILE:O	1:B:640:ALA:C	2.64	0.41
1:A:83:ILE:N	1:A:83:ILE:CD1	2.84	0.41
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.21	0.41
1:A:571:ASN:HD22	1:A:571:ASN:HA	1.66	0.41
1:B:91:HIS:O	1:B:92:ILE:C	2.62	0.41
1:B:477:TYR:CA	1:B:529:ILE:HD13	2.51	0.41
1:B:498:ARG:NH2	1:B:540:LYS:HE3	2.21	0.41
1:B:160:LEU:O	1:B:165:GLN:HB2	2.21	0.40
1:B:322:ILE:HD13	1:B:376:LEU:HD21	2.03	0.40
1:B:533:GLN:HE21	1:B:533:GLN:HB2	1.74	0.40
1:A:48:VAL:HG12	1:A:85:ASP:OD1	2.21	0.40
1:A:321:ARG:O	1:A:321:ARG:CG	2.68	0.40
1:B:54:VAL:O	1:B:58:ALA:HB2	2.20	0.40
1:B:663:SER:O	1:B:664:ARG:C	2.64	0.40
1:B:118:TYR:N	1:B:118:TYR:CD1	2.89	0.40
1:B:436:TYR:HA	1:B:503:ILE:O	2.21	0.40
1:B:695:TYR:O	1:B:696:ALA:C	2.64	0.40
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.21	0.40
1:A:285:LEU:CD2	1:A:290:ARG:HD3	2.51	0.40
1:B:66:VAL:O	1:B:67:PRO:C	2.64	0.40
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.36	0.40
1:B:698:TYR:CE1	1:B:702:LYS:HG3	2.56	0.40
1:A:223:TYR:CD2	1:A:229:HIS:HB3	2.56	0.40
1:A:264:MET:HE2	1:A:264:MET:HB3	1.99	0.40
1:A:433:ASN:O	1:A:435:ILE:CD1	2.70	0.40
1:B:39:ILE:CG2	1:B:43:ILE:HD12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	729/776 (94%)	634 (87%)	73 (10%)	22 (3%)	3	8
1	B	732/776 (94%)	633 (86%)	83 (11%)	16 (2%)	5	12
2	C	7/20 (35%)	3 (43%)	3 (43%)	1 (14%)	0	0
2	D	7/20 (35%)	2 (29%)	4 (57%)	1 (14%)	0	0
All	All	1475/1592 (93%)	1272 (86%)	163 (11%)	40 (3%)	4	9

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLY
1	A	198	PRO
1	A	324	ILE
1	A	327	SER
1	A	700	LEU
1	A	726	THR
1	B	53	ALA
1	B	97	LEU
1	B	326	SER
1	B	758	ASN
1	A	51	GLU
1	A	188	LEU
1	A	209	ASN
1	A	460	ASN
1	A	473	LYS
1	A	641	GLU
1	A	675	VAL
1	B	64	GLU
1	B	251	GLU
1	B	664	ARG
1	B	722	GLY
2	C	12	PRO
2	D	12	PRO
1	A	347	ASP
1	A	702	LYS
1	B	123	GLU
1	A	41	LYS
1	A	125	TYR

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	578	LYS
1	A	592	ALA
1	B	41	LYS
1	B	349	LEU
1	B	609	ASN
1	A	179	ASN
1	B	210	SER
1	B	250	GLN
1	B	616	LYS
1	A	36	LEU
1	B	138	VAL

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	672/710 (95%)	609 (91%)	63 (9%)	8	18
1	B	675/710 (95%)	622 (92%)	53 (8%)	11	24
2	C	9/17 (53%)	7 (78%)	2 (22%)	1	0
2	D	9/17 (53%)	8 (89%)	1 (11%)	6	12
All	All	1365/1454 (94%)	1246 (91%)	119 (9%)	9	21

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	30	LYS
1	A	46	ILE
1	A	64	GLU
1	A	88	ILE
1	A	102	LYS
1	A	103	LYS
1	A	107	ILE
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	193	GLN
1	A	196	GLU
1	A	207	GLU
1	A	215	GLU
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	263	ARG
1	A	265	LEU
1	A	275	LYS
1	A	285	LEU
1	A	294	LYS
1	A	296	LEU
1	A	301	GLU
1	A	304	LYS
1	A	314	GLU
1	A	322	ILE
1	A	368	LEU
1	A	372	GLU
1	A	408	VAL
1	A	434	LYS
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	460	ASN
1	A	462	LYS
1	A	491	ARG
1	A	494	LEU
1	A	499	LEU
1	A	505	LEU
1	A	522	GLN
1	A	555	ILE
1	A	564	LEU
1	A	566	ILE
1	A	578	LYS
1	A	580	THR
1	A	581	LYS
1	A	582	LEU
1	A	619	THR
1	A	635	THR
1	A	636	LEU

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Mol	Chain	Res	Type
1	A	639	ILE
1	A	644	THR
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	692	VAL
1	A	702	LYS
1	A	703	ASN
1	A	733	GLU
1	A	739	GLU
1	A	761	LYS
1	A	764	GLN
1	B	65	LYS
1	B	66	VAL
1	B	68	SER
1	B	77	ILE
1	B	90	LYS
1	B	97	LEU
1	B	99	GLU
1	B	107	ILE
1	B	129	LEU
1	B	145	LEU
1	B	146	ASN
1	B	156	SER
1	B	165	GLN
1	B	203	VAL
1	B	228	GLN
1	B	233	LEU
1	B	238	PRO
1	B	256	LEU
1	B	292	LEU
1	B	304	LYS
1	B	305	ASP
1	B	314	GLU
1	B	323	GLN
1	B	345	ILE
1	B	350	SER
1	B	355	GLU
1	B	366	ASN
1	B	391	ARG
1	B	425	GLN
1	B	430	THR

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Mol	Chain	Res	Type
1	B	435	ILE
1	B	446	LEU
1	B	467	ILE
1	B	478	SER
1	B	496	ASN
1	B	515	GLU
1	B	516	ASN
1	B	520	ILE
1	B	538	SER
1	B	557	THR
1	B	608	ASN
1	B	611	GLN
1	B	613	ASP
1	B	616	LYS
1	B	636	LEU
1	B	639	ILE
1	B	679	ASN
1	B	682	GLU
1	B	710	ASN
1	B	712	LYS
1	B	733	GLU
1	B	758	ASN
1	B	769	GLN
2	C	13	MET
2	C	15	PRO
2	D	13	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	140	ASN
1	A	164	ASN
1	A	186	GLN
1	A	193	GLN
1	A	214	GLN
1	A	242	ASN
1	A	253	ASN
1	A	262	GLN
1	A	276	GLN
1	A	277	HIS

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	390	GLN
1	A	393	GLN
1	A	411	GLN
1	A	417	GLN
1	A	440	ASN
1	A	460	ASN
1	A	469	ASN
1	A	474	ASN
1	A	522	GLN
1	A	524	ASN
1	A	537	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	608	ASN
1	A	646	GLN
1	A	652	GLN
1	A	654	HIS
1	A	679	ASN
1	A	703	ASN
1	A	710	ASN
1	A	745	HIS
1	A	749	HIS
1	A	767	ASN
1	B	91	HIS
1	B	146	ASN
1	B	164	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	208	GLN
1	B	214	GLN
1	B	228	GLN
1	B	242	ASN
1	B	262	GLN
1	B	276	GLN
1	B	277	HIS
1	B	297	GLN
1	B	313	GLN
1	B	390	GLN

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Mol	Chain	Res	Type
1	B	411	GLN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	474	ASN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	608	ASN
1	B	638	ASN
1	B	645	HIS
1	B	646	GLN
1	B	654	HIS
1	B	669	HIS
1	B	679	ASN
1	B	690	HIS
1	B	710	ASN
1	B	756	GLN
1	B	758	ASN
1	B	767	ASN
1	B	769	GLN
1	B	775	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	733/776 (94%)	0.53	81 (11%) 10 8	13, 43, 108, 126	0
1	B	736/776 (94%)	0.39	61 (8%) 17 13	13, 40, 95, 115	0
2	C	9/20 (45%)	4.32	8 (88%) 0 0	94, 101, 104, 107	0
2	D	9/20 (45%)	4.15	8 (88%) 0 0	93, 101, 104, 107	0
All	All	1487/1592 (93%)	0.51	158 (10%) 11 9	13, 42, 103, 126	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	GLU	7.2
2	D	10	PRO	6.4
1	A	349	LEU	6.1
2	D	9	TYR	6.0
2	C	16	THR	5.8
1	B	357	LEU	5.4
2	C	12	PRO	5.3
1	B	349	LEU	5.1
2	C	8	VAL	5.0
1	A	367	PRO	4.9
2	C	10	PRO	4.8
1	B	137	TYR	4.8
2	C	15	PRO	4.7
1	B	35	HIS	4.5
2	D	15	PRO	4.5
1	A	322	ILE	4.4
1	A	310	SER	4.4
1	A	345	ILE	4.4
2	C	9	TYR	4.3
2	C	11	TYR	4.3
2	D	16	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	8	VAL	4.2
1	A	31	THR	4.1
1	A	308	ILE	4.0
1	B	350	SER	4.0
1	A	324	ILE	4.0
1	A	344	ASP	3.8
1	B	351	GLU	3.8
2	D	12	PRO	3.8
1	A	368	LEU	3.6
1	B	366	ASN	3.5
1	B	50	GLY	3.5
1	A	369	SER	3.5
1	A	55	LYS	3.5
1	B	104	ILE	3.5
1	A	94	LEU	3.4
1	B	34	GLU	3.4
1	A	137	TYR	3.4
1	A	35	HIS	3.3
2	D	14	GLU	3.3
1	B	326	SER	3.2
1	B	113	LEU	3.2
1	A	46	ILE	3.2
1	A	343	ILE	3.2
1	A	330	LEU	3.1
1	A	706	ASP	3.1
1	A	327	SER	3.1
1	B	115	HIS	3.1
1	B	324	ILE	3.1
1	A	316	LYS	3.1
1	A	311	LEU	3.1
2	D	11	TYR	3.1
1	B	36	LEU	3.1
1	B	141	THR	3.1
1	B	352	GLU	3.0
1	A	329	PHE	3.0
1	A	140	ASN	3.0
1	B	305	ASP	3.0
1	A	337	PHE	3.0
1	A	104	ILE	2.9
1	A	318	LEU	2.9
1	A	321	ARG	2.9
1	B	353	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLU	2.9
1	B	112	ALA	2.9
1	A	340	LYS	2.9
1	B	93	SER	2.9
1	A	341	LEU	2.9
2	C	14	GLU	2.8
1	B	43	ILE	2.8
1	B	348	SER	2.8
1	B	96	ALA	2.8
1	A	313	GLN	2.7
1	A	314	GLU	2.7
1	B	730	ARG	2.7
1	A	96	ALA	2.7
1	B	59	ALA	2.7
1	A	326	SER	2.7
1	B	98	SER	2.7
1	A	99	GLU	2.7
1	A	50	GLY	2.7
1	A	702	LYS	2.7
1	A	713	LYS	2.7
1	A	709	THR	2.7
1	B	704	GLN	2.7
1	B	41	LYS	2.6
1	A	98	SER	2.6
1	A	28	ARG	2.6
1	A	48	VAL	2.6
1	A	136	ASP	2.6
1	B	42	HIS	2.6
1	B	97	LEU	2.6
1	A	348	SER	2.6
1	A	97	LEU	2.6
1	A	707	LEU	2.6
1	B	356	LEU	2.6
1	A	43	ILE	2.6
1	B	323	GLN	2.6
1	B	705	SER	2.5
1	A	101	LYS	2.5
1	A	307	ILE	2.5
1	A	676	GLU	2.5
1	B	33	GLU	2.5
1	B	135	GLU	2.5
1	B	329	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	712	LYS	2.5
1	B	114	LEU	2.5
1	B	101	LYS	2.5
1	B	136	ASP	2.5
1	B	125	TYR	2.5
1	B	52	GLU	2.5
1	B	208	GLN	2.5
1	A	309	HIS	2.5
1	A	44	VAL	2.4
1	B	134	SER	2.4
1	A	180	ALA	2.4
1	B	710	ASN	2.4
1	A	710	ASN	2.4
1	B	54	VAL	2.4
1	A	27	GLU	2.4
1	A	705	SER	2.4
1	A	39	ILE	2.4
1	A	703	ASN	2.3
1	B	678	ARG	2.3
1	B	139	GLU	2.3
1	B	345	ILE	2.3
1	A	347	ASP	2.3
1	A	319	LEU	2.3
1	A	700	LEU	2.3
1	A	49	LYS	2.3
1	B	51	GLU	2.2
1	A	45	LYS	2.2
1	A	342	GLN	2.2
1	A	678	ARG	2.2
1	A	199	THR	2.2
1	B	89	THR	2.2
1	B	99	GLU	2.2
1	A	323	GLN	2.2
1	A	320	LYS	2.2
1	A	32	GLN	2.2
1	A	36	LEU	2.2
1	B	775	ASN	2.1
1	A	718	PHE	2.1
1	B	711	SER	2.1
1	A	84	VAL	2.1
1	B	354	LYS	2.1
1	A	185	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	315	GLU	2.1
1	B	140	ASN	2.1
1	A	85	ASP	2.1
1	B	706	ASP	2.1
1	A	111	ASP	2.1
1	A	198	PRO	2.0
1	B	330	LEU	2.0
1	A	458	THR	2.0
1	B	368	LEU	2.0
1	B	53	ALA	2.0
1	A	328	ASP	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 oligosaccharides 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.