



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:50 PM UTC

PDB ID : 2YWB / pdb_00002ywb
Title : Crystal structure of GMP synthetase from *Thermus thermophilus*
Authors : Baba, S.; Kanagawa, M.; Yanai, H.; Ishii, T.; Kuramitsu, S.; Yokoyama, S.; Sampei, G.; Kawai, G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-04-20
Resolution : 2.10 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

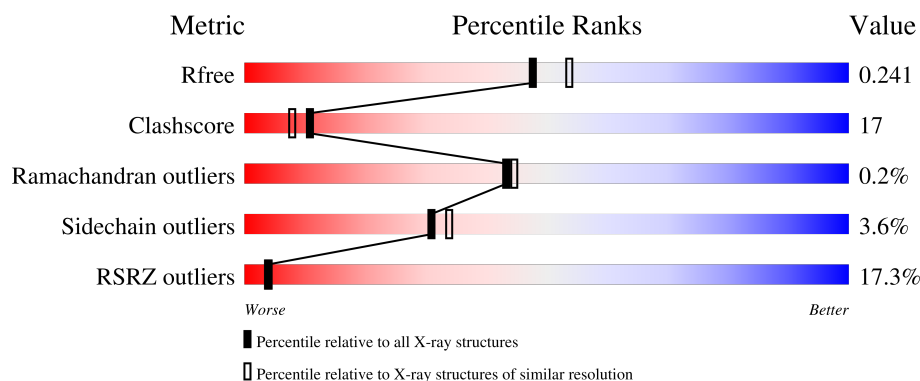
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	503	14% 67% 24% 6%
1	B	503	14% 60% 30% 8%
1	C	503	18% 64% 26% 7%
1	D	503	18% 59% 30% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15065 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 GMP synthase [glutamine-hydrolyzing].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3718	2382	658	672	6			
1	B	463	Total	C	N	O	S	0	0	0
			3656	2344	650	656	6			
1	C	466	Total	C	N	O	S	0	0	0
			3676	2355	653	662	6			
1	D	463	Total	C	N	O	S	0	0	0
			3659	2347	650	656	6			

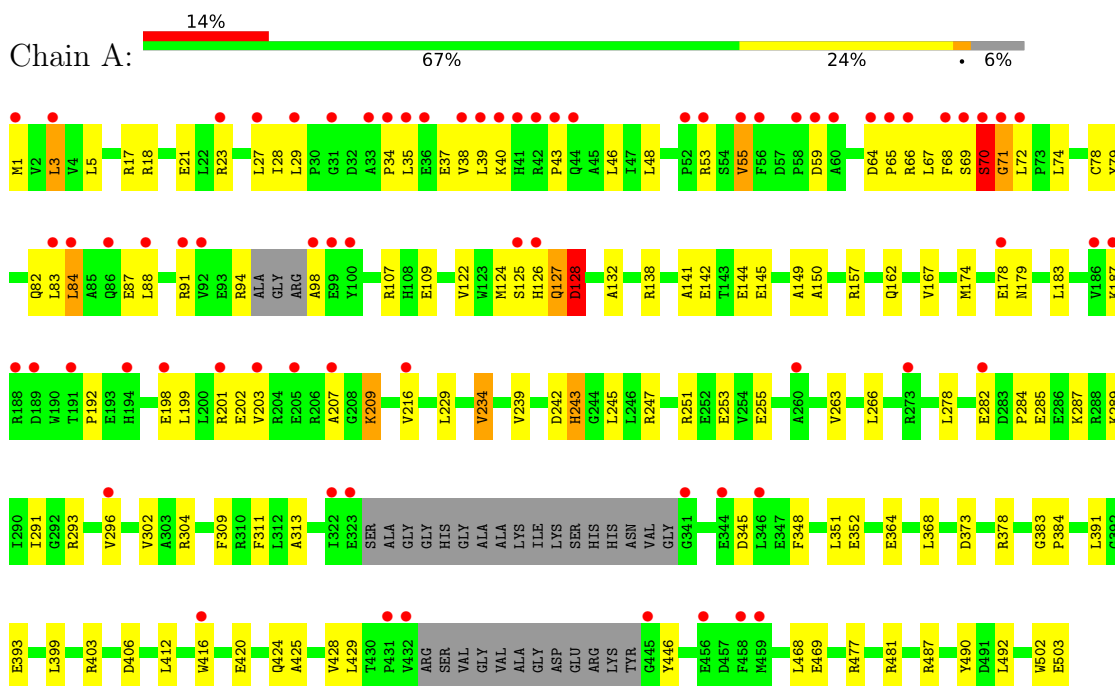
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	101	Total	O	0	0
			101	101		
2	C	85	Total	O	0	0
			85	85		
2	D	71	Total	O	0	0
			71	71		

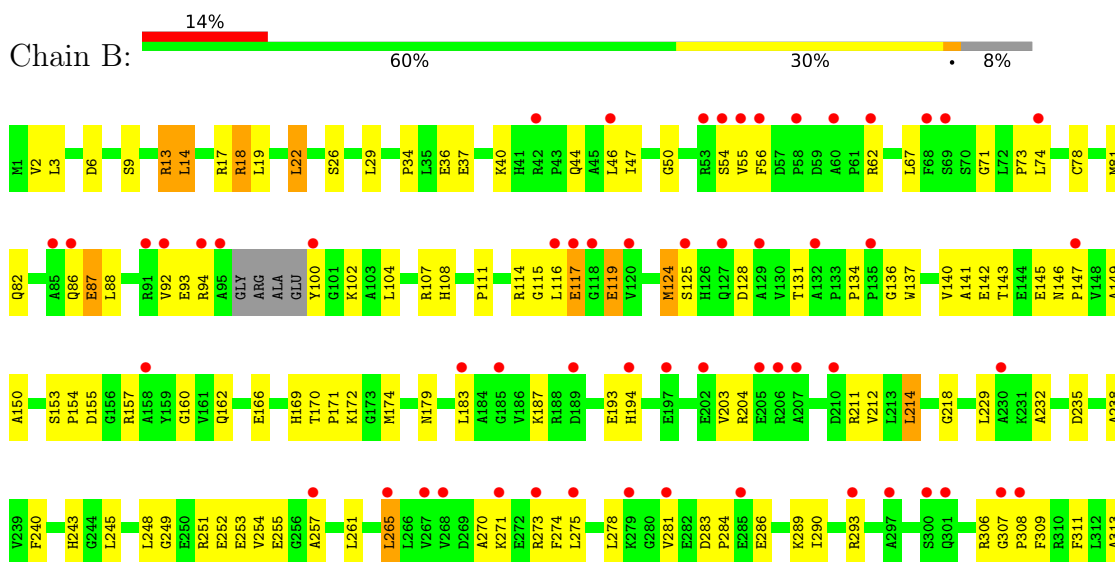
3 Residue-property plots

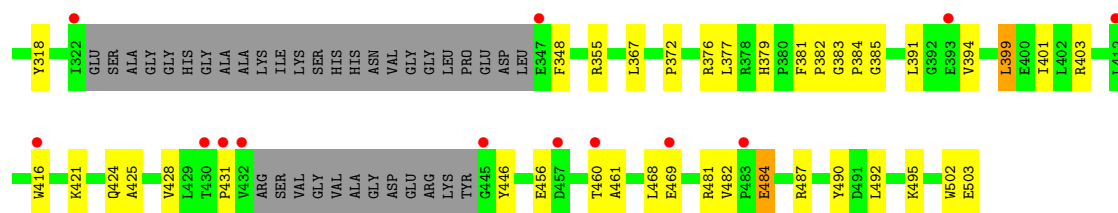
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

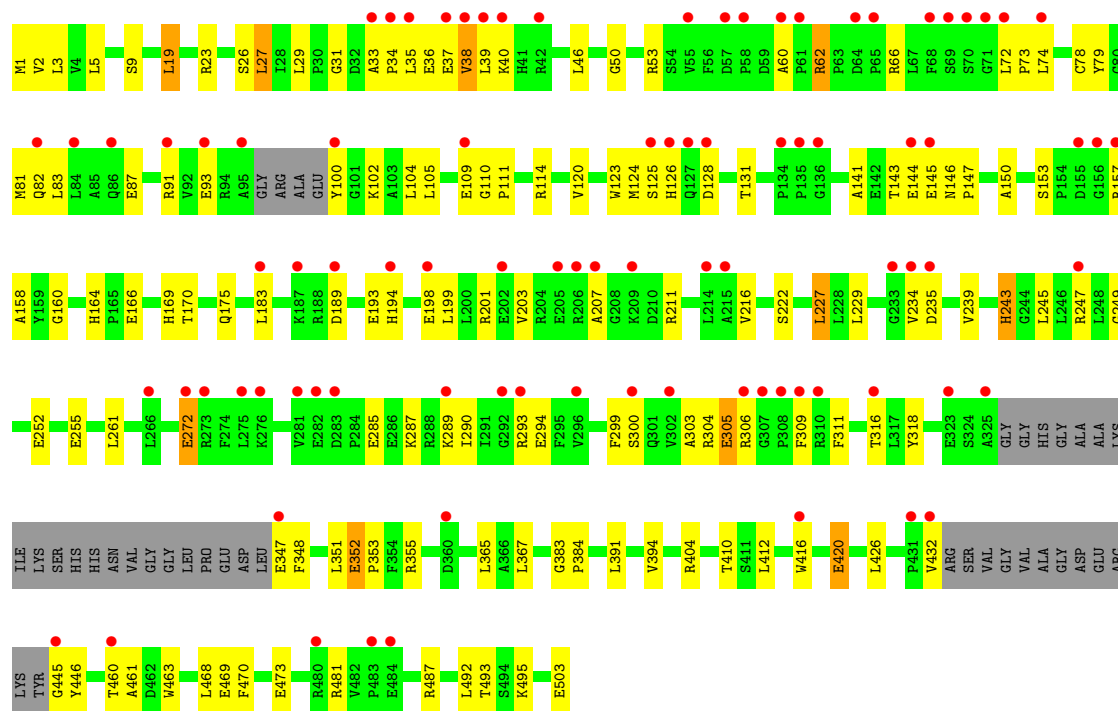


• Molecule 1: GMP synthase [glutamine-hydrolyzing]

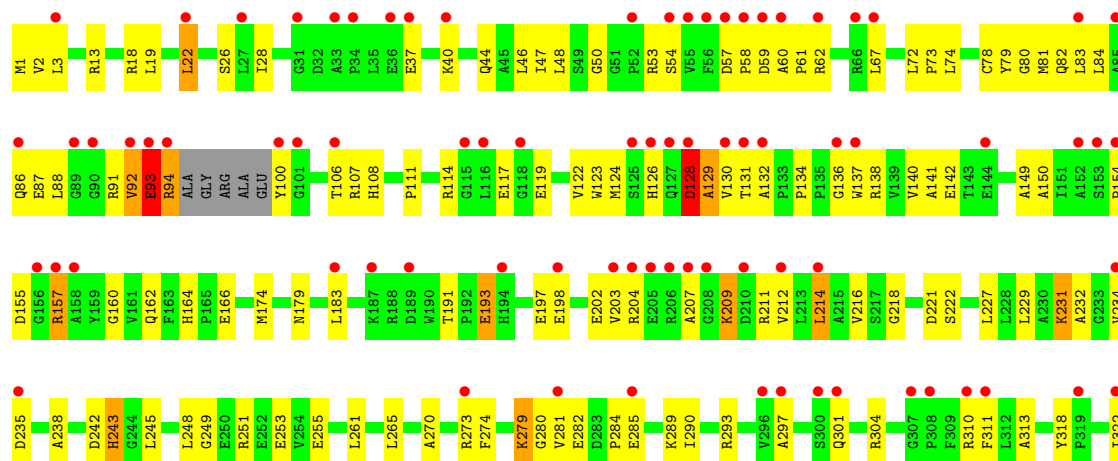


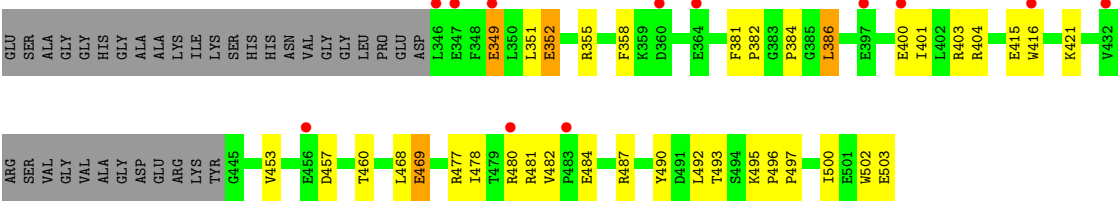


• Molecule 1: GMP synthase [glutamine-hydrolyzing]



• Molecule 1: GMP synthase [glutamine-hydrolyzing]





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.95Å 114.85Å 160.03Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	43.28 – 2.10 43.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (43.28-2.10) 98.2 (43.28-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.272 0.243 , 0.241	Depositor DCC
R_{free} test set	7310 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15065	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.43	0/3795	0.91	7/5146 (0.1%)
1	B	0.40	0/3732	0.91	13/5060 (0.3%)
1	C	0.41	0/3752	0.88	8/5087 (0.2%)
1	D	0.40	0/3735	0.94	17/5064 (0.3%)
All	All	0.41	0/15014	0.91	45/20357 (0.2%)

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	4
1	D	0	3
All	All	0	7

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	GLU	O-C-N	-10.36	111.33	122.94
1	A	127	GLN	O-C-N	9.93	136.21	123.01
1	B	116	LEU	O-C-N	9.04	133.18	122.24
1	A	126	HIS	O-C-N	-7.15	113.56	122.35
1	B	22	LEU	CA-C-N	7.06	132.17	122.07
1	B	22	LEU	C-N-CA	7.06	132.17	122.07
1	D	128	ASP	O-C-N	-7.04	113.23	122.59
1	D	93	GLU	CA-C-N	6.96	134.23	121.70
1	D	93	GLU	C-N-CA	6.96	134.23	121.70
1	D	482	VAL	CA-C-N	6.41	127.85	119.84
1	D	482	VAL	C-N-CA	6.41	127.85	119.84
1	D	457	ASP	CA-C-N	6.27	132.39	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	457	ASP	C-N-CA	6.27	132.39	122.61
1	C	352	GLU	CA-C-N	6.19	125.81	119.56
1	C	352	GLU	C-N-CA	6.19	125.81	119.56
1	B	218	GLY	N-CA-C	-6.19	106.58	114.37
1	D	352	GLU	CA-C-N	6.04	125.66	119.56
1	D	352	GLU	C-N-CA	6.04	125.66	119.56
1	B	153	SER	CA-C-N	6.03	125.74	119.05
1	B	153	SER	C-N-CA	6.03	125.74	119.05
1	A	70	SER	O-C-N	-5.94	115.22	122.05
1	D	265	LEU	N-CA-C	5.88	119.05	109.59
1	D	92	VAL	O-C-N	5.82	129.02	123.03
1	B	265	LEU	N-CA-C	5.74	119.17	109.76
1	D	478	ILE	N-CA-C	5.64	116.42	110.72
1	D	218	GLY	N-CA-C	-5.62	107.28	114.37
1	C	463	TRP	N-CA-C	-5.51	102.24	110.23
1	C	143	THR	N-CA-C	-5.50	101.15	109.85
1	A	128	ASP	O-C-N	-5.48	115.30	122.59
1	B	124	MET	N-CA-C	5.40	118.12	110.50
1	B	146	ASN	CA-C-N	5.37	125.04	119.56
1	B	146	ASN	C-N-CA	5.37	125.04	119.56
1	C	170	THR	N-CA-C	-5.31	97.24	108.39
1	A	352	GLU	CA-C-N	5.27	125.08	119.28
1	A	352	GLU	C-N-CA	5.27	125.08	119.28
1	D	358	PHE	N-CA-C	-5.26	102.73	110.52
1	C	365	LEU	N-CA-C	-5.25	105.64	111.36
1	A	125	SER	N-CA-C	-5.17	101.28	109.76
1	D	129	ALA	CA-C-N	-5.16	115.92	122.43
1	D	129	ALA	C-N-CA	-5.16	115.92	122.43
1	B	6	ASP	N-CA-C	5.13	116.67	108.41
1	C	126	HIS	CA-C-N	5.12	128.82	121.50
1	C	126	HIS	C-N-CA	5.12	128.82	121.50
1	B	170	THR	CA-C-N	5.06	126.17	119.84
1	B	170	THR	C-N-CA	5.06	126.17	119.84

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	23	ARG	Sidechain
1	A	69	SER	Mainchain
1	A	70	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	D	128	ASP	Mainchain
1	D	93	GLU	Peptide,Mainchain

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	3718	0	3787	104	0
1	B	3656	0	3733	133	0
1	C	3676	0	3749	125	0
1	D	3659	0	3739	159	0
2	A	99	0	0	5	0
2	B	101	0	0	8	0
2	C	85	0	0	9	0
2	D	71	0	0	3	0
All	All	15065	0	15008	492	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 17.

All (492) 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:94:ARG:HH11	1:D:94:ARG:HG3	1.15	1.05
1:C:82:GLN:HE22	1:C:128:ASP:HB2	1.15	1.03
1:C:3:LEU:HD21	1:C:29:LEU:HD12	1.41	1.02
1:A:3:LEU:HD11	1:A:29:LEU:HB2	1.44	0.97
1:D:111:PRO:HB2	1:D:183:LEU:HD21	1.47	0.95
1:A:3:LEU:HD21	1:A:29:LEU:HD13	1.47	0.94
1:B:248:LEU:HG	1:B:403:ARG:HG2	1.50	0.91
1:D:46:LEU:HB2	1:D:74:LEU:HD23	1.51	0.91
1:C:82:GLN:NE2	1:C:128:ASP:HB2	1.85	0.90
1:C:62:ARG:HH11	1:C:62:ARG:HB3	1.36	0.90
1:B:17:ARG:HD2	2:B:583:HOH:O	1.72	0.88
1:C:111:PRO:HB2	1:C:183:LEU:HD21	1.58	0.85
1:A:468:LEU:HD21	1:B:468:LEU:HD21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:C	1:A:72:LEU:H	1.85	0.83
1:B:115:GLY:HA2	1:B:117:GLU:OE2	1.79	0.82
1:B:111:PRO:HB2	1:B:183:LEU:CD2	2.09	0.82
1:C:62:ARG:HB3	1:C:62:ARG:NH1	1.95	0.82
1:A:287:LYS:O	1:A:291:ILE:HG12	1.80	0.81
1:D:94:ARG:HG3	1:D:94:ARG:NH1	1.83	0.80
1:C:468:LEU:HD21	1:D:468:LEU:HD21	1.64	0.79
1:A:278:LEU:HD11	1:A:291:ILE:HD11	1.66	0.78
1:C:1:MET:HE1	1:C:3:LEU:HD13	1.65	0.78
1:B:111:PRO:HB2	1:B:183:LEU:HD21	1.67	0.77
1:D:111:PRO:HA	1:D:114:ARG:HG3	1.67	0.76
1:A:242:ASP:OD2	1:A:251:ARG:HD3	1.85	0.76
1:D:82:GLN:HE22	1:D:128:ASP:CB	1.99	0.75
1:A:412:LEU:HD21	1:A:477:ARG:NH1	2.02	0.75
1:D:204:ARG:HG3	1:D:232:ALA:HB1	1.68	0.75
1:A:477:ARG:HG3	1:A:481:ARG:NH1	2.01	0.75
1:D:82:GLN:HE22	1:D:128:ASP:HB2	1.52	0.73
1:B:278:LEU:O	1:B:281:VAL:HG12	1.87	0.73
1:D:243:HIS:HD2	1:D:245:LEU:H	1.36	0.73
1:A:481:ARG:HE	1:C:104:LEU:HD21	1.55	0.72
1:B:401:ILE:HG12	1:B:484:GLU:HG3	1.72	0.72
1:B:179:ASN:O	1:B:183:LEU:HG	1.90	0.71
1:B:214:LEU:HD13	1:B:238:ALA:HA	1.71	0.71
1:C:416:TRP:HH2	1:C:469:GLU:OE1	1.72	0.71
1:A:424:GLN:HE21	1:A:425:ALA:H	1.38	0.71
1:C:207:ALA:HA	1:C:311:PHE:CE2	2.26	0.70
1:A:203:VAL:HG12	1:A:234:VAL:HG11	1.74	0.70
1:B:119:GLU:HG2	1:D:481:ARG:NH1	2.07	0.69
1:A:70:SER:C	1:A:72:LEU:N	2.47	0.69
1:A:216:VAL:HG13	2:A:573:HOH:O	1.94	0.68
1:C:198:GLU:HG3	1:C:201:ARG:NH2	2.08	0.68
1:C:203:VAL:HG12	1:C:234:VAL:HG11	1.76	0.68
1:A:37:GLU:O	1:A:40:LYS:HG2	1.94	0.67
1:C:91:ARG:HH11	1:C:91:ARG:HG2	1.60	0.67
1:C:81:MET:HG3	1:C:160:GLY:HA3	1.77	0.67
1:B:421:LYS:O	1:D:421:LYS:HE3	1.95	0.66
1:B:248:LEU:HG	1:B:403:ARG:CG	2.23	0.66
1:C:193:GLU:HG2	1:C:194:HIS:N	2.09	0.66
1:B:119:GLU:HG2	1:D:481:ARG:CZ	2.26	0.66
1:B:136:GLY:O	1:B:154:PRO:HG3	1.95	0.66
1:D:46:LEU:HB2	1:D:74:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HG3	1:A:201:ARG:HH12	1.61	0.65
1:D:204:ARG:HH21	1:D:232:ALA:HA	1.60	0.65
1:D:242:ASP:OD2	1:D:251:ARG:HD3	1.97	0.65
1:A:71:GLY:O	1:A:157:ARG:HD2	1.97	0.65
1:D:249:GLY:O	1:D:253:GLU:HG3	1.96	0.65
1:C:198:GLU:HG3	1:C:201:ARG:HH22	1.62	0.64
1:D:1:MET:N	1:D:44:GLN:HE21	1.96	0.64
1:A:70:SER:OG	1:A:72:LEU:HB2	1.97	0.64
1:D:141:ALA:HB3	1:D:150:ALA:HB3	1.79	0.64
1:A:91:ARG:HB3	1:A:132:ALA:HB3	1.78	0.64
1:D:212:VAL:HG22	1:D:235:ASP:O	1.97	0.64
1:A:247:ARG:NH1	1:A:406:ASP:OD2	2.31	0.64
1:C:102:LYS:HE2	1:C:169:HIS:HD2	1.62	0.64
1:C:416:TRP:HZ3	2:C:572:HOH:O	1.81	0.64
1:C:316:THR:HG21	1:C:352:GLU:OE2	1.98	0.64
1:D:477:ARG:HD2	1:D:481:ARG:NE	2.12	0.64
1:B:270:ALA:HB1	1:B:273:ARG:HD3	1.80	0.63
1:B:94:ARG:HA	1:B:128:ASP:OD1	1.98	0.63
1:B:46:LEU:CD1	1:B:67:LEU:HD11	2.29	0.63
1:A:17:ARG:O	1:A:21:GLU:HG3	1.99	0.63
1:B:384:PRO:HG3	2:B:555:HOH:O	1.99	0.62
1:A:35:LEU:HD22	1:A:66:ARG:HB2	1.81	0.62
1:B:111:PRO:HB2	1:B:183:LEU:HD22	1.80	0.62
1:D:142:GLU:HA	1:D:149:ALA:CB	2.30	0.62
1:D:204:ARG:HE	1:D:232:ALA:HA	1.63	0.62
1:D:203:VAL:HG11	1:D:229:LEU:HD23	1.80	0.62
1:D:285:GLU:O	1:D:289:LYS:HG3	2.01	0.61
1:A:364:GLU:O	1:A:368:LEU:HD13	2.00	0.61
1:B:93:GLU:CD	1:B:131:THR:HG21	2.26	0.61
1:C:198:GLU:HA	1:C:201:ARG:NH1	2.16	0.60
1:C:53:ARG:HD2	1:C:60:ALA:HA	1.83	0.60
1:D:214:LEU:HD13	1:D:238:ALA:HA	1.84	0.60
1:B:14:LEU:O	1:B:18:ARG:HG2	2.01	0.59
1:D:243:HIS:CD2	1:D:245:LEU:H	2.17	0.59
1:C:144:GLU:HG3	1:C:145:GLU:HG2	1.83	0.59
1:D:248:LEU:HD13	1:D:403:ARG:HG2	1.84	0.59
1:A:490:TYR:HB2	1:B:492:LEU:HD11	1.83	0.59
1:C:109:GLU:CD	1:C:110:GLY:H	2.09	0.59
1:B:240:PHE:HB2	1:B:265:LEU:HD11	1.85	0.59
1:B:37:GLU:HA	1:B:40:LYS:NZ	2.18	0.59
1:B:100:TYR:HB3	1:B:124:MET:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD22	1:D:117:GLU:HB3	1.84	0.59
1:C:416:TRP:CH2	1:C:469:GLU:OE1	2.56	0.59
1:B:119:GLU:HG2	1:D:481:ARG:HD3	1.84	0.58
1:B:78:CYS:SG	1:B:125:SER:HB2	2.43	0.58
1:B:249:GLY:O	1:B:253:GLU:HG3	2.03	0.58
1:C:416:TRP:HE3	2:C:564:HOH:O	1.87	0.58
1:C:460:THR:HG23	1:C:495:LYS:O	2.04	0.58
1:B:104:LEU:HD21	1:D:481:ARG:NH2	2.19	0.58
1:C:141:ALA:HB3	1:C:150:ALA:HB3	1.85	0.58
1:A:373:ASP:OD1	1:C:23:ARG:NH1	2.31	0.58
1:C:3:LEU:HD11	1:C:29:LEU:HG	1.86	0.58
1:B:141:ALA:HB3	1:B:150:ALA:HB3	1.86	0.58
1:D:94:ARG:NH1	1:D:94:ARG:CG	2.61	0.57
1:B:142:GLU:HG2	1:B:147:PRO:O	2.05	0.57
1:C:309:PHE:HB2	1:C:348:PHE:HE1	1.69	0.57
1:C:3:LEU:HD12	1:C:27:LEU:O	2.04	0.57
1:B:115:GLY:CA	1:B:117:GLU:OE2	2.51	0.57
1:C:211:ARG:HB3	1:C:309:PHE:CD1	2.40	0.57
1:D:155:ASP:CG	1:D:157:ARG:HB2	2.30	0.57
1:B:214:LEU:HD13	1:B:214:LEU:O	2.05	0.57
1:C:3:LEU:HD21	1:C:29:LEU:CD1	2.26	0.57
1:D:304:ARG:HB3	1:D:304:ARG:NH1	2.20	0.57
1:A:207:ALA:HA	1:A:311:PHE:CE2	2.40	0.56
1:B:155:ASP:OD2	1:B:157:ARG:HD3	2.04	0.56
1:A:1:MET:HG3	1:A:43:PRO:HA	1.87	0.56
1:C:412:LEU:HG	1:C:470:PHE:CE1	2.40	0.56
1:B:240:PHE:HE2	1:B:254:VAL:HB	1.70	0.56
1:A:35:LEU:HD22	1:A:66:ARG:CB	2.36	0.56
1:A:46:LEU:HD12	1:A:74:LEU:HD21	1.86	0.56
1:B:424:GLN:HE21	1:B:425:ALA:H	1.53	0.56
1:A:304:ARG:HD3	1:A:345:ASP:OD2	2.05	0.56
1:B:211:ARG:HD3	1:B:307:GLY:HA2	1.87	0.56
1:D:53:ARG:HD2	1:D:61:PRO:HD3	1.87	0.56
1:D:136:GLY:O	1:D:154:PRO:HG3	2.05	0.56
1:D:453:VAL:HG21	1:D:500:ILE:HD12	1.88	0.56
1:B:306:ARG:HD3	2:B:568:HOH:O	2.05	0.56
1:D:81:MET:HE3	1:D:130:VAL:CG2	2.36	0.56
1:D:231:LYS:HE3	1:D:231:LYS:HA	1.88	0.55
1:B:18:ARG:HD2	1:B:166:GLU:O	2.06	0.55
1:B:44:GLN:HE22	1:B:187:LYS:HG3	1.70	0.55
1:B:484:GLU:CD	1:B:484:GLU:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:O	1:C:38:VAL:HG13	2.06	0.55
1:A:378:ARG:HB3	1:A:378:ARG:NH1	2.21	0.55
1:B:56:PHE:CZ	1:B:92:VAL:HG23	2.41	0.55
1:C:412:LEU:HG	1:C:470:PHE:HE1	1.72	0.55
1:D:48:LEU:HD11	1:D:74:LEU:HD22	1.89	0.55
1:A:35:LEU:O	1:A:38:VAL:HG22	2.05	0.55
1:D:81:MET:HE1	1:D:162:GLN:HB2	1.88	0.55
1:D:204:ARG:NH2	1:D:232:ALA:HA	2.21	0.55
1:D:207:ALA:HA	1:D:311:PHE:CE2	2.41	0.55
1:D:209:LYS:NZ	1:D:209:LYS:HB3	2.21	0.55
1:A:481:ARG:HD2	2:A:594:HOH:O	2.06	0.55
1:C:111:PRO:HA	1:C:114:ARG:HG3	1.88	0.55
1:D:204:ARG:HE	1:D:232:ALA:CA	2.20	0.55
1:B:481:ARG:HG2	1:B:481:ARG:HH11	1.72	0.55
1:C:481:ARG:HG2	1:C:481:ARG:HH11	1.71	0.55
1:B:284:PRO:HB3	1:B:503:GLU:HB2	1.88	0.55
1:C:243:HIS:CD2	1:C:245:LEU:H	2.25	0.54
1:A:243:HIS:CD2	1:A:245:LEU:H	2.25	0.54
1:B:252:GLU:HG3	2:B:530:HOH:O	2.07	0.54
1:C:412:LEU:HD11	1:C:473:GLU:OE1	2.06	0.54
1:A:209:LYS:HB3	1:A:209:LYS:NZ	2.21	0.54
1:A:309:PHE:HB2	1:A:348:PHE:CE1	2.42	0.54
1:B:394:VAL:HG13	1:B:399:LEU:HD13	1.89	0.54
1:B:460:THR:HG23	1:B:495:LYS:O	2.07	0.54
1:B:34:PRO:HB2	1:B:36:GLU:CD	2.33	0.54
1:B:141:ALA:C	1:B:149:ALA:HB3	2.33	0.54
1:B:379:HIS:HD2	2:B:603:HOH:O	1.89	0.54
1:D:134:PRO:HB2	1:D:137:TRP:CD1	2.43	0.54
1:B:203:VAL:HG21	1:B:229:LEU:HD23	1.89	0.54
1:A:373:ASP:CG	1:C:23:ARG:HH22	2.16	0.54
1:D:108:HIS:HA	1:D:140:VAL:O	2.08	0.54
1:D:81:MET:HG3	1:D:160:GLY:HA3	1.89	0.54
1:B:257:ALA:O	1:B:261:LEU:HD13	2.08	0.53
1:A:378:ARG:HB3	1:A:378:ARG:HH11	1.73	0.53
1:C:153:SER:HB3	1:C:158:ALA:HB3	1.90	0.53
1:C:383:GLY:N	1:C:384:PRO:HD2	2.22	0.53
1:B:143:THR:HG22	1:B:145:GLU:H	1.71	0.53
1:C:73:PRO:HA	1:C:157:ARG:O	2.09	0.53
1:C:272:GLU:CD	1:C:272:GLU:H	2.17	0.53
1:C:306:ARG:HG3	1:C:306:ARG:HH11	1.74	0.53
1:A:68:PHE:HE2	1:A:87:GLU:OE2	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:PRO:HB2	1:B:384:PRO:HD2	1.91	0.53
1:C:293:ARG:CG	1:C:294:GLU:N	2.71	0.53
1:C:287:LYS:HE2	1:C:394:VAL:HG23	1.90	0.53
1:B:214:LEU:HB3	1:B:313:ALA:HB3	1.91	0.52
1:C:1:MET:HE1	1:C:3:LEU:CD1	2.36	0.52
1:A:48:LEU:HD12	1:A:48:LEU:N	2.24	0.52
1:D:111:PRO:CB	1:D:183:LEU:HD21	2.30	0.52
1:D:93:GLU:HB2	1:D:131:THR:OG1	2.09	0.52
1:D:107:ARG:HB2	1:D:142:GLU:HG2	1.91	0.52
1:C:78:CYS:SG	1:C:125:SER:HB2	2.49	0.52
1:C:229:LEU:HD22	1:C:234:VAL:HG21	1.92	0.52
1:D:204:ARG:NE	1:D:232:ALA:HA	2.24	0.52
1:D:281:VAL:HG21	1:D:290:ILE:HD12	1.90	0.52
1:C:420:GLU:HG3	2:C:523:HOH:O	2.08	0.52
1:D:477:ARG:HD2	1:D:481:ARG:CZ	2.39	0.52
1:A:203:VAL:HG11	1:A:229:LEU:HD23	1.92	0.52
1:C:37:GLU:O	1:C:40:LYS:HB3	2.10	0.52
1:D:106:THR:HG22	1:D:142:GLU:O	2.10	0.52
1:B:13:ARG:HG3	1:B:13:ARG:HH11	1.75	0.52
1:C:82:GLN:NE2	1:C:128:ASP:CB	2.68	0.52
1:D:179:ASN:O	1:D:183:LEU:HG	2.10	0.51
1:A:70:SER:O	1:A:72:LEU:N	2.43	0.51
1:C:211:ARG:HD2	1:C:235:ASP:OD1	2.11	0.51
1:A:98:ALA:HB2	1:A:127:GLN:NE2	2.25	0.51
1:A:284:PRO:HB3	1:A:503:GLU:HB2	1.92	0.51
1:C:83:LEU:O	1:C:87:GLU:HG3	2.11	0.51
1:D:157:ARG:HH11	1:D:157:ARG:HG3	1.75	0.51
1:D:141:ALA:HB3	1:D:150:ALA:CB	2.39	0.51
1:D:142:GLU:HA	1:D:149:ALA:HB2	1.91	0.51
1:D:204:ARG:CG	1:D:232:ALA:HB1	2.38	0.51
1:A:492:LEU:HD11	1:B:490:TYR:HB2	1.92	0.51
1:B:119:GLU:OE2	1:D:481:ARG:HD3	2.11	0.51
1:B:248:LEU:HD22	1:D:117:GLU:CB	2.41	0.51
1:D:281:VAL:HG21	1:D:290:ILE:CD1	2.41	0.51
1:D:214:LEU:HB3	1:D:313:ALA:HB3	1.93	0.51
1:C:102:LYS:HG3	1:C:123:TRP:HZ3	1.75	0.51
1:B:55:VAL:HG11	1:B:82:GLN:HB2	1.92	0.50
1:C:391:LEU:HD12	1:C:503:GLU:OE2	2.11	0.50
1:B:18:ARG:HD3	1:B:174:MET:SD	2.50	0.50
1:B:416:TRP:CH2	1:B:469:GLU:OE1	2.64	0.50
1:C:252:GLU:HG3	2:C:574:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HG	1:B:403:ARG:CD	2.41	0.50
1:D:214:LEU:HD22	1:D:214:LEU:C	2.36	0.50
1:D:54:SER:O	1:D:57:ASP:HB3	2.11	0.50
1:D:86:GLN:HG3	1:D:87:GLU:HG2	1.94	0.50
1:B:431:PRO:HA	1:B:446:TYR:CD1	2.47	0.50
1:A:91:ARG:NH1	1:A:91:ARG:HB2	2.27	0.50
1:A:309:PHE:HB2	1:A:348:PHE:HE1	1.75	0.50
1:C:164:HIS:HD2	1:C:166:GLU:OE2	1.95	0.50
1:B:416:TRP:HE3	2:D:551:HOH:O	1.95	0.49
1:C:285:GLU:O	1:C:289:LYS:HG3	2.12	0.49
1:A:282:GLU:OE2	1:A:393:GLU:HB2	2.12	0.49
1:B:73:PRO:HA	1:B:157:ARG:O	2.13	0.49
1:B:78:CYS:O	1:B:82:GLN:HG2	2.11	0.49
1:A:68:PHE:CE2	1:A:87:GLU:OE2	2.66	0.49
2:B:594:HOH:O	1:D:416:TRP:HE3	1.95	0.49
1:C:300:SER:O	1:C:303:ALA:HB3	2.12	0.49
1:B:54:SER:C	1:B:56:PHE:H	2.20	0.49
1:B:93:GLU:OE2	1:B:131:THR:HG21	2.13	0.49
1:B:401:ILE:CG1	1:B:484:GLU:HG3	2.42	0.49
1:D:73:PRO:HG3	1:D:157:ARG:NH1	2.28	0.49
1:D:214:LEU:HD13	1:D:214:LEU:O	2.12	0.49
1:C:189:ASP:HB2	2:C:520:HOH:O	2.11	0.49
1:C:272:GLU:CD	1:C:272:GLU:N	2.71	0.49
1:D:270:ALA:O	1:D:274:PHE:HD2	1.95	0.49
1:D:304:ARG:HB3	1:D:304:ARG:HH11	1.76	0.49
1:C:3:LEU:HB3	1:C:46:LEU:HD23	1.94	0.49
1:D:13:ARG:HD2	2:D:509:HOH:O	2.12	0.49
1:B:482:VAL:HG12	1:B:484:GLU:HG2	1.94	0.49
1:D:381:PHE:HZ	1:D:386:LEU:HD13	1.78	0.49
1:C:93:GLU:CD	1:C:131:THR:HG21	2.38	0.49
1:A:5:LEU:CD1	1:A:67:LEU:HD21	2.43	0.48
1:B:62:ARG:HH12	1:B:86:GLN:NE2	2.11	0.48
1:B:204:ARG:HH21	1:B:232:ALA:HA	1.77	0.48
1:B:270:ALA:CB	1:B:273:ARG:HD3	2.42	0.48
1:D:142:GLU:HA	1:D:149:ALA:HB3	1.95	0.48
1:C:35:LEU:HD22	1:C:66:ARG:HB2	1.96	0.48
1:C:46:LEU:HD12	1:C:74:LEU:HD21	1.95	0.48
1:D:1:MET:H3	1:D:44:GLN:HE21	1.59	0.48
1:D:18:ARG:O	1:D:22:LEU:HD22	2.12	0.48
1:B:307:GLY:HA3	1:B:308:PRO:C	2.38	0.48
1:C:460:THR:HG22	1:C:461:ALA:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLY:O	1:D:84:LEU:HD13	2.14	0.48
1:B:162:GLN:O	1:B:162:GLN:HG3	2.14	0.48
1:C:105:LEU:HD12	1:C:120:VAL:HG11	1.94	0.48
1:A:285:GLU:O	1:A:289:LYS:HG2	2.14	0.48
1:A:141:ALA:HB3	1:A:150:ALA:HB3	1.95	0.48
1:B:108:HIS:HA	1:B:140:VAL:O	2.13	0.48
1:D:94:ARG:HH11	1:D:94:ARG:CG	2.00	0.48
1:A:399:LEU:O	1:A:403:ARG:HG3	2.14	0.48
1:B:19:LEU:HD11	1:B:47:ILE:HD12	1.96	0.48
1:D:198:GLU:HG3	1:D:202:GLU:OE2	2.14	0.48
1:D:400:GLU:O	1:D:404:ARG:HG3	2.14	0.48
1:C:5:LEU:HB3	1:C:31:GLY:HA2	1.96	0.47
1:D:304:ARG:HH11	1:D:304:ARG:CB	2.27	0.47
1:A:84:LEU:HD12	1:A:88:LEU:HD12	1.95	0.47
1:B:55:VAL:HG11	1:B:82:GLN:CB	2.45	0.47
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.24	0.47
1:B:372:PRO:HB2	1:D:22:LEU:HD12	1.95	0.47
1:A:55:VAL:HG21	1:A:82:GLN:HB3	1.97	0.47
1:A:239:VAL:HG21	1:A:302:VAL:HG11	1.96	0.47
1:A:391:LEU:HD13	1:A:428:VAL:CG1	2.44	0.47
1:B:460:THR:HG22	1:B:461:ALA:N	2.29	0.47
1:D:301:GLN:HA	1:D:304:ARG:HH12	1.80	0.47
1:A:179:ASN:O	1:A:183:LEU:HG	2.14	0.47
1:C:243:HIS:HD2	1:C:245:LEU:H	1.62	0.47
1:D:480:ARG:HG3	1:D:480:ARG:HH11	1.79	0.47
1:C:351:LEU:HD22	1:C:353:PRO:HG3	1.97	0.47
1:D:91:ARG:HB3	1:D:132:ALA:HB3	1.96	0.47
1:D:310:ARG:HH11	1:D:310:ARG:HG2	1.79	0.47
1:C:5:LEU:HD21	1:C:46:LEU:HD22	1.97	0.47
1:C:290:ILE:O	1:C:293:ARG:HG2	2.14	0.47
1:D:22:LEU:HD22	1:D:174:MET:HE3	1.95	0.47
1:D:81:MET:HE3	1:D:130:VAL:HG21	1.96	0.47
1:C:309:PHE:HB2	1:C:348:PHE:CE1	2.49	0.47
1:D:82:GLN:NE2	1:D:128:ASP:HB2	2.27	0.47
1:D:164:HIS:HD2	1:D:166:GLU:OE2	1.98	0.47
1:D:279:LYS:HD2	1:D:280:GLY:N	2.30	0.47
1:C:72:LEU:O	1:C:74:LEU:HG	2.15	0.47
1:C:109:GLU:CG	1:C:110:GLY:N	2.78	0.46
1:D:92:VAL:HG23	1:D:129:ALA:O	2.15	0.46
1:A:198:GLU:O	1:A:202:GLU:HG3	2.15	0.46
1:C:203:VAL:HG11	1:C:229:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LYS:O	1:B:275:LEU:HD23	2.15	0.46
1:D:1:MET:HE1	1:D:3:LEU:HG	1.96	0.46
1:D:37:GLU:O	1:D:40:LYS:HG2	2.15	0.46
1:A:293:ARG:O	1:A:296:VAL:HG22	2.16	0.46
1:B:22:LEU:HD21	1:B:174:MET:HE3	1.97	0.46
1:A:53:ARG:HD3	1:A:59:ASP:O	2.16	0.46
1:A:424:GLN:HE21	1:A:425:ALA:N	2.09	0.46
1:B:2:VAL:O	1:B:26:SER:HA	2.16	0.46
1:B:251:ARG:HD2	1:B:255:GLU:OE2	2.16	0.46
1:D:48:LEU:HD12	1:D:48:LEU:N	2.31	0.46
1:A:420:GLU:HG2	2:A:596:HOH:O	2.15	0.46
1:D:62:ARG:NH2	1:D:86:GLN:HE22	2.13	0.46
1:D:141:ALA:C	1:D:149:ALA:HB3	2.40	0.46
1:B:37:GLU:HA	1:B:40:LYS:HZ3	1.81	0.46
1:C:46:LEU:HD12	1:C:74:LEU:CD2	2.46	0.46
1:C:316:THR:OG1	1:C:352:GLU:HB3	2.16	0.46
1:A:412:LEU:O	1:A:416:TRP:HD1	1.99	0.46
1:B:243:HIS:CD2	1:B:245:LEU:H	2.34	0.46
1:C:35:LEU:O	1:C:39:LEU:HG	2.16	0.46
1:C:247:ARG:HD3	2:C:550:HOH:O	2.15	0.46
1:D:58:PRO:C	1:D:60:ALA:H	2.24	0.46
1:B:3:LEU:HD11	1:B:29:LEU:CD1	2.46	0.46
1:C:78:CYS:O	1:C:79:TYR:C	2.59	0.45
1:B:81:MET:HE2	1:B:162:GLN:NE2	2.31	0.45
1:A:416:TRP:CH2	1:A:469:GLU:OE1	2.70	0.45
1:C:93:GLU:OE1	1:C:131:THR:HG21	2.16	0.45
1:A:46:LEU:HB2	1:A:74:LEU:HD23	1.99	0.45
1:A:469:GLU:HG3	1:D:469:GLU:HG3	1.98	0.45
1:B:391:LEU:HD13	1:B:428:VAL:CG1	2.46	0.45
1:D:310:ARG:HG3	1:D:311:PHE:CD2	2.51	0.45
1:A:78:CYS:O	1:A:82:GLN:HG3	2.17	0.45
1:C:293:ARG:HG3	1:C:294:GLU:N	2.31	0.45
1:D:18:ARG:HA	1:D:174:MET:HE1	1.99	0.45
1:C:432:VAL:HG12	1:C:445:GLY:C	2.42	0.45
1:A:46:LEU:HD12	1:A:74:LEU:CD2	2.47	0.45
1:D:28:ILE:HD12	1:D:322:ILE:HD13	1.98	0.45
1:D:83:LEU:O	1:D:87:GLU:HG3	2.16	0.45
1:B:399:LEU:O	1:B:403:ARG:HB2	2.17	0.45
1:C:100:TYR:HB3	1:C:124:MET:O	2.16	0.45
1:C:318:TYR:HA	1:C:355:ARG:O	2.16	0.45
1:D:46:LEU:HD13	1:D:67:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:HE22	1:A:128:ASP:HB2	1.81	0.45
1:A:253:GLU:HG2	1:C:175:GLN:CD	2.42	0.45
1:C:404:ARG:NH2	1:C:481:ARG:O	2.50	0.45
1:C:481:ARG:HD2	2:C:563:HOH:O	2.17	0.45
1:D:2:VAL:O	1:D:26:SER:HA	2.16	0.45
1:D:78:CYS:O	1:D:82:GLN:HG3	2.17	0.45
1:D:203:VAL:HG12	1:D:234:VAL:HG21	1.99	0.45
1:D:460:THR:HG23	1:D:495:LYS:O	2.16	0.45
1:D:212:VAL:HG12	1:D:311:PHE:HB2	1.99	0.44
1:B:211:ARG:HG3	1:B:235:ASP:OD2	2.17	0.44
1:B:17:ARG:CD	2:B:583:HOH:O	2.48	0.44
1:B:169:HIS:C	1:B:171:PRO:HD3	2.42	0.44
1:B:193:GLU:HG2	1:B:194:HIS:CD2	2.52	0.44
1:B:211:ARG:HG3	1:B:211:ARG:HH11	1.80	0.44
1:B:245:LEU:HD23	1:B:399:LEU:HD21	1.99	0.44
1:B:318:TYR:HA	1:B:355:ARG:O	2.17	0.44
1:A:84:LEU:HD13	1:A:84:LEU:HA	1.80	0.44
1:C:306:ARG:HG3	1:C:306:ARG:NH1	2.32	0.44
1:A:53:ARG:NH1	1:A:59:ASP:O	2.50	0.44
1:A:82:GLN:NE2	1:A:128:ASP:HB2	2.32	0.44
1:D:86:GLN:HG3	1:D:87:GLU:CG	2.47	0.44
1:D:293:ARG:HG3	1:D:293:ARG:HH11	1.82	0.44
1:A:28:ILE:O	1:A:29:LEU:HD12	2.18	0.44
1:A:122:VAL:HG23	1:A:124:MET:HG2	1.99	0.44
1:B:193:GLU:HG2	1:B:194:HIS:N	2.32	0.44
1:B:214:LEU:CD1	1:B:238:ALA:HA	2.42	0.44
1:B:134:PRO:HB2	1:B:137:TRP:CD1	2.53	0.44
1:C:492:LEU:HD11	1:D:490:TYR:HB2	2.00	0.44
1:D:401:ILE:HD11	1:D:484:GLU:HG2	2.00	0.44
1:A:167:VAL:HG22	2:A:576:HOH:O	2.17	0.44
1:D:46:LEU:HD11	1:D:72:LEU:HD12	2.00	0.44
1:C:199:LEU:O	1:C:203:VAL:HG23	2.18	0.43
1:D:82:GLN:NE2	1:D:128:ASP:CB	2.75	0.43
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.88	0.43
1:A:313:ALA:HA	1:A:351:LEU:O	2.18	0.43
1:C:46:LEU:HB2	1:C:74:LEU:CD2	2.47	0.43
1:D:138:ARG:HH11	1:D:138:ARG:HG3	1.83	0.43
1:D:50:GLY:HA2	1:D:79:TYR:HB3	2.00	0.43
1:D:496:PRO:HB2	1:D:497:PRO:HA	2.00	0.43
1:A:251:ARG:NH1	1:A:255:GLU:OE2	2.51	0.43
1:A:487:ARG:HD3	1:B:502:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ALA:O	1:B:274:PHE:HD2	2.01	0.43
1:D:58:PRO:HG2	1:D:59:ASP:H	1.82	0.43
1:A:229:LEU:HD22	1:A:234:VAL:HG21	2.00	0.43
1:C:91:ARG:CG	1:C:91:ARG:NH1	2.82	0.43
1:C:198:GLU:HA	1:C:201:ARG:CZ	2.48	0.43
1:D:94:ARG:NH2	1:D:126:HIS:O	2.52	0.43
1:B:381:PHE:CE2	1:B:385:GLY:HA2	2.52	0.43
1:B:481:ARG:NE	1:D:119:GLU:OE1	2.52	0.43
1:C:157:ARG:NH1	1:C:157:ARG:HG2	2.34	0.43
1:C:216:VAL:HA	1:C:222:SER:HB2	2.00	0.43
1:B:71:GLY:O	1:B:157:ARG:NH2	2.44	0.43
1:B:119:GLU:HG2	1:D:481:ARG:CD	2.48	0.43
1:D:138:ARG:HG3	1:D:138:ARG:NH1	2.33	0.43
1:B:107:ARG:O	1:B:141:ALA:HA	2.17	0.43
1:C:100:TYR:HB2	1:C:123:TRP:CE2	2.53	0.43
1:D:162:GLN:O	1:D:162:GLN:HG3	2.18	0.43
1:A:416:TRP:HE3	2:A:581:HOH:O	2.01	0.43
1:C:487:ARG:HD3	1:D:502:TRP:CE2	2.54	0.43
1:A:383:GLY:N	1:A:384:PRO:HD2	2.33	0.43
1:B:114:ARG:HH21	1:D:255:GLU:HG3	1.83	0.43
1:B:243:HIS:HE1	1:B:383:GLY:O	2.02	0.43
1:C:19:LEU:HD23	1:C:26:SER:HB3	2.01	0.43
1:C:304:ARG:O	1:C:305:GLU:HG3	2.19	0.43
1:D:100:TYR:HB2	1:D:123:TRP:CZ2	2.54	0.43
1:A:429:LEU:HD11	1:A:446:TYR:HB3	2.01	0.42
1:B:37:GLU:HA	1:B:40:LYS:HZ2	1.84	0.42
1:B:87:GLU:O	1:B:88:LEU:HD23	2.19	0.42
1:A:18:ARG:HD2	1:A:174:MET:SD	2.59	0.42
1:A:35:LEU:O	1:A:39:LEU:HG	2.20	0.42
1:A:64:ASP:O	1:A:67:LEU:HB2	2.20	0.42
1:A:199:LEU:O	1:A:203:VAL:HG23	2.19	0.42
1:A:34:PRO:HG2	1:A:37:GLU:HB3	2.01	0.42
1:D:155:ASP:OD2	1:D:157:ARG:HB2	2.18	0.42
1:C:9:SER:HB2	1:C:50:GLY:C	2.45	0.42
1:D:46:LEU:HD12	1:D:74:LEU:HD21	2.02	0.42
1:A:64:ASP:O	1:A:65:PRO:C	2.61	0.42
1:A:91:ARG:CB	1:A:132:ALA:HB3	2.49	0.42
1:C:252:GLU:HA	1:C:255:GLU:OE2	2.19	0.42
1:D:216:VAL:HA	1:D:222:SER:HB2	2.01	0.42
1:A:477:ARG:O	1:A:481:ARG:HG2	2.20	0.42
1:B:212:VAL:HG22	1:B:311:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:HB2	1:C:74:LEU:HD22	2.02	0.42
1:C:146:ASN:HA	1:C:147:PRO:HD2	1.94	0.42
1:D:279:LYS:HD2	1:D:279:LYS:C	2.44	0.42
1:A:162:GLN:HG3	1:A:162:GLN:O	2.20	0.42
1:A:502:TRP:CZ2	1:B:487:ARG:HD3	2.55	0.42
1:C:239:VAL:HB	1:C:299:PHE:HE1	1.84	0.42
1:D:221:ASP:HB2	2:D:518:HOH:O	2.20	0.42
1:B:289:LYS:O	1:B:293:ARG:HG3	2.18	0.42
1:D:352:GLU:HG3	1:D:355:ARG:HD2	2.02	0.42
1:C:249:GLY:HA2	2:C:574:HOH:O	2.20	0.41
1:D:284:PRO:HB3	1:D:503:GLU:HB2	2.00	0.41
1:A:46:LEU:HB2	1:A:74:LEU:CD2	2.50	0.41
1:C:383:GLY:N	1:C:384:PRO:CD	2.84	0.41
1:C:468:LEU:HD21	1:D:468:LEU:CD2	2.44	0.41
1:D:122:VAL:HG23	1:D:124:MET:HG2	2.01	0.41
1:D:301:GLN:HA	1:D:304:ARG:NH1	2.34	0.41
1:B:155:ASP:OD2	1:B:157:ARG:HB2	2.20	0.41
1:B:283:ASP:HB3	1:B:286:GLU:HB2	2.01	0.41
1:C:481:ARG:HG2	1:C:481:ARG:NH1	2.35	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.86	0.41
1:C:109:GLU:HG3	1:C:110:GLY:N	2.35	0.41
1:D:1:MET:SD	1:D:1:MET:C	3.04	0.41
1:D:57:ASP:HB3	1:D:60:ALA:HB2	2.02	0.41
1:D:193:GLU:O	1:D:197:GLU:HG3	2.20	0.41
1:D:313:ALA:HA	1:D:351:LEU:O	2.20	0.41
1:B:367:LEU:HB2	1:B:376:ARG:NE	2.35	0.41
1:D:78:CYS:O	1:D:79:TYR:C	2.64	0.41
1:D:477:ARG:HH11	1:D:481:ARG:NH2	2.19	0.41
1:B:81:MET:HG3	1:B:160:GLY:HA3	2.02	0.41
1:B:383:GLY:N	1:B:384:PRO:CD	2.82	0.41
1:C:432:VAL:HG12	1:C:446:TYR:N	2.34	0.41
1:D:57:ASP:CG	1:D:58:PRO:HD2	2.45	0.41
1:C:33:ALA:HA	1:C:34:PRO:HD3	1.90	0.41
1:D:211:ARG:HD2	1:D:235:ASP:OD1	2.19	0.41
1:A:79:TYR:CE2	1:A:83:LEU:HD11	2.56	0.41
1:A:94:ARG:NH1	1:A:94:ARG:HG2	2.36	0.41
1:A:107:ARG:O	1:A:141:ALA:HA	2.21	0.41
1:B:9:SER:HB2	1:B:50:GLY:C	2.46	0.41
1:B:54:SER:C	1:B:56:PHE:N	2.79	0.41
1:B:290:ILE:HA	1:B:293:ARG:NH1	2.35	0.41
1:C:2:VAL:O	1:C:26:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ARG:NH1	2:C:541:HOH:O	2.54	0.41
1:A:243:HIS:HD2	1:A:245:LEU:H	1.67	0.41
1:B:141:ALA:HB3	1:B:150:ALA:CB	2.51	0.41
1:B:240:PHE:C	1:B:240:PHE:CD1	2.99	0.41
1:D:84:LEU:O	1:D:88:LEU:HB2	2.21	0.41
1:D:137:TRP:CD1	1:D:154:PRO:HD3	2.56	0.41
1:D:349:GLU:OE1	1:D:349:GLU:HA	2.21	0.41
1:C:426:LEU:HD12	1:C:426:LEU:C	2.46	0.40
1:D:209:LYS:HB3	1:D:209:LYS:HZ2	1.86	0.40
1:D:382:PRO:HB2	1:D:384:PRO:HD2	2.03	0.40
1:A:239:VAL:CG2	1:A:302:VAL:HG11	2.51	0.40
1:B:309:PHE:HB2	1:B:348:PHE:CE1	2.56	0.40
1:B:481:ARG:CD	1:D:119:GLU:OE1	2.70	0.40
1:C:1:MET:C	1:C:1:MET:SD	3.04	0.40
1:D:191:THR:HB	1:D:193:GLU:OE1	2.21	0.40
1:A:142:GLU:HA	1:A:149:ALA:CB	2.51	0.40
1:B:376:ARG:NH1	1:B:377:LEU:HD21	2.36	0.40
1:B:460:THR:CG2	1:B:461:ALA:N	2.83	0.40
1:C:227:LEU:HD21	1:C:261:LEU:HD13	2.04	0.40
1:B:172:LYS:HA	2:B:528:HOH:O	2.20	0.40
1:D:318:TYR:HA	1:D:355:ARG:O	2.21	0.40
1:A:192:PRO:HG3	1:C:367:LEU:HD22	2.04	0.40
1:B:102:LYS:HE2	1:D:415:GLU:OE2	2.21	0.40
1:C:35:LEU:HA	1:C:38:VAL:CG1	2.52	0.40
1:D:19:LEU:HD11	1:D:47:ILE:HD12	2.02	0.40
1:D:60:ALA:HA	1:D:61:PRO:HD3	1.90	0.40
1:D:82:GLN:HE22	1:D:128:ASP:HB3	1.82	0.40
1:D:273:ARG:HH22	1:D:297:ALA:HB1	1.86	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	463/503 (92%)	445 (96%)	17 (4%)	1 (0%)	43	44
1	B	455/503 (90%)	441 (97%)	13 (3%)	1 (0%)	43	44
1	C	458/503 (91%)	441 (96%)	16 (4%)	1 (0%)	43	44
1	D	455/503 (90%)	438 (96%)	17 (4%)	0	100	100
All	All	1831/2012 (91%)	1765 (96%)	63 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLY
1	C	305	GLU
1	B	87	GLU

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	389/409 (95%)	375 (96%)	14 (4%)	31	34
1	B	382/409 (93%)	372 (97%)	10 (3%)	40	46
1	C	384/409 (94%)	372 (97%)	12 (3%)	35	39
1	D	383/409 (94%)	364 (95%)	19 (5%)	22	22
All	All	1538/1636 (94%)	1483 (96%)	55 (4%)	31	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	55	VAL
1	A	84	LEU
1	A	109	GLU
1	A	138	ARG
1	A	144	GLU
1	A	145	GLU
1	A	178	GLU

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Mol	Chain	Res	Type
1	A	187	LYS
1	A	209	LYS
1	A	234	VAL
1	A	243	HIS
1	A	263	VAL
1	A	266	LEU
1	B	13	ARG
1	B	14	LEU
1	B	18	ARG
1	B	74	LEU
1	B	117	GLU
1	B	119	GLU
1	B	214	LEU
1	B	399	LEU
1	B	456	GLU
1	B	484	GLU
1	C	19	LEU
1	C	27	LEU
1	C	36	GLU
1	C	38	VAL
1	C	62	ARG
1	C	227	LEU
1	C	243	HIS
1	C	272	GLU
1	C	347	GLU
1	C	410	THR
1	C	420	GLU
1	C	493	THR
1	D	22	LEU
1	D	93	GLU
1	D	94	ARG
1	D	157	ARG
1	D	193	GLU
1	D	209	LYS
1	D	214	LEU
1	D	227	LEU
1	D	231	LYS
1	D	243	HIS
1	D	261	LEU
1	D	279	LYS
1	D	282	GLU
1	D	349	GLU

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Mol	Chain	Res	Type
1	D	386	LEU
1	D	469	GLU
1	D	487	ARG
1	D	492	LEU
1	D	493	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	108	HIS
1	A	121	GLN
1	A	127	GLN
1	A	179	ASN
1	A	243	HIS
1	A	314	GLN
1	A	424	GLN
1	B	41	HIS
1	B	86	GLN
1	B	121	GLN
1	B	126	HIS
1	B	162	GLN
1	B	243	HIS
1	B	264	ASN
1	B	379	HIS
1	B	424	GLN
1	C	41	HIS
1	C	44	GLN
1	C	82	GLN
1	C	164	HIS
1	C	169	HIS
1	C	243	HIS
1	D	10	GLN
1	D	44	GLN
1	D	82	GLN
1	D	164	HIS
1	D	243	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	471/503 (93%)	0.87	72 (15%) 5 5	23, 41, 83, 109	0
1	B	463/503 (92%)	0.91	70 (15%) 5 5	24, 46, 78, 96	0
1	C	466/503 (92%)	0.97	89 (19%) 3 3	21, 45, 82, 113	0
1	D	463/503 (92%)	1.14	91 (19%) 3 3	23, 48, 86, 112	0
All	All	1863/2012 (92%)	0.97	322 (17%) 4 4	21, 45, 82, 113	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	SER	6.7
1	C	95	ALA	6.5
1	A	38	VAL	5.7
1	D	204	ARG	5.5
1	A	416	TRP	5.5
1	D	194	HIS	5.5
1	C	125	SER	5.0
1	D	55	VAL	5.0
1	A	33	ALA	4.7
1	D	58	PRO	4.6
1	A	39	LEU	4.5
1	B	95	ALA	4.5
1	C	100	TYR	4.3
1	A	71	GLY	4.3
1	C	445	GLY	4.2
1	D	56	PHE	4.2
1	C	325	ALA	4.2
1	A	458	PHE	4.2
1	A	296	VAL	4.1
1	C	60	ALA	4.1
1	A	35	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	432	VAL	4.1
1	D	94	ARG	4.0
1	C	308	PRO	4.0
1	D	57	ASP	4.0
1	B	125	SER	4.0
1	A	445	GLY	4.0
1	A	41	HIS	4.0
1	D	54	SER	4.0
1	B	58	PRO	4.0
1	D	127	GLN	3.9
1	B	307	GLY	3.9
1	D	346	LEU	3.9
1	D	100	TYR	3.9
1	A	70	SER	3.9
1	D	157	ARG	3.9
1	A	126	HIS	3.8
1	C	432	VAL	3.8
1	B	127	GLN	3.8
1	D	125	SER	3.8
1	B	445	GLY	3.8
1	D	235	ASP	3.7
1	B	483	PRO	3.7
1	D	34	PRO	3.7
1	B	117	GLU	3.7
1	D	300	SER	3.7
1	B	183	LEU	3.6
1	B	308	PRO	3.6
1	A	59	ASP	3.6
1	B	118	GLY	3.6
1	C	71	GLY	3.6
1	A	36	GLU	3.5
1	B	275	LEU	3.5
1	A	125	SER	3.5
1	D	206	ARG	3.5
1	B	56	PHE	3.5
1	B	60	ALA	3.5
1	C	58	PRO	3.5
1	D	183	LEU	3.5
1	D	189	ASP	3.5
1	B	194	HIS	3.5
1	D	432	VAL	3.5
1	D	416	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	311	PHE	3.4
1	A	459	MET	3.4
1	B	100	TYR	3.4
1	D	126	HIS	3.4
1	D	131	THR	3.4
1	A	60	ALA	3.4
1	C	205	GLU	3.4
1	D	456	GLU	3.4
1	B	273	ARG	3.4
1	A	198	GLU	3.4
1	C	323	GLU	3.4
1	D	308	PRO	3.4
1	D	207	ALA	3.4
1	D	22	LEU	3.4
1	D	144	GLU	3.3
1	A	86	GLN	3.3
1	B	293	ARG	3.3
1	A	64	ASP	3.2
1	C	128	ASP	3.2
1	D	128	ASP	3.2
1	C	307	GLY	3.2
1	B	416	TRP	3.2
1	C	293	ARG	3.2
1	A	344	GLU	3.2
1	B	205	GLU	3.2
1	C	144	GLU	3.2
1	A	55	VAL	3.2
1	B	129	ALA	3.2
1	A	29	LEU	3.2
1	D	89	GLY	3.2
1	C	296	VAL	3.1
1	A	3	LEU	3.1
1	D	285	GLU	3.1
1	A	68	PHE	3.1
1	B	432	VAL	3.1
1	D	158	ALA	3.1
1	C	273	ARG	3.1
1	D	137	TRP	3.1
1	C	70	SER	3.1
1	D	198	GLU	3.1
1	C	126	HIS	3.1
1	D	93	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	212	VAL	3.1
1	B	116	LEU	3.1
1	D	322	ILE	3.1
1	A	323	GLU	3.0
1	C	347	GLU	3.0
1	C	33	ALA	3.0
1	A	1	MET	3.0
1	C	157	ARG	3.0
1	D	273	ARG	3.0
1	A	431	PRO	3.0
1	B	207	ALA	3.0
1	D	31	GLY	3.0
1	D	90	GLY	3.0
1	C	145	GLU	3.0
1	A	58	PRO	3.0
1	D	86	GLN	3.0
1	D	301	GLN	3.0
1	A	186	VAL	3.0
1	C	55	VAL	3.0
1	D	92	VAL	3.0
1	D	234	VAL	3.0
1	C	134	PRO	3.0
1	A	100	TYR	3.0
1	B	68	PHE	3.0
1	B	206	ARG	2.9
1	B	393	GLU	2.9
1	C	40	LYS	2.9
1	C	247	ARG	2.9
1	A	346	LEU	2.9
1	B	86	GLN	2.9
1	D	480	ARG	2.9
1	A	31	GLY	2.9
1	A	88	LEU	2.9
1	D	136	GLY	2.9
1	C	460	THR	2.9
1	D	106	THR	2.9
1	A	65	PRO	2.9
1	A	194	HIS	2.9
1	D	115	GLY	2.9
1	A	205	GLU	2.8
1	A	456	GLU	2.8
1	B	297	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	397	GLU	2.8
1	A	34	PRO	2.8
1	A	66	ARG	2.8
1	C	198	GLU	2.8
1	B	46	LEU	2.8
1	C	480	ARG	2.7
1	A	99	GLU	2.7
1	C	209	LYS	2.7
1	C	34	PRO	2.7
1	C	206	ARG	2.7
1	B	55	VAL	2.7
1	C	38	VAL	2.7
1	A	189	ASP	2.7
1	B	189	ASP	2.7
1	A	341	GLY	2.7
1	C	86	GLN	2.7
1	C	109	GLU	2.7
1	D	400	GLU	2.7
1	D	210	ASP	2.7
1	C	127	GLN	2.7
1	B	197	GLU	2.7
1	B	53	ARG	2.7
1	A	43	PRO	2.6
1	C	483	PRO	2.6
1	C	289	LYS	2.6
1	A	23	ARG	2.6
1	B	460	THR	2.6
1	C	360	ASP	2.6
1	D	59	ASP	2.6
1	B	91	ARG	2.6
1	C	82	GLN	2.6
1	A	84	LEU	2.6
1	B	271	LYS	2.6
1	C	135	PRO	2.6
1	C	283	ASP	2.6
1	D	360	ASP	2.6
1	D	130	VAL	2.6
1	D	203	VAL	2.6
1	A	178	GLU	2.6
1	A	27	LEU	2.6
1	C	309	PHE	2.5
1	B	279	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	300	SER	2.5
1	C	183	LEU	2.5
1	C	416	TRP	2.5
1	D	296	VAL	2.5
1	D	483	PRO	2.5
1	B	185	GLY	2.5
1	C	234	VAL	2.5
1	D	154	PRO	2.5
1	A	83	LEU	2.5
1	C	69	SER	2.4
1	D	85	ALA	2.4
1	D	297	ALA	2.4
1	C	266	LEU	2.4
1	C	276	LYS	2.4
1	C	189	ASP	2.4
1	B	69	SER	2.4
1	B	265	LEU	2.4
1	B	347	GLU	2.4
1	D	347	GLU	2.4
1	B	281	VAL	2.4
1	D	153	SER	2.4
1	A	40	LYS	2.4
1	C	61	PRO	2.4
1	C	272	GLU	2.4
1	C	194	HIS	2.4
1	B	158	ALA	2.3
1	D	205	GLU	2.3
1	D	83	LEU	2.3
1	C	292	GLY	2.3
1	C	155	ASP	2.3
1	D	62	ARG	2.3
1	B	267	VAL	2.3
1	C	316	THR	2.3
1	C	93	GLU	2.3
1	D	319	PRO	2.3
1	A	72	LEU	2.3
1	B	74	LEU	2.3
1	D	214	LEU	2.3
1	B	322	ILE	2.3
1	A	92	VAL	2.3
1	B	92	VAL	2.3
1	B	135	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	65	PRO	2.3
1	A	98	ALA	2.3
1	A	188	ARG	2.3
1	D	208	GLY	2.3
1	D	40	LYS	2.3
1	D	36	GLU	2.3
1	C	302	VAL	2.3
1	C	91	ARG	2.3
1	C	156	GLY	2.3
1	D	187	LYS	2.3
1	C	214	LEU	2.3
1	C	484	GLU	2.2
1	B	120	VAL	2.2
1	A	53	ARG	2.2
1	B	85	ALA	2.2
1	B	230	ALA	2.2
1	C	136	GLY	2.2
1	D	118	GLY	2.2
1	C	39	LEU	2.2
1	C	84	LEU	2.2
1	B	301	GLN	2.2
1	B	62	ARG	2.2
1	D	66	ARG	2.2
1	D	281	VAL	2.2
1	C	57	ASP	2.2
1	D	156	GLY	2.2
1	C	207	ALA	2.2
1	D	60	ALA	2.2
1	D	349	GLU	2.2
1	C	74	LEU	2.2
1	A	42	ARG	2.2
1	C	187	LYS	2.2
1	A	322	ILE	2.2
1	B	210	ASP	2.2
1	A	282	GLU	2.2
1	B	285	GLU	2.2
1	C	233	GLY	2.2
1	D	364	GLU	2.2
1	C	215	ALA	2.2
1	D	33	ALA	2.2
1	C	72	LEU	2.2
1	C	235	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	52	PRO	2.1
1	C	37	GLU	2.1
1	C	68	PHE	2.1
1	A	44	GLN	2.1
1	D	101	GLY	2.1
1	D	132	ALA	2.1
1	A	273	ARG	2.1
1	B	94	ARG	2.1
1	C	275	LEU	2.1
1	A	216	VAL	2.1
1	B	268	VAL	2.1
1	D	307	GLY	2.1
1	C	306	ARG	2.1
1	B	257	ALA	2.1
1	A	187	LYS	2.1
1	C	35	LEU	2.1
1	D	67	LEU	2.1
1	B	457	ASP	2.1
1	B	431	PRO	2.1
1	C	431	PRO	2.1
1	A	91	ARG	2.1
1	D	310	ARG	2.1
1	A	56	PHE	2.1
1	A	203	VAL	2.1
1	C	281	VAL	2.1
1	A	260	ALA	2.1
1	B	412	LEU	2.1
1	D	3	LEU	2.1
1	D	116	LEU	2.1
1	B	202	GLU	2.1
1	C	202	GLU	2.1
1	A	201	ARG	2.1
1	C	42	ARG	2.1
1	C	64	ASP	2.0
1	B	42	ARG	2.0
1	C	310	ARG	2.0
1	A	191	THR	2.0
1	B	147	PRO	2.0
1	B	469	GLU	2.0
1	C	282	GLU	2.0
1	D	37	GLU	2.0
1	B	54	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	300	SER	2.0
1	A	207	ALA	2.0
1	B	132	ALA	2.0
1	D	152	ALA	2.0
1	D	27	LEU	2.0
1	A	52	PRO	2.0
1	B	430	THR	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.