



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2018 – 04:47 PM EDT

PDB ID : 5F7C
Title : Crystal structure of Family 31 alpha-glucosidase (BT_0339) from Bacteroides thetaiotaomicron
Authors : Chaudet, M.M.; Rose, D.R.
Deposited on : 2015-12-07
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031172
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

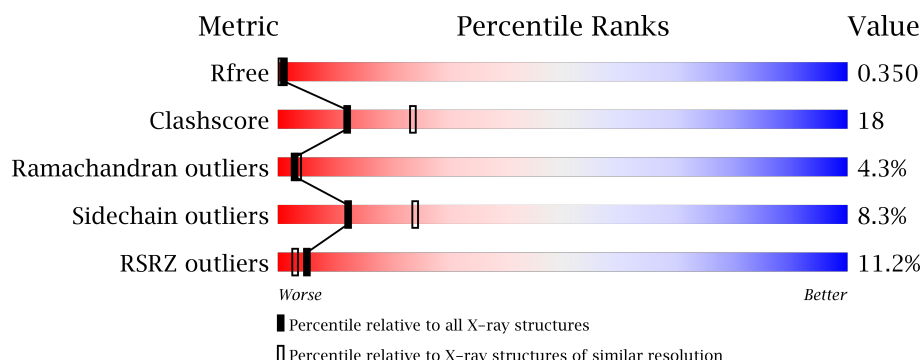
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	<div> <div>5%</div> <div>50% 26% 6% 18%</div> </div>
1	B	761	<div> <div>16%</div> <div>53% 22% 5% 20%</div> </div>
1	C	761	<div> <div>6%</div> <div>57% 23% 17%</div> </div>
1	D	761	<div> <div>9%</div> <div>51% 26% 18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34019 atoms, of which 14026 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	625	Total	C	H	N	O	S	0	0	0
			8422	3229	3426	837	901	29			
1	B	611	Total	C	H	N	O	S	0	0	0
			8403	3150	3512	832	881	28			
1	C	632	Total	C	H	N	O	S	0	0	0
			8637	3278	3548	865	917	29			
1	D	623	Total	C	H	N	O	S	0	0	0
			8490	3185	3540	840	895	30			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	PHE	conflict	UNP Q8AAX3
A	13	PHE	LEU	conflict	UNP Q8AAX3
A	750	HIS	-	expression tag	UNP Q8AAX3
A	751	HIS	-	expression tag	UNP Q8AAX3
A	752	HIS	-	expression tag	UNP Q8AAX3
A	753	HIS	-	expression tag	UNP Q8AAX3
A	754	HIS	-	expression tag	UNP Q8AAX3
A	755	HIS	-	expression tag	UNP Q8AAX3
A	756	LEU	-	expression tag	UNP Q8AAX3
A	757	ARG	-	expression tag	UNP Q8AAX3
A	758	VAL	-	expression tag	UNP Q8AAX3
A	759	PRO	-	expression tag	UNP Q8AAX3
A	760	ARG	-	expression tag	UNP Q8AAX3
A	761	GLY	-	expression tag	UNP Q8AAX3
A	762	SER	-	expression tag	UNP Q8AAX3
B	12	LEU	PHE	conflict	UNP Q8AAX3
B	13	PHE	LEU	conflict	UNP Q8AAX3
B	750	HIS	-	expression tag	UNP Q8AAX3
B	751	HIS	-	expression tag	UNP Q8AAX3
B	752	HIS	-	expression tag	UNP Q8AAX3
B	753	HIS	-	expression tag	UNP Q8AAX3

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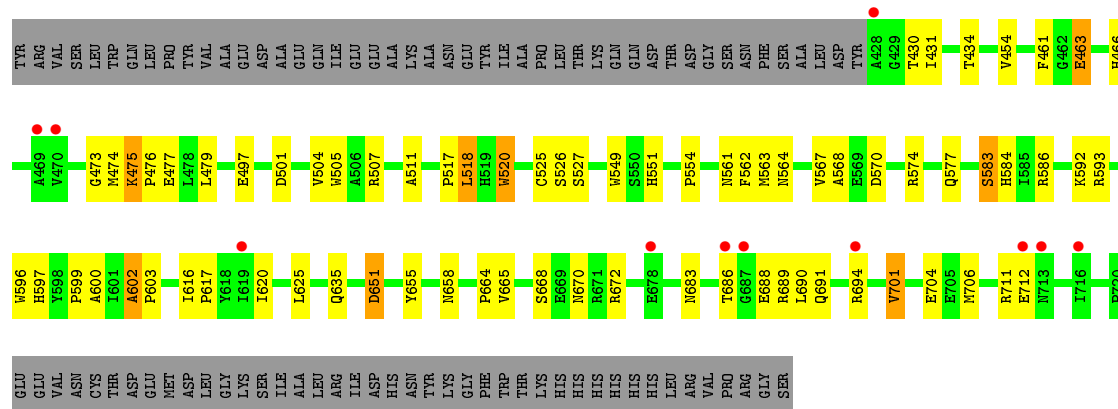
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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP Q8AAX3
B	755	HIS	-	expression tag	UNP Q8AAX3
B	756	LEU	-	expression tag	UNP Q8AAX3
B	757	ARG	-	expression tag	UNP Q8AAX3
B	758	VAL	-	expression tag	UNP Q8AAX3
B	759	PRO	-	expression tag	UNP Q8AAX3
B	760	ARG	-	expression tag	UNP Q8AAX3
B	761	GLY	-	expression tag	UNP Q8AAX3
B	762	SER	-	expression tag	UNP Q8AAX3
C	12	LEU	PHE	conflict	UNP Q8AAX3
C	13	PHE	LEU	conflict	UNP Q8AAX3
C	750	HIS	-	expression tag	UNP Q8AAX3
C	751	HIS	-	expression tag	UNP Q8AAX3
C	752	HIS	-	expression tag	UNP Q8AAX3
C	753	HIS	-	expression tag	UNP Q8AAX3
C	754	HIS	-	expression tag	UNP Q8AAX3
C	755	HIS	-	expression tag	UNP Q8AAX3
C	756	LEU	-	expression tag	UNP Q8AAX3
C	757	ARG	-	expression tag	UNP Q8AAX3
C	758	VAL	-	expression tag	UNP Q8AAX3
C	759	PRO	-	expression tag	UNP Q8AAX3
C	760	ARG	-	expression tag	UNP Q8AAX3
C	761	GLY	-	expression tag	UNP Q8AAX3
C	762	SER	-	expression tag	UNP Q8AAX3
D	12	LEU	PHE	conflict	UNP Q8AAX3
D	13	PHE	LEU	conflict	UNP Q8AAX3
D	750	HIS	-	expression tag	UNP Q8AAX3
D	751	HIS	-	expression tag	UNP Q8AAX3
D	752	HIS	-	expression tag	UNP Q8AAX3
D	753	HIS	-	expression tag	UNP Q8AAX3
D	754	HIS	-	expression tag	UNP Q8AAX3
D	755	HIS	-	expression tag	UNP Q8AAX3
D	756	LEU	-	expression tag	UNP Q8AAX3
D	757	ARG	-	expression tag	UNP Q8AAX3
D	758	VAL	-	expression tag	UNP Q8AAX3
D	759	PRO	-	expression tag	UNP Q8AAX3
D	760	ARG	-	expression tag	UNP Q8AAX3
D	761	GLY	-	expression tag	UNP Q8AAX3
D	762	SER	-	expression tag	UNP Q8AAX3

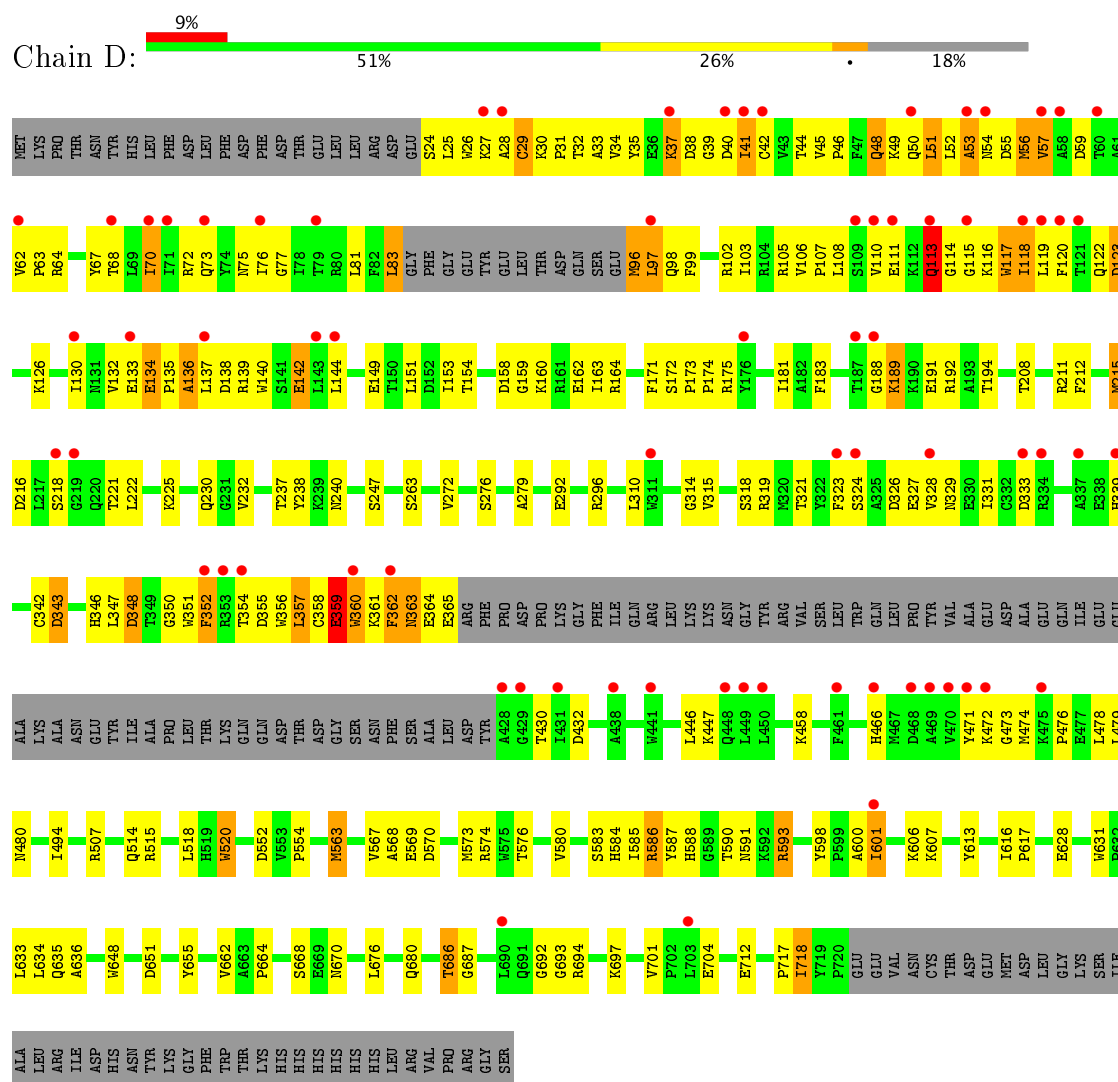
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	9	Total 9	O 9	0	0
2	C	18	Total 18	O 18	0	0
2	D	17	Total 17	O 17	0	0





• Molecule 1: Alpha-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.34Å 75.00Å 232.86Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	48.81 – 2.60 48.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.60) 100.0 (48.81-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.302 , 0.349 0.306 , 0.350	Depositor DCC
R_{free} test set	2000 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	34019	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.66	1/5147 (0.0%)	0.58	1/7000 (0.0%)
1	B	0.71	2/5035 (0.0%)	0.48	1/6839 (0.0%)
1	C	0.74	2/5240 (0.0%)	0.55	1/7115 (0.0%)
1	D	0.74	2/5092 (0.0%)	0.54	1/6917 (0.0%)
All	All	0.71	7/20514 (0.0%)	0.54	4/27871 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	SER	CA-CB	-37.04	0.97	1.52
1	B	324	SER	CA-CB	-37.03	0.97	1.52
1	D	324	SER	CA-CB	-36.99	0.97	1.52
1	C	324	SER	CA-CB	-36.97	0.97	1.52
1	B	117	TRP	CA-CB	-25.68	0.97	1.53
1	C	117	TRP	CA-CB	-25.66	0.97	1.53
1	D	117	TRP	CA-CB	-25.66	0.97	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	PRO	N-CA-CB	5.63	110.06	103.30
1	D	476	PRO	N-CA-CB	5.57	109.99	103.30
1	A	476	PRO	N-CA-CB	5.31	109.67	103.30
1	C	476	PRO	N-CA-CB	5.24	109.58	103.30

There are no chirality outliers.

There are no planarity outliers.

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	4996	3426	4731	213	0
1	B	4891	3512	4668	166	0
1	C	5089	3548	4863	161	0
1	D	4950	3540	4704	182	0
2	A	23	0	0	0	0
2	B	9	0	0	0	0
2	C	18	0	0	0	0
2	D	17	0	0	2	0
All	All	19993	14026	18966	711	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 18.

All (711) 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:49:LYS:HB2	1:D:64:ARG:HG2	1.26	1.12
1:A:14:ASP:HA	1:A:15:PHE:HB2	1.17	1.12
1:A:49:LYS:HB2	1:A:64:ARG:HD2	1.39	1.03
1:A:14:ASP:CA	1:A:15:PHE:HB2	1.94	0.98
1:A:37:LYS:HB2	1:A:39:GLY:H	1.26	0.96
1:A:136:ALA:HA	1:A:137:LEU:HG	1.49	0.92
1:A:36:GLU:CB	1:A:37:LYS:HG3	2.01	0.90
1:A:14:ASP:HA	1:A:15:PHE:CB	2.00	0.90
1:D:362:PHE:HB3	1:D:363:ASN:C	1.93	0.89
1:A:86:GLY:HA3	1:A:87:GLU:HG2	1.55	0.89
1:A:30:LYS:HE2	1:A:133:GLU:HG2	1.53	0.87
1:C:356:TRP:HA	1:C:357:LEU:HB2	1.55	0.87
1:A:37:LYS:HB2	1:A:39:GLY:N	1.90	0.87
1:A:652:ASP:OD2	1:A:672:ARG:NH2	2.09	0.86
1:A:315:VAL:HG22	1:A:342:CYS:HA	1.57	0.86
1:D:24:SER:N	2:D:801:HOH:O	2.09	0.85
1:A:21:ARG:HH12	1:A:186:ARG:HH11	1.26	0.83
1:D:49:LYS:CB	1:D:64:ARG:HG2	2.08	0.82
1:A:119:LEU:HD12	1:A:128:ALA:HB3	1.61	0.82
1:B:49:LYS:HE3	1:B:58:ALA:HB1	1.60	0.82
1:D:507:ARG:HB2	1:D:520:TRP:CZ3	2.13	0.82
1:A:430:THR:HG1	1:A:466:HIS:HD1	1.26	0.82
1:B:191:GLU:HG3	1:B:192:ARG:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:MET:HG3	1:A:479:LEU:HB2	1.61	0.81
1:D:49:LYS:HB2	1:D:64:ARG:CG	2.08	0.81
1:A:691:GLN:HB3	1:A:694:ARG:HE	1.45	0.81
1:A:136:ALA:HA	1:A:137:LEU:CG	2.10	0.80
1:C:507:ARG:HB2	1:C:520:TRP:CH2	2.16	0.80
1:B:350:GLY:HA2	1:B:352:PHE:H	1.46	0.80
1:B:57:VAL:HG12	1:B:58:ALA:H	1.45	0.80
1:B:238:TYR:CD2	1:B:507:ARG:HD3	2.16	0.80
1:A:664:PRO:O	1:A:672:ARG:NH1	2.15	0.80
1:D:362:PHE:HB3	1:D:363:ASN:CA	2.12	0.79
1:A:136:ALA:HA	1:A:137:LEU:CB	2.13	0.78
1:D:97:LEU:HD23	1:D:98:GLN:HG3	1.66	0.77
1:A:33:ALA:HB3	1:A:45:VAL:CG1	2.14	0.77
1:B:53:ALA:HA	1:B:54:ASN:HB3	1.64	0.77
1:C:574:ARG:NH2	1:C:670:ASN:OD1	2.18	0.77
1:A:136:ALA:HB1	1:A:137:LEU:HB2	1.65	0.76
1:A:49:LYS:HE2	1:A:58:ALA:HB1	1.66	0.76
1:C:191:GLU:HG3	1:C:192:ARG:HE	1.49	0.76
1:B:28:ALA:HA	1:B:48:GLN:HG3	1.66	0.76
1:B:29:CYS:SG	1:B:49:LYS:HG3	2.26	0.76
1:D:430:THR:OG1	1:D:466:HIS:ND1	2.19	0.76
1:D:113:GLN:HE21	1:D:119:LEU:HD21	1.51	0.75
1:A:12:LEU:HD12	1:A:13:PHE:N	2.02	0.75
1:C:664:PRO:O	1:C:672:ARG:NH1	2.20	0.75
1:D:318:SER:HB2	1:D:346:HIS:HB3	1.69	0.75
1:A:507:ARG:HB2	1:A:520:TRP:CH2	2.22	0.75
1:D:119:LEU:HD13	1:D:120:PHE:N	2.01	0.75
1:B:118:ILE:HG13	1:B:133:GLU:CG	2.17	0.74
1:B:564:ASN:HB3	1:D:139:ARG:HA	1.67	0.74
1:C:75:ASN:ND2	1:C:107:PRO:HD2	2.02	0.74
1:D:113:GLN:HG3	1:D:114:GLY:HA2	1.70	0.73
1:A:46:PRO:HD2	1:A:67:TYR:O	1.88	0.73
1:A:686:THR:O	1:A:688:GLU:N	2.22	0.73
1:D:99:PHE:O	1:D:515:ARG:NH2	2.21	0.73
1:A:136:ALA:CB	1:A:137:LEU:HB2	2.18	0.73
1:B:587:TYR:HB3	1:B:593:ARG:HG2	1.71	0.73
1:B:318:SER:HB2	1:B:346:HIS:HB3	1.71	0.72
1:C:318:SER:HB2	1:C:346:HIS:HB3	1.71	0.72
1:B:49:LYS:HB3	1:B:64:ARG:HG2	1.71	0.72
1:D:31:PRO:HA	1:D:46:PRO:HA	1.70	0.72
1:D:134:GLU:N	1:D:135:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:TYR:CD2	1:D:507:ARG:HD3	2.24	0.72
1:C:691:GLN:OE1	1:C:694:ARG:NH2	2.23	0.72
1:A:136:ALA:CA	1:A:137:LEU:HB2	2.19	0.72
1:D:97:LEU:HG	1:D:98:GLN:HA	1.70	0.71
1:C:362:PHE:O	1:C:364:GLU:N	2.22	0.71
1:A:348:ASP:OD2	1:A:349:THR:HG23	1.91	0.71
1:A:712:GLU:O	1:A:713:ASN:HB2	1.90	0.71
1:C:430:THR:HG1	1:C:466:HIS:HD1	0.72	0.71
1:C:689:ARG:NH2	1:C:712:GLU:OE2	2.23	0.70
1:C:191:GLU:HA	1:C:279:ALA:HB2	1.73	0.70
1:D:46:PRO:HD2	1:D:67:TYR:O	1.91	0.70
1:C:116:LYS:HD2	1:C:120:PHE:CE2	2.26	0.70
1:D:119:LEU:HD12	1:D:130:ILE:HD13	1.72	0.70
1:A:86:GLY:HA3	1:A:87:GLU:CG	2.21	0.70
1:A:49:LYS:HB2	1:A:64:ARG:CD	2.19	0.69
1:A:17:THR:N	1:A:19:LEU:H	1.90	0.69
1:A:574:ARG:NH2	1:A:670:ASN:OD1	2.26	0.69
1:D:29:CYS:HB3	1:D:149:GLU:HB2	1.75	0.69
1:B:350:GLY:HA2	1:B:351:TRP:CB	2.22	0.69
1:C:35:TYR:CG	1:C:119:LEU:HG	2.27	0.69
1:D:72:ARG:HD3	1:D:108:LEU:HD22	1.75	0.69
1:C:353:ARG:HA	1:C:362:PHE:CD2	2.28	0.68
1:C:430:THR:OG1	1:C:466:HIS:ND1	2.10	0.68
1:B:42:CYS:SG	1:B:111:GLU:HG2	2.33	0.68
1:D:328:VAL:CG2	1:D:347:LEU:HD11	2.24	0.68
1:B:118:ILE:HG13	1:B:133:GLU:HG3	1.75	0.68
1:A:37:LYS:HB2	1:A:38:ASP:CA	2.24	0.68
1:A:507:ARG:HB2	1:A:520:TRP:CZ3	2.29	0.68
1:C:106:VAL:N	1:C:107:PRO:HD3	2.08	0.68
1:A:336:ARG:NH1	1:A:340:TYR:O	2.27	0.67
1:C:44:THR:O	1:C:46:PRO:HD3	1.94	0.67
1:D:111:GLU:OE2	1:D:111:GLU:N	2.26	0.67
1:D:507:ARG:HB2	1:D:520:TRP:CH2	2.28	0.67
1:B:475:LYS:HE3	1:B:478:LEU:HG	1.74	0.67
1:A:124:GLY:HA2	1:A:125:THR:O	1.95	0.67
1:A:338:GLU:O	1:A:606:LYS:NZ	2.23	0.67
1:A:43:VAL:HB	1:A:70:ILE:HG22	1.76	0.67
1:B:315:VAL:HG13	1:B:342:CYS:HA	1.75	0.67
1:C:704:GLU:OE1	1:C:704:GLU:N	2.27	0.67
1:D:32:THR:N	1:D:45:VAL:O	2.27	0.67
1:B:29:CYS:HB3	1:B:149:GLU:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:OE2	1:B:507:ARG:HD2	1.95	0.66
1:A:27:LYS:HB2	1:A:51:LEU:HD21	1.76	0.66
1:D:154:THR:HG23	1:D:164:ARG:HB3	1.76	0.66
1:A:30:LYS:HG3	1:A:149:GLU:HB3	1.78	0.66
1:C:51:LEU:HG	1:C:56:MET:SD	2.36	0.66
1:B:46:PRO:HD2	1:B:67:TYR:O	1.95	0.66
1:D:686:THR:OG1	1:D:687:GLY:N	2.27	0.66
1:A:191:GLU:HA	1:A:279:ALA:HB2	1.77	0.65
1:C:43:VAL:HG13	1:C:68:THR:HG23	1.79	0.65
1:D:41:ILE:HG13	1:D:70:ILE:HD12	1.78	0.65
1:C:31:PRO:HA	1:C:46:PRO:HA	1.78	0.65
1:C:35:TYR:CD1	1:C:119:LEU:HG	2.31	0.65
1:D:35:TYR:HB3	1:D:119:LEU:HG	1.77	0.65
1:B:191:GLU:HA	1:B:279:ALA:HB2	1.79	0.65
1:B:49:LYS:CB	1:B:64:ARG:HG2	2.26	0.65
1:A:86:GLY:N	1:A:87:GLU:HB2	2.12	0.65
1:C:51:LEU:HD12	1:C:56:MET:HG2	1.79	0.65
1:A:318:SER:HB2	1:A:346:HIS:HB3	1.79	0.65
1:A:54:ASN:HA	1:A:55:ASP:HB3	1.79	0.65
1:C:103:ILE:HG22	1:C:104:ARG:H	1.59	0.65
1:B:192:ARG:HA	1:B:276:SER:O	1.97	0.65
1:C:22:ASP:O	1:C:187:THR:N	2.30	0.65
1:A:18:GLU:OE2	1:A:20:LEU:HB2	1.96	0.65
1:D:32:THR:HB	1:D:45:VAL:HG13	1.78	0.64
1:D:447:LYS:HB2	1:D:494:ILE:HD11	1.79	0.64
1:D:144:LEU:HD12	1:D:173:PRO:HD2	1.79	0.64
1:C:38:ASP:O	1:C:40:ASP:N	2.30	0.64
1:A:37:LYS:HD3	1:A:40:ASP:H	1.62	0.64
1:A:51:LEU:HG	1:A:56:MET:SD	2.37	0.64
1:C:51:LEU:HD13	1:C:58:ALA:HA	1.78	0.64
1:D:97:LEU:CB	1:D:98:GLN:HA	2.28	0.64
1:A:37:LYS:HB2	1:A:38:ASP:HA	1.79	0.64
1:C:22:ASP:HB3	1:C:187:THR:HA	1.80	0.64
1:D:25:LEU:HD23	1:D:56:MET:CE	2.28	0.64
1:A:435:TYR:O	1:A:437:LYS:N	2.31	0.63
1:B:576:THR:O	1:B:580:VAL:HG23	1.99	0.63
1:A:121:THR:O	1:A:123:ASP:HB3	1.99	0.63
1:B:49:LYS:HD3	1:B:50:GLN:N	2.12	0.63
1:C:75:ASN:CG	1:C:107:PRO:HD2	2.18	0.63
1:B:682:VAL:HG13	1:B:710:VAL:HG23	1.79	0.63
1:C:507:ARG:HB2	1:C:520:TRP:CZ3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ILE:HG23	1:C:596:TRP:CH2	2.32	0.63
1:A:325:ALA:O	1:A:329:ASN:ND2	2.23	0.63
1:D:328:VAL:HG21	1:D:347:LEU:HD11	1.80	0.63
1:D:49:LYS:HD3	1:D:64:ARG:HE	1.63	0.63
1:A:136:ALA:CA	1:A:137:LEU:CB	2.77	0.63
1:A:86:GLY:HA3	1:A:87:GLU:CB	2.29	0.62
1:B:30:LYS:HG3	1:B:132:VAL:HG12	1.80	0.62
1:B:507:ARG:HB2	1:B:520:TRP:CZ3	2.34	0.62
1:D:97:LEU:CG	1:D:98:GLN:HA	2.29	0.62
1:A:86:GLY:CA	1:A:87:GLU:HB2	2.29	0.62
1:D:352:PHE:HA	1:D:361:LYS:HA	1.81	0.62
1:C:23:GLU:HA	1:C:185:LYS:O	1.99	0.62
1:B:49:LYS:HZ2	1:B:50:GLN:H	1.48	0.62
1:D:34:VAL:CB	1:D:45:VAL:HG12	2.30	0.62
1:B:35:TYR:CZ	1:B:119:LEU:HD13	2.35	0.62
1:C:322:TYR:O	1:C:350:GLY:HA3	2.00	0.61
1:A:203:GLU:OE1	1:A:246:SER:OG	2.19	0.61
1:A:37:LYS:CB	1:A:38:ASP:HA	2.29	0.61
1:C:310:LEU:HD13	1:C:620:ILE:HD11	1.83	0.61
1:D:52:LEU:HD22	1:D:57:VAL:CG1	2.29	0.61
1:A:37:LYS:HG2	1:A:40:ASP:CA	2.30	0.61
1:D:552:ASP:OD1	1:D:586:ARG:NH1	2.33	0.61
1:A:136:ALA:HA	1:A:137:LEU:HB2	1.80	0.61
1:A:50:GLN:HB3	1:A:62:VAL:HG11	1.82	0.61
1:A:124:GLY:HA2	1:A:125:THR:C	2.20	0.61
1:C:103:ILE:HG22	1:C:104:ARG:N	2.16	0.61
1:C:116:LYS:HD2	1:C:120:PHE:HE2	1.65	0.61
1:B:64:ARG:NH1	1:B:149:GLU:OE1	2.33	0.60
1:D:362:PHE:HB2	1:D:364:GLU:HG3	1.82	0.60
1:B:350:GLY:HA2	1:B:352:PHE:N	2.15	0.60
1:B:44:THR:HG23	1:B:69:LEU:HB3	1.83	0.60
1:C:53:ALA:N	1:C:54:ASN:HB2	2.15	0.60
1:B:35:TYR:CD1	1:B:119:LEU:HD22	2.36	0.60
1:B:122:GLN:HB3	1:B:125:THR:CG2	2.31	0.60
1:B:186:ARG:HD2	1:B:187:THR:HG23	1.82	0.60
1:B:53:ALA:HB1	1:B:54:ASN:C	2.21	0.60
1:B:601:ILE:HD12	1:B:601:ILE:O	2.01	0.60
1:A:192:ARG:HA	1:A:276:SER:O	2.01	0.60
1:C:364:GLU:C	1:C:365:GLU:HG2	2.19	0.60
1:A:30:LYS:HD3	1:A:133:GLU:OE1	2.02	0.60
1:A:475:LYS:NZ	1:A:475:LYS:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:O	1:B:108:LEU:HD12	2.02	0.60
1:B:49:LYS:HG2	1:B:64:ARG:NE	2.17	0.60
1:A:30:LYS:CE	1:A:133:GLU:HG2	2.31	0.59
1:D:27:LYS:HG2	1:D:50:GLN:HG2	1.84	0.59
1:B:49:LYS:HE3	1:B:58:ALA:CB	2.30	0.59
1:D:569:GLU:HB3	1:D:601:ILE:HG13	1.83	0.59
1:D:49:LYS:HE2	1:D:64:ARG:HH21	1.67	0.59
1:C:103:ILE:HG13	1:C:300:ASP:HA	1.84	0.59
1:C:683:ASN:OD1	1:C:686:THR:N	2.35	0.59
1:B:151:LEU:HD23	1:B:181:ILE:HD12	1.85	0.59
1:A:360:TRP:O	1:A:362:PHE:N	2.36	0.59
1:B:49:LYS:HB3	1:B:64:ARG:CG	2.31	0.59
1:A:86:GLY:CA	1:A:87:GLU:CB	2.81	0.58
1:D:35:TYR:CD2	1:D:119:LEU:HB2	2.38	0.58
1:D:563:MET:HG3	1:D:590:THR:HB	1.85	0.58
1:B:151:LEU:CD2	1:B:181:ILE:HD12	2.33	0.58
1:D:171:PHE:HB3	1:D:175:ARG:HB3	1.86	0.58
1:A:17:THR:H	1:A:19:LEU:H	1.50	0.58
1:A:211:ARG:NH2	1:A:240:ASN:OD1	2.36	0.58
1:B:69:LEU:HB2	1:B:83:LEU:HD12	1.85	0.58
1:D:35:TYR:CG	1:D:119:LEU:HG	2.38	0.58
1:D:598:TYR:O	1:D:601:ILE:HB	2.02	0.58
1:B:450:LEU:HB3	1:B:498:VAL:HG21	1.86	0.58
1:C:118:ILE:HD11	1:C:120:PHE:CZ	2.39	0.58
1:C:315:VAL:HG13	1:C:342:CYS:HA	1.85	0.58
1:A:139:ARG:HA	1:C:564:ASN:OD1	2.04	0.58
1:A:245:LEU:HB3	1:A:291:MET:HE1	1.85	0.58
1:B:154:THR:HG23	1:B:164:ARG:HB3	1.85	0.58
1:C:315:VAL:CG1	1:C:342:CYS:HA	2.33	0.58
1:D:587:TYR:HB3	1:D:593:ARG:HG2	1.86	0.58
1:A:315:VAL:CG2	1:A:342:CYS:HA	2.30	0.58
1:B:475:LYS:H	1:B:475:LYS:HD3	1.69	0.58
1:B:40:ASP:CB	1:B:110:VAL:HG12	2.34	0.58
1:A:359:GLU:O	1:A:361:LYS:N	2.36	0.57
1:A:713:ASN:OD1	1:B:658:ASN:ND2	2.37	0.57
1:C:35:TYR:CD2	1:C:119:LEU:HG	2.39	0.57
1:D:113:GLN:NE2	1:D:119:LEU:HD21	2.19	0.57
1:B:50:GLN:CB	1:B:58:ALA:HA	2.34	0.57
1:B:564:ASN:ND2	1:D:140:TRP:O	2.37	0.57
1:A:175:ARG:NE	1:C:230:GLN:OE1	2.34	0.57
1:A:715:VAL:HG11	1:B:715:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:CYS:SG	1:B:345:ILE:HG21	2.45	0.57
1:D:118:ILE:H	1:D:118:ILE:HD13	1.70	0.57
1:D:68:THR:O	1:D:83:LEU:HD22	2.05	0.57
1:A:244:TYR:CZ	1:A:272:VAL:HG11	2.40	0.57
1:A:336:ARG:N	1:A:336:ARG:HD2	2.20	0.57
1:B:601:ILE:HG23	1:B:703:LEU:HD21	1.87	0.57
1:D:151:LEU:CD2	1:D:181:ILE:HD12	2.34	0.57
1:B:652:ASP:OD2	1:B:672:ARG:NH2	2.38	0.56
1:A:37:LYS:HG2	1:A:40:ASP:HA	1.86	0.56
1:D:191:GLU:HG3	1:D:192:ARG:HG3	1.85	0.56
1:D:192:ARG:HA	1:D:276:SER:O	2.05	0.56
1:D:191:GLU:HA	1:D:279:ALA:HB2	1.87	0.56
1:B:355:ASP:CB	1:B:356:TRP:HA	2.33	0.56
1:A:627:VAL:HG23	1:A:628:GLU:HG2	1.85	0.56
1:A:49:LYS:HD3	1:A:64:ARG:HD3	1.86	0.56
1:A:598:TYR:O	1:A:601:ILE:HG22	2.06	0.56
1:D:662:VAL:HG12	1:D:664:PRO:HD3	1.88	0.56
1:B:323:PHE:O	1:B:324:SER:CB	2.47	0.56
1:B:98:GLN:HG3	1:B:99:PHE:N	2.21	0.56
1:D:315:VAL:HG22	1:D:342:CYS:HA	1.86	0.56
1:D:31:PRO:HD3	1:D:151:LEU:HD12	1.87	0.56
1:A:69:LEU:HD11	1:A:81:LEU:HD12	1.88	0.56
1:C:191:GLU:CG	1:C:192:ARG:HE	2.17	0.56
1:D:75:ASN:ND2	1:D:105:ARG:O	2.38	0.56
1:A:123:ASP:OD1	1:A:125:THR:HG21	2.05	0.55
1:B:435:TYR:CG	1:B:472:LYS:HD2	2.41	0.55
1:D:97:LEU:HD23	1:D:98:GLN:CG	2.37	0.55
1:A:211:ARG:NH1	1:A:237:THR:OG1	2.36	0.55
1:D:35:TYR:CD2	1:D:119:LEU:HD23	2.42	0.55
1:D:52:LEU:HD22	1:D:57:VAL:HG11	1.88	0.55
1:C:26:TRP:NE1	1:C:185:LYS:HD3	2.21	0.55
1:B:315:VAL:CG1	1:B:342:CYS:HA	2.36	0.55
1:D:354:THR:O	1:D:356:TRP:HA	2.06	0.55
1:D:362:PHE:HB3	1:D:363:ASN:CB	2.36	0.55
1:A:686:THR:O	1:A:686:THR:OG1	2.10	0.55
1:C:583:SER:OG	1:C:584:HIS:ND1	2.38	0.55
1:A:332:CYS:SG	1:A:345:ILE:HG13	2.47	0.55
1:C:192:ARG:HA	1:C:276:SER:O	2.07	0.55
1:C:474:MET:HE2	1:C:479:LEU:HD13	1.88	0.55
1:B:171:PHE:HB3	1:B:175:ARG:HB3	1.89	0.54
1:C:161:ARG:O	1:C:162:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:HD3	1:B:50:GLN:CB	2.37	0.54
1:C:43:VAL:HG13	1:C:68:THR:CG2	2.37	0.54
1:D:329:ASN:O	1:D:333:ASP:HB2	2.07	0.54
1:D:49:LYS:CD	1:D:64:ARG:HE	2.20	0.54
1:A:37:LYS:CB	1:A:39:GLY:H	2.11	0.54
1:B:178:GLY:O	1:B:179:LEU:HD23	2.08	0.54
1:C:525:CYS:O	1:C:527:SER:N	2.41	0.54
1:C:635:GLN:HB2	1:C:655:TYR:HB2	1.90	0.54
1:D:122:GLN:HG2	1:D:123:ASP:H	1.73	0.54
1:C:184:CYS:HB2	1:C:192:ARG:HB2	1.89	0.54
1:D:211:ARG:NH2	1:D:240:ASN:OD1	2.35	0.54
1:C:53:ALA:CA	1:C:54:ASN:HB2	2.38	0.53
1:D:25:LEU:HD23	1:D:56:MET:HE3	1.89	0.53
1:A:338:GLU:O	1:A:339:HIS:HB2	2.08	0.53
1:C:32:THR:N	1:C:45:VAL:O	2.39	0.53
1:A:31:PRO:HG2	1:A:130:ILE:HG21	1.91	0.53
1:A:580:VAL:O	1:A:612:ARG:NH1	2.41	0.53
1:B:691:GLN:OE1	1:B:691:GLN:N	2.37	0.53
1:C:106:VAL:N	1:C:107:PRO:CD	2.72	0.53
1:D:25:LEU:HD23	1:D:56:MET:HE1	1.89	0.53
1:D:73:GLN:N	1:D:111:GLU:OE1	2.37	0.53
1:A:474:MET:CG	1:A:479:LEU:HB2	2.37	0.53
1:B:507:ARG:HB2	1:B:520:TRP:CH2	2.44	0.53
1:C:193:ALA:HB2	1:C:279:ALA:HA	1.91	0.53
1:B:465:ILE:HD12	1:B:480:ASN:HA	1.91	0.53
1:B:658:ASN:ND2	1:B:711:ARG:HH22	2.06	0.53
1:C:144:LEU:HG	1:C:172:SER:CB	2.39	0.53
1:C:688:GLU:HG2	1:C:690:LEU:CD2	2.39	0.53
1:D:53:ALA:HA	1:D:54:ASN:HB3	1.90	0.53
1:A:69:LEU:HD11	1:A:81:LEU:CD1	2.39	0.53
1:B:432:ASP:OD2	1:B:472:LYS:HE2	2.09	0.53
1:D:53:ALA:CA	1:D:54:ASN:HB3	2.38	0.53
1:B:122:GLN:HB3	1:B:125:THR:HG23	1.90	0.53
1:B:31:PRO:O	1:B:33:ALA:N	2.42	0.53
1:C:358:CYS:O	1:C:360:TRP:N	2.42	0.53
1:A:212:PHE:CE1	1:A:232:VAL:HG22	2.45	0.52
1:B:30:LYS:O	1:B:32:THR:N	2.42	0.52
1:C:327:GLU:O	1:C:331:ILE:HG13	2.09	0.52
1:B:115:GLY:HA2	1:B:119:LEU:HD23	1.90	0.52
1:D:35:TYR:CE2	1:D:119:LEU:HB2	2.44	0.52
1:A:18:GLU:CD	1:A:18:GLU:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASP:HA	1:A:19:LEU:HA	1.91	0.52
1:B:53:ALA:HB1	1:B:54:ASN:O	2.09	0.52
1:A:474:MET:HE3	1:A:479:LEU:HD13	1.91	0.52
1:A:49:LYS:HD3	1:A:64:ARG:CD	2.40	0.52
1:A:26:TRP:CE2	1:A:50:GLN:HB2	2.45	0.52
1:C:184:CYS:O	1:C:191:GLU:N	2.42	0.52
1:D:136:ALA:O	1:D:138:ASP:N	2.40	0.52
1:D:430:THR:HG1	1:D:466:HIS:HD1	1.41	0.52
1:A:579:GLY:O	1:A:582:THR:OG1	2.25	0.52
1:A:82:PHE:CZ	1:A:89:GLU:HA	2.45	0.52
1:B:185:LYS:NZ	1:B:188:GLY:O	2.25	0.52
1:C:328:VAL:HG13	1:C:345:ILE:HG21	1.91	0.52
1:D:570:ASP:OD2	1:D:668:SER:OG	2.15	0.52
1:A:361:LYS:O	1:A:362:PHE:CB	2.58	0.52
1:A:475:LYS:HB3	1:A:475:LYS:HZ3	1.73	0.52
1:A:138:ASP:O	1:A:139:ARG:HB2	2.10	0.52
1:D:478:LEU:N	1:D:478:LEU:HD22	2.25	0.52
1:A:292:GLU:HG3	1:A:631:TRP:CE2	2.45	0.52
1:C:54:ASN:O	1:C:55:ASP:HB2	2.10	0.52
1:A:16:ASP:HB2	1:A:19:LEU:HD13	1.92	0.51
1:C:358:CYS:C	1:C:360:TRP:H	2.13	0.51
1:C:474:MET:HG3	1:C:479:LEU:HB2	1.90	0.51
1:C:144:LEU:HG	1:C:172:SER:HB3	1.91	0.51
1:A:314:GLY:HA3	1:A:343:ASP:HB2	1.93	0.51
1:D:116:LYS:O	1:D:117:TRP:CB	2.51	0.51
1:D:134:GLU:H	1:D:135:PRO:HD2	1.74	0.51
1:C:25:LEU:HD13	1:C:26:TRP:N	2.25	0.51
1:D:53:ALA:HA	1:D:54:ASN:C	2.30	0.51
1:D:600:ALA:HA	1:D:601:ILE:HB	1.91	0.51
1:B:59:ASP:OD1	1:B:62:VAL:HG22	2.10	0.51
1:C:365:GLU:O	1:C:366:ARG:HB2	2.10	0.51
1:B:49:LYS:HZ2	1:B:50:GLN:N	2.07	0.51
1:A:317:MET:HB3	1:A:345:ILE:HD13	1.92	0.51
1:C:116:LYS:O	1:C:117:TRP:CB	2.52	0.51
1:C:191:GLU:OE1	1:C:192:ARG:NE	2.44	0.51
1:C:362:PHE:C	1:C:364:GLU:H	2.13	0.51
1:A:18:GLU:N	1:A:18:GLU:OE1	2.32	0.51
1:A:31:PRO:HB3	1:A:44:THR:CG2	2.40	0.51
1:C:355:ASP:HB3	1:C:356:TRP:CD1	2.45	0.51
1:C:37:LYS:HB2	1:C:113:GLN:CG	2.40	0.51
1:B:332:CYS:SG	1:B:345:ILE:HD12	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:CYS:SG	1:C:345:ILE:HG13	2.51	0.50
1:A:430:THR:OG1	1:A:466:HIS:ND1	2.26	0.50
1:C:331:ILE:HG23	1:C:596:TRP:HH2	1.72	0.50
1:A:576:THR:HG22	1:A:587:TYR:OH	2.12	0.50
1:B:189:LYS:HB2	1:B:189:LYS:NZ	2.27	0.50
1:B:225:LYS:NZ	1:B:226:ASN:O	2.43	0.50
1:D:35:TYR:CB	1:D:119:LEU:HG	2.40	0.50
1:A:244:TYR:CE2	1:A:272:VAL:HG11	2.46	0.50
1:C:351:TRP:H	1:C:351:TRP:HD1	1.56	0.50
1:C:689:ARG:NH2	1:C:712:GLU:HB2	2.27	0.50
1:D:29:CYS:HB3	1:D:149:GLU:CB	2.39	0.50
1:D:31:PRO:HB3	1:D:44:THR:CG2	2.41	0.50
1:A:430:THR:HG1	1:A:466:HIS:CE1	2.30	0.50
1:B:348:ASP:O	1:B:350:GLY:N	2.43	0.50
1:B:614:SER:O	1:B:718:ILE:HG23	2.11	0.50
1:D:119:LEU:HD13	1:D:120:PHE:CA	2.41	0.50
1:A:573:MET:SD	1:A:601:ILE:HG13	2.51	0.50
1:B:563:MET:HG2	1:D:142:GLU:H	1.77	0.50
1:B:49:LYS:CE	1:B:58:ALA:HB1	2.37	0.50
1:C:116:LYS:HZ3	1:C:120:PHE:HD2	1.59	0.50
1:A:21:ARG:HH12	1:A:186:ARG:NH1	2.02	0.49
1:B:118:ILE:CG1	1:B:133:GLU:HG3	2.41	0.49
1:B:53:ALA:HA	1:B:54:ASN:CB	2.35	0.49
1:B:99:PHE:HB3	1:B:485:LEU:CD2	2.41	0.49
1:D:693:GLY:O	1:D:694:ARG:HD3	2.11	0.49
1:A:137:LEU:O	1:A:138:ASP:HB2	2.13	0.49
1:C:355:ASP:C	1:C:356:TRP:CD1	2.85	0.49
1:A:51:LEU:HD13	1:A:58:ALA:HA	1.95	0.49
1:A:82:PHE:CE2	1:A:89:GLU:HA	2.47	0.49
1:B:158:ASP:OD2	1:B:161:ARG:HB2	2.12	0.49
1:B:477:GLU:O	1:B:478:LEU:HD22	2.13	0.49
1:D:238:TYR:HD2	1:D:507:ARG:HD3	1.75	0.49
1:B:122:GLN:HB3	1:B:125:THR:HG22	1.94	0.49
1:B:31:PRO:HD2	1:B:132:VAL:HG12	1.93	0.49
1:D:97:LEU:CB	1:D:98:GLN:CA	2.91	0.49
1:B:465:ILE:H	1:B:465:ILE:HD13	1.77	0.49
1:C:331:ILE:HG23	1:C:596:TRP:CZ2	2.48	0.49
1:D:189:LYS:N	1:D:189:LYS:HD2	2.27	0.49
1:D:473:GLY:O	1:D:474:MET:HB3	2.13	0.49
1:B:350:GLY:CA	1:B:351:TRP:CB	2.91	0.49
1:C:121:THR:HB	1:C:128:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:HG2	1:D:50:GLN:CG	2.43	0.49
1:A:299:ARG:NH1	1:A:629:SER:O	2.46	0.49
1:A:551:HIS:CD2	1:A:578:PHE:CE2	3.01	0.49
1:B:118:ILE:N	1:B:118:ILE:HD12	2.28	0.49
1:B:163:ILE:HD11	1:B:197:PHE:CG	2.48	0.49
1:B:69:LEU:HD13	1:B:83:LEU:HB2	1.95	0.49
1:A:144:LEU:HD23	1:C:562:PHE:CG	2.47	0.49
1:D:97:LEU:CD2	1:D:98:GLN:HG3	2.40	0.49
1:A:338:GLU:HB3	1:A:340:TYR:CE2	2.48	0.49
1:B:186:ARG:CD	1:B:187:THR:HG23	2.42	0.49
1:C:658:ASN:O	1:C:711:ARG:NH2	2.46	0.49
1:D:480:ASN:HB3	2:D:805:HOH:O	2.11	0.49
1:D:573:MET:HG2	1:D:601:ILE:HD12	1.95	0.49
1:C:22:ASP:O	1:C:186:ARG:HA	2.12	0.48
1:D:576:THR:O	1:D:580:VAL:HG23	2.12	0.48
1:A:37:LYS:HD2	1:A:38:ASP:HA	1.95	0.48
1:B:30:LYS:HE2	1:B:149:GLU:OE2	2.14	0.48
1:B:667:ASN:O	1:B:668:SER:CB	2.61	0.48
1:C:475:LYS:HB3	1:C:477:GLU:CD	2.34	0.48
1:D:583:SER:OG	1:D:584:HIS:ND1	2.42	0.48
1:A:124:GLY:N	1:A:125:THR:OG1	2.46	0.48
1:C:123:ASP:N	1:C:125:THR:N	2.62	0.48
1:A:474:MET:CE	1:A:479:LEU:HD13	2.44	0.48
1:A:560:PRO:O	1:A:561:ASN:CB	2.62	0.48
1:D:211:ARG:HD3	1:D:222:LEU:HD22	1.94	0.48
1:D:588:HIS:N	1:D:593:ARG:HD2	2.29	0.48
1:B:551:HIS:CD2	1:B:575:TRP:HE1	2.31	0.48
1:C:37:LYS:HE3	1:C:38:ASP:O	2.13	0.48
1:D:144:LEU:HG	1:D:172:SER:OG	2.14	0.48
1:D:216:ASP:OD1	1:D:218:SER:OG	2.31	0.48
1:D:221:THR:HA	1:D:263:SER:HA	1.94	0.48
1:A:37:LYS:HB3	1:A:41:ILE:O	2.14	0.48
1:B:31:PRO:HG3	1:B:151:LEU:CD1	2.44	0.48
1:D:25:LEU:HD12	1:D:26:TRP:H	1.79	0.48
1:D:318:SER:OG	1:D:319:ARG:N	2.45	0.48
1:A:691:GLN:HB3	1:A:694:ARG:NE	2.23	0.48
1:B:594:GLU:HG2	1:B:596:TRP:CZ2	2.49	0.48
1:B:635:GLN:HB2	1:B:655:TYR:HB2	1.96	0.48
1:C:160:LYS:HB3	1:C:160:LYS:NZ	2.29	0.48
1:A:37:LYS:HB3	1:A:41:ILE:H	1.79	0.48
1:A:617:PRO:HB2	1:A:717:PRO:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:CYS:HB2	1:B:192:ARG:HB2	1.94	0.48
1:B:629:SER:OG	1:B:630:GLY:N	2.47	0.48
1:B:664:PRO:O	1:B:672:ARG:NH1	2.44	0.48
1:A:221:THR:HA	1:A:263:SER:HA	1.95	0.48
1:A:35:TYR:CZ	1:A:43:VAL:HG22	2.49	0.48
1:C:35:TYR:CE1	1:C:119:LEU:HG	2.48	0.48
1:C:254:TYR:O	1:C:256:THR:N	2.46	0.48
1:C:577:GLN:CB	1:C:706:MET:HE3	2.44	0.48
1:D:326:ASP:OD2	1:D:326:ASP:N	2.47	0.48
1:A:33:ALA:HB3	1:A:45:VAL:HG11	1.92	0.47
1:A:583:SER:OG	1:A:584:HIS:ND1	2.46	0.47
1:C:40:ASP:O	1:C:111:GLU:HB2	2.13	0.47
1:C:309:PRO:HG3	1:C:501:ASP:HB3	1.96	0.47
1:A:144:LEU:HD22	1:C:563:MET:HE1	1.96	0.47
1:D:45:VAL:O	1:D:45:VAL:HG13	2.13	0.47
1:D:49:LYS:CE	1:D:64:ARG:HH21	2.26	0.47
1:C:53:ALA:HA	1:C:54:ASN:C	2.34	0.47
1:C:570:ASP:OD2	1:C:668:SER:OG	2.16	0.47
1:D:113:GLN:CG	1:D:114:GLY:HA2	2.44	0.47
1:D:215:MET:CE	1:D:636:ALA:HB1	2.44	0.47
1:B:616:ILE:N	1:B:617:PRO:HD2	2.29	0.47
1:B:686:THR:OG1	1:B:687:GLY:N	2.46	0.47
1:D:355:ASP:HA	1:D:356:TRP:HA	1.58	0.47
1:A:126:LYS:HD2	1:A:126:LYS:O	2.14	0.47
1:A:302:THR:OG1	1:A:514:GLN:NE2	2.47	0.47
1:D:326:ASP:HA	1:D:327:GLU:C	2.35	0.47
1:D:327:GLU:HA	1:D:331:ILE:HD13	1.97	0.47
1:B:57:VAL:HG12	1:B:58:ALA:N	2.22	0.47
1:D:432:ASP:OD1	1:D:471:TYR:HB3	2.14	0.47
1:C:102:ARG:C	1:C:103:ILE:HG12	2.35	0.47
1:C:191:GLU:CA	1:C:279:ALA:HB2	2.43	0.47
1:C:349:THR:HG21	1:C:356:TRP:CH2	2.50	0.47
1:D:247:SER:HA	1:D:648:TRP:CZ2	2.50	0.47
1:A:49:LYS:HB3	1:A:49:LYS:NZ	2.29	0.47
1:B:30:LYS:HB2	1:B:149:GLU:HB2	1.97	0.47
1:A:572:TYR:O	1:A:576:THR:HG23	2.15	0.46
1:C:592:LYS:HD3	1:C:597:HIS:HB3	1.97	0.46
1:C:599:PRO:HA	1:C:602:ALA:CB	2.45	0.46
1:D:35:TYR:HD2	1:D:119:LEU:HD23	1.77	0.46
1:A:87:GLU:HB3	1:A:88:TYR:CD1	2.51	0.46
1:D:680:GLN:HB2	1:D:712:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:53:ALA:HB3	2.15	0.46
1:C:26:TRP:CE2	1:C:185:LYS:HD3	2.50	0.46
1:A:171:PHE:HB3	1:A:175:ARG:HB3	1.98	0.46
1:A:328:VAL:HG21	1:A:347:LEU:HD11	1.98	0.46
1:A:552:ASP:OD1	1:A:586:ARG:NH1	2.47	0.46
1:B:477:GLU:C	1:B:478:LEU:HD22	2.35	0.46
1:C:686:THR:CG2	1:C:688:GLU:HB2	2.46	0.46
1:C:44:THR:HG23	1:C:69:LEU:O	2.16	0.46
1:D:53:ALA:N	1:D:54:ASN:HB3	2.30	0.46
1:C:134:GLU:HB2	1:C:135:PRO:C	2.36	0.46
1:A:151:LEU:CD2	1:A:181:ILE:HD12	2.45	0.46
1:B:456:CYS:SG	1:B:457:ILE:N	2.88	0.46
1:B:562:PHE:CE1	1:B:590:THR:HG21	2.51	0.46
1:A:15:PHE:O	1:A:16:ASP:HB3	2.15	0.46
1:A:200:ARG:HB3	1:A:201:PRO:HD2	1.98	0.46
1:B:223:PHE:O	1:B:225:LYS:N	2.49	0.46
1:B:517:PRO:HA	1:B:518:LEU:HA	1.79	0.46
1:C:434:THR:HG21	1:C:474:MET:HE2	1.98	0.46
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.81	0.46
1:A:36:GLU:HA	1:A:37:LYS:HA	1.66	0.46
1:A:616:ILE:HB	1:A:617:PRO:HD3	1.96	0.46
1:A:618:TYR:CD1	1:A:716:ILE:HG23	2.51	0.46
1:D:574:ARG:NH2	1:D:670:ASN:OD1	2.45	0.46
1:A:54:ASN:CA	1:A:55:ASP:HB3	2.45	0.45
1:B:445:LEU:O	1:B:448:GLN:HG2	2.16	0.45
1:A:475:LYS:HE2	1:A:477:GLU:OE2	2.17	0.45
1:B:316:TRP:CE3	1:B:344:VAL:HG11	2.51	0.45
1:D:563:MET:HA	1:D:590:THR:HB	1.98	0.45
1:A:613:TYR:HA	1:A:616:ILE:HG12	1.98	0.45
1:D:717:PRO:O	1:D:718:ILE:HG23	2.17	0.45
1:A:212:PHE:CD1	1:A:232:VAL:HG22	2.52	0.45
1:A:505:TRP:CD1	1:A:520:TRP:CE3	3.04	0.45
1:B:573:MET:SD	1:B:601:ILE:HG21	2.57	0.45
1:D:118:ILE:O	1:D:118:ILE:HG12	2.14	0.45
1:A:347:LEU:N	1:A:347:LEU:HD22	2.32	0.45
1:C:31:PRO:O	1:C:33:ALA:N	2.50	0.45
1:A:567:VAL:O	1:A:568:ALA:HB3	2.17	0.45
1:B:49:LYS:HB3	1:B:64:ARG:CB	2.47	0.45
1:C:191:GLU:HG3	1:C:192:ARG:NE	2.26	0.45
1:C:46:PRO:HD2	1:C:67:TYR:O	2.15	0.45
1:A:37:LYS:N	1:A:38:ASP:HA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ALA:HB2	1:B:279:ALA:HA	1.98	0.45
1:C:211:ARG:NH1	1:C:237:THR:HG21	2.32	0.45
1:D:208:THR:HG21	1:D:222:LEU:HD13	1.98	0.45
1:D:446:LEU:HD12	1:D:494:ILE:HG21	1.99	0.45
1:D:474:MET:SD	1:D:479:LEU:HA	2.56	0.45
1:D:55:ASP:HA	1:D:56:MET:HA	1.55	0.45
1:A:190:LYS:HE3	1:A:190:LYS:HB2	1.53	0.45
1:A:319:ARG:O	1:A:321:THR:HA	2.17	0.45
1:B:177:ASP:OD1	1:B:267:HIS:NE2	2.50	0.45
1:C:181:ILE:HG12	1:C:195:LEU:HD23	1.99	0.45
1:D:613:TYR:HA	1:D:616:ILE:HG12	1.98	0.45
1:A:32:THR:O	1:A:33:ALA:HB2	2.17	0.45
1:B:118:ILE:HG13	1:B:133:GLU:HG2	1.96	0.45
1:D:348:ASP:OD1	1:D:458:LYS:NZ	2.34	0.45
1:A:232:VAL:O	1:A:232:VAL:HG13	2.17	0.44
1:B:350:GLY:CA	1:B:352:PHE:H	2.23	0.44
1:C:475:LYS:HB3	1:C:477:GLU:OE1	2.17	0.44
1:A:599:PRO:C	1:A:601:ILE:H	2.20	0.44
1:B:38:ASP:O	1:B:40:ASP:N	2.50	0.44
1:C:22:ASP:HB3	1:C:187:THR:CA	2.47	0.44
1:D:153:ILE:O	1:D:164:ARG:HB2	2.18	0.44
1:C:125:THR:N	1:C:126:LYS:HA	2.31	0.44
1:C:434:THR:CG2	1:C:474:MET:HE2	2.47	0.44
1:D:158:ASP:OD1	1:D:159:GLY:N	2.51	0.44
1:D:40:ASP:CB	1:D:110:VAL:HG12	2.47	0.44
1:D:49:LYS:CG	1:D:64:ARG:HG2	2.47	0.44
1:D:133:GLU:O	1:D:134:GLU:HB2	2.17	0.44
1:A:18:GLU:CD	1:A:18:GLU:N	2.71	0.44
1:B:239:LYS:HE2	1:B:519:HIS:HB3	2.00	0.44
1:B:83:LEU:HB3	1:B:281:LEU:HD11	2.00	0.44
1:C:475:LYS:HB3	1:C:477:GLU:OE2	2.18	0.44
1:C:49:LYS:HD3	1:C:64:ARG:HG2	1.99	0.44
1:D:616:ILE:N	1:D:617:PRO:CD	2.81	0.44
1:D:676:LEU:O	1:D:693:GLY:HA2	2.18	0.44
1:D:97:LEU:HB3	1:D:98:GLN:CA	2.48	0.44
1:A:88:TYR:O	1:A:89:GLU:HB2	2.17	0.44
1:D:352:PHE:CE2	1:D:358:CYS:HA	2.53	0.44
1:B:49:LYS:HB2	1:B:49:LYS:HZ3	1.83	0.44
1:D:119:LEU:HB3	1:D:130:ILE:HB	2.00	0.44
1:D:339:HIS:HB2	1:D:606:LYS:HE3	1.98	0.44
1:B:658:ASN:HD21	1:B:711:ARG:HH22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:THR:HG22	1:C:431:ILE:N	2.33	0.44
1:C:434:THR:CG2	1:C:479:LEU:HD13	2.47	0.43
1:C:599:PRO:HA	1:C:602:ALA:HB2	2.00	0.43
1:C:688:GLU:HG2	1:C:690:LEU:HD22	2.00	0.43
1:D:160:LYS:HE2	1:D:160:LYS:HB3	1.78	0.43
1:D:53:ALA:CA	1:D:54:ASN:CB	2.96	0.43
1:D:62:VAL:HG23	1:D:63:PRO:HD2	2.00	0.43
1:B:113:GLN:HG3	1:B:120:PHE:O	2.18	0.43
1:B:212:PHE:CE1	1:B:232:VAL:HG23	2.53	0.43
1:B:211:ARG:HD2	1:B:237:THR:HG21	1.99	0.43
1:C:115:GLY:O	1:C:116:LYS:HB3	2.17	0.43
1:C:665:VAL:HG21	1:C:701:VAL:CG2	2.49	0.43
1:D:362:PHE:CB	1:D:363:ASN:CB	2.96	0.43
1:A:223:PHE:O	1:A:225:LYS:N	2.52	0.43
1:B:49:LYS:HB2	1:B:49:LYS:NZ	2.33	0.43
1:D:188:GLY:C	1:D:189:LYS:HD2	2.38	0.43
1:D:314:GLY:HA3	1:D:343:ASP:HB2	2.00	0.43
1:B:135:PRO:O	1:B:137:LEU:HD22	2.18	0.43
1:A:316:TRP:CE2	1:A:344:VAL:HG21	2.53	0.43
1:A:358:CYS:O	1:A:359:GLU:HB3	2.18	0.43
1:B:441:TRP:O	1:B:445:LEU:N	2.46	0.43
1:B:291:MET:HB3	1:B:639:LEU:HD23	2.00	0.43
1:B:83:LEU:C	1:B:83:LEU:HD23	2.38	0.43
1:C:474:MET:CE	1:C:479:LEU:HD13	2.48	0.43
1:D:359:GLU:O	1:D:360:TRP:CB	2.67	0.43
1:D:583:SER:HG	1:D:584:HIS:HD1	1.58	0.43
1:C:318:SER:OG	1:C:319:ARG:N	2.52	0.43
1:B:72:ARG:NH2	1:B:108:LEU:HD22	2.34	0.43
1:D:212:PHE:CZ	1:D:232:VAL:HG23	2.54	0.43
1:A:316:TRP:CE3	1:A:344:VAL:HG11	2.54	0.43
1:A:350:GLY:HA2	1:A:355:ASP:HA	2.00	0.43
1:B:116:LYS:O	1:B:118:ILE:N	2.52	0.43
1:D:364:GLU:O	1:D:365:GLU:HB2	2.19	0.43
1:D:215:MET:HE3	1:D:636:ALA:HB1	2.00	0.43
1:A:37:LYS:HB3	1:A:41:ILE:N	2.34	0.42
1:A:211:ARG:HH12	1:A:237:THR:CB	2.32	0.42
1:A:602:ALA:N	1:A:603:PRO:CD	2.82	0.42
1:C:54:ASN:HB3	1:C:55:ASP:H	1.62	0.42
1:C:154:THR:HG23	1:C:164:ARG:HB3	2.02	0.42
1:C:549:TRP:CZ3	1:C:551:HIS:HD2	2.36	0.42
1:D:52:LEU:CD1	1:D:59:ASP:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ILE:HD11	1:B:467:MET:SD	2.60	0.42
1:B:601:ILE:H	1:B:601:ILE:HG13	1.71	0.42
1:C:561:ASN:OD1	1:C:564:ASN:HB2	2.19	0.42
1:D:30:LYS:NZ	1:D:132:VAL:O	2.52	0.42
1:A:224:LEU:HB2	1:A:260:SER:HB2	2.02	0.42
1:A:245:LEU:HD13	1:A:291:MET:HE2	2.00	0.42
1:A:37:LYS:H	1:A:38:ASP:HA	1.85	0.42
1:B:118:ILE:HD12	1:B:118:ILE:H	1.83	0.42
1:B:191:GLU:CA	1:B:279:ALA:HB2	2.49	0.42
1:B:592:LYS:H	1:B:592:LYS:HD2	1.85	0.42
1:B:175:ARG:NE	1:D:230:GLN:OE1	2.52	0.42
1:D:321:THR:HG21	1:D:350:GLY:H	1.84	0.42
1:D:28:ALA:HB2	1:D:48:GLN:NE2	2.34	0.42
1:A:144:LEU:HD21	1:A:172:SER:HB3	2.01	0.42
1:B:190:LYS:HD3	1:B:190:LYS:H	1.85	0.42
1:A:309:PRO:HG3	1:A:501:ASP:HB3	2.01	0.42
1:A:551:HIS:HE1	1:A:579:GLY:HA2	1.84	0.42
1:A:676:LEU:HD11	1:A:690:LEU:HD13	2.01	0.42
1:B:352:PHE:C	1:B:354:THR:H	2.23	0.42
1:C:688:GLU:HG2	1:C:690:LEU:HD21	2.02	0.42
1:D:130:ILE:HD12	1:D:130:ILE:N	2.34	0.42
1:D:211:ARG:NH1	1:D:237:THR:OG1	2.52	0.42
1:A:118:ILE:O	1:A:119:LEU:HD23	2.19	0.42
1:A:517:PRO:HA	1:A:518:LEU:HA	1.84	0.42
1:C:505:TRP:CD1	1:C:520:TRP:CE3	3.08	0.42
1:C:53:ALA:H	1:C:54:ASN:HB2	1.85	0.42
1:C:567:VAL:O	1:C:568:ALA:HB3	2.20	0.42
1:C:616:ILE:N	1:C:617:PRO:HD2	2.33	0.42
1:D:48:GLN:HG2	1:D:183:PHE:HE2	1.85	0.42
1:D:635:GLN:HB2	1:D:655:TYR:HB2	2.02	0.42
1:D:76:ILE:HD12	1:D:106:VAL:HG12	2.01	0.42
1:A:23:GLU:HA	1:A:185:LYS:O	2.19	0.42
1:C:158:ASP:HB2	1:C:287:ALA:HB1	2.01	0.42
1:C:232:VAL:HG13	1:C:232:VAL:O	2.20	0.42
1:C:463:GLU:OE1	1:C:507:ARG:NH2	2.53	0.42
1:A:173:PRO:O	1:A:176:TYR:HE1	2.03	0.42
1:C:602:ALA:HB3	1:C:603:PRO:HD3	2.01	0.42
1:A:27:LYS:O	1:A:48:GLN:HA	2.20	0.41
1:A:561:ASN:CG	1:A:564:ASN:HB2	2.40	0.41
1:B:465:ILE:HD12	1:B:480:ASN:HD22	1.85	0.41
1:B:55:ASP:N	1:B:55:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TYR:CZ	1:C:272:VAL:HG11	2.54	0.41
1:C:517:PRO:HA	1:C:518:LEU:HA	1.84	0.41
1:C:651:ASP:OD2	1:C:651:ASP:N	2.52	0.41
1:D:292:GLU:HG3	1:D:631:TRP:CE2	2.54	0.41
1:A:57:VAL:HG22	1:A:58:ALA:N	2.35	0.41
1:C:115:GLY:HA2	1:C:119:LEU:HD13	2.02	0.41
1:C:353:ARG:HA	1:C:362:PHE:HD2	1.83	0.41
1:A:144:LEU:HD22	1:C:563:MET:CE	2.50	0.41
1:A:326:ASP:O	1:A:330:GLU:HG3	2.19	0.41
1:A:367:PHE:CD2	1:A:368:PRO:HD2	2.55	0.41
1:A:51:LEU:HD22	1:A:51:LEU:N	2.34	0.41
1:B:49:LYS:C	1:B:49:LYS:HD3	2.41	0.41
1:C:686:THR:HG21	1:C:688:GLU:HB2	2.03	0.41
1:D:26:TRP:HA	1:D:50:GLN:HB2	2.02	0.41
1:A:126:LYS:C	1:A:126:LYS:HD2	2.41	0.41
1:A:163:ILE:HD11	1:A:197:PHE:CD2	2.54	0.41
1:A:553:VAL:HA	1:A:554:PRO:HA	1.89	0.41
1:B:31:PRO:HD2	1:B:132:VAL:CG1	2.49	0.41
1:C:212:PHE:CE1	1:C:232:VAL:HG22	2.55	0.41
1:D:113:GLN:CB	1:D:114:GLY:CA	2.97	0.41
1:A:614:SER:O	1:A:718:ILE:HB	2.19	0.41
1:B:125:THR:HA	1:B:126:LYS:HA	1.89	0.41
1:B:601:ILE:O	1:B:602:ALA:CB	2.67	0.41
1:A:241:ILE:CG2	1:A:243:PHE:HB3	2.51	0.41
1:B:139:ARG:HD2	1:B:139:ARG:HA	1.69	0.41
1:B:450:LEU:CB	1:B:498:VAL:HG21	2.51	0.41
1:B:594:GLU:HA	1:B:595:PRO:HD3	1.83	0.41
1:C:134:GLU:HB2	1:C:135:PRO:CA	2.51	0.41
1:C:348:ASP:C	1:C:350:GLY:H	2.23	0.41
1:D:135:PRO:O	1:D:136:ALA:HB2	2.20	0.41
1:B:493:GLU:O	1:B:497:GLU:HB2	2.20	0.41
1:A:27:LYS:HG3	1:A:179:LEU:HD22	2.02	0.41
1:A:17:THR:HA	1:A:18:GLU:HA	1.79	0.41
1:A:361:LYS:O	1:A:362:PHE:HB2	2.21	0.41
1:B:224:LEU:N	1:B:260:SER:O	2.54	0.41
1:C:357:LEU:HD23	1:C:359:GLU:H	1.86	0.41
1:D:37:LYS:HA	1:D:42:CYS:HA	2.03	0.41
1:D:347:LEU:N	1:D:347:LEU:HD22	2.35	0.41
1:C:319:ARG:HG2	1:C:320:MET:N	2.36	0.41
1:C:242:PRO:HD2	1:C:511:ALA:HB2	2.03	0.41
1:A:594:GLU:HA	1:A:595:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ILE:N	1:A:617:PRO:CD	2.84	0.41
1:B:701:VAL:HG11	1:B:707:PRO:HD3	2.03	0.41
1:B:83:LEU:HB3	1:B:281:LEU:CD1	2.50	0.41
1:D:134:GLU:N	1:D:135:PRO:CD	2.80	0.41
1:A:173:PRO:N	1:A:174:PRO:CD	2.84	0.40
1:A:30:LYS:HD3	1:A:133:GLU:CD	2.41	0.40
1:A:315:VAL:HA	1:A:585:ILE:HG23	2.02	0.40
1:A:717:PRO:C	1:A:718:ILE:HG22	2.42	0.40
1:B:27:LYS:O	1:B:48:GLN:HA	2.21	0.40
1:B:600:ALA:HA	1:B:601:ILE:C	2.42	0.40
1:C:461:PHE:H	1:C:507:ARG:NH1	2.19	0.40
1:D:72:ARG:HH11	1:D:108:LEU:HD13	1.86	0.40
1:A:338:GLU:HB3	1:A:340:TYR:CD2	2.55	0.40
1:B:204:CYS:HB2	1:B:648:TRP:CE3	2.56	0.40
1:D:292:GLU:OE1	1:D:296:ARG:NH2	2.53	0.40
1:D:315:VAL:HA	1:D:585:ILE:HG23	2.04	0.40
1:D:75:ASN:N	1:D:75:ASN:OD1	2.53	0.40
1:D:96:MET:HB3	1:D:97:LEU:H	1.65	0.40
1:A:144:LEU:CD2	1:A:172:SER:HB3	2.51	0.40
1:A:30:LYS:HE3	1:A:149:GLU:HG2	2.03	0.40
1:B:207:GLY:O	1:B:208:THR:OG1	2.27	0.40
1:C:349:THR:HG21	1:C:356:TRP:CZ2	2.56	0.40
1:C:505:TRP:CZ2	1:C:586:ARG:HD2	2.56	0.40
1:C:41:ILE:HG21	1:C:72:ARG:HE	1.86	0.40
1:D:173:PRO:N	1:D:174:PRO:CD	2.84	0.40
1:D:51:LEU:O	1:D:52:LEU:HB2	2.21	0.40
1:B:435:TYR:CD2	1:B:438:ALA:HB2	2.55	0.40
1:D:49:LYS:NZ	1:D:64:ARG:HH21	2.20	0.40
1:A:458:LYS:HA	1:A:505:TRP:HB3	2.03	0.40
1:A:54:ASN:HA	1:A:55:ASP:HA	1.98	0.40
1:C:41:ILE:HG22	1:C:72:ARG:HD3	2.02	0.40
1:D:352:PHE:N	1:D:352:PHE:CD1	2.89	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	619/761 (81%)	518 (84%)	71 (12%)	30 (5%)	2	3
1	B	605/761 (80%)	523 (86%)	59 (10%)	23 (4%)	3	4
1	C	626/761 (82%)	537 (86%)	66 (10%)	23 (4%)	4	5
1	D	617/761 (81%)	532 (86%)	55 (9%)	30 (5%)	2	3
All	All	2467/3044 (81%)	2110 (86%)	251 (10%)	106 (4%)	3	3

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	133	GLU
1	A	137	LEU
1	A	142	GLU
1	A	162	GLU
1	A	355	ASP
1	A	359	GLU
1	A	360	TRP
1	A	361	LYS
1	A	362	PHE
1	A	687	GLY
1	A	713	ASN
1	B	31	PRO
1	B	32	THR
1	B	51	LEU
1	B	107	PRO
1	B	142	GLU
1	B	602	ALA
1	C	55	ASP
1	C	105	ARG
1	C	116	LYS
1	C	142	GLU
1	C	357	LEU
1	C	359	GLU
1	C	363	ASN
1	D	103	ILE
1	D	107	PRO
1	D	134	GLU

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Mol	Chain	Res	Type
1	D	136	ALA
1	D	137	LEU
1	D	142	GLU
1	D	351	TRP
1	D	359	GLU
1	D	360	TRP
1	A	15	PHE
1	A	54	ASN
1	A	86	GLY
1	A	123	ASP
1	A	124	GLY
1	A	138	ASP
1	A	437	LYS
1	A	561	ASN
1	B	39	GLY
1	B	349	THR
1	C	32	THR
1	C	39	GLY
1	C	57	VAL
1	C	98	GLN
1	C	143	LEU
1	C	366	ARG
1	C	526	SER
1	D	33	ALA
1	D	38	ASP
1	D	357	LEU
1	A	715	VAL
1	B	104	ARG
1	B	117	TRP
1	B	668	SER
1	C	351	TRP
1	C	356	TRP
1	D	51	LEU
1	D	53	ALA
1	D	113	GLN
1	D	323	PHE
1	D	362	PHE
1	D	568	ALA
1	D	601	ILE
1	D	686	THR
1	A	161	ARG
1	A	255	HIS

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Mol	Chain	Res	Type
1	A	568	ALA
1	B	34	VAL
1	B	55	ASP
1	B	123	ASP
1	B	140	TRP
1	B	160	LYS
1	B	324	SER
1	C	53	ALA
1	C	140	TRP
1	C	600	ALA
1	C	602	ALA
1	D	123	ASP
1	D	363	ASN
1	D	472	LYS
1	A	139	ARG
1	A	714	ALA
1	B	224	LEU
1	B	354	THR
1	C	102	ARG
1	D	57	VAL
1	D	718	ILE
1	A	85	PHE
1	B	599	PRO
1	D	39	GLY
1	D	77	GLY
1	D	692	GLY
1	B	76	ILE
1	A	367	PHE
1	A	554	PRO
1	D	115	GLY
1	A	436	PRO
1	C	473	GLY
1	B	57	VAL
1	B	554	PRO
1	C	554	PRO
1	D	554	PRO

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	512/663 (77%)	460 (90%)	52 (10%)	8	15
1	B	504/663 (76%)	460 (91%)	44 (9%)	11	22
1	C	527/663 (80%)	495 (94%)	32 (6%)	20	41
1	D	507/663 (76%)	464 (92%)	43 (8%)	12	23
All	All	2050/2652 (77%)	1879 (92%)	171 (8%)	12	24

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	PHE
1	A	15	PHE
1	A	18	GLU
1	A	20	LEU
1	A	21	ARG
1	A	43	VAL
1	A	48	GLN
1	A	52	LEU
1	A	68	THR
1	A	75	ASN
1	A	83	LEU
1	A	87	GLU
1	A	123	ASP
1	A	126	LYS
1	A	144	LEU
1	A	158	ASP
1	A	161	ARG
1	A	163	ILE
1	A	200	ARG
1	A	215	MET
1	A	232	VAL
1	A	241	ILE
1	A	249	MET
1	A	269	THR
1	A	278	GLN
1	A	280	MET
1	A	338	GLU
1	A	342	CYS
1	A	343	ASP

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Mol	Chain	Res	Type
1	A	362	PHE
1	A	367	PHE
1	A	449	LEU
1	A	474	MET
1	A	475	LYS
1	A	494	ILE
1	A	504	VAL
1	A	518	LEU
1	A	520	TRP
1	A	551	HIS
1	A	563	MET
1	A	574	ARG
1	A	583	SER
1	A	593	ARG
1	A	634	LEU
1	A	651	ASP
1	A	672	ARG
1	A	680	GLN
1	A	697	LYS
1	A	711	ARG
1	A	715	VAL
1	A	718	ILE
1	B	44	THR
1	B	48	GLN
1	B	49	LYS
1	B	72	ARG
1	B	79	THR
1	B	102	ARG
1	B	111	GLU
1	B	123	ASP
1	B	125	THR
1	B	137	LEU
1	B	160	LYS
1	B	163	ILE
1	B	177	ASP
1	B	186	ARG
1	B	189	LYS
1	B	190	LYS
1	B	195	LEU
1	B	200	ARG
1	B	281	LEU
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	330	GLU
1	B	334	ARG
1	B	343	ASP
1	B	345	ILE
1	B	354	THR
1	B	430	THR
1	B	445	LEU
1	B	465	ILE
1	B	472	LYS
1	B	475	LYS
1	B	518	LEU
1	B	520	TRP
1	B	559	LEU
1	B	564	ASN
1	B	592	LYS
1	B	593	ARG
1	B	614	SER
1	B	625	LEU
1	B	634	LEU
1	B	651	ASP
1	B	667	ASN
1	B	669	GLU
1	B	710	VAL
1	B	713	ASN
1	C	35	TYR
1	C	44	THR
1	C	70	ILE
1	C	83	LEU
1	C	102	ARG
1	C	113	GLN
1	C	122	GLN
1	C	137	LEU
1	C	140	TRP
1	C	163	ILE
1	C	192	ARG
1	C	194	THR
1	C	195	LEU
1	C	208	THR
1	C	225	LYS
1	C	232	VAL
1	C	261	LYS
1	C	348	ASP

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Mol	Chain	Res	Type
1	C	351	TRP
1	C	356	TRP
1	C	454	VAL
1	C	463	GLU
1	C	475	LYS
1	C	497	GLU
1	C	504	VAL
1	C	518	LEU
1	C	520	TRP
1	C	583	SER
1	C	593	ARG
1	C	625	LEU
1	C	651	ASP
1	C	701	VAL
1	D	29	CYS
1	D	37	LYS
1	D	41	ILE
1	D	48	GLN
1	D	56	MET
1	D	70	ILE
1	D	81	LEU
1	D	83	LEU
1	D	96	MET
1	D	97	LEU
1	D	102	ARG
1	D	113	GLN
1	D	118	ILE
1	D	126	LYS
1	D	162	GLU
1	D	163	ILE
1	D	189	LYS
1	D	194	THR
1	D	215	MET
1	D	225	LYS
1	D	272	VAL
1	D	310	LEU
1	D	343	ASP
1	D	348	ASP
1	D	352	PHE
1	D	357	LEU
1	D	359	GLU
1	D	514	GLN

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Mol	Chain	Res	Type
1	D	518	LEU
1	D	520	TRP
1	D	563	MET
1	D	567	VAL
1	D	586	ARG
1	D	591	ASN
1	D	593	ARG
1	D	607	LYS
1	D	628	GLU
1	D	633	LEU
1	D	634	LEU
1	D	651	ASP
1	D	697	LYS
1	D	701	VAL
1	D	704	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	B	255	HIS
1	B	551	HIS
1	B	591	ASN
1	B	649	HIS
1	D	113	GLN
1	D	259	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	625/761 (82%)	0.47	38 (6%) 21 15	22, 45, 78, 95	0
1	B	611/761 (80%)	1.21	125 (20%) 1 0	47, 64, 88, 96	0
1	C	632/761 (83%)	0.62	45 (7%) 16 11	25, 49, 83, 95	0
1	D	623/761 (81%)	0.82	71 (11%) 5 3	32, 53, 87, 101	0
All	All	2491/3044 (81%)	0.78	279 (11%) 5 3	22, 56, 85, 101	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	GLY	7.6
1	D	113	GLN	6.7
1	B	59	ASP	6.5
1	B	468	ASP	6.5
1	B	52	LEU	6.3
1	B	62	VAL	6.3
1	D	119	LEU	6.2
1	C	337	ALA	6.2
1	A	470	VAL	6.1
1	D	470	VAL	6.1
1	B	117	TRP	5.8
1	C	54	ASN	5.7
1	D	323	PHE	5.7
1	B	323	PHE	5.5
1	B	439	THR	5.4
1	B	58	ALA	5.4
1	B	601	ILE	5.3
1	D	53	ALA	5.3
1	C	120	PHE	5.3
1	B	689	ARG	5.2
1	D	468	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	5.2
1	D	352	PHE	5.0
1	B	442	TYR	5.0
1	B	27	LYS	5.0
1	B	29	CYS	4.9
1	B	470	VAL	4.8
1	D	188	GLY	4.8
1	B	566	ILE	4.8
1	D	471	TYR	4.8
1	A	54	ASN	4.8
1	B	437	LYS	4.8
1	B	110	VAL	4.7
1	D	54	ASN	4.6
1	B	718	ILE	4.5
1	B	122	GLN	4.4
1	A	477	GLU	4.4
1	B	143	LEU	4.4
1	B	472	LYS	4.3
1	B	69	LEU	4.3
1	D	120	PHE	4.3
1	D	328	VAL	4.2
1	A	691	GLN	4.1
1	D	40	ASP	4.1
1	B	51	LEU	4.1
1	D	71	ILE	4.1
1	B	60	THR	4.1
1	B	130	ILE	4.1
1	D	360	TRP	4.0
1	B	65	GLU	3.9
1	C	713	ASN	3.9
1	B	142	GLU	3.8
1	B	186	ARG	3.8
1	D	601	ILE	3.8
1	D	143	LEU	3.8
1	C	356	TRP	3.8
1	C	40	ASP	3.8
1	B	68	THR	3.7
1	C	99	PHE	3.7
1	B	434	THR	3.6
1	B	487	TYR	3.6
1	B	218	SER	3.5
1	B	627	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	110	VAL	3.5
1	D	337	ALA	3.4
1	B	120	PHE	3.4
1	B	177	ASP	3.4
1	B	719	TYR	3.4
1	D	130	ILE	3.4
1	A	720	PRO	3.4
1	B	454	VAL	3.4
1	C	57	VAL	3.4
1	D	133	GLU	3.4
1	A	13	PHE	3.3
1	A	62	VAL	3.3
1	C	33	ALA	3.3
1	B	118	ILE	3.3
1	B	137	LEU	3.3
1	D	60	THR	3.3
1	B	127	ARG	3.3
1	D	354	THR	3.3
1	B	351	TRP	3.2
1	C	35	TYR	3.2
1	B	354	THR	3.2
1	B	28	ALA	3.2
1	B	211	ARG	3.2
1	B	49	LYS	3.1
1	B	44	THR	3.1
1	B	310	LEU	3.1
1	A	466	HIS	3.1
1	D	27	LYS	3.1
1	B	455	THR	3.1
1	C	323	PHE	3.1
1	D	450	LEU	3.1
1	D	187	THR	3.0
1	B	161	ARG	3.0
1	B	435	TYR	3.0
1	B	337	ALA	3.0
1	B	604	LEU	3.0
1	A	129	VAL	3.0
1	D	334	ARG	3.0
1	D	449	LEU	3.0
1	D	466	HIS	3.0
1	B	694	ARG	3.0
1	B	313	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	478	LEU	3.0
1	B	53	ALA	3.0
1	C	619	ILE	2.9
1	D	333	ASP	2.9
1	B	26	TRP	2.9
1	C	360	TRP	2.9
1	B	35	TYR	2.9
1	B	116	LYS	2.9
1	D	62	VAL	2.9
1	B	140	TRP	2.9
1	A	144	LEU	2.9
1	B	265	ALA	2.9
1	C	70	ILE	2.9
1	B	469	ALA	2.9
1	D	41	ILE	2.8
1	D	429	GLY	2.8
1	D	475	LYS	2.8
1	B	123	ASP	2.8
1	C	350	GLY	2.8
1	B	81	LEU	2.8
1	A	20	LEU	2.8
1	B	289	ASP	2.8
1	B	451	ASP	2.8
1	D	218	SER	2.8
1	D	339	HIS	2.8
1	D	469	ALA	2.7
1	B	453	GLY	2.7
1	C	686	THR	2.7
1	D	144	LEU	2.7
1	C	134	GLU	2.7
1	D	311	TRP	2.7
1	A	52	LEU	2.7
1	A	150	THR	2.7
1	B	334	ARG	2.7
1	B	680	GLN	2.7
1	C	119	LEU	2.7
1	A	42	CYS	2.7
1	B	219	GLY	2.7
1	D	73	GLN	2.7
1	D	690	LEU	2.7
1	A	188	GLY	2.6
1	C	113	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	431	ILE	2.6
1	B	715	VAL	2.6
1	A	70	ILE	2.6
1	B	125	THR	2.6
1	A	12	LEU	2.6
1	B	155	LEU	2.6
1	D	111	GLU	2.6
1	A	140	TRP	2.6
1	B	157	PRO	2.6
1	B	220	GLN	2.6
1	B	691	GLN	2.6
1	A	187	THR	2.5
1	A	686	THR	2.5
1	B	181	ILE	2.5
1	B	720	PRO	2.5
1	B	676	LEU	2.5
1	D	703	LEU	2.5
1	C	32	THR	2.5
1	A	125	THR	2.5
1	C	470	VAL	2.5
1	B	667	ASN	2.5
1	C	97	LEU	2.5
1	D	448	GLN	2.5
1	B	671	ARG	2.5
1	A	368	PRO	2.5
1	B	431	ILE	2.5
1	B	43	VAL	2.5
1	C	56	MET	2.5
1	A	124	GLY	2.4
1	B	465	ILE	2.4
1	D	70	ILE	2.4
1	C	328	VAL	2.4
1	B	438	ALA	2.4
1	C	121	THR	2.4
1	B	352	PHE	2.4
1	B	251	GLY	2.4
1	C	125	THR	2.4
1	C	469	ALA	2.4
1	D	137	LEU	2.4
1	D	438	ALA	2.4
1	D	50	GLN	2.4
1	D	441	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	ALA	2.4
1	A	132	VAL	2.4
1	B	82	PHE	2.4
1	D	461	PHE	2.4
1	B	149	GLU	2.4
1	D	428	ALA	2.4
1	D	324	SER	2.4
1	D	37	LYS	2.4
1	C	31	PRO	2.4
1	D	109	SER	2.4
1	B	111	GLU	2.4
1	B	189	LYS	2.3
1	C	30	LYS	2.3
1	D	118	ILE	2.3
1	D	353	ARG	2.3
1	A	49	LYS	2.3
1	B	173	PRO	2.3
1	B	141	SER	2.3
1	C	678	GLU	2.3
1	B	41	ILE	2.3
1	B	150	THR	2.3
1	D	431	ILE	2.3
1	B	475	LYS	2.3
1	A	604	LEU	2.3
1	D	28	ALA	2.3
1	A	328	VAL	2.3
1	B	477	GLU	2.3
1	B	36	GLU	2.3
1	A	689	ARG	2.3
1	B	690	LEU	2.3
1	A	435	TYR	2.3
1	B	42	CYS	2.3
1	C	716	ILE	2.3
1	C	687	GLY	2.2
1	D	362	PHE	2.2
1	B	229	GLY	2.2
1	B	319	ARG	2.2
1	C	694	ARG	2.2
1	A	269	THR	2.2
1	A	45	VAL	2.2
1	B	34	VAL	2.2
1	C	25	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	176	TYR	2.2
1	B	57	VAL	2.2
1	A	46	PRO	2.2
1	B	490	ALA	2.2
1	A	471	TYR	2.2
1	B	471	TYR	2.2
1	B	234	ASN	2.2
1	C	50	GLN	2.2
1	C	712	GLU	2.2
1	D	42	CYS	2.2
1	D	115	GLY	2.2
1	D	76	ILE	2.1
1	D	58	ALA	2.1
1	A	24	SER	2.1
1	C	46	PRO	2.1
1	C	150	THR	2.1
1	B	204	CYS	2.1
1	D	57	VAL	2.1
1	B	446	LEU	2.1
1	B	709	TYR	2.1
1	C	428	ALA	2.1
1	B	713	ASN	2.1
1	B	271	SER	2.1
1	D	219	GLY	2.1
1	C	53	ALA	2.1
1	D	68	THR	2.1
1	C	366	ARG	2.1
1	B	712	GLU	2.1
1	D	97	LEU	2.1
1	B	603	PRO	2.1
1	C	104	ARG	2.1
1	B	134	GLU	2.1
1	B	688	GLU	2.1
1	B	217	LEU	2.1
1	B	703	LEU	2.1
1	B	654	TYR	2.1
1	D	79	THR	2.1
1	A	17	THR	2.0
1	B	185	LYS	2.0
1	D	110	VAL	2.0
1	C	340	TYR	2.0
1	A	219	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	231	GLY	2.0
1	B	537	GLY	2.0
1	B	572	TYR	2.0
1	D	121	THR	2.0
1	C	107	PRO	2.0
1	D	472	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.