



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 05:44 PM EDT

PDB ID : 8SAO
Title : Crystal structure of class III lanthipeptide synthetase ThurKC in complex with ThurA1 leader peptide
Authors : Hernandez Garcia, A.; Nair, S.K.
Deposited on : 2023-04-01
Resolution : 2.50 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

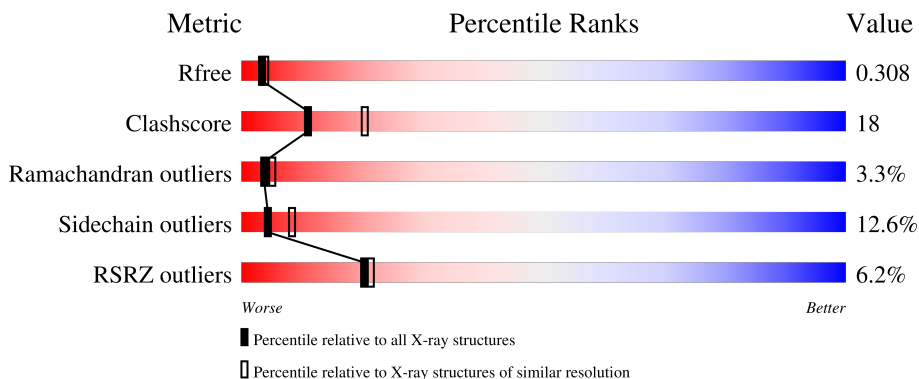
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	14	
1	C	14	
2	B	859	
2	D	859	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13859 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 Class III lanthipeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	14	109	68	19	21	1	0	0	0
1	C	14	109	68	19	21	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	ALA	-	expression tag	UNP A0A7U1BAR4
C	-29	ALA	-	expression tag	UNP A0A7U1BAR4

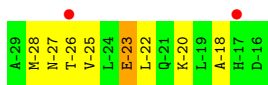
- Molecule 2 is a protein called Class III lanthionine synthetase LanKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	845	6821	4379	1128	1292	22	0	0	0
2	D	845	6820	4380	1128	1290	22	0	0	0

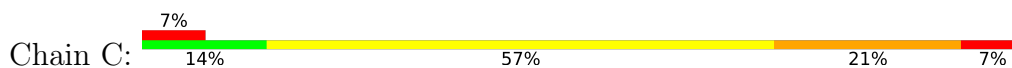
3 Residue-property plots [i](#)

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.

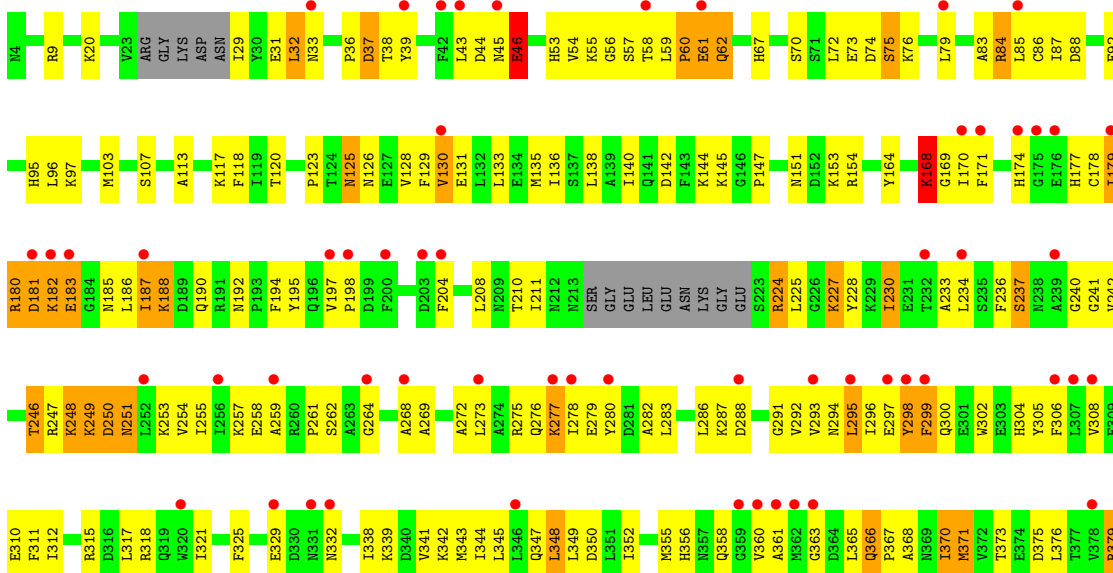
- Molecule 1: Class III lanthipeptide

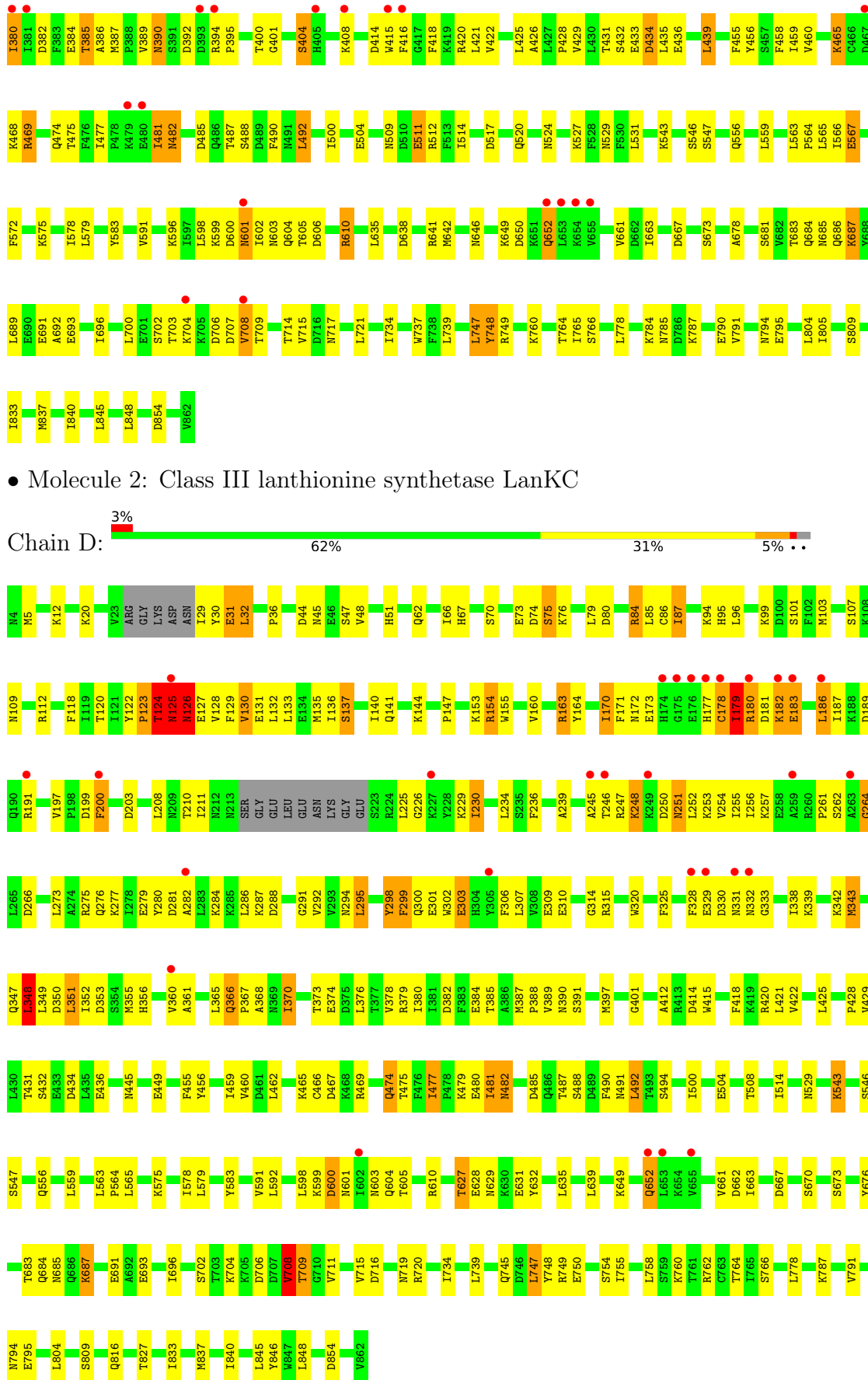


- Molecule 1: Class III lanthipeptide



- Molecule 2: Class III lanthionine synthetase LanKC





● Molecule 2: Class III lanthionine synthetase LanKC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 52.90Å 233.42Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	232.25 – 2.50 232.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (232.25-2.50) 96.9 (232.25-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.52Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.246 , 0.307 0.245 , 0.308	Depositor DCC
R_{free} test set	3260 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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	0.30	0/109	0.64	0/146
1	C	0.30	0/109	0.68	0/146
2	B	0.29	0/6954	0.69	2/9383 (0.0%)
2	D	0.31	0/6953	0.70	1/9382 (0.0%)
All	All	0.30	0/14125	0.69	3/19057 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	794	ASN	CB-CA-C	5.74	121.87	110.40
2	B	33	ASN	CB-CA-C	5.53	121.47	110.40
2	D	627	THR	CB-CA-C	-5.18	97.61	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LYS	Peptide
2	D	600	ASP	Peptide
2	D	604	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	109	0	114	7	0
1	C	109	0	114	20	0
2	B	6821	0	6812	255	0
2	D	6820	0	6817	239	0
All	All	13859	0	13857	502	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 (502) 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)
2:B:83:ALA:O	2:B:87:ILE:HG12	1.49	1.12
2:B:404:SER:HB3	2:B:416:PHE:HE2	0.99	1.08
2:B:404:SER:HB3	2:B:416:PHE:CE2	1.92	1.04
2:B:650:ASP:OD2	2:B:652:GLN:HG2	1.58	1.03
1:C:-28:MET:HB2	2:D:302:TRP:CD1	1.93	1.03
2:D:178:CYS:HB2	2:D:189:ASP:HB3	1.42	0.98
2:D:627:THR:O	2:D:627:THR:OG1	1.76	0.97
2:B:401:GLY:HA2	2:B:431:THR:O	1.65	0.96
2:D:137:SER:HG	2:D:155:TRP:HZ3	0.95	0.94
2:D:172:ASN:HB3	2:D:179:ILE:HD13	1.48	0.94
2:D:36:PRO:HG2	2:D:87:ILE:HG21	1.50	0.93
2:B:420:ARG:HE	2:B:431:THR:HG22	1.34	0.93
2:D:85:LEU:O	2:D:85:LEU:HD23	1.68	0.91
2:D:420:ARG:HE	2:D:431:THR:HG22	1.32	0.91
2:D:401:GLY:HA2	2:D:431:THR:O	1.72	0.90
2:D:295:LEU:HD23	2:D:295:LEU:H	1.33	0.90
2:D:627:THR:O	2:D:629:ASN:N	2.07	0.86
2:D:266:ASP:OD2	2:D:275:ARG:HD3	1.77	0.85
2:D:481:ILE:HG22	2:D:482:ASN:H	1.42	0.83
2:B:254:VAL:HA	2:B:311:PHE:HB2	1.59	0.83
2:B:168:LYS:HG2	2:B:169:GLY:H	1.41	0.83
2:B:247:ARG:HG3	2:B:249:LYS:HZ2	1.43	0.82
2:D:791:VAL:O	2:D:795:GLU:HG3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-27:ASN:O	1:A:-23:GLU:HB3	1.81	0.81
2:B:286:LEU:HD23	2:B:358:GLN:HG3	1.62	0.81
2:D:477:ILE:O	2:D:477:ILE:HG13	1.80	0.80
1:C:-28:MET:CB	2:D:302:TRP:CD1	2.65	0.80
2:B:760:LYS:HD3	2:B:795:GLU:OE1	1.81	0.79
2:B:404:SER:CB	2:B:416:PHE:HE2	1.92	0.79
2:B:299:PHE:CE1	2:B:306:PHE:HB2	2.18	0.79
2:D:125:ASN:O	2:D:127:GLU:N	2.15	0.78
2:B:131:GLU:O	2:B:135:MET:HG3	1.83	0.78
1:A:-25:VAL:HG11	2:B:302:TRP:CE3	2.20	0.76
1:C:-25:VAL:HG21	2:D:302:TRP:CB	2.15	0.76
2:B:465:LYS:O	2:B:468:LYS:HB2	1.86	0.76
2:B:456:TYR:O	2:B:460:VAL:HG23	1.87	0.75
2:D:171:PHE:HD1	2:D:177:HIS:HA	1.51	0.75
2:D:181:ASP:HA	2:D:186:LEU:HA	1.68	0.75
2:D:163:ARG:NH2	2:D:189:ASP:OD1	2.19	0.75
2:D:31:GLU:O	2:D:32:LEU:HB2	1.87	0.74
2:D:295:LEU:HD23	2:D:295:LEU:N	2.02	0.74
2:B:455:PHE:CE1	2:B:459:ILE:HD11	2.23	0.74
2:D:361:ALA:HB2	2:D:389:VAL:HG12	1.69	0.74
2:D:208:LEU:HA	2:D:211:ILE:HG22	1.69	0.73
2:D:180:ARG:HG2	2:D:189:ASP:HB2	1.71	0.72
1:A:-26:THR:HA	1:A:-23:GLU:HG2	1.71	0.72
2:B:737:TRP:HE1	2:B:784:LYS:CE	2.03	0.72
2:D:29:ILE:HG22	2:D:30:TYR:H	1.55	0.72
2:B:358:GLN:HB2	2:B:360:VAL:HG12	1.72	0.72
2:D:816:GLN:HG2	2:D:827:THR:HG21	1.72	0.72
2:B:60:PRO:HB2	2:B:62:GLN:O	1.90	0.71
2:B:329:GLU:HB3	2:B:760:LYS:HB3	1.72	0.71
2:B:125:ASN:CG	2:B:126:ASN:H	1.93	0.71
2:D:137:SER:OG	2:D:155:TRP:HZ3	1.70	0.71
2:B:345:LEU:HD11	2:B:425:LEU:HD13	1.71	0.71
2:D:66:ILE:HD12	2:D:133:LEU:CD2	2.22	0.70
2:D:420:ARG:HE	2:D:431:THR:CG2	2.05	0.70
2:B:599:LYS:HD3	2:B:635:LEU:HD13	1.73	0.70
2:D:171:PHE:CD1	2:D:177:HIS:HA	2.26	0.70
2:D:126:ASN:HD22	2:D:126:ASN:H	1.40	0.70
1:A:-28:MET:HB3	2:B:302:TRP:NE1	2.07	0.70
2:B:420:ARG:HE	2:B:431:THR:CG2	2.04	0.70
2:D:284:LYS:HA	2:D:287:LYS:HG3	1.73	0.70
1:C:-29:ALA:C	1:C:-27:ASN:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:LYS:O	2:D:280:TYR:N	2.24	0.69
2:B:37:ASP:C	2:B:39:TYR:H	1.96	0.69
2:D:456:TYR:O	2:D:460:VAL:HG23	1.93	0.69
1:C:-25:VAL:HG21	2:D:302:TRP:HB2	1.74	0.69
2:D:348:LEU:HD22	2:D:378:VAL:HG11	1.75	0.69
2:B:130:VAL:HG12	2:B:130:VAL:O	1.93	0.69
2:D:455:PHE:CE1	2:D:459:ILE:HD11	2.27	0.69
2:B:181:ASP:HB2	2:B:187:ILE:HG12	1.76	0.68
2:D:130:VAL:HG12	2:D:130:VAL:O	1.92	0.68
2:B:60:PRO:C	2:B:62:GLN:H	1.96	0.68
2:D:48:VAL:HG22	2:D:101:SER:HB3	1.75	0.68
2:D:208:LEU:HA	2:D:211:ILE:CG2	2.24	0.68
1:C:-22:LEU:HA	1:C:-19:LEU:HD12	1.76	0.67
2:B:345:LEU:HD21	2:B:422:VAL:HA	1.78	0.66
1:A:-28:MET:HB3	2:B:302:TRP:CE2	2.31	0.66
2:B:348:LEU:O	2:B:352:ILE:HG13	1.96	0.66
2:D:421:LEU:HD12	2:D:425:LEU:HD23	1.77	0.66
2:B:566:ILE:O	2:B:575:LYS:NZ	2.27	0.65
2:B:421:LEU:HD11	2:B:425:LEU:HD11	1.78	0.65
2:D:292:VAL:HG22	2:D:355:MET:HE2	1.79	0.65
2:D:126:ASN:HD22	2:D:126:ASN:N	1.91	0.65
2:B:246:THR:HG23	2:B:253:LYS:HG3	1.79	0.64
2:B:524:ASN:HB3	2:B:567:GLU:OE2	1.97	0.64
2:D:279:GLU:O	2:D:279:GLU:HG2	1.97	0.64
2:D:663:ILE:HD11	2:D:716:ASP:HA	1.78	0.64
2:B:287:LYS:HE3	2:B:294:ASN:HB3	1.79	0.64
2:B:349:LEU:HD11	2:B:469:ARG:HH21	1.61	0.64
2:B:421:LEU:O	2:B:425:LEU:HD12	1.97	0.64
2:B:279:GLU:HG2	2:B:279:GLU:O	1.97	0.64
1:C:-21:GLN:HB3	2:D:112:ARG:HH12	1.62	0.64
2:D:348:LEU:HB3	2:D:418:PHE:CE1	2.33	0.64
2:B:604:GLN:HG3	2:B:606:ASP:H	1.63	0.63
2:B:73:GLU:HG2	2:B:74:ASP:N	2.14	0.63
2:B:228:TYR:CD2	2:B:247:ARG:HB2	2.33	0.63
2:B:431:THR:HG21	2:B:436:GLU:OE1	1.99	0.63
2:B:418:PHE:O	2:B:422:VAL:HG23	1.98	0.62
2:D:598:LEU:HD23	2:D:598:LEU:O	1.99	0.62
2:B:73:GLU:HG2	2:B:74:ASP:H	1.64	0.62
2:B:684:GLN:HA	2:B:684:GLN:OE1	2.00	0.62
2:B:55:LYS:HG2	2:B:56:GLY:H	1.65	0.62
1:C:-21:GLN:HB3	2:D:112:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:LEU:HD23	2:B:598:LEU:O	2.00	0.61
2:B:123:PRO:HB2	2:B:128:VAL:HG23	1.83	0.61
2:D:348:LEU:HB3	2:D:418:PHE:HE1	1.64	0.61
2:D:170:ILE:O	2:D:179:ILE:HG12	2.01	0.61
2:B:255:ILE:HG12	2:B:311:PHE:HD1	1.65	0.61
2:D:154:ARG:NH2	2:D:303:GLU:OE1	2.33	0.61
2:D:315:ARG:HH21	2:D:320:TRP:HD1	1.48	0.61
2:B:297:GLU:HG3	2:B:298:TYR:H	1.66	0.61
2:B:182:LYS:HG2	2:B:183:GLU:N	2.13	0.61
2:B:142:ASP:HB3	2:D:284:LYS:HZ1	1.65	0.61
2:D:343:MET:O	2:D:347:GLN:HG3	2.00	0.61
2:D:329:GLU:HB3	2:D:760:LYS:HB3	1.83	0.61
1:C:-28:MET:CB	2:D:302:TRP:HD1	2.14	0.60
2:D:66:ILE:HD12	2:D:133:LEU:HD21	1.83	0.60
2:D:684:GLN:OE1	2:D:684:GLN:HA	2.01	0.60
2:D:66:ILE:CD1	2:D:133:LEU:HD21	2.32	0.60
2:B:421:LEU:CD1	2:B:425:LEU:HD11	2.31	0.60
2:D:504:GLU:HG2	2:D:547:SER:OG	2.02	0.60
2:B:39:TYR:HA	2:B:53:HIS:O	2.01	0.59
2:D:389:VAL:O	2:D:390:ASN:HB2	2.00	0.59
2:D:418:PHE:O	2:D:422:VAL:HG23	2.01	0.59
2:B:178:CYS:HA	2:B:188:LYS:HA	1.84	0.59
2:D:226:GLY:O	2:D:248:LYS:NZ	2.34	0.59
2:D:420:ARG:NE	2:D:431:THR:HG22	2.12	0.59
2:B:638:ASP:OD1	2:B:641:ARG:NH2	2.35	0.59
2:B:696:ILE:CD1	2:B:739:LEU:HD22	2.32	0.59
2:D:291:GLY:HA3	2:D:351:LEU:HD11	1.85	0.59
2:D:123:PRO:HB2	2:D:128:VAL:HG23	1.83	0.59
2:B:142:ASP:HB3	2:D:284:LYS:NZ	2.17	0.59
2:D:348:LEU:HD21	2:D:370:ILE:HG21	1.84	0.59
2:D:431:THR:HG21	2:D:436:GLU:OE1	2.02	0.59
2:D:734:ILE:HD11	2:D:778:LEU:HD13	1.84	0.59
2:D:66:ILE:HD12	2:D:133:LEU:HD23	1.85	0.59
2:D:353:ASP:OD2	2:D:469:ARG:NH2	2.36	0.59
2:D:129:PHE:C	2:D:131:GLU:H	2.06	0.59
2:D:245:ALA:HB2	2:D:256:ILE:HD11	1.84	0.59
2:B:315:ARG:O	2:B:371:MET:HG3	2.02	0.58
2:B:349:LEU:CD1	2:B:469:ARG:HH21	2.16	0.58
2:D:421:LEU:CD1	2:D:425:LEU:HD23	2.33	0.58
2:B:145:LYS:HD3	2:B:154:ARG:NH2	2.18	0.58
2:B:129:PHE:C	2:B:131:GLU:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:CYS:HB3	2:B:186:LEU:O	2.04	0.58
2:B:255:ILE:HG12	2:B:311:PHE:CD1	2.38	0.58
2:D:284:LYS:HA	2:D:287:LYS:CG	2.33	0.58
2:D:314:GLY:O	2:D:315:ARG:HG3	2.04	0.58
2:B:685:ASN:OD1	2:B:687:LYS:HD2	2.04	0.58
2:D:163:ARG:HH11	2:D:163:ARG:CG	2.17	0.58
2:B:250:ASP:O	2:B:251:ASN:HB2	2.04	0.57
2:B:61:GLU:HG2	2:B:180:ARG:HG3	1.86	0.57
2:B:296:ILE:HB	2:B:308:VAL:HB	1.85	0.57
2:B:344:ILE:HD11	2:B:376:LEU:HD12	1.86	0.57
2:B:247:ARG:HG3	2:B:249:LYS:NZ	2.18	0.57
2:B:504:GLU:HG2	2:B:547:SER:OG	2.05	0.57
2:B:686:GLN:HE22	2:B:689:LEU:HD23	1.68	0.57
2:B:286:LEU:CD2	2:B:358:GLN:HG3	2.34	0.57
2:B:297:GLU:O	2:B:298:TYR:HB2	2.04	0.57
2:D:182:LYS:HG3	2:D:183:GLU:N	2.19	0.57
2:B:61:GLU:HA	2:B:168:LYS:NZ	2.20	0.57
2:B:195:TYR:CE2	2:B:197:VAL:HG22	2.40	0.56
2:B:325:PHE:CE2	2:B:428:PRO:HD3	2.40	0.56
2:B:275:ARG:HD2	2:B:384:GLU:HB3	1.87	0.56
2:D:320:TRP:HZ3	2:D:425:LEU:CD1	2.19	0.56
2:D:366:GLN:HB2	2:D:367:PRO:HD2	1.86	0.56
2:D:29:ILE:HG22	2:D:30:TYR:N	2.19	0.56
2:D:421:LEU:CD1	2:D:425:LEU:CD2	2.83	0.56
2:D:481:ILE:HG22	2:D:482:ASN:N	2.15	0.56
2:B:37:ASP:C	2:B:39:TYR:N	2.60	0.56
2:B:389:VAL:O	2:B:390:ASN:HB2	2.05	0.55
2:D:178:CYS:SG	2:D:179:ILE:N	2.78	0.55
2:D:685:ASN:OD1	2:D:687:LYS:HD2	2.05	0.55
2:B:511:GLU:OE2	2:B:527:LYS:HE3	2.05	0.55
2:B:103:MET:O	2:B:107:SER:HB3	2.06	0.55
2:B:247:ARG:CG	2:B:249:LYS:HZ2	2.16	0.55
2:B:338:ILE:HG23	2:B:455:PHE:HD2	1.72	0.55
1:A:-18:ALA:O	2:B:233:ALA:HB3	2.06	0.55
1:C:-29:ALA:C	1:C:-27:ASN:N	2.59	0.55
1:C:-17:HIS:CG	1:C:-16:ASP:H	2.25	0.55
2:B:352:ILE:O	2:B:356:HIS:HD2	1.89	0.55
2:D:103:MET:O	2:D:107:SER:HB3	2.07	0.55
2:B:300:GLN:O	2:B:300:GLN:HG2	2.07	0.54
2:B:178:CYS:SG	2:B:188:LYS:HA	2.48	0.54
2:D:421:LEU:HD11	2:D:425:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ILE:HD13	2:B:179:ILE:HA	1.88	0.54
2:B:420:ARG:NE	2:B:431:THR:HG22	2.13	0.54
2:D:352:ILE:HB	2:D:415:TRP:CH2	2.43	0.54
2:B:749:ARG:O	2:B:749:ARG:HD3	2.07	0.54
2:D:315:ARG:NH2	2:D:320:TRP:HD1	2.05	0.54
2:D:62:GLN:HE22	2:D:180:ARG:HH22	1.54	0.54
2:D:66:ILE:CD1	2:D:133:LEU:CD2	2.86	0.54
2:B:230:ILE:O	2:B:230:ILE:CG2	2.56	0.53
2:B:341:VAL:HG13	2:B:345:LEU:HD13	1.90	0.53
2:B:125:ASN:CG	2:B:126:ASN:N	2.61	0.53
2:B:299:PHE:CZ	2:B:306:PHE:HB2	2.43	0.53
2:D:429:VAL:HG22	2:D:764:THR:O	2.09	0.53
2:D:164:TYR:HE1	2:D:180:ARG:NH1	2.07	0.53
2:D:136:ILE:O	2:D:140:ILE:HG12	2.09	0.53
2:B:692:ALA:O	2:B:696:ILE:HG13	2.09	0.52
1:C:-28:MET:HB2	2:D:302:TRP:NE1	2.22	0.52
2:B:392:ASP:HB3	2:B:408:LYS:O	2.10	0.52
2:D:137:SER:OG	2:D:155:TRP:CZ3	2.52	0.52
2:D:325:PHE:CE2	2:D:428:PRO:HD3	2.44	0.52
2:D:421:LEU:HD11	2:D:425:LEU:CD2	2.40	0.52
2:B:366:GLN:HB2	2:B:367:PRO:HD2	1.92	0.52
2:D:44:ASP:HB3	2:D:47:SER:HB2	1.92	0.52
2:D:300:GLN:HG2	2:D:300:GLN:O	2.10	0.52
2:D:87:ILE:N	2:D:87:ILE:HD13	2.24	0.52
2:B:31:GLU:O	2:B:32:LEU:CB	2.58	0.51
1:C:-21:GLN:HA	2:D:236:PHE:CZ	2.45	0.51
2:B:370:ILE:HD13	2:B:380:ILE:HG13	1.91	0.51
2:B:833:ILE:O	2:B:837:MET:HG3	2.10	0.51
2:B:181:ASP:N	2:B:185:ASN:HA	2.25	0.51
2:B:603:ASN:CG	2:B:642:MET:HG3	2.31	0.51
2:B:734:ILE:HD11	2:B:778:LEU:HD13	1.91	0.51
2:B:277:LYS:HA	2:B:280:TYR:HB3	1.92	0.51
2:B:352:ILE:HB	2:B:415:TRP:CH2	2.46	0.51
2:B:170:ILE:HG22	2:B:178:CYS:HB2	1.92	0.51
2:D:62:GLN:HE22	2:D:180:ARG:NH2	2.08	0.51
2:D:500:ILE:HD13	2:D:833:ILE:HD13	1.93	0.51
2:B:343:MET:O	2:B:347:GLN:HG3	2.10	0.51
2:D:575:LYS:O	2:D:579:LEU:HG	2.11	0.51
2:D:79:LEU:HD11	2:D:95:HIS:CD2	2.46	0.51
2:D:543:LYS:HG3	2:D:846:TYR:OH	2.11	0.51
2:B:36:PRO:HG2	2:B:87:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LYS:HG2	2:B:249:LYS:H	1.75	0.51
2:B:338:ILE:HG23	2:B:455:PHE:CD2	2.46	0.51
2:D:279:GLU:OE2	2:D:309:GLU:OE2	2.30	0.51
2:D:84:ARG:C	2:D:86:CYS:H	2.14	0.50
2:B:366:GLN:OE1	2:B:368:ALA:HB3	2.11	0.50
2:B:169:GLY:C	2:B:170:ILE:HG13	2.30	0.50
2:B:241:GLY:H	2:B:258:GLU:HB3	1.76	0.50
2:D:598:LEU:HD23	2:D:598:LEU:C	2.32	0.50
2:D:833:ILE:O	2:D:837:MET:HG3	2.11	0.50
2:B:500:ILE:HD13	2:B:833:ILE:HD13	1.93	0.50
2:D:676:TYR:CZ	2:D:691:GLU:HG2	2.46	0.50
1:C:-19:LEU:O	2:D:236:PHE:HE2	1.95	0.50
2:D:257:LYS:O	2:D:276:GLN:NE2	2.45	0.50
2:D:284:LYS:NZ	2:D:284:LYS:CB	2.75	0.50
2:B:136:ILE:O	2:B:140:ILE:HG12	2.11	0.50
2:D:284:LYS:HG2	2:D:287:LYS:HD3	1.94	0.50
2:D:355:MET:HE3	2:D:380:ILE:HD12	1.94	0.50
2:B:130:VAL:HG22	2:B:208:LEU:HD21	1.94	0.50
2:D:412:ALA:CB	2:D:474:GLN:OE1	2.59	0.50
2:D:749:ARG:O	2:D:749:ARG:HD3	2.11	0.50
2:D:348:LEU:HD22	2:D:378:VAL:CG1	2.42	0.50
2:B:228:TYR:HD2	2:B:247:ARG:HB2	1.76	0.49
2:B:363:GLY:HA3	2:B:385:THR:HB	1.93	0.49
2:B:575:LYS:O	2:B:579:LEU:HG	2.12	0.49
2:B:747:LEU:HB3	2:B:748:TYR:CD2	2.46	0.49
2:D:352:ILE:O	2:D:356:HIS:HB2	2.12	0.49
2:B:268:ALA:O	2:B:269:ALA:HB3	2.12	0.49
2:D:563:LEU:HB3	2:D:564:PRO:HD3	1.94	0.49
2:B:429:VAL:HG22	2:B:764:THR:O	2.12	0.49
2:D:421:LEU:HD12	2:D:425:LEU:CD2	2.43	0.49
2:B:84:ARG:C	2:B:86:CYS:H	2.16	0.49
2:D:702:SER:O	2:D:715:VAL:HG12	2.12	0.49
2:B:236:PHE:O	2:B:237:SER:HB3	2.11	0.49
2:B:737:TRP:HE1	2:B:784:LYS:HE2	1.77	0.49
2:D:445:ASN:O	2:D:449:GLU:HG2	2.13	0.49
2:B:361:ALA:O	2:B:386:ALA:HA	2.12	0.49
2:D:488:SER:HB3	2:D:490:PHE:CE1	2.47	0.49
2:B:583:TYR:HB2	2:B:591:VAL:HG21	1.94	0.49
2:D:180:ARG:CZ	2:D:180:ARG:HB2	2.43	0.49
2:D:366:GLN:OE1	2:D:368:ALA:HB3	2.13	0.49
2:B:130:VAL:O	2:B:130:VAL:CG1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ILE:HG23	2:B:180:ARG:HD2	1.95	0.49
2:B:604:GLN:CD	2:B:605:THR:H	2.16	0.49
2:D:279:GLU:O	2:D:279:GLU:CG	2.60	0.49
2:B:248:LYS:O	2:B:249:LYS:HE3	2.13	0.48
2:B:610:ARG:HD2	2:B:667:ASP:OD1	2.12	0.48
2:D:181:ASP:OD1	2:D:186:LEU:HB3	2.12	0.48
2:D:328:PHE:CE1	2:D:709:THR:HB	2.47	0.48
1:C:-17:HIS:CD2	1:C:-16:ASP:H	2.31	0.48
2:D:250:ASP:OD1	2:D:252:LEU:HB2	2.13	0.48
2:D:292:VAL:O	2:D:379:ARG:NH2	2.40	0.48
2:D:338:ILE:HG23	2:D:455:PHE:CD2	2.48	0.48
2:D:747:LEU:HB3	2:D:748:TYR:CD2	2.48	0.48
2:B:702:SER:O	2:B:715:VAL:HG12	2.13	0.48
2:D:70:SER:O	2:D:147:PRO:HD2	2.14	0.48
2:D:292:VAL:CG2	2:D:355:MET:HE2	2.42	0.48
2:D:845:LEU:HB3	2:D:848:LEU:HD12	1.95	0.48
2:B:67:HIS:HD2	2:B:120:THR:OG1	1.96	0.48
2:B:563:LEU:HB3	2:B:564:PRO:HD3	1.95	0.48
2:B:257:LYS:O	2:B:276:GLN:NE2	2.46	0.48
2:D:30:TYR:HB3	2:D:79:LEU:CD2	2.43	0.48
2:D:85:LEU:HD11	2:D:135:MET:O	2.13	0.48
2:D:163:ARG:HH11	2:D:163:ARG:HG3	1.79	0.48
2:D:755:ILE:O	2:D:758:LEU:HB2	2.13	0.48
2:B:361:ALA:HB1	2:B:414:ASP:OD2	2.13	0.48
2:B:182:LYS:HG2	2:B:183:GLU:HG2	1.96	0.48
2:D:62:GLN:NE2	2:D:180:ARG:HH22	2.12	0.48
2:D:280:TYR:C	2:D:282:ALA:H	2.17	0.48
2:B:358:GLN:HB2	2:B:360:VAL:CG1	2.43	0.47
2:B:598:LEU:HA	2:B:601:ASN:HB2	1.95	0.47
2:D:125:ASN:C	2:D:127:GLU:H	2.13	0.47
2:B:683:THR:O	2:B:684:GLN:HB2	2.14	0.47
2:D:598:LEU:C	2:D:600:ASP:H	2.18	0.47
2:B:282:ALA:O	2:B:286:LEU:HD12	2.14	0.47
2:B:291:GLY:O	2:B:379:ARG:HB3	2.14	0.47
2:B:349:LEU:HD11	2:B:469:ARG:NH2	2.27	0.47
2:B:455:PHE:O	2:B:459:ILE:HG12	2.13	0.47
2:B:599:LYS:CD	2:B:635:LEU:HD13	2.43	0.47
2:D:683:THR:O	2:D:684:GLN:HB2	2.15	0.47
2:B:693:GLU:HA	2:B:696:ILE:HD12	1.97	0.47
2:D:164:TYR:HE1	2:D:180:ARG:CZ	2.26	0.47
2:D:347:GLN:O	2:D:350:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLU:OE1	2:B:46:GLU:HA	2.14	0.47
2:B:600:ASP:O	2:B:601:ASN:C	2.52	0.47
2:D:583:TYR:HB2	2:D:591:VAL:HG21	1.96	0.47
2:B:60:PRO:C	2:B:62:GLN:N	2.67	0.47
2:B:276:GLN:O	2:B:280:TYR:HB2	2.15	0.47
2:D:31:GLU:O	2:D:32:LEU:CB	2.58	0.47
2:D:44:ASP:HB3	2:D:47:SER:CB	2.45	0.47
2:D:599:LYS:HB2	2:D:635:LEU:HD13	1.97	0.47
2:D:30:TYR:CE1	2:D:75:SER:HB3	2.49	0.47
2:B:439:LEU:HD11	2:B:805:ILE:HD11	1.96	0.47
2:B:180:ARG:H	2:B:180:ARG:HG2	1.51	0.46
2:B:79:LEU:HD11	2:B:95:HIS:CD2	2.51	0.46
2:B:131:GLU:HB3	2:B:135:MET:CE	2.45	0.46
2:D:124:THR:O	2:D:125:ASN:C	2.53	0.46
2:D:455:PHE:O	2:D:459:ILE:HG12	2.15	0.46
2:D:652:GLN:HE22	2:D:662:ASP:HB2	1.80	0.46
2:B:188:LYS:HE3	2:B:190:GLN:HG2	1.98	0.46
2:B:686:GLN:NE2	2:B:689:LEU:HD23	2.30	0.46
2:B:168:LYS:CG	2:B:169:GLY:H	2.20	0.46
2:D:229:LYS:HB2	2:D:248:LYS:HE2	1.98	0.46
2:D:432:SER:C	2:D:434:ASP:H	2.19	0.46
2:B:421:LEU:HD12	2:B:425:LEU:CD1	2.45	0.46
2:B:678:ALA:O	2:B:681:SER:OG	2.29	0.46
2:B:432:SER:C	2:B:434:ASP:H	2.19	0.46
2:B:492:LEU:HD23	2:B:840:ILE:CD1	2.46	0.46
2:D:347:GLN:O	2:D:349:LEU:N	2.49	0.46
2:B:318:ARG:HH21	2:B:368:ALA:HB2	1.80	0.46
2:B:416:PHE:O	2:B:416:PHE:CD1	2.69	0.46
2:B:605:THR:HA	2:B:646:ASN:OD1	2.15	0.46
2:D:329:GLU:OE2	2:D:762:ARG:NH2	2.49	0.46
2:D:355:MET:CE	2:D:380:ILE:HD12	2.46	0.46
2:B:421:LEU:CD1	2:B:425:LEU:CD1	2.93	0.46
2:B:208:LEU:HA	2:B:211:ILE:HG12	1.97	0.45
2:B:228:TYR:CE2	2:B:247:ARG:HB2	2.52	0.45
2:D:230:ILE:HG22	2:D:230:ILE:O	2.16	0.45
2:B:181:ASP:HB3	2:B:185:ASN:H	1.81	0.45
2:B:236:PHE:O	2:B:237:SER:CB	2.63	0.45
2:D:30:TYR:HE1	2:D:75:SER:HB3	1.82	0.45
2:D:94:LYS:HE2	2:D:122:TYR:OH	2.16	0.45
2:D:164:TYR:CE1	2:D:180:ARG:NH1	2.84	0.45
2:B:83:ALA:O	2:B:87:ILE:CG1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:TYR:HD1	2:D:306:PHE:O	1.99	0.45
2:D:492:LEU:HD23	2:D:840:ILE:CD1	2.46	0.45
2:B:84:ARG:HA	2:B:84:ARG:HD3	1.71	0.45
2:B:96:LEU:HD12	2:B:118:PHE:HD1	1.81	0.45
2:B:145:LYS:HD3	2:B:154:ARG:HH21	1.80	0.45
2:B:291:GLY:O	2:B:379:ARG:CB	2.65	0.45
2:D:123:PRO:O	2:D:124:THR:CB	2.65	0.45
2:D:559:LEU:HD21	2:D:578:ILE:HG23	1.97	0.45
2:B:317:LEU:O	2:B:321:ILE:HG12	2.17	0.45
2:B:435:LEU:O	2:B:439:LEU:HD12	2.17	0.45
2:B:703:THR:HA	2:B:714:THR:HA	1.99	0.45
2:B:706:ASP:O	2:B:709:THR:O	2.35	0.45
2:D:123:PRO:HB3	2:D:132:LEU:HD12	1.98	0.45
2:D:154:ARG:HH22	2:D:303:GLU:CD	2.19	0.45
2:D:279:GLU:OE1	2:D:384:GLU:HG2	2.16	0.45
2:B:512:ARG:HG2	2:B:527:LYS:HG2	1.97	0.45
2:B:234:LEU:HB2	2:B:242:VAL:HG12	1.98	0.45
2:B:294:ASN:O	2:B:310:GLU:HB3	2.17	0.45
2:D:361:ALA:HB1	2:D:414:ASP:OD1	2.17	0.45
2:D:388:PRO:HG2	2:D:391:SER:HB2	1.99	0.45
2:D:418:PHE:HD2	2:D:466:CYS:SG	2.40	0.45
2:B:73:GLU:OE1	2:B:73:GLU:N	2.31	0.44
2:B:347:GLN:O	2:B:349:LEU:N	2.50	0.44
2:B:352:ILE:O	2:B:356:HIS:CD2	2.69	0.44
2:B:704:LYS:HE2	2:B:715:VAL:HG21	1.99	0.44
2:B:845:LEU:HB3	2:B:848:LEU:HD12	1.98	0.44
2:D:73:GLU:HG2	2:D:74:ASP:H	1.82	0.44
2:D:339:LYS:O	2:D:342:LYS:HB2	2.17	0.44
2:B:276:GLN:OE1	2:B:305:TYR:HB3	2.17	0.44
2:D:610:ARG:HD2	2:D:667:ASP:OD1	2.17	0.44
2:B:259:ALA:HB1	2:B:272:ALA:O	2.17	0.44
2:B:394:ARG:HG2	2:B:395:PRO:HD2	1.98	0.44
2:D:76:LYS:HD2	2:D:76:LYS:HA	1.77	0.44
2:B:488:SER:HB3	2:B:490:PHE:CE1	2.52	0.44
2:B:492:LEU:HD23	2:B:840:ILE:HD13	1.98	0.44
2:D:96:LEU:HD12	2:D:118:PHE:HD1	1.82	0.44
2:D:247:ARG:NH2	2:D:250:ASP:OD2	2.49	0.44
2:D:298:TYR:O	2:D:299:PHE:HB3	2.18	0.44
1:C:-25:VAL:HG21	2:D:302:TRP:CG	2.51	0.44
2:B:278:ILE:C	2:B:280:TYR:H	2.19	0.44
1:A:-22:LEU:C	1:A:-20:LYS:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ASP:H	2:B:185:ASN:HA	1.82	0.44
2:B:559:LEU:HD21	2:B:578:ILE:HG23	1.99	0.44
2:D:180:ARG:NH1	2:D:180:ARG:HB2	2.33	0.44
2:D:182:LYS:HB2	2:D:200:PHE:CZ	2.53	0.44
2:B:60:PRO:O	2:B:62:GLN:N	2.48	0.44
2:B:292:VAL:HG22	2:B:355:MET:HE2	1.99	0.44
2:B:455:PHE:HE1	2:B:459:ILE:HD11	1.78	0.44
2:D:320:TRP:HZ3	2:D:425:LEU:HD13	1.81	0.44
2:D:67:HIS:HD2	2:D:120:THR:OG1	2.01	0.43
2:D:245:ALA:HB3	2:D:254:VAL:HG23	2.00	0.43
2:B:54:VAL:HG23	2:B:92:GLU:HG2	1.99	0.43
2:B:347:GLN:O	2:B:350:ASP:N	2.45	0.43
2:D:66:ILE:HD11	2:D:129:PHE:CE1	2.54	0.43
2:D:492:LEU:HD23	2:D:840:ILE:HD13	1.99	0.43
1:C:-28:MET:HB3	2:D:302:TRP:HD1	1.83	0.43
2:B:125:ASN:O	2:B:128:VAL:HG22	2.18	0.43
2:D:130:VAL:O	2:D:130:VAL:CG1	2.62	0.43
2:D:32:LEU:HD22	2:D:84:ARG:HH12	1.83	0.43
2:B:182:LYS:HB3	2:B:182:LYS:HE3	1.72	0.43
2:B:610:ARG:NH1	2:B:667:ASP:OD2	2.51	0.43
2:B:693:GLU:HG2	2:B:739:LEU:HD21	2.01	0.43
2:D:29:ILE:CG2	2:D:30:TYR:H	2.26	0.43
2:D:74:ASP:O	2:D:75:SER:C	2.56	0.43
2:D:277:LYS:O	2:D:280:TYR:HB2	2.17	0.43
2:D:592:LEU:HA	2:D:592:LEU:HD12	1.74	0.43
2:B:61:GLU:HA	2:B:168:LYS:HZ3	1.83	0.43
2:B:295:LEU:H	2:B:295:LEU:HG	1.69	0.43
2:B:292:VAL:HG12	2:B:293:VAL:N	2.34	0.43
2:B:312:ILE:HD13	2:B:379:ARG:HG3	1.99	0.43
2:D:277:LYS:O	2:D:280:TYR:CB	2.67	0.43
2:B:204:PHE:CE2	2:B:208:LEU:HD11	2.54	0.43
2:D:474:GLN:HE21	2:D:474:GLN:HB2	1.66	0.43
2:D:529:ASN:OD1	2:D:529:ASN:C	2.57	0.43
2:B:312:ILE:HG21	2:B:379:ARG:HG3	2.01	0.42
2:D:179:ILE:HA	2:D:187:ILE:O	2.18	0.42
2:D:328:PHE:CD1	2:D:709:THR:HB	2.54	0.42
2:D:401:GLY:O	2:D:420:ARG:HG2	2.18	0.42
2:D:163:ARG:CG	2:D:163:ARG:NH1	2.82	0.42
2:D:239:ALA:HB2	2:D:264:GLY:HA3	2.01	0.42
2:B:415:TRP:HZ3	2:B:418:PHE:CD2	2.38	0.42
2:B:517:ASP:O	2:B:520:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ILE:HG12	2:B:455:PHE:CD2	2.54	0.42
2:D:480:GLU:CD	2:D:480:GLU:H	2.23	0.42
2:B:481:ILE:HB	2:B:482:ASN:H	1.64	0.42
2:B:113:ALA:O	2:B:117:LYS:NZ	2.53	0.42
2:B:237:SER:O	2:B:240:GLY:O	2.38	0.42
2:D:389:VAL:O	2:D:390:ASN:CB	2.67	0.42
1:C:-22:LEU:O	2:D:236:PHE:HZ	2.01	0.42
2:D:280:TYR:HE1	2:D:307:LEU:HD13	1.84	0.42
2:B:339:LYS:O	2:B:342:LYS:HB2	2.20	0.42
2:D:706:ASP:OD1	2:D:708:VAL:HG23	2.20	0.42
2:B:598:LEU:HD23	2:B:598:LEU:C	2.39	0.42
2:D:563:LEU:N	2:D:564:PRO:CD	2.83	0.41
1:C:-24:LEU:HD12	1:C:-24:LEU:HA	1.91	0.41
2:B:179:ILE:N	2:B:187:ILE:O	2.49	0.41
2:B:250:ASP:O	2:B:251:ASN:CB	2.69	0.41
2:B:342:LYS:HE2	2:B:458:PHE:CD2	2.54	0.41
2:B:465:LYS:HE3	2:B:465:LYS:HB2	1.83	0.41
2:B:604:GLN:CG	2:B:605:THR:N	2.83	0.41
2:B:700:LEU:O	2:B:703:THR:OG1	2.31	0.41
2:D:286:LEU:HB3	2:D:292:VAL:HG21	2.01	0.41
2:D:709:THR:OG1	2:D:711:VAL:HG13	2.19	0.41
2:B:37:ASP:O	2:B:39:TYR:N	2.53	0.41
2:B:61:GLU:CG	2:B:180:ARG:HG3	2.49	0.41
2:B:62:GLN:HG3	2:B:164:TYR:OH	2.21	0.41
2:B:74:ASP:OD2	2:B:144:LYS:HB3	2.21	0.41
2:B:277:LYS:HA	2:B:280:TYR:CB	2.49	0.41
2:B:717:ASN:OD1	2:B:717:ASN:N	2.53	0.41
2:D:261:PRO:O	2:D:262:SER:HB2	2.21	0.41
2:D:401:GLY:CA	2:D:431:THR:O	2.57	0.41
2:D:129:PHE:C	2:D:131:GLU:N	2.73	0.41
2:D:284:LYS:HB3	2:D:284:LYS:HZ3	1.84	0.41
2:D:598:LEU:O	2:D:600:ASP:N	2.53	0.41
2:B:426:ALA:HB2	2:B:455:PHE:HE1	1.86	0.41
2:D:178:CYS:O	2:D:179:ILE:O	2.38	0.41
2:D:603:ASN:HD21	2:D:639:LEU:HD21	1.84	0.41
2:B:74:ASP:O	2:B:76:LYS:N	2.54	0.41
2:B:129:PHE:C	2:B:131:GLU:N	2.74	0.41
2:B:341:VAL:O	2:B:345:LEU:HB2	2.20	0.41
2:B:380:ILE:O	2:B:380:ILE:CG2	2.68	0.41
2:D:422:VAL:HG12	2:D:459:ILE:HG23	2.02	0.41
2:D:491:ASN:HB3	2:D:494:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-23:GLU:C	1:C:-21:GLN:H	2.24	0.41
2:B:72:LEU:O	2:B:75:SER:HB2	2.21	0.41
2:B:261:PRO:O	2:B:262:SER:HB2	2.21	0.41
2:B:297:GLU:O	2:B:298:TYR:CB	2.67	0.41
2:B:747:LEU:O	2:B:749:ARG:N	2.54	0.41
2:D:123:PRO:O	2:D:124:THR:HB	2.21	0.41
2:D:361:ALA:HB1	2:D:414:ASP:CG	2.41	0.41
2:D:693:GLU:HG2	2:D:739:LEU:HD21	2.03	0.41
2:B:70:SER:O	2:B:147:PRO:HD2	2.21	0.41
2:B:349:LEU:O	2:B:415:TRP:HH2	2.04	0.41
2:B:531:LEU:HB2	2:B:572:PHE:HB3	2.03	0.41
2:B:563:LEU:N	2:B:564:PRO:CD	2.84	0.41
2:B:790:GLU:HG2	2:B:791:VAL:H	1.86	0.41
2:D:374:GLU:C	2:D:376:LEU:H	2.24	0.41
2:D:745:GLN:HB2	2:D:747:LEU:HD22	2.03	0.40
2:D:804:LEU:HD12	2:D:804:LEU:HA	1.81	0.40
2:B:151:ASN:ND2	2:B:192:ASN:H	2.20	0.40
2:B:224:ARG:HH12	2:B:227:LYS:HE2	1.86	0.40
2:D:99:LYS:O	2:D:103:MET:HG2	2.21	0.40
2:D:147:PRO:HD3	2:D:262:SER:HB3	2.03	0.40
2:B:125:ASN:O	2:B:128:VAL:CG2	2.70	0.40
2:B:421:LEU:HD12	2:B:425:LEU:HD12	2.04	0.40
2:B:529:ASN:OD1	2:B:529:ASN:C	2.60	0.40
2:D:234:LEU:HD23	2:D:234:LEU:HA	1.90	0.40
2:D:177:HIS:HE1	2:D:191:ARG:NH1	2.19	0.40
2:D:592:LEU:HD12	2:D:632:TYR:OH	2.21	0.40
2:B:188:LYS:CE	2:B:190:GLN:HG2	2.50	0.40
2:D:598:LEU:C	2:D:600:ASP:N	2.75	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	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
1	C	12/14 (86%)	9 (75%)	1 (8%)	2 (17%)	0	0
2	B	839/859 (98%)	715 (85%)	95 (11%)	29 (4%)	3	4
2	D	839/859 (98%)	733 (87%)	81 (10%)	25 (3%)	4	6
All	All	1702/1746 (98%)	1467 (86%)	179 (10%)	56 (3%)	4	5

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	LEU
2	B	38	THR
2	B	62	GLN
2	B	75	SER
2	B	187	ILE
2	B	198	PRO
2	B	237	SER
2	B	251	ASN
2	B	264	GLY
2	B	298	TYR
2	B	481	ILE
2	B	482	ASN
2	B	708	VAL
2	D	32	LEU
2	D	75	SER
2	D	123	PRO
2	D	124	THR
2	D	126	ASN
2	D	178	CYS
2	D	179	ILE
2	D	251	ASN
2	D	264	GLY
2	D	481	ILE
2	D	482	ASN
2	D	601	ASN
2	D	628	GLU
1	C	-28	MET
2	B	46	GLU
2	B	61	GLU
2	B	130	VAL
2	D	130	VAL
2	D	183	GLU
2	D	331	ASN

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Mol	Chain	Res	Type
2	D	348	LEU
2	D	708	VAL
1	C	-17	HIS
2	B	181	ASP
2	B	348	LEU
2	B	382	ASP
2	B	601	ASN
2	B	748	TYR
2	D	125	ASN
2	D	382	ASP
2	D	508	THR
2	B	168	LYS
2	B	250	ASP
2	B	390	ASN
2	D	333	GLY
2	B	58	THR
2	B	249	LYS
2	D	31	GLU
2	B	60	PRO
2	B	304	HIS
2	B	332	ASN
2	D	299	PHE
2	D	332	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	12/12 (100%)	11 (92%)	1 (8%)	11	22
1	C	12/12 (100%)	8 (67%)	4 (33%)	0	0
2	B	752/765 (98%)	660 (88%)	92 (12%)	5	9
2	D	752/765 (98%)	657 (87%)	95 (13%)	4	8
All	All	1528/1554 (98%)	1336 (87%)	192 (13%)	4	8

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-23	GLU
1	C	-26	THR
1	C	-24	LEU
1	C	-19	LEU
1	C	-17	HIS
2	B	9	ARG
2	B	20	LYS
2	B	29	ILE
2	B	37	ASP
2	B	43	LEU
2	B	44	ASP
2	B	45	ASN
2	B	46	GLU
2	B	57	SER
2	B	59	LEU
2	B	84	ARG
2	B	85	LEU
2	B	88	ASP
2	B	97	LYS
2	B	125	ASN
2	B	133	LEU
2	B	138	LEU
2	B	153	LYS
2	B	168	LYS
2	B	171	PHE
2	B	174	HIS
2	B	177	HIS
2	B	179	ILE
2	B	180	ARG
2	B	182	LYS
2	B	183	GLU
2	B	188	LYS
2	B	194	PHE
2	B	210	THR
2	B	224	ARG
2	B	225	LEU
2	B	227	LYS
2	B	230	ILE
2	B	246	THR
2	B	273	LEU
2	B	277	LYS
2	B	283	LEU
2	B	288	ASP

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Mol	Chain	Res	Type
2	B	295	LEU
2	B	299	PHE
2	B	365	LEU
2	B	366	GLN
2	B	370	ILE
2	B	371	MET
2	B	373	THR
2	B	375	ASP
2	B	379	ARG
2	B	380	ILE
2	B	385	THR
2	B	387	MET
2	B	400	THR
2	B	404	SER
2	B	433	GLU
2	B	434	ASP
2	B	439	LEU
2	B	465	LYS
2	B	469	ARG
2	B	474	GLN
2	B	475	THR
2	B	477	ILE
2	B	485	ASP
2	B	487	THR
2	B	492	LEU
2	B	509	ASN
2	B	511	GLU
2	B	514	ILE
2	B	543	LYS
2	B	546	SER
2	B	556	GLN
2	B	565	LEU
2	B	567	GLU
2	B	596	LYS
2	B	602	ILE
2	B	610	ARG
2	B	649	LYS
2	B	652	GLN
2	B	661	VAL
2	B	663	ILE
2	B	673	SER
2	B	687	LYS

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Mol	Chain	Res	Type
2	B	691	GLU
2	B	707	ASP
2	B	708	VAL
2	B	721	LEU
2	B	747	LEU
2	B	765	ILE
2	B	766	SER
2	B	785	ASN
2	B	787	LYS
2	B	804	LEU
2	B	809	SER
2	B	854	ASP
2	D	5	MET
2	D	12	LYS
2	D	20	LYS
2	D	45	ASN
2	D	51	HIS
2	D	80	ASP
2	D	84	ARG
2	D	87	ILE
2	D	109	ASN
2	D	124	THR
2	D	125	ASN
2	D	126	ASN
2	D	137	SER
2	D	141	GLN
2	D	144	LYS
2	D	153	LYS
2	D	154	ARG
2	D	160	VAL
2	D	163	ARG
2	D	170	ILE
2	D	173	GLU
2	D	179	ILE
2	D	180	ARG
2	D	182	LYS
2	D	186	LEU
2	D	197	VAL
2	D	199	ASP
2	D	200	PHE
2	D	203	ASP
2	D	210	THR

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Mol	Chain	Res	Type
2	D	225	LEU
2	D	230	ILE
2	D	246	THR
2	D	248	LYS
2	D	251	ASN
2	D	253	LYS
2	D	255	ILE
2	D	273	LEU
2	D	281	ASP
2	D	288	ASP
2	D	294	ASN
2	D	295	LEU
2	D	298	TYR
2	D	301	GLU
2	D	303	GLU
2	D	310	GLU
2	D	330	ASP
2	D	343	MET
2	D	348	LEU
2	D	351	LEU
2	D	360	VAL
2	D	365	LEU
2	D	366	GLN
2	D	370	ILE
2	D	373	THR
2	D	385	THR
2	D	387	MET
2	D	397	MET
2	D	462	LEU
2	D	465	LYS
2	D	467	ASP
2	D	474	GLN
2	D	475	THR
2	D	477	ILE
2	D	479	LYS
2	D	485	ASP
2	D	487	THR
2	D	492	LEU
2	D	514	ILE
2	D	543	LYS
2	D	546	SER
2	D	556	GLN

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Mol	Chain	Res	Type
2	D	565	LEU
2	D	605	THR
2	D	631	GLU
2	D	649	LYS
2	D	652	GLN
2	D	661	VAL
2	D	670	SER
2	D	673	SER
2	D	687	LYS
2	D	696	ILE
2	D	704	LYS
2	D	708	VAL
2	D	709	THR
2	D	719	ASN
2	D	720	ARG
2	D	747	LEU
2	D	750	GLU
2	D	754	SER
2	D	766	SER
2	D	787	LYS
2	D	794	ASN
2	D	809	SER
2	D	854	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	-17	HIS
2	B	14	ASN
2	B	151	ASN
2	B	357	ASN
2	B	440	GLN
2	B	450	ASN
2	B	686	GLN
2	D	14	ASN
2	D	53	HIS
2	D	62	GLN
2	D	126	ASN
2	D	151	ASN
2	D	177	HIS
2	D	213	ASN
2	D	300	GLN

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Mol	Chain	Res	Type
2	D	357	ASN
2	D	440	GLN
2	D	450	ASN
2	D	603	ASN
2	D	652	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	14/14 (100%)	1.17	2 (14%) 2 2	74, 88, 136, 147	0
1	C	14/14 (100%)	0.52	1 (7%) 16 16	75, 86, 108, 113	0
2	B	845/859 (98%)	0.46	75 (8%) 9 9	24, 66, 116, 149	0
2	D	845/859 (98%)	0.14	29 (3%) 45 48	16, 53, 92, 156	0
All	All	1718/1746 (98%)	0.31	107 (6%) 20 21	16, 59, 109, 156	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	176	GLU	9.9
2	B	176	GLU	8.2
2	B	308	VAL	8.0
2	B	653	LEU	6.7
2	D	175	GLY	6.3
2	D	653	LEU	5.4
2	B	320	TRP	5.3
2	B	378	VAL	5.2
2	D	602	ILE	4.7
2	B	181	ASP	4.4
2	B	293	VAL	4.4
2	B	277	LYS	4.3
2	D	655	VAL	4.3
2	B	307	LEU	4.3
2	B	171	PHE	4.1
2	D	652	GLN	4.1
1	A	-17	HIS	4.0
2	D	332	ASN	3.9
2	B	329	GLU	3.9
2	B	256	ILE	3.9
2	D	180	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	346	LEU	3.8
2	B	393	ASP	3.8
2	D	246	THR	3.8
2	B	288	ASP	3.7
2	B	708	VAL	3.6
2	B	361	ALA	3.4
2	B	264	GLY	3.4
2	B	183	GLU	3.4
2	D	200	PHE	3.3
2	B	360	VAL	3.3
2	B	297	GLU	3.3
2	B	306	PHE	3.3
2	B	479	LYS	3.3
2	B	175	GLY	3.2
2	B	187	ILE	3.2
2	D	174	HIS	3.2
2	B	182	LYS	3.1
2	B	280	TYR	3.1
2	B	197	VAL	3.0
2	B	299	PHE	3.0
2	B	42	PHE	3.0
2	B	85	LEU	3.0
2	B	331	ASN	3.0
2	B	43	LEU	2.9
2	B	405	HIS	2.9
2	B	467	ASP	2.8
2	B	363	GLY	2.8
2	D	328	PHE	2.8
2	B	252	LEU	2.8
2	B	601	ASN	2.8
2	B	655	VAL	2.8
2	D	177	HIS	2.8
2	B	295	LEU	2.8
2	B	652	GLN	2.8
2	B	79	LEU	2.8
2	B	203	ASP	2.7
2	B	39	TYR	2.7
2	D	305	TYR	2.7
2	B	268	ALA	2.6
2	B	362	MET	2.6
2	D	125	ASN	2.6
2	B	273	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	232	THR	2.6
2	B	380	ILE	2.6
2	B	704	LYS	2.6
2	B	332	ASN	2.6
2	B	278	ILE	2.5
2	D	360	VAL	2.5
2	B	179	ILE	2.5
2	B	408	LYS	2.5
2	D	331	ASN	2.5
2	B	480	GLU	2.5
2	B	234	LEU	2.4
2	B	58	THR	2.4
2	B	298	TYR	2.4
2	B	61	GLU	2.4
2	B	170	ILE	2.3
2	B	416	PHE	2.3
2	B	259	ALA	2.3
2	B	45	ASN	2.3
2	D	329	GLU	2.3
2	B	130	VAL	2.3
2	D	183	GLU	2.3
2	D	182	LYS	2.3
2	B	200	PHE	2.3
2	B	239	ALA	2.3
2	B	174	HIS	2.3
2	D	186	LEU	2.2
2	D	178	CYS	2.2
1	A	-26	THR	2.2
2	D	227	LYS	2.2
2	B	394	ARG	2.2
2	B	415	TRP	2.2
2	D	282	ALA	2.2
2	D	191	ARG	2.2
2	D	263	ALA	2.2
2	B	359	GLY	2.1
2	B	204	PHE	2.1
2	B	198	PRO	2.1
2	B	654	LYS	2.1
1	C	-28	MET	2.1
2	D	245	ALA	2.0
2	B	33	ASN	2.0
2	B	381	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	249	LYS	2.0
2	D	259	ALA	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 monosaccharides 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.