



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:21 PM UTC

PDB ID : 8SAO / pdb_00008sao
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

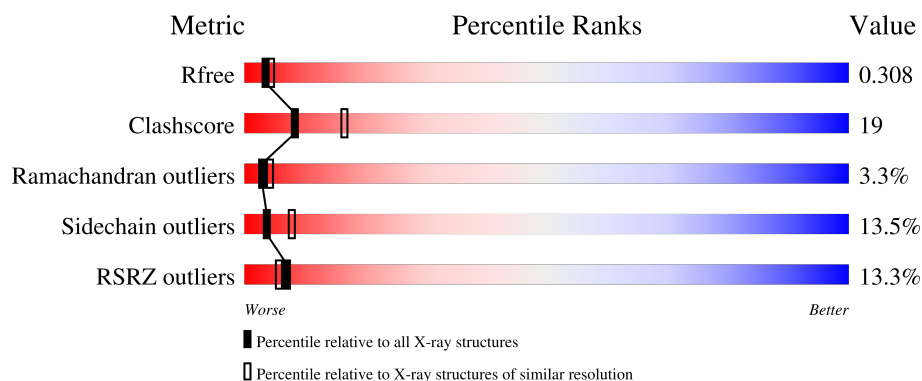
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	43% 43% 43% 14%
1	C	14	29% 14% 50% 36%
2	B	859	17% 57% 34% 8%
2	D	859	9% 60% 31% 6%

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
1	A	14	Total	C	N	O	S	0	0	0
			109	68	19	21	1			
1	C	14	Total	C	N	O	S	0	0	0
			109	68	19	21	1			

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

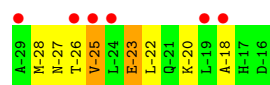
- Molecule 2 is a protein called Class III lanthionine synthetase LanKC.

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

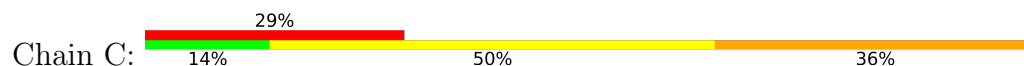
3 Residue-property plots [i](#)

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.

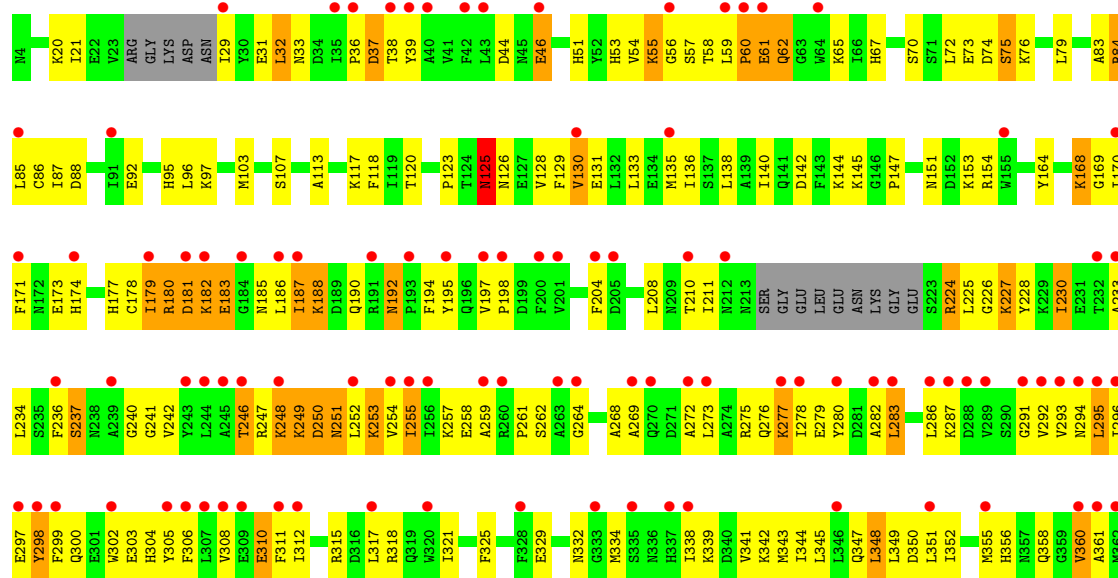
- Molecule 1: Class III lanthipeptide

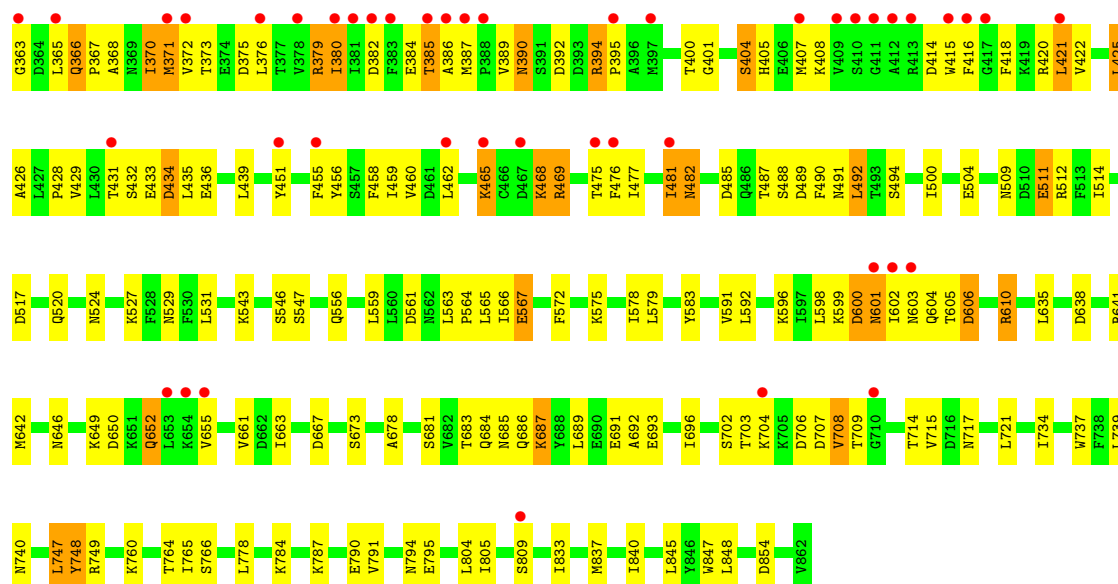


- Molecule 1: Class III lanthipeptide



- Molecule 2: Class III lanthionine synthetase LanKC





• Molecule 2: Class III lanthionine synthetase LanKC



S754	I755		L758	S759	K760	T761	R762	C763	T764	I765	S766		L778		K787		V791		N794	E795		L804		S809		Q816		T827		I833		M837		I840		L845	Y846	W847	L848		D854		Y862
------	------	--	------	------	------	------	------	------	------	------	------	--	------	--	------	--	------	--	------	------	--	------	--	------	--	------	--	------	--	------	--	------	--	------	--	------	------	------	------	--	------	--	------

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)	Xtriage
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 (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13859	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/109	1.01	0/146
1	C	0.46	0/109	1.12	0/146
2	B	0.45	0/6954	1.07	14/9383 (0.1%)
2	D	0.46	0/6953	1.07	5/9382 (0.1%)
All	All	0.46	0/14125	1.07	19/19057 (0.1%)

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 (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	627	THR	CB-CA-C	-8.37	97.61	111.51
2	D	48	VAL	N-CA-C	-7.78	106.32	113.71
2	D	350	ASP	CB-CA-C	-6.61	100.51	110.88
2	D	606	ASP	CA-CB-CG	6.54	119.14	112.60
2	B	606	ASP	CA-CB-CG	6.14	118.74	112.60
2	B	55	LYS	CB-CA-C	-5.94	109.70	116.54
2	B	794	ASN	CB-CA-C	5.83	121.87	110.67
2	B	405	HIS	CB-CA-C	5.65	118.17	111.22
2	B	33	ASN	CB-CA-C	5.55	121.47	110.42
2	D	740	ASN	CB-CA-C	5.53	119.97	110.79
2	B	561	ASP	CA-CB-CG	-5.41	107.19	112.60
2	B	600	ASP	CA-CB-CG	5.40	118.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	740	ASN	CB-CA-C	5.29	119.57	110.79
2	B	125	ASN	CA-C-N	5.13	128.80	120.60
2	B	125	ASN	C-N-CA	5.13	128.80	120.60
2	B	226	GLY	CA-C-N	5.04	127.29	120.38
2	B	226	GLY	C-N-CA	5.04	127.29	120.38
2	B	283	LEU	CA-C-N	5.01	127.25	120.44
2	B	283	LEU	C-N-CA	5.01	127.25	120.44

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	9	0
1	C	109	0	114	20	0
2	B	6821	0	6812	266	0
2	D	6820	0	6817	257	0
All	All	13859	0	13857	532	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 19.

All (532) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:247:ARG:HG3	2:B:249:LYS:HZ2	1.34	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:D:791:VAL:O	2:D:795:GLU:HG3	1.80	0.82
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:D:355:MET:HE1	2:D:380:ILE:HD12	1.64	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:B:334:MET:HE3	2:B:451:TYR:CE1	2.18	0.79
2:D:125:ASN:O	2:D:127:GLU:N	2.15	0.78
2:B:131:GLU:HB3	2:B:135:MET:HE3	1.65	0.78
2:B:131:GLU:O	2:B:135:MET:HG3	1.83	0.78
2:B:292:VAL:HG22	2:B:355:MET:HE2	1.66	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:125:ASN:CG	2:B:126:ASN:H	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:GLU:O	2:D:32:LEU:HB2	1.87	0.74
1:C:-29:ALA:C	1:C:-27:ASN:H	1.95	0.74
2:D:295:LEU:HD23	2:D:295:LEU:N	2.02	0.74
2:B:37:ASP:C	2:B:39:TYR:H	1.96	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:B:60:PRO:C	2:B:62:GLN:H	1.96	0.72
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: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:B:603:ASN:HB3	2:B:642:MET:HE2	1.73	0.70
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
2:D:277:LYS:O	2:D:280:TYR:N	2.24	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: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: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:130:VAL:HG12	2:B:130:VAL:O	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:142:ASP:HB3	2:D:284:LYS:HZ1	1.62	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:D:129:PHE:C	2:D:131:GLU:H	2.06	0.63
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:129:PHE:C	2:B:131:GLU:H	2.07	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
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:D:292:VAL:HG22	2:D:355:MET:HE2	1.83	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:334:MET:HE3	2:D:451:TYR:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:ARG:CG	2:B:249:LYS:HZ2	2.12	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:B:351:LEU:HG	2:B:355:MET:HE3	1.84	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
1:C:-29:ALA:C	1:C:-27:ASN:N	2.59	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: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:37:ASP:C	2:B:39:TYR:N	2.60	0.58
2:B:145:LYS:HD3	2:B:154:ARG:NH2	2.18	0.58
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:125:ASN:CG	2:B:126:ASN:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:84:ARG:C	2:D:86:CYS:H	2.14	0.55
2:B:338:ILE:HG23	2:B:455:PHE:HD2	1.72	0.55
2:B:603:ASN:CG	2:B:642:MET:HG3	2.31	0.55
2:D:598:LEU:HD23	2:D:598:LEU:C	2.32	0.55
1:A:-18:ALA:O	2:B:233:ALA:HB3	2.06	0.55
2:B:169:GLY:C	2:B:170:ILE:HG13	2.30	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
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:604:GLN:CD	2:B:605:THR:H	2.16	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:ARG:C	2:B:86:CYS:H	2.16	0.52
2:D:280:TYR:C	2:D:282:ALA:H	2.17	0.52
2:D:125:ASN:C	2:D:127:GLU:H	2.13	0.52
2:B:692:ALA:O	2:B:696:ILE:HG13	2.09	0.52
2:D:598:LEU:C	2:D:600:ASP:H	2.18	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:B:600:ASP:O	2:B:601:ASN:C	2.52	0.52
2:B:60:PRO:C	2:B:62:GLN:N	2.67	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: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:124:THR:O	2:D:125:ASN:C	2.53	0.51
2:D:575:LYS:O	2:D:579:LEU:HG	2.11	0.51
2:B:302:TRP:CG	2:B:303:GLU:H	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:SER:C	2:B:434:ASP:H	2.19	0.50
2:B:366:GLN:OE1	2:B:368:ALA:HB3	2.11	0.50
2:B:241:GLY:H	2:B:258:GLU:HB3	1.76	0.50
2:D:99:LYS:HE2	2:D:103:MET:HE2	1.93	0.50
2:D:154:ARG:HH22	2:D:303:GLU:CD	2.19	0.50
2:D:432:SER:C	2:D:434:ASP:H	2.19	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:B:130:VAL:HG22	2:B:208:LEU:HD21	1.94	0.50
2:D:371:MET:HE2	2:D:381:ILE:HD13	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:278:ILE:C	2:B:280:TYR:H	2.19	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:D:702:SER:O	2:D:715:VAL:HG12	2.12	0.49
2:B:61:GLU:HA	2:B:168:LYS:HZ3	1.78	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
2:B:170:ILE:HG23	2:B:180:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:GLU:O	2:D:279:GLU:CG	2.60	0.49
1:A:-22:LEU:C	1:A:-20:LYS:H	2.20	0.48
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: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:B:678:ALA:O	2:B:681:SER:OG	2.29	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:D:74:ASP:O	2:D:75:SER:C	2.56	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: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: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:529:ASN:OD1	2:D:529:ASN:C	2.57	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
2:D:583:TYR:HB2	2:D:591:VAL:HG21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ASP:HB3	2:D:47:SER:CB	2.45	0.47
2:D:480:GLU:CD	2:D:480:GLU:H	2.23	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:D:678:ALA:O	2:D:681:SER:OG	2.30	0.47
2:B:439:LEU:HD11	2:B:805:ILE:HD11	1.96	0.47
2:B:683:THR:O	2:B:684:GLN:HB2	2.14	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:598:LEU:HD23	2:B:598:LEU:C	2.39	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:B:421:LEU:HD12	2:B:425:LEU:CD1	2.45	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:129:PHE:C	2:D:131:GLU:N	2.73	0.46
2:D:329:GLU:OE2	2:D:762:ARG:NH2	2.49	0.46
2:B:129:PHE:C	2:B:131:GLU:N	2.74	0.46
2:B:247:ARG:HG3	2:B:249:LYS:NZ	2.18	0.46
2:B:421:LEU:CD1	2:B:425:LEU:CD1	2.93	0.46
2:D:361:ALA:HB1	2:D:414:ASP:CG	2.41	0.45
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:374:GLU:C	2:D:376:LEU:H	2.24	0.45
2:B:407:MET:HE1	2:B:476:PHE:CD1	2.51	0.45
2:D:230:ILE:O	2:D:230:ILE:HG22	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
2:B:529:ASN:C	2:B:529:ASN:OD1	2.60	0.45
2:D:298:TYR:HD1	2:D:306:PHE:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:284:LYS:HB3	2:D:284:LYS:HZ3	1.81	0.45
2:D:598:LEU:C	2:D:600:ASP:N	2.75	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
1:C:-23:GLU:C	1:C:-21:GLN:H	2.24	0.44
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:212:ASN:O	2:D:213:ASN:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:LYS:NZ	2:D:303:GLU:OE1	2.44	0.44
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
1:A:-22:LEU:C	1:A:-20:LYS:N	2.76	0.44
2:D:182:LYS:HB2	2:D:200:PHE:CZ	2.53	0.44
2:D:847:TRP:CD1	2:D:847:TRP:H	2.35	0.44
2:B:60:PRO:O	2:B:62:GLN:N	2.48	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:B:61:GLU:C	2:B:62:GLN:HG2	2.43	0.43
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: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: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:330:ASP:O	2:D:331:ASN:C	2.61	0.43
2:B:847:TRP:CD1	2:B:847:TRP:H	2.37	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: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:489:ASP:OD2	2:D:494:SER:OG	2.33	0.42
2:B:371:MET:HE2	2:B:371:MET:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:223:SER:C	2:D:225:LEU:H	2.27	0.42
2:B:338:ILE:HG12	2:B:455:PHE:CD2	2.54	0.42
1:A:-28:MET:HE2	2:B:302:TRP:HE1	1.84	0.42
2:B:74:ASP:O	2:B:75:SER:C	2.63	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
2:D:704:LYS:HD2	2:D:704:LYS:C	2.45	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:432:SER:C	2:D:434:ASP:N	2.78	0.42
2:D:706:ASP:OD1	2:D:708:VAL:HG23	2.20	0.42
2:D:84:ARG:C	2:D:86:CYS:N	2.78	0.41
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: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:489:ASP:OD2	2:B:494:SER:OG	2.34	0.41
2:D:347:GLN:O	2:D:348:LEU:C	2.63	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:5:MET:HE2	2:D:5:MET:O	2.19	0.41
2:D:278:ILE:C	2:D:280:TYR:H	2.29	0.41
2:D:401:GLY:CA	2:D:431:THR:O	2.57	0.41
2:D:261:PRO:O	2:D:262:SER:HB2	2.21	0.41
2:D:598:LEU:O	2:D:600:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ALA:HB2	2:B:455:PHE:HE1	1.86	0.41
2:B:432:SER:C	2:B:434:ASP:N	2.79	0.41
2:D:178:CYS:O	2:D:179:ILE:O	2.38	0.41
2:D:598:LEU:C	2:D:598:LEU:CD2	2.93	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:D:507:LEU:C	2:D:508:THR:O	2.62	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
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: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:11:LEU:O	2:D:12:LYS:C	2.64	0.40
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:B:491:ASN:OD1	2:B:491:ASN:C	2.65	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:D:234:LEU:HD23	2:D:234:LEU:HA	1.90	0.40
2:D:483:LEU:C	2:D:485:ASP:H	2.29	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

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	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%)	3	5
All	All	1702/1746 (98%)	1467 (86%)	179 (10%)	56 (3%)	3	4

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	10 (83%)	2 (17%)	2	4
1	C	12/12 (100%)	8 (67%)	4 (33%)	0	0
2	B	752/765 (98%)	651 (87%)	101 (13%)	4	8
2	D	752/765 (98%)	653 (87%)	99 (13%)	4	8
All	All	1528/1554 (98%)	1322 (86%)	206 (14%)	4	8

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-25	VAL
1	A	-23	GLU
1	C	-26	THR
1	C	-25	VAL
1	C	-24	LEU
1	C	-19	LEU
2	B	20	LYS
2	B	21	ILE
2	B	29	ILE
2	B	37	ASP
2	B	44	ASP
2	B	46	GLU
2	B	51	HIS
2	B	57	SER
2	B	59	LEU
2	B	65	LYS
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	171	PHE
2	B	173	GLU
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

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Mol	Chain	Res	Type
2	B	192	ASN
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	252	LEU
2	B	253	LYS
2	B	255	ILE
2	B	273	LEU
2	B	277	LYS
2	B	283	LEU
2	B	295	LEU
2	B	310	GLU
2	B	360	VAL
2	B	365	LEU
2	B	366	GLN
2	B	370	ILE
2	B	371	MET
2	B	372	VAL
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	394	ARG
2	B	400	THR
2	B	404	SER
2	B	421	LEU
2	B	425	LEU
2	B	433	GLU
2	B	434	ASP
2	B	462	LEU
2	B	465	LYS
2	B	468	LYS
2	B	469	ARG
2	B	475	THR
2	B	477	ILE
2	B	485	ASP

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Mol	Chain	Res	Type
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	592	LEU
2	B	596	LYS
2	B	602	ILE
2	B	610	ARG
2	B	649	LYS
2	B	652	GLN
2	B	655	VAL
2	B	661	VAL
2	B	663	ILE
2	B	673	SER
2	B	687	LYS
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	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	32	LEU
2	D	45	ASN
2	D	51	HIS
2	D	84	ARG
2	D	87	ILE
2	D	109	ASN
2	D	124	THR

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Mol	Chain	Res	Type
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	183	GLU
2	D	186	LEU
2	D	187	ILE
2	D	197	VAL
2	D	199	ASP
2	D	200	PHE
2	D	203	ASP
2	D	210	THR
2	D	224	ARG
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	284	LYS
2	D	287	LYS
2	D	288	ASP
2	D	294	ASN
2	D	295	LEU
2	D	300	GLN
2	D	303	GLU
2	D	310	GLU
2	D	343	MET
2	D	348	LEU

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Mol	Chain	Res	Type
2	D	351	LEU
2	D	354	SER
2	D	360	VAL
2	D	365	LEU
2	D	366	GLN
2	D	370	ILE
2	D	373	THR
2	D	376	LEU
2	D	385	THR
2	D	387	MET
2	D	460	VAL
2	D	462	LEU
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
2	D	565	LEU
2	D	605	THR
2	D	631	GLU
2	D	644	LYS
2	D	649	LYS
2	D	652	GLN
2	D	655	VAL
2	D	661	VAL
2	D	670	SER
2	D	673	SER
2	D	696	ILE
2	D	704	LYS
2	D	708	VAL
2	D	709	THR
2	D	720	ARG
2	D	747	LEU
2	D	750	GLU
2	D	754	SER

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Mol	Chain	Res	Type
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-17	HIS
1	C	-17	HIS
2	B	14	ASN
2	B	109	ASN
2	B	151	ASN
2	B	185	ASN
2	B	300	GLN
2	B	357	ASN
2	B	440	GLN
2	B	450	ASN
2	B	604	GLN
2	B	652	GLN
2	B	686	GLN
2	B	719	ASN
2	D	8	HIS
2	D	14	ASN
2	D	62	GLN
2	D	109	ASN
2	D	126	ASN
2	D	151	ASN
2	D	177	HIS
2	D	270	GLN
2	D	357	ASN
2	D	440	GLN
2	D	450	ASN
2	D	603	ASN
2	D	652	GLN
2	D	713	GLN
2	D	719	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	14/14 (100%)	1.84	6 (42%) 0 0	74, 88, 136, 147	0
1	C	14/14 (100%)	1.52	4 (28%) 1 1	75, 86, 108, 113	0
2	B	845/859 (98%)	0.96	143 (16%) 4 3	24, 66, 116, 149	0
2	D	845/859 (98%)	0.52	75 (8%) 15 13	16, 53, 92, 156	0
All	All	1718/1746 (98%)	0.75	228 (13%) 7 6	16, 59, 109, 156	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	320	TRP	6.1
2	B	42	PHE	5.3
2	B	29	ILE	5.1
2	D	176	GLU	5.0
2	B	308	VAL	5.0
2	D	602	ILE	4.8
2	B	481	ILE	4.6
2	D	180	ARG	4.4
2	B	361	ALA	4.4
2	B	85	LEU	4.3
2	D	125	ASN	4.3
2	B	256	ILE	4.2
2	B	378	VAL	4.1
2	B	43	LEU	4.1
2	B	602	ILE	4.1
1	A	-19	LEU	4.1
2	D	329	GLU	4.0
2	B	264	GLY	4.0
2	B	273	LEU	3.9
2	B	307	LEU	3.8
2	D	653	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	346	LEU	3.8
2	B	655	VAL	3.7
2	B	411	GLY	3.7
2	B	246	THR	3.6
2	B	170	ILE	3.6
2	B	278	ILE	3.6
2	B	380	ILE	3.6
2	D	481	ILE	3.6
2	B	296	ILE	3.5
2	B	293	VAL	3.5
2	D	29	ILE	3.5
2	B	416	PHE	3.5
2	D	328	PHE	3.5
2	D	174	HIS	3.5
2	B	289	VAL	3.5
2	B	306	PHE	3.5
2	B	415	TRP	3.5
2	D	186	LEU	3.4
1	C	-28	MET	3.4
2	B	186	LEU	3.4
2	B	243	TYR	3.3
1	C	-29	ALA	3.3
2	B	259	ALA	3.3
2	B	38	THR	3.2
2	B	710	GLY	3.2
2	B	381	ILE	3.2
2	B	386	ALA	3.2
2	D	655	VAL	3.2
2	B	248	LYS	3.1
2	B	198	PRO	3.1
2	B	376	LEU	3.1
2	D	603	ASN	3.1
2	B	233	ALA	3.1
2	B	302	TRP	3.1
2	D	179	ILE	3.1
2	D	135	MET	3.0
2	D	184	GLY	3.0
2	B	282	ALA	3.0
2	B	288	ASP	3.0
2	B	179	ILE	3.0
2	B	130	VAL	2.9
2	B	286	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	305	TYR	2.9
2	D	200	PHE	2.9
2	B	363	GLY	2.9
2	D	178	CYS	2.9
2	B	252	LEU	2.9
2	D	32	LEU	2.9
2	D	299	PHE	2.9
2	B	60	PRO	2.9
2	D	155	TRP	2.9
2	D	228	TYR	2.9
2	B	362	MET	2.9
2	B	245	ALA	2.9
2	B	407	MET	2.9
2	D	305	TYR	2.9
2	D	124	THR	2.8
2	D	306	PHE	2.8
2	B	360	VAL	2.8
2	B	385	THR	2.8
2	B	351	LEU	2.8
2	B	277	LYS	2.8
2	B	382	ASP	2.8
2	B	254	VAL	2.8
2	B	232	THR	2.8
2	B	272	ALA	2.8
2	D	171	PHE	2.8
2	B	197	VAL	2.7
2	B	295	LEU	2.7
2	B	91	ILE	2.7
2	D	87	ILE	2.7
2	D	320	TRP	2.7
2	B	291	GLY	2.7
2	D	333	GLY	2.7
2	B	312	ILE	2.7
2	D	293	VAL	2.7
2	B	263	ALA	2.7
2	B	299	PHE	2.7
2	B	603	ASN	2.7
2	D	654	LYS	2.7
2	B	46	GLU	2.7
2	D	83	ALA	2.6
2	B	383	PHE	2.6
2	B	309	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	-18	ALA	2.6
2	D	282	ALA	2.6
2	B	39	TYR	2.6
2	B	387	MET	2.6
2	B	653	LEU	2.6
2	B	409	VAL	2.6
2	B	601	ASN	2.6
2	B	181	ASP	2.6
1	A	-26	THR	2.6
2	B	388	PRO	2.5
2	D	175	GLY	2.5
2	B	365	LEU	2.5
2	D	182	LYS	2.5
2	B	191	ARG	2.5
2	B	255	ILE	2.5
1	A	-24	LEU	2.5
2	B	283	LEU	2.5
2	B	412	ALA	2.5
2	B	280	TYR	2.5
2	B	204	PHE	2.5
2	D	273	LEU	2.5
2	D	289	VAL	2.5
1	A	-29	ALA	2.5
2	B	244	LEU	2.5
2	B	455	PHE	2.5
2	B	475	THR	2.5
2	D	210	THR	2.5
2	D	146	GLY	2.4
2	B	205	ASP	2.4
2	D	234	LEU	2.4
2	B	64	TRP	2.4
2	D	302	TRP	2.4
2	B	397	MET	2.4
2	D	5	MET	2.4
2	B	431	THR	2.4
2	B	297	GLU	2.4
2	D	414	ASP	2.4
2	B	195	TYR	2.4
2	B	236	PHE	2.4
2	B	465	LYS	2.4
2	B	35	ILE	2.4
2	B	292	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	360	VAL	2.4
2	B	467	ASP	2.3
2	B	200	PHE	2.3
2	B	395	PRO	2.3
2	D	239	ALA	2.3
2	B	270	GLN	2.3
2	B	337	HIS	2.3
2	B	182	LYS	2.3
1	C	-24	LEU	2.3
2	D	187	ILE	2.3
2	D	651	LYS	2.3
2	B	328	PHE	2.3
2	B	476	PHE	2.3
1	C	-27	ASN	2.2
2	D	280	TYR	2.3
2	B	184	GLY	2.2
2	B	317	LEU	2.2
2	D	295	LEU	2.2
2	B	201	VAL	2.2
2	D	378	VAL	2.2
2	B	269	ALA	2.2
2	B	174	HIS	2.2
2	D	246	THR	2.2
2	D	475	THR	2.2
2	B	335	SER	2.2
2	D	183	GLU	2.2
2	B	311	PHE	2.2
2	D	383	PHE	2.2
2	B	40	ALA	2.2
2	B	298	TYR	2.2
2	B	451	TYR	2.2
2	D	604	GLN	2.2
2	B	417	GLY	2.2
2	D	286	LEU	2.2
2	D	391	SER	2.2
2	B	260	ARG	2.2
2	B	239	ALA	2.2
2	D	332	ASN	2.2
2	D	601	ASN	2.2
2	B	135	MET	2.2
2	B	355	MET	2.2
2	B	338	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	312	ILE	2.2
2	D	55	LYS	2.2
2	B	59	LEU	2.1
2	B	187	ILE	2.1
2	D	181	ASP	2.1
2	B	654	LYS	2.1
2	B	171	PHE	2.1
2	D	415	TRP	2.1
2	D	476	PHE	2.1
2	B	212	ASN	2.1
2	D	307	LEU	2.1
2	B	372	VAL	2.1
2	B	56	GLY	2.1
2	D	211	ILE	2.1
2	D	380	ILE	2.1
2	B	371	MET	2.1
2	D	177	HIS	2.1
2	B	462	LEU	2.1
2	D	348	LEU	2.1
2	B	210	THR	2.1
2	B	704	LYS	2.1
2	B	410	SER	2.1
2	B	193	PRO	2.1
2	D	455	PHE	2.0
2	D	263	ALA	2.0
2	B	294	ASN	2.0
2	D	369	ASN	2.0
2	B	61	GLU	2.0
2	B	333	GLY	2.0
2	B	809	SER	2.0
2	D	397	MET	2.0
1	A	-25	VAL	2.0
2	B	413	ARG	2.0
2	B	421	LEU	2.0
2	B	287	LYS	2.0
2	D	109	ASN	2.0
2	D	477	ILE	2.0
2	B	155	TRP	2.0
2	B	36	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.