



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:21 PM GMT

PDB ID : 4LDS
Title : The inward-facing structure of the glucose transporter from *Staphylococcus epidermidis*
Authors : Choe, J.; Aleshin, A.; Iancu, C.V.
Deposited on : 2013-06-25
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

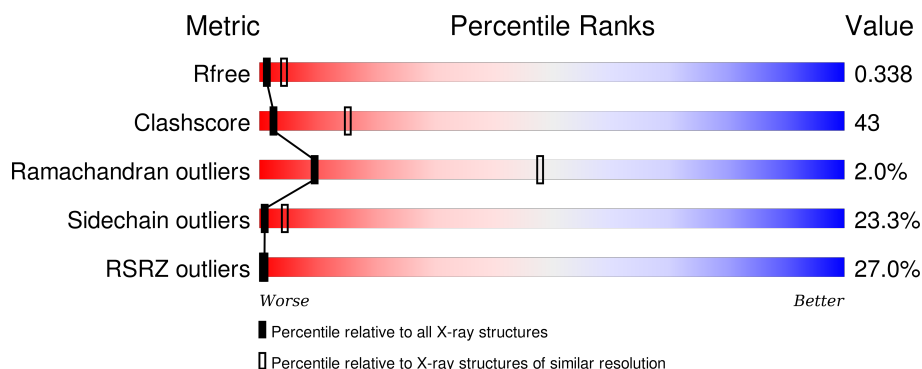
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	446	<div> <div>28%</div> <div>30% 49% 14% • 6%</div> </div>
1	B	446	<div> <div>23%</div> <div>35% 47% 11% • 6%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6388 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.

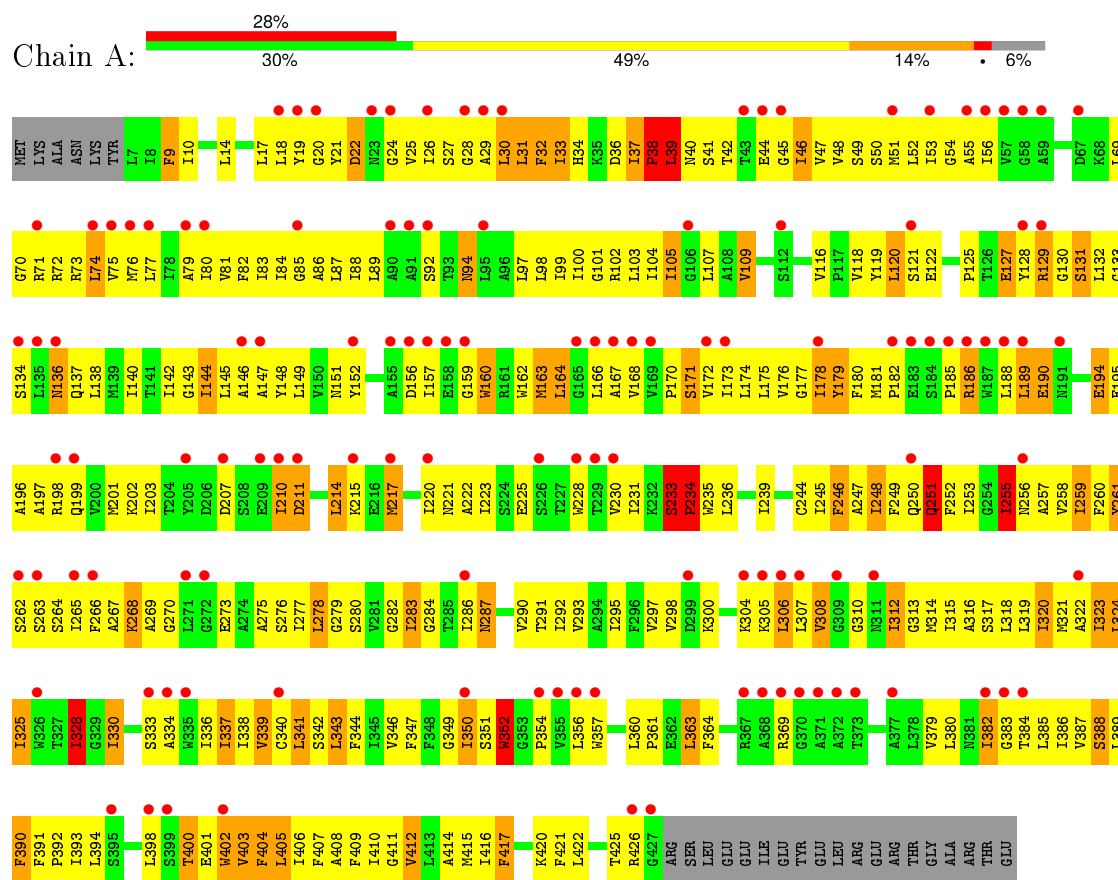
- Molecule 1 is a protein called Bicyclomycin resistance protein TcaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			
1	B	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			

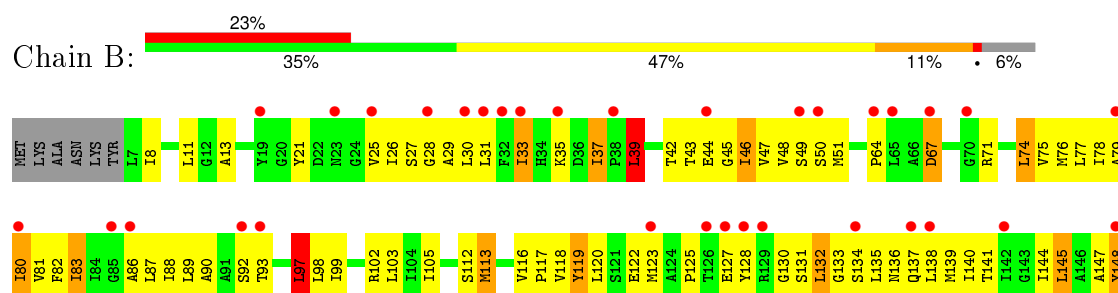
3 Residue-property plots

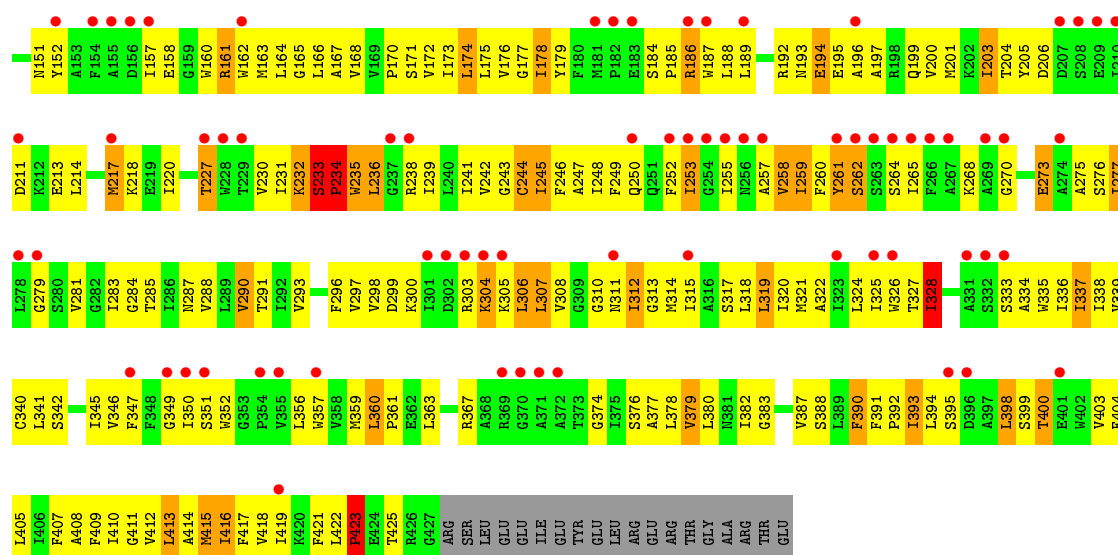
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Bicyclomycin resistance protein TcaB



• Molecule 1: Bicyclomycin resistance protein TcaB





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.07Å 118.85Å 160.05Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	19.90 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.90-3.20) 98.4 (19.90-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.302 , 0.341 0.296 , 0.338	Depositor DCC
R_{free} test set	1945 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 8.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	16 of 38905 reflections (0.041%)	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.75	1/3258 (0.0%)	0.98	8/4431 (0.2%)
1	B	0.57	0/3258	0.85	4/4431 (0.1%)
All	All	0.67	1/6516 (0.0%)	0.92	12/8862 (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
1	A	0	2
1	B	0	5
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	TRP	CB-CG	-5.71	1.40	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	GLY	N-CA-C	7.80	132.61	113.10
1	A	39	LEU	CA-CB-CG	6.36	129.92	115.30
1	A	31	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	314	MET	CB-CG-SD	5.95	130.25	112.40
1	B	39	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	255	ILE	CB-CA-C	-5.57	100.46	111.60
1	A	251	GLN	N-CA-C	5.34	125.42	111.00
1	A	38	PRO	N-CA-C	5.29	125.85	112.10
1	A	341	LEU	CA-CB-CG	-5.24	103.26	115.30
1	B	205	TYR	N-CA-C	5.06	124.67	111.00
1	A	402	TRP	N-CA-C	5.06	124.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PRO	Peptide
1	A	400	THR	Peptide
1	B	206	ASP	Peptide
1	B	233	SER	Peptide
1	B	234	PRO	Peptide
1	B	399	SER	Peptide
1	B	423	PRO	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	3194	0	3399	306	0
1	B	3194	0	3399	262	0
All	All	6388	0	6798	563	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 43.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HG2	1:B:217:MET:HG2	1.32	1.04
1:B:92:SER:HA	1:B:97:LEU:HD11	1.38	1.01
1:A:330:ILE:HA	1:A:333:SER:HB3	1.49	0.94
1:A:324:LEU:HD11	1:A:336:ILE:HB	1.52	0.90
1:A:283:ILE:HD11	1:A:342:SER:HA	1.53	0.89
1:A:163:MET:HA	1:A:166:LEU:HB2	1.54	0.88
1:A:318:LEU:HD23	1:A:404:PHE:HB3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD11	1:A:171:SER:HA	1.54	0.86
1:B:351:SER:HG	1:B:352:TRP:HD1	1.22	0.86
1:B:253:ILE:HG13	1:B:410:ILE:HG22	1.57	0.84
1:B:315:ILE:HG23	1:B:408:ALA:HB1	1.61	0.82
1:A:185:PRO:HA	1:A:188:LEU:HD12	1.62	0.81
1:B:172:VAL:HA	1:B:175:LEU:HB2	1.61	0.80
1:B:334:ALA:HA	1:B:337:ILE:HB	1.61	0.80
1:A:82:PHE:HB3	1:A:171:SER:HB2	1.64	0.80
1:A:25:VAL:HG13	1:A:160:TRP:HH2	1.47	0.79
1:A:83:ILE:HA	1:A:168:VAL:HG22	1.65	0.79
1:B:411:GLY:O	1:B:415:MET:HB2	1.83	0.78
1:A:351:SER:HB2	1:A:352:TRP:CD1	2.19	0.78
1:A:130:GLY:O	1:A:133:GLY:N	2.16	0.77
1:A:409:PHE:HA	1:A:412:VAL:HB	1.66	0.77
1:B:35:LYS:HB3	1:B:157:ILE:HD11	1.66	0.77
1:A:76:MET:SD	1:A:178:ILE:HB	2.25	0.76
1:A:388:SER:OG	1:A:389:LEU:N	2.15	0.76
1:B:186:ARG:HG3	1:B:189:LEU:HD12	1.69	0.75
1:B:234:PRO:HB2	1:B:238:ARG:HH21	1.50	0.75
1:A:276:SER:O	1:A:280:SER:OG	2.03	0.74
1:A:284:GLY:O	1:A:287:ASN:ND2	2.20	0.74
1:B:409:PHE:HA	1:B:412:VAL:HB	1.68	0.74
1:A:30:LEU:HG	1:A:264:SER:HB2	1.68	0.74
1:B:241:ILE:HA	1:B:244:CYS:HB2	1.70	0.74
1:B:318:LEU:HD23	1:B:404:PHE:HD1	1.53	0.73
1:A:406:ILE:O	1:A:409:PHE:N	2.22	0.73
1:A:25:VAL:HG22	1:A:160:TRP:HZ3	1.54	0.72
1:A:246:PHE:CE2	1:A:356:LEU:HG	2.23	0.72
1:A:387:VAL:HG13	1:A:391:PHE:HD2	1.54	0.72
1:A:87:LEU:HG	1:A:168:VAL:HG21	1.69	0.72
1:A:312:ILE:HG12	1:B:320:ILE:HG12	1.72	0.72
1:A:131:SER:O	1:A:134:SER:OG	2.07	0.72
1:A:387:VAL:HG13	1:A:391:PHE:CD2	2.25	0.71
1:A:266:PHE:CE1	1:A:338:ILE:HA	2.25	0.71
1:B:398:LEU:HD12	1:B:400:THR:HB	1.73	0.71
1:B:227:THR:HG21	1:B:367:ARG:HH11	1.55	0.71
1:A:315:ILE:HA	1:A:318:LEU:HB2	1.71	0.71
1:B:265:ILE:HD13	1:B:337:ILE:HD13	1.72	0.70
1:A:253:ILE:HD11	1:A:410:ILE:HG22	1.74	0.70
1:A:323:ILE:HG21	1:B:415:MET:HE3	1.73	0.70
1:A:346:VAL:O	1:A:350:ILE:HG12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HB3	1:A:157:ILE:HD11	1.73	0.69
1:A:25:VAL:HG13	1:A:160:TRP:CH2	2.27	0.69
1:A:217:MET:HA	1:A:220:ILE:HG12	1.75	0.69
1:B:175:LEU:HG	1:B:179:TYR:HE1	1.58	0.68
1:A:351:SER:HB2	1:A:352:TRP:HD1	1.57	0.68
1:B:87:LEU:HG	1:B:168:VAL:HG21	1.76	0.68
1:A:273:GLU:O	1:A:276:SER:N	2.27	0.67
1:A:246:PHE:CZ	1:A:360:LEU:HG	2.29	0.67
1:A:207:ASP:HA	1:A:210:ILE:HG12	1.75	0.67
1:B:158:GLU:HG2	1:B:161:ARG:HH21	1.59	0.67
1:A:89:LEU:HB3	1:A:164:LEU:HD12	1.77	0.67
1:B:395:SER:HA	1:B:400:THR:HG21	1.76	0.67
1:B:324:LEU:HB3	1:B:333:SER:HB2	1.77	0.66
1:B:394:LEU:HD13	1:B:398:LEU:HD11	1.77	0.66
1:A:265:ILE:O	1:A:269:ALA:HB3	1.95	0.66
1:B:141:THR:HG22	1:B:288:VAL:HG22	1.78	0.66
1:A:244:CYS:HB3	1:A:379:VAL:HG11	1.78	0.65
1:A:283:ILE:HA	1:A:286:ILE:HD12	1.78	0.65
1:B:407:PHE:HA	1:B:410:ILE:HB	1.79	0.65
1:B:171:SER:O	1:B:175:LEU:N	2.30	0.65
1:A:145:LEU:HD23	1:A:284:GLY:HA3	1.79	0.65
1:B:27:SER:HA	1:B:260:PHE:HA	1.79	0.65
1:A:322:ALA:HB1	1:A:401:GLU:HG2	1.78	0.65
1:B:253:ILE:HG23	1:B:407:PHE:HB3	1.79	0.65
1:B:308:VAL:HG22	1:B:418:VAL:HG11	1.79	0.64
1:B:122:GLU:HG2	1:B:186:ARG:HB2	1.79	0.64
1:A:266:PHE:HB3	1:A:275:ALA:O	1.98	0.64
1:A:257:ALA:HB2	1:A:387:VAL:HG12	1.79	0.64
1:A:146:ALA:HA	1:A:149:LEU:HD13	1.80	0.64
1:B:44:GLU:HA	1:B:47:VAL:HB	1.79	0.64
1:A:89:LEU:HD13	1:A:101:GLY:HA3	1.79	0.63
1:A:317:SER:HA	1:A:320:ILE:HG22	1.80	0.63
1:B:21:TYR:HA	1:B:147:ALA:HB2	1.81	0.63
1:A:84:ILE:HG22	1:A:104:ILE:HG21	1.79	0.62
1:A:323:ILE:HG21	1:B:415:MET:CE	2.28	0.62
1:B:176:VAL:HA	1:B:179:TYR:HB2	1.81	0.62
1:B:335:TRP:O	1:B:338:ILE:HB	1.99	0.62
1:A:80:ILE:HA	1:A:83:ILE:HG22	1.81	0.62
1:B:26:ILE:HG13	1:B:29:ALA:HB3	1.82	0.62
1:A:92:SER:HA	1:A:97:LEU:HD21	1.81	0.62
1:A:151:ASN:HA	1:A:163:MET:SD	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ILE:HD13	1:B:412:VAL:HG23	1.82	0.62
1:B:200:VAL:HA	1:B:203:ILE:HB	1.82	0.62
1:A:152:TYR:CZ	1:A:273:GLU:HB2	2.34	0.62
1:A:403:VAL:O	1:A:406:ILE:N	2.33	0.62
1:A:75:VAL:HG21	1:A:119:TYR:CG	2.35	0.62
1:A:189:LEU:HD11	1:A:214:LEU:HD22	1.82	0.62
1:A:312:ILE:HG23	1:B:320:ILE:HD11	1.80	0.62
1:A:72:ARG:NH2	1:A:181:MET:O	2.33	0.62
1:A:159:GLY:O	1:A:162:TRP:HB3	1.99	0.61
1:B:400:THR:OG1	1:B:400:THR:O	2.17	0.61
1:A:100:ILE:HA	1:A:103:LEU:HD12	1.81	0.61
1:A:257:ALA:HB2	1:A:387:VAL:CG1	2.32	0.60
1:B:45:GLY:O	1:B:49:SER:OG	2.09	0.60
1:B:255:ILE:HA	1:B:258:VAL:HB	1.83	0.60
1:A:51:MET:HA	1:A:102:ARG:O	2.01	0.60
1:A:306:LEU:O	1:A:351:SER:OG	2.16	0.60
1:B:325:ILE:HG21	1:B:400:THR:O	2.02	0.60
1:B:79:ALA:HB2	1:B:178:ILE:HD12	1.83	0.60
1:A:275:ALA:O	1:A:279:GLY:HA3	2.02	0.60
1:A:334:ALA:HA	1:A:337:ILE:HB	1.82	0.60
1:A:144:ILE:O	1:A:147:ALA:HB3	2.01	0.60
1:A:47:VAL:O	1:A:50:SER:OG	2.16	0.60
1:A:249:PHE:HD2	1:A:414:ALA:HB2	1.67	0.60
1:B:158:GLU:HA	1:B:161:ARG:NE	2.17	0.59
1:A:79:ALA:O	1:A:82:PHE:HB2	2.02	0.59
1:B:315:ILE:HG12	1:B:408:ALA:O	2.03	0.59
1:A:45:GLY:O	1:A:49:SER:OG	2.14	0.59
1:A:118:VAL:HA	1:A:121:SER:HB3	1.84	0.59
1:B:46:ILE:HA	1:B:49:SER:HB2	1.85	0.59
1:B:42:THR:HA	1:B:393:ILE:HG22	1.85	0.59
1:A:175:LEU:HG	1:A:179:TYR:CE1	2.38	0.59
1:B:170:PRO:HA	1:B:173:ILE:HG12	1.85	0.59
1:B:334:ALA:C	1:B:337:ILE:H	2.05	0.59
1:A:42:THR:HG22	1:A:393:ILE:HB	1.83	0.59
1:A:20:GLY:O	1:A:144:ILE:HG13	2.03	0.59
1:A:256:ASN:O	1:A:260:PHE:HE1	1.84	0.59
1:A:318:LEU:HD13	1:A:408:ALA:HA	1.85	0.58
1:B:26:ILE:HD11	1:B:48:VAL:HG22	1.84	0.58
1:A:352:TRP:HE3	1:A:356:LEU:HD22	1.68	0.58
1:B:214:LEU:O	1:B:218:LYS:HB2	2.03	0.58
1:A:310:GLY:O	1:A:347:PHE:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HA	1:A:44:GLU:CD	2.24	0.58
1:A:266:PHE:O	1:A:270:GLY:HA3	2.03	0.58
1:A:253:ILE:CD1	1:A:410:ILE:HG22	2.33	0.58
1:B:253:ILE:HD13	1:B:314:MET:HE1	1.86	0.58
1:A:409:PHE:CA	1:A:412:VAL:HB	2.34	0.58
1:A:173:ILE:O	1:A:177:GLY:N	2.35	0.58
1:A:51:MET:HB2	1:A:102:ARG:HE	1.68	0.58
1:B:313:GLY:HA3	1:B:347:PHE:CD2	2.38	0.58
1:B:318:LEU:HB3	1:B:404:PHE:HB3	1.85	0.57
1:B:383:GLY:O	1:B:387:VAL:HG23	2.04	0.57
1:A:315:ILE:HD11	1:A:411:GLY:O	2.04	0.57
1:B:123:MET:HE1	1:B:200:VAL:HG11	1.87	0.57
1:A:273:GLU:C	1:A:276:SER:H	2.08	0.57
1:B:233:SER:HB3	1:B:234:PRO:HD3	1.86	0.57
1:A:28:GLY:O	1:A:31:LEU:HB3	2.04	0.57
1:A:79:ALA:HA	1:A:82:PHE:HD2	1.69	0.57
1:B:306:LEU:HD22	1:B:351:SER:HB3	1.87	0.57
1:B:253:ILE:CG1	1:B:410:ILE:HG22	2.32	0.57
1:A:336:ILE:O	1:A:339:VAL:HB	2.03	0.57
1:A:9:PHE:CE1	1:A:120:LEU:HG	2.40	0.57
1:B:185:PRO:HA	1:B:188:LEU:HD12	1.86	0.57
1:B:144:ILE:HG23	1:B:148:TYR:CE2	2.40	0.57
1:A:313:GLY:O	1:A:316:ALA:HB3	2.04	0.57
1:B:311:ASN:HB3	1:B:415:MET:SD	2.45	0.57
1:B:407:PHE:HD1	1:B:410:ILE:HD12	1.70	0.57
1:B:252:PHE:CZ	1:B:383:GLY:HA2	2.40	0.57
1:B:284:GLY:O	1:B:288:VAL:HG23	2.05	0.56
1:A:321:MET:HE2	1:A:340:CYS:HB3	1.87	0.56
1:A:258:VAL:O	1:A:262:SER:OG	2.21	0.56
1:A:247:ALA:O	1:A:380:LEU:HD12	2.05	0.56
1:A:352:TRP:CE3	1:A:356:LEU:HD22	2.40	0.56
1:B:359:MET:O	1:B:363:LEU:HG	2.05	0.56
1:B:174:LEU:HD13	1:B:177:GLY:HA3	1.87	0.56
1:B:51:MET:HB2	1:B:102:ARG:HD3	1.87	0.56
1:A:315:ILE:HG23	1:A:408:ALA:HB1	1.88	0.56
1:A:128:TYR:HB3	1:A:132:LEU:HD11	1.88	0.56
1:A:24:GLY:O	1:A:27:SER:HB3	2.05	0.56
1:A:300:LYS:O	1:A:426:ARG:NH1	2.39	0.56
1:A:261:TYR:OH	1:A:403:VAL:HG21	2.05	0.56
1:A:307:LEU:HD11	1:A:356:LEU:HD13	1.86	0.56
1:B:387:VAL:HA	1:B:391:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:PHE:HA	1:B:421:PHE:HD2	1.71	0.56
1:A:389:LEU:O	1:A:393:ILE:HG23	2.06	0.55
1:B:413:LEU:HD23	1:B:416:ILE:HG21	1.87	0.55
1:B:125:PRO:HA	1:B:186:ARG:HH22	1.72	0.55
1:A:27:SER:HA	1:A:260:PHE:HA	1.87	0.55
1:A:85:GLY:O	1:A:89:LEU:HB2	2.07	0.55
1:A:176:VAL:HA	1:A:179:TYR:CG	2.42	0.55
1:B:112:SER:OG	1:B:113:MET:N	2.40	0.55
1:A:246:PHE:CE2	1:A:360:LEU:HG	2.42	0.55
1:B:86:ALA:O	1:B:164:LEU:HB3	2.07	0.55
1:B:141:THR:HG21	1:B:288:VAL:HA	1.89	0.55
1:B:419:ILE:O	1:B:423:PRO:HG3	2.07	0.55
1:B:374:GLY:O	1:B:377:ALA:HB3	2.06	0.55
1:A:29:ALA:O	1:A:32:PHE:N	2.41	0.54
1:B:242:VAL:O	1:B:245:ILE:HG22	2.07	0.54
1:B:257:ALA:HA	1:B:260:PHE:CD2	2.43	0.54
1:A:160:TRP:HA	1:A:163:MET:HG2	1.89	0.54
1:A:77:LEU:O	1:A:81:VAL:HG23	2.07	0.54
1:B:287:ASN:HA	1:B:290:VAL:HG12	1.88	0.54
1:B:125:PRO:HA	1:B:186:ARG:NH2	2.23	0.54
1:B:43:THR:HA	1:B:46:ILE:HB	1.89	0.54
1:B:246:PHE:HD1	1:B:417:PHE:CE1	2.26	0.54
1:A:352:TRP:CD1	1:A:352:TRP:N	2.76	0.54
1:A:390:PHE:HB3	1:A:391:PHE:CD1	2.42	0.54
1:A:343:LEU:O	1:A:346:VAL:N	2.40	0.54
1:B:308:VAL:HG22	1:B:418:VAL:CG1	2.37	0.54
1:B:71:ARG:O	1:B:75:VAL:HG23	2.08	0.54
1:A:122:GLU:HG2	1:A:186:ARG:HB3	1.90	0.54
1:B:170:PRO:O	1:B:174:LEU:N	2.41	0.54
1:A:321:MET:SD	1:A:337:ILE:HG12	2.47	0.53
1:B:137:GLN:O	1:B:140:ILE:HB	2.08	0.53
1:A:175:LEU:HA	1:A:178:ILE:HD12	1.90	0.53
1:B:307:LEU:HA	1:B:351:SER:OG	2.08	0.53
1:B:234:PRO:O	1:B:236:LEU:N	2.41	0.53
1:B:378:LEU:O	1:B:382:ILE:HG13	2.08	0.53
1:A:26:ILE:HG12	1:A:48:VAL:CG2	2.38	0.53
1:A:315:ILE:HG22	1:A:319:LEU:HD12	1.89	0.53
1:A:405:LEU:O	1:A:408:ALA:HB3	2.09	0.53
1:B:80:ILE:HG13	1:B:175:LEU:HD11	1.89	0.53
1:B:249:PHE:CZ	1:B:413:LEU:HD22	2.44	0.53
1:B:233:SER:HB3	1:B:234:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TRP:O	1:B:360:LEU:N	2.41	0.53
1:A:252:PHE:HB3	1:A:410:ILE:HG21	1.91	0.53
1:A:19:TYR:CE1	1:A:109:VAL:HG13	2.44	0.53
1:A:143:GLY:O	1:A:147:ALA:HB2	2.09	0.52
1:B:259:ILE:HA	1:B:262:SER:HB3	1.91	0.52
1:A:409:PHE:C	1:A:412:VAL:HB	2.30	0.52
1:B:313:GLY:HA3	1:B:347:PHE:CE2	2.45	0.52
1:B:130:GLY:O	1:B:133:GLY:N	2.42	0.52
1:A:28:GLY:HA3	1:A:151:ASN:CG	2.30	0.52
1:A:211:ASP:O	1:A:215:LYS:HB2	2.09	0.52
1:B:187:TRP:HE3	1:B:188:LEU:HG	1.75	0.52
1:B:324:LEU:HD11	1:B:336:ILE:HD12	1.92	0.52
1:A:22:ASP:OD2	1:A:105:ILE:HG23	2.09	0.52
1:A:339:VAL:O	1:A:342:SER:N	2.43	0.52
1:A:318:LEU:CD2	1:A:404:PHE:HB3	2.35	0.52
1:B:152:TYR:HE1	1:B:273:GLU:HB2	1.75	0.52
1:A:261:TYR:O	1:A:264:SER:HB3	2.10	0.51
1:A:341:LEU:O	1:A:344:PHE:N	2.43	0.51
1:B:26:ILE:HA	1:B:29:ALA:HB3	1.92	0.51
1:A:46:ILE:O	1:A:49:SER:HB2	2.09	0.51
1:B:21:TYR:HE1	1:B:167:ALA:HB2	1.75	0.51
1:A:54:GLY:HA3	1:A:103:LEU:O	2.10	0.51
1:B:99:ILE:O	1:B:103:LEU:HG	2.10	0.51
1:A:246:PHE:CD2	1:A:356:LEU:HG	2.46	0.51
1:B:148:TYR:OH	1:B:284:GLY:HA3	2.11	0.51
1:A:47:VAL:HG21	1:A:98:LEU:HD13	1.91	0.51
1:B:287:ASN:O	1:B:291:THR:HG23	2.11	0.51
1:A:339:VAL:O	1:A:343:LEU:HD22	2.10	0.51
1:B:326:TRP:O	1:B:328:ILE:N	2.44	0.51
1:B:196:ALA:HA	1:B:199:GLN:HB2	1.93	0.51
1:A:318:LEU:HB3	1:A:408:ALA:HB2	1.91	0.51
1:A:320:ILE:O	1:A:324:LEU:HB2	2.10	0.51
1:B:315:ILE:HD11	1:B:411:GLY:C	2.31	0.51
1:A:390:PHE:O	1:A:393:ILE:HG12	2.10	0.51
1:B:75:VAL:HB	1:B:178:ILE:HG21	1.93	0.51
1:A:266:PHE:HZ	1:A:341:LEU:HD23	1.75	0.51
1:B:141:THR:O	1:B:144:ILE:HG22	2.11	0.51
1:A:33:ILE:HD12	1:A:34:HIS:H	1.75	0.51
1:A:404:PHE:CD1	1:A:404:PHE:N	2.77	0.51
1:B:414:ALA:O	1:B:418:VAL:HG23	2.10	0.51
1:B:173:ILE:HA	1:B:176:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLY:HA2	1:B:347:PHE:CD1	2.46	0.51
1:B:296:PHE:CE1	1:B:300:LYS:HD2	2.45	0.51
1:A:266:PHE:CZ	1:A:341:LEU:HD23	2.46	0.50
1:B:132:LEU:O	1:B:135:LEU:HB3	2.12	0.50
1:B:335:TRP:O	1:B:339:VAL:HG23	2.11	0.50
1:B:248:ILE:HG23	1:B:252:PHE:CD2	2.46	0.50
1:A:10:ILE:O	1:A:14:LEU:HG	2.12	0.50
1:B:93:THR:H	1:B:97:LEU:HG	1.76	0.50
1:B:273:GLU:O	1:B:276:SER:N	2.36	0.50
1:B:74:LEU:O	1:B:78:ILE:HG13	2.12	0.50
1:A:30:LEU:HD12	1:A:33:ILE:HG12	1.94	0.50
1:A:261:TYR:HA	1:A:264:SER:HB3	1.94	0.50
1:A:404:PHE:HA	1:A:407:PHE:HB2	1.94	0.50
1:B:360:LEU:HB3	1:B:361:PRO:HD3	1.93	0.50
1:B:131:SER:O	1:B:134:SER:OG	2.25	0.50
1:A:308:VAL:HG22	1:A:415:MET:HE1	1.94	0.50
1:A:308:VAL:O	1:A:312:ILE:HB	2.11	0.49
1:B:145:LEU:HD23	1:B:288:VAL:HG21	1.95	0.49
1:A:190:GLU:HG3	1:A:221:ASN:HB3	1.94	0.49
1:B:357:TRP:O	1:B:361:PRO:HD2	2.13	0.49
1:A:25:VAL:HG22	1:A:160:TRP:CZ3	2.41	0.49
1:A:325:ILE:HG12	1:A:333:SER:OG	2.12	0.49
1:A:172:VAL:O	1:A:175:LEU:HB3	2.11	0.49
1:B:90:ALA:O	1:B:161:ARG:HB3	2.11	0.49
1:B:86:ALA:HA	1:B:164:LEU:HD12	1.92	0.49
1:B:315:ILE:HA	1:B:318:LEU:HD12	1.93	0.49
1:B:234:PRO:HB2	1:B:238:ARG:NH2	2.22	0.49
1:B:44:GLU:O	1:B:48:VAL:HG23	2.12	0.49
1:B:76:MET:SD	1:B:178:ILE:HB	2.52	0.49
1:A:236:LEU:HD12	1:A:236:LEU:H	1.77	0.49
1:B:189:LEU:HD22	1:B:218:LYS:HZ2	1.78	0.49
1:B:303:ARG:HG2	1:B:359:MET:HG2	1.94	0.49
1:B:232:LYS:HD2	1:B:233:SER:HB2	1.95	0.48
1:B:193:ASN:O	1:B:195:GLU:N	2.46	0.48
1:A:263:SER:OG	1:A:280:SER:OG	2.31	0.48
1:A:336:ILE:C	1:A:339:VAL:HB	2.32	0.48
1:B:26:ILE:HG23	1:B:260:PHE:CE1	2.48	0.48
1:B:187:TRP:CE3	1:B:188:LEU:HG	2.48	0.48
1:B:87:LEU:CG	1:B:168:VAL:HG21	2.43	0.48
1:B:26:ILE:HA	1:B:29:ALA:CB	2.44	0.48
1:B:151:ASN:N	1:B:163:MET:HE1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HA	1:A:38:PRO:HG2	1.95	0.48
1:B:174:LEU:HA	1:B:174:LEU:HD13	1.66	0.48
1:B:27:SER:HB2	1:B:259:ILE:HD12	1.94	0.48
1:A:357:TRP:HZ2	1:A:380:LEU:HD22	1.77	0.48
1:A:186:ARG:HA	1:A:189:LEU:HB2	1.96	0.48
1:A:188:LEU:HD13	1:A:196:ALA:HB3	1.96	0.48
1:B:26:ILE:HG21	1:B:51:MET:SD	2.54	0.48
1:B:125:PRO:HB3	1:B:213:GLU:CD	2.34	0.48
1:A:26:ILE:HD13	1:A:102:ARG:NH1	2.29	0.48
1:A:308:VAL:HA	1:A:415:MET:SD	2.53	0.48
1:A:41:SER:O	1:A:44:GLU:HB2	2.14	0.48
1:B:152:TYR:CE1	1:B:273:GLU:HB2	2.49	0.48
1:B:37:ILE:HG22	1:B:39:LEU:HD12	1.96	0.48
1:B:185:PRO:O	1:B:197:ALA:HB2	2.14	0.47
1:A:321:MET:HB2	1:A:321:MET:HE2	1.74	0.47
1:A:86:ALA:HB3	1:A:168:VAL:HG23	1.96	0.47
1:A:409:PHE:HD1	1:A:412:VAL:HG21	1.79	0.47
1:B:13:ALA:O	1:B:139:MET:HG2	2.13	0.47
1:A:409:PHE:HA	1:A:412:VAL:CB	2.38	0.47
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.70	0.47
1:B:334:ALA:O	1:B:337:ILE:N	2.47	0.47
1:A:305:LYS:HA	1:A:308:VAL:HB	1.96	0.47
1:A:258:VAL:O	1:A:262:SER:CB	2.62	0.47
1:A:190:GLU:HG3	1:A:221:ASN:CG	2.35	0.47
1:A:290:VAL:HG11	1:A:349:GLY:HA3	1.96	0.47
1:A:251:GLN:NE2	1:A:256:ASN:HB2	2.29	0.47
1:A:26:ILE:HG23	1:A:260:PHE:CG	2.50	0.47
1:A:52:LEU:HA	1:A:55:ALA:HB3	1.96	0.47
1:B:249:PHE:HD2	1:B:417:PHE:CD2	2.33	0.47
1:A:416:ILE:O	1:A:420:LYS:HB2	2.15	0.47
1:B:122:GLU:HB3	1:B:186:ARG:H	1.80	0.47
1:A:164:LEU:O	1:A:167:ALA:HB3	2.14	0.47
1:A:27:SER:HB3	1:A:148:TYR:HB3	1.96	0.47
1:B:307:LEU:HA	1:B:351:SER:HG	1.79	0.47
1:B:189:LEU:HD22	1:B:218:LYS:NZ	2.29	0.47
1:A:264:SER:O	1:A:268:LYS:HB2	2.15	0.47
1:B:253:ILE:HG21	1:B:314:MET:HE3	1.96	0.47
1:B:379:VAL:HA	1:B:382:ILE:HD12	1.97	0.47
1:A:407:PHE:HA	1:A:410:ILE:HG13	1.96	0.47
1:B:290:VAL:CG1	1:B:349:GLY:HA3	2.45	0.47
1:A:265:ILE:O	1:A:270:GLY:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:C	1:A:127:GLU:H	2.17	0.47
1:A:400:THR:HB	1:A:402:TRP:HB2	1.97	0.46
1:B:415:MET:HA	1:B:418:VAL:HB	1.96	0.46
1:B:26:ILE:HD12	1:B:102:ARG:HH11	1.81	0.46
1:A:69:LEU:HD22	1:A:73:ARG:HH21	1.80	0.46
1:B:235:TRP:H	1:B:238:ARG:HH21	1.62	0.46
1:B:336:ILE:HA	1:B:339:VAL:HG23	1.97	0.46
1:B:379:VAL:O	1:B:382:ILE:HB	2.15	0.46
1:B:307:LEU:HD13	1:B:356:LEU:HD11	1.97	0.46
1:B:326:TRP:C	1:B:328:ILE:H	2.18	0.46
1:A:199:GLN:O	1:A:202:LYS:HB2	2.15	0.46
1:A:417:PHE:C	1:A:417:PHE:CD1	2.89	0.46
1:A:26:ILE:HG23	1:A:260:PHE:HB3	1.97	0.46
1:A:318:LEU:HD13	1:A:407:PHE:O	2.15	0.46
1:A:174:LEU:O	1:A:178:ILE:HG13	2.15	0.46
1:B:173:ILE:O	1:B:177:GLY:N	2.48	0.46
1:B:322:ALA:O	1:B:325:ILE:HB	2.15	0.46
1:B:261:TYR:HA	1:B:264:SER:HB3	1.97	0.46
1:A:84:ILE:O	1:A:88:ILE:HB	2.16	0.46
1:A:148:TYR:HE1	1:A:280:SER:C	2.19	0.46
1:A:26:ILE:HG23	1:A:260:PHE:CB	2.46	0.46
1:B:307:LEU:HD12	1:B:418:VAL:HG22	1.98	0.46
1:A:181:MET:HA	1:A:182:PRO:HD3	1.66	0.46
1:B:326:TRP:O	1:B:328:ILE:HD12	2.16	0.46
1:B:297:VAL:HA	1:B:300:LYS:HB3	1.98	0.46
1:A:198:ARG:O	1:A:201:MET:HB2	2.16	0.46
1:B:86:ALA:N	1:B:105:ILE:HD11	2.31	0.46
1:B:148:TYR:HE1	1:B:281:VAL:HG13	1.80	0.46
1:B:312:ILE:HG22	1:B:313:GLY:N	2.30	0.46
1:B:351:SER:OG	1:B:352:TRP:HD1	1.92	0.45
1:A:89:LEU:HD21	1:A:102:ARG:HG2	1.97	0.45
1:A:26:ILE:HG12	1:A:48:VAL:HG21	1.97	0.45
1:A:321:MET:HG2	1:A:404:PHE:CD1	2.52	0.45
1:A:89:LEU:HB3	1:A:164:LEU:CD1	2.46	0.45
1:B:175:LEU:O	1:B:179:TYR:HD1	2.00	0.45
1:B:43:THR:O	1:B:47:VAL:HG23	2.15	0.45
1:B:188:LEU:HD13	1:B:197:ALA:N	2.31	0.45
1:A:400:THR:C	1:A:402:TRP:N	2.66	0.45
1:B:415:MET:O	1:B:418:VAL:HB	2.17	0.45
1:B:26:ILE:HG21	1:B:51:MET:HE1	1.99	0.45
1:A:236:LEU:O	1:A:239:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PRO:HA	1:B:67:ASP:HB2	1.97	0.45
1:A:26:ILE:HA	1:A:29:ALA:HB3	1.99	0.45
1:B:265:ILE:HG22	1:B:268:LYS:HB3	1.99	0.45
1:A:279:GLY:O	1:A:283:ILE:HB	2.17	0.45
1:A:133:GLY:O	1:A:136:ASN:HB3	2.16	0.45
1:A:21:TYR:HA	1:A:147:ALA:HB2	1.98	0.45
1:A:402:TRP:O	1:A:406:ILE:HG12	2.16	0.45
1:A:94:ASN:N	1:A:94:ASN:OD1	2.50	0.45
1:B:160:TRP:O	1:B:163:MET:HG2	2.17	0.45
1:B:118:VAL:O	1:B:122:GLU:HG3	2.17	0.45
1:A:160:TRP:CA	1:A:163:MET:HG2	2.47	0.45
1:A:307:LEU:HD13	1:A:352:TRP:CH2	2.52	0.45
1:B:235:TRP:CH2	1:B:236:LEU:HD11	2.52	0.45
1:B:144:ILE:HG23	1:B:148:TYR:CZ	2.52	0.45
1:A:248:ILE:HD11	1:A:382:ILE:HG22	1.98	0.45
1:A:144:ILE:HG22	1:A:145:LEU:N	2.31	0.45
1:A:324:LEU:HD12	1:A:340:CYS:SG	2.57	0.45
1:B:138:LEU:HA	1:B:141:THR:OG1	2.17	0.45
1:B:29:ALA:O	1:B:33:ILE:HG23	2.17	0.45
1:A:31:LEU:HD11	1:A:152:TYR:CG	2.52	0.44
1:A:325:ILE:O	1:A:328:ILE:N	2.44	0.44
1:A:21:TYR:OH	1:A:167:ALA:HB2	2.17	0.44
1:A:259:ILE:HG23	1:A:260:PHE:H	1.81	0.44
1:A:176:VAL:HA	1:A:179:TYR:CD2	2.52	0.44
1:B:347:PHE:CE1	1:B:350:ILE:HD11	2.51	0.44
1:B:184:SER:HA	1:B:185:PRO:HD3	1.81	0.44
1:B:21:TYR:CZ	1:B:25:VAL:HG21	2.53	0.44
1:B:75:VAL:HG12	1:B:178:ILE:HD13	1.99	0.44
1:B:77:LEU:O	1:B:81:VAL:HG23	2.16	0.44
1:B:304:LYS:HE3	1:B:305:LYS:HE3	1.99	0.44
1:A:24:GLY:O	1:A:148:TYR:HB3	2.16	0.44
1:A:37:ILE:N	1:A:38:PRO:HD3	2.31	0.44
1:A:351:SER:CB	1:A:352:TRP:CD1	2.97	0.44
1:A:138:LEU:HD11	1:A:295:ILE:HD11	2.00	0.44
1:B:117:PRO:HA	1:B:120:LEU:HB3	1.99	0.44
1:A:164:LEU:HA	1:A:164:LEU:HD22	1.64	0.44
1:B:51:MET:SD	1:B:102:ARG:NH1	2.91	0.44
1:A:100:ILE:O	1:A:103:LEU:HB2	2.18	0.44
1:B:246:PHE:HB2	1:B:417:PHE:CZ	2.53	0.44
1:A:334:ALA:O	1:A:337:ILE:N	2.49	0.44
1:A:189:LEU:HD21	1:A:214:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:PHE:O	1:B:250:GLN:HB3	2.18	0.44
1:B:122:GLU:HB3	1:B:185:PRO:HD2	1.99	0.44
1:B:403:VAL:HG13	1:B:407:PHE:CE2	2.53	0.44
1:B:246:PHE:HB2	1:B:417:PHE:HZ	1.83	0.44
1:B:321:MET:HB2	1:B:340:CYS:HB3	1.99	0.44
1:A:164:LEU:HD22	1:A:167:ALA:HB2	1.99	0.43
1:A:410:ILE:C	1:A:412:VAL:H	2.20	0.43
1:A:87:LEU:CG	1:A:168:VAL:HG21	2.44	0.43
1:A:188:LEU:HB2	1:A:197:ALA:HB2	2.00	0.43
1:A:386:ILE:O	1:A:390:PHE:HB2	2.18	0.43
1:A:194:GLU:O	1:A:197:ALA:HB3	2.18	0.43
1:B:21:TYR:CD2	1:B:147:ALA:HA	2.53	0.43
1:B:89:LEU:HD12	1:B:89:LEU:HA	1.54	0.43
1:A:267:ALA:HB2	1:A:273:GLU:HA	2.00	0.43
1:A:336:ILE:O	1:A:340:CYS:SG	2.64	0.43
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.69	0.43
1:A:228:TRP:HE3	1:A:231:ILE:HG13	1.82	0.43
1:B:194:GLU:O	1:B:197:ALA:HB3	2.18	0.43
1:B:27:SER:OG	1:B:28:GLY:N	2.51	0.43
1:A:104:ILE:HA	1:A:107:LEU:HD12	2.00	0.43
1:A:230:VAL:O	1:A:236:LEU:HD13	2.19	0.43
1:A:83:ILE:HG13	1:A:168:VAL:HG13	2.01	0.43
1:A:52:LEU:HB2	1:A:385:LEU:HG	2.00	0.43
1:B:249:PHE:HD2	1:B:417:PHE:HD2	1.67	0.43
1:B:79:ALA:HB2	1:B:178:ILE:CD1	2.47	0.43
1:B:163:MET:HA	1:B:166:LEU:HB2	2.01	0.43
1:A:26:ILE:HG12	1:A:48:VAL:HG22	2.01	0.43
1:A:186:ARG:NH1	1:A:201:MET:SD	2.89	0.43
1:A:280:SER:O	1:A:283:ILE:HG22	2.18	0.43
1:B:318:LEU:HD22	1:B:404:PHE:HA	2.01	0.43
1:A:79:ALA:HB3	1:A:175:LEU:HD13	2.01	0.43
1:A:189:LEU:HA	1:A:194:GLU:HB2	2.01	0.43
1:B:145:LEU:HA	1:B:148:TYR:CE1	2.54	0.43
1:A:315:ILE:HG23	1:A:408:ALA:CB	2.48	0.43
1:A:252:PHE:HE1	1:A:383:GLY:HA2	1.84	0.43
1:B:315:ILE:O	1:B:319:LEU:HD12	2.19	0.43
1:B:417:PHE:HA	1:B:421:PHE:CD2	2.53	0.43
1:B:326:TRP:C	1:B:328:ILE:N	2.72	0.43
1:A:70:GLY:O	1:A:74:LEU:HB2	2.19	0.43
1:A:222:ALA:O	1:A:225:GLU:HB2	2.19	0.43
1:A:287:ASN:O	1:A:291:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:HB2	1:B:398:LEU:HD21	2.00	0.42
1:B:257:ALA:HB1	1:B:261:TYR:CE2	2.54	0.42
1:B:247:ALA:HA	1:B:250:GLN:OE1	2.19	0.42
1:A:234:PRO:O	1:A:236:LEU:N	2.52	0.42
1:A:278:LEU:HA	1:A:278:LEU:HD13	1.81	0.42
1:B:125:PRO:HB2	1:B:128:TYR:HD2	1.84	0.42
1:A:350:ILE:HG12	1:A:350:ILE:H	1.66	0.42
1:A:168:VAL:HA	1:A:171:SER:HB3	2.00	0.42
1:A:92:SER:HA	1:A:97:LEU:HD11	2.01	0.42
1:B:248:ILE:HG23	1:B:252:PHE:CE2	2.54	0.42
1:A:321:MET:SD	1:A:337:ILE:HD11	2.59	0.42
1:A:87:LEU:HG	1:A:168:VAL:CG2	2.44	0.42
1:B:296:PHE:CD1	1:B:300:LYS:HD2	2.55	0.42
1:B:88:ILE:HD13	1:B:88:ILE:HA	1.93	0.42
1:A:145:LEU:O	1:A:149:LEU:HB2	2.18	0.42
1:A:253:ILE:HD12	1:A:253:ILE:N	2.35	0.42
1:A:343:LEU:HD22	1:A:343:LEU:H	1.84	0.42
1:A:72:ARG:HG3	1:A:182:PRO:O	2.19	0.42
1:B:307:LEU:HB2	1:B:352:TRP:NE1	2.34	0.42
1:B:415:MET:O	1:B:419:ILE:HG13	2.20	0.42
1:B:413:LEU:HA	1:B:416:ILE:HB	2.01	0.42
1:A:146:ALA:O	1:A:149:LEU:HB3	2.20	0.42
1:A:315:ILE:HG23	1:A:408:ALA:CA	2.49	0.42
1:A:341:LEU:HA	1:A:341:LEU:HD12	1.58	0.42
1:A:307:LEU:HD22	1:A:352:TRP:CD2	2.55	0.42
1:B:71:ARG:HB3	1:B:119:TYR:CD2	2.54	0.42
1:A:400:THR:HB	1:A:402:TRP:N	2.35	0.42
1:A:308:VAL:HG13	1:A:415:MET:HE2	2.01	0.42
1:B:359:MET:O	1:B:363:LEU:N	2.53	0.42
1:A:259:ILE:HG23	1:A:260:PHE:N	2.34	0.42
1:B:152:TYR:HD2	1:B:277:ILE:HD12	1.85	0.42
1:A:417:PHE:O	1:A:421:PHE:HD1	2.03	0.42
1:B:345:ILE:HA	1:B:345:ILE:HD13	1.82	0.42
1:B:290:VAL:O	1:B:293:VAL:HG12	2.19	0.42
1:A:42:THR:HA	1:A:393:ILE:HG22	2.02	0.42
1:A:217:MET:SD	1:A:220:ILE:HD11	2.60	0.42
1:B:75:VAL:HG12	1:B:178:ILE:CD1	2.50	0.42
1:B:275:ALA:O	1:B:279:GLY:HA3	2.20	0.42
1:B:217:MET:HG3	1:B:217:MET:O	2.18	0.41
1:A:152:TYR:CG	1:A:152:TYR:O	2.72	0.41
1:A:318:LEU:HD13	1:A:407:PHE:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD21	1:A:214:LEU:HD13	2.01	0.41
1:A:388:SER:O	1:A:392:PRO:HD2	2.20	0.41
1:B:46:ILE:HA	1:B:49:SER:CB	2.48	0.41
1:A:152:TYR:CE2	1:A:273:GLU:O	2.73	0.41
1:A:38:PRO:C	1:A:39:LEU:HD13	2.39	0.41
1:B:235:TRP:N	1:B:238:ARG:HH21	2.18	0.41
1:B:148:TYR:CD1	1:B:281:VAL:HG22	2.55	0.41
1:B:261:TYR:CE2	1:B:392:PRO:HG3	2.55	0.41
1:B:390:PHE:O	1:B:393:ILE:HG23	2.20	0.41
1:A:361:PRO:O	1:A:369:ARG:NH2	2.53	0.41
1:A:26:ILE:O	1:A:260:PHE:HB2	2.21	0.41
1:B:175:LEU:HG	1:B:179:TYR:CE1	2.47	0.41
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.77	0.41
1:A:52:LEU:O	1:A:56:ILE:HG13	2.21	0.41
1:B:376:SER:O	1:B:380:LEU:HB2	2.20	0.41
1:A:160:TRP:CZ3	1:A:164:LEU:HD23	2.54	0.41
1:A:315:ILE:HG12	1:A:408:ALA:O	2.20	0.41
1:B:83:ILE:HA	1:B:168:VAL:HG22	2.02	0.41
1:A:385:LEU:HA	1:A:388:SER:HB3	2.03	0.41
1:A:233:SER:CB	1:A:234:PRO:HD2	2.50	0.41
1:A:19:TYR:HE1	1:A:109:VAL:HG13	1.82	0.41
1:A:36:ASP:OD1	1:A:157:ILE:HG13	2.20	0.41
1:A:282:GLY:O	1:A:286:ILE:HG13	2.21	0.41
1:B:148:TYR:CE1	1:B:281:VAL:HA	2.55	0.41
1:B:261:TYR:CD2	1:B:392:PRO:HG3	2.55	0.41
1:A:363:LEU:HD13	1:A:364:PHE:CE1	2.55	0.41
1:B:93:THR:H	1:B:97:LEU:CG	2.34	0.41
1:A:251:GLN:OE1	1:A:384:THR:HG22	2.21	0.41
1:B:83:ILE:N	1:B:171:SER:OG	2.53	0.41
1:B:243:GLY:HA2	1:B:246:PHE:HB3	2.03	0.41
1:B:342:SER:O	1:B:346:VAL:HG23	2.20	0.41
1:B:97:LEU:HD12	1:B:97:LEU:C	2.40	0.41
1:B:161:ARG:O	1:B:164:LEU:HB2	2.20	0.41
1:B:133:GLY:O	1:B:136:ASN:HB3	2.21	0.41
1:A:340:CYS:HA	1:A:343:LEU:HD23	2.03	0.41
1:B:311:ASN:HA	1:B:314:MET:HE2	2.03	0.41
1:A:307:LEU:HB3	1:A:352:TRP:CZ2	2.56	0.41
1:A:293:VAL:O	1:A:297:VAL:HG22	2.21	0.41
1:B:298:VAL:HG23	1:B:299:ASP:OD1	2.21	0.41
1:A:32:PHE:HD1	1:A:32:PHE:HA	1.68	0.41
1:B:75:VAL:O	1:B:178:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HB	1:A:402:TRP:CA	2.51	0.40
1:B:30:LEU:HD22	1:B:260:PHE:HB3	2.01	0.40
1:B:45:GLY:HA2	1:B:388:SER:O	2.20	0.40
1:A:255:ILE:HA	1:A:258:VAL:HB	2.03	0.40
1:A:416:ILE:HG23	1:B:327:THR:HG22	2.02	0.40
1:A:251:GLN:HG2	1:A:384:THR:HA	2.03	0.40
1:A:401:GLU:OE2	1:A:405:LEU:HD12	2.21	0.40
1:A:411:GLY:HA2	1:A:414:ALA:HB3	2.03	0.40
1:B:165:GLY:O	1:B:168:VAL:HB	2.21	0.40
1:A:170:PRO:O	1:A:173:ILE:HG12	2.21	0.40
1:B:116:VAL:HB	1:B:117:PRO:HD3	2.02	0.40
1:A:304:LYS:O	1:A:307:LEU:HB2	2.22	0.40
1:A:128:TYR:O	1:A:132:LEU:HG	2.21	0.40
1:A:130:GLY:O	1:A:132:LEU:N	2.55	0.40
1:B:394:LEU:O	1:B:398:LEU:HG	2.20	0.40
1:A:190:GLU:HG3	1:A:221:ASN:CB	2.52	0.40
1:A:175:LEU:O	1:A:179:TYR:N	2.55	0.40
1:B:318:LEU:HB3	1:B:404:PHE:O	2.21	0.40
1:A:385:LEU:HD23	1:A:385:LEU:O	2.22	0.40
1:A:318:LEU:HD13	1:A:408:ALA:CA	2.51	0.40
1:B:311:ASN:O	1:B:315:ILE:HG13	2.21	0.40
1:B:238:ARG:O	1:B:242:VAL:HG23	2.22	0.40
1:A:313:GLY:HA2	1:A:316:ALA:CB	2.52	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	419/446 (94%)	350 (84%)	58 (14%)	11 (3%)	7 40
1	B	419/446 (94%)	355 (85%)	58 (14%)	6 (1%)	14 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	838/892 (94%)	705 (84%)	116 (14%)	17 (2%)	9 48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	235	TRP
1	B	234	PRO
1	B	328	ILE
1	B	194	GLU
1	B	235	TRP
1	A	129	ARG
1	A	131	SER
1	B	233	SER
1	A	403	VAL
1	A	233	SER
1	A	38	PRO
1	A	354	PRO
1	A	328	ILE
1	A	339	VAL
1	B	423	PRO
1	A	308	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/363 (94%)	256 (75%)	85 (25%)	1 3
1	B	341/363 (94%)	267 (78%)	74 (22%)	1 6
All	All	682/726 (94%)	523 (77%)	159 (23%)	1 4

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE

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Mol	Chain	Res	Type
1	A	17	LEU
1	A	22	ASP
1	A	30	LEU
1	A	32	PHE
1	A	33	ILE
1	A	37	ILE
1	A	39	LEU
1	A	40	ASN
1	A	46	ILE
1	A	53	ILE
1	A	71	ARG
1	A	74	LEU
1	A	94	ASN
1	A	99	ILE
1	A	105	ILE
1	A	109	VAL
1	A	116	VAL
1	A	120	LEU
1	A	127	GLU
1	A	129	ARG
1	A	136	ASN
1	A	137	GLN
1	A	140	ILE
1	A	142	ILE
1	A	144	ILE
1	A	156	ASP
1	A	160	TRP
1	A	163	MET
1	A	164	LEU
1	A	171	SER
1	A	178	ILE
1	A	179	TYR
1	A	180	PHE
1	A	186	ARG
1	A	189	LEU
1	A	190	GLU
1	A	194	GLU
1	A	195	GLU
1	A	203	ILE
1	A	210	ILE
1	A	211	ASP
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	217	MET
1	A	223	ILE
1	A	233	SER
1	A	245	ILE
1	A	246	PHE
1	A	248	ILE
1	A	250	GLN
1	A	251	GLN
1	A	255	ILE
1	A	259	ILE
1	A	261	TYR
1	A	268	LYS
1	A	277	ILE
1	A	278	LEU
1	A	283	ILE
1	A	287	ASN
1	A	292	ILE
1	A	298	VAL
1	A	306	LEU
1	A	312	ILE
1	A	320	ILE
1	A	323	ILE
1	A	324	LEU
1	A	325	ILE
1	A	328	ILE
1	A	330	ILE
1	A	337	ILE
1	A	343	LEU
1	A	350	ILE
1	A	352	TRP
1	A	363	LEU
1	A	382	ILE
1	A	388	SER
1	A	390	PHE
1	A	394	LEU
1	A	398	LEU
1	A	404	PHE
1	A	405	LEU
1	A	412	VAL
1	A	417	PHE
1	A	422	LEU
1	A	425	THR

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Mol	Chain	Res	Type
1	B	8	ILE
1	B	11	LEU
1	B	31	LEU
1	B	33	ILE
1	B	37	ILE
1	B	39	LEU
1	B	46	ILE
1	B	50	SER
1	B	67	ASP
1	B	74	LEU
1	B	80	ILE
1	B	82	PHE
1	B	83	ILE
1	B	97	LEU
1	B	98	LEU
1	B	113	MET
1	B	119	TYR
1	B	127	GLU
1	B	132	LEU
1	B	145	LEU
1	B	148	TYR
1	B	161	ARG
1	B	162	TRP
1	B	174	LEU
1	B	178	ILE
1	B	186	ARG
1	B	192	ARG
1	B	201	MET
1	B	203	ILE
1	B	204	THR
1	B	211	ASP
1	B	217	MET
1	B	220	ILE
1	B	227	THR
1	B	230	VAL
1	B	231	ILE
1	B	232	LYS
1	B	233	SER
1	B	236	LEU
1	B	239	ILE
1	B	244	CYS
1	B	245	ILE

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Mol	Chain	Res	Type
1	B	253	ILE
1	B	258	VAL
1	B	259	ILE
1	B	261	TYR
1	B	262	SER
1	B	273	GLU
1	B	277	ILE
1	B	283	ILE
1	B	285	THR
1	B	290	VAL
1	B	304	LYS
1	B	306	LEU
1	B	307	LEU
1	B	312	ILE
1	B	317	SER
1	B	319	LEU
1	B	328	ILE
1	B	337	ILE
1	B	341	LEU
1	B	360	LEU
1	B	379	VAL
1	B	390	PHE
1	B	393	ILE
1	B	398	LEU
1	B	400	THR
1	B	405	LEU
1	B	413	LEU
1	B	415	MET
1	B	416	ILE
1	B	422	LEU
1	B	423	PRO
1	B	425	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	421/446 (94%)	1.62	123 (29%) 1 0	10, 149, 347, 447	0
1	B	421/446 (94%)	1.40	104 (24%) 1 1	10, 224, 394, 532	0
All	All	842/892 (94%)	1.51	227 (26%) 1 0	10, 185, 372, 532	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	SER	23.0
1	B	207	ASP	16.3
1	A	427	GLY	15.5
1	B	371	ALA	14.5
1	A	370	GLY	14.4
1	A	399	SER	11.2
1	B	209	GLU	10.7
1	A	128	TYR	10.7
1	A	182	PRO	9.8
1	A	371	ALA	9.8
1	A	228	TRP	9.3
1	A	91	ALA	8.9
1	B	93	THR	8.4
1	B	156	ASP	8.3
1	B	262	SER	7.8
1	B	370	GLY	7.4
1	A	165	GLY	7.1
1	B	157	ILE	6.9
1	B	155	ALA	6.8
1	A	183	GLU	6.8
1	B	228	TRP	6.7
1	B	217	MET	6.6
1	A	187	TRP	6.6
1	A	158	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	VAL	6.4
1	A	185	PRO	6.4
1	B	227	THR	6.3
1	B	67	ASP	6.1
1	A	256	ASN	6.1
1	A	58	GLY	6.0
1	A	90	ALA	5.9
1	B	19	TYR	5.9
1	A	129	ARG	5.8
1	B	332	SER	5.8
1	B	372	ALA	5.8
1	B	127	GLU	5.7
1	B	302	ASP	5.5
1	A	121	SER	5.4
1	A	156	ASP	5.3
1	B	396	ASP	5.2
1	B	237	GLY	5.0
1	A	229	THR	5.0
1	B	183	GLU	4.9
1	B	266	PHE	4.8
1	B	80	ILE	4.8
1	A	157	ILE	4.7
1	A	357	TRP	4.7
1	B	148	TYR	4.7
1	B	31	LEU	4.5
1	A	56	ILE	4.5
1	B	350	ILE	4.5
1	B	152	TYR	4.5
1	A	211	ASP	4.5
1	B	129	ARG	4.5
1	B	264	SER	4.5
1	B	79	ALA	4.5
1	B	267	ALA	4.5
1	A	24	GLY	4.5
1	A	205	TYR	4.4
1	A	186	ARG	4.4
1	A	20	GLY	4.3
1	A	92	SER	4.3
1	B	50	SER	4.3
1	A	77	LEU	4.3
1	B	419	ILE	4.3
1	B	270	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	49	SER	4.3
1	B	92	SER	4.3
1	A	207	ASP	4.2
1	A	306	LEU	4.2
1	A	95	LEU	4.2
1	B	326	TRP	4.1
1	B	311	ASN	4.1
1	A	57	VAL	4.1
1	B	269	ALA	4.1
1	A	369	ARG	4.0
1	A	29	ALA	4.0
1	A	30	LEU	4.0
1	A	166	LEU	4.0
1	A	59	ALA	4.0
1	B	355	VAL	4.0
1	B	274	ALA	3.9
1	B	256	ASN	3.9
1	B	261	TYR	3.9
1	A	44	GLU	3.8
1	A	55	ALA	3.8
1	A	354	PRO	3.7
1	A	262	SER	3.7
1	B	254	GLY	3.7
1	A	304	LYS	3.6
1	A	85	GLY	3.6
1	A	272	GLY	3.6
1	B	349	GLY	3.6
1	A	167	ALA	3.6
1	B	301	ILE	3.6
1	B	128	TYR	3.6
1	B	331	ALA	3.6
1	B	28	GLY	3.5
1	A	384	THR	3.5
1	A	372	ALA	3.5
1	A	76	MET	3.5
1	A	74	LEU	3.5
1	B	304	LYS	3.5
1	B	354	PRO	3.5
1	A	136	ASN	3.4
1	A	188	LEU	3.4
1	A	356	LEU	3.4
1	B	126	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	257	ALA	3.4
1	B	263	SER	3.4
1	A	28	GLY	3.4
1	B	142	ILE	3.3
1	A	395	SER	3.3
1	B	44	GLU	3.3
1	A	377	ALA	3.3
1	A	155	ALA	3.3
1	B	253	ILE	3.2
1	B	30	LEU	3.2
1	A	112	SER	3.2
1	A	191	ASN	3.2
1	B	325	ILE	3.1
1	B	196	ALA	3.1
1	A	230	VAL	3.1
1	A	367	ARG	3.1
1	A	335	TRP	3.1
1	A	368	ALA	3.1
1	B	23	ASN	3.1
1	B	181	MET	3.1
1	A	271	LEU	3.1
1	A	350	ILE	3.1
1	B	187	TRP	3.1
1	B	279	GLY	3.0
1	A	23	ASN	3.0
1	A	334	ALA	3.0
1	A	134	SER	3.0
1	B	333	SER	2.9
1	A	355	VAL	2.9
1	B	351	SER	2.9
1	B	401	GLU	2.9
1	A	135	LEU	2.9
1	B	137	GLN	2.9
1	A	305	LYS	2.9
1	A	311	ASN	2.9
1	A	79	ALA	2.8
1	B	265	ILE	2.8
1	B	210	ILE	2.8
1	B	70	GLY	2.7
1	A	402	TRP	2.7
1	A	51	MET	2.7
1	A	210	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	18	LEU	2.6
1	A	326	TRP	2.6
1	B	35	LYS	2.6
1	A	220	ILE	2.6
1	A	71	ARG	2.6
1	B	395	SER	2.6
1	B	32	PHE	2.6
1	B	138	LEU	2.6
1	A	147	ALA	2.6
1	A	184	SER	2.6
1	B	33	ILE	2.6
1	A	67	ASP	2.6
1	B	154	PHE	2.6
1	B	86	ALA	2.5
1	A	209	GLU	2.5
1	A	333	SER	2.5
1	A	53	ILE	2.5
1	A	19	TYR	2.5
1	A	307	LEU	2.5
1	B	182	PRO	2.5
1	A	340	CYS	2.4
1	A	198	ARG	2.4
1	A	146	ALA	2.4
1	A	426	ARG	2.4
1	B	229	THR	2.4
1	A	80	ILE	2.4
1	B	38	PRO	2.4
1	B	85	GLY	2.4
1	A	152	TYR	2.4
1	A	286	ILE	2.4
1	B	25	VAL	2.4
1	B	238	ARG	2.3
1	B	357	TRP	2.3
1	B	250	GLN	2.3
1	B	278	LEU	2.3
1	A	226	SER	2.3
1	A	398	LEU	2.3
1	A	299	ASP	2.3
1	B	123	MET	2.3
1	B	252	PHE	2.3
1	B	255	ILE	2.3
1	B	134	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	186	ARG	2.3
1	A	199	GLN	2.3
1	A	75	VAL	2.3
1	A	106	GLY	2.3
1	A	250	GLN	2.3
1	A	43	THR	2.3
1	B	369	ARG	2.2
1	B	303	ARG	2.2
1	A	169	VAL	2.2
1	A	322	ALA	2.2
1	B	305	LYS	2.2
1	B	162	TRP	2.2
1	A	309	GLY	2.2
1	A	265	ILE	2.2
1	A	383	GLY	2.1
1	A	373	THR	2.1
1	A	178	ILE	2.1
1	B	189	LEU	2.1
1	A	26	ILE	2.1
1	A	172	VAL	2.1
1	A	382	ILE	2.1
1	A	266	PHE	2.1
1	B	64	PRO	2.1
1	B	65	LEU	2.1
1	B	347	PHE	2.1
1	B	211	ASP	2.1
1	B	315	ILE	2.1
1	B	323	ILE	2.1
1	A	217	MET	2.1
1	A	189	LEU	2.1
1	A	45	GLY	2.1
1	A	215	LYS	2.0
1	A	263	SER	2.0
1	A	159	GLY	2.0
1	A	173	ILE	2.0

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

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.