



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:26 PM UTC

PDB ID : 5LQ3 / pdb_00005lq3
Title : Structures and transport dynamics of the Campylobacter jejuni multidrug efflux pump CmeB
Authors : Su, C.C.
Deposited on : 2016-08-15
Resolution : 3.55 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

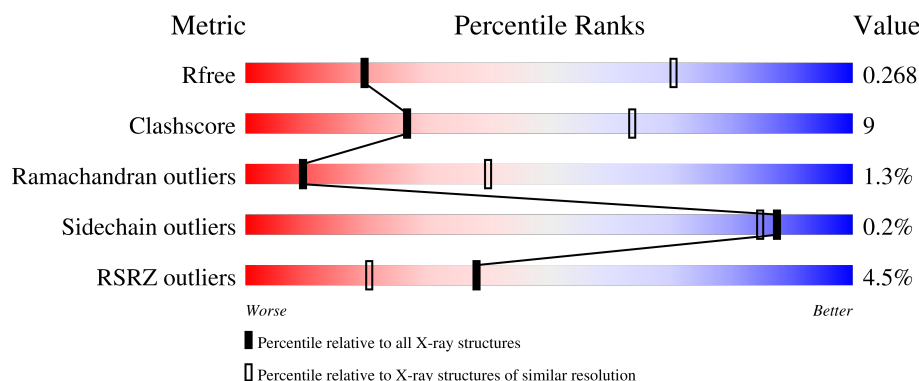
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	1035	5% 78% 21%
1	B	1035	8% 75% 24%
1	C	1035	3% 78% 21%
1	D	1035	3% 78% 21%
1	E	1035	4% 72% 26%

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Mol	Chain	Length	Quality of chain
1	F	1035	4% 78% 22%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 47878 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.

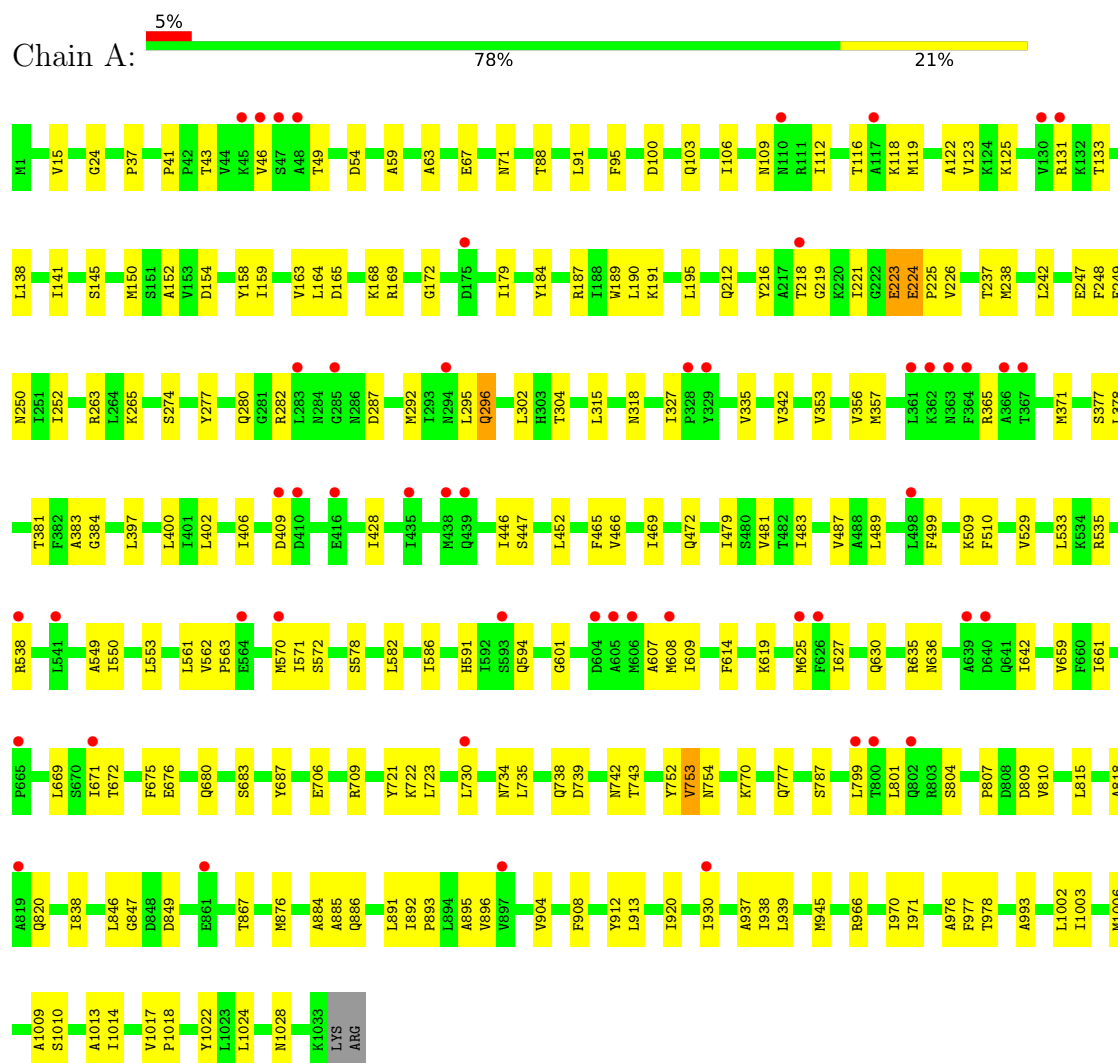
- Molecule 1 is a protein called CmeB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1033	Total	C	N	O	S	0	0	0
			7973	5155	1301	1485	32			
1	B	1033	Total	C	N	O	S	0	0	0
			7973	5155	1301	1485	32			
1	C	1035	Total	C	N	O	S	0	0	0
			7993	5167	1307	1487	32			
1	D	1033	Total	C	N	O	S	0	0	0
			7973	5155	1301	1485	32			
1	E	1033	Total	C	N	O	S	0	0	0
			7973	5155	1301	1485	32			
1	F	1035	Total	C	N	O	S	0	0	0
			7993	5167	1307	1487	32			

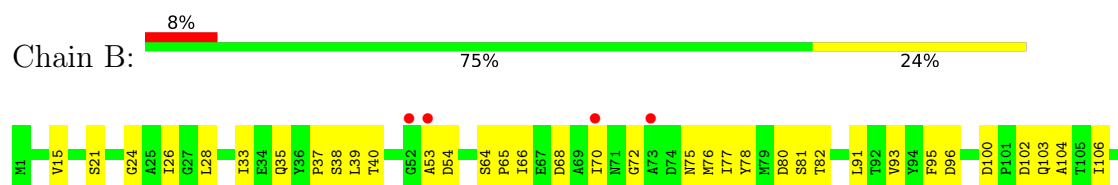
3 Residue-property plots

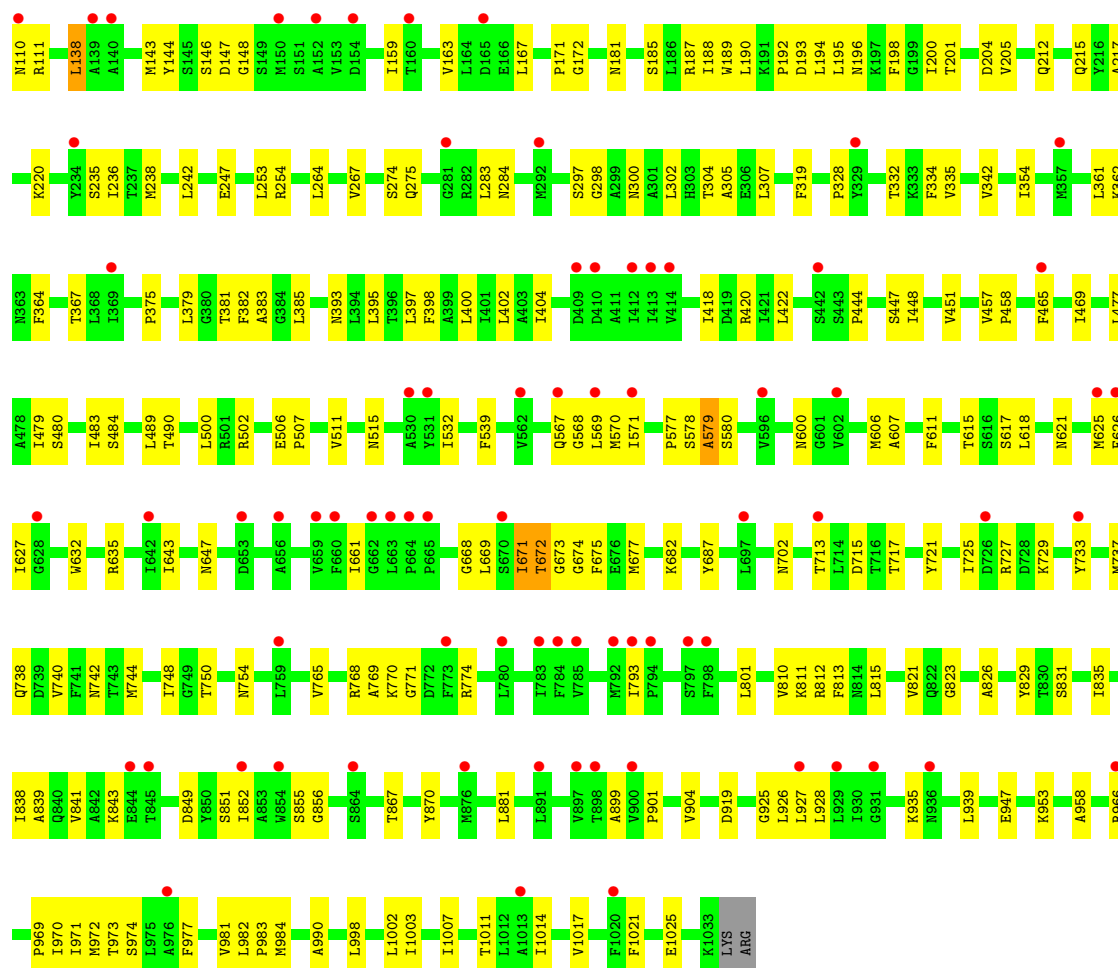
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CmeB

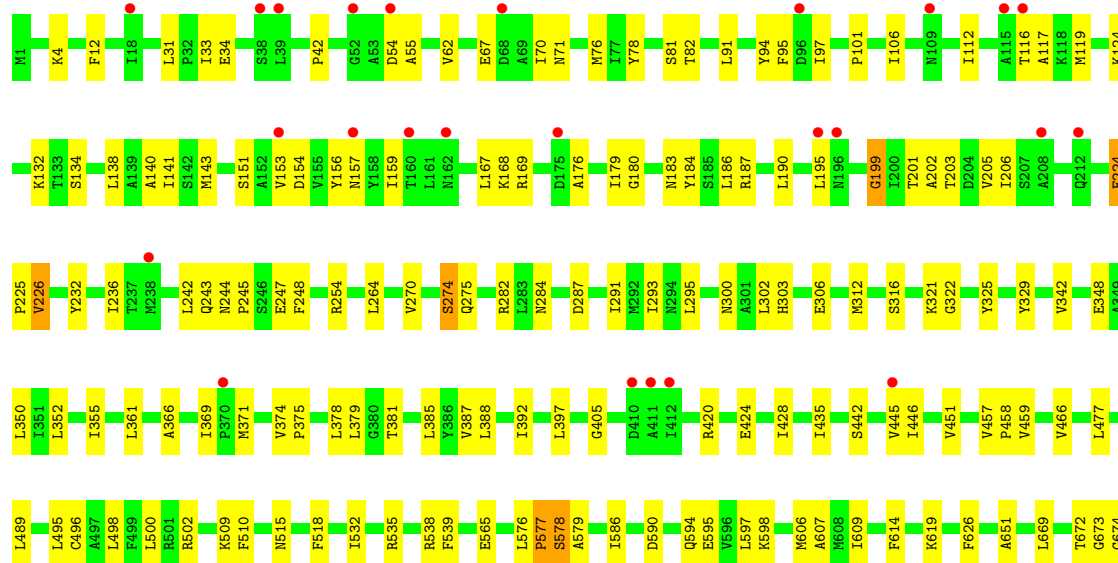
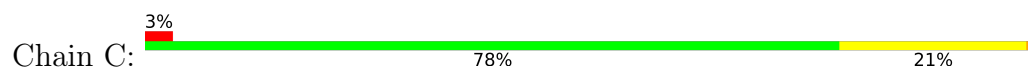


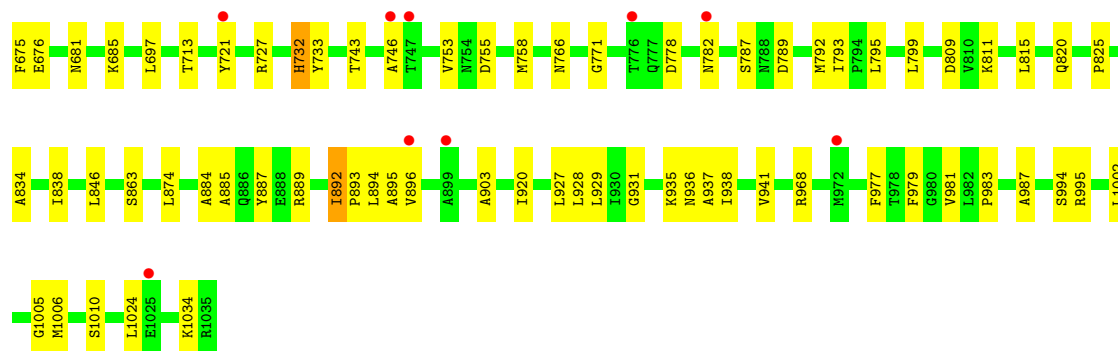
• Molecule 1: CmeB



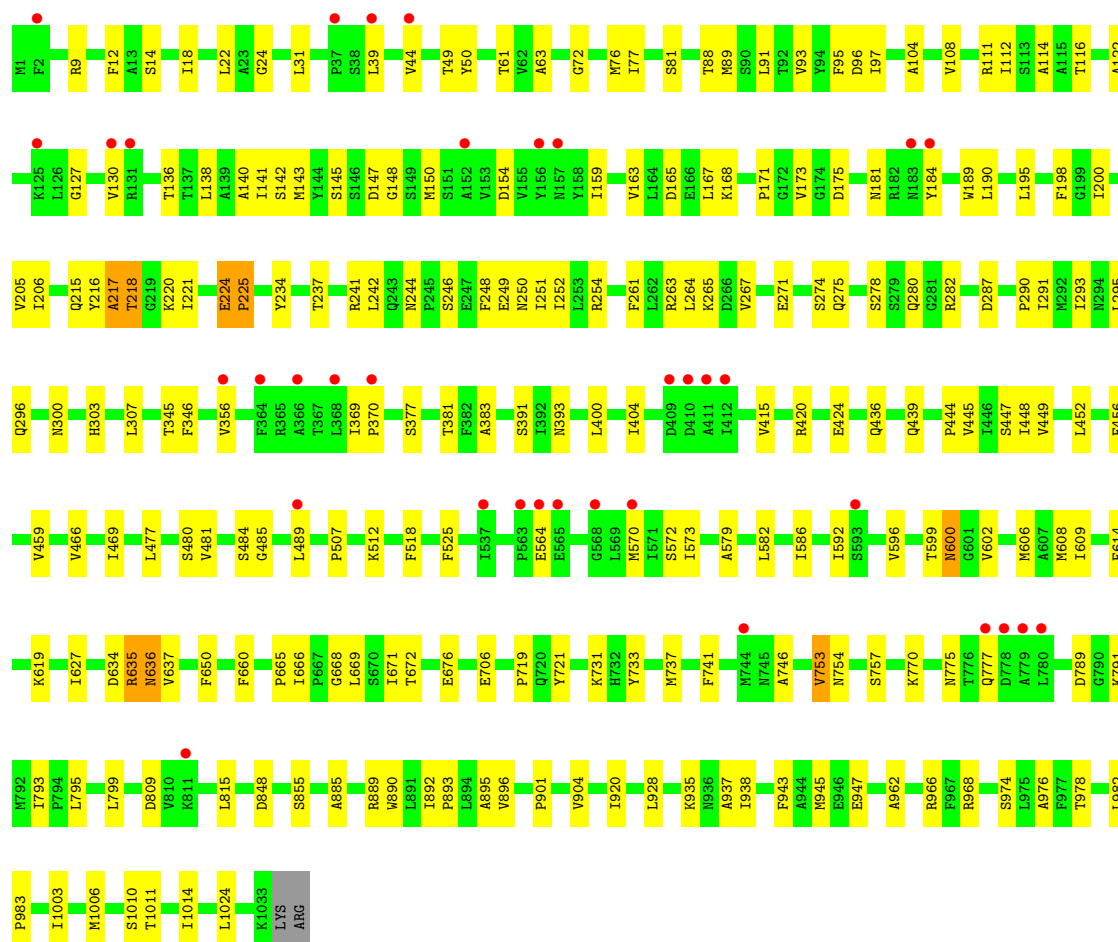
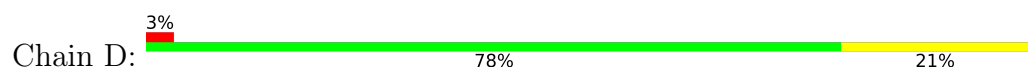


• Molecule 1: CmeB

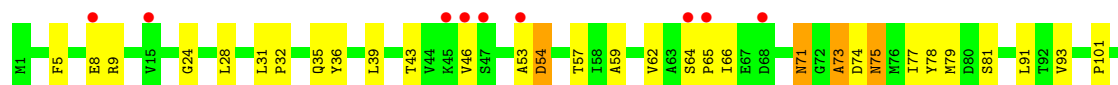
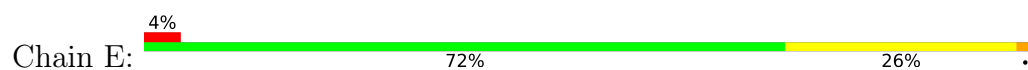


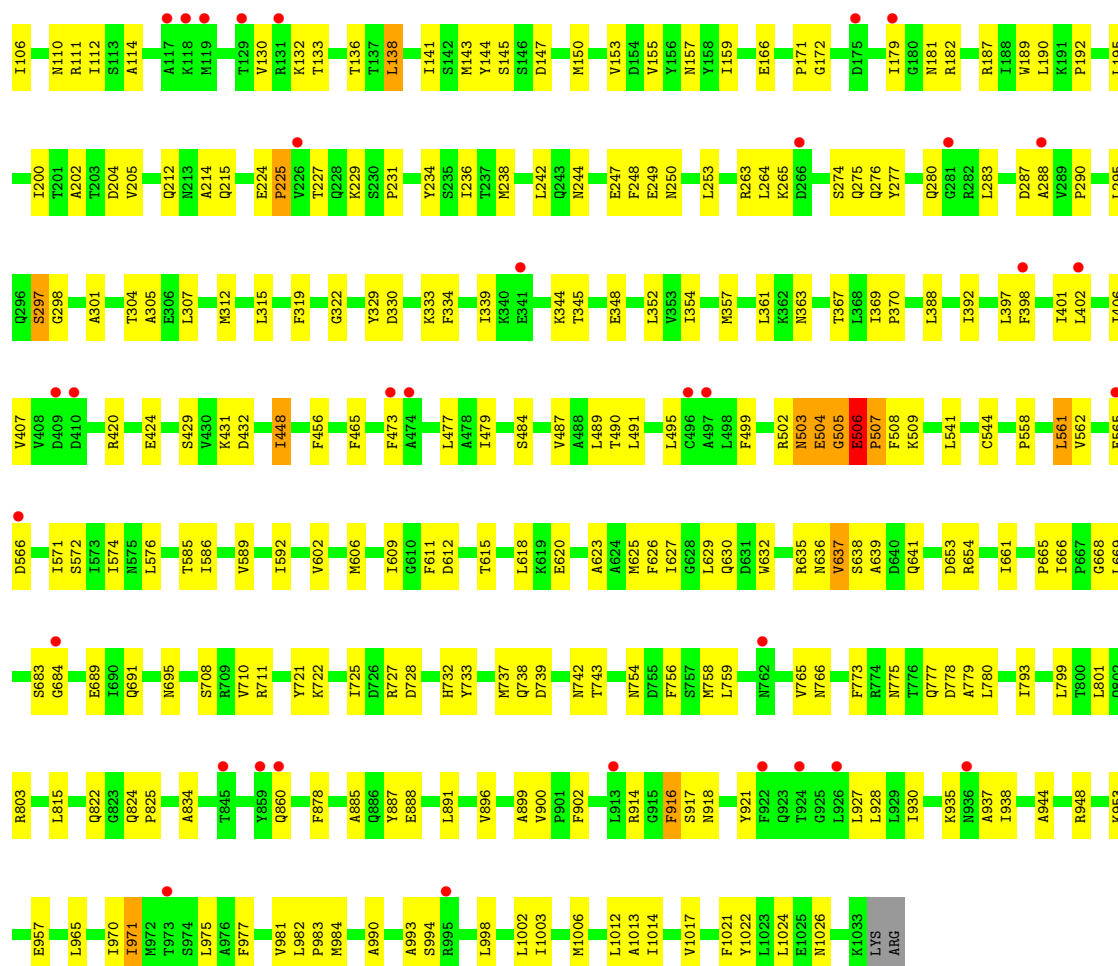


• Molecule 1: CmeB

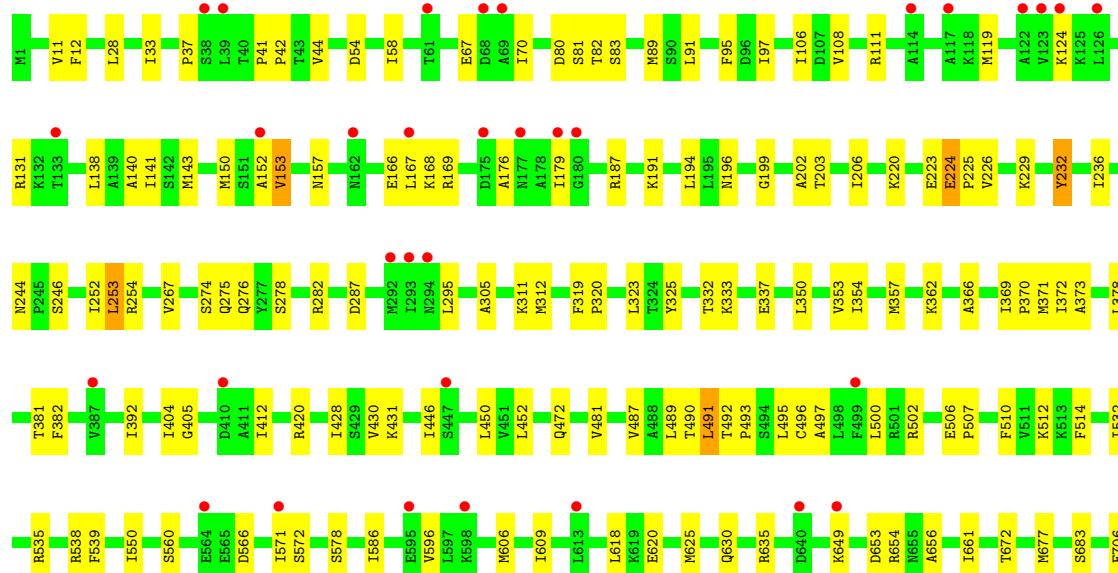
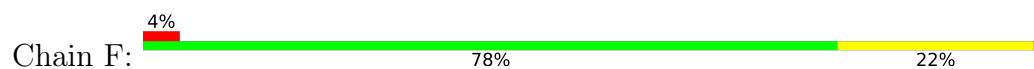


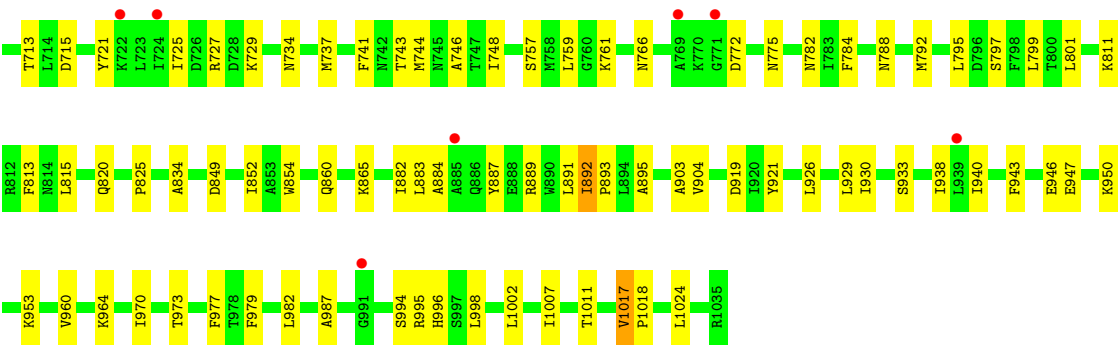
• Molecule 1: CmeB





• Molecule 1: CmeB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	120.87Å 127.99Å 169.61Å 99.79° 99.45° 84.95°	Depositor
Resolution (Å)	90.27 – 3.55 90.27 – 3.55	Depositor EDS
% Data completeness (in resolution range)	89.5 (90.27-3.55) 91.2 (90.27-3.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.268 0.229 , 0.268	Depositor DCC
R_{free} test set	5494 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	47878	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	0.10	0/8129	0.29	0/11032
1	B	0.11	0/8129	0.31	0/11032
1	C	0.13	1/8149 (0.0%)	0.29	0/11057
1	D	0.11	0/8129	0.30	0/11032
1	E	0.12	0/8129	0.38	3/11032 (0.0%)
1	F	0.10	0/8149	0.29	0/11057
All	All	0.11	1/48814 (0.0%)	0.31	3/66242 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	732	HIS	CE1-NE2	-5.82	1.26	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	505	GLY	N-CA-C	16.76	131.94	112.50
1	E	506	GLU	N-CA-C	6.07	115.94	108.11
1	E	504	GLU	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7973	0	8119	148	0
1	B	7973	0	8119	170	0
1	C	7993	0	8145	148	0
1	D	7973	0	8119	150	0
1	E	7973	0	8119	195	0
1	F	7993	0	8145	142	0
All	All	47878	0	48766	894	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 9.

All (894) 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:81:SER:HB3	1:B:91:LEU:HD23	1.31	1.12
1:A:671:ILE:HD12	1:A:672:THR:H	1.31	0.95
1:D:224:GLU:HB3	1:D:225:PRO:HD3	1.53	0.91
1:C:62:VAL:HA	1:C:119:MET:HE1	1.60	0.83
1:A:586:ILE:HG12	1:A:609:ILE:HD12	1.60	0.82
1:C:929:LEU:HD21	1:C:1005:GLY:HA3	1.62	0.80
1:C:224:GLU:HB3	1:C:225:PRO:HD3	1.65	0.79
1:A:189:TRP:HB3	1:A:770:LYS:HB2	1.66	0.77
1:E:507:PRO:HD2	1:E:508:PHE:H	1.49	0.76
1:C:903:ALA:HB1	1:C:929:LEU:HG	1.68	0.75
1:F:630:GLN:O	1:F:635:ARG:NH1	2.22	0.72
1:B:236:ILE:HG22	1:C:721:TYR:HB2	1.71	0.72
1:D:198:PHE:O	1:D:254:ARG:NH2	2.21	0.72
1:A:671:ILE:HD12	1:A:672:THR:N	2.04	0.72
1:C:42:PRO:HG2	1:C:95:PHE:HB2	1.72	0.71
1:F:199:GLY:H	1:F:254:ARG:HH22	1.38	0.71
1:F:507:PRO:HB2	1:F:512:LYS:HB2	1.72	0.71
1:E:363:ASN:HB3	1:E:503:ASN:HB3	1.72	0.70
1:B:570:MET:HB2	1:B:627:ILE:HB	1.72	0.70
1:D:61:THR:HG21	1:F:757:SER:HB3	1.73	0.70
1:A:184:TYR:HA	1:A:274:SER:HA	1.74	0.70
1:B:981:VAL:HB	1:B:984:MET:HE2	1.74	0.70
1:F:152:ALA:O	1:F:276:GLN:NE2	2.24	0.70
1:A:165:ASP:HB2	1:B:815:LEU:HD13	1.74	0.69
1:A:250:ASN:HA	1:A:263:ARG:HD3	1.75	0.69
1:D:189:TRP:HB3	1:D:770:LYS:HB2	1.74	0.69
1:A:721:TYR:HB2	1:C:236:ILE:HG22	1.75	0.69
1:F:1017:VAL:HG23	1:F:1018:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:ARG:NH1	1:F:287:ASP:OD1	2.27	0.68
1:A:71:ASN:ND2	1:C:169:ARG:O	2.26	0.67
1:E:507:PRO:O	1:E:508:PHE:HB2	1.94	0.67
1:A:138:LEU:HD22	1:A:295:LEU:HD23	1.74	0.67
1:A:659:VAL:HG22	1:A:709:ARG:HH21	1.60	0.67
1:B:21:SER:HA	1:B:379:LEU:HD22	1.75	0.67
1:D:159:ILE:HA	1:D:163:VAL:HB	1.77	0.67
1:A:619:LYS:NZ	1:A:809:ASP:OD2	2.20	0.66
1:D:224:GLU:HB3	1:D:225:PRO:CD	2.25	0.66
1:A:277:TYR:HB3	1:C:224:GLU:HG2	1.76	0.66
1:F:490:THR:O	1:F:492:THR:N	2.28	0.66
1:A:735:LEU:HD23	1:A:787:SER:HA	1.78	0.66
1:E:143:MET:HE2	1:E:312:MET:HE1	1.78	0.66
1:E:565:GLU:HB2	1:E:993:ALA:HB2	1.78	0.66
1:E:625:MET:HE3	1:E:627:ILE:HD11	1.78	0.66
1:B:669:LEU:HD13	1:B:672:THR:HA	1.76	0.66
1:D:263:ARG:NH2	1:E:728:ASP:OD2	2.28	0.66
1:F:729:LYS:NZ	1:F:797:SER:O	2.29	0.66
1:C:889:ARG:HD2	1:C:892:ILE:HD13	1.77	0.65
1:A:571:ILE:HD11	1:A:672:THR:HG22	1.76	0.65
1:D:753:VAL:HG13	1:D:754:ASN:H	1.61	0.65
1:E:244:ASN:HB2	1:E:247:GLU:HG3	1.77	0.65
1:A:216:TYR:H	1:A:238:MET:HE3	1.61	0.65
1:E:190:LEU:HB3	1:E:195:LEU:HD11	1.78	0.65
1:E:171:PRO:HD2	1:E:307:LEU:HD13	1.78	0.65
1:E:509:LYS:HD3	1:E:509:LYS:H	1.61	0.65
1:F:571:ILE:HD11	1:F:672:THR:HG22	1.76	0.65
1:F:202:ALA:HB3	1:F:743:THR:HG22	1.79	0.65
1:F:560:SER:O	1:F:865:LYS:NZ	2.29	0.65
1:E:280:GLN:NE2	1:E:287:ASP:OD2	2.30	0.65
1:E:344:LYS:NZ	1:E:348:GLU:OE2	2.28	0.65
1:A:106:ILE:HB	1:C:106:ILE:HG21	1.79	0.65
1:A:43:THR:OG1	1:A:133:THR:O	2.14	0.64
1:B:81:SER:HB3	1:B:91:LEU:CD2	2.19	0.64
1:B:448:ILE:HG21	1:B:935:LYS:HE2	1.79	0.64
1:C:676:GLU:OE2	1:C:820:GLN:NE2	2.30	0.64
1:E:138:LEU:HD21	1:E:305:ALA:HB2	1.79	0.64
1:A:249:GLU:HB3	1:A:265:LYS:HB3	1.79	0.64
1:C:138:LEU:HB2	1:C:295:LEU:HB2	1.79	0.64
1:E:46:VAL:HG22	1:E:130:VAL:HG12	1.80	0.64
1:F:947:GLU:HB3	1:F:953:LYS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLY:HA2	1:B:383:ALA:HB2	1.80	0.64
1:B:750:THR:OG1	1:B:768:ARG:NH1	2.31	0.64
1:A:24:GLY:HA2	1:A:383:ALA:HB2	1.80	0.64
1:A:466:VAL:HG11	1:A:867:THR:HG21	1.79	0.64
1:E:733:TYR:HB3	1:E:793:ILE:HD13	1.80	0.63
1:E:238:MET:HE3	1:F:725:ILE:HD11	1.79	0.63
1:F:677:MET:HE3	1:F:852:ILE:HG13	1.81	0.63
1:D:885:ALA:HB1	1:F:12:PHE:HD1	1.64	0.63
1:C:184:TYR:HE1	1:C:274:SER:H	1.47	0.63
1:E:566:ASP:HB2	1:E:639:ALA:HB2	1.80	0.63
1:F:431:LYS:HA	1:F:497:ALA:HB1	1.80	0.63
1:B:192:PRO:O	1:B:196:ASN:ND2	2.24	0.62
1:C:778:ASP:O	1:C:782:ASN:ND2	2.31	0.62
1:D:619:LYS:NZ	1:D:809:ASP:OD2	2.30	0.62
1:E:181:ASN:OD1	1:E:275:GLN:NE2	2.32	0.62
1:E:611:PHE:HA	1:E:618:LEU:HA	1.81	0.62
1:D:676:GLU:HG2	1:D:855:SER:HB3	1.81	0.62
1:D:249:GLU:HB3	1:D:265:LYS:HB3	1.80	0.62
1:E:507:PRO:CD	1:E:508:PHE:H	2.12	0.62
1:F:428:ILE:O	1:F:502:ARG:NH2	2.33	0.62
1:D:445:VAL:HG21	1:D:489:LEU:HD21	1.82	0.62
1:A:190:LEU:O	1:A:770:LYS:N	2.33	0.62
1:E:914:ARG:HD2	1:E:916:PHE:HE2	1.65	0.62
1:B:826:ALA:HB3	1:B:829:TYR:HD2	1.65	0.61
1:D:586:ILE:HG12	1:D:609:ILE:HG21	1.82	0.61
1:A:1017:VAL:HG23	1:A:1018:PRO:HD3	1.81	0.61
1:E:236:ILE:HG22	1:F:721:TYR:HB2	1.80	0.61
1:F:929:LEU:HD21	1:F:1002:LEU:HA	1.81	0.61
1:E:721:TYR:HB3	1:E:801:LEU:HG	1.83	0.61
1:A:152:ALA:HB2	1:A:287:ASP:HB3	1.83	0.61
1:B:70:ILE:HA	1:B:76:MET:HE1	1.81	0.61
1:D:50:TYR:HE1	1:D:122:ALA:HB3	1.64	0.61
1:E:420:ARG:HD2	1:E:965:LEU:HD22	1.82	0.61
1:F:535:ARG:HB3	1:F:538:ARG:HD2	1.83	0.61
1:D:184:TYR:HA	1:D:274:SER:HA	1.82	0.60
1:D:234:TYR:HE2	1:E:803:ARG:HH21	1.48	0.60
1:E:571:ILE:HG13	1:E:661:ILE:HG13	1.83	0.60
1:C:282:ARG:HB2	1:C:607:ALA:HB3	1.83	0.60
1:E:330:ASP:HB3	1:E:333:LYS:HB2	1.82	0.60
1:A:224:GLU:O	1:A:226:VAL:N	2.33	0.60
1:D:775:ASN:ND2	1:D:777:GLN:OE1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:PHE:HA	1:B:618:LEU:HA	1.83	0.60
1:D:244:ASN:OD1	1:D:246:SER:OG	2.18	0.60
1:F:187:ARG:HG2	1:F:766:ASN:HB2	1.82	0.60
1:A:342:VAL:HG11	1:A:397:LEU:HB3	1.83	0.60
1:C:242:LEU:HD22	1:C:247:GLU:HB3	1.84	0.60
1:E:141:ILE:HG21	1:E:312:MET:HE2	1.84	0.60
1:F:203:THR:HG23	1:F:743:THR:HG23	1.84	0.60
1:C:159:ILE:HG23	1:C:291:ILE:HD11	1.82	0.60
1:B:82:THR:HG22	1:B:811:LYS:HG2	1.84	0.60
1:D:241:ARG:NH1	1:D:757:SER:OG	2.34	0.60
1:C:1006:MET:O	1:C:1010:SER:OG	2.17	0.59
1:D:815:LEU:O	1:F:169:ARG:NH2	2.35	0.59
1:A:223:GLU:OE2	1:B:768:ARG:NH1	2.35	0.59
1:A:402:LEU:HD11	1:A:1002:LEU:HD21	1.84	0.59
1:D:974:SER:HA	1:D:1006:MET:HE3	1.84	0.59
1:E:606:MET:O	1:E:626:PHE:N	2.36	0.59
1:A:447:SER:HB3	1:A:938:ILE:HD13	1.85	0.59
1:F:446:ILE:HD11	1:F:489:LEU:HD11	1.83	0.59
1:C:224:GLU:HB3	1:C:225:PRO:CD	2.30	0.59
1:E:35:GLN:HG3	1:E:36:TYR:HD1	1.68	0.59
1:C:143:MET:HB2	1:C:159:ILE:HD11	1.85	0.59
1:A:280:GLN:HB3	1:A:609:ILE:HD11	1.83	0.58
1:E:388:LEU:HD12	1:E:479:ILE:HD11	1.84	0.58
1:E:666:ILE:HG22	1:E:668:GLY:H	1.68	0.58
1:C:168:LYS:HG2	1:C:176:ALA:H	1.68	0.58
1:C:202:ALA:HB3	1:C:743:THR:HG22	1.84	0.58
1:F:42:PRO:HG2	1:F:95:PHE:HB2	1.84	0.58
1:A:118:LYS:HG3	1:C:183:ASN:HD21	1.68	0.58
1:F:119:MET:HB2	1:F:124:LYS:HE2	1.84	0.58
1:F:987:ALA:HB1	1:F:995:ARG:HH21	1.68	0.58
1:A:884:ALA:HA	1:A:893:PRO:HG3	1.86	0.58
1:C:894:LEU:HD12	1:C:1024:LEU:HD11	1.86	0.58
1:C:369:ILE:HD12	1:C:495:LEU:HB3	1.86	0.58
1:B:100:ASP:HB3	1:B:103:GLN:HB3	1.86	0.57
1:F:487:VAL:HG13	1:F:491:LEU:HD23	1.85	0.57
1:C:282:ARG:NH1	1:C:287:ASP:OD1	2.37	0.57
1:A:190:LEU:HB3	1:A:195:LEU:HD11	1.87	0.57
1:B:146:SER:O	1:B:148:GLY:N	2.37	0.57
1:A:377:SER:O	1:A:381:THR:OG1	2.21	0.57
1:D:721:TYR:HB2	1:F:236:ILE:HG22	1.85	0.57
1:C:371:MET:HE3	1:C:374:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:SER:O	1:D:381:THR:OG1	2.21	0.57
1:E:981:VAL:HB	1:E:984:MET:HE2	1.87	0.57
1:C:199:GLY:O	1:C:254:ARG:NH2	2.37	0.57
1:E:253:LEU:HD11	1:E:264:LEU:HD12	1.87	0.57
1:F:405:GLY:HA3	1:F:977:PHE:HA	1.87	0.57
1:C:576:LEU:O	1:C:578:SER:N	2.37	0.57
1:C:203:THR:HG23	1:C:743:THR:HG23	1.86	0.56
1:B:138:LEU:HD21	1:B:305:ALA:HB2	1.87	0.56
1:C:4:LYS:HG3	1:C:435:ILE:HD12	1.87	0.56
1:B:342:VAL:HG21	1:B:397:LEU:HB2	1.86	0.56
1:D:206:ILE:HD11	1:D:746:ALA:HB2	1.86	0.56
1:B:744:MET:HE3	1:B:748:ILE:HD11	1.87	0.56
1:C:892:ILE:H	1:C:893:PRO:HD2	1.70	0.56
1:A:739:ASP:O	1:A:743:THR:OG1	2.21	0.56
1:E:465:PHE:HB3	1:E:860:GLN:HB3	1.87	0.56
1:A:553:LEU:HD22	1:A:908:PHE:HB3	1.87	0.56
1:C:935:LYS:NZ	1:C:936:ASN:OD1	2.38	0.56
1:E:5:PHE:HE1	1:E:9:ARG:HD2	1.69	0.56
1:E:402:LEU:HD21	1:E:998:LEU:HD21	1.86	0.56
1:C:153:VAL:O	1:C:157:ASN:ND2	2.38	0.56
1:D:599:THR:HG22	1:D:600:ASN:H	1.69	0.56
1:E:914:ARG:HD2	1:E:916:PHE:CE2	2.42	0.55
1:F:82:THR:HB	1:F:811:LYS:HE3	1.87	0.55
1:A:141:ILE:HG23	1:A:327:ILE:HG12	1.88	0.55
1:F:979:PHE:HA	1:F:982:LEU:HB2	1.88	0.55
1:A:683:SER:HB3	1:A:849:ASP:HB2	1.88	0.55
1:B:489:LEU:HD12	1:B:490:THR:HG23	1.88	0.55
1:C:300:ASN:HB3	1:C:303:HIS:HB3	1.88	0.55
1:F:887:TYR:HE2	1:F:938:ILE:HD11	1.71	0.55
1:A:145:SER:HB2	1:A:150:MET:HB2	1.87	0.55
1:B:106:ILE:HG21	1:C:106:ILE:HD13	1.88	0.55
1:C:577:PRO:O	1:C:579:ALA:N	2.39	0.55
1:B:395:LEU:HD13	1:B:469:ILE:HG23	1.88	0.55
1:C:496:CYS:HA	1:C:500:LEU:HD23	1.86	0.55
1:B:39:LEU:HD13	1:B:465:PHE:HE1	1.72	0.55
1:D:136:THR:HG21	1:D:668:GLY:HA2	1.88	0.55
1:E:283:LEU:HG	1:E:288:ALA:HB2	1.89	0.55
1:F:168:LYS:HG2	1:F:176:ALA:H	1.71	0.55
1:C:977:PHE:CD2	1:C:1006:MET:HG2	2.42	0.55
1:A:630:GLN:HB2	1:A:635:ARG:HD3	1.88	0.55
1:C:981:VAL:HG11	1:C:1002:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLY:HA2	1:D:383:ALA:HB2	1.88	0.55
1:D:224:GLU:HG3	1:E:277:TYR:CD1	2.42	0.55
1:E:638:SER:OG	1:E:641:GLN:HB2	2.06	0.55
1:D:195:LEU:HD23	1:D:267:VAL:HB	1.90	0.54
1:D:215:GLN:NE2	1:E:57:THR:OG1	2.40	0.54
1:A:179:ILE:HD12	1:A:608:MET:HG2	1.88	0.54
1:A:687:TYR:CZ	1:A:810:VAL:HG13	2.43	0.54
1:B:733:TYR:HB3	1:B:793:ILE:HD13	1.88	0.54
1:E:145:SER:HB3	1:E:150:MET:HB2	1.88	0.54
1:E:1002:LEU:HD12	1:E:1003:ILE:HD12	1.89	0.54
1:A:119:MET:HE1	1:A:123:VAL:HB	1.90	0.54
1:B:402:LEU:HB3	1:B:928:LEU:HD22	1.88	0.54
1:D:391:SER:O	1:D:393:ASN:ND2	2.40	0.54
1:F:795:LEU:HB3	1:F:799:LEU:HD12	1.88	0.54
1:D:635:ARG:HG3	1:D:637:VAL:H	1.72	0.54
1:A:365:ARG:NH1	1:A:499:PHE:O	2.38	0.54
1:C:151:SER:OG	1:C:154:ASP:OD2	2.26	0.54
1:D:44:VAL:HG12	1:D:93:VAL:HB	1.89	0.54
1:D:81:SER:HB3	1:D:91:LEU:HD13	1.88	0.54
1:C:787:SER:OG	1:C:789:ASP:OD1	2.25	0.54
1:D:127:GLY:HA3	1:E:114:ALA:HA	1.89	0.54
1:D:167:LEU:HD13	1:D:293:ILE:HD11	1.89	0.54
1:F:903:ALA:HB1	1:F:929:LEU:HD12	1.90	0.54
1:E:172:GLY:HA3	1:E:304:THR:HG21	1.89	0.54
1:E:187:ARG:HG2	1:E:766:ASN:HB2	1.89	0.54
1:F:366:ALA:HB2	1:F:500:LEU:HD11	1.90	0.54
1:A:970:ILE:HG22	1:A:971:ILE:HD12	1.90	0.54
1:C:138:LEU:HD22	1:C:295:LEU:HD13	1.89	0.54
1:C:82:THR:HB	1:C:811:LYS:HE3	1.89	0.54
1:D:143:MET:HB2	1:D:159:ILE:HD11	1.90	0.54
1:A:469:ILE:HD12	1:A:920:ILE:HD13	1.89	0.53
1:C:428:ILE:O	1:C:502:ARG:NH2	2.41	0.53
1:D:889:ARG:NH2	1:D:892:ILE:HD13	2.23	0.53
1:E:891:LEU:HB3	1:E:1024:LEU:HD22	1.91	0.53
1:C:459:VAL:HG11	1:C:927:LEU:HD13	1.89	0.53
1:D:130:VAL:O	1:E:110:ASN:ND2	2.39	0.53
1:E:35:GLN:HG3	1:E:36:TYR:CD1	2.43	0.53
1:D:282:ARG:NH1	1:D:287:ASP:OD1	2.41	0.53
1:E:79:MET:HB3	1:E:93:VAL:HA	1.90	0.53
1:A:15:VAL:HG13	1:B:881:LEU:HB3	1.88	0.53
1:A:553:LEU:HD21	1:A:912:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:PRO:HB2	1:E:132:LYS:HD3	1.90	0.53
1:C:140:ALA:HB3	1:C:329:TYR:HB3	1.89	0.53
1:E:31:LEU:HD23	1:E:32:PRO:HD2	1.90	0.53
1:F:140:ALA:HB1	1:F:606:MET:HE1	1.90	0.53
1:D:481:VAL:HA	1:D:484:SER:HB3	1.90	0.53
1:F:450:LEU:HB3	1:F:882:ILE:HG21	1.91	0.53
1:A:601:GLY:HA3	1:A:642:ILE:HD11	1.91	0.53
1:C:352:LEU:HD22	1:C:979:PHE:HD2	1.74	0.53
1:E:407:VAL:HG22	1:E:484:SER:HB2	1.90	0.53
1:E:602:VAL:HA	1:E:629:LEU:HA	1.90	0.53
1:C:405:GLY:HA3	1:C:977:PHE:HA	1.90	0.53
1:C:466:VAL:HG22	1:C:920:ILE:HD11	1.91	0.53
1:F:744:MET:HE3	1:F:748:ILE:HD11	1.90	0.53
1:A:561:LEU:HD12	1:A:562:VAL:HG12	1.91	0.53
1:A:179:ILE:HD11	1:A:292:MET:HG3	1.90	0.52
1:C:167:LEU:HD13	1:C:293:ILE:HD11	1.90	0.52
1:E:35:GLN:HE22	1:E:334:PHE:HE2	1.57	0.52
1:F:83:SER:HB3	1:F:89:MET:HG2	1.91	0.52
1:F:196:ASN:ND2	1:F:782:ASN:O	2.39	0.52
1:F:353:VAL:HG21	1:F:404:ILE:HG22	1.90	0.52
1:D:943:PHE:HD2	1:D:962:ALA:HA	1.75	0.52
1:D:896:VAL:HG13	1:D:937:ALA:HB3	1.92	0.52
1:A:131:ARG:HB3	1:B:111:ARG:HH12	1.75	0.52
1:E:429:SER:OG	1:E:432:ASP:OD2	2.28	0.52
1:D:9:ARG:HG2	1:E:888:GLU:OE2	2.09	0.52
1:F:987:ALA:O	1:F:996:HIS:NE2	2.37	0.52
1:B:511:VAL:O	1:B:515:ASN:ND2	2.31	0.52
1:F:44:VAL:HG21	1:F:108:VAL:HG21	1.91	0.52
1:A:116:THR:HA	1:A:119:MET:HG3	1.92	0.52
1:C:977:PHE:HD2	1:C:1006:MET:HG2	1.75	0.52
1:E:212:GLN:O	1:F:727:ARG:NH1	2.39	0.52
1:B:328:PRO:HB2	1:B:626:PHE:HE2	1.74	0.52
1:C:697:LEU:HD12	1:C:846:LEU:HD11	1.91	0.52
1:D:296:GLN:HE22	1:E:74:ASP:HA	1.73	0.52
1:B:615:THR:HG23	1:B:617:SER:H	1.75	0.52
1:B:982:LEU:N	1:B:983:PRO:HD2	2.25	0.52
1:F:892:ILE:H	1:F:893:PRO:HD2	1.74	0.52
1:B:397:LEU:HA	1:B:400:LEU:HD22	1.92	0.51
1:C:33:ILE:HD13	1:C:392:ILE:HB	1.92	0.51
1:D:147:ASP:OD1	1:D:148:GLY:N	2.38	0.51
1:D:168:LYS:NZ	1:D:175:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:758:MET:HG2	1:E:759:LEU:HG	1.91	0.51
1:A:37:PRO:HG3	1:A:472:GLN:HG3	1.91	0.51
1:C:190:LEU:HD13	1:C:195:LEU:HD11	1.92	0.51
1:A:237:THR:HA	1:B:54:ASP:HB3	1.91	0.51
1:D:596:VAL:O	1:D:602:VAL:HG21	2.11	0.51
1:F:150:MET:HE1	1:F:320:PRO:HG2	1.92	0.51
1:A:159:ILE:HG22	1:A:164:LEU:HB2	1.92	0.51
1:A:218:THR:HG23	1:A:219:GLY:H	1.75	0.51
1:A:447:SER:OG	1:A:886:GLN:OE1	2.25	0.51
1:C:515:ASN:OD1	1:C:968:ARG:NH2	2.43	0.51
1:D:159:ILE:HD13	1:D:291:ILE:HD11	1.92	0.51
1:E:402:LEU:HD22	1:E:928:LEU:HD22	1.92	0.51
1:F:727:ARG:NH1	1:F:737:MET:SD	2.84	0.51
1:B:904:VAL:HG12	1:B:926:LEU:HD11	1.93	0.51
1:F:801:LEU:H	1:F:801:LEU:HD23	1.76	0.51
1:B:398:PHE:CZ	1:B:998:LEU:HD22	2.46	0.51
1:E:283:LEU:HA	1:E:606:MET:HA	1.92	0.51
1:A:723:LEU:HD22	1:A:799:LEU:HB3	1.92	0.51
1:B:737:MET:HA	1:B:740:VAL:HG12	1.93	0.51
1:D:518:PHE:HZ	1:D:968:ARG:HA	1.76	0.51
1:E:406:ILE:HD12	1:E:477:LEU:HD22	1.91	0.51
1:E:448:ILE:HG12	1:E:935:LYS:HG3	1.92	0.51
1:E:507:PRO:CD	1:E:508:PHE:N	2.73	0.51
1:E:242:LEU:HB2	1:E:248:PHE:CE1	2.45	0.51
1:E:339:ILE:HG12	1:E:397:LEU:HD21	1.92	0.51
1:E:572:SER:HB2	1:E:625:MET:HB3	1.92	0.51
1:D:12:PHE:CD2	1:E:885:ALA:HB1	2.46	0.51
1:D:76:MET:HA	1:D:95:PHE:HA	1.93	0.51
1:D:377:SER:OG	1:D:480:SER:O	2.28	0.51
1:E:392:ILE:HG23	1:E:397:LEU:HD11	1.93	0.51
1:A:706:GLU:N	1:A:706:GLU:OE1	2.43	0.50
1:B:375:PRO:O	1:B:379:LEU:HB2	2.11	0.50
1:B:675:PHE:HE2	1:B:821:VAL:HG12	1.75	0.50
1:C:302:LEU:HD12	1:C:302:LEU:H	1.75	0.50
1:E:143:MET:HE1	1:E:319:PHE:HZ	1.76	0.50
1:E:502:ARG:O	1:E:504:GLU:N	2.44	0.50
1:A:282:ARG:HB2	1:A:607:ALA:HB3	1.93	0.50
1:C:140:ALA:HB1	1:C:606:MET:HE1	1.93	0.50
1:D:706:GLU:N	1:D:706:GLU:OE1	2.45	0.50
1:D:795:LEU:HB3	1:D:799:LEU:HD12	1.93	0.50
1:F:354:ILE:HG12	1:F:371:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:ILE:HG12	1:F:609:ILE:HG21	1.92	0.50
1:A:446:ILE:HD11	1:A:489:LEU:HD11	1.93	0.50
1:A:753:VAL:HG22	1:A:754:ASN:H	1.76	0.50
1:B:66:ILE:HG22	1:B:815:LEU:HD23	1.92	0.50
1:B:721:TYR:HB3	1:B:801:LEU:HD11	1.94	0.50
1:A:891:LEU:HD23	1:A:1028:ASN:HD21	1.75	0.50
1:B:200:ILE:HG21	1:B:253:LEU:HD13	1.94	0.50
1:B:532:ILE:HG23	1:B:539:PHE:CG	2.47	0.50
1:C:451:VAL:HG12	1:C:931:GLY:HA2	1.92	0.50
1:E:665:PRO:HD2	1:E:669:LEU:HD11	1.93	0.50
1:B:382:PHE:HE1	1:B:400:LEU:HD21	1.76	0.50
1:B:422:LEU:O	1:B:502:ARG:NH2	2.45	0.50
1:D:733:TYR:HB3	1:D:793:ILE:HG12	1.93	0.50
1:E:106:ILE:HG21	1:F:106:ILE:HD12	1.92	0.50
1:A:582:LEU:O	1:A:586:ILE:HG13	2.12	0.50
1:C:378:LEU:O	1:C:381:THR:HG22	2.12	0.50
1:D:224:GLU:HG3	1:E:277:TYR:HD1	1.77	0.50
1:D:300:ASN:OD1	1:D:303:HIS:N	2.40	0.50
1:C:795:LEU:HB3	1:C:799:LEU:HD12	1.94	0.50
1:E:66:ILE:HG12	1:E:79:MET:HE1	1.94	0.50
1:B:188:ILE:HD13	1:B:264:LEU:HD21	1.93	0.49
1:B:217:ALA:HB3	1:B:238:MET:HB3	1.93	0.49
1:B:947:GLU:HG3	1:B:953:LYS:HD2	1.93	0.49
1:E:948:ARG:NH1	1:E:953:LYS:O	2.45	0.49
1:B:901:PRO:HA	1:B:904:VAL:HG22	1.93	0.49
1:C:681:ASN:OD1	1:C:685:LYS:N	2.38	0.49
1:C:477:LEU:HD13	1:C:928:LEU:HD13	1.94	0.49
1:C:884:ALA:HB2	1:C:893:PRO:HG3	1.93	0.49
1:E:54:ASP:OD2	1:E:57:THR:OG1	2.29	0.49
1:E:112:ILE:C	1:E:114:ALA:H	2.21	0.49
1:E:777:GLN:O	1:E:777:GLN:NE2	2.44	0.49
1:B:682:LYS:HE2	1:B:851:SER:HB2	1.94	0.49
1:C:81:SER:HB3	1:C:91:LEU:HD13	1.94	0.49
1:E:618:LEU:H	1:E:618:LEU:HD23	1.77	0.49
1:E:1022:TYR:O	1:E:1026:ASN:ND2	2.46	0.49
1:F:166:GLU:HG3	1:F:311:LYS:HE2	1.95	0.49
1:A:252:ILE:HG22	1:A:263:ARG:HG2	1.94	0.49
1:C:590:ASP:O	1:C:594:GLN:HB2	2.13	0.49
1:D:448:ILE:HG12	1:D:935:LYS:HG3	1.93	0.49
1:E:576:LEU:HD13	1:E:585:THR:HG23	1.95	0.49
1:B:826:ALA:HB3	1:B:829:TYR:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:960:VAL:HG12	1:F:964:LYS:HE2	1.95	0.49
1:E:64:SER:HB3	1:E:65:PRO:HD3	1.95	0.49
1:E:977:PHE:O	1:E:981:VAL:HG22	2.12	0.49
1:F:566:ASP:OD1	1:F:635:ARG:NH2	2.46	0.49
1:F:903:ALA:HB2	1:F:933:SER:HB3	1.93	0.49
1:C:54:ASP:OD1	1:C:55:ALA:N	2.46	0.49
1:C:201:THR:HB	1:C:792:MET:HE1	1.93	0.49
1:D:150:MET:O	1:D:154:ASP:HB2	2.12	0.49
1:D:237:THR:HG23	1:E:722:LYS:HA	1.94	0.49
1:E:357:MET:HE2	1:E:361:LEU:HD22	1.95	0.49
1:F:138:LEU:HD22	1:F:295:LEU:HD13	1.95	0.49
1:A:977:PHE:HD2	1:A:1006:MET:HG2	1.78	0.49
1:C:535:ARG:HB2	1:C:538:ARG:HG2	1.94	0.49
1:C:614:PHE:HE1	1:C:672:THR:HG21	1.78	0.49
1:C:887:TYR:HE2	1:C:938:ILE:HD11	1.77	0.49
1:D:72:GLY:O	1:D:111:ARG:NH2	2.46	0.49
1:D:190:LEU:HD21	1:D:205:VAL:HG11	1.95	0.48
1:E:227:THR:OG1	1:F:772:ASP:OD2	2.23	0.48
1:B:187:ARG:HD3	1:B:189:TRP:CZ2	2.48	0.48
1:E:295:LEU:HD22	1:E:301:ALA:HB2	1.94	0.48
1:E:369:ILE:HB	1:E:370:PRO:HD3	1.95	0.48
1:E:541:LEU:HA	1:E:544:CYS:SG	2.53	0.48
1:B:91:LEU:C	1:B:91:LEU:HD13	2.37	0.48
1:B:838:ILE:HA	1:B:841:VAL:HG22	1.96	0.48
1:D:171:PRO:HD2	1:D:307:LEU:HD13	1.94	0.48
1:F:319:PHE:HB3	1:F:323:LEU:HB3	1.96	0.48
1:A:302:LEU:HD21	1:A:335:VAL:HB	1.95	0.48
1:A:912:TYR:HD1	1:A:913:LEU:HD12	1.78	0.48
1:B:190:LEU:HD21	1:B:205:VAL:HG11	1.96	0.48
1:C:224:GLU:CB	1:C:225:PRO:HD3	2.41	0.48
1:C:274:SER:OG	1:C:275:GLN:N	2.46	0.48
1:B:402:LEU:HD21	1:B:998:LEU:HD21	1.95	0.48
1:C:565:GLU:OE2	1:C:994:SER:N	2.44	0.48
1:D:142:SER:HB2	1:D:606:MET:SD	2.53	0.48
1:E:505:GLY:C	1:E:506:GLU:HG3	2.39	0.48
1:E:725:ILE:HD11	1:E:727:ARG:CZ	2.43	0.48
1:B:738:GLN:O	1:B:742:ASN:HB2	2.13	0.48
1:F:143:MET:HG2	1:F:325:TYR:HB3	1.96	0.48
1:A:122:ALA:HA	1:A:125:LYS:HD2	1.96	0.48
1:A:187:ARG:NE	1:A:274:SER:O	2.39	0.48
1:A:212:GLN:HA	1:B:737:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:HD11	1:C:112:ILE:HD11	1.94	0.48
1:C:71:ASN:HA	1:C:76:MET:HE1	1.95	0.48
1:B:64:SER:HB3	1:B:65:PRO:HD3	1.95	0.48
1:D:63:ALA:HA	1:D:89:MET:HE2	1.95	0.48
1:D:436:GLN:HA	1:D:439:GLN:HG3	1.95	0.48
1:E:66:ILE:HG23	1:E:815:LEU:HD22	1.95	0.48
1:F:706:GLU:OE1	1:F:706:GLU:N	2.46	0.48
1:A:570:MET:HG3	1:A:627:ILE:HB	1.96	0.48
1:B:571:ILE:HG13	1:B:661:ILE:HG13	1.96	0.48
1:C:895:ALA:HB2	1:C:1024:LEU:HD12	1.95	0.48
1:D:356:VAL:HG11	1:D:976:ALA:HA	1.95	0.48
1:E:900:VAL:HG13	1:E:930:ILE:HG12	1.95	0.48
1:B:632:TRP:HA	1:B:635:ARG:HG2	1.95	0.47
1:D:261:PHE:HZ	1:E:732:HIS:HB2	1.79	0.47
1:D:346:PHE:CD2	1:D:404:ILE:HD11	2.48	0.47
1:D:477:LEU:HD13	1:D:928:LEU:HD13	1.95	0.47
1:D:525:PHE:HE1	1:D:1014:ILE:HG13	1.78	0.47
1:E:297:SER:OG	1:E:298:GLY:N	2.46	0.47
1:F:572:SER:HB3	1:F:625:MET:HB2	1.96	0.47
1:B:970:ILE:HG21	1:B:1014:ILE:HG21	1.95	0.47
1:D:63:ALA:HB2	1:D:89:MET:HG3	1.95	0.47
1:E:74:ASP:O	1:E:75:ASN:HB3	2.15	0.47
1:F:153:VAL:O	1:F:157:ASN:ND2	2.34	0.47
1:F:220:LYS:HE2	1:F:223:GLU:HB2	1.96	0.47
1:A:169:ARG:HG3	1:B:76:MET:HE3	1.95	0.47
1:D:242:LEU:HB2	1:D:248:PHE:CE1	2.49	0.47
1:F:357:MET:HE3	1:F:370:PRO:HG2	1.96	0.47
1:F:865:LYS:HA	1:F:865:LYS:HD2	1.65	0.47
1:A:163:VAL:HA	1:A:315:LEU:HD13	1.96	0.47
1:B:364:PHE:O	1:B:367:THR:HG22	2.14	0.47
1:C:101:PRO:HB2	1:C:132:LYS:HG3	1.97	0.47
1:C:446:ILE:HD11	1:C:489:LEU:HD11	1.95	0.47
1:D:731:LYS:HB2	1:F:252:ILE:HD12	1.96	0.47
1:E:505:GLY:C	1:E:506:GLU:CG	2.88	0.47
1:E:982:LEU:N	1:E:983:PRO:HD2	2.30	0.47
1:F:253:LEU:HD12	1:F:267:VAL:HG11	1.97	0.47
1:C:206:ILE:HD11	1:C:746:ALA:HB2	1.96	0.47
1:E:691:GLN:NE2	1:E:695:ASN:OD1	2.48	0.47
1:F:305:ALA:HB2	1:F:332:THR:HG21	1.95	0.47
1:F:977:PHE:HZ	1:F:1002:LEU:HD23	1.80	0.47
1:C:595:GLU:HA	1:C:598:LYS:HZ3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:LYS:HD3	1:C:809:ASP:OD1	2.15	0.47
1:C:987:ALA:HB1	1:C:995:ARG:HH21	1.79	0.47
1:A:242:LEU:HD22	1:A:247:GLU:HB3	1.96	0.47
1:B:72:GLY:HA3	1:B:75:ASN:HB2	1.96	0.47
1:B:393:ASN:O	1:B:397:LEU:HG	2.14	0.47
1:B:839:ALA:O	1:B:843:LYS:HG2	2.14	0.47
1:D:39:LEU:HD21	1:D:469:ILE:HG13	1.97	0.47
1:D:449:VAL:HG21	1:D:485:GLY:HA3	1.96	0.47
1:D:895:ALA:HB2	1:D:1024:LEU:HD12	1.97	0.47
1:E:81:SER:HB3	1:E:91:LEU:HD13	1.95	0.47
1:E:586:ILE:HA	1:E:609:ILE:HD13	1.97	0.47
1:F:224:GLU:HB3	1:F:225:PRO:HD2	1.96	0.47
1:F:490:THR:O	1:F:493:PRO:HD2	2.15	0.47
1:F:784:PHE:HB3	1:F:792:MET:HB3	1.97	0.47
1:A:46:VAL:HB	1:A:91:LEU:HB3	1.97	0.47
1:A:465:PHE:HE2	1:A:561:LEU:HD11	1.80	0.47
1:D:737:MET:HE3	1:D:741:PHE:HE1	1.80	0.47
1:E:179:ILE:HD11	1:E:290:PRO:HB2	1.96	0.47
1:E:234:TYR:OH	1:F:775:ASN:O	2.33	0.47
1:E:249:GLU:HB3	1:E:265:LYS:HB3	1.96	0.47
1:F:373:ALA:HA	1:F:487:VAL:HG11	1.96	0.47
1:B:198:PHE:O	1:B:254:ARG:NH1	2.48	0.47
1:C:825:PRO:HB3	1:C:834:ALA:HB2	1.95	0.47
1:E:756:PHE:CE2	1:E:758:MET:HB2	2.50	0.47
1:B:35:GLN:HE22	1:B:334:PHE:HE2	1.63	0.47
1:B:671:ILE:HG23	1:B:674:GLY:H	1.80	0.47
1:B:925:GLY:HA3	1:B:1002:LEU:HD23	1.97	0.47
1:C:284:ASN:HA	1:C:597:LEU:HD11	1.97	0.47
1:E:71:ASN:HB3	1:E:111:ARG:CZ	2.44	0.47
1:E:635:ARG:NE	1:E:637:VAL:HA	2.29	0.47
1:A:801:LEU:H	1:A:801:LEU:HD23	1.80	0.46
1:D:140:ALA:HB1	1:D:606:MET:HE1	1.97	0.46
1:C:119:MET:HE2	1:C:119:MET:HA	1.97	0.46
1:E:711:ARG:NH2	1:E:822:GLN:OE1	2.48	0.46
1:E:778:ASP:C	1:E:780:LEU:H	2.22	0.46
1:E:970:ILE:HG21	1:E:1014:ILE:HG21	1.98	0.46
1:A:59:ALA:HA	1:A:63:ALA:HB3	1.97	0.46
1:A:614:PHE:CE1	1:A:671:ILE:HD13	2.51	0.46
1:B:625:MET:HE3	1:B:627:ILE:HD11	1.97	0.46
1:B:812:ARG:NH2	1:B:815:LEU:O	2.48	0.46
1:C:225:PRO:HD2	1:C:226:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:TYR:CD2	1:C:626:PHE:HB3	2.51	0.46
1:F:206:ILE:HD11	1:F:746:ALA:HB2	1.96	0.46
1:F:578:SER:HB3	1:F:715:ASP:OD2	2.16	0.46
1:F:895:ALA:HB2	1:F:1024:LEU:HD12	1.97	0.46
1:A:676:GLU:CD	1:A:820:GLN:HE21	2.23	0.46
1:D:570:MET:HG3	1:D:627:ILE:HB	1.96	0.46
1:D:943:PHE:O	1:D:947:GLU:HG2	2.15	0.46
1:E:187:ARG:HD3	1:E:189:TRP:CH2	2.51	0.46
1:E:345:THR:HG21	1:E:401:ILE:HG23	1.98	0.46
1:A:49:THR:HG22	1:A:88:THR:HG22	1.97	0.46
1:A:738:GLN:O	1:A:742:ASN:ND2	2.38	0.46
1:B:677:MET:HG3	1:B:821:VAL:HB	1.97	0.46
1:B:831:SER:O	1:B:835:ILE:HG12	2.15	0.46
1:E:144:TYR:CG	1:E:283:LEU:HD21	2.50	0.46
1:C:342:VAL:HG11	1:C:397:LEU:HB3	1.98	0.46
1:E:953:LYS:HD3	1:E:957:GLU:HB3	1.97	0.46
1:A:242:LEU:HB2	1:A:248:PHE:CE2	2.51	0.46
1:B:65:PRO:HA	1:B:68:ASP:HB3	1.97	0.46
1:B:418:ILE:C	1:B:420:ARG:H	2.23	0.46
1:C:117:ALA:C	1:C:119:MET:H	2.23	0.46
1:F:141:ILE:HG21	1:F:312:MET:HE2	1.96	0.46
1:F:350:LEU:O	1:F:354:ILE:HG13	2.15	0.46
1:F:532:ILE:HG12	1:F:539:PHE:CZ	2.51	0.46
1:A:353:VAL:HA	1:A:356:VAL:HG12	1.98	0.46
1:A:1010:SER:O	1:A:1014:ILE:HG12	2.16	0.46
1:B:39:LEU:HD13	1:B:465:PHE:CE1	2.51	0.46
1:B:144:TYR:CD1	1:B:283:LEU:HD21	2.51	0.46
1:B:1007:ILE:O	1:B:1011:THR:OG1	2.22	0.46
1:C:1034:LYS:HE2	1:C:1034:LYS:HB3	1.82	0.46
1:D:138:LEU:HD22	1:D:295:LEU:HG	1.98	0.46
1:D:217:ALA:O	1:D:218:THR:HB	2.16	0.46
1:E:574:ILE:HB	1:E:623:ALA:HB3	1.97	0.46
1:F:759:LEU:HD23	1:F:759:LEU:HA	1.81	0.46
1:A:777:GLN:CD	1:A:777:GLN:H	2.23	0.46
1:D:165:ASP:HB3	1:E:815:LEU:HD12	1.98	0.46
1:D:190:LEU:O	1:D:770:LYS:N	2.39	0.46
1:D:892:ILE:HG21	1:D:945:MET:SD	2.56	0.46
1:E:592:ILE:HG22	1:E:625:MET:HE1	1.97	0.46
1:A:158:TYR:OH	1:A:318:ASN:O	2.32	0.45
1:C:67:GLU:HB3	1:C:815:LEU:HD23	1.98	0.45
1:D:114:ALA:HB1	1:F:131:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ARG:NE	1:E:276:GLN:O	2.49	0.45
1:E:495:LEU:HD22	1:E:499:PHE:HE2	1.82	0.45
1:E:738:GLN:O	1:E:742:ASN:ND2	2.28	0.45
1:B:354:ILE:HA	1:B:367:THR:OG1	2.16	0.45
1:B:715:ASP:OD1	1:B:717:THR:OG1	2.30	0.45
1:C:392:ILE:HG23	1:C:397:LEU:HD21	1.98	0.45
1:D:252:ILE:HG22	1:D:263:ARG:HG2	1.97	0.45
1:D:456:PHE:HA	1:D:459:VAL:HG22	1.97	0.45
1:F:70:ILE:O	1:F:111:ARG:NH1	2.50	0.45
1:F:276:GLN:C	1:F:278:SER:H	2.24	0.45
1:F:653:ASP:HB3	1:F:656:ALA:O	2.16	0.45
1:D:466:VAL:HG23	1:D:920:ILE:HD11	1.98	0.45
1:D:665:PRO:HG2	1:D:666:ILE:HD12	1.99	0.45
1:A:661:ILE:HD12	1:A:672:THR:HG21	1.98	0.45
1:A:815:LEU:O	1:C:169:ARG:NH2	2.49	0.45
1:A:895:ALA:HB2	1:A:1024:LEU:HD12	1.98	0.45
1:B:361:LEU:O	1:B:362:LYS:HB2	2.15	0.45
1:B:1002:LEU:HD12	1:B:1003:ILE:HD12	1.97	0.45
1:E:361:LEU:O	1:E:363:ASN:N	2.48	0.45
1:B:143:MET:HE1	1:B:319:PHE:CZ	2.51	0.45
1:D:44:VAL:HG11	1:D:108:VAL:HG21	1.98	0.45
1:F:825:PRO:HB3	1:F:834:ALA:HB2	1.98	0.45
1:C:31:LEU:HD11	1:C:385:LEU:HB2	1.98	0.45
1:E:192:PRO:HD2	1:E:773:PHE:CG	2.51	0.45
1:E:8:GLU:HG2	1:E:431:LYS:HE2	1.97	0.45
1:E:632:TRP:CE2	1:E:990:ALA:HB2	2.52	0.45
1:E:635:ARG:HG3	1:E:637:VAL:HG12	1.98	0.45
1:A:295:LEU:HD13	1:A:296:GLN:N	2.32	0.45
1:E:632:TRP:HA	1:E:635:ARG:NH1	2.32	0.45
1:A:41:PRO:HB3	1:A:95:PHE:O	2.16	0.45
1:A:106:ILE:HG21	1:B:106:ILE:HD12	1.98	0.45
1:A:846:LEU:HB3	1:A:847:GLY:H	1.64	0.45
1:B:77:ILE:HG13	1:B:78:TYR:H	1.80	0.45
1:B:163:VAL:O	1:B:167:LEU:HB2	2.17	0.45
1:C:532:ILE:HG23	1:C:539:PHE:CG	2.51	0.45
1:C:675:PHE:CZ	1:C:838:ILE:HG13	2.52	0.45
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.99	0.45
1:D:369:ILE:HB	1:D:370:PRO:HD3	1.99	0.45
1:E:187:ARG:HD3	1:E:189:TRP:CZ2	2.52	0.45
1:F:191:LYS:HD2	1:F:194:LEU:HD22	1.99	0.45
1:B:33:ILE:HG21	1:B:302:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:LEU:HB2	1:E:477:LEU:HD21	1.98	0.45
1:E:612:ASP:HB3	1:E:615:THR:HG22	1.98	0.45
1:B:91:LEU:CD1	1:B:93:VAL:HG23	2.47	0.44
1:C:787:SER:HB3	1:C:793:ILE:HD11	1.99	0.44
1:F:54:ASP:O	1:F:58:ILE:HG13	2.17	0.44
1:F:81:SER:HB3	1:F:91:LEU:HD13	1.98	0.44
1:F:452:LEU:HD22	1:F:481:VAL:HG21	1.97	0.44
1:B:457:VAL:N	1:B:458:PRO:HD2	2.33	0.44
1:C:375:PRO:O	1:C:379:LEU:HB2	2.16	0.44
1:C:896:VAL:HG13	1:C:937:ALA:HB3	1.99	0.44
1:D:145:SER:HB2	1:D:150:MET:HB2	1.98	0.44
1:D:251:ILE:O	1:D:264:LEU:N	2.50	0.44
1:E:143:MET:HE1	1:E:319:PHE:CZ	2.52	0.44
1:E:147:ASP:HB2	1:E:322:GLY:HA3	2.00	0.44
1:C:141:ILE:N	1:C:291:ILE:O	2.51	0.44
1:D:592:ILE:HG23	1:D:650:PHE:CE2	2.53	0.44
1:D:901:PRO:HA	1:D:904:VAL:HG22	1.99	0.44
1:F:37:PRO:HG3	1:F:472:GLN:HG3	1.99	0.44
1:F:661:ILE:HG21	1:F:672:THR:HB	1.99	0.44
1:F:677:MET:HB2	1:F:854:TRP:CE3	2.53	0.44
1:A:226:VAL:HG12	1:B:771:GLY:HA3	2.00	0.44
1:B:189:TRP:HZ3	1:B:768:ARG:HG2	1.82	0.44
1:B:687:TYR:OH	1:B:810:VAL:HG13	2.17	0.44
1:C:442:SER:O	1:C:446:ILE:HG12	2.18	0.44
1:C:755:ASP:OD1	1:C:755:ASP:N	2.49	0.44
1:E:39:LEU:HG	1:E:465:PHE:HE2	1.82	0.44
1:F:683:SER:HB3	1:F:849:ASP:HB2	1.99	0.44
1:A:356:VAL:HG11	1:A:976:ALA:HA	1.99	0.44
1:A:572:SER:OG	1:A:625:MET:HB3	2.18	0.44
1:B:444:PRO:O	1:B:447:SER:N	2.51	0.44
1:B:577:PRO:O	1:B:580:SER:OG	2.30	0.44
1:C:352:LEU:HD23	1:C:355:ILE:HD11	2.00	0.44
1:D:452:LEU:HD13	1:D:481:VAL:HG21	2.00	0.44
1:F:412:ILE:HD11	1:F:973:THR:HA	1.99	0.44
1:A:563:PRO:HB2	1:A:993:ALA:HB1	2.00	0.44
1:C:245:PRO:HD3	1:C:758:MET:SD	2.57	0.44
1:C:361:LEU:HD23	1:C:366:ALA:O	2.17	0.44
1:E:558:PRO:O	1:E:917:SER:HB2	2.18	0.44
1:E:896:VAL:HG13	1:E:937:ALA:HB3	1.99	0.44
1:B:713:THR:OG1	1:B:811:LYS:NZ	2.51	0.44
1:B:855:SER:OG	1:B:856:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ILE:HG13	1:E:721:TYR:HD2	1.83	0.44
1:D:280:GLN:HG2	1:D:282:ARG:HH12	1.83	0.44
1:D:573:ILE:HG12	1:D:614:PHE:HE2	1.82	0.44
1:F:492:THR:O	1:F:496:CYS:HB2	2.16	0.44
1:F:550:ILE:HD13	1:F:904:VAL:HG13	1.99	0.44
1:A:402:LEU:HD11	1:A:1002:LEU:CD2	2.47	0.44
1:A:509:LYS:HG3	1:A:510:PHE:H	1.82	0.44
1:B:643:ILE:O	1:B:647:ASN:ND2	2.32	0.44
1:B:725:ILE:H	1:B:725:ILE:HG13	1.65	0.44
1:B:283:LEU:HB3	1:B:606:MET:HG3	2.00	0.44
1:D:666:ILE:HD13	1:D:669:LEU:HD12	2.00	0.44
1:E:487:VAL:HG13	1:E:491:LEU:HB3	2.00	0.44
1:F:943:PHE:O	1:F:947:GLU:HG2	2.18	0.44
1:A:815:LEU:HB3	1:C:169:ARG:NH2	2.33	0.43
1:B:28:LEU:HD11	1:B:382:PHE:CD2	2.53	0.43
1:B:75:ASN:O	1:B:96:ASP:HB2	2.18	0.43
1:C:509:LYS:HD2	1:C:510:PHE:N	2.33	0.43
1:C:586:ILE:HG12	1:C:609:ILE:HG21	2.00	0.43
1:D:189:TRP:NE1	1:D:271:GLU:OE2	2.47	0.43
1:E:73:ALA:C	1:E:75:ASN:H	2.26	0.43
1:E:153:VAL:O	1:E:157:ASN:ND2	2.44	0.43
1:B:171:PRO:HD2	1:B:307:LEU:HD13	1.99	0.43
1:B:300:ASN:O	1:B:304:THR:HG23	2.18	0.43
1:D:49:THR:HG22	1:D:88:THR:HG22	1.99	0.43
1:D:95:PHE:CZ	1:D:104:ALA:HB1	2.54	0.43
1:D:400:LEU:O	1:D:404:ILE:HG13	2.19	0.43
1:E:77:ILE:HG13	1:E:78:TYR:H	1.83	0.43
1:E:205:VAL:HG13	1:E:264:LEU:HD11	2.00	0.43
1:F:510:PHE:O	1:F:514:PHE:N	2.42	0.43
1:F:649:LYS:HB2	1:F:649:LYS:HE2	1.86	0.43
1:A:378:LEU:HD22	1:A:400:LEU:HD22	2.01	0.43
1:B:297:SER:OG	1:B:298:GLY:N	2.51	0.43
1:B:444:PRO:O	1:B:448:ILE:N	2.48	0.43
1:B:465:PHE:CE1	1:B:668:GLY:HA3	2.53	0.43
1:D:848:ASP:OD1	1:D:848:ASP:N	2.52	0.43
1:D:1010:SER:O	1:D:1014:ILE:HG12	2.18	0.43
1:E:754:ASN:H	1:E:765:VAL:HG12	1.83	0.43
1:A:896:VAL:HG13	1:A:937:ALA:HB3	2.00	0.43
1:B:444:PRO:C	1:B:448:ILE:HD13	2.44	0.43
1:B:578:SER:HA	1:B:621:ASN:HD22	1.84	0.43
1:C:248:PHE:O	1:C:264:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:653:ASP:CG	1:E:654:ARG:H	2.24	0.43
1:B:939:LEU:HB3	1:B:966:ARG:HD2	2.00	0.43
1:C:518:PHE:HE2	1:C:968:ARG:HG3	1.83	0.43
1:D:141:ILE:HB	1:D:291:ILE:HB	2.00	0.43
1:D:447:SER:HB3	1:D:938:ILE:HD13	1.99	0.43
1:D:890:TRP:CE2	1:F:11:VAL:HG13	2.53	0.43
1:E:238:MET:HE2	1:F:741:PHE:CE1	2.54	0.43
1:E:250:ASN:HA	1:E:263:ARG:HD3	2.00	0.43
1:F:33:ILE:HD13	1:F:392:ILE:HB	2.01	0.43
1:F:596:VAL:HG21	1:F:625:MET:HE1	2.01	0.43
1:F:620:GLU:H	1:F:620:GLU:CD	2.26	0.43
1:A:730:LEU:HD12	1:A:730:LEU:HA	1.86	0.43
1:A:885:ALA:HB1	1:C:12:PHE:CD2	2.54	0.43
1:A:939:LEU:O	1:A:966:ARG:HG3	2.18	0.43
1:B:332:THR:HA	1:B:335:VAL:HG12	2.01	0.43
1:B:632:TRP:CZ2	1:B:990:ALA:HB2	2.54	0.43
1:B:927:LEU:HD23	1:B:927:LEU:HA	1.92	0.43
1:C:733:TYR:HB3	1:C:793:ILE:HD13	2.01	0.43
1:D:181:ASN:O	1:D:275:GLN:HB3	2.19	0.43
1:D:579:ALA:HB2	1:D:719:PRO:HG3	2.01	0.43
1:E:155:VAL:O	1:E:159:ILE:HG12	2.19	0.43
1:E:354:ILE:HG12	1:E:367:THR:HG23	2.01	0.43
1:E:489:LEU:HD12	1:E:490:THR:HG23	2.01	0.43
1:B:970:ILE:HG22	1:B:971:ILE:HD12	2.01	0.43
1:D:525:PHE:CE1	1:D:1014:ILE:HG13	2.54	0.43
1:D:671:ILE:HD12	1:D:672:THR:N	2.34	0.43
1:E:200:ILE:HG23	1:E:204:ASP:HB2	2.01	0.43
1:E:224:GLU:O	1:E:225:PRO:C	2.62	0.43
1:B:402:LEU:HB2	1:B:477:LEU:HD21	2.01	0.43
1:B:579:ALA:O	1:B:621:ASN:HB3	2.19	0.43
1:F:41:PRO:HB3	1:F:95:PHE:O	2.19	0.43
1:F:734:ASN:OD1	1:F:788:ASN:HB2	2.18	0.43
1:F:998:LEU:O	1:F:1002:LEU:HD13	2.19	0.43
1:A:465:PHE:CE2	1:A:561:LEU:HD11	2.53	0.42
1:B:480:SER:O	1:B:484:SER:OG	2.32	0.42
1:B:998:LEU:O	1:B:1002:LEU:HG	2.19	0.42
1:D:507:PRO:HB2	1:D:512:LYS:HB2	2.00	0.42
1:A:752:TYR:O	1:A:753:VAL:HG12	2.18	0.42
1:B:68:ASP:OD2	1:B:111:ARG:HG3	2.20	0.42
1:B:185:SER:HB3	1:B:274:SER:O	2.19	0.42
1:B:418:ILE:HG21	1:B:500:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLU:HB2	1:E:315:LEU:HD11	2.01	0.42
1:E:899:ALA:HB2	1:E:1017:VAL:HG22	2.01	0.42
1:F:369:ILE:HD12	1:F:495:LEU:HB3	2.01	0.42
1:A:54:ASP:OD1	1:A:54:ASP:N	2.37	0.42
1:A:221:ILE:HG13	1:B:721:TYR:HD2	1.85	0.42
1:A:384:GLY:HA3	1:A:479:ILE:HD13	2.00	0.42
1:C:134:SER:HB3	1:C:295:LEU:O	2.20	0.42
1:C:672:THR:OG1	1:C:673:GLY:N	2.52	0.42
1:D:943:PHE:HB2	1:D:966:ARG:HE	1.84	0.42
1:E:775:ASN:ND2	1:E:775:ASN:O	2.52	0.42
1:E:825:PRO:HB3	1:E:834:ALA:HB2	2.01	0.42
1:E:902:PHE:CD1	1:E:1012:LEU:HB3	2.54	0.42
1:F:199:GLY:O	1:F:254:ARG:NH1	2.51	0.42
1:B:102:ASP:OD1	1:B:102:ASP:N	2.52	0.42
1:B:159:ILE:HA	1:B:163:VAL:HG22	2.00	0.42
1:B:190:LEU:HB2	1:B:769:ALA:HA	2.01	0.42
1:C:316:SER:HB3	1:C:325:TYR:HE1	1.84	0.42
1:C:321:LYS:HB3	1:C:322:GLY:H	1.63	0.42
1:E:242:LEU:HD23	1:E:247:GLU:HB3	2.00	0.42
1:F:946:GLU:HG3	1:F:950:LYS:HE2	2.02	0.42
1:A:67:GLU:HB3	1:A:815:LEU:HD23	2.02	0.42
1:A:753:VAL:HG22	1:A:754:ASN:HD22	1.84	0.42
1:C:190:LEU:HD21	1:C:205:VAL:HG11	2.01	0.42
1:E:5:PHE:CE1	1:E:9:ARG:HD2	2.53	0.42
1:E:708:SER:OG	1:E:824:GLN:HG3	2.20	0.42
1:E:981:VAL:HG23	1:E:1003:ILE:HD11	2.00	0.42
1:A:150:MET:O	1:A:154:ASP:HB2	2.20	0.42
1:A:680:GLN:HB3	1:A:818:ALA:HB2	2.02	0.42
1:B:201:THR:HG23	1:B:204:ASP:H	1.84	0.42
1:C:116:THR:O	1:C:119:MET:HB2	2.20	0.42
1:C:874:LEU:HA	1:C:874:LEU:HD23	1.84	0.42
1:D:345:THR:HG23	1:D:983:PRO:HB2	2.01	0.42
1:F:926:LEU:O	1:F:930:ILE:HG13	2.20	0.42
1:D:892:ILE:N	1:D:893:PRO:HD2	2.35	0.42
1:E:971:ILE:O	1:E:975:LEU:HB2	2.19	0.42
1:F:884:ALA:HB2	1:F:893:PRO:HG3	2.02	0.42
1:A:191:LYS:HE3	1:A:191:LYS:HB2	1.91	0.42
1:B:973:THR:HG23	1:B:974:SER:N	2.35	0.42
1:D:278:SER:HA	1:D:582:LEU:HD22	2.02	0.42
1:D:789:ASP:HB2	1:D:791:LYS:HG3	2.02	0.42
1:E:39:LEU:HG	1:E:465:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ALA:HB3	1:E:743:THR:HG23	2.01	0.42
1:B:567:GLN:O	1:B:569:LEU:N	2.53	0.42
1:B:671:ILE:O	1:B:672:THR:HG22	2.20	0.42
1:C:374:VAL:HB	1:C:375:PRO:HD3	2.02	0.42
1:C:509:LYS:H	1:C:509:LYS:HG3	1.68	0.42
1:D:77:ILE:HD11	1:D:96:ASP:HA	2.01	0.42
1:E:138:LEU:HD12	1:E:295:LEU:HB2	2.01	0.42
1:F:223:GLU:HG2	1:F:224:GLU:HG3	2.02	0.42
1:A:357:MET:SD	1:A:371:MET:HE2	2.60	0.42
1:B:385:LEU:HD23	1:B:479:ILE:HD12	2.01	0.42
1:B:400:LEU:O	1:B:404:ILE:HG13	2.20	0.42
1:B:768:ARG:HG3	1:B:769:ALA:O	2.20	0.42
1:B:852:ILE:H	1:B:852:ILE:HD12	1.84	0.42
1:B:899:ALA:HB2	1:B:1017:VAL:HG22	2.01	0.42
1:C:302:LEU:O	1:C:306:GLU:HG3	2.20	0.42
1:D:572:SER:HB3	1:D:660:PHE:CD2	2.55	0.42
1:E:43:THR:OG1	1:E:133:THR:OG1	2.15	0.42
1:F:921:TYR:HE2	1:F:994:SER:HB3	1.84	0.42
1:B:849:ASP:OD1	1:B:849:ASP:N	2.53	0.41
1:C:442:SER:O	1:C:445:VAL:HG22	2.20	0.41
1:C:713:THR:OG1	1:C:820:GLN:HB3	2.20	0.41
1:D:635:ARG:O	1:D:636:ASN:HB3	2.20	0.41
1:E:329:TYR:HD2	1:E:626:PHE:HZ	1.67	0.41
1:E:398:PHE:HB3	1:E:473:PHE:HE1	1.84	0.41
1:E:636:ASN:O	1:E:637:VAL:HG22	2.19	0.41
1:F:167:LEU:HD21	1:F:312:MET:SD	2.59	0.41
1:F:430:VAL:HG12	1:F:497:ALA:HA	2.01	0.41
1:A:406:ILE:O	1:A:409:ASP:HB2	2.20	0.41
1:A:483:ILE:O	1:A:487:VAL:HG23	2.21	0.41
1:C:348:GLU:HG3	1:C:983:PRO:HB3	2.02	0.41
1:D:195:LEU:HB3	1:D:200:ILE:O	2.20	0.41
1:E:561:LEU:HB3	1:E:562:VAL:H	1.65	0.41
1:F:67:GLU:HB3	1:F:815:LEU:HD23	2.02	0.41
1:A:109:ASN:ND2	1:B:110:ASN:OD1	2.28	0.41
1:A:112:ILE:O	1:A:116:THR:OG1	2.35	0.41
1:A:452:LEU:HD12	1:A:481:VAL:HG11	2.03	0.41
1:A:535:ARG:HA	1:A:538:ARG:HH11	1.85	0.41
1:B:193:ASP:OD1	1:B:194:LEU:N	2.53	0.41
1:B:242:LEU:HD22	1:B:247:GLU:HB3	2.02	0.41
1:B:381:THR:HA	1:B:483:ILE:HD12	2.03	0.41
1:B:674:GLY:HA3	1:B:823:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:GLU:HB3	1:B:958:ALA:HB1	2.02	0.41
1:C:179:ILE:HD13	1:C:179:ILE:HA	1.91	0.41
1:D:978:THR:HG23	1:D:1003:ILE:HG13	2.01	0.41
1:E:24:GLY:O	1:E:28:LEU:HB2	2.20	0.41
1:A:159:ILE:HA	1:A:163:VAL:HB	2.02	0.41
1:B:24:GLY:HA3	1:B:379:LEU:HD23	2.03	0.41
1:B:190:LEU:O	1:B:770:LYS:N	2.41	0.41
1:B:195:LEU:HD12	1:B:267:VAL:HB	2.02	0.41
1:E:629:LEU:HD12	1:E:630:GLN:O	2.20	0.41
1:F:761:LYS:HE2	1:F:761:LYS:HB3	1.89	0.41
1:A:428:ILE:HD12	1:A:428:ILE:HA	1.94	0.41
1:A:509:LYS:HG3	1:A:510:PHE:N	2.36	0.41
1:A:671:ILE:H	1:A:671:ILE:HG13	1.70	0.41
1:B:220:LYS:HG2	1:B:235:SER:HB3	2.03	0.41
1:B:702:ASN:O	1:B:702:ASN:ND2	2.54	0.41
1:D:250:ASN:HA	1:D:263:ARG:HD3	2.01	0.41
1:D:982:LEU:HB3	1:D:983:PRO:HD3	2.01	0.41
1:E:669:LEU:H	1:E:669:LEU:HD23	1.86	0.41
1:F:244:ASN:OD1	1:F:246:SER:OG	2.19	0.41
1:A:164:LEU:HD21	1:A:168:LYS:HE2	2.03	0.41
1:A:225:PRO:HG2	1:B:774:ARG:NH1	2.35	0.41
1:A:591:HIS:NE2	1:E:689:GLU:HG2	2.35	0.41
1:C:78:TYR:CZ	1:C:94:TYR:HD2	2.39	0.41
1:C:97:ILE:HD12	1:C:97:ILE:H	1.86	0.41
1:C:143:MET:HG2	1:C:325:TYR:HB3	2.03	0.41
1:C:186:LEU:HD11	1:C:270:VAL:HG12	2.01	0.41
1:C:243:GLN:HG3	1:C:244:ASN:HD22	1.85	0.41
1:D:220:LYS:NZ	1:E:620:GLU:OE1	2.54	0.41
1:F:420:ARG:HE	1:F:420:ARG:HB3	1.71	0.41
1:A:533:LEU:HD22	1:A:1022:TYR:HD2	1.86	0.41
1:B:970:ILE:O	1:B:973:THR:HG22	2.21	0.41
1:B:977:PHE:O	1:B:981:VAL:HG22	2.21	0.41
1:C:938:ILE:HD12	1:C:938:ILE:HA	1.94	0.41
1:E:589:VAL:HG21	1:E:609:ILE:HG12	2.03	0.41
1:A:978:THR:HG23	1:A:1003:ILE:HG13	2.02	0.41
1:B:506:GLU:HA	1:B:507:PRO:HD3	1.92	0.41
1:C:578:SER:OG	1:C:579:ALA:N	2.54	0.41
1:D:97:ILE:HD12	1:D:97:ILE:H	1.85	0.41
1:D:112:ILE:O	1:D:116:THR:OG1	2.36	0.41
1:E:887:TYR:OH	1:E:938:ILE:O	2.39	0.41
1:F:80:ASP:HB3	1:F:813:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLU:HB3	1:F:225:PRO:CD	2.51	0.41
1:A:100:ASP:HB3	1:A:103:GLN:HB3	2.03	0.41
1:A:154:ASP:OD1	1:A:154:ASP:N	2.54	0.41
1:A:172:GLY:HA3	1:A:304:THR:HG21	2.03	0.41
1:B:80:ASP:HB3	1:B:813:PHE:HD1	1.86	0.41
1:B:607:ALA:HA	1:B:625:MET:HA	2.03	0.41
1:B:981:VAL:HG23	1:B:1003:ILE:HD11	2.03	0.41
1:C:457:VAL:HG12	1:C:458:PRO:HD3	2.02	0.41
1:D:31:LEU:HD22	1:D:391:SER:HA	2.03	0.41
1:D:216:TYR:CE2	1:E:737:MET:HG2	2.55	0.41
1:D:221:ILE:HG13	1:E:721:TYR:CD2	2.56	0.41
1:D:290:PRO:HG3	1:D:608:MET:HG3	2.02	0.41
1:D:370:PRO:HG3	1:D:415:VAL:HG21	2.03	0.41
1:D:420:ARG:O	1:D:424:GLU:HB2	2.21	0.41
1:D:444:PRO:O	1:D:448:ILE:HG13	2.21	0.41
1:E:635:ARG:HE	1:E:637:VAL:HA	1.86	0.41
1:E:921:TYR:CD2	1:E:994:SER:HB3	2.56	0.41
1:F:97:ILE:HD11	1:F:860:GLN:HE22	1.86	0.41
1:F:179:ILE:O	1:F:618:LEU:HD21	2.21	0.41
1:F:883:LEU:HB2	1:F:893:PRO:HB3	2.03	0.41
1:F:977:PHE:CZ	1:F:1002:LEU:HD23	2.56	0.41
1:A:549:ALA:O	1:A:553:LEU:HB2	2.21	0.41
1:A:722:LYS:HE2	1:A:804:SER:HB2	2.03	0.41
1:B:754:ASN:O	1:B:765:VAL:HG22	2.21	0.41
1:D:579:ALA:O	1:F:232:TYR:HA	2.21	0.41
1:F:713:THR:OG1	1:F:820:GLN:HB3	2.21	0.41
1:F:889:ARG:HG2	1:F:891:LEU:HD23	2.03	0.41
1:F:940:ILE:HG13	1:F:970:ILE:HD11	2.02	0.41
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.89	0.40
1:A:876:MET:HG2	1:A:930:ILE:HD11	2.03	0.40
1:B:212:GLN:O	1:C:727:ARG:NH1	2.54	0.40
1:B:448:ILE:HA	1:B:451:VAL:HG12	2.04	0.40
1:B:600:ASN:H	1:B:600:ASN:HD22	1.68	0.40
1:B:1021:PHE:O	1:B:1025:GLU:HB2	2.21	0.40
1:C:116:THR:O	1:C:124:LYS:HE2	2.21	0.40
1:C:420:ARG:O	1:C:424:GLU:HG2	2.21	0.40
1:D:190:LEU:HB3	1:D:195:LEU:HD11	2.03	0.40
1:E:59:ALA:HA	1:E:62:VAL:HG12	2.02	0.40
1:E:780:LEU:HD21	1:E:799:LEU:HB3	2.03	0.40
1:E:944:ALA:HB1	1:E:1021:PHE:CE2	2.56	0.40
1:F:80:ASP:HB3	1:F:813:PHE:HD1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:PHE:CE2	1:A:838:ILE:HG13	2.56	0.40
1:A:846:LEU:HD13	1:A:846:LEU:HA	1.94	0.40
1:B:302:LEU:HD11	1:B:335:VAL:HG13	2.02	0.40
1:C:156:TYR:CE1	1:C:274:SER:HA	2.57	0.40
1:C:187:ARG:HG2	1:C:766:ASN:HB2	2.03	0.40
1:C:350:LEU:HD21	1:C:374:VAL:HG11	2.03	0.40
1:D:573:ILE:HG12	1:D:614:PHE:CE2	2.56	0.40
1:D:669:LEU:HD23	1:D:669:LEU:HA	1.97	0.40
1:F:28:LEU:HD13	1:F:382:PHE:CD2	2.56	0.40
1:F:229:LYS:HA	1:F:229:LYS:HD3	1.86	0.40
1:B:725:ILE:HD13	1:B:727:ARG:HG2	2.02	0.40
1:B:729:LYS:O	1:B:733:TYR:HD1	2.04	0.40
1:C:34:GLU:HG2	1:C:300:ASN:ND2	2.36	0.40
1:C:141:ILE:HD13	1:C:312:MET:HG3	2.03	0.40
1:D:167:LEU:O	1:D:173:VAL:HG21	2.21	0.40
1:D:564:GLU:HG2	1:D:665:PRO:HD3	2.04	0.40
1:E:352:LEU:HD13	1:E:352:LEU:HA	1.94	0.40
1:F:274:SER:OG	1:F:275:GLN:N	2.53	0.40
1:F:333:LYS:O	1:F:337:GLU:HG2	2.20	0.40
1:A:529:VAL:O	1:A:533:LEU:HG	2.22	0.40
1:A:1009:ALA:O	1:A:1013:ALA:HB3	2.22	0.40
1:B:95:PHE:CE1	1:B:104:ALA:HB1	2.57	0.40
1:B:172:GLY:HA3	1:B:304:THR:CG2	2.52	0.40
1:B:867:THR:HG23	1:B:870:TYR:HE1	1.87	0.40
1:B:969:PRO:HA	1:B:972:MET:HG2	2.02	0.40
1:C:387:VAL:HG23	1:C:388:LEU:HG	2.03	0.40
1:D:22:LEU:HD22	1:E:878:PHE:HE1	1.86	0.40
1:E:136:THR:HG23	1:E:295:LEU:HB3	2.03	0.40
1:E:420:ARG:O	1:E:424:GLU:HG2	2.20	0.40
1:E:902:PHE:HB3	1:E:1013:ALA:HB2	2.03	0.40
1:F:560:SER:HB3	1:F:919:ASP:HB3	2.03	0.40
1:F:1007:ILE:O	1:F:1011:THR:OG1	2.25	0.40
1:A:550:ILE:HD13	1:A:904:VAL:HG13	2.04	0.40
1:A:721:TYR:O	1:C:236:ILE:HA	2.22	0.40
1:A:892:ILE:HG21	1:A:945:MET:SD	2.61	0.40
1:B:15:VAL:HG21	1:C:885:ALA:HB2	2.04	0.40
1:B:939:LEU:HD13	1:B:966:ARG:NH1	2.36	0.40
1:D:14:SER:O	1:D:18:ILE:HG13	2.21	0.40
1:D:634:ASP:OD1	1:D:634:ASP:N	2.54	0.40
1:D:945:MET:HE2	1:D:945:MET:HB3	1.96	0.40
1:E:283:LEU:HB3	1:E:606:MET:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:PHE:HE1	1:E:927:LEU:HB3	1.86	0.40
1:E:739:ASP:OD1	1:E:739:ASP:N	2.53	0.40
1:E:918:ASN:ND2	1:E:918:ASN:O	2.55	0.40
1:E:1006:MET:HA	1:E:1006:MET:HE3	2.04	0.40
1:F:378:LEU:O	1:F:381:THR:HG22	2.21	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	1031/1035 (100%)	954 (92%)	70 (7%)	7 (1%)	18	51
1	B	1031/1035 (100%)	944 (92%)	71 (7%)	16 (2%)	7	36
1	C	1033/1035 (100%)	951 (92%)	66 (6%)	16 (2%)	8	37
1	D	1031/1035 (100%)	932 (90%)	90 (9%)	9 (1%)	14	47
1	E	1031/1035 (100%)	950 (92%)	59 (6%)	22 (2%)	5	31
1	F	1033/1035 (100%)	949 (92%)	74 (7%)	10 (1%)	12	45
All	All	6190/6210 (100%)	5680 (92%)	430 (7%)	80 (1%)	9	40

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	753	VAL
1	B	37	PRO
1	B	40	THR
1	C	224	GLU
1	C	226	VAL
1	C	578	SER
1	C	669	LEU

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Mol	Chain	Res	Type
1	D	217	ALA
1	D	218	THR
1	D	636	ASN
1	D	753	VAL
1	E	53	ALA
1	E	73	ALA
1	E	75	ASN
1	E	214	ALA
1	E	215	GLN
1	E	225	PRO
1	E	916	PHE
1	F	226	VAL
1	A	636	ASN
1	B	38	SER
1	B	138	LEU
1	B	284	ASN
1	B	568	GLY
1	B	671	ILE
1	B	672	THR
1	C	180	GLY
1	C	274	SER
1	C	674	GLY
1	C	863	SER
1	D	600	ASN
1	E	71	ASN
1	E	231	PRO
1	E	297	SER
1	E	503	ASN
1	E	637	VAL
1	F	491	LEU
1	A	223	GLU
1	B	147	ASP
1	B	579	ALA
1	C	232	TYR
1	C	498	LEU
1	D	225	PRO
1	E	54	ASP
1	E	229	LYS
1	E	507	PRO
1	E	684	GLY
1	E	779	ALA
1	F	654	ARG

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	578	SER
1	B	215	GLN
1	B	919	ASP
1	C	651	ALA
1	D	224	GLU
1	D	635	ARG
1	E	138	LEU
1	E	274	SER
1	E	561	LEU
1	A	807	PRO
1	B	53	ALA
1	B	181	ASN
1	B	275	GLN
1	D	1011	THR
1	F	153	VAL
1	F	232	TYR
1	F	362	LYS
1	F	506	GLU
1	B	673	GLY
1	C	577	PRO
1	C	753	VAL
1	C	892	ILE
1	E	683	SER
1	F	224	GLU
1	F	253	LEU
1	E	710	VAL
1	C	199	GLY
1	C	771	GLY
1	A	224	GLU
1	F	892	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	869/871 (100%)	867 (100%)	2 (0%)	87 85
1	B	869/871 (100%)	868 (100%)	1 (0%)	88 87
1	C	871/871 (100%)	870 (100%)	1 (0%)	88 87
1	D	869/871 (100%)	869 (100%)	0	100 100
1	E	869/871 (100%)	866 (100%)	3 (0%)	86 82
1	F	871/871 (100%)	869 (100%)	2 (0%)	87 85
All	All	5218/5226 (100%)	5209 (100%)	9 (0%)	87 85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	734	ASN
1	B	26	ILE
1	C	732	HIS
1	E	448	ILE
1	E	506	GLU
1	E	971	ILE
1	F	372	ILE
1	F	1017	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	243	GLN
1	A	275	GLN
1	A	655	ASN
1	A	745	ASN
1	A	782	ASN
1	A	820	GLN
1	A	822	GLN
1	A	860	GLN
1	A	1028	ASN
1	B	35	GLN
1	B	284	ASN
1	B	417	ASN

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Mol	Chain	Res	Type
1	B	472	GLN
1	B	575	ASN
1	B	636	ASN
1	B	702	ASN
1	B	775	ASN
1	C	109	ASN
1	C	417	ASN
1	C	575	ASN
1	C	600	ASN
1	C	636	ASN
1	C	655	ASN
1	C	680	GLN
1	D	162	ASN
1	D	183	ASN
1	D	296	GLN
1	D	417	ASN
1	D	720	GLN
1	D	736	ASN
1	D	923	GLN
1	E	35	GLN
1	E	276	GLN
1	E	630	GLN
1	E	691	GLN
1	E	695	ASN
1	E	766	ASN
1	E	777	GLN
1	E	788	ASN
1	E	802	GLN
1	F	177	ASN
1	F	250	ASN
1	F	257	ASN
1	F	280	GLN
1	F	680	GLN
1	F	788	ASN
1	F	820	GLN
1	F	822	GLN
1	F	936	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 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	1033/1035 (99%)	0.43	51 (4%)	35 19	70, 94, 119, 168	0
1	B	1033/1035 (99%)	0.57	79 (7%)	20 12	73, 110, 157, 178	0
1	C	1035/1035 (100%)	0.29	34 (3%)	49 27	64, 95, 130, 158	0
1	D	1033/1035 (99%)	0.35	35 (3%)	48 26	72, 96, 118, 159	0
1	E	1033/1035 (99%)	0.39	43 (4%)	40 21	70, 103, 138, 163	0
1	F	1035/1035 (100%)	0.35	40 (3%)	43 23	64, 88, 129, 163	0
All	All	6202/6210 (99%)	0.40	282 (4%)	38 20	64, 98, 135, 178	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	564	GLU	7.1
1	B	784	PHE	6.3
1	B	845	THR	5.6
1	B	663	LEU	5.6
1	C	410	ASP	5.3
1	B	626	PHE	5.3
1	E	117	ALA	5.2
1	F	294	ASN	5.2
1	B	898	THR	4.7
1	F	175	ASP	4.6
1	F	292	MET	4.6
1	A	362	LYS	4.6
1	A	363	ASN	4.6
1	A	285	GLY	4.6
1	B	292	MET	4.5
1	E	68	ASP	4.5
1	A	861	GLU	4.4
1	E	175	ASP	4.4
1	B	412	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	489	LEU	4.2
1	B	653	ASP	4.2
1	B	897	VAL	4.2
1	F	122	ALA	4.2
1	B	530	ALA	4.1
1	B	569	LEU	4.1
1	E	860	GLN	4.1
1	A	800	THR	4.1
1	A	361	LEU	4.1
1	A	416	GLU	4.0
1	D	410	ASP	4.0
1	F	885	ALA	4.0
1	E	129	THR	3.9
1	A	439	GLN	3.9
1	E	64	SER	3.9
1	A	438	MET	3.9
1	F	177	ASN	3.9
1	A	364	PHE	3.8
1	D	778	ASP	3.7
1	E	409	ASP	3.7
1	A	435	ILE	3.6
1	B	656	ALA	3.6
1	D	2	PHE	3.6
1	F	38	SER	3.6
1	A	175	ASP	3.5
1	B	602	VAL	3.5
1	B	140	ALA	3.5
1	F	769	ALA	3.4
1	F	613	LEU	3.4
1	A	564	GLU	3.4
1	C	175	ASP	3.4
1	A	48	ALA	3.4
1	C	52	GLY	3.4
1	E	845	THR	3.4
1	B	410	ASP	3.4
1	B	931	GLY	3.3
1	A	45	LYS	3.3
1	D	125	LYS	3.3
1	F	114	ALA	3.3
1	E	762	ASN	3.3
1	B	369	ILE	3.3
1	D	570	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	117	ALA	3.3
1	E	922	PHE	3.3
1	C	776	THR	3.3
1	C	212	GLN	3.3
1	D	366	ALA	3.3
1	C	747	THR	3.3
1	E	118	LYS	3.2
1	A	283	LEU	3.2
1	A	640	ASP	3.2
1	B	662	GLY	3.2
1	D	370	PRO	3.2
1	B	733	TYR	3.2
1	B	976	ALA	3.2
1	E	936	ASN	3.2
1	A	604	ASP	3.2
1	F	124	LYS	3.1
1	D	780	LEU	3.1
1	B	625	MET	3.1
1	B	414	VAL	3.1
1	B	773	PHE	3.1
1	A	328	PRO	3.1
1	D	565	GLU	3.1
1	B	642	ILE	3.0
1	C	153	VAL	3.0
1	F	117	ALA	3.0
1	A	606	MET	3.0
1	D	37	PRO	3.0
1	A	409	ASP	3.0
1	F	180	GLY	3.0
1	C	109	ASN	3.0
1	D	184	TYR	3.0
1	D	368	LEU	3.0
1	F	162	ASN	3.0
1	B	357	MET	3.0
1	A	541	LEU	3.0
1	E	496	CYS	2.9
1	B	139	ALA	2.9
1	A	730	LEU	2.9
1	B	876	MET	2.9
1	B	329	TYR	2.9
1	F	595	GLU	2.9
1	D	777	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	697	LEU	2.9
1	E	8	GLU	2.9
1	A	671	ILE	2.9
1	B	793	ILE	2.9
1	A	639	ALA	2.8
1	D	364	PHE	2.8
1	B	664	PRO	2.8
1	C	370	PRO	2.8
1	B	596	VAL	2.8
1	F	69	ALA	2.8
1	A	625	MET	2.8
1	E	473	PHE	2.8
1	A	131	ARG	2.8
1	D	568	GLY	2.8
1	D	131	ARG	2.8
1	A	130	VAL	2.8
1	E	46	VAL	2.8
1	B	152	ALA	2.8
1	A	799	LEU	2.7
1	C	195	LEU	2.7
1	C	972	MET	2.7
1	B	713	THR	2.7
1	F	167	LEU	2.7
1	A	665	PRO	2.7
1	C	721	TYR	2.7
1	E	913	LEU	2.7
1	D	779	ALA	2.7
1	A	110	ASN	2.7
1	B	52	GLY	2.7
1	B	53	ALA	2.7
1	F	598	LYS	2.7
1	B	670	SER	2.7
1	B	165	ASP	2.6
1	F	991	GLY	2.6
1	C	39	LEU	2.6
1	E	398	PHE	2.6
1	B	110	ASN	2.6
1	B	785	VAL	2.6
1	C	411	ALA	2.6
1	D	152	ALA	2.6
1	B	409	ASP	2.6
1	C	196	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	356	VAL	2.6
1	F	179	ILE	2.6
1	E	45	LYS	2.6
1	E	859	TYR	2.6
1	B	792	MET	2.6
1	A	626	PHE	2.5
1	A	218	THR	2.5
1	C	38	SER	2.5
1	F	123	VAL	2.5
1	C	157	ASN	2.5
1	D	183	ASN	2.5
1	E	924	THR	2.5
1	A	593	SER	2.5
1	B	234	TYR	2.5
1	E	226	VAL	2.5
1	F	939	LEU	2.5
1	B	852	ILE	2.5
1	D	537	ILE	2.5
1	B	281	GLY	2.5
1	F	447	SER	2.5
1	C	208	ALA	2.5
1	B	794	PRO	2.5
1	A	410	ASP	2.5
1	E	281	GLY	2.5
1	C	116	THR	2.5
1	B	150	MET	2.5
1	B	797	SER	2.5
1	E	341	GLU	2.4
1	C	54	ASP	2.4
1	E	266	ASP	2.4
1	F	564	GLU	2.4
1	B	759	LEU	2.4
1	B	966	ARG	2.4
1	E	566	ASP	2.4
1	F	387	VAL	2.4
1	B	798	PHE	2.4
1	B	929	LEU	2.4
1	E	402	LEU	2.4
1	C	782	ASN	2.4
1	B	665	PRO	2.4
1	D	563	PRO	2.4
1	F	649	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	39	LEU	2.4
1	C	1025	GLU	2.4
1	A	294	ASN	2.4
1	A	570	MET	2.3
1	F	722	LYS	2.3
1	F	152	ALA	2.3
1	E	684	GLY	2.3
1	B	900	VAL	2.3
1	D	44	VAL	2.3
1	F	133	THR	2.3
1	C	115	ALA	2.3
1	D	39	LEU	2.3
1	F	293	ILE	2.3
1	B	660	PHE	2.3
1	D	411	ALA	2.3
1	F	68	ASP	2.3
1	B	160	THR	2.3
1	E	995	ARG	2.3
1	B	891	LEU	2.3
1	D	412	ILE	2.3
1	F	640	ASP	2.3
1	B	571	ILE	2.2
1	F	571	ILE	2.2
1	A	46	VAL	2.2
1	C	896	VAL	2.2
1	F	410	ASP	2.2
1	C	162	ASN	2.2
1	B	1020	PHE	2.2
1	E	47	SER	2.2
1	F	61	THR	2.2
1	B	465	PHE	2.2
1	C	96	ASP	2.2
1	E	410	ASP	2.2
1	E	53	ALA	2.2
1	A	329	TYR	2.2
1	A	608	MET	2.2
1	F	771	GLY	2.2
1	C	68	ASP	2.2
1	D	157	ASN	2.2
1	A	605	ALA	2.2
1	C	238	MET	2.2
1	B	864	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	844	GLU	2.2
1	B	70	ILE	2.2
1	A	366	ALA	2.2
1	B	73	ALA	2.2
1	B	1013	ALA	2.2
1	C	412	ILE	2.2
1	F	499	PHE	2.2
1	E	474	ALA	2.1
1	F	724	ILE	2.1
1	D	811	LYS	2.1
1	B	567	GLN	2.1
1	B	854	TRP	2.1
1	C	445	VAL	2.1
1	B	780	LEU	2.1
1	A	819	ALA	2.1
1	C	899	ALA	2.1
1	B	413	ILE	2.1
1	E	65	PRO	2.1
1	D	744	MET	2.1
1	A	538	ARG	2.1
1	E	497	ALA	2.1
1	B	936	ASN	2.1
1	B	927	LEU	2.1
1	E	119	MET	2.1
1	A	367	THR	2.1
1	E	565	GLU	2.1
1	A	930	ILE	2.1
1	B	783	ILE	2.1
1	B	562	VAL	2.1
1	E	926	LEU	2.1
1	B	628	GLY	2.1
1	C	160	THR	2.1
1	E	973	THR	2.1
1	A	47	SER	2.1
1	A	802	GLN	2.1
1	B	154	ASP	2.0
1	D	409	ASP	2.0
1	E	179	ILE	2.0
1	A	498	LEU	2.0
1	F	126	LEU	2.0
1	D	130	VAL	2.0
1	B	531	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	156	TYR	2.0
1	C	18	ILE	2.0
1	E	131	ARG	2.0
1	B	726	ASP	2.0
1	B	442	SER	2.0
1	B	659	VAL	2.0
1	E	15	VAL	2.0
1	C	746	ALA	2.0
1	D	593	SER	2.0
1	E	288	ALA	2.0
1	A	897	VAL	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.