Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FEM
Title	:	Structure of the synthase subunit Pdx1.1 (Snz1) of PLP synthase from Saccharomyces cerevisiae
Authors	:	Strohmeier, M.; Windeisen, V.; Sinning, I.; Tews, I.
Deposited on	:	2008-11-30
Resolution	:	3.02 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 ①) were used in the production of this report:

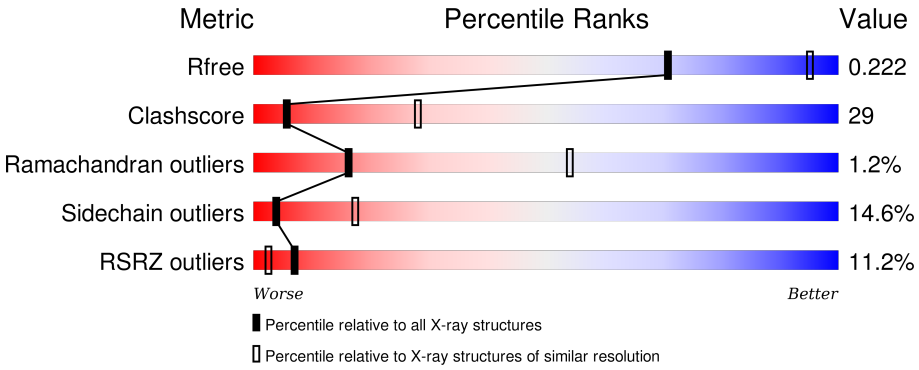
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 <=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	297	3% 49% 39% 6% • 5%
1	B	297	8% 49% 39% 5% • 5%
1	C	297	12% 52% 37% 6% • 5%
1	D	297	18% 49% 39% 5% • 5%
1	E	297	13% 50% 38% 5% • 5%

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Mol	Chain	Length	Quality of chain
1	F	297	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12600 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 Pyridoxine biosynthesis protein SNZ1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	B	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	C	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	D	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	E	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	F	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			

- Molecule 2 is water.

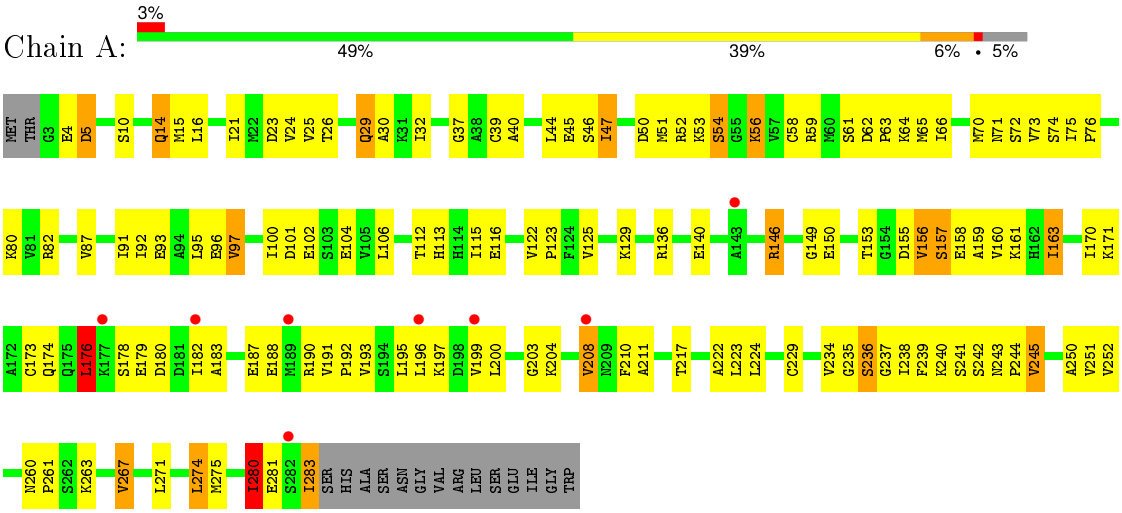
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	E	1	Total	O	0	0
			1	1		
2	F	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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.

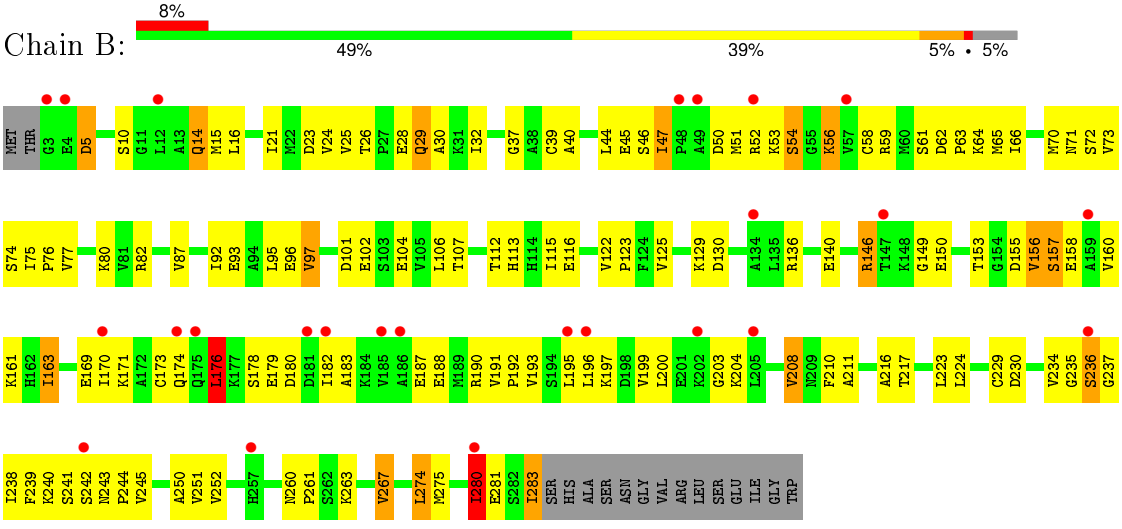
- Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain A:



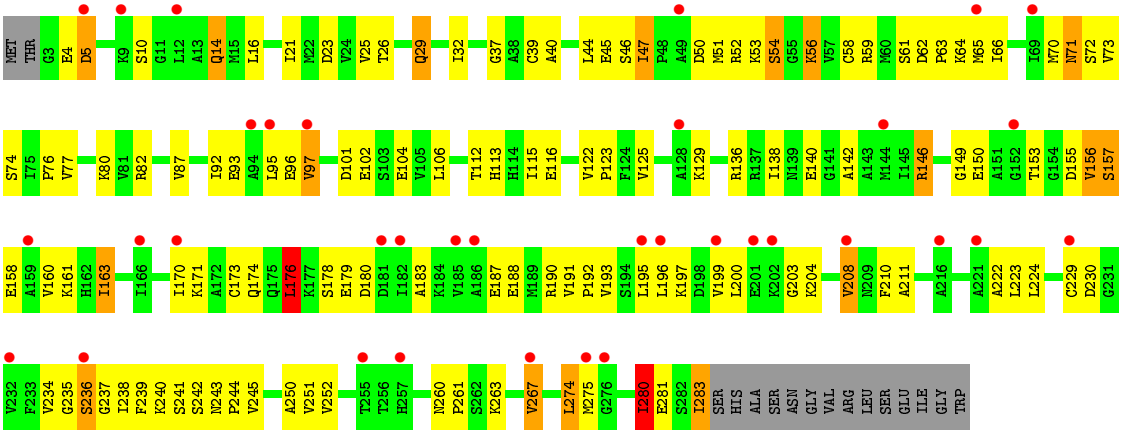
- Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain B:



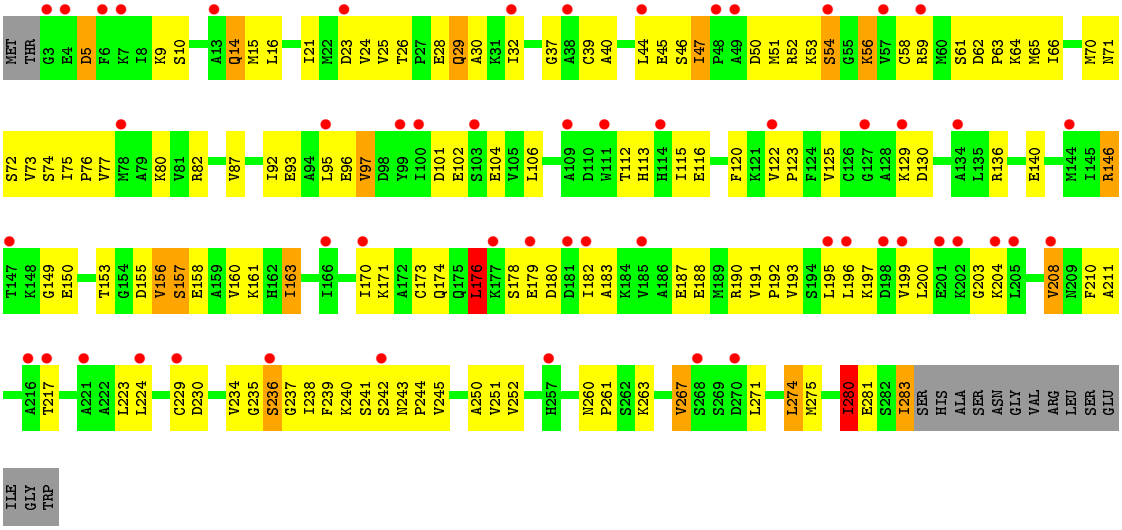
- Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain C:



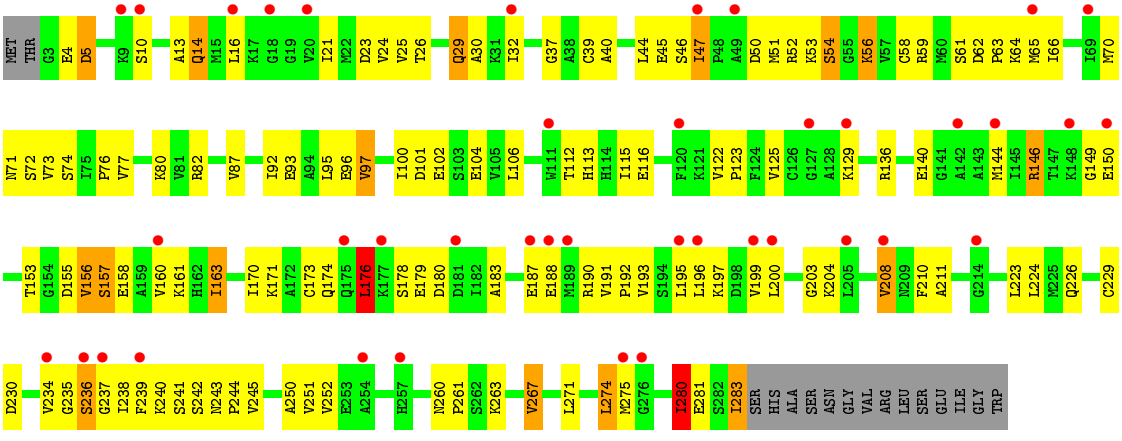
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain D:



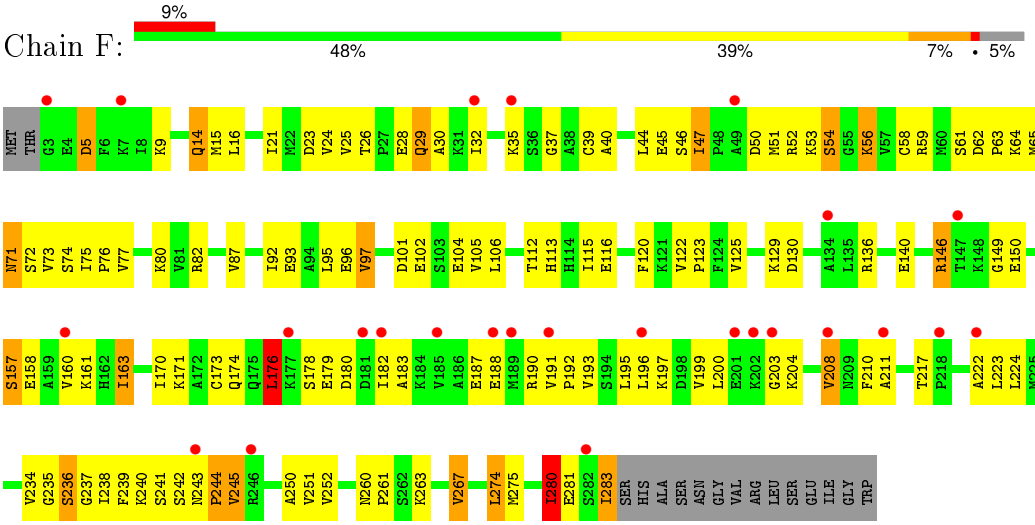
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain E:



• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	154.07Å 154.22Å 154.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.02 19.79 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.02) 99.2 (19.79-3.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.162 , 0.181 0.224 , 0.222	Depositor DCC
R_{free} test set	2009 reflections (2.89%)	DCC
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.5	EDS
Estimated twinning fraction	0.470 for H,K,L 0.298 for K,-L,-H 0.231 for -L,-H,K 0.149 for -h,l,k 0.149 for -l,-k,-h 0.149 for k,h,-l 0.348 for k,l,h 0.348 for l,h,k	Xtriage
Reported twinning fraction	0.470 for H,K,L 0.298 for K,-L,-H 0.231 for -L,-H,K	Depositor
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Outliers	0 of 71521 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12600	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/2125	0.67	0/2861
1	B	0.53	0/2125	0.69	0/2861
1	C	0.51	0/2125	0.68	0/2861
1	D	0.53	0/2125	0.69	0/2861
1	E	0.51	0/2125	0.68	0/2861
1	F	0.53	0/2125	0.69	0/2861
All	All	0.52	0/12750	0.68	0/17166

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	LEU	Peptide
1	B	176	LEU	Peptide
1	C	176	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	D	176	LEU	Peptide
1	E	176	LEU	Peptide
1	F	176	LEU	Peptide

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	2099	0	2162	130	0
1	B	2099	0	2162	132	1
1	C	2099	0	2162	122	0
1	D	2099	0	2162	129	0
1	E	2099	0	2162	129	0
1	F	2099	0	2162	129	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	12600	0	12972	747	1

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 29.

All (747) 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:173:CYS:O	1:B:176:LEU:HD22	1.29	1.32
1:F:173:CYS:O	1:F:176:LEU:HD22	1.31	1.29
1:D:173:CYS:O	1:D:176:LEU:HD22	1.28	1.26
1:A:173:CYS:O	1:A:176:LEU:HD22	1.31	1.25
1:C:173:CYS:O	1:C:176:LEU:HD22	1.29	1.23
1:E:173:CYS:O	1:E:176:LEU:HD22	1.32	1.22
1:E:92:ILE:HG23	1:E:97:VAL:HG21	1.41	1.03
1:B:92:ILE:HG23	1:B:97:VAL:HG21	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HG23	1:C:97:VAL:HG21	1.42	1.00
1:B:92:ILE:CG2	1:B:97:VAL:HG21	1.94	0.98
1:D:92:ILE:HG23	1:D:97:VAL:HG21	1.46	0.98
1:C:92:ILE:CG2	1:C:97:VAL:HG21	1.93	0.97
1:E:92:ILE:CG2	1:E:97:VAL:HG21	1.94	0.97
1:F:92:ILE:CG2	1:F:97:VAL:HG21	1.95	0.96
1:F:92:ILE:HG23	1:F:97:VAL:HG21	1.44	0.96
1:A:92:ILE:CG2	1:A:97:VAL:HG21	1.96	0.96
1:D:211:ALA:HB1	1:D:224:LEU:HD13	1.47	0.96
1:A:92:ILE:HG23	1:A:97:VAL:HG21	1.46	0.95
1:F:211:ALA:HB1	1:F:224:LEU:HD13	1.48	0.95
1:D:92:ILE:CG2	1:D:97:VAL:HG21	1.95	0.95
1:A:211:ALA:HB1	1:A:224:LEU:HD13	1.51	0.93
1:E:211:ALA:HB1	1:E:224:LEU:HD13	1.49	0.93
1:C:211:ALA:HB1	1:C:224:LEU:HD13	1.50	0.93
1:B:211:ALA:HB1	1:B:224:LEU:HD13	1.49	0.92
1:D:163:ILE:HD13	1:D:229:CYS:SG	2.09	0.92
1:C:163:ILE:HD13	1:C:229:CYS:SG	2.12	0.90
1:B:47:ILE:HD12	1:B:47:ILE:H	1.38	0.89
1:A:47:ILE:H	1:A:47:ILE:HD12	1.38	0.88
1:B:163:ILE:HD13	1:B:229:CYS:SG	2.14	0.88
1:C:47:ILE:HD12	1:C:47:ILE:H	1.39	0.87
1:E:174:GLN:HA	1:E:200:LEU:HD22	1.56	0.87
1:E:92:ILE:HG23	1:E:97:VAL:CG2	2.05	0.86
1:F:174:GLN:HA	1:F:200:LEU:HD22	1.57	0.86
1:A:174:GLN:HA	1:A:200:LEU:HD22	1.58	0.85
1:B:92:ILE:HG23	1:B:97:VAL:CG2	2.06	0.85
1:E:47:ILE:H	1:E:47:ILE:HD12	1.40	0.85
1:B:174:GLN:HA	1:B:200:LEU:HD22	1.58	0.84
1:C:92:ILE:HG23	1:C:97:VAL:CG2	2.07	0.84
1:D:92:ILE:HG23	1:D:97:VAL:CG2	2.07	0.84
1:F:47:ILE:H	1:F:47:ILE:HD12	1.42	0.84
1:F:92:ILE:HG23	1:F:97:VAL:CG2	2.08	0.83
1:D:174:GLN:HA	1:D:200:LEU:HD22	1.58	0.83
1:C:174:GLN:HA	1:C:200:LEU:HD22	1.59	0.83
1:D:47:ILE:HD12	1:D:47:ILE:H	1.42	0.82
1:A:92:ILE:HG23	1:A:97:VAL:CG2	2.10	0.81
1:F:163:ILE:HD13	1:F:229:CYS:SG	2.22	0.80
1:F:283:ILE:HG22	1:F:283:ILE:O	1.82	0.80
1:F:280:ILE:HG22	1:F:281:GLU:N	1.96	0.80
1:C:280:ILE:HG22	1:C:281:GLU:N	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:HD13	1:C:50:ASP:OD2	1.85	0.77
1:A:280:ILE:HG22	1:A:281:GLU:N	1.97	0.77
1:E:280:ILE:HG22	1:E:281:GLU:N	2.00	0.77
1:D:47:ILE:HD13	1:D:50:ASP:OD2	1.86	0.76
1:D:280:ILE:HG22	1:D:281:GLU:N	2.00	0.75
1:E:163:ILE:HD13	1:E:229:CYS:SG	2.26	0.75
1:E:283:ILE:HG22	1:E:283:ILE:O	1.83	0.75
1:D:211:ALA:CB	1:D:224:LEU:HD13	2.16	0.75
1:A:163:ILE:HD13	1:A:229:CYS:SG	2.27	0.75
1:C:274:LEU:HD12	1:C:274:LEU:H	1.51	0.75
1:A:47:ILE:HD13	1:A:50:ASP:OD2	1.87	0.75
1:A:59:ARG:HG2	1:A:82:ARG:CZ	2.17	0.74
1:F:283:ILE:CG2	1:F:283:ILE:O	2.35	0.74
1:F:47:ILE:HD13	1:F:50:ASP:OD2	1.87	0.74
1:B:280:ILE:HG22	1:B:281:GLU:N	2.01	0.74
1:F:211:ALA:CB	1:F:224:LEU:HD13	2.17	0.73
1:E:47:ILE:HD13	1:E:50:ASP:OD2	1.87	0.73
1:C:283:ILE:O	1:C:283:ILE:CG2	2.35	0.73
1:C:59:ARG:HG2	1:C:82:ARG:CZ	2.18	0.73
1:A:283:ILE:CG2	1:A:283:ILE:O	2.36	0.73
1:E:283:ILE:O	1:E:283:ILE:CG2	2.36	0.73
1:C:211:ALA:CB	1:C:224:LEU:HD13	2.19	0.73
1:C:283:ILE:HG22	1:C:283:ILE:O	1.89	0.72
1:B:92:ILE:CG2	1:B:97:VAL:CG2	2.67	0.72
1:B:59:ARG:HG2	1:B:82:ARG:CZ	2.19	0.71
1:A:283:ILE:HG22	1:A:283:ILE:O	1.89	0.71
1:F:44:LEU:O	1:F:44:LEU:HD12	1.90	0.71
1:E:176:LEU:HD23	1:E:176:LEU:O	1.91	0.71
1:F:59:ARG:HG2	1:F:82:ARG:CZ	2.20	0.71
1:D:274:LEU:H	1:D:274:LEU:HD12	1.54	0.70
1:D:59:ARG:HG2	1:D:82:ARG:CZ	2.22	0.70
1:E:59:ARG:HG2	1:E:82:ARG:CZ	2.21	0.70
1:F:274:LEU:H	1:F:274:LEU:HD12	1.57	0.70
1:B:283:ILE:O	1:B:283:ILE:HG22	1.91	0.70
1:B:211:ALA:CB	1:B:224:LEU:HD13	2.20	0.70
1:C:92:ILE:CG2	1:C:97:VAL:CG2	2.68	0.70
1:F:54:SER:HB2	1:F:56:LYS:H	1.56	0.70
1:D:242:SER:C	1:D:243:ASN:HD22	1.94	0.70
1:D:176:LEU:HD23	1:D:176:LEU:O	1.90	0.70
1:E:92:ILE:CG2	1:E:97:VAL:CG2	2.68	0.70
1:D:54:SER:HB2	1:D:56:LYS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:SER:HB2	1:E:56:LYS:H	1.57	0.69
1:A:87:VAL:HG21	1:F:223:LEU:HA	1.72	0.69
1:E:211:ALA:CB	1:E:224:LEU:HD13	2.19	0.69
1:B:54:SER:HB2	1:B:56:LYS:H	1.57	0.69
1:A:54:SER:HB2	1:A:56:LYS:H	1.58	0.69
1:C:54:SER:HB2	1:C:56:LYS:H	1.55	0.69
1:D:196:LEU:CD2	1:D:200:LEU:HD11	2.23	0.69
1:F:242:SER:C	1:F:243:ASN:HD22	1.96	0.69
1:B:47:ILE:HD13	1:B:50:ASP:OD2	1.93	0.68
1:B:47:ILE:HD12	1:B:47:ILE:N	2.07	0.68
1:A:47:ILE:N	1:A:47:ILE:HD12	2.08	0.68
1:C:183:ALA:O	1:C:187:GLU:HG3	1.94	0.68
1:A:274:LEU:HD12	1:A:274:LEU:H	1.57	0.68
1:C:16:LEU:HD22	1:C:39:CYS:SG	2.34	0.68
1:D:283:ILE:O	1:D:283:ILE:HG22	1.94	0.68
1:B:283:ILE:O	1:B:283:ILE:CG2	2.41	0.67
1:B:242:SER:C	1:B:243:ASN:HD22	1.96	0.67
1:B:274:LEU:H	1:B:274:LEU:HD12	1.59	0.67
1:E:274:LEU:HD12	1:E:274:LEU:H	1.58	0.67
1:D:223:LEU:HA	1:E:87:VAL:HG21	1.76	0.67
1:A:242:SER:C	1:A:243:ASN:HD22	1.97	0.67
1:F:92:ILE:CG2	1:F:97:VAL:CG2	2.69	0.67
1:A:16:LEU:HD22	1:A:39:CYS:SG	2.34	0.67
1:D:92:ILE:CG2	1:D:97:VAL:CG2	2.68	0.66
1:A:176:LEU:HD23	1:A:176:LEU:O	1.96	0.66
1:E:196:LEU:CD2	1:E:200:LEU:HD11	2.26	0.66
1:B:196:LEU:CD2	1:B:200:LEU:HD11	2.26	0.66
1:C:47:ILE:HD12	1:C:47:ILE:N	2.09	0.65
1:A:196:LEU:CD2	1:A:200:LEU:HD11	2.26	0.65
1:F:196:LEU:CD2	1:F:200:LEU:HD11	2.27	0.65
1:F:16:LEU:HD22	1:F:39:CYS:SG	2.37	0.65
1:D:183:ALA:O	1:D:187:GLU:HG3	1.97	0.65
1:C:156:VAL:O	1:C:160:VAL:HG13	1.97	0.64
1:E:223:LEU:HA	1:F:87:VAL:HG21	1.79	0.64
1:E:242:SER:C	1:E:243:ASN:HD22	2.00	0.64
1:D:47:ILE:O	1:D:51:MET:HG3	1.98	0.64
1:B:16:LEU:HD22	1:B:39:CYS:SG	2.38	0.64
1:E:183:ALA:O	1:E:187:GLU:HG3	1.96	0.64
1:A:234:VAL:HG11	1:A:238:ILE:CD1	2.28	0.64
1:A:211:ALA:CB	1:A:224:LEU:HD13	2.25	0.64
1:E:234:VAL:HG11	1:E:238:ILE:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:O	1:C:14:GLN:HB2	1.98	0.64
1:F:47:ILE:N	1:F:47:ILE:HD12	2.12	0.63
1:D:47:ILE:HD12	1:D:47:ILE:N	2.12	0.63
1:A:122:VAL:HG13	1:A:123:PRO:HD2	1.80	0.63
1:A:183:ALA:O	1:A:187:GLU:HG3	1.98	0.63
1:A:92:ILE:CG2	1:A:97:VAL:CG2	2.70	0.63
1:F:183:ALA:O	1:F:187:GLU:HG3	1.98	0.63
1:B:183:ALA:O	1:B:187:GLU:HG3	1.97	0.63
1:D:234:VAL:HG11	1:D:238:ILE:CD1	2.28	0.63
1:C:242:SER:C	1:C:243:ASN:HD22	2.02	0.63
1:E:47:ILE:HD12	1:E:47:ILE:N	2.10	0.63
1:F:176:LEU:HD23	1:F:176:LEU:O	1.98	0.63
1:A:174:GLN:CA	1:A:200:LEU:HD22	2.29	0.63
1:C:196:LEU:CD2	1:C:200:LEU:HD11	2.27	0.63
1:D:283:ILE:CG2	1:D:283:ILE:O	2.46	0.63
1:B:29:GLN:HG2	1:B:239:PHE:CZ	2.34	0.62
1:A:10:SER:O	1:A:14:GLN:HB2	1.99	0.62
1:D:122:VAL:HG13	1:D:123:PRO:HD2	1.81	0.62
1:C:199:VAL:O	1:C:203:GLY:N	2.32	0.62
1:B:174:GLN:CA	1:B:200:LEU:HD22	2.29	0.62
1:E:174:GLN:CA	1:E:200:LEU:HD22	2.28	0.62
1:D:250:ALA:HB1	1:D:267:VAL:HG23	1.82	0.62
1:F:174:GLN:CA	1:F:200:LEU:HD22	2.29	0.62
1:C:223:LEU:HA	1:D:87:VAL:HG21	1.80	0.62
1:B:176:LEU:HD23	1:B:176:LEU:O	2.00	0.62
1:B:199:VAL:O	1:B:203:GLY:N	2.31	0.62
1:E:72:SER:O	1:E:73:VAL:HG12	1.99	0.61
1:E:122:VAL:HG13	1:E:123:PRO:HD2	1.81	0.61
1:D:199:VAL:O	1:D:203:GLY:N	2.33	0.61
1:B:122:VAL:HG13	1:B:123:PRO:HD2	1.81	0.61
1:D:174:GLN:CA	1:D:200:LEU:HD22	2.30	0.61
1:B:44:LEU:HD12	1:B:44:LEU:O	2.00	0.61
1:E:16:LEU:HD22	1:E:39:CYS:SG	2.41	0.61
1:C:174:GLN:CA	1:C:200:LEU:HD22	2.30	0.61
1:C:160:VAL:HG22	1:C:161:LYS:N	2.16	0.61
1:E:149:GLY:HA2	1:E:158:GLU:HB3	1.82	0.61
1:E:176:LEU:HD23	1:E:176:LEU:C	2.22	0.60
1:C:149:GLY:HA2	1:C:158:GLU:HB3	1.82	0.60
1:F:149:GLY:HA2	1:F:158:GLU:HB3	1.83	0.60
1:C:176:LEU:HD23	1:C:176:LEU:O	2.00	0.60
1:E:199:VAL:O	1:E:203:GLY:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ASN:HB3	1:F:263:LYS:HB3	1.84	0.60
1:E:93:GLU:CG	1:E:122:VAL:HG23	2.32	0.60
1:B:93:GLU:CG	1:B:122:VAL:HG23	2.31	0.60
1:B:149:GLY:HA2	1:B:158:GLU:HB3	1.82	0.60
1:C:122:VAL:HG13	1:C:123:PRO:HD2	1.82	0.60
1:B:191:VAL:HG13	1:B:192:PRO:HD2	1.84	0.60
1:A:149:GLY:HA2	1:A:158:GLU:HB3	1.82	0.60
1:B:260:ASN:HB3	1:B:263:LYS:HB3	1.84	0.60
1:F:122:VAL:HG13	1:F:123:PRO:HD2	1.83	0.60
1:E:10:SER:O	1:E:14:GLN:HB2	2.01	0.60
1:B:92:ILE:O	1:B:97:VAL:HG22	2.02	0.60
1:B:223:LEU:HA	1:C:87:VAL:HG21	1.83	0.60
1:D:149:GLY:HA2	1:D:158:GLU:HB3	1.83	0.60
1:C:92:ILE:O	1:C:97:VAL:HG22	2.02	0.60
1:C:234:VAL:HG11	1:C:238:ILE:CD1	2.32	0.60
1:C:191:VAL:HG13	1:C:192:PRO:HD2	1.84	0.60
1:F:70:MET:HE1	1:F:97:VAL:HG13	1.84	0.59
1:D:250:ALA:CB	1:D:267:VAL:HG23	2.32	0.59
1:D:16:LEU:HD22	1:D:39:CYS:SG	2.41	0.59
1:E:260:ASN:HB3	1:E:263:LYS:HB3	1.83	0.59
1:B:217:THR:HG21	1:C:59:ARG:HD2	1.83	0.59
1:A:260:ASN:HB3	1:A:263:LYS:HB3	1.84	0.59
1:A:199:VAL:O	1:A:203:GLY:N	2.34	0.59
1:C:260:ASN:HB3	1:C:263:LYS:HB3	1.84	0.59
1:A:280:ILE:CG2	1:A:281:GLU:N	2.66	0.59
1:D:260:ASN:HB3	1:D:263:LYS:HB3	1.84	0.59
1:D:112:THR:HG22	1:D:113:HIS:CD2	2.37	0.59
1:C:62:ASP:O	1:C:65:MET:HB3	2.02	0.59
1:B:47:ILE:O	1:B:51:MET:HG3	2.02	0.59
1:D:72:SER:O	1:D:73:VAL:HG12	2.03	0.59
1:F:156:VAL:O	1:F:160:VAL:HG13	2.03	0.59
1:E:44:LEU:HD13	1:E:46:SER:O	2.02	0.59
1:E:155:ASP:HB3	1:E:280:ILE:HD12	1.85	0.59
1:F:199:VAL:O	1:F:203:GLY:N	2.35	0.58
1:A:156:VAL:O	1:A:157:SER:C	2.41	0.58
1:B:72:SER:O	1:B:73:VAL:HG12	2.02	0.58
1:D:176:LEU:HD23	1:D:176:LEU:C	2.23	0.58
1:C:160:VAL:CG2	1:C:161:LYS:N	2.67	0.58
1:F:62:ASP:O	1:F:65:MET:HB3	2.04	0.58
1:A:160:VAL:HG22	1:A:161:LYS:N	2.19	0.58
1:F:44:LEU:HD13	1:F:46:SER:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ALA:HB1	1:B:267:VAL:HG23	1.86	0.58
1:D:44:LEU:HD12	1:D:44:LEU:O	2.03	0.58
1:D:160:VAL:HG22	1:D:161:LYS:N	2.17	0.58
1:B:234:VAL:HG11	1:B:238:ILE:CD1	2.34	0.58
1:C:44:LEU:HD13	1:C:46:SER:O	2.03	0.58
1:B:70:MET:HE1	1:B:97:VAL:HG13	1.86	0.57
1:B:156:VAL:O	1:B:160:VAL:HG13	2.04	0.57
1:E:92:ILE:O	1:E:97:VAL:HG22	2.04	0.57
1:A:93:GLU:CG	1:A:122:VAL:HG23	2.35	0.57
1:A:250:ALA:HB1	1:A:267:VAL:HG23	1.87	0.57
1:F:112:THR:HG22	1:F:113:HIS:CD2	2.39	0.57
1:D:62:ASP:O	1:D:65:MET:HB3	2.04	0.57
1:D:242:SER:C	1:D:243:ASN:ND2	2.58	0.57
1:E:44:LEU:HD12	1:E:44:LEU:O	2.04	0.57
1:A:44:LEU:O	1:A:44:LEU:HD12	2.04	0.57
1:A:44:LEU:HD13	1:A:46:SER:O	2.04	0.57
1:F:280:ILE:CG2	1:F:281:GLU:N	2.65	0.57
1:A:176:LEU:HD23	1:A:176:LEU:C	2.24	0.57
1:B:45:GLU:HA	1:B:65:MET:HE3	1.85	0.57
1:D:280:ILE:CG2	1:D:281:GLU:N	2.68	0.57
1:D:93:GLU:CG	1:D:122:VAL:HG23	2.35	0.57
1:B:62:ASP:O	1:B:65:MET:HB3	2.04	0.57
1:C:250:ALA:HB1	1:C:267:VAL:HG23	1.86	0.57
1:A:191:VAL:HG13	1:A:192:PRO:HD2	1.86	0.57
1:E:156:VAL:O	1:E:160:VAL:HG13	2.05	0.57
1:D:155:ASP:HB3	1:D:280:ILE:HD12	1.87	0.57
1:B:160:VAL:HG22	1:B:161:LYS:N	2.20	0.56
1:C:160:VAL:O	1:C:163:ILE:HG22	2.03	0.56
1:B:29:GLN:HG2	1:B:239:PHE:CE1	2.40	0.56
1:C:250:ALA:CB	1:C:267:VAL:HG23	2.35	0.56
1:B:250:ALA:CB	1:B:267:VAL:HG23	2.35	0.56
1:E:62:ASP:O	1:E:65:MET:HB3	2.05	0.56
1:A:62:ASP:O	1:A:65:MET:HB3	2.05	0.56
1:A:104:GLU:OE2	1:A:146:ARG:NH2	2.38	0.56
1:B:24:VAL:HG11	1:B:30:ALA:HA	1.88	0.56
1:A:155:ASP:HB3	1:A:280:ILE:HD12	1.87	0.56
1:F:93:GLU:CG	1:F:122:VAL:HG23	2.35	0.56
1:A:250:ALA:CB	1:A:267:VAL:HG23	2.36	0.56
1:D:32:ILE:HG23	1:D:245:VAL:HG22	1.86	0.56
1:F:176:LEU:HD23	1:F:176:LEU:C	2.26	0.56
1:A:87:VAL:CG2	1:F:223:LEU:HA	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:GLU:HA	1:F:65:MET:HE3	1.87	0.56
1:C:54:SER:HB2	1:C:56:LYS:N	2.20	0.56
1:A:21:ILE:HD11	1:A:210:PHE:CE2	2.41	0.56
1:D:156:VAL:O	1:D:160:VAL:HG13	2.06	0.56
1:E:280:ILE:CG2	1:E:281:GLU:N	2.68	0.56
1:A:92:ILE:O	1:A:97:VAL:HG22	2.06	0.55
1:E:54:SER:HB2	1:E:56:LYS:N	2.22	0.55
1:F:234:VAL:HG11	1:F:238:ILE:CD1	2.36	0.55
1:C:93:GLU:CG	1:C:122:VAL:HG23	2.35	0.55
1:C:29:GLN:HG2	1:C:239:PHE:CE1	2.41	0.55
1:A:112:THR:HG22	1:A:113:HIS:CD2	2.41	0.55
1:C:70:MET:HE1	1:C:97:VAL:HG13	1.88	0.55
1:E:160:VAL:HG22	1:E:161:LYS:N	2.21	0.55
1:A:47:ILE:O	1:A:51:MET:HG3	2.06	0.55
1:E:47:ILE:O	1:E:51:MET:HG3	2.05	0.55
1:D:44:LEU:HD13	1:D:46:SER:O	2.07	0.55
1:B:112:THR:HG22	1:B:113:HIS:CD2	2.41	0.55
1:E:191:VAL:HG13	1:E:192:PRO:HD2	1.87	0.55
1:A:242:SER:C	1:A:243:ASN:ND2	2.60	0.55
1:C:32:ILE:HG23	1:C:245:VAL:HG22	1.87	0.55
1:F:51:MET:HE2	1:F:58:CYS:HB3	1.87	0.55
1:F:242:SER:C	1:F:243:ASN:ND2	2.59	0.55
1:D:37:GLY:HA3	1:D:252:VAL:HG11	1.88	0.55
1:E:160:VAL:O	1:E:163:ILE:HG22	2.07	0.55
1:C:37:GLY:HA3	1:C:252:VAL:HG11	1.89	0.55
1:C:72:SER:O	1:C:73:VAL:HG12	2.06	0.55
1:E:66:ILE:HG22	1:E:70:MET:HE3	1.89	0.55
1:C:47:ILE:O	1:C:51:MET:HG3	2.06	0.55
1:D:235:GLY:O	1:D:236:SER:C	2.45	0.55
1:B:155:ASP:HB3	1:B:280:ILE:HD12	1.87	0.55
1:F:191:VAL:HG13	1:F:192:PRO:HD2	1.87	0.55
1:D:29:GLN:HG2	1:D:239:PHE:CZ	2.42	0.55
1:C:112:THR:HG22	1:C:113:HIS:CD2	2.42	0.55
1:D:92:ILE:O	1:D:97:VAL:HG22	2.06	0.55
1:F:155:ASP:HB3	1:F:280:ILE:HD12	1.88	0.55
1:E:112:THR:HG22	1:E:113:HIS:CD2	2.42	0.55
1:F:21:ILE:HD11	1:F:210:PHE:CE2	2.41	0.55
1:B:160:VAL:CG2	1:B:161:LYS:N	2.70	0.55
1:D:160:VAL:CG2	1:D:161:LYS:N	2.70	0.55
1:F:54:SER:HB2	1:F:56:LYS:N	2.22	0.55
1:B:280:ILE:CG2	1:B:281:GLU:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:SER:C	1:B:243:ASN:ND2	2.60	0.55
1:E:250:ALA:HB1	1:E:267:VAL:HG23	1.88	0.55
1:E:70:MET:HE1	1:E:97:VAL:HG13	1.89	0.54
1:A:160:VAL:CG2	1:A:161:LYS:N	2.70	0.54
1:F:47:ILE:O	1:F:51:MET:HG3	2.06	0.54
1:A:59:ARG:HD2	1:F:217:THR:HG21	1.89	0.54
1:C:45:GLU:HA	1:C:65:MET:HE3	1.89	0.54
1:B:54:SER:HB2	1:B:56:LYS:N	2.22	0.54
1:A:54:SER:HB2	1:A:56:LYS:N	2.22	0.54
1:C:176:LEU:HD23	1:C:176:LEU:C	2.28	0.54
1:D:54:SER:HB2	1:D:56:LYS:N	2.22	0.54
1:A:223:LEU:HA	1:B:87:VAL:HG21	1.90	0.54
1:F:92:ILE:O	1:F:97:VAL:HG22	2.08	0.54
1:F:234:VAL:HG12	1:F:235:GLY:N	2.23	0.54
1:C:195:LEU:O	1:C:196:LEU:C	2.46	0.54
1:B:44:LEU:HD13	1:B:46:SER:O	2.07	0.54
1:D:21:ILE:HD11	1:D:210:PHE:CE2	2.42	0.54
1:E:29:GLN:HG2	1:E:239:PHE:CE1	2.42	0.54
1:E:21:ILE:HD11	1:E:210:PHE:CE2	2.42	0.54
1:F:160:VAL:HG22	1:F:161:LYS:N	2.22	0.54
1:F:72:SER:O	1:F:73:VAL:HG12	2.07	0.54
1:D:80:LYS:HB3	1:D:106:LEU:HD11	1.89	0.54
1:C:21:ILE:HD11	1:C:210:PHE:CE2	2.42	0.54
1:F:104:GLU:OE2	1:F:146:ARG:NH2	2.41	0.54
1:D:45:GLU:HA	1:D:65:MET:HE3	1.90	0.54
1:A:37:GLY:HA3	1:A:252:VAL:HG11	1.89	0.54
1:E:37:GLY:HA3	1:E:252:VAL:HG11	1.90	0.54
1:C:104:GLU:OE2	1:C:146:ARG:NH2	2.40	0.53
1:B:176:LEU:HD23	1:B:176:LEU:C	2.27	0.53
1:E:250:ALA:CB	1:E:267:VAL:HG23	2.39	0.53
1:A:45:GLU:HA	1:A:65:MET:HE3	1.89	0.53
1:A:72:SER:O	1:A:73:VAL:HG12	2.08	0.53
1:F:29:GLN:HG2	1:F:239:PHE:CZ	2.44	0.53
1:D:191:VAL:HG13	1:D:192:PRO:HD2	1.90	0.53
1:B:101:ASP:HA	1:B:125:VAL:HG13	1.90	0.53
1:F:160:VAL:O	1:F:163:ILE:HG22	2.08	0.53
1:B:21:ILE:HD11	1:B:210:PHE:CE2	2.44	0.53
1:E:101:ASP:HA	1:E:125:VAL:HG13	1.90	0.53
1:A:70:MET:HE1	1:A:97:VAL:HG13	1.90	0.53
1:A:29:GLN:HG2	1:A:239:PHE:CE1	2.43	0.53
1:A:160:VAL:O	1:A:163:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:O	1:B:163:ILE:HG22	2.08	0.53
1:B:93:GLU:HG3	1:B:122:VAL:HG23	1.91	0.53
1:E:5:ASP:N	1:E:5:ASP:OD1	2.38	0.53
1:E:195:LEU:O	1:E:196:LEU:C	2.46	0.53
1:F:37:GLY:HA3	1:F:252:VAL:HG11	1.90	0.53
1:D:29:GLN:HG2	1:D:239:PHE:CE1	2.44	0.53
1:B:104:GLU:OE2	1:B:146:ARG:NH2	2.42	0.53
1:C:155:ASP:HB3	1:C:280:ILE:HD12	1.90	0.52
1:C:242:SER:C	1:C:243:ASN:ND2	2.62	0.52
1:D:70:MET:HE1	1:D:97:VAL:HG13	1.90	0.52
1:A:156:VAL:O	1:A:160:VAL:HG13	2.08	0.52
1:D:195:LEU:O	1:D:196:LEU:C	2.47	0.52
1:D:150:GLU:HB3	1:D:153:THR:HG21	1.92	0.52
1:B:45:GLU:HG2	1:B:61:SER:OG	2.10	0.52
1:C:5:ASP:N	1:C:5:ASP:OD1	2.36	0.52
1:E:242:SER:C	1:E:243:ASN:ND2	2.63	0.52
1:E:45:GLU:HA	1:E:65:MET:HE3	1.92	0.52
1:D:217:THR:HG21	1:E:59:ARG:HD2	1.91	0.52
1:C:44:LEU:O	1:C:44:LEU:HD12	2.09	0.52
1:A:45:GLU:HG2	1:A:61:SER:OG	2.10	0.52
1:F:195:LEU:O	1:F:196:LEU:C	2.48	0.52
1:A:193:VAL:O	1:A:197:LYS:HB2	2.10	0.52
1:C:80:LYS:HB3	1:C:106:LEU:HD11	1.92	0.52
1:F:66:ILE:HG22	1:F:70:MET:HE3	1.92	0.52
1:A:47:ILE:H	1:A:47:ILE:CD1	2.15	0.52
1:E:160:VAL:CG2	1:E:161:LYS:N	2.72	0.51
1:B:37:GLY:HA3	1:B:252:VAL:HG11	1.91	0.51
1:E:72:SER:C	1:E:73:VAL:CG1	2.78	0.51
1:C:193:VAL:O	1:C:197:LYS:HB2	2.10	0.51
1:E:63:PRO:O	1:E:64:LYS:C	2.48	0.51
1:B:32:ILE:HG23	1:B:245:VAL:HG22	1.91	0.51
1:B:195:LEU:O	1:B:196:LEU:C	2.49	0.51
1:A:29:GLN:HG2	1:A:239:PHE:CZ	2.46	0.51
1:F:156:VAL:O	1:F:157:SER:C	2.48	0.51
1:B:235:GLY:O	1:B:236:SER:C	2.49	0.51
1:A:195:LEU:O	1:A:196:LEU:C	2.48	0.51
1:B:93:GLU:HG2	1:B:122:VAL:HG23	1.93	0.51
1:D:72:SER:C	1:D:73:VAL:CG1	2.79	0.51
1:B:80:LYS:HB3	1:B:106:LEU:HD11	1.92	0.51
1:D:193:VAL:O	1:D:197:LYS:HB2	2.11	0.51
1:F:250:ALA:CB	1:F:267:VAL:HG23	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:GLY:O	1:F:236:SER:C	2.48	0.51
1:A:80:LYS:HB3	1:A:106:LEU:HD11	1.93	0.51
1:E:122:VAL:CG1	1:E:123:PRO:HD2	2.41	0.51
1:E:93:GLU:HG3	1:E:122:VAL:HG23	1.92	0.51
1:F:250:ALA:HB1	1:F:267:VAL:HG23	1.91	0.51
1:E:47:ILE:H	1:E:47:ILE:CD1	2.17	0.51
1:D:280:ILE:O	1:D:283:ILE:HB	2.11	0.51
1:B:5:ASP:N	1:B:5:ASP:OD1	2.43	0.51
1:A:95:LEU:O	1:A:96:GLU:HB2	2.11	0.51
1:D:160:VAL:O	1:D:163:ILE:HG22	2.11	0.51
1:A:234:VAL:HG12	1:A:235:GLY:N	2.26	0.51
1:A:235:GLY:O	1:A:236:SER:C	2.49	0.51
1:D:122:VAL:CG1	1:D:123:PRO:HD2	2.41	0.51
1:E:193:VAL:O	1:E:197:LYS:HB2	2.11	0.50
1:B:95:LEU:O	1:B:96:GLU:HB2	2.10	0.50
1:F:66:ILE:HG22	1:F:70:MET:CE	2.42	0.50
1:A:211:ALA:HB2	1:A:229:CYS:SG	2.52	0.50
1:C:51:MET:HB3	1:C:58:CYS:SG	2.51	0.50
1:D:45:GLU:HG2	1:D:61:SER:OG	2.11	0.50
1:D:101:ASP:HA	1:D:125:VAL:HG13	1.93	0.50
1:C:280:ILE:O	1:C:283:ILE:HB	2.12	0.50
1:C:223:LEU:HA	1:D:87:VAL:CG2	2.40	0.50
1:B:193:VAL:O	1:B:197:LYS:HB2	2.12	0.50
1:E:211:ALA:HB2	1:E:229:CYS:SG	2.51	0.50
1:A:23:ASP:HB2	1:A:235:GLY:HA2	1.93	0.50
1:F:24:VAL:HG11	1:F:30:ALA:HA	1.93	0.50
1:B:156:VAL:O	1:B:157:SER:C	2.49	0.50
1:B:72:SER:C	1:B:73:VAL:CG1	2.80	0.50
1:E:47:ILE:CG2	1:E:236:SER:HB3	2.41	0.50
1:E:51:MET:HB3	1:E:58:CYS:SG	2.52	0.50
1:B:66:ILE:HG22	1:B:70:MET:CE	2.42	0.50
1:E:95:LEU:O	1:E:96:GLU:HB2	2.11	0.50
1:E:32:ILE:HG23	1:E:245:VAL:HG22	1.93	0.50
1:A:101:ASP:HA	1:A:125:VAL:HG13	1.93	0.50
1:F:160:VAL:CG2	1:F:161:LYS:N	2.74	0.49
1:E:156:VAL:O	1:E:157:SER:C	2.48	0.49
1:C:156:VAL:O	1:C:157:SER:C	2.51	0.49
1:B:47:ILE:CG2	1:B:236:SER:HB3	2.42	0.49
1:D:51:MET:HE2	1:D:58:CYS:HB3	1.94	0.49
1:E:223:LEU:HA	1:F:87:VAL:CG2	2.42	0.49
1:C:29:GLN:HG2	1:C:239:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLU:HB3	1:B:153:THR:HG21	1.93	0.49
1:D:95:LEU:O	1:D:96:GLU:HB2	2.11	0.49
1:D:104:GLU:OE2	1:D:146:ARG:NH2	2.45	0.49
1:E:150:GLU:HB3	1:E:153:THR:HG21	1.94	0.49
1:B:23:ASP:HB2	1:B:235:GLY:HA2	1.94	0.49
1:D:63:PRO:O	1:D:64:LYS:C	2.51	0.49
1:A:32:ILE:HG23	1:A:245:VAL:HG22	1.93	0.49
1:D:156:VAL:O	1:D:157:SER:C	2.51	0.49
1:B:51:MET:HE2	1:B:58:CYS:HB3	1.94	0.49
1:F:47:ILE:CG2	1:F:236:SER:HB3	2.43	0.49
1:B:267:VAL:HG23	1:B:267:VAL:O	2.13	0.49
1:F:193:VAL:O	1:F:197:LYS:HB2	2.11	0.49
1:B:25:VAL:HG12	1:B:26:THR:HG23	1.95	0.49
1:E:104:GLU:OE2	1:E:146:ARG:NH2	2.46	0.49
1:E:235:GLY:O	1:E:236:SER:C	2.50	0.49
1:A:5:ASP:N	1:A:5:ASP:OD1	2.37	0.49
1:D:267:VAL:O	1:D:267:VAL:HG23	2.11	0.49
1:F:72:SER:C	1:F:73:VAL:CG1	2.80	0.49
1:A:150:GLU:HB3	1:A:153:THR:HG21	1.93	0.49
1:E:234:VAL:HG11	1:E:238:ILE:HD12	1.93	0.49
1:D:93:GLU:HG3	1:D:122:VAL:HG23	1.94	0.49
1:A:234:VAL:HG11	1:A:238:ILE:HD12	1.93	0.49
1:A:47:ILE:CG2	1:A:236:SER:HB3	2.43	0.49
1:E:51:MET:HE2	1:E:58:CYS:HB3	1.94	0.49
1:E:93:GLU:HG2	1:E:122:VAL:HG23	1.94	0.49
1:C:72:SER:C	1:C:73:VAL:CG1	2.81	0.49
1:E:29:GLN:HG2	1:E:239:PHE:CZ	2.47	0.49
1:F:101:ASP:HA	1:F:125:VAL:HG13	1.93	0.49
1:D:5:ASP:OD1	1:D:5:ASP:N	2.45	0.49
1:B:63:PRO:O	1:B:64:LYS:C	2.51	0.49
1:B:234:VAL:HG12	1:B:235:GLY:N	2.27	0.49
1:B:47:ILE:H	1:B:47:ILE:CD1	2.15	0.49
1:F:280:ILE:O	1:F:283:ILE:HB	2.13	0.49
1:E:223:LEU:CA	1:F:87:VAL:HG21	2.42	0.49
1:E:45:GLU:HG2	1:E:61:SER:OG	2.13	0.49
1:A:237:GLY:HA3	1:A:240:LYS:HB2	1.95	0.49
1:F:23:ASP:HB2	1:F:235:GLY:HA2	1.95	0.48
1:E:280:ILE:O	1:E:283:ILE:HB	2.12	0.48
1:A:66:ILE:HG22	1:A:70:MET:HE3	1.95	0.48
1:D:47:ILE:CG2	1:D:236:SER:HB3	2.43	0.48
1:A:122:VAL:CG1	1:A:123:PRO:HD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLU:HG2	1:C:61:SER:OG	2.12	0.48
1:A:93:GLU:HG2	1:A:122:VAL:HG23	1.95	0.48
1:D:267:VAL:O	1:D:267:VAL:CG2	2.60	0.48
1:C:237:GLY:HA3	1:C:240:LYS:HB2	1.95	0.48
1:A:63:PRO:O	1:A:64:LYS:C	2.50	0.48
1:D:237:GLY:HA3	1:D:240:LYS:HB2	1.94	0.48
1:A:23:ASP:HB2	1:A:235:GLY:CA	2.43	0.48
1:E:51:MET:O	1:E:54:SER:OG	2.32	0.48
1:D:51:MET:HB3	1:D:58:CYS:SG	2.54	0.48
1:F:9:LYS:NZ	1:F:120:PHE:O	2.37	0.48
1:B:280:ILE:O	1:B:283:ILE:HB	2.13	0.48
1:F:44:LEU:C	1:F:44:LEU:HD12	2.34	0.48
1:B:122:VAL:CG1	1:B:123:PRO:HD2	2.42	0.48
1:C:93:GLU:HG2	1:C:122:VAL:HG23	1.95	0.48
1:C:235:GLY:O	1:C:236:SER:C	2.52	0.48
1:A:150:GLU:HB3	1:A:153:THR:CG2	2.44	0.48
1:D:66:ILE:HG22	1:D:70:MET:HE3	1.95	0.48
1:A:51:MET:HE2	1:A:58:CYS:HB3	1.96	0.48
1:F:45:GLU:HG2	1:F:61:SER:OG	2.13	0.48
1:C:63:PRO:O	1:C:64:LYS:C	2.51	0.48
1:B:196:LEU:O	1:B:200:LEU:HG	2.14	0.48
1:D:23:ASP:HB2	1:D:235:GLY:HA2	1.95	0.48
1:A:280:ILE:O	1:A:283:ILE:HB	2.14	0.48
1:F:80:LYS:HB3	1:F:106:LEU:HD11	1.95	0.48
1:C:47:ILE:CG2	1:C:236:SER:HB3	2.43	0.48
1:D:234:VAL:HG11	1:D:238:ILE:HD12	1.94	0.48
1:A:234:VAL:HG21	1:A:251:VAL:HG11	1.96	0.47
1:C:223:LEU:CA	1:D:87:VAL:HG21	2.43	0.47
1:F:93:GLU:HG2	1:F:122:VAL:HG23	1.96	0.47
1:C:51:MET:HE2	1:C:58:CYS:HB3	1.95	0.47
1:D:47:ILE:CD1	1:D:47:ILE:H	2.20	0.47
1:A:260:ASN:O	1:A:261:PRO:C	2.52	0.47
1:B:237:GLY:HA3	1:B:240:LYS:HB2	1.95	0.47
1:F:5:ASP:OD1	1:F:5:ASP:N	2.46	0.47
1:B:51:MET:O	1:B:54:SER:OG	2.33	0.47
1:B:40:ALA:HB2	1:B:76:PRO:HG2	1.96	0.47
1:E:237:GLY:HA3	1:E:240:LYS:HB2	1.95	0.47
1:B:66:ILE:HG22	1:B:70:MET:HE3	1.96	0.47
1:C:51:MET:O	1:C:54:SER:OG	2.32	0.47
1:E:234:VAL:HG12	1:E:235:GLY:N	2.28	0.47
1:C:93:GLU:HG3	1:C:122:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLU:OE2	1:B:115:ILE:HG13	2.14	0.47
1:B:23:ASP:HB2	1:B:235:GLY:CA	2.45	0.47
1:A:51:MET:HB3	1:A:58:CYS:SG	2.54	0.47
1:A:217:THR:HG21	1:B:59:ARG:HD2	1.96	0.47
1:D:72:SER:C	1:D:73:VAL:HG12	2.35	0.47
1:F:40:ALA:HB2	1:F:76:PRO:HG2	1.97	0.47
1:E:24:VAL:HG11	1:E:30:ALA:HA	1.95	0.47
1:C:122:VAL:CG1	1:C:123:PRO:HD2	2.44	0.47
1:B:267:VAL:O	1:B:267:VAL:CG2	2.61	0.47
1:C:234:VAL:HG21	1:C:251:VAL:HG11	1.96	0.47
1:A:87:VAL:HG21	1:F:223:LEU:CA	2.42	0.47
1:E:72:SER:C	1:E:73:VAL:HG12	2.35	0.47
1:F:122:VAL:CG1	1:F:123:PRO:HD2	2.44	0.47
1:C:267:VAL:HG23	1:C:267:VAL:O	2.15	0.47
1:F:29:GLN:HG2	1:F:239:PHE:CE1	2.50	0.47
1:D:101:ASP:CB	1:D:125:VAL:HG13	2.44	0.47
1:F:95:LEU:O	1:F:96:GLU:HB2	2.14	0.47
1:C:101:ASP:HA	1:C:125:VAL:HG13	1.96	0.47
1:B:29:GLN:HG2	1:B:239:PHE:CE2	2.49	0.47
1:F:93:GLU:HG3	1:F:122:VAL:HG23	1.96	0.47
1:D:150:GLU:HB3	1:D:153:THR:CG2	2.44	0.47
1:B:150:GLU:HB3	1:B:153:THR:CG2	2.44	0.47
1:C:23:ASP:HB2	1:C:235:GLY:HA2	1.97	0.47
1:F:196:LEU:O	1:F:200:LEU:HG	2.15	0.47
1:A:100:ILE:O	1:A:125:VAL:HG12	2.14	0.47
1:D:28:GLU:O	1:D:32:ILE:HG12	2.15	0.47
1:C:47:ILE:H	1:C:47:ILE:CD1	2.17	0.47
1:F:234:VAL:HG21	1:F:251:VAL:HG11	1.96	0.47
1:E:267:VAL:O	1:E:267:VAL:HG23	2.13	0.47
1:C:267:VAL:CG2	1:C:267:VAL:O	2.63	0.47
1:C:150:GLU:HB3	1:C:153:THR:HG21	1.96	0.47
1:F:63:PRO:O	1:F:64:LYS:C	2.53	0.47
1:C:66:ILE:HG22	1:C:70:MET:CE	2.45	0.46
1:C:234:VAL:HG12	1:C:235:GLY:N	2.30	0.46
1:E:80:LYS:HB3	1:E:106:LEU:HD11	1.96	0.46
1:A:93:GLU:HG3	1:A:122:VAL:HG23	1.95	0.46
1:D:234:VAL:HG21	1:D:251:VAL:HG11	1.97	0.46
1:E:150:GLU:HB3	1:E:153:THR:CG2	2.46	0.46
1:F:237:GLY:HA3	1:F:240:LYS:HB2	1.96	0.46
1:F:28:GLU:O	1:F:32:ILE:HG12	2.16	0.46
1:B:216:ALA:HB3	1:C:59:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:VAL:O	1:E:267:VAL:CG2	2.63	0.46
1:C:150:GLU:HB3	1:C:153:THR:CG2	2.46	0.46
1:C:66:ILE:HG22	1:C:70:MET:HE3	1.98	0.46
1:F:70:MET:HE1	1:F:97:VAL:CG1	2.45	0.46
1:A:47:ILE:CD1	1:A:47:ILE:N	2.75	0.46
1:A:196:LEU:O	1:A:200:LEU:HG	2.16	0.46
1:A:72:SER:C	1:A:73:VAL:CG1	2.83	0.46
1:C:95:LEU:O	1:C:96:GLU:HB2	2.14	0.46
1:D:9:LYS:NZ	1:D:120:PHE:O	2.35	0.46
1:F:226:GLN:HB3	1:F:226:GLN:HE21	1.63	0.46
1:D:196:LEU:HD21	1:D:200:LEU:HD11	1.96	0.46
1:D:234:VAL:HG12	1:D:235:GLY:N	2.29	0.46
1:D:101:ASP:HB2	1:D:125:VAL:CG1	2.46	0.46
1:E:14:GLN:HA	1:E:208:VAL:CG2	2.46	0.45
1:D:24:VAL:HG11	1:D:30:ALA:HA	1.97	0.45
1:E:66:ILE:HG22	1:E:70:MET:CE	2.47	0.45
1:E:170:ILE:O	1:E:174:GLN:HB2	2.16	0.45
1:A:170:ILE:O	1:A:174:GLN:HB2	2.15	0.45
1:B:72:SER:C	1:B:73:VAL:HG12	2.36	0.45
1:A:222:ALA:HB3	1:B:87:VAL:HG11	1.99	0.45
1:F:72:SER:C	1:F:73:VAL:HG12	2.36	0.45
1:E:23:ASP:HB2	1:E:235:GLY:HA2	1.97	0.45
1:D:234:VAL:CG1	1:D:238:ILE:HD12	2.46	0.45
1:F:32:ILE:HG23	1:F:245:VAL:HG22	1.96	0.45
1:E:234:VAL:HG21	1:E:251:VAL:HG11	1.97	0.45
1:B:260:ASN:O	1:B:261:PRO:C	2.55	0.45
1:E:234:VAL:CG1	1:E:238:ILE:HD12	2.46	0.45
1:F:23:ASP:HB2	1:F:235:GLY:CA	2.46	0.45
1:D:196:LEU:O	1:D:200:LEU:HG	2.16	0.45
1:D:23:ASP:HB2	1:D:235:GLY:CA	2.47	0.45
1:D:93:GLU:HG2	1:D:122:VAL:HG23	1.97	0.45
1:E:13:ALA:HB1	1:E:144:MET:HB2	1.99	0.45
1:A:102:GLU:OE2	1:A:115:ILE:HG13	2.17	0.45
1:E:23:ASP:HB2	1:E:235:GLY:CA	2.47	0.45
1:C:23:ASP:HB2	1:C:235:GLY:CA	2.47	0.45
1:C:280:ILE:CG2	1:C:281:GLU:N	2.67	0.45
1:D:44:LEU:HD12	1:D:44:LEU:C	2.38	0.45
1:C:72:SER:C	1:C:73:VAL:HG12	2.37	0.45
1:A:66:ILE:HG22	1:A:70:MET:CE	2.47	0.45
1:C:170:ILE:O	1:C:174:GLN:HB2	2.17	0.45
1:B:92:ILE:HG23	1:B:97:VAL:HG22	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ILE:HG22	1:D:70:MET:CE	2.45	0.44
1:D:250:ALA:HB1	1:D:267:VAL:CG2	2.46	0.44
1:A:234:VAL:CG1	1:A:238:ILE:HD12	2.47	0.44
1:D:51:MET:O	1:D:54:SER:OG	2.35	0.44
1:C:208:VAL:HG12	1:C:230:ASP:CB	2.48	0.44
1:A:40:ALA:HB2	1:A:76:PRO:HG2	1.99	0.44
1:B:93:GLU:HG3	1:B:122:VAL:CG2	2.48	0.44
1:B:234:VAL:HG11	1:B:238:ILE:HD12	2.00	0.44
1:C:234:VAL:HG11	1:C:238:ILE:HD12	1.98	0.44
1:A:14:GLN:HA	1:A:208:VAL:CG2	2.47	0.44
1:E:70:MET:CE	1:E:97:VAL:HG13	2.48	0.44
1:E:196:LEU:O	1:E:200:LEU:HG	2.17	0.44
1:C:250:ALA:HB1	1:C:267:VAL:CG2	2.47	0.44
1:C:101:ASP:CB	1:C:125:VAL:HG13	2.48	0.44
1:A:87:VAL:HG11	1:F:222:ALA:HB3	1.98	0.44
1:F:136:ARG:O	1:F:140:GLU:HB2	2.18	0.44
1:B:51:MET:HB3	1:B:58:CYS:SG	2.57	0.44
1:F:260:ASN:O	1:F:261:PRO:C	2.56	0.44
1:A:101:ASP:CB	1:A:125:VAL:HG13	2.48	0.44
1:A:91:ILE:O	1:A:91:ILE:CG2	2.66	0.44
1:E:260:ASN:O	1:E:261:PRO:C	2.56	0.44
1:E:40:ALA:HB2	1:E:76:PRO:HG2	2.00	0.44
1:A:51:MET:O	1:A:54:SER:OG	2.35	0.44
1:F:234:VAL:CG1	1:F:235:GLY:N	2.81	0.44
1:A:24:VAL:HG11	1:A:30:ALA:HA	1.99	0.44
1:B:29:GLN:CG	1:B:239:PHE:CE1	3.01	0.43
1:E:136:ARG:O	1:E:140:GLU:HB2	2.18	0.43
1:C:102:GLU:OE2	1:C:115:ILE:HG13	2.18	0.43
1:F:170:ILE:O	1:F:174:GLN:HB2	2.18	0.43
1:C:196:LEU:O	1:C:200:LEU:HG	2.17	0.43
1:C:280:ILE:O	1:C:281:GLU:C	2.57	0.43
1:B:70:MET:HB3	1:B:77:VAL:HG11	1.99	0.43
1:B:47:ILE:N	1:B:47:ILE:CD1	2.75	0.43
1:D:170:ILE:O	1:D:174:GLN:HB2	2.19	0.43
1:B:101:ASP:CB	1:B:125:VAL:HG13	2.48	0.43
1:E:101:ASP:CB	1:E:125:VAL:HG13	2.47	0.43
1:C:160:VAL:HG22	1:C:161:LYS:H	1.80	0.43
1:F:101:ASP:CB	1:F:125:VAL:HG13	2.48	0.43
1:E:92:ILE:HG22	1:E:100:ILE:HD11	2.01	0.43
1:F:70:MET:HB3	1:F:77:VAL:HG11	1.99	0.43
1:E:93:GLU:HG3	1:E:122:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD12	1:B:44:LEU:C	2.37	0.43
1:C:260:ASN:O	1:C:261:PRO:C	2.57	0.43
1:C:40:ALA:HB2	1:C:76:PRO:HG2	2.00	0.43
1:D:10:SER:O	1:D:14:GLN:HB2	2.19	0.43
1:F:150:GLU:HB3	1:F:153:THR:HG21	2.01	0.43
1:E:100:ILE:O	1:E:125:VAL:HG12	2.19	0.43
1:F:51:MET:O	1:F:54:SER:OG	2.36	0.43
1:B:260:ASN:O	1:B:263:LYS:N	2.51	0.43
1:D:102:GLU:OE2	1:D:115:ILE:HG13	2.19	0.43
1:F:211:ALA:HB2	1:F:229:CYS:SG	2.58	0.43
1:C:101:ASP:HB2	1:C:125:VAL:CG1	2.49	0.43
1:B:208:VAL:HG12	1:B:230:ASP:CB	2.49	0.43
1:D:25:VAL:HG12	1:D:26:THR:HG23	2.00	0.43
1:B:196:LEU:HD21	1:B:200:LEU:HD11	1.98	0.43
1:F:234:VAL:HG11	1:F:238:ILE:HD12	2.01	0.43
1:B:250:ALA:HB1	1:B:267:VAL:CG2	2.48	0.43
1:A:101:ASP:HB2	1:A:125:VAL:CG1	2.48	0.43
1:F:208:VAL:HG12	1:F:230:ASP:CB	2.48	0.43
1:F:51:MET:HB3	1:F:58:CYS:SG	2.58	0.43
1:E:260:ASN:O	1:E:263:LYS:N	2.52	0.43
1:C:260:ASN:O	1:C:263:LYS:N	2.52	0.43
1:F:267:VAL:O	1:F:267:VAL:HG23	2.18	0.43
1:F:150:GLU:HB3	1:F:153:THR:CG2	2.49	0.43
1:F:14:GLN:HA	1:F:208:VAL:HG21	2.01	0.43
1:F:71:ASN:HD22	1:F:71:ASN:HA	1.68	0.43
1:A:182:ILE:O	1:A:183:ALA:C	2.58	0.42
1:C:222:ALA:HB3	1:D:87:VAL:HG11	2.00	0.42
1:B:28:GLU:O	1:B:32:ILE:HG12	2.19	0.42
1:A:91:ILE:O	1:A:91:ILE:HG22	2.18	0.42
1:D:130:ASP:C	1:D:130:ASP:OD1	2.57	0.42
1:B:234:VAL:HG21	1:B:251:VAL:HG11	2.01	0.42
1:E:196:LEU:HD21	1:E:200:LEU:HD11	2.00	0.42
1:D:223:LEU:HA	1:E:87:VAL:CG2	2.46	0.42
1:C:70:MET:HA	1:C:77:VAL:HG21	2.01	0.42
1:D:40:ALA:HB2	1:D:76:PRO:HG2	2.00	0.42
1:E:25:VAL:HG12	1:E:26:THR:HG23	2.02	0.42
1:B:70:MET:HA	1:B:77:VAL:HG21	2.02	0.42
1:A:158:GLU:O	1:A:159:ALA:C	2.57	0.42
1:B:136:ARG:O	1:B:140:GLU:HB2	2.20	0.42
1:A:234:VAL:CG1	1:A:235:GLY:N	2.82	0.42
1:B:182:ILE:O	1:B:183:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLU:HG3	1:D:122:VAL:CG2	2.50	0.42
1:D:263:LYS:O	1:D:267:VAL:HG12	2.18	0.42
1:F:260:ASN:O	1:F:263:LYS:N	2.53	0.42
1:F:101:ASP:HB2	1:F:125:VAL:CG1	2.50	0.42
1:F:25:VAL:HG12	1:F:26:THR:HG23	2.02	0.42
1:E:92:ILE:HG23	1:E:97:VAL:HG22	1.99	0.42
1:C:71:ASN:HA	1:C:71:ASN:HD22	1.67	0.42
1:A:136:ARG:O	1:A:140:GLU:HB2	2.19	0.42
1:E:101:ASP:HB2	1:E:125:VAL:CG1	2.49	0.42
1:C:274:LEU:N	1:C:274:LEU:HD12	2.29	0.42
1:D:271:LEU:HD12	1:D:271:LEU:HA	1.88	0.42
1:A:260:ASN:O	1:A:263:LYS:N	2.53	0.42
1:E:271:LEU:HA	1:E:271:LEU:HD12	1.88	0.42
1:B:70:MET:HE1	1:B:97:VAL:CG1	2.49	0.41
1:C:70:MET:CE	1:C:97:VAL:HG13	2.50	0.41
1:F:70:MET:HA	1:F:77:VAL:HG21	2.02	0.41
1:A:125:VAL:CG2	1:A:146:ARG:HG2	2.50	0.41
1:D:208:VAL:HG12	1:D:230:ASP:CB	2.50	0.41
1:A:196:LEU:HD21	1:A:200:LEU:HD11	2.00	0.41
1:B:170:ILE:O	1:B:174:GLN:HB2	2.20	0.41
1:A:75:ILE:HB	1:A:76:PRO:HD2	2.02	0.41
1:B:160:VAL:HG22	1:B:161:LYS:H	1.84	0.41
1:D:47:ILE:CD1	1:D:47:ILE:N	2.79	0.41
1:D:182:ILE:O	1:D:183:ALA:C	2.59	0.41
1:A:267:VAL:HG23	1:A:267:VAL:O	2.19	0.41
1:A:223:LEU:HA	1:B:87:VAL:CG2	2.49	0.41
1:C:136:ARG:O	1:C:140:GLU:HB2	2.20	0.41
1:A:160:VAL:HG22	1:A:161:LYS:H	1.86	0.41
1:B:75:ILE:HB	1:B:76:PRO:HD2	2.02	0.41
1:B:70:MET:CE	1:B:97:VAL:HG13	2.50	0.41
1:D:70:MET:HA	1:D:77:VAL:HG21	2.03	0.41
1:F:70:MET:CE	1:F:97:VAL:HG13	2.51	0.41
1:A:25:VAL:HG12	1:A:26:THR:HG23	2.02	0.41
1:D:136:ARG:O	1:D:140:GLU:HB2	2.20	0.41
1:F:102:GLU:OE2	1:F:115:ILE:HG13	2.21	0.41
1:B:101:ASP:HB2	1:B:125:VAL:CG1	2.50	0.41
1:F:47:ILE:N	1:F:47:ILE:CD1	2.78	0.41
1:D:196:LEU:CD2	1:D:200:LEU:CD1	2.97	0.41
1:F:105:VAL:O	1:F:105:VAL:HG12	2.21	0.41
1:E:226:GLN:HB3	1:E:226:GLN:HE21	1.65	0.41
1:A:58:CYS:O	1:A:106:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:LYS:O	1:E:267:VAL:HG12	2.21	0.41
1:C:29:GLN:HG2	1:C:239:PHE:CD1	2.56	0.41
1:F:267:VAL:CG2	1:F:267:VAL:O	2.68	0.41
1:A:70:MET:CE	1:A:97:VAL:HG13	2.51	0.41
1:B:211:ALA:HB2	1:B:229:CYS:SG	2.61	0.41
1:C:234:VAL:CG1	1:C:238:ILE:HD12	2.51	0.41
1:D:280:ILE:O	1:D:281:GLU:C	2.58	0.41
1:E:44:LEU:C	1:E:44:LEU:HD12	2.41	0.41
1:A:223:LEU:CA	1:B:87:VAL:HG21	2.50	0.41
1:A:72:SER:C	1:A:73:VAL:HG12	2.40	0.41
1:B:10:SER:O	1:B:14:GLN:HB2	2.21	0.41
1:E:163:ILE:HD13	1:E:229:CYS:HG	1.81	0.41
1:F:182:ILE:O	1:F:183:ALA:C	2.59	0.41
1:A:14:GLN:HA	1:A:208:VAL:HG21	2.03	0.41
1:C:93:GLU:HG3	1:C:122:VAL:CG2	2.51	0.41
1:D:260:ASN:O	1:D:263:LYS:N	2.54	0.40
1:D:75:ILE:HB	1:D:76:PRO:HD2	2.03	0.40
1:C:25:VAL:HG12	1:C:26:THR:HG23	2.03	0.40
1:D:234:VAL:HG11	1:D:238:ILE:HD11	2.01	0.40
1:A:250:ALA:HB1	1:A:267:VAL:CG2	2.49	0.40
1:F:244:PRO:O	1:F:245:VAL:C	2.60	0.40
1:C:138:ILE:HA	1:C:142:ALA:HB3	2.03	0.40
1:E:102:GLU:OE2	1:E:115:ILE:HG13	2.21	0.40
1:A:271:LEU:HA	1:A:271:LEU:HD12	1.92	0.40
1:E:280:ILE:O	1:E:283:ILE:N	2.50	0.40
1:B:82:ARG:HD2	1:B:107:THR:O	2.22	0.40
1:B:223:LEU:HA	1:C:87:VAL:CG2	2.51	0.40
1:C:263:LYS:O	1:C:267:VAL:HG12	2.21	0.40
1:E:58:CYS:O	1:E:106:LEU:HB3	2.22	0.40
1:D:260:ASN:O	1:D:261:PRO:C	2.59	0.40
1:E:208:VAL:HG12	1:E:230:ASP:CB	2.51	0.40
1:E:29:GLN:HG2	1:E:239:PHE:CD1	2.56	0.40
1:F:75:ILE:HB	1:F:76:PRO:HD2	2.04	0.40
1:F:14:GLN:HA	1:F:208:VAL:CG2	2.51	0.40
1:E:70:MET:HA	1:E:77:VAL:HG21	2.04	0.40
1:F:70:MET:CE	1:F:97:VAL:CG1	3.00	0.40
1:E:234:VAL:CG1	1:E:235:GLY:N	2.85	0.40
1:B:169:GLU:O	1:B:170:ILE:C	2.59	0.40
1:D:54:SER:HB2	1:D:56:LYS:CG	2.52	0.40
1:D:243:ASN:N	1:D:243:ASN:ND2	2.69	0.40
1:B:130:ASP:OD1	1:B:130:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ASP:C	1:F:130:ASP:OD1	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PRO:CD	1:F:35:LYS:NZ[3_655]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/297 (94%)	242 (87%)	33 (12%)	4 (1%)	14	50
1	B	279/297 (94%)	239 (86%)	37 (13%)	3 (1%)	17	56
1	C	279/297 (94%)	241 (86%)	35 (12%)	3 (1%)	17	56
1	D	279/297 (94%)	242 (87%)	34 (12%)	3 (1%)	17	56
1	E	279/297 (94%)	238 (85%)	38 (14%)	3 (1%)	17	56
1	F	279/297 (94%)	240 (86%)	35 (12%)	4 (1%)	14	50
All	All	1674/1782 (94%)	1442 (86%)	212 (13%)	20 (1%)	16	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	SER
1	B	236	SER
1	C	236	SER
1	D	236	SER
1	E	236	SER
1	F	236	SER
1	A	244	PRO

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Mol	Chain	Res	Type
1	C	244	PRO
1	F	244	PRO
1	A	280	ILE
1	D	244	PRO
1	D	280	ILE
1	E	244	PRO
1	B	244	PRO
1	E	280	ILE
1	A	245	VAL
1	B	280	ILE
1	C	280	ILE
1	F	245	VAL
1	F	280	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/242 (95%)	195 (85%)	34 (15%)	4 17
1	B	229/242 (95%)	196 (86%)	33 (14%)	4 18
1	C	229/242 (95%)	196 (86%)	33 (14%)	4 18
1	D	229/242 (95%)	196 (86%)	33 (14%)	4 18
1	E	229/242 (95%)	196 (86%)	33 (14%)	4 18
1	F	229/242 (95%)	195 (85%)	34 (15%)	4 17
All	All	1374/1452 (95%)	1174 (85%)	200 (15%)	4 17

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	5	ASP
1	A	14	GLN
1	A	15	MET
1	A	29	GLN

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Mol	Chain	Res	Type
1	A	47	ILE
1	A	52	ARG
1	A	53	LYS
1	A	54	SER
1	A	56	LYS
1	A	71	ASN
1	A	74	SER
1	A	97	VAL
1	A	116	GLU
1	A	129	LYS
1	A	146	ARG
1	A	156	VAL
1	A	157	SER
1	A	163	ILE
1	A	171	LYS
1	A	176	LEU
1	A	178	SER
1	A	179	GLU
1	A	180	ASP
1	A	188	GLU
1	A	190	ARG
1	A	204	LYS
1	A	208	VAL
1	A	241	SER
1	A	267	VAL
1	A	274	LEU
1	A	275	MET
1	A	280	ILE
1	A	283	ILE
1	B	5	ASP
1	B	14	GLN
1	B	15	MET
1	B	29	GLN
1	B	47	ILE
1	B	52	ARG
1	B	53	LYS
1	B	54	SER
1	B	56	LYS
1	B	71	ASN
1	B	74	SER
1	B	97	VAL
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	129	LYS
1	B	146	ARG
1	B	156	VAL
1	B	157	SER
1	B	163	ILE
1	B	171	LYS
1	B	176	LEU
1	B	178	SER
1	B	179	GLU
1	B	180	ASP
1	B	188	GLU
1	B	190	ARG
1	B	204	LYS
1	B	208	VAL
1	B	241	SER
1	B	267	VAL
1	B	274	LEU
1	B	275	MET
1	B	280	ILE
1	B	283	ILE
1	C	4	GLU
1	C	5	ASP
1	C	14	GLN
1	C	29	GLN
1	C	47	ILE
1	C	52	ARG
1	C	53	LYS
1	C	54	SER
1	C	56	LYS
1	C	71	ASN
1	C	74	SER
1	C	97	VAL
1	C	116	GLU
1	C	129	LYS
1	C	146	ARG
1	C	156	VAL
1	C	157	SER
1	C	163	ILE
1	C	171	LYS
1	C	176	LEU
1	C	178	SER
1	C	179	GLU

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Mol	Chain	Res	Type
1	C	180	ASP
1	C	188	GLU
1	C	190	ARG
1	C	204	LYS
1	C	208	VAL
1	C	241	SER
1	C	267	VAL
1	C	274	LEU
1	C	275	MET
1	C	280	ILE
1	C	283	ILE
1	D	5	ASP
1	D	14	GLN
1	D	15	MET
1	D	29	GLN
1	D	47	ILE
1	D	52	ARG
1	D	53	LYS
1	D	54	SER
1	D	56	LYS
1	D	71	ASN
1	D	74	SER
1	D	97	VAL
1	D	116	GLU
1	D	129	LYS
1	D	146	ARG
1	D	156	VAL
1	D	157	SER
1	D	163	ILE
1	D	171	LYS
1	D	176	LEU
1	D	178	SER
1	D	179	GLU
1	D	180	ASP
1	D	188	GLU
1	D	190	ARG
1	D	204	LYS
1	D	208	VAL
1	D	241	SER
1	D	267	VAL
1	D	274	LEU
1	D	275	MET

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Mol	Chain	Res	Type
1	D	280	ILE
1	D	283	ILE
1	E	4	GLU
1	E	5	ASP
1	E	14	GLN
1	E	29	GLN
1	E	47	ILE
1	E	52	ARG
1	E	53	LYS
1	E	54	SER
1	E	56	LYS
1	E	71	ASN
1	E	74	SER
1	E	97	VAL
1	E	116	GLU
1	E	129	LYS
1	E	146	ARG
1	E	156	VAL
1	E	157	SER
1	E	163	ILE
1	E	171	LYS
1	E	176	LEU
1	E	178	SER
1	E	179	GLU
1	E	180	ASP
1	E	188	GLU
1	E	190	ARG
1	E	204	LYS
1	E	208	VAL
1	E	241	SER
1	E	267	VAL
1	E	274	LEU
1	E	275	MET
1	E	280	ILE
1	E	283	ILE
1	F	5	ASP
1	F	14	GLN
1	F	15	MET
1	F	29	GLN
1	F	47	ILE
1	F	52	ARG
1	F	53	LYS

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Mol	Chain	Res	Type
1	F	54	SER
1	F	56	LYS
1	F	71	ASN
1	F	74	SER
1	F	97	VAL
1	F	116	GLU
1	F	129	LYS
1	F	146	ARG
1	F	156	VAL
1	F	157	SER
1	F	163	ILE
1	F	171	LYS
1	F	176	LEU
1	F	178	SER
1	F	179	GLU
1	F	180	ASP
1	F	188	GLU
1	F	190	ARG
1	F	204	LYS
1	F	208	VAL
1	F	226	GLN
1	F	241	SER
1	F	267	VAL
1	F	274	LEU
1	F	275	MET
1	F	280	ILE
1	F	283	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	90	GLN
1	A	113	HIS
1	A	226	GLN
1	A	243	ASN
1	B	14	GLN
1	B	90	GLN
1	B	226	GLN
1	B	243	ASN
1	C	14	GLN
1	C	90	GLN

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Mol	Chain	Res	Type
1	C	226	GLN
1	C	243	ASN
1	D	14	GLN
1	D	90	GLN
1	D	226	GLN
1	D	243	ASN
1	E	14	GLN
1	E	90	GLN
1	E	226	GLN
1	E	243	ASN
1	F	14	GLN
1	F	90	GLN
1	F	226	GLN
1	F	243	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	281/297 (94%)	0.69	8 (2%) 56 27	7, 39, 56, 67	0
1	B	281/297 (94%)	0.93	25 (8%) 12 4	7, 39, 56, 67	0
1	C	281/297 (94%)	1.10	35 (12%) 5 2	7, 39, 56, 67	0
1	D	281/297 (94%)	1.33	54 (19%) 2 1	7, 39, 56, 67	0
1	E	281/297 (94%)	1.08	40 (14%) 4 1	7, 39, 56, 67	0
1	F	281/297 (94%)	0.96	27 (9%) 10 4	7, 39, 56, 67	0
All	All	1686/1782 (94%)	1.02	189 (11%) 7 2	7, 39, 57, 67	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	LEU	4.9
1	E	196	LEU	4.9
1	D	195	LEU	4.8
1	B	49	ALA	4.5
1	D	49	ALA	4.3
1	C	216	ALA	4.2
1	E	49	ALA	4.1
1	E	236	SER	4.0
1	F	189	MET	4.0
1	C	5	ASP	3.9
1	D	54	SER	3.8
1	A	143	ALA	3.8
1	F	7	LYS	3.8
1	D	182	ILE	3.8
1	F	201	GLU	3.7
1	D	198	ASP	3.7
1	D	216	ALA	3.7
1	E	47	ILE	3.7
1	B	48	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	196	LEU	3.7
1	F	181	ASP	3.6
1	C	236	SER	3.6
1	F	35	LYS	3.5
1	B	159	ALA	3.5
1	E	9	LYS	3.4
1	E	181	ASP	3.4
1	D	201	GLU	3.4
1	D	196	LEU	3.4
1	D	199	VAL	3.3
1	E	69	ILE	3.3
1	C	144	MET	3.3
1	F	69	ILE	3.2
1	C	94	ALA	3.2
1	B	181	ASP	3.2
1	F	182	ILE	3.2
1	D	170	ILE	3.2
1	D	7	LYS	3.1
1	B	4	GLU	3.1
1	E	276	GLY	3.1
1	E	177	LYS	3.1
1	D	48	PRO	3.1
1	D	122	VAL	3.1
1	D	208	VAL	3.1
1	F	196	LEU	3.1
1	B	195	LEU	3.0
1	F	177	LYS	3.0
1	D	181	ASP	3.0
1	D	268	SER	2.9
1	D	224	LEU	2.8
1	B	147	THR	2.8
1	E	195	LEU	2.8
1	F	49	ALA	2.8
1	D	202	LYS	2.7
1	B	175	GLN	2.7
1	D	114	HIS	2.7
1	D	257	HIS	2.7
1	C	267	VAL	2.7
1	E	65	MET	2.7
1	D	129	LYS	2.7
1	E	144	MET	2.7
1	C	208	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	3	GLY	2.7
1	D	44	LEU	2.7
1	C	170	ILE	2.7
1	F	218	PRO	2.6
1	C	185	VAL	2.6
1	D	242	SER	2.6
1	D	127	GLY	2.6
1	D	32	ILE	2.6
1	A	182	ILE	2.6
1	B	186	ALA	2.6
1	C	221	ALA	2.6
1	E	16	LEU	2.6
1	C	181	ASP	2.6
1	D	4	GLU	2.6
1	E	129	LYS	2.6
1	E	10	SER	2.6
1	E	237	GLY	2.6
1	E	32	ILE	2.6
1	C	9	LYS	2.5
1	D	95	LEU	2.5
1	B	242	SER	2.5
1	D	236	SER	2.5
1	C	182	ILE	2.5
1	B	52	ARG	2.5
1	B	257	HIS	2.5
1	E	142	ALA	2.5
1	C	257	HIS	2.5
1	C	275	MET	2.5
1	C	97	VAL	2.5
1	E	214	GLY	2.5
1	F	3	GLY	2.5
1	D	147	THR	2.4
1	F	134	ALA	2.4
1	D	185	VAL	2.4
1	F	203	GLY	2.4
1	F	191	VAL	2.4
1	F	208	VAL	2.4
1	A	282	SER	2.4
1	F	246	ARG	2.4
1	D	229	CYS	2.4
1	C	95	LEU	2.4
1	B	57	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	144	MET	2.4
1	E	275	MET	2.4
1	E	188	GLU	2.4
1	C	69	ILE	2.3
1	E	205	LEU	2.3
1	F	185	VAL	2.3
1	B	202	LYS	2.3
1	C	152	GLY	2.3
1	E	239	PHE	2.3
1	E	189	MET	2.3
1	A	196	LEU	2.3
1	D	103	SER	2.3
1	D	221	ALA	2.3
1	D	99	TYR	2.3
1	C	49	ALA	2.3
1	C	166	ILE	2.3
1	D	57	VAL	2.3
1	C	12	LEU	2.3
1	D	6	PHE	2.3
1	B	134	ALA	2.3
1	D	59	ARG	2.3
1	C	201	GLU	2.3
1	D	166	ILE	2.3
1	D	78	MET	2.3
1	C	196	LEU	2.3
1	C	199	VAL	2.3
1	C	229	CYS	2.3
1	E	175	GLN	2.2
1	B	182	ILE	2.2
1	D	134	ALA	2.2
1	B	236	SER	2.2
1	A	208	VAL	2.2
1	C	255	THR	2.2
1	D	217	THR	2.2
1	F	147	THR	2.2
1	E	160	VAL	2.2
1	D	177	LYS	2.2
1	F	188	GLU	2.2
1	D	38	ALA	2.2
1	E	234	VAL	2.2
1	B	12	LEU	2.2
1	E	257	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLY	2.2
1	B	185	VAL	2.2
1	C	65	MET	2.2
1	F	243	ASN	2.2
1	D	205	LEU	2.1
1	E	200	LEU	2.1
1	A	199	VAL	2.1
1	D	100	ILE	2.1
1	E	208	VAL	2.1
1	C	159	ALA	2.1
1	C	202	LYS	2.1
1	E	254	ALA	2.1
1	F	222	ALA	2.1
1	F	202	LYS	2.1
1	F	282	SER	2.1
1	D	204	LYS	2.1
1	E	127	GLY	2.1
1	E	199	VAL	2.1
1	C	128	ALA	2.1
1	D	13	ALA	2.1
1	B	174	GLN	2.1
1	D	179	GLU	2.1
1	F	211	ALA	2.1
1	D	23	ASP	2.1
1	E	111	TRP	2.1
1	F	32	ILE	2.1
1	C	232	VAL	2.1
1	E	20	VAL	2.1
1	D	270	ASP	2.1
1	E	120	PHE	2.1
1	E	18	GLY	2.1
1	B	170	ILE	2.0
1	B	280	ILE	2.0
1	B	205	LEU	2.0
1	E	187	GLU	2.0
1	A	177	LYS	2.0
1	C	276	GLY	2.0
1	D	111	TRP	2.0
1	C	186	ALA	2.0
1	E	148	LYS	2.0
1	E	150	GLU	2.0
1	F	160	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	189	MET	2.0
1	D	109	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.