Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:18 PM GMT

PDB ID	:	4HVZ
Title	:	Crystal structure of brucella abortus immunogenic BP26 protein
Authors	:	Kim, D.; Park, J.; Oh, B.; Song, J.
Deposited on	:	2012-11-07
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

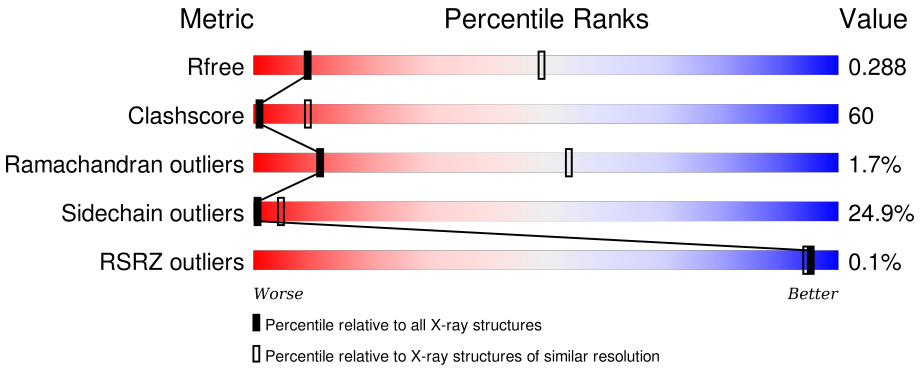
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	224	35% 44% 15%
1	B	224	26% 57% 10%
1	C	224	25% 50% 19%
1	D	224	29% 45% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6340 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 26 kDa periplasmic immunogenic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	B	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	C	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			
1	D	214	Total	C	N	O	S	0	0	0
			1585	981	282	313	9			

There are 8 discrepancies between the modelled and reference sequences:

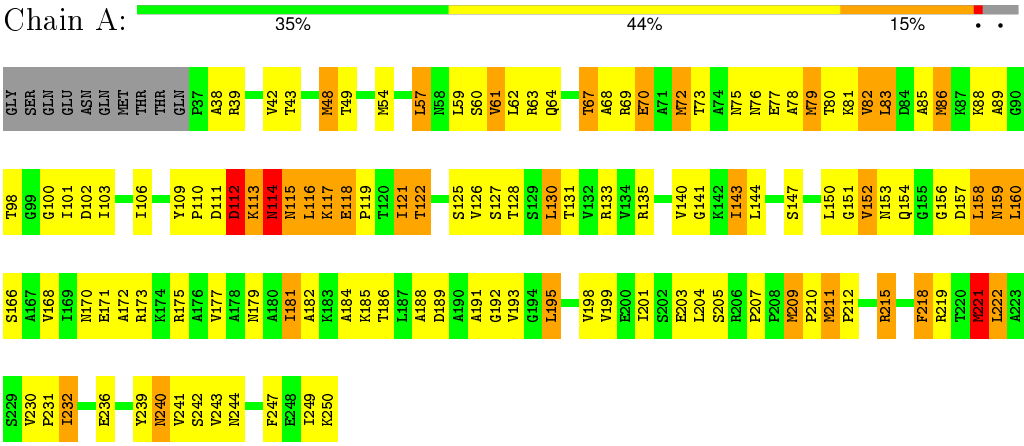
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	EXPRESSION TAG	UNP Q44642
A	28	SER	-	EXPRESSION TAG	UNP Q44642
B	27	GLY	-	EXPRESSION TAG	UNP Q44642
B	28	SER	-	EXPRESSION TAG	UNP Q44642
C	27	GLY	-	EXPRESSION TAG	UNP Q44642
C	28	SER	-	EXPRESSION TAG	UNP Q44642
D	27	GLY	-	EXPRESSION TAG	UNP Q44642
D	28	SER	-	EXPRESSION TAG	UNP Q44642

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.

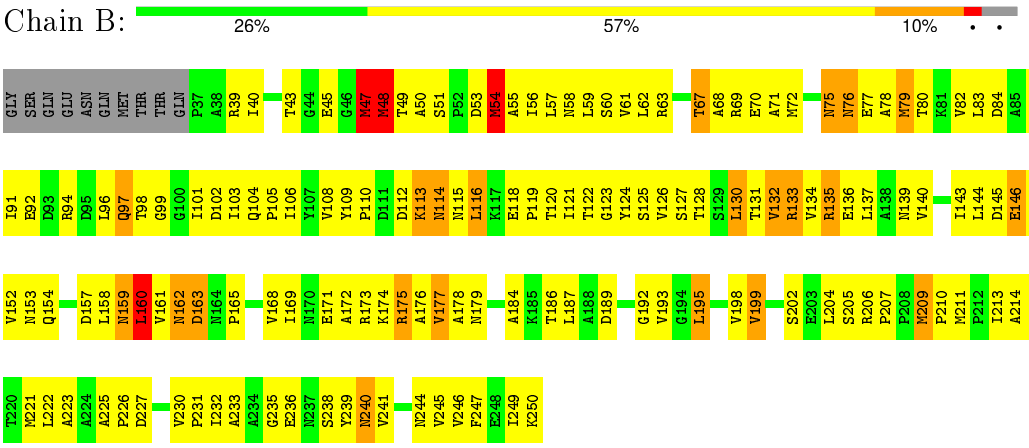
- Molecule 1: 26 kDa periplasmic immunogenic protein

Chain A:



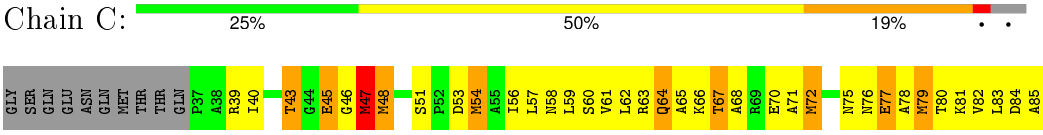
- Molecule 1: 26 kDa periplasmic immunogenic protein

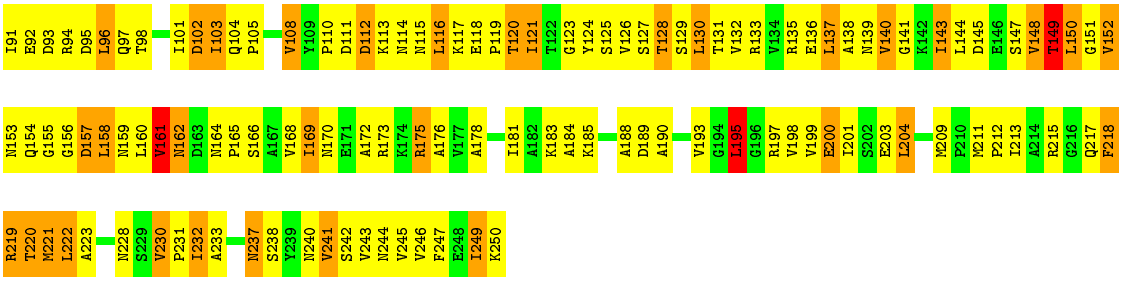
Chain B:



- Molecule 1: 26 kDa periplasmic immunogenic protein

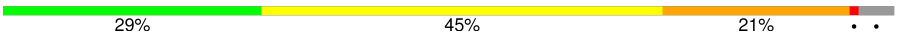
Chain C:

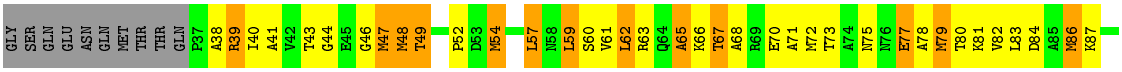


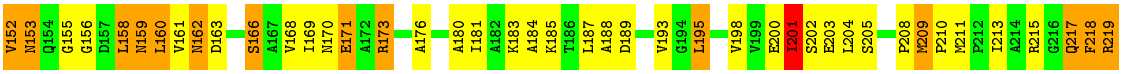


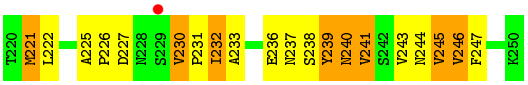
• Molecule 1: 26 kDa periplasmic immunogenic protein

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	203.09Å 203.09Å 207.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.50 42.02 – 3.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.96-3.50) 88.8 (42.02-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.45 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.283 0.242 , 0.288	Depositor DCC
R_{free} test set	2448 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	117.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 83.3	EDS
Estimated twinning fraction	0.000 for -l,-k,-h 0.011 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 26996 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6340	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	0.88	7/1602 (0.4%)	0.89	0/2172
1	B	0.89	7/1602 (0.4%)	0.89	1/2172 (0.0%)
1	C	0.92	9/1602 (0.6%)	0.98	3/2172 (0.1%)
1	D	0.93	9/1602 (0.6%)	0.98	3/2172 (0.1%)
All	All	0.91	32/6408 (0.5%)	0.93	7/8688 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	3
All	All	0	6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	MET	CG-SD	8.33	2.02	1.81
1	B	209	MET	CG-SD	7.92	2.01	1.81
1	A	86	MET	CG-SD	7.83	2.01	1.81
1	D	79	MET	CG-SD	7.65	2.01	1.81
1	A	221	MET	CG-SD	7.59	2.00	1.81
1	A	72	MET	CG-SD	7.40	2.00	1.81
1	B	79	MET	CG-SD	7.31	2.00	1.81
1	A	79	MET	CG-SD	7.17	1.99	1.81
1	C	72	MET	CG-SD	7.11	1.99	1.81
1	D	86	MET	CG-SD	7.02	1.99	1.81
1	C	86	MET	CG-SD	7.01	1.99	1.81
1	A	48	MET	CG-SD	6.67	1.98	1.81
1	C	209	MET	CG-SD	6.65	1.98	1.81
1	C	79	MET	CG-SD	6.57	1.98	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	MET	CG-SD	6.49	1.98	1.81
1	B	221	MET	CG-SD	6.40	1.97	1.81
1	B	47	MET	CG-SD	6.38	1.97	1.81
1	B	86	MET	CG-SD	6.32	1.97	1.81
1	B	48	MET	CG-SD	6.26	1.97	1.81
1	A	54	MET	CG-SD	6.21	1.97	1.81
1	D	209	MET	CG-SD	6.21	1.97	1.81
1	C	221	MET	CG-SD	5.96	1.96	1.81
1	D	221	MET	CG-SD	5.93	1.96	1.81
1	C	48	MET	CG-SD	5.88	1.96	1.81
1	C	211	MET	CG-SD	5.83	1.96	1.81
1	D	211	MET	CG-SD	5.83	1.96	1.81
1	C	47	MET	CG-SD	5.79	1.96	1.81
1	B	54	MET	CG-SD	5.76	1.96	1.81
1	A	211	MET	CG-SD	5.59	1.95	1.81
1	D	72	MET	CG-SD	5.30	1.95	1.81
1	D	47	MET	CG-SD	5.24	1.94	1.81
1	D	48	MET	CG-SD	5.09	1.94	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	158	LEU	CA-CB-CG	-8.83	95.00	115.30
1	C	195	LEU	CA-CB-CG	7.09	131.62	115.30
1	D	137	LEU	CA-CB-CG	6.45	130.14	115.30
1	C	46	GLY	N-CA-C	-6.36	97.20	113.10
1	C	204	LEU	CA-CB-CG	-6.10	101.28	115.30
1	B	160	LEU	CA-CB-CG	5.67	128.33	115.30
1	D	201	ILE	CB-CA-C	-5.66	100.28	111.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASP	Peptide
1	A	114	ASN	Peptide
1	A	228	ASN	Peptide
1	D	112	ASP	Peptide
1	D	217	GLN	Peptide
1	D	65	ALA	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	1585	0	1629	199	0
1	B	1585	0	1629	200	1
1	C	1585	0	1629	227	3
1	D	1585	0	1629	224	3
All	All	6340	0	6516	776	4

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 60.

All (776) 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:A:86:MET:SD	1:A:86:MET:CG	2.01	1.47
1:B:209:MET:CG	1:B:209:MET:SD	2.01	1.47
1:D:54:MET:SD	1:D:54:MET:CG	2.02	1.44
1:B:118:GLU:HG3	1:B:119:PRO:HD2	1.27	1.14
1:A:62:LEU:HB3	1:A:127:SER:HB2	1.28	1.14
1:B:47:MET:HE2	1:B:47:MET:HA	1.27	1.13
1:C:103:ILE:H	1:C:103:ILE:CD1	1.62	1.10
1:C:175:ARG:HH11	1:C:175:ARG:HB2	1.13	1.06
1:D:65:ALA:HB2	1:D:71:ALA:CB	1.85	1.05
1:C:103:ILE:HD12	1:C:103:ILE:N	1.64	1.05
1:C:103:ILE:HG23	1:C:126:VAL:CG2	1.87	1.05
1:D:65:ALA:CB	1:D:71:ALA:HB2	1.87	1.04
1:D:98:THR:HG22	1:D:130:LEU:HA	1.38	1.04
1:A:83:LEU:HD12	1:A:83:LEU:H	1.20	1.04
1:C:175:ARG:NH1	1:C:175:ARG:HB2	1.73	1.02
1:D:91:ILE:HD11	1:D:143:ILE:HG21	1.41	1.02
1:A:182:ALA:HA	1:A:185:LYS:HE2	1.39	1.01
1:A:59:LEU:HB3	1:A:152:VAL:HG11	1.40	1.00
1:C:67:THR:HG22	1:C:70:GLU:OE1	1.60	0.99
1:B:103:ILE:H	1:C:158:LEU:HD21	1.23	0.99
1:A:61:VAL:HG23	1:A:152:VAL:HG22	1.42	0.99
1:A:121:ILE:HD12	1:A:121:ILE:H	1.24	0.98
1:C:175:ARG:CB	1:C:175:ARG:HH11	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLY:O	1:D:152:VAL:HG22	1.63	0.98
1:D:63:ARG:HH12	1:D:81:LYS:NZ	1.61	0.98
1:D:63:ARG:HH12	1:D:81:LYS:HZ1	1.00	0.97
1:C:152:VAL:HG12	1:C:153:ASN:N	1.82	0.95
1:C:114:ASN:HB3	1:C:116:LEU:CD1	1.96	0.95
1:C:103:ILE:H	1:C:103:ILE:HD12	0.81	0.95
1:A:230:VAL:HG12	1:A:231:PRO:HD2	1.46	0.95
1:A:193:VAL:HG11	1:A:249:ILE:HG23	1.46	0.95
1:C:79:MET:O	1:C:82:VAL:HG12	1.65	0.94
1:A:161:VAL:HG23	1:A:162:ASN:N	1.82	0.94
1:C:101:ILE:HD13	1:C:128:THR:HB	1.46	0.94
1:B:91:ILE:HD11	1:B:143:ILE:HD12	1.48	0.94
1:D:65:ALA:HB2	1:D:71:ALA:HB2	0.95	0.94
1:D:200:GLU:HB3	1:D:246:VAL:HG23	1.47	0.93
1:A:91:ILE:HG13	1:A:96:LEU:HD11	1.51	0.93
1:C:114:ASN:HB3	1:C:116:LEU:HD11	1.51	0.92
1:B:218:PHE:HD1	1:B:219:ARG:H	1.00	0.92
1:D:134:VAL:HG11	1:D:140:VAL:HG23	1.53	0.90
1:B:210:PRO:HB3	1:B:239:TYR:CE2	2.08	0.89
1:C:108:VAL:HG23	1:C:120:THR:HG23	1.54	0.89
1:C:91:ILE:HG23	1:C:96:LEU:HD23	1.52	0.89
1:D:140:VAL:HA	1:D:143:ILE:CD1	2.04	0.88
1:B:218:PHE:HD1	1:B:219:ARG:N	1.71	0.87
1:B:108:VAL:O	1:B:119:PRO:HA	1.75	0.86
1:B:47:MET:CE	1:B:47:MET:HA	2.04	0.86
1:D:115:ASN:C	1:D:117:LYS:H	1.78	0.86
1:C:61:VAL:HG22	1:C:128:THR:O	1.74	0.85
1:C:64:GLN:HB3	1:C:125:SER:HA	1.59	0.84
1:D:77:GLU:OE1	1:D:78:ALA:N	2.11	0.84
1:A:189:ASP:O	1:A:192:GLY:N	2.12	0.83
1:A:131:THR:HG23	1:B:233:ALA:HB2	1.60	0.83
1:D:200:GLU:HB3	1:D:246:VAL:CG2	2.09	0.83
1:C:157:ASP:HB3	1:D:218:PHE:CZ	2.13	0.83
1:B:110:PRO:HA	1:B:114:ASN:ND2	1.94	0.82
1:D:65:ALA:HB1	1:D:67:THR:H	1.44	0.82
1:D:67:THR:HG23	1:D:70:GLU:HB3	1.60	0.82
1:C:152:VAL:HG12	1:C:153:ASN:H	1.43	0.82
1:C:218:PHE:CE2	1:C:219:ARG:HG2	2.15	0.82
1:A:67:THR:HG22	1:A:70:GLU:OE1	1.79	0.82
1:A:121:ILE:HD11	1:B:154:GLN:NE2	1.94	0.82
1:D:57:LEU:HD21	1:D:132:VAL:HB	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:HD21	1:C:128:THR:HG22	1.43	0.81
1:D:198:VAL:HG22	1:D:247:PHE:CE2	2.15	0.81
1:D:63:ARG:NH2	1:D:81:LYS:HZ2	1.78	0.81
1:D:147:SER:O	1:D:150:LEU:N	2.14	0.81
1:A:181:ILE:HG22	1:A:182:ALA:N	1.96	0.80
1:D:59:LEU:HD13	1:D:130:LEU:HD23	1.64	0.80
1:C:103:ILE:HG23	1:C:126:VAL:HG23	1.63	0.80
1:C:103:ILE:HG23	1:C:126:VAL:HG22	1.63	0.80
1:B:169:ILE:HD11	1:B:239:TYR:CD2	2.15	0.80
1:B:133:ARG:HH21	1:C:231:PRO:HD3	1.44	0.80
1:D:48:MET:HG2	1:D:168:VAL:HG23	1.64	0.80
1:C:147:SER:HB3	1:C:152:VAL:HG11	1.62	0.80
1:B:233:ALA:O	1:B:236:GLU:HB2	1.81	0.80
1:A:60:SER:O	1:A:152:VAL:HG13	1.81	0.79
1:D:237:ASN:HB3	1:D:239:TYR:HE1	1.48	0.79
1:B:48:MET:HA	1:B:48:MET:CE	2.13	0.79
1:D:63:ARG:HH22	1:D:81:LYS:HZ2	1.28	0.79
1:B:131:THR:CG2	1:C:233:ALA:HA	2.14	0.78
1:C:63:ARG:HH12	1:C:81:LYS:NZ	1.81	0.78
1:A:114:ASN:O	1:A:115:ASN:HB2	1.83	0.78
1:A:67:THR:HG22	1:A:70:GLU:CG	2.13	0.78
1:B:105:PRO:HG3	1:C:154:GLN:NE2	1.98	0.78
1:B:60:SER:H	1:B:153:ASN:ND2	1.81	0.78
1:B:45:GLU:OE1	1:B:45:GLU:N	2.16	0.78
1:B:57:LEU:HB3	1:B:59:LEU:HD21	1.65	0.77
1:B:102:ASP:OD2	1:C:158:LEU:HD11	1.84	0.77
1:D:198:VAL:HG22	1:D:247:PHE:CD2	2.19	0.77
1:B:159:ASN:N	1:B:159:ASN:OD1	2.11	0.77
1:A:83:LEU:N	1:A:83:LEU:HD12	1.99	0.77
1:D:63:ARG:NH1	1:D:81:LYS:NZ	2.32	0.77
1:C:215:ARG:O	1:C:218:PHE:CD2	2.37	0.77
1:A:101:ILE:CG2	1:B:160:LEU:HD21	2.15	0.77
1:B:233:ALA:N	1:B:236:GLU:OE2	2.17	0.77
1:A:102:ASP:OD1	1:A:102:ASP:O	2.03	0.77
1:D:92:GLU:HG3	1:D:93:ASP:H	1.50	0.77
1:D:59:LEU:HD12	1:D:130:LEU:O	1.84	0.77
1:D:109:TYR:CE2	1:D:119:PRO:HG2	2.20	0.77
1:C:45:GLU:HB2	1:C:241:VAL:O	1.83	0.77
1:B:103:ILE:N	1:C:158:LEU:HD21	2.00	0.76
1:D:96:LEU:HD21	1:D:132:VAL:HG22	1.67	0.76
1:C:123:GLY:O	1:C:124:TYR:CD1	2.37	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:O	1:C:116:LEU:HD12	1.86	0.76
1:C:157:ASP:HB3	1:D:218:PHE:HZ	1.50	0.76
1:C:105:PRO:HG3	1:D:155:GLY:HA3	1.68	0.76
1:B:189:ASP:O	1:B:192:GLY:N	2.18	0.75
1:A:210:PRO:O	1:A:212:PRO:HD3	1.86	0.75
1:A:82:VAL:HG22	1:A:150:LEU:HD13	1.68	0.75
1:C:130:LEU:HD21	1:C:132:VAL:HG23	1.69	0.75
1:B:152:VAL:HG12	1:B:153:ASN:ND2	2.02	0.75
1:A:165:PRO:O	1:A:168:VAL:N	2.19	0.75
1:D:63:ARG:HH22	1:D:81:LYS:NZ	1.85	0.74
1:A:43:THR:HG22	1:A:244:ASN:OD1	1.87	0.74
1:B:116:LEU:HD22	1:B:116:LEU:O	1.87	0.74
1:A:166:SER:O	1:A:170:ASN:HB2	1.87	0.74
1:B:109:TYR:CD2	1:B:119:PRO:HB3	2.22	0.73
1:A:57:LEU:HD23	1:A:57:LEU:N	2.02	0.73
1:A:102:ASP:HB2	1:B:158:LEU:HD21	1.69	0.73
1:C:60:SER:H	1:C:153:ASN:ND2	1.87	0.73
1:A:230:VAL:HG12	1:A:231:PRO:CD	2.18	0.73
1:D:92:GLU:HG3	1:D:93:ASP:N	2.03	0.73
1:A:67:THR:HG22	1:A:70:GLU:HG2	1.70	0.72
1:A:193:VAL:HG11	1:A:249:ILE:CG2	2.17	0.72
1:A:103:ILE:HG22	1:A:126:VAL:HG22	1.71	0.71
1:B:72:MET:O	1:B:76:ASN:N	2.22	0.71
1:D:109:TYR:HE2	1:D:119:PRO:HG2	1.55	0.71
1:C:63:ARG:HH12	1:C:81:LYS:HZ1	1.36	0.71
1:B:161:VAL:HG22	1:B:162:ASN:H	1.56	0.71
1:D:48:MET:CE	1:D:171:GLU:HB3	2.21	0.71
1:D:48:MET:CE	1:D:171:GLU:HG2	2.21	0.71
1:D:80:THR:HA	1:D:83:LEU:HB2	1.73	0.70
1:B:240:ASN:N	1:B:240:ASN:OD1	2.24	0.70
1:B:48:MET:HA	1:B:48:MET:HE3	1.72	0.70
1:B:56:ILE:O	1:B:159:ASN:ND2	2.25	0.70
1:C:143:ILE:HD12	1:C:143:ILE:O	1.92	0.70
1:D:140:VAL:HA	1:D:143:ILE:HD11	1.74	0.69
1:D:57:LEU:CD2	1:D:132:VAL:HB	2.22	0.69
1:B:91:ILE:CG2	1:B:96:LEU:HD11	2.24	0.68
1:D:115:ASN:C	1:D:117:LYS:N	2.47	0.68
1:A:110:PRO:N	1:A:116:LEU:HD11	2.08	0.68
1:A:193:VAL:CG1	1:A:249:ILE:HG23	2.21	0.67
1:D:109:TYR:CD2	1:D:119:PRO:CG	2.77	0.67
1:D:233:ALA:O	1:D:236:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:HD11	1:D:158:LEU:HD13	1.76	0.67
1:A:63:ARG:NH2	1:A:81:LYS:HZ2	1.91	0.67
1:D:46:GLY:H	1:D:176:ALA:HB2	1.59	0.67
1:C:101:ILE:CD1	1:C:128:THR:HB	2.23	0.67
1:A:78:ALA:HA	1:A:81:LYS:HE3	1.75	0.67
1:D:63:ARG:NH1	1:D:81:LYS:HZ1	1.83	0.67
1:B:131:THR:HG21	1:C:232:ILE:O	1.94	0.67
1:C:79:MET:CE	1:C:128:THR:HG23	2.24	0.67
1:D:140:VAL:HA	1:D:143:ILE:HD12	1.76	0.67
1:D:48:MET:HG3	1:D:49:THR:H	1.60	0.67
1:D:146:GLU:O	1:D:150:LEU:HG	1.95	0.67
1:C:61:VAL:O	1:C:127:SER:OG	2.08	0.67
1:C:123:GLY:C	1:C:124:TYR:CD1	2.68	0.67
1:A:240:ASN:OD1	1:A:240:ASN:N	2.26	0.67
1:D:97:GLN:HG3	1:D:98:THR:N	2.08	0.67
1:B:63:ARG:HH11	1:B:78:ALA:HB2	1.58	0.67
1:D:49:THR:HG21	1:D:232:ILE:HD12	1.77	0.67
1:C:181:ILE:CG2	1:C:185:LYS:HE3	2.25	0.67
1:C:130:LEU:CD2	1:C:132:VAL:HG23	2.25	0.66
1:C:154:GLN:OE1	1:C:155:GLY:N	2.28	0.66
1:D:219:ARG:O	1:D:222:LEU:N	2.28	0.66
1:A:131:THR:HG23	1:B:233:ALA:CB	2.25	0.66
1:C:68:ALA:O	1:C:71:ALA:HB3	1.94	0.66
1:D:41:ALA:HB2	1:D:246:VAL:HG13	1.78	0.66
1:B:59:LEU:HA	1:B:153:ASN:HD21	1.61	0.66
1:C:82:VAL:HG23	1:C:150:LEU:CD2	2.25	0.66
1:A:218:PHE:H	1:A:218:PHE:HD2	1.44	0.66
1:C:128:THR:OG1	1:C:129:SER:N	2.23	0.66
1:B:210:PRO:HB3	1:B:239:TYR:CZ	2.30	0.66
1:A:243:VAL:HG23	1:A:244:ASN:N	2.11	0.66
1:D:59:LEU:CD1	1:D:130:LEU:HD23	2.26	0.66
1:B:116:LEU:O	1:B:118:GLU:HB2	1.95	0.66
1:B:131:THR:HG21	1:C:233:ALA:HA	1.77	0.66
1:A:219:ARG:HA	1:A:222:LEU:HD11	1.77	0.65
1:B:59:LEU:CA	1:B:153:ASN:HD21	2.09	0.65
1:A:98:THR:HG23	1:A:130:LEU:HD12	1.77	0.65
1:C:82:VAL:O	1:C:85:ALA:HB3	1.97	0.65
1:B:61:VAL:HG11	1:B:82:VAL:HG11	1.79	0.65
1:A:91:ILE:CG1	1:A:96:LEU:HD11	2.26	0.65
1:B:118:GLU:HG3	1:B:119:PRO:CD	2.16	0.65
1:C:131:THR:OG1	1:D:233:ALA:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:O	1:C:139:ASN:N	2.30	0.65
1:C:54:MET:HE1	1:C:133:ARG:HG2	1.79	0.65
1:D:65:ALA:CB	1:D:67:THR:H	2.09	0.64
1:C:54:MET:CE	1:C:133:ARG:HG2	2.27	0.64
1:C:53:ASP:HB2	1:C:162:ASN:HA	1.79	0.64
1:D:98:THR:HB	1:D:129:SER:O	1.97	0.64
1:D:77:GLU:CD	1:D:78:ALA:N	2.50	0.64
1:B:171:GLU:OE2	1:B:175:ARG:HD3	1.96	0.64
1:B:43:THR:HG22	1:B:244:ASN:OD1	1.97	0.64
1:D:49:THR:HG21	1:D:232:ILE:CD1	2.27	0.64
1:C:110:PRO:HA	1:C:116:LEU:HD11	1.80	0.64
1:C:184:ALA:HB1	1:C:195:LEU:HD21	1.80	0.64
1:C:78:ALA:HA	1:C:81:LYS:HE3	1.80	0.64
1:A:49:THR:HG21	1:A:232:ILE:HD11	1.80	0.64
1:C:218:PHE:CD2	1:C:219:ARG:HG2	2.33	0.63
1:D:98:THR:HG22	1:D:130:LEU:CA	2.23	0.63
1:B:91:ILE:HG21	1:B:96:LEU:HD11	1.80	0.63
1:B:225:ALA:HB1	1:B:226:PRO:HD2	1.81	0.63
1:C:110:PRO:HA	1:C:116:LEU:CD1	2.28	0.63
1:C:217:GLN:HB3	1:C:221:MET:HG2	1.79	0.63
1:B:157:ASP:O	1:B:159:ASN:OD1	2.17	0.63
1:A:163:ASP:O	1:A:165:PRO:HD3	1.97	0.63
1:D:123:GLY:C	1:D:124:TYR:HD1	2.02	0.63
1:B:140:VAL:HA	1:B:143:ILE:HG22	1.81	0.63
1:D:184:ALA:HB2	1:D:247:PHE:HE1	1.63	0.63
1:B:133:ARG:NH2	1:C:231:PRO:HD3	2.14	0.63
1:C:124:TYR:OH	1:D:148:VAL:HG21	1.99	0.63
1:D:82:VAL:HG23	1:D:150:LEU:HD12	1.79	0.63
1:D:106:ILE:HD11	1:D:124:TYR:C	2.18	0.62
1:C:61:VAL:O	1:C:61:VAL:HG23	2.00	0.62
1:D:109:TYR:CE2	1:D:119:PRO:CG	2.82	0.62
1:D:48:MET:HE2	1:D:171:GLU:HG2	1.82	0.62
1:C:112:ASP:C	1:C:112:ASP:OD1	2.37	0.62
1:A:215:ARG:O	1:A:218:PHE:CD2	2.52	0.62
1:A:173:ARG:HD2	1:B:186:THR:HG21	1.82	0.62
1:C:60:SER:H	1:C:153:ASN:HD21	1.46	0.62
1:A:86:MET:HA	1:A:89:ALA:HB3	1.82	0.62
1:D:108:VAL:HG12	1:D:120:THR:O	2.00	0.62
1:D:118:GLU:HG3	1:D:119:PRO:O	1.99	0.62
1:A:195:LEU:C	1:A:195:LEU:HD12	2.19	0.62
1:B:168:VAL:HG12	1:B:169:ILE:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ALA:O	1:B:71:ALA:HB3	2.00	0.61
1:C:45:GLU:HB3	1:C:242:SER:HA	1.81	0.61
1:C:139:ASN:O	1:C:143:ILE:HG23	2.00	0.61
1:D:103:ILE:HG23	1:D:126:VAL:CG2	2.30	0.61
1:A:59:LEU:HB3	1:A:152:VAL:CG1	2.24	0.61
1:D:150:LEU:N	1:D:150:LEU:HD23	2.15	0.61
1:A:63:ARG:HH22	1:A:81:LYS:NZ	1.99	0.61
1:C:230:VAL:HG12	1:C:231:PRO:HD2	1.81	0.61
1:B:131:THR:HG23	1:C:233:ALA:HA	1.81	0.61
1:D:110:PRO:HA	1:D:114:ASN:HB3	1.82	0.61
1:B:47:MET:HE1	1:B:240:ASN:CG	2.20	0.61
1:C:150:LEU:HD12	1:C:151:GLY:N	2.16	0.61
1:C:68:ALA:HB3	1:D:145:ASP:OD2	2.00	0.61
1:C:199:VAL:HG12	1:C:246:VAL:O	2.00	0.61
1:C:147:SER:O	1:C:152:VAL:HB	2.00	0.61
1:B:218:PHE:CD1	1:B:219:ARG:N	2.56	0.61
1:A:91:ILE:CG2	1:A:143:ILE:HD11	2.31	0.60
1:D:110:PRO:HG3	1:D:118:GLU:O	2.00	0.60
1:D:66:LYS:O	1:D:66:LYS:HG2	2.01	0.60
1:C:45:GLU:N	1:C:45:GLU:OE1	2.35	0.60
1:A:63:ARG:HH12	1:A:81:LYS:HZ1	1.50	0.60
1:A:173:ARG:NH1	1:A:203:GLU:OE2	2.34	0.60
1:A:158:LEU:HD13	1:A:158:LEU:H	1.67	0.60
1:D:61:VAL:HG12	1:D:152:VAL:HG12	1.84	0.60
1:C:120:THR:OG1	1:C:121:ILE:N	2.35	0.60
1:D:48:MET:HG3	1:D:49:THR:N	2.17	0.60
1:A:85:ALA:O	1:A:88:LYS:HG3	2.02	0.59
1:C:111:ASP:H	1:C:114:ASN:HB2	1.68	0.59
1:A:80:THR:HA	1:A:83:LEU:CD1	2.33	0.59
1:A:101:ILE:HG23	1:B:160:LEU:HD21	1.82	0.59
1:A:160:LEU:HD23	1:A:160:LEU:H	1.67	0.59
1:A:153:ASN:OD1	1:A:154:GLN:N	2.36	0.59
1:B:118:GLU:CG	1:B:119:PRO:HD2	2.19	0.59
1:C:103:ILE:N	1:C:103:ILE:CD1	2.38	0.59
1:D:48:MET:HE1	1:D:171:GLU:HG2	1.85	0.59
1:B:57:LEU:HB2	1:B:132:VAL:HG22	1.83	0.59
1:B:67:THR:HG23	1:B:70:GLU:OE1	2.03	0.59
1:D:184:ALA:HB1	1:D:195:LEU:HD11	1.85	0.59
1:A:62:LEU:HB3	1:A:127:SER:CB	2.19	0.59
1:A:181:ILE:CG2	1:A:182:ALA:N	2.66	0.59
1:B:92:GLU:HG3	1:B:94:ARG:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLY:H	1:D:176:ALA:CB	2.15	0.59
1:A:179:ASN:OD1	1:A:179:ASN:C	2.41	0.59
1:B:53:ASP:OD1	1:B:162:ASN:HA	2.02	0.58
1:C:101:ILE:HD13	1:C:128:THR:CB	2.26	0.58
1:C:91:ILE:CG2	1:C:96:LEU:HD23	2.29	0.58
1:A:109:TYR:HD2	1:A:119:PRO:HG3	1.68	0.58
1:C:145:ASP:O	1:C:149:THR:OG1	2.19	0.58
1:D:240:ASN:OD1	1:D:240:ASN:N	2.37	0.58
1:C:101:ILE:HD12	1:C:127:SER:O	2.04	0.58
1:D:184:ALA:CB	1:D:247:PHE:CE1	2.86	0.58
1:B:59:LEU:HB3	1:B:153:ASN:HD21	1.67	0.58
1:B:47:MET:O	1:B:48:MET:HG2	2.03	0.58
1:A:163:ASP:O	1:A:165:PRO:CD	2.51	0.58
1:C:169:ILE:HG22	1:C:170:ASN:N	2.19	0.58
1:D:139:ASN:O	1:D:143:ILE:HD11	2.03	0.58
1:A:189:ASP:O	1:A:191:ALA:N	2.36	0.58
1:B:63:ARG:HH11	1:B:78:ALA:CB	2.17	0.58
1:A:114:ASN:O	1:A:115:ASN:CB	2.50	0.58
1:D:201:ILE:HD13	1:D:245:VAL:HG13	1.85	0.58
1:B:116:LEU:HD13	1:B:118:GLU:HB3	1.86	0.57
1:D:61:VAL:O	1:D:61:VAL:HG23	2.03	0.57
1:D:78:ALA:O	1:D:81:LYS:HB2	2.04	0.57
1:A:182:ALA:CA	1:A:185:LYS:HE2	2.26	0.57
1:A:147:SER:O	1:A:151:GLY:O	2.21	0.57
1:A:158:LEU:HD13	1:A:158:LEU:N	2.18	0.57
1:B:97:GLN:O	1:B:130:LEU:HD12	2.04	0.57
1:A:131:THR:HG21	1:B:232:ILE:O	2.04	0.57
1:C:82:VAL:HG23	1:C:150:LEU:HD22	1.86	0.57
1:A:121:ILE:N	1:A:121:ILE:HD12	2.07	0.57
1:A:182:ALA:HA	1:A:185:LYS:CE	2.26	0.57
1:C:108:VAL:CG2	1:C:120:THR:HG23	2.32	0.57
1:D:188:ALA:HB1	1:D:193:VAL:HG23	1.87	0.57
1:A:80:THR:HA	1:A:83:LEU:HD11	1.86	0.57
1:D:109:TYR:HD2	1:D:119:PRO:CG	2.17	0.57
1:A:117:LYS:O	1:A:117:LYS:HG3	2.04	0.57
1:B:123:GLY:C	1:B:124:TYR:CD1	2.77	0.57
1:A:198:VAL:O	1:A:198:VAL:HG12	2.05	0.57
1:D:63:ARG:NH2	1:D:81:LYS:NZ	2.49	0.57
1:A:110:PRO:CA	1:A:116:LEU:HD11	2.35	0.57
1:B:250:LYS:O	1:B:250:LYS:HD3	2.05	0.56
1:D:98:THR:CG2	1:D:130:LEU:HA	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:HG23	1:C:96:LEU:CD2	2.29	0.56
1:D:114:ASN:ND2	1:D:117:LYS:HG2	2.21	0.56
1:A:207:PRO:HG3	1:B:45:GLU:OE2	2.06	0.56
1:A:218:PHE:CD2	1:A:218:PHE:N	2.72	0.56
1:B:114:ASN:O	1:B:115:ASN:CG	2.43	0.56
1:B:91:ILE:HD11	1:B:143:ILE:CD1	2.30	0.56
1:C:184:ALA:HB1	1:C:195:LEU:CD2	2.35	0.56
1:A:67:THR:HG22	1:A:70:GLU:CD	2.25	0.56
1:D:43:THR:HG22	1:D:244:ASN:OD1	2.05	0.56
1:C:61:VAL:CG2	1:C:128:THR:H	2.19	0.56
1:B:54:MET:CE	1:B:135:ARG:HA	2.35	0.56
1:C:98:THR:HG22	1:C:130:LEU:HB2	1.87	0.56
1:D:103:ILE:HG23	1:D:126:VAL:HG23	1.88	0.56
1:D:63:ARG:CZ	1:D:81:LYS:HZ2	2.19	0.56
1:A:111:ASP:O	1:A:114:ASN:N	2.38	0.56
1:D:202:SER:HB2	1:D:204:LEU:HD11	1.87	0.56
1:D:204:LEU:HD12	1:D:204:LEU:N	2.21	0.56
1:D:109:TYR:CD2	1:D:119:PRO:HB3	2.40	0.55
1:D:215:ARG:O	1:D:218:PHE:CG	2.60	0.55
1:D:57:LEU:CD2	1:D:132:VAL:O	2.53	0.55
1:A:154:GLN:NE2	1:A:157:ASP:OD2	2.40	0.55
1:B:134:VAL:HG22	1:B:143:ILE:HD13	1.89	0.55
1:A:49:THR:HG21	1:A:232:ILE:CD1	2.36	0.55
1:C:82:VAL:HG23	1:C:150:LEU:HD21	1.87	0.55
1:C:111:ASP:O	1:C:114:ASN:HB2	2.06	0.55
1:C:114:ASN:HB3	1:C:116:LEU:HD12	1.85	0.55
1:D:184:ALA:HB2	1:D:247:PHE:CE1	2.40	0.55
1:A:209:MET:HE2	1:A:209:MET:C	2.27	0.55
1:C:130:LEU:C	1:C:130:LEU:HD23	2.26	0.55
1:A:109:TYR:CD2	1:A:119:PRO:HG3	2.42	0.55
1:A:133:ARG:CZ	1:B:231:PRO:HG3	2.36	0.55
1:A:184:ALA:HB1	1:A:195:LEU:HD22	1.89	0.55
1:D:203:GLU:O	1:D:203:GLU:HG3	2.07	0.55
1:C:103:ILE:CD1	1:D:158:LEU:HD13	2.36	0.55
1:C:155:GLY:C	1:C:157:ASP:H	2.10	0.55
1:A:117:LYS:CG	1:A:117:LYS:O	2.54	0.55
1:B:101:ILE:HD11	1:B:126:VAL:CG1	2.37	0.55
1:B:173:ARG:O	1:B:176:ALA:HB3	2.06	0.55
1:A:152:VAL:HG12	1:A:152:VAL:O	2.05	0.55
1:B:161:VAL:HG22	1:B:162:ASN:N	2.22	0.55
1:B:58:ASN:C	1:B:59:LEU:HD23	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:NH2	1:A:81:LYS:NZ	2.54	0.55
1:C:114:ASN:CB	1:C:116:LEU:HD11	2.33	0.55
1:B:163:ASP:C	1:B:165:PRO:HD3	2.27	0.54
1:C:95:ASP:OD2	1:C:133:ARG:HD2	2.07	0.54
1:C:152:VAL:CG1	1:C:153:ASN:N	2.53	0.54
1:C:82:VAL:HG13	1:C:83:LEU:N	2.22	0.54
1:D:109:TYR:CD2	1:D:119:PRO:CB	2.90	0.54
1:C:45:GLU:CB	1:C:241:VAL:O	2.53	0.54
1:A:91:ILE:HG23	1:A:143:ILE:HD11	1.89	0.54
1:C:133:ARG:HH21	1:D:231:PRO:HD3	1.72	0.54
1:C:218:PHE:N	1:C:218:PHE:CD2	2.75	0.54
1:D:217:GLN:O	1:D:218:PHE:C	2.45	0.54
1:B:184:ALA:HB2	1:B:247:PHE:CE1	2.43	0.54
1:D:147:SER:O	1:D:149:THR:N	2.41	0.54
1:D:108:VAL:O	1:D:119:PRO:HB3	2.07	0.54
1:B:101:ILE:HD11	1:B:126:VAL:HG13	1.90	0.54
1:C:159:ASN:O	1:C:160:LEU:HD23	2.07	0.54
1:D:87:LYS:NZ	1:D:93:ASP:OD1	2.22	0.54
1:B:108:VAL:HG12	1:B:109:TYR:N	2.22	0.54
1:B:161:VAL:HG13	1:B:162:ASN:N	2.23	0.54
1:D:198:VAL:CG2	1:D:247:PHE:CE2	2.90	0.54
1:D:38:ALA:C	1:D:39:ARG:HG2	2.28	0.54
1:A:121:ILE:HD11	1:B:154:GLN:HE22	1.72	0.54
1:C:218:PHE:N	1:C:218:PHE:HD2	2.05	0.54
1:C:152:VAL:HG12	1:C:153:ASN:CG	2.28	0.54
1:C:64:GLN:CB	1:C:125:SER:HA	2.34	0.54
1:A:63:ARG:HD2	1:A:78:ALA:CB	2.37	0.54
1:D:151:GLY:O	1:D:152:VAL:CG2	2.47	0.53
1:B:210:PRO:HD2	1:C:223:ALA:HB1	1.90	0.53
1:A:110:PRO:CD	1:A:116:LEU:HD11	2.38	0.53
1:D:137:LEU:O	1:D:139:ASN:N	2.41	0.53
1:D:47:MET:HG2	1:D:48:MET:N	2.21	0.53
1:D:44:GLY:HA3	1:D:180:ALA:HB2	1.89	0.53
1:C:212:PRO:HA	1:C:237:ASN:OD1	2.08	0.53
1:A:103:ILE:CG2	1:A:126:VAL:HG22	2.38	0.53
1:A:76:ASN:O	1:A:79:MET:HB3	2.07	0.53
1:A:68:ALA:HB3	1:B:145:ASP:OD1	2.08	0.53
1:B:145:ASP:O	1:B:148:VAL:HG12	2.08	0.53
1:D:238:SER:C	1:D:239:TYR:HD1	2.12	0.53
1:A:68:ALA:HB2	1:B:144:LEU:HD23	1.88	0.53
1:D:109:TYR:HD2	1:D:119:PRO:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:O	1:A:70:GLU:HG3	2.09	0.53
1:D:48:MET:HE2	1:D:171:GLU:HB3	1.90	0.53
1:C:56:ILE:O	1:C:159:ASN:HB2	2.09	0.53
1:B:110:PRO:HA	1:B:114:ASN:CG	2.29	0.53
1:D:239:TYR:N	1:D:239:TYR:HD1	2.06	0.53
1:B:184:ALA:HB1	1:B:195:LEU:HD21	1.91	0.52
1:C:144:LEU:O	1:C:147:SER:N	2.41	0.52
1:D:46:GLY:N	1:D:176:ALA:HA	2.24	0.52
1:C:195:LEU:HD22	1:C:247:PHE:CG	2.44	0.52
1:A:114:ASN:HA	1:A:116:LEU:HD23	1.90	0.52
1:A:101:ILE:HG22	1:B:160:LEU:CD2	2.39	0.52
1:B:68:ALA:HA	1:B:71:ALA:HB2	1.91	0.52
1:A:116:LEU:HD12	1:A:118:GLU:O	2.09	0.52
1:B:59:LEU:CB	1:B:153:ASN:HD21	2.23	0.52
1:C:161:VAL:HG12	1:C:162:ASN:H	1.74	0.52
1:C:47:MET:HE3	1:C:240:ASN:HD22	1.75	0.52
1:C:135:ARG:O	1:C:136:GLU:HB2	2.09	0.52
1:A:100:GLY:HA3	1:B:235:GLY:HA3	1.90	0.52
1:B:211:MET:HB2	1:B:238:SER:O	2.09	0.52
1:B:168:VAL:HG12	1:B:169:ILE:HD13	1.92	0.52
1:C:43:THR:HB	1:C:244:ASN:OD1	2.10	0.52
1:D:49:THR:OG1	1:D:236:GLU:OE1	2.26	0.52
1:A:159:ASN:O	1:A:161:VAL:CG1	2.58	0.52
1:D:52:PRO:HB3	1:D:160:LEU:HB2	1.91	0.52
1:D:213:ILE:CD1	1:D:236:GLU:O	2.58	0.51
1:A:110:PRO:HD3	1:A:116:LEU:CD1	2.40	0.51
1:C:148:VAL:HG12	1:C:149:THR:N	2.25	0.51
1:D:106:ILE:HD12	1:D:125:SER:HB2	1.92	0.51
1:A:207:PRO:CG	1:B:45:GLU:OE2	2.59	0.51
1:C:123:GLY:C	1:C:124:TYR:HD1	2.11	0.51
1:A:78:ALA:HA	1:A:81:LYS:HG3	1.92	0.51
1:D:203:GLU:HB3	1:D:243:VAL:HG23	1.93	0.51
1:C:57:LEU:HD12	1:C:57:LEU:N	2.24	0.51
1:B:103:ILE:H	1:C:158:LEU:CD2	2.10	0.51
1:D:184:ALA:O	1:D:187:LEU:HB2	2.10	0.51
1:B:49:THR:HG21	1:B:232:ILE:CD1	2.41	0.51
1:C:80:THR:HA	1:C:83:LEU:HD12	1.92	0.51
1:A:61:VAL:CG1	1:A:61:VAL:O	2.59	0.51
1:C:175:ARG:NH1	1:C:175:ARG:CB	2.52	0.51
1:C:147:SER:HA	1:C:152:VAL:HG21	1.93	0.51
1:B:169:ILE:CD1	1:B:239:TYR:CD2	2.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:MET:HB3	1:A:91:ILE:HD11	1.92	0.51
1:A:61:VAL:HG23	1:A:152:VAL:CG2	2.29	0.51
1:A:121:ILE:CD1	1:A:121:ILE:H	1.99	0.51
1:B:82:VAL:HG23	1:B:150:LEU:HD22	1.92	0.51
1:A:49:THR:CG2	1:A:232:ILE:HD11	2.40	0.51
1:B:215:ARG:O	1:B:218:PHE:HB3	2.11	0.50
1:B:68:ALA:O	1:B:71:ALA:CB	2.60	0.50
1:B:63:ARG:HD3	1:B:78:ALA:HB2	1.93	0.50
1:C:199:VAL:N	1:C:246:VAL:O	2.36	0.50
1:D:239:TYR:N	1:D:239:TYR:CD1	2.77	0.50
1:A:131:THR:CG2	1:B:233:ALA:HB2	2.37	0.50
1:C:64:GLN:HB3	1:C:125:SER:CA	2.36	0.50
1:C:95:ASP:OD1	1:C:135:ARG:HD2	2.12	0.50
1:A:111:ASP:H	1:A:114:ASN:HB3	1.76	0.50
1:A:77:GLU:O	1:A:81:LYS:HG3	2.12	0.50
1:B:124:TYR:OH	1:C:148:VAL:CG2	2.60	0.50
1:D:41:ALA:CB	1:D:246:VAL:HG13	2.41	0.50
1:C:178:ALA:HA	1:C:181:ILE:HD12	1.93	0.50
1:B:123:GLY:O	1:B:124:TYR:CD1	2.65	0.50
1:C:173:ARG:NH1	1:C:203:GLU:OE1	2.43	0.50
1:B:249:ILE:HG22	1:B:250:LYS:N	2.26	0.50
1:A:151:GLY:C	1:A:152:VAL:HG23	2.31	0.50
1:B:102:ASP:CG	1:C:158:LEU:HD11	2.33	0.50
1:D:213:ILE:N	1:D:213:ILE:HD12	2.26	0.50
1:C:131:THR:OG1	1:D:233:ALA:CB	2.59	0.50
1:A:218:PHE:N	1:A:218:PHE:HD2	2.07	0.50
1:D:116:LEU:O	1:D:118:GLU:N	2.37	0.49
1:D:123:GLY:C	1:D:124:TYR:CD1	2.84	0.49
1:D:153:ASN:OD1	1:D:156:GLY:N	2.45	0.49
1:D:116:LEU:C	1:D:118:GLU:H	2.14	0.49
1:C:56:ILE:HD12	1:D:222:LEU:HD13	1.94	0.49
1:C:117:LYS:O	1:C:118:GLU:HG3	2.12	0.49
1:A:111:ASP:O	1:A:114:ASN:HB3	2.12	0.49
1:C:193:VAL:HB	1:C:249:ILE:CG2	2.43	0.49
1:C:172:ALA:O	1:C:173:ARG:C	2.50	0.49
1:C:188:ALA:HB1	1:C:193:VAL:O	2.12	0.49
1:D:62:LEU:O	1:D:62:LEU:HD13	2.12	0.49
1:B:216:GLY:C	1:B:218:PHE:H	2.13	0.49
1:B:106:ILE:HD11	1:B:125:SER:HB2	1.94	0.49
1:C:39:ARG:HA	1:C:247:PHE:O	2.13	0.49
1:A:86:MET:O	1:A:89:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PHE:O	1:B:222:LEU:HD13	2.12	0.49
1:B:168:VAL:HG11	1:B:239:TYR:CD1	2.46	0.49
1:D:217:GLN:HB3	1:D:221:MET:HG2	1.94	0.49
1:B:55:ALA:HB3	1:B:134:VAL:HB	1.94	0.49
1:A:198:VAL:HG22	1:A:247:PHE:CD2	2.48	0.49
1:D:59:LEU:HD12	1:D:59:LEU:H	1.77	0.49
1:A:177:VAL:HG12	1:A:181:ILE:HD12	1.94	0.49
1:D:109:TYR:HD2	1:D:119:PRO:CB	2.25	0.49
1:A:111:ASP:O	1:A:114:ASN:CB	2.61	0.49
1:B:144:LEU:O	1:B:147:SER:HB2	2.13	0.49
1:D:122:THR:OG1	1:D:122:THR:O	2.31	0.49
1:C:152:VAL:CG1	1:C:153:ASN:H	2.11	0.48
1:B:54:MET:HA	1:B:54:MET:HE2	1.95	0.48
1:C:164:ASN:HB2	1:D:227:ASP:OD2	2.13	0.48
1:C:58:ASN:C	1:C:59:LEU:HD23	2.34	0.48
1:A:101:ILE:CG2	1:B:160:LEU:CD2	2.90	0.48
1:C:121:ILE:N	1:C:121:ILE:HD13	2.28	0.48
1:B:112:ASP:O	1:B:113:LYS:HB2	2.13	0.48
1:A:67:THR:CG2	1:A:70:GLU:HG2	2.43	0.48
1:B:53:ASP:O	1:B:54:MET:HE3	2.12	0.48
1:A:204:LEU:HA	1:B:43:THR:HG23	1.95	0.48
1:A:158:LEU:N	1:A:158:LEU:HD22	2.29	0.48
1:C:204:LEU:HD23	1:D:43:THR:HG23	1.95	0.48
1:B:114:ASN:O	1:B:115:ASN:OD1	2.31	0.48
1:B:59:LEU:HB3	1:B:152:VAL:CG1	2.44	0.48
1:A:207:PRO:HB3	1:B:45:GLU:OE2	2.13	0.48
1:B:206:ARG:HB2	1:B:206:ARG:NH1	2.28	0.48
1:C:75:ASN:O	1:C:76:ASN:C	2.52	0.48
1:B:216:GLY:HA2	1:B:218:PHE:CD2	2.48	0.48
1:D:82:VAL:CG2	1:D:150:LEU:HD12	2.43	0.48
1:A:249:ILE:O	1:A:250:LYS:HB2	2.14	0.48
1:B:60:SER:H	1:B:153:ASN:HD22	1.59	0.48
1:B:79:MET:HE3	1:B:98:THR:HG21	1.95	0.48
1:D:166:SER:O	1:D:170:ASN:HB2	2.14	0.48
1:C:72:MET:O	1:C:75:ASN:HB3	2.14	0.48
1:D:48:MET:HE2	1:D:171:GLU:CG	2.43	0.48
1:B:61:VAL:O	1:B:61:VAL:HG23	2.14	0.48
1:A:154:GLN:CD	1:A:157:ASP:OD2	2.52	0.48
1:B:214:ALA:HB3	1:B:217:GLN:CG	2.44	0.48
1:D:60:SER:O	1:D:152:VAL:HA	2.14	0.47
1:C:111:ASP:OD1	1:C:112:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:THR:CB	1:D:232:ILE:HD11	2.44	0.47
1:A:57:LEU:CD2	1:A:57:LEU:N	2.72	0.47
1:C:170:ASN:O	1:C:173:ARG:HB3	2.14	0.47
1:B:159:ASN:O	1:B:160:LEU:HD12	2.14	0.47
1:D:161:VAL:HG22	1:D:162:ASN:H	1.80	0.47
1:D:200:GLU:CB	1:D:246:VAL:HG23	2.33	0.47
1:C:91:ILE:HG13	1:C:92:GLU:H	1.79	0.47
1:D:46:GLY:N	1:D:176:ALA:HB2	2.29	0.47
1:A:153:ASN:CG	1:A:154:GLN:H	2.16	0.47
1:C:149:THR:H	1:C:149:THR:HG1	1.44	0.47
1:C:114:ASN:HD22	1:C:116:LEU:HD11	1.80	0.47
1:D:96:LEU:HA	1:D:96:LEU:HD23	1.63	0.47
1:D:67:THR:HG23	1:D:70:GLU:CB	2.39	0.47
1:C:152:VAL:HG13	1:C:153:ASN:ND2	2.30	0.47
1:B:204:LEU:HA	1:C:43:THR:CG2	2.44	0.47
1:D:159:ASN:C	1:D:160:LEU:HD23	2.34	0.47
1:C:151:GLY:O	1:C:152:VAL:HB	2.14	0.47
1:C:215:ARG:O	1:C:218:PHE:CG	2.67	0.47
1:D:57:LEU:HD21	1:D:132:VAL:CB	2.35	0.47
1:D:57:LEU:HD23	1:D:57:LEU:H	1.79	0.47
1:A:82:VAL:CG2	1:A:150:LEU:HD13	2.41	0.47
1:D:159:ASN:N	1:D:159:ASN:OD1	2.48	0.47
1:B:162:ASN:O	1:B:165:PRO:HG3	2.15	0.47
1:D:181:ILE:HA	1:D:247:PHE:CZ	2.49	0.47
1:C:103:ILE:HD13	1:D:158:LEU:HD12	1.97	0.47
1:B:110:PRO:HG3	1:B:118:GLU:CA	2.44	0.47
1:A:110:PRO:HD3	1:A:116:LEU:HD11	1.98	0.46
1:C:162:ASN:N	1:C:162:ASN:OD1	2.48	0.46
1:C:111:ASP:H	1:C:114:ASN:CB	2.28	0.46
1:D:185:LYS:HD2	1:D:189:ASP:OD1	2.15	0.46
1:C:48:MET:HE1	1:C:175:ARG:NH1	2.30	0.46
1:C:139:ASN:O	1:C:143:ILE:CG2	2.63	0.46
1:A:121:ILE:N	1:A:121:ILE:CD1	2.70	0.46
1:A:111:ASP:N	1:A:114:ASN:HB3	2.29	0.46
1:D:46:GLY:N	1:D:176:ALA:CB	2.78	0.46
1:D:195:LEU:HD21	1:D:247:PHE:CG	2.51	0.46
1:A:165:PRO:O	1:A:166:SER:C	2.54	0.46
1:A:72:MET:O	1:A:75:ASN:HB3	2.15	0.46
1:D:209:MET:O	1:D:210:PRO:C	2.53	0.46
1:C:105:PRO:HG3	1:D:155:GLY:CA	2.40	0.46
1:C:103:ILE:CD1	1:D:158:LEU:CD1	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:THR:OG1	1:D:68:ALA:N	2.49	0.46
1:C:144:LEU:O	1:C:147:SER:HB2	2.15	0.46
1:A:232:ILE:HD12	1:A:236:GLU:OE1	2.16	0.46
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.41	0.46
1:D:128:THR:HG22	1:D:129:SER:N	2.30	0.46
1:C:57:LEU:CD1	1:C:57:LEU:N	2.79	0.46
1:C:60:SER:O	1:C:152:VAL:HA	2.16	0.46
1:B:68:ALA:O	1:B:71:ALA:N	2.48	0.46
1:C:157:ASP:CB	1:D:218:PHE:CZ	2.92	0.46
1:B:59:LEU:HB3	1:B:152:VAL:HG11	1.98	0.46
1:B:53:ASP:O	1:B:54:MET:CE	2.63	0.46
1:B:62:LEU:HB3	1:B:127:SER:HB3	1.97	0.46
1:D:63:ARG:CZ	1:D:81:LYS:NZ	2.77	0.46
1:D:106:ILE:CD1	1:D:125:SER:HB2	2.46	0.46
1:A:184:ALA:HB3	1:A:195:LEU:HD21	1.98	0.46
1:A:113:LYS:O	1:A:113:LYS:HG3	2.16	0.46
1:C:79:MET:O	1:C:82:VAL:N	2.50	0.45
1:A:243:VAL:CG2	1:A:244:ASN:N	2.78	0.45
1:C:54:MET:HE1	1:C:133:ARG:CG	2.44	0.45
1:B:49:THR:HG22	1:B:238:SER:HB3	1.98	0.45
1:D:106:ILE:HD11	1:D:124:TYR:O	2.15	0.45
1:A:140:VAL:HG12	1:A:141:GLY:N	2.31	0.45
1:C:67:THR:CG2	1:C:70:GLU:OE1	2.49	0.45
1:A:67:THR:CG2	1:A:70:GLU:OE1	2.57	0.45
1:B:175:ARG:O	1:B:179:ASN:N	2.44	0.45
1:B:98:THR:HG22	1:B:130:LEU:HB2	1.98	0.45
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.58	0.45
1:C:59:LEU:HD11	1:C:147:SER:OG	2.17	0.45
1:D:57:LEU:HD23	1:D:57:LEU:N	2.31	0.45
1:B:79:MET:HE1	1:B:130:LEU:HB2	1.98	0.45
1:A:198:VAL:CG2	1:A:247:PHE:CD2	2.99	0.45
1:C:220:THR:O	1:C:223:ALA:HB3	2.16	0.45
1:D:114:ASN:O	1:D:115:ASN:CB	2.64	0.45
1:C:67:THR:HG1	1:C:68:ALA:H	1.65	0.45
1:B:110:PRO:HG3	1:B:118:GLU:N	2.32	0.45
1:C:103:ILE:CG2	1:C:126:VAL:HG23	2.39	0.45
1:A:173:ARG:NH1	1:A:203:GLU:OE1	2.50	0.45
1:A:158:LEU:HA	1:A:160:LEU:HD21	1.99	0.45
1:A:68:ALA:HB3	1:B:145:ASP:CG	2.37	0.45
1:C:67:THR:OG1	1:D:145:ASP:OD1	2.34	0.45
1:B:54:MET:HE2	1:B:135:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:O	1:B:218:PHE:CD2	2.70	0.45
1:C:98:THR:HG22	1:C:130:LEU:CB	2.47	0.45
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.67	0.45
1:C:48:MET:CG	1:C:168:VAL:HG13	2.47	0.45
1:A:204:LEU:HD23	1:B:43:THR:HG23	1.98	0.45
1:D:84:ASP:C	1:D:86:MET:N	2.70	0.45
1:B:101:ILE:CG2	1:C:160:LEU:HD11	2.47	0.45
1:D:217:GLN:HB3	1:D:221:MET:CG	2.47	0.45
1:D:48:MET:CE	1:D:171:GLU:CB	2.94	0.45
1:D:48:MET:HE2	1:D:171:GLU:CB	2.46	0.45
1:C:45:GLU:HA	1:C:176:ALA:HB1	1.98	0.45
1:C:97:GLN:HG3	1:C:98:THR:N	2.31	0.45
1:B:169:ILE:O	1:B:172:ALA:N	2.49	0.44
1:B:72:MET:O	1:B:75:ASN:N	2.50	0.44
1:C:94:ARG:O	1:D:231:PRO:HD3	2.16	0.44
1:C:165:PRO:CD	1:C:166:SER:H	2.29	0.44
1:D:147:SER:C	1:D:149:THR:N	2.69	0.44
1:C:47:MET:HE2	1:C:47:MET:HB2	1.84	0.44
1:D:98:THR:HG21	1:D:130:LEU:HB2	1.99	0.44
1:D:151:GLY:C	1:D:152:VAL:HG13	2.37	0.44
1:B:62:LEU:HD12	1:B:125:SER:OG	2.16	0.44
1:A:88:LYS:HG3	1:A:89:ALA:N	2.31	0.44
1:D:149:THR:HB	1:D:150:LEU:HD23	1.99	0.44
1:C:217:GLN:O	1:C:218:PHE:C	2.55	0.44
1:C:48:MET:HE1	1:C:175:ARG:HH12	1.83	0.44
1:B:161:VAL:HG13	1:B:162:ASN:C	2.38	0.44
1:D:114:ASN:O	1:D:115:ASN:HB2	2.17	0.44
1:B:146:GLU:OE1	1:B:150:LEU:CD1	2.66	0.44
1:A:144:LEU:O	1:A:147:SER:OG	2.31	0.44
1:C:213:ILE:HG12	1:C:221:MET:HG3	1.98	0.44
1:A:91:ILE:CD1	1:A:96:LEU:HD11	2.48	0.44
1:A:230:VAL:CG1	1:A:231:PRO:HD2	2.33	0.44
1:D:219:ARG:O	1:D:221:MET:N	2.51	0.44
1:D:57:LEU:N	1:D:57:LEU:CD2	2.80	0.44
1:A:209:MET:HG2	1:A:210:PRO:HD2	1.99	0.44
1:B:102:ASP:OD2	1:C:158:LEU:CD1	2.60	0.44
1:B:205:SER:O	1:B:207:PRO:HD3	2.17	0.44
1:A:171:GLU:O	1:A:175:ARG:HG2	2.16	0.44
1:C:241:VAL:CG2	1:C:242:SER:N	2.81	0.44
1:B:177:VAL:HG11	1:C:190:ALA:CB	2.48	0.44
1:A:159:ASN:O	1:A:161:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:TYR:HD2	1:D:119:PRO:HG3	1.83	0.43
1:B:115:ASN:HB3	1:B:116:LEU:H	1.66	0.43
1:A:161:VAL:HG23	1:A:162:ASN:O	2.19	0.43
1:A:184:ALA:CB	1:A:195:LEU:CD2	2.96	0.43
1:C:152:VAL:CG1	1:C:153:ASN:CG	2.86	0.43
1:C:83:LEU:O	1:C:86:MET:N	2.49	0.43
1:A:103:ILE:H	1:B:158:LEU:HG	1.83	0.43
1:D:100:GLY:C	1:D:101:ILE:HG12	2.38	0.43
1:C:48:MET:CE	1:C:175:ARG:NH1	2.81	0.43
1:A:98:THR:CG2	1:A:130:LEU:HD12	2.45	0.43
1:D:230:VAL:HG12	1:D:231:PRO:HD2	2.00	0.43
1:B:186:THR:HG22	1:B:187:LEU:N	2.33	0.43
1:C:240:ASN:OD1	1:C:240:ASN:C	2.57	0.43
1:C:140:VAL:CG1	1:C:141:GLY:N	2.81	0.43
1:C:221:MET:O	1:C:222:LEU:C	2.56	0.43
1:C:104:GLN:OE1	1:C:105:PRO:HD2	2.19	0.43
1:B:82:VAL:HG23	1:B:150:LEU:CD2	2.49	0.43
1:D:62:LEU:HD12	1:D:62:LEU:H	1.83	0.43
1:A:175:ARG:HH21	1:A:226:PRO:HG3	1.83	0.43
1:A:221:MET:O	1:A:224:ALA:N	2.51	0.43
1:C:201:ILE:O	1:D:40:ILE:HA	2.18	0.43
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.19	0.43
1:B:63:ARG:HD2	1:B:78:ALA:HB1	2.00	0.43
1:C:169:ILE:O	1:C:172:ALA:HB3	2.18	0.43
1:C:75:ASN:O	1:C:77:GLU:N	2.51	0.43
1:B:62:LEU:HA	1:B:126:VAL:O	2.18	0.43
1:C:94:ARG:NH1	1:C:94:ARG:HB2	2.34	0.43
1:A:91:ILE:HG21	1:A:143:ILE:CD1	2.48	0.43
1:B:213:ILE:HG13	1:B:236:GLU:O	2.19	0.43
1:B:54:MET:HG3	1:B:55:ALA:H	1.84	0.43
1:D:41:ALA:HB2	1:D:246:VAL:CG1	2.47	0.43
1:D:109:TYR:HA	1:D:110:PRO:HD2	1.77	0.43
1:B:104:GLN:HA	1:B:105:PRO:HD2	1.89	0.43
1:C:131:THR:HG1	1:D:233:ALA:HB2	1.84	0.43
1:A:165:PRO:HD2	1:B:227:ASP:OD1	2.19	0.43
1:C:93:ASP:OD1	1:C:94:ARG:N	2.52	0.43
1:A:131:THR:CG2	1:B:233:ALA:CB	2.97	0.43
1:A:133:ARG:NH2	1:B:231:PRO:HG3	2.34	0.43
1:A:172:ALA:O	1:A:175:ARG:HB2	2.19	0.43
1:C:57:LEU:HB3	1:C:59:LEU:HD21	2.00	0.42
1:D:61:VAL:O	1:D:75:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:HA	1:A:165:PRO:HD2	1.84	0.42
1:D:225:ALA:O	1:D:226:PRO:C	2.56	0.42
1:A:156:GLY:O	1:A:159:ASN:OD1	2.36	0.42
1:B:91:ILE:HG22	1:B:92:GLU:O	2.20	0.42
1:D:218:PHE:HB3	1:D:219:ARG:H	1.27	0.42
1:B:45:GLU:HA	1:B:241:VAL:O	2.19	0.42
1:C:184:ALA:CB	1:C:195:LEU:HD21	2.47	0.42
1:B:174:LYS:O	1:B:178:ALA:CB	2.67	0.42
1:B:48:MET:HE2	1:B:49:THR:H	1.84	0.42
1:D:48:MET:CE	1:D:171:GLU:CG	2.94	0.42
1:A:122:THR:O	1:A:122:THR:HG23	2.19	0.42
1:C:84:ASP:HB3	1:C:88:LYS:HE3	2.00	0.42
1:D:59:LEU:O	1:D:130:LEU:O	2.37	0.42
1:C:92:GLU:O	1:C:96:LEU:HG	2.20	0.42
1:A:100:GLY:CA	1:B:235:GLY:HA3	2.49	0.42
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.71	0.42
1:B:199:VAL:HG23	1:B:246:VAL:HG12	2.01	0.42
1:C:62:LEU:HA	1:C:127:SER:OG	2.19	0.42
1:C:63:ARG:HH12	1:C:81:LYS:HZ2	1.62	0.42
1:D:63:ARG:HD2	1:D:78:ALA:CB	2.50	0.42
1:C:103:ILE:HD13	1:D:158:LEU:CD1	2.49	0.42
1:C:133:ARG:NH2	1:D:231:PRO:HD3	2.34	0.42
1:C:118:GLU:HA	1:C:119:PRO:HD3	1.66	0.42
1:D:136:GLU:HA	1:D:136:GLU:OE1	2.19	0.42
1:D:104:GLN:HA	1:D:105:PRO:HD2	1.80	0.42
1:B:108:VAL:CG1	1:B:109:TYR:N	2.82	0.42
1:D:140:VAL:O	1:D:143:ILE:HD12	2.20	0.42
1:C:121:ILE:CD1	1:C:121:ILE:N	2.80	0.42
1:A:218:PHE:O	1:A:222:LEU:HG	2.20	0.42
1:D:79:MET:HE2	1:D:130:LEU:HD13	2.02	0.42
1:C:150:LEU:CD1	1:C:152:VAL:HG23	2.50	0.42
1:B:169:ILE:HD13	1:B:169:ILE:N	2.34	0.42
1:D:87:LYS:C	1:D:90:GLY:H	2.23	0.42
1:A:204:LEU:CD2	1:B:43:THR:HG23	2.49	0.42
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.85	0.42
1:A:59:LEU:HD13	1:A:147:SER:HB2	2.01	0.42
1:A:210:PRO:O	1:A:212:PRO:CD	2.63	0.42
1:A:75:ASN:O	1:A:76:ASN:C	2.57	0.42
1:C:82:VAL:CG1	1:C:83:LEU:N	2.81	0.42
1:C:137:LEU:O	1:C:138:ALA:C	2.57	0.42
1:A:78:ALA:O	1:A:81:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLY:O	1:C:158:LEU:N	2.53	0.41
1:D:63:ARG:NH1	1:D:81:LYS:HZ2	2.13	0.41
1:D:198:VAL:CG2	1:D:247:PHE:CD2	2.98	0.41
1:B:57:LEU:HA	1:B:57:LEU:HD13	1.88	0.41
1:A:209:MET:HE2	1:A:209:MET:HB3	1.77	0.41
1:D:124:TYR:N	1:D:124:TYR:CD1	2.88	0.41
1:D:208:PRO:HB3	1:D:240:ASN:O	2.20	0.41
1:B:204:LEU:HA	1:C:43:THR:HG23	2.01	0.41
1:A:188:ALA:HB1	1:A:193:VAL:O	2.20	0.41
1:D:96:LEU:HD23	1:D:131:THR:O	2.19	0.41
1:C:137:LEU:C	1:C:139:ASN:N	2.72	0.41
1:C:135:ARG:O	1:C:136:GLU:CB	2.66	0.41
1:C:200:GLU:HG3	1:C:201:ILE:N	2.34	0.41
1:A:106:ILE:HD11	1:A:125:SER:HB2	2.01	0.41
1:A:102:ASP:OD1	1:A:102:ASP:C	2.58	0.41
1:A:79:MET:HA	1:A:79:MET:CE	2.50	0.41
1:A:38:ALA:HB1	1:A:249:ILE:HB	2.02	0.41
1:A:201:ILE:HB	1:B:40:ILE:HG23	2.02	0.41
1:B:48:MET:O	1:B:238:SER:HA	2.21	0.41
1:A:185:LYS:O	1:A:186:THR:C	2.58	0.41
1:A:159:ASN:O	1:A:161:VAL:HG13	2.21	0.41
1:B:98:THR:HB	1:B:99:GLY:H	1.77	0.41
1:D:153:ASN:OD1	1:D:156:GLY:HA2	2.21	0.41
1:B:49:THR:O	1:B:50:ALA:HB2	2.21	0.41
1:C:75:ASN:C	1:C:77:GLU:N	2.72	0.41
1:D:110:PRO:CA	1:D:114:ASN:HB3	2.51	0.41
1:D:57:LEU:HD21	1:D:132:VAL:CG1	2.49	0.41
1:D:46:GLY:HA3	1:D:176:ALA:N	2.36	0.41
1:D:173:ARG:HA	1:D:241:VAL:HG11	2.02	0.41
1:C:72:MET:CE	1:D:140:VAL:HG12	2.51	0.41
1:C:65:ALA:O	1:C:67:THR:N	2.54	0.41
1:B:54:MET:O	1:B:137:LEU:HD13	2.21	0.41
1:B:91:ILE:HG22	1:B:96:LEU:HD11	2.02	0.41
1:B:71:ALA:HB1	1:B:126:VAL:CG2	2.51	0.41
1:A:154:GLN:HA	1:A:154:GLN:NE2	2.35	0.41
1:B:184:ALA:CB	1:B:247:PHE:CE1	3.04	0.41
1:A:85:ALA:O	1:A:89:ALA:HB2	2.21	0.41
1:A:230:VAL:CG1	1:A:231:PRO:CD	2.96	0.41
1:D:110:PRO:HA	1:D:114:ASN:CB	2.49	0.41
1:D:49:THR:HG21	1:D:232:ILE:HD11	2.03	0.41
1:A:184:ALA:CB	1:A:195:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:O	1:B:40:ILE:HA	2.21	0.41
1:C:62:LEU:O	1:C:63:ARG:HG2	2.21	0.40
1:B:121:ILE:HD11	1:B:124:TYR:CZ	2.56	0.40
1:B:140:VAL:HA	1:B:143:ILE:CG2	2.50	0.40
1:D:169:ILE:HG12	1:D:239:TYR:HD2	1.87	0.40
1:A:210:PRO:CG	1:B:223:ALA:HB1	2.52	0.40
1:D:79:MET:HE3	1:D:82:VAL:HG13	2.04	0.40
1:A:117:LYS:O	1:A:118:GLU:C	2.57	0.40
1:A:209:MET:O	1:A:211:MET:N	2.54	0.40
1:A:112:ASP:O	1:A:113:LYS:CB	2.69	0.40
1:A:241:VAL:HG12	1:A:242:SER:N	2.35	0.40
1:D:160:LEU:H	1:D:160:LEU:HG	1.70	0.40
1:C:219:ARG:HG3	1:C:220:THR:H	1.87	0.40
1:A:239:TYR:N	1:A:239:TYR:CD1	2.89	0.40
1:B:88:LYS:C	1:B:90:GLY:N	2.75	0.40

All (4) 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:C:113:LYS:NZ	1:D:127:SER:O[8_554]	1.85	0.35
1:C:102:ASP:O	1:D:113:LYS:NZ[8_554]	1.88	0.32
1:B:114:ASN:OD1	1:B:215:ARG:NH2[10_555]	2.05	0.15
1:C:127:SER:O	1:D:113:LYS:NZ[8_554]	2.09	0.11

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	212/224 (95%)	182 (86%)	26 (12%)	4 (2%)	10 51
1	B	212/224 (95%)	191 (90%)	21 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	212/224 (95%)	186 (88%)	21 (10%)	5 (2%)	7 47
1	D	212/224 (95%)	181 (85%)	26 (12%)	5 (2%)	7 47
All	All	848/896 (95%)	740 (87%)	94 (11%)	14 (2%)	11 54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	VAL
1	D	114	ASN
1	D	152	VAL
1	C	152	VAL
1	D	115	ASN
1	D	117	LYS
1	A	114	ASN
1	A	115	ASN
1	A	118	GLU
1	C	157	ASP
1	C	149	THR
1	D	116	LEU
1	C	148	VAL
1	C	161	VAL

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	171/180 (95%)	132 (77%)	39 (23%)	1 6
1	B	171/180 (95%)	130 (76%)	41 (24%)	1 5
1	C	171/180 (95%)	121 (71%)	50 (29%)	0 3
1	D	171/180 (95%)	131 (77%)	40 (23%)	1 5
All	All	684/720 (95%)	514 (75%)	170 (25%)	1 5

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	42	VAL
1	A	48	MET
1	A	57	LEU
1	A	61	VAL
1	A	64	GLN
1	A	67	THR
1	A	69	ARG
1	A	70	GLU
1	A	73	THR
1	A	82	VAL
1	A	83	LEU
1	A	92	GLU
1	A	112	ASP
1	A	113	LYS
1	A	116	LEU
1	A	117	LYS
1	A	121	ILE
1	A	122	THR
1	A	128	THR
1	A	130	LEU
1	A	135	ARG
1	A	143	ILE
1	A	158	LEU
1	A	159	ASN
1	A	160	LEU
1	A	161	VAL
1	A	162	ASN
1	A	181	ILE
1	A	195	LEU
1	A	199	VAL
1	A	205	SER
1	A	209	MET
1	A	215	ARG
1	A	218	PHE
1	A	221	MET
1	A	222	LEU
1	A	232	ILE
1	A	240	ASN
1	B	39	ARG
1	B	47	MET
1	B	48	MET
1	B	51	SER

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Mol	Chain	Res	Type
1	B	54	MET
1	B	67	THR
1	B	69	ARG
1	B	75	ASN
1	B	76	ASN
1	B	77	GLU
1	B	80	THR
1	B	84	ASP
1	B	97	GLN
1	B	113	LYS
1	B	114	ASN
1	B	116	LEU
1	B	120	THR
1	B	122	THR
1	B	128	THR
1	B	130	LEU
1	B	132	VAL
1	B	133	ARG
1	B	135	ARG
1	B	136	GLU
1	B	139	ASN
1	B	146	GLU
1	B	159	ASN
1	B	160	LEU
1	B	162	ASN
1	B	163	ASP
1	B	175	ARG
1	B	177	VAL
1	B	193	VAL
1	B	195	LEU
1	B	198	VAL
1	B	199	VAL
1	B	202	SER
1	B	218	PHE
1	B	230	VAL
1	B	240	ASN
1	B	245	VAL
1	C	40	ILE
1	C	43	THR
1	C	45	GLU
1	C	47	MET
1	C	51	SER

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Mol	Chain	Res	Type
1	C	64	GLN
1	C	66	LYS
1	C	67	THR
1	C	77	GLU
1	C	96	LEU
1	C	102	ASP
1	C	103	ILE
1	C	108	VAL
1	C	112	ASP
1	C	115	ASN
1	C	116	LEU
1	C	120	THR
1	C	121	ILE
1	C	128	THR
1	C	130	LEU
1	C	137	LEU
1	C	140	VAL
1	C	143	ILE
1	C	149	THR
1	C	150	LEU
1	C	158	LEU
1	C	161	VAL
1	C	162	ASN
1	C	169	ILE
1	C	175	ARG
1	C	183	LYS
1	C	189	ASP
1	C	195	LEU
1	C	197	ARG
1	C	198	VAL
1	C	200	GLU
1	C	218	PHE
1	C	219	ARG
1	C	220	THR
1	C	222	LEU
1	C	228	ASN
1	C	230	VAL
1	C	232	ILE
1	C	237	ASN
1	C	238	SER
1	C	241	VAL
1	C	243	VAL

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Mol	Chain	Res	Type
1	C	245	VAL
1	C	249	ILE
1	C	250	LYS
1	D	39	ARG
1	D	49	THR
1	D	57	LEU
1	D	59	LEU
1	D	62	LEU
1	D	67	THR
1	D	73	THR
1	D	77	GLU
1	D	101	ILE
1	D	106	ILE
1	D	112	ASP
1	D	116	LEU
1	D	120	THR
1	D	121	ILE
1	D	122	THR
1	D	130	LEU
1	D	140	VAL
1	D	143	ILE
1	D	150	LEU
1	D	153	ASN
1	D	159	ASN
1	D	160	LEU
1	D	162	ASN
1	D	163	ASP
1	D	166	SER
1	D	171	GLU
1	D	173	ARG
1	D	183	LYS
1	D	195	LEU
1	D	201	ILE
1	D	205	SER
1	D	218	PHE
1	D	219	ARG
1	D	230	VAL
1	D	232	ILE
1	D	239	TYR
1	D	240	ASN
1	D	241	VAL
1	D	245	VAL

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Mol	Chain	Res	Type
1	D	246	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	B	114	ASN
1	B	153	ASN
1	C	75	ASN
1	C	153	ASN
1	C	240	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	214/224 (95%)	-0.37	0	100	100	83, 122, 157, 173	0
1	B	214/224 (95%)	-0.27	0	100	100	79, 122, 163, 187	0
1	C	214/224 (95%)	-0.41	0	100	100	78, 118, 157, 176	0
1	D	214/224 (95%)	-0.38	1 (0%)	91	88	77, 120, 155, 166	0
All	All	856/896 (95%)	-0.36	1 (0%)	95	94	77, 121, 158, 187	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	SER	2.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.