Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 PM GMT

PDB ID	:	4KEV
Title	:	Crystal structure of SsoPox W263L
Authors	:	Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.
Deposited on	:	2013-04-26
Resolution	:	2.65 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:

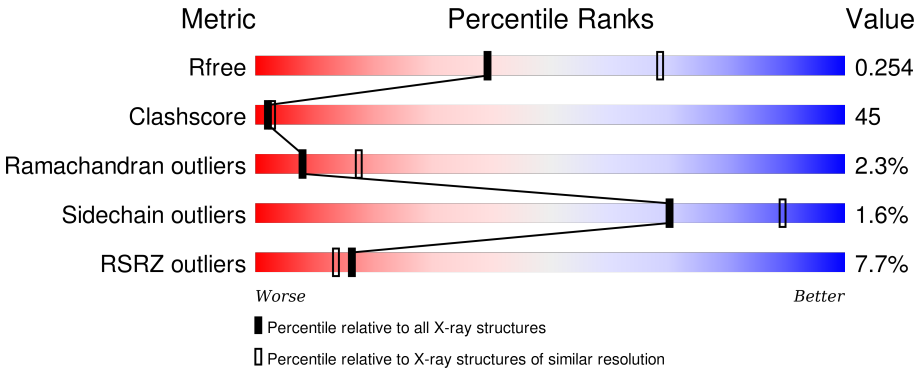
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	314	4% 46% 50% ·
1	B	314	6% 47% 51% ·
1	C	314	8% 48% 49% ·
1	D	314	13% 43% 53% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	KCX	D	137	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10258 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 Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	1	0
			2515	1615	425	468	7			
1	B	314	Total	C	N	O	S	0	0	0
			2507	1607	425	468	7			
1	C	314	Total	C	N	O	S	0	1	0
			2518	1616	426	469	7			
1	D	314	Total	C	N	O	S	0	1	0
			2518	1613	429	469	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	TRP	ENGINEERED MUTATION	UNP Q97VT7
B	263	LEU	TRP	ENGINEERED MUTATION	UNP Q97VT7
C	263	LEU	TRP	ENGINEERED MUTATION	UNP Q97VT7
D	263	LEU	TRP	ENGINEERED MUTATION	UNP Q97VT7

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Co 1 1	0	0
3	A	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0

- Molecule 4 is water.

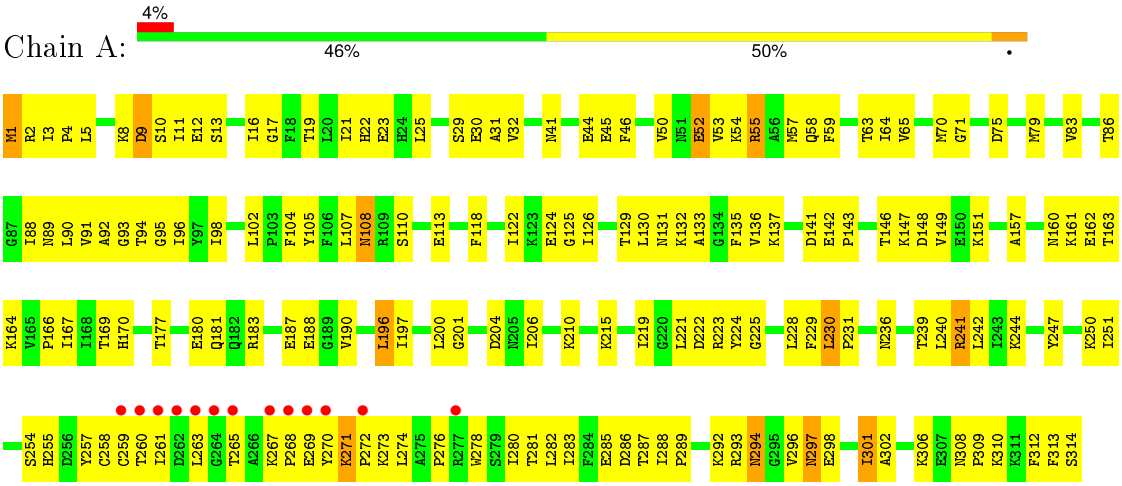
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	57	Total O 57 57	0	0
4	C	31	Total O 31 31	0	0
4	D	29	Total O 29 29	0	0

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.

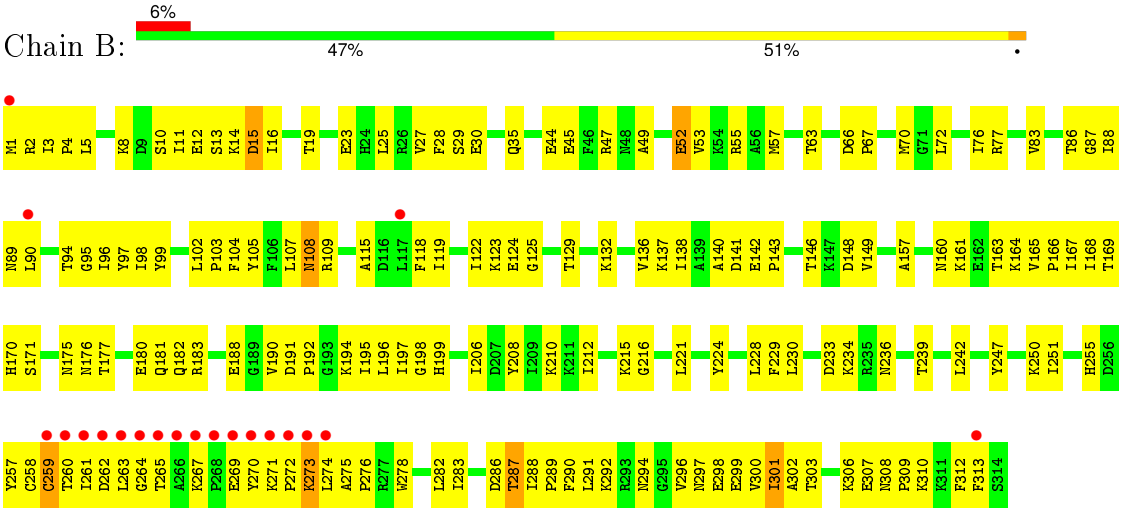
- Molecule 1: Aryldialkylphosphatase

Chain A:



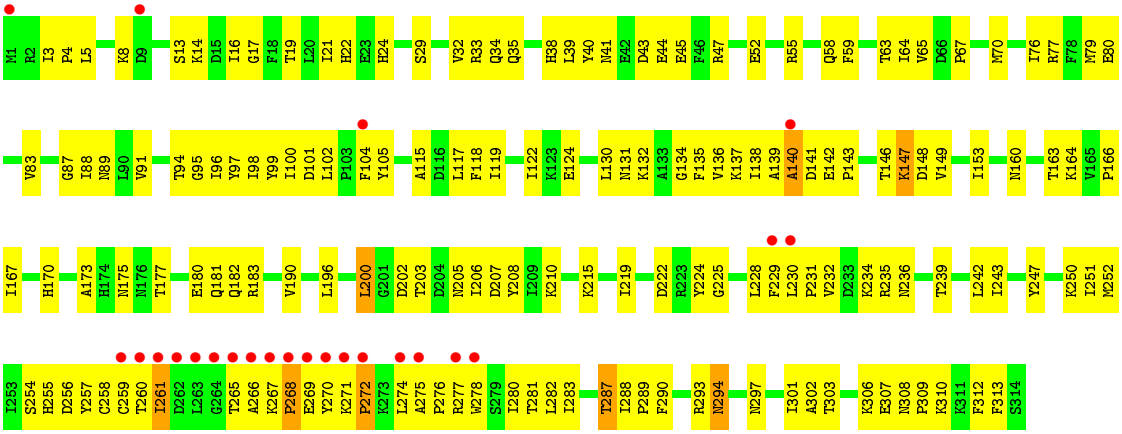
- Molecule 1: Aryldialkylphosphatase

Chain B:

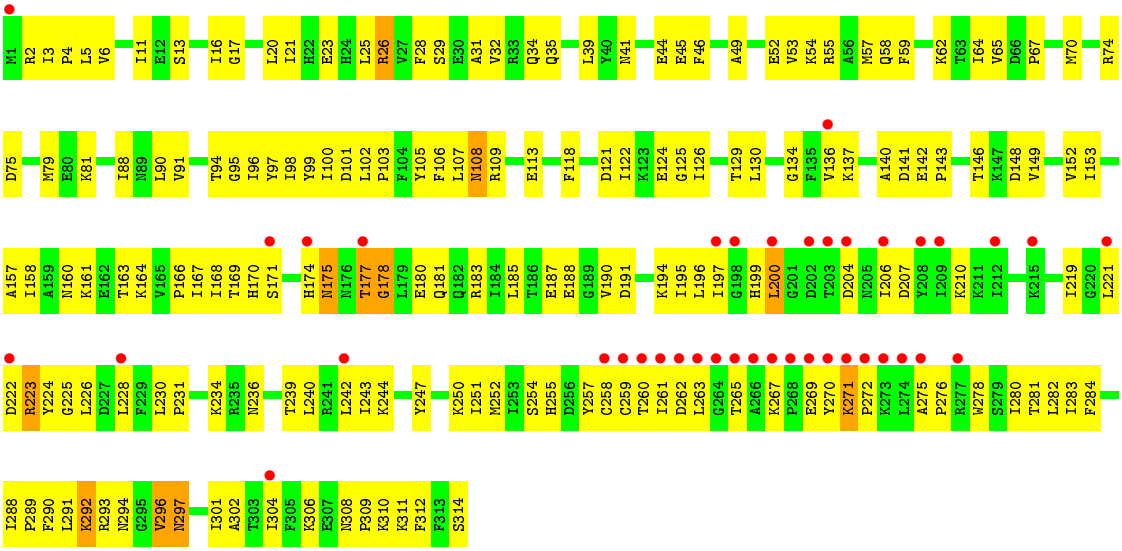


- Molecule 1: Aryldialkylphosphatase

Chain C:



- Molecule 1: Aryldialkylphosphatase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.91Å 105.08Å 153.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 2.65 46.10 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.14-2.65) 99.2 (46.10-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.203 , 0.250 0.206 , 0.254	Depositor DCC
R_{free} test set	2015 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 39816 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10258	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CO, FE2, KCX

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	0.21	0/2555	0.37	0/3449
1	B	0.21	0/2543	0.37	0/3433
1	C	0.21	0/2555	0.36	0/3449
1	D	0.21	0/2554	0.36	0/3447
All	All	0.21	0/10207	0.37	0/13778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2515	0	2551	252	1
1	B	2507	0	2542	225	1
1	C	2518	0	2550	202	0
1	D	2518	0	2554	260	0
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
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	75	0	0	11	0
4	B	57	0	0	10	0
4	C	31	0	0	10	0
4	D	29	0	0	7	0
All	All	10258	0	10197	910	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 45.

All (910) 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:102:LEU:CD2	1:B:148:ASP:HB3	1.59	1.30
1:B:29:SER:HB3	4:B:527:HOH:O	1.37	1.24
1:A:296:VAL:HB	4:A:566:HOH:O	1.11	1.24
1:C:52:GLU:HG3	1:C:280:ILE:HG21	1.23	1.21
1:C:102:LEU:CD1	1:C:148:ASP:HB3	1.74	1.15
1:D:129:THR:HB	4:D:509:HOH:O	1.47	1.15
1:B:102:LEU:HD22	1:B:148:ASP:HB3	1.27	1.13
1:B:291:LEU:HB3	1:B:296:VAL:HG11	1.19	1.13
1:A:19:THR:HG22	1:A:63:THR:HB	1.16	1.13
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.25	1.12
1:D:29:SER:HB2	1:D:32:VAL:HG12	1.29	1.11
1:B:301:ILE:HD12	1:B:302:ALA:N	1.65	1.10
1:A:55:ARG:HH11	1:A:55:ARG:CG	1.66	1.08
1:D:221:LEU:HD13	1:D:239:THR:HG22	1.34	1.07
1:A:206:ILE:HD11	1:A:242:LEU:CD2	1.84	1.06
1:B:2:ARG:HH21	1:B:13:SER:HB2	1.18	1.06
1:D:292:LYS:H	1:D:296:VAL:CG1	1.67	1.06
1:D:26[A]:ARG:HH11	1:D:26[A]:ARG:CG	1.66	1.06
1:A:98:ILE:HD13	1:A:102:LEU:HD12	1.37	1.05
1:A:19:THR:CG2	1:A:63:THR:HB	1.84	1.05
1:A:98:ILE:CD1	1:A:102:LEU:HD12	1.86	1.05
1:A:55:ARG:HH11	1:A:55:ARG:HG2	0.89	1.04
1:A:221:LEU:HD13	1:A:239:THR:HG22	1.40	1.03
1:B:176:ASN:HA	1:B:208:TYR:OH	1.58	1.03
1:B:221:LEU:HD13	1:B:239:THR:HG22	1.38	1.02
1:B:55:ARG:HD3	4:B:544:HOH:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLU:HG3	1:C:280:ILE:CG2	1.90	1.01
1:A:102:LEU:HD13	1:A:148:ASP:HB3	1.04	1.00
1:D:99:TYR:CD1	1:D:141:ASP:HB2	1.96	1.00
1:A:55:ARG:NH1	1:A:55:ARG:HG2	1.67	1.00
1:A:25:LEU:HD11	1:A:90:LEU:HD11	1.44	0.99
1:A:102:LEU:CD1	1:A:148:ASP:HB3	1.92	0.99
1:A:258:CYS:HB2	1:A:261:ILE:CG1	1.93	0.99
1:D:21:ILE:HA	1:D:65:VAL:CG1	1.92	0.99
1:D:291:LEU:O	1:D:292:LYS:HB3	1.63	0.98
1:B:291:LEU:O	1:B:296:VAL:HG12	1.61	0.98
1:D:219:ILE:HD11	1:D:251:ILE:HG12	1.45	0.97
1:A:129:THR:HG22	1:A:131:ASN:H	1.28	0.97
1:D:297:ASN:H	1:D:297:ASN:HD22	0.98	0.97
1:C:301:ILE:HD12	1:C:302:ALA:N	1.79	0.96
1:A:255:HIS:NE2	1:A:283:ILE:HG23	1.81	0.95
1:D:26[A]:ARG:HH11	1:D:26[A]:ARG:HG3	1.31	0.95
1:C:70:MET:CE	1:C:96:ILE:HG23	1.97	0.95
1:A:98:ILE:CD1	1:A:102:LEU:CD1	2.46	0.94
1:A:45:GLU:HG2	1:A:260:THR:HG21	1.49	0.94
1:D:206:ILE:HG13	1:D:210:LYS:HE3	1.50	0.94
1:B:102:LEU:CD2	1:B:148:ASP:CB	2.46	0.94
1:D:29:SER:HB2	1:D:32:VAL:CG1	1.96	0.94
1:A:301:ILE:C	1:A:301:ILE:HD12	1.88	0.93
1:C:45:GLU:HG2	1:C:260:THR:HG21	1.49	0.93
1:A:258:CYS:HB2	1:A:261:ILE:HG12	1.48	0.92
1:D:292:LYS:N	1:D:296:VAL:CG1	2.33	0.92
1:C:180:GLU:OE2	1:C:183:ARG:NH1	2.02	0.92
1:B:273:LYS:H	1:B:276:PRO:HG3	1.33	0.92
1:D:301:ILE:HD12	1:D:302:ALA:N	1.84	0.91
1:A:161:LYS:NZ	1:A:188:GLU:O	2.04	0.91
1:C:102:LEU:HD13	1:C:148:ASP:HB3	1.50	0.91
1:B:228:LEU:HD11	1:B:274:LEU:HD22	1.48	0.91
1:A:102:LEU:HD13	1:A:148:ASP:CB	1.98	0.90
1:A:219:ILE:O	1:A:219:ILE:HD12	1.71	0.90
1:D:283:ILE:HD12	1:D:284:PHE:N	1.86	0.90
1:B:146:THR:OG1	1:B:149:VAL:HG23	1.71	0.90
1:B:291:LEU:C	1:B:296:VAL:CG1	2.41	0.90
1:B:176:ASN:ND2	1:B:208:TYR:CE2	2.40	0.89
1:B:107:LEU:O	1:B:108:ASN:HB2	1.69	0.89
1:A:98:ILE:HD13	1:A:102:LEU:CD1	2.03	0.89
1:C:267:LYS:HB3	1:C:268:PRO:HD2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:HG13	1:C:101:ASP:H	1.38	0.89
1:B:261:ILE:HD11	1:B:263:LEU:HD12	1.53	0.88
1:D:292:LYS:H	1:D:296:VAL:HG12	1.39	0.88
1:D:21:ILE:HA	1:D:65:VAL:HG12	1.52	0.88
1:D:100:ILE:HG23	1:D:101:ASP:H	1.38	0.88
1:D:21:ILE:HD12	1:D:65:VAL:HG11	1.54	0.87
1:D:224:TYR:HE2	1:D:236:ASN:ND2	1.73	0.87
1:A:206:ILE:CD1	1:A:242:LEU:HD21	2.05	0.87
1:C:29:SER:HB3	4:C:518:HOH:O	1.75	0.87
1:B:291:LEU:CB	1:B:296:VAL:HG11	2.04	0.86
1:D:149:VAL:O	1:D:152:VAL:HG12	1.74	0.86
1:C:182:GLN:HE22	1:C:215:LYS:HB2	1.41	0.86
1:A:206:ILE:HD11	1:A:242:LEU:HD23	1.56	0.86
1:D:206:ILE:HD11	1:D:242:LEU:CD2	2.06	0.86
1:A:306:LYS:HD2	4:A:558:HOH:O	1.76	0.85
1:D:46:PHE:CE1	1:D:81:LYS:HG2	2.12	0.85
1:C:277:ARG:O	1:C:282:LEU:HD12	1.76	0.84
1:D:297:ASN:HD22	1:D:297:ASN:N	1.74	0.84
1:B:271:LYS:HB3	1:B:272:PRO:CD	2.08	0.84
1:A:206:ILE:CD1	1:A:242:LEU:CD2	2.56	0.84
1:C:271:LYS:HB3	1:C:272:PRO:HD3	1.60	0.84
1:C:282:LEU:HD23	1:C:282:LEU:O	1.78	0.83
1:B:206:ILE:HD11	1:B:242:LEU:CD2	2.08	0.83
1:A:301:ILE:HD12	1:A:302:ALA:N	1.93	0.83
1:A:104[B]:PHE:HD2	1:B:263:LEU:HD23	1.41	0.83
1:D:301:ILE:HD12	1:D:301:ILE:C	1.98	0.82
1:B:301:ILE:C	1:B:301:ILE:HD12	1.99	0.82
1:B:138:ILE:HD12	1:B:138:ILE:C	2.00	0.82
1:B:206:ILE:HD11	1:B:242:LEU:HD23	1.60	0.82
1:A:258:CYS:CB	1:A:261:ILE:HG12	2.07	0.82
1:D:292:LYS:N	1:D:296:VAL:HG13	1.95	0.82
1:D:297:ASN:H	1:D:297:ASN:ND2	1.77	0.81
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.14	0.81
1:C:301:ILE:HD12	1:C:301:ILE:C	2.01	0.81
1:D:107:LEU:O	1:D:108:ASN:HB2	1.80	0.81
1:A:19:THR:HG22	1:A:63:THR:CB	2.07	0.81
1:A:228:LEU:HD13	1:A:228:LEU:O	1.80	0.81
1:B:233:ASP:HB3	4:B:540:HOH:O	1.79	0.80
1:A:161:LYS:CE	1:A:188:GLU:O	2.28	0.80
1:D:230:LEU:HD12	1:D:231:PRO:HD2	1.61	0.80
1:A:225:GLY:HA3	1:A:278:TRP:HD1	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:O	1:C:65:VAL:HG13	1.80	0.80
1:B:14:LYS:O	1:B:16:ILE:N	2.15	0.80
1:C:288:ILE:HB	1:C:289:PRO:HD3	1.62	0.80
1:A:5:LEU:HD21	1:A:11:ILE:HG12	1.62	0.80
1:B:102:LEU:HD23	1:B:148:ASP:HB3	1.61	0.79
1:C:98:ILE:O	1:C:98:ILE:HD12	1.81	0.79
1:C:70:MET:HE2	1:C:96:ILE:HG23	1.62	0.79
1:B:176:ASN:ND2	1:B:208:TYR:HE2	1.78	0.79
1:A:219:ILE:CD1	1:A:251:ILE:HA	2.12	0.79
1:C:52:GLU:OE2	1:C:280:ILE:HG22	1.82	0.79
1:B:2:ARG:O	1:B:2:ARG:HD2	1.82	0.79
1:D:288:ILE:HB	1:D:289:PRO:HD3	1.65	0.79
1:B:2:ARG:NH2	1:B:13:SER:HB2	1.97	0.79
1:C:70:MET:HE1	1:C:96:ILE:HG23	1.62	0.79
1:C:21:ILE:HD12	1:C:65:VAL:HG11	1.63	0.79
1:A:110:SER:OG	1:A:113:GLU:HG3	1.81	0.79
1:A:230:LEU:HD12	1:A:231:PRO:HD2	1.64	0.79
1:A:282:LEU:O	1:A:282:LEU:HD13	1.82	0.79
1:D:99:TYR:CE1	1:D:141:ASP:HB2	2.16	0.79
1:D:26[A]:ARG:HH11	1:D:26[A]:ARG:HG2	1.46	0.78
1:B:57:MET:HE3	1:B:88:ILE:HB	1.65	0.78
1:A:267:LYS:HZ3	1:B:109:ARG:CZ	1.96	0.78
1:B:57:MET:CE	1:B:88:ILE:HB	2.15	0.77
1:A:296:VAL:O	1:A:297:ASN:CG	2.23	0.77
1:D:196:LEU:C	1:D:196:LEU:HD23	2.04	0.76
1:C:21:ILE:HA	1:C:65:VAL:CG1	2.16	0.76
1:C:102:LEU:HD12	1:C:148:ASP:HB3	1.67	0.76
1:D:100:ILE:HG23	1:D:101:ASP:N	2.01	0.76
1:A:219:ILE:HD11	1:A:251:ILE:HA	1.67	0.76
1:B:301:ILE:CD1	1:B:302:ALA:N	2.48	0.76
1:B:3:ILE:HG22	1:B:11:ILE:O	1.85	0.76
1:D:21:ILE:CA	1:D:65:VAL:CG1	2.64	0.76
1:D:206:ILE:CG1	1:D:210:LYS:HE3	2.16	0.76
1:D:102:LEU:HD12	1:D:103:PRO:HD2	1.69	0.75
1:A:58:GLN:HG3	1:C:58:GLN:O	1.87	0.75
1:A:21:ILE:HA	1:A:65:VAL:HG22	1.68	0.74
1:A:281:THR:O	1:A:281:THR:HG22	1.86	0.74
1:C:267:LYS:HD2	4:C:520:HOH:O	1.86	0.74
1:C:100:ILE:HG13	1:C:101:ASP:N	2.03	0.74
1:A:9:ASP:O	1:A:10:SER:HB3	1.86	0.74
1:B:163:THR:O	1:B:164:LYS:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD11	1:B:274:LEU:CD2	2.19	0.73
1:D:142:GLU:N	1:D:143:PRO:HD2	2.03	0.73
1:C:39:LEU:HD13	1:D:105:TYR:OH	1.87	0.73
1:B:228:LEU:HD22	1:B:228:LEU:H	1.53	0.73
1:D:290:PHE:HA	1:D:293:ARG:NH2	2.04	0.73
1:A:263:LEU:HG	1:A:265:THR:H	1.51	0.73
1:A:288:ILE:HB	1:A:289:PRO:HD3	1.69	0.73
1:B:272:PRO:O	1:B:273:LYS:HB2	1.87	0.72
1:A:137:KCX:OQ1	1:A:170:HIS:HB2	1.88	0.72
1:B:291:LEU:O	1:B:296:VAL:CG1	2.36	0.72
1:C:104[B]:PHE:CD1	1:D:263:LEU:HD23	2.25	0.72
1:D:21:ILE:HA	1:D:65:VAL:HG11	1.70	0.72
1:D:291:LEU:O	1:D:292:LYS:CB	2.36	0.72
1:A:21:ILE:HD12	1:A:65:VAL:HG21	1.72	0.72
1:A:224:TYR:HE1	1:A:236:ASN:OD1	1.72	0.72
1:D:283:ILE:HD12	1:D:283:ILE:C	2.09	0.72
1:D:26[A]:ARG:HH22	1:D:75:ASP:CB	2.02	0.72
1:B:228:LEU:CD1	1:B:274:LEU:HD22	2.19	0.72
1:C:302:ALA:O	1:C:306:LYS:HB2	1.90	0.71
1:C:258:CYS:O	1:C:261:ILE:N	2.23	0.71
1:D:2:ARG:HE	1:D:314:SER:HA	1.53	0.71
1:B:302:ALA:O	1:B:306:LYS:HB2	1.89	0.71
1:D:100:ILE:HD12	1:D:146:THR:HG21	1.72	0.71
1:D:25:LEU:O	1:D:259:CYS:HB2	1.89	0.71
1:A:129:THR:HG22	1:A:130:LEU:N	2.05	0.71
1:A:163:THR:O	1:A:164:LYS:HB2	1.91	0.71
1:A:257:TYR:HA	1:A:278:TRP:CZ2	2.26	0.71
1:D:224:TYR:CE2	1:D:236:ASN:ND2	2.57	0.71
1:A:267:LYS:NZ	1:B:109:ARG:CZ	2.54	0.71
1:B:175:ASN:OD1	1:B:177:THR:HG23	1.91	0.70
1:D:160:ASN:ND2	1:D:190:VAL:HG13	2.05	0.70
1:A:206:ILE:HD12	1:A:242:LEU:HD21	1.71	0.70
1:B:258:CYS:HB2	1:B:261:ILE:HB	1.72	0.70
1:D:206:ILE:HD11	1:D:242:LEU:HD21	1.73	0.70
1:A:296:VAL:HG23	1:A:297:ASN:H	1.54	0.70
1:C:105:TYR:HD2	1:D:262:ASP:OD1	1.73	0.70
1:B:291:LEU:HB3	1:B:296:VAL:CG1	2.11	0.70
1:C:267:LYS:HB3	1:C:268:PRO:CD	2.21	0.70
1:B:102:LEU:HD23	1:B:148:ASP:CB	2.17	0.70
1:A:17:GLY:O	1:A:19:THR:HG23	1.91	0.70
1:A:257:TYR:CE1	1:A:278:TRP:O	2.45	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLU:HG3	4:B:545:HOH:O	1.92	0.70
1:B:138:ILE:HD12	1:B:138:ILE:O	1.91	0.70
1:B:170:HIS:ND1	1:B:199:HIS:CD2	2.60	0.70
1:D:99:TYR:CD1	1:D:141:ASP:CB	2.74	0.69
1:C:182:GLN:NE2	1:C:215:LYS:HB2	2.06	0.69
1:A:183:ARG:O	1:A:187:GLU:HG3	1.91	0.69
1:A:225:GLY:HA3	1:A:278:TRP:CD1	2.27	0.69
1:A:296:VAL:HG23	1:A:297:ASN:N	2.07	0.69
1:B:136:VAL:CG1	1:B:167:ILE:HG12	2.23	0.69
1:C:29:SER:HB2	1:C:32:VAL:HG22	1.73	0.69
1:C:230:LEU:CD1	1:C:234:LYS:HD3	2.23	0.69
1:D:21:ILE:C	1:D:65:VAL:CG1	2.61	0.69
1:B:4:PRO:C	1:B:5:LEU:HD12	2.12	0.69
1:D:222:ASP:O	1:D:223:ARG:HG3	1.91	0.69
1:A:53:VAL:O	1:A:57:MET:HG3	1.91	0.69
1:C:137:KCX:OQ2	1:C:170:HIS:HB2	1.92	0.69
1:D:174:HIS:O	1:D:175:ASN:HB3	1.91	0.69
1:C:260:THR:HG22	1:C:260:THR:O	1.93	0.69
1:A:104[B]:PHE:CD2	1:B:263:LEU:HD23	2.27	0.69
1:B:299:GLU:OE1	1:B:299:GLU:N	2.27	0.68
1:C:52:GLU:CG	1:C:280:ILE:CG2	2.70	0.68
1:B:221:LEU:CD1	1:B:239:THR:HG22	2.21	0.68
1:A:267:LYS:HD2	1:A:270:TYR:HE1	1.57	0.68
1:D:26[A]:ARG:CG	1:D:26[A]:ARG:NH1	2.39	0.68
1:A:95:GLY:HA2	1:A:118:PHE:CE1	2.29	0.68
1:D:282:LEU:C	1:D:282:LEU:HD13	2.13	0.68
1:D:230:LEU:HD11	1:D:234:LYS:HD3	1.74	0.67
1:A:52:GLU:OE2	1:A:52:GLU:HA	1.94	0.67
1:D:11:ILE:C	1:D:11:ILE:HD12	2.14	0.67
1:D:107:LEU:O	1:D:108:ASN:CB	2.42	0.67
1:A:224:TYR:OH	1:A:239:THR:HG21	1.93	0.67
1:A:29:SER:HB2	1:A:32:VAL:HG22	1.75	0.67
1:C:24:HIS:CE1	1:C:67:PRO:HG2	2.29	0.67
1:B:161:LYS:NZ	1:B:161:LYS:HB2	2.10	0.67
1:A:301:ILE:C	1:A:301:ILE:CD1	2.62	0.67
1:C:196:LEU:C	1:C:196:LEU:HD23	2.15	0.67
1:B:247:TYR:O	1:B:251:ILE:HG13	1.95	0.67
1:B:271:LYS:CB	1:B:272:PRO:HD3	2.14	0.66
1:C:303:THR:HA	1:C:307:GLU:HB2	1.75	0.66
1:D:102:LEU:CD1	1:D:103:PRO:HD2	2.25	0.66
1:D:222:ASP:O	1:D:223:ARG:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:TYR:HH	1:D:99:TYR:HH	1.40	0.66
1:A:308:ASN:HB2	1:A:309:PRO:HD3	1.76	0.66
1:A:265:THR:O	1:A:265:THR:HG22	1.93	0.66
1:C:230:LEU:HD11	1:C:234:LYS:HD3	1.77	0.66
1:A:130:LEU:HD22	1:A:130:LEU:N	2.11	0.66
1:D:206:ILE:CD1	1:D:242:LEU:HD21	2.25	0.66
1:D:11:ILE:O	1:D:11:ILE:HD12	1.96	0.66
1:B:45:GLU:HG2	1:B:260:THR:HG21	1.78	0.66
1:D:3:ILE:HG13	1:D:11:ILE:CD1	2.25	0.66
1:C:142:GLU:HB3	1:C:143:PRO:HD3	1.77	0.66
1:B:160:ASN:OD1	1:B:190:VAL:HG13	1.96	0.66
1:A:271:LYS:HB3	1:A:272:PRO:HD3	1.78	0.65
1:C:104[A]:PHE:CE1	1:D:99:TYR:HD2	2.15	0.65
1:D:26[B]:ARG:HE	1:D:28:PHE:HE2	1.45	0.65
1:C:45:GLU:HG2	1:C:260:THR:CG2	2.24	0.65
1:D:225:GLY:O	1:D:275:ALA:HB1	1.96	0.65
1:B:301:ILE:HD12	1:B:302:ALA:CA	2.27	0.65
1:A:273:LYS:C	1:A:274:LEU:HD12	2.16	0.65
1:D:196:LEU:CD2	1:D:196:LEU:C	2.64	0.65
1:A:221:LEU:CD1	1:A:239:THR:HG22	2.21	0.65
1:D:158:ILE:HA	1:D:161:LYS:NZ	2.10	0.65
1:C:261:ILE:O	1:C:261:ILE:HG23	1.95	0.65
1:B:195:ILE:HG22	1:B:196:LEU:N	2.11	0.65
1:C:175:ASN:ND2	1:C:177:THR:HG23	2.12	0.65
1:B:206:ILE:CD1	1:B:242:LEU:HD21	2.28	0.64
1:D:228:LEU:C	1:D:228:LEU:HD13	2.18	0.64
1:A:46:PHE:O	1:A:50:VAL:HG23	1.97	0.64
1:B:163:THR:C	1:B:164:LYS:HD2	2.17	0.64
1:D:149:VAL:O	1:D:153:ILE:HG13	1.97	0.64
1:A:11:ILE:HD11	1:A:16:ILE:HG22	1.79	0.64
1:B:161:LYS:HZ2	1:B:161:LYS:HB2	1.63	0.64
1:A:296:VAL:O	1:A:297:ASN:CB	2.45	0.64
1:A:258:CYS:HB2	1:A:261:ILE:CD1	2.27	0.64
1:A:270:TYR:O	1:A:274:LEU:HD13	1.97	0.64
1:C:88:ILE:HG12	1:C:89:ASN:N	2.13	0.64
1:A:228:LEU:HD13	1:A:228:LEU:C	2.18	0.64
1:D:302:ALA:O	1:D:306:LYS:HB2	1.98	0.63
1:A:129:THR:HG22	1:A:131:ASN:N	2.08	0.63
1:A:267:LYS:HD2	1:A:270:TYR:CE1	2.33	0.63
1:B:182:GLN:HE22	1:B:215:LYS:HB2	1.63	0.63
1:C:280:ILE:O	1:C:280:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG23	1:B:3:ILE:O	1.97	0.63
1:C:219:ILE:HG12	1:C:250:LYS:O	1.98	0.63
1:A:129:THR:CG2	1:A:130:LEU:N	2.61	0.63
1:A:1:MET:O	1:A:2:ARG:HB3	1.97	0.63
1:A:13:SER:OG	1:A:314:SER:HB3	1.99	0.63
1:D:29:SER:CB	1:D:32:VAL:HG12	2.18	0.63
1:B:157:ALA:HB1	1:B:188:GLU:HB3	1.81	0.63
1:A:261:ILE:HG22	1:A:263:LEU:H	1.62	0.63
1:A:21:ILE:HA	1:A:65:VAL:CG2	2.28	0.63
1:D:194:LYS:HE2	4:D:507:HOH:O	1.99	0.63
1:B:196:LEU:C	1:B:196:LEU:HD23	2.18	0.63
1:B:288:ILE:HB	1:B:289:PRO:HD3	1.81	0.63
1:B:125:GLY:HA3	1:B:129:THR:O	1.97	0.63
1:C:206:ILE:HD11	1:C:242:LEU:HD23	1.80	0.63
1:C:260:THR:O	1:C:261:ILE:C	2.36	0.63
1:B:124:GLU:HA	1:B:124:GLU:OE1	1.98	0.63
1:D:219:ILE:HG12	1:D:250:LYS:O	1.99	0.62
1:C:104[A]:PHE:CE1	1:D:99:TYR:CD2	2.87	0.62
1:A:107:LEU:HD12	1:B:263:LEU:HD22	1.81	0.62
1:D:26[A]:ARG:HG3	1:D:26[A]:ARG:NH1	2.04	0.62
1:A:29:SER:O	1:A:32:VAL:HG22	1.98	0.62
1:D:221:LEU:CD1	1:D:239:THR:HG22	2.22	0.62
1:D:283:ILE:HD11	1:D:284:PHE:CD2	2.34	0.62
1:A:52:GLU:OE2	1:A:52:GLU:CA	2.48	0.62
1:A:105:TYR:HD2	1:B:262:ASP:OD1	1.83	0.62
1:A:271:LYS:HD2	1:A:271:LYS:C	2.20	0.62
1:D:130:LEU:HD23	4:D:512:HOH:O	1.98	0.62
1:D:239:THR:O	1:D:243:ILE:HG13	2.00	0.62
1:D:129:THR:HG23	4:D:512:HOH:O	2.00	0.62
1:D:158:ILE:HA	1:D:161:LYS:HZ3	1.63	0.62
1:C:247:TYR:O	1:C:251:ILE:HG13	2.00	0.62
1:B:291:LEU:C	1:B:296:VAL:HG12	2.11	0.62
1:C:257:TYR:HA	1:C:278:TRP:CZ2	2.35	0.62
1:C:21:ILE:C	1:C:65:VAL:HG13	2.19	0.62
1:A:267:LYS:C	1:A:269:GLU:H	2.03	0.62
1:D:26[A]:ARG:HH22	1:D:75:ASP:HB3	1.65	0.61
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.33	0.61
1:D:57:MET:HG2	1:D:88:ILE:HD13	1.81	0.61
1:A:282:LEU:HD13	1:A:282:LEU:C	2.20	0.61
1:B:176:ASN:CA	1:B:208:TYR:OH	2.44	0.61
1:B:206:ILE:CD1	1:B:242:LEU:CD2	2.77	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:HD2	4:A:568:HOH:O	1.83	0.61
1:D:204:ASP:OD2	1:D:234:LYS:HE3	2.00	0.61
1:D:283:ILE:HD11	1:D:284:PHE:CE2	2.35	0.61
1:D:247:TYR:O	1:D:251:ILE:HG13	2.01	0.61
1:D:224:TYR:HE2	1:D:236:ASN:HD21	1.47	0.61
1:B:263:LEU:HB3	1:B:265:THR:HG22	1.83	0.61
1:D:169:THR:OG1	1:D:197:ILE:HA	2.01	0.61
1:D:271:LYS:HB3	1:D:272:PRO:HD3	1.82	0.61
1:A:229:PHE:O	1:A:230:LEU:HB2	1.99	0.61
1:B:14:LYS:O	1:B:15:ASP:C	2.40	0.61
1:C:99:TYR:CE1	1:C:141:ASP:HB2	2.37	0.60
1:B:258:CYS:C	1:B:260:THR:H	2.04	0.60
1:C:282:LEU:HD23	1:C:282:LEU:C	2.22	0.60
1:A:50:VAL:HG12	1:A:54:LYS:HE3	1.83	0.60
1:A:98:ILE:CD1	1:A:102:LEU:HD11	2.30	0.60
1:A:219:ILE:HD11	1:A:251:ILE:HG12	1.82	0.60
1:D:255:HIS:CE1	1:D:283:ILE:HG13	2.36	0.60
1:D:222:ASP:O	1:D:223:ARG:HB2	2.01	0.60
1:A:104[B]:PHE:HE2	1:B:262:ASP:HB3	1.65	0.60
1:B:255:HIS:NE2	1:B:283:ILE:HG23	2.16	0.60
1:D:90:LEU:HD13	1:D:90:LEU:C	2.21	0.60
1:B:141:ASP:CG	1:B:142:GLU:H	2.04	0.60
1:A:296:VAL:CB	4:A:566:HOH:O	1.93	0.60
1:C:102:LEU:HD13	1:C:148:ASP:CB	2.29	0.60
1:D:3:ILE:HG13	1:D:11:ILE:HD11	1.84	0.60
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.36	0.60
1:C:261:ILE:HD12	1:C:271:LYS:HE2	1.84	0.60
1:C:294:ASN:HD22	1:C:294:ASN:N	1.99	0.60
1:A:161:LYS:HE3	1:A:188:GLU:O	2.02	0.60
1:B:228:LEU:HD22	1:B:228:LEU:N	2.16	0.60
1:A:104[B]:PHE:CE2	1:B:262:ASP:HB3	2.35	0.60
1:B:95:GLY:HA2	1:B:118:PHE:CE1	2.36	0.60
1:B:308:ASN:HB2	1:B:309:PRO:HD3	1.83	0.59
1:B:272:PRO:O	1:B:273:LYS:CB	2.50	0.59
1:B:258:CYS:O	1:B:260:THR:N	2.35	0.59
1:B:282:LEU:HD13	1:B:282:LEU:O	2.02	0.59
1:B:138:ILE:C	1:B:138:ILE:CD1	2.70	0.59
1:C:196:LEU:C	1:C:196:LEU:CD2	2.70	0.59
1:C:265:THR:HG23	1:C:266:ALA:N	2.17	0.59
1:A:59:PHE:HE2	1:C:59:PHE:CE2	2.21	0.59
1:A:157:ALA:O	1:A:161:LYS:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:VAL:CG1	1:D:195:ILE:HD11	2.32	0.59
1:D:13:SER:OG	1:D:314:SER:HB3	2.02	0.59
1:C:301:ILE:CD1	1:C:301:ILE:C	2.71	0.59
1:A:270:TYR:HB3	1:A:274:LEU:HD22	1.84	0.59
1:D:4:PRO:C	1:D:5:LEU:HD12	2.23	0.59
1:B:258:CYS:C	1:B:260:THR:N	2.55	0.59
1:A:294:ASN:N	1:A:294:ASN:HD22	1.99	0.59
1:C:275:ALA:HB1	1:C:278:TRP:HB2	1.85	0.59
1:A:118:PHE:O	1:A:122:ILE:HG13	2.03	0.59
1:D:20:LEU:O	1:D:65:VAL:HG12	2.03	0.58
1:D:181:GLN:O	1:D:185:LEU:HG	2.02	0.58
1:B:98:ILE:HD13	1:B:102:LEU:HD13	1.85	0.58
1:C:21:ILE:O	1:C:65:VAL:CG1	2.51	0.58
1:B:228:LEU:CD2	1:B:228:LEU:H	2.16	0.58
1:A:219:ILE:O	1:A:219:ILE:CD1	2.48	0.58
1:D:21:ILE:C	1:D:65:VAL:HG13	2.24	0.58
1:A:70:MET:CE	1:A:96:ILE:HG23	2.32	0.58
1:C:55:ARG:NH2	1:C:281:THR:OG1	2.36	0.58
1:A:188:GLU:HA	1:A:188:GLU:OE2	2.04	0.58
1:B:94:THR:O	1:B:136:VAL:HA	2.04	0.58
1:D:188:GLU:O	1:D:188:GLU:HG3	2.03	0.58
1:D:121:ASP:HB3	1:D:126:ILE:HG12	1.84	0.58
1:C:255:HIS:NE2	1:C:283:ILE:HG23	2.19	0.58
1:B:4:PRO:HB3	1:B:132:LYS:HB2	1.85	0.58
1:B:163:THR:C	1:B:164:LYS:CD	2.72	0.58
1:C:206:ILE:HD11	1:C:242:LEU:CD2	2.34	0.58
1:A:21:ILE:O	1:A:65:VAL:CG2	2.51	0.58
1:B:52:GLU:CG	4:B:545:HOH:O	2.49	0.58
1:D:180:GLU:OE2	1:D:183:ARG:NH1	2.37	0.58
1:D:206:ILE:HD11	1:D:242:LEU:HD23	1.84	0.57
1:C:228:LEU:HD11	1:C:274:LEU:HD13	1.86	0.57
1:B:123:LYS:O	1:B:132:LYS:HE3	2.04	0.57
1:C:79:MET:CE	4:C:508:HOH:O	2.52	0.57
1:C:160:ASN:ND2	1:C:190:VAL:HG13	2.19	0.57
1:B:107:LEU:O	1:B:108:ASN:CB	2.46	0.57
1:D:297:ASN:ND2	1:D:297:ASN:N	2.44	0.57
1:C:70:MET:HE1	1:C:96:ILE:CG2	2.31	0.57
1:A:219:ILE:HD12	1:A:251:ILE:HA	1.85	0.57
1:C:136:VAL:CG1	1:C:167:ILE:HG12	2.33	0.57
1:C:65:VAL:HG23	1:C:135:PHE:CE1	2.39	0.57
1:B:182:GLN:NE2	1:B:215:LYS:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PRO:CB	1:C:132:LYS:HB2	2.34	0.57
1:B:228:LEU:HD22	1:B:274:LEU:O	2.03	0.57
1:A:215:LYS:HD3	4:A:552:HOH:O	2.04	0.57
1:B:275:ALA:HB1	1:B:278:TRP:HB2	1.87	0.57
1:A:108:ASN:HD22	1:A:108:ASN:C	2.07	0.57
1:B:157:ALA:HB3	1:B:188:GLU:HG2	1.86	0.57
1:D:70:MET:CE	1:D:96:ILE:HG23	2.34	0.57
1:D:163:THR:O	1:D:164:LYS:HB2	2.04	0.57
1:C:147:LYS:HD2	1:C:147:LYS:H	1.70	0.57
1:B:163:THR:O	1:B:164:LYS:CB	2.53	0.57
1:D:16:ILE:HD12	1:D:309:PRO:HB2	1.87	0.57
1:A:59:PHE:CE2	1:C:59:PHE:CE2	2.92	0.56
1:D:102:LEU:CG	1:D:103:PRO:HD2	2.35	0.56
1:C:308:ASN:HB2	1:C:309:PRO:HD3	1.87	0.56
1:D:222:ASP:O	1:D:223:ARG:CG	2.53	0.56
1:B:297:ASN:OD1	1:B:300:VAL:HG23	2.06	0.56
1:B:102:LEU:HD23	1:B:148:ASP:CG	2.25	0.56
1:C:166:PRO:HB2	1:C:312:PHE:CE2	2.40	0.56
1:D:191:ASP:HB2	1:D:194:LYS:HD3	1.88	0.56
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.40	0.56
1:D:52:GLU:HG3	1:D:280:ILE:CG2	2.35	0.56
1:B:264:GLY:O	1:B:267:LYS:HG3	2.06	0.56
1:B:196:LEU:C	1:B:196:LEU:CD2	2.74	0.56
1:D:21:ILE:O	1:D:21:ILE:HG13	2.06	0.55
1:C:200:LEU:HD12	1:C:200:LEU:C	2.27	0.55
1:C:33:ARG:NH1	1:C:40:TYR:CG	2.75	0.55
1:A:142:GLU:HB3	1:A:143:PRO:HD3	1.87	0.55
1:A:224:TYR:CE1	1:A:236:ASN:OD1	2.58	0.55
1:B:298:GLU:O	1:B:301:ILE:HG13	2.07	0.55
1:B:270:TYR:O	1:B:274:LEU:HD12	2.05	0.55
1:B:16:ILE:HG21	4:B:530:HOH:O	2.06	0.55
1:D:308:ASN:HB2	1:D:309:PRO:HD3	1.88	0.55
1:D:100:ILE:CG2	1:D:101:ASP:H	2.15	0.55
1:B:206:ILE:CG1	1:B:210:LYS:HE3	2.37	0.55
1:B:161:LYS:NZ	1:B:161:LYS:CB	2.69	0.55
1:C:52:GLU:CD	1:C:280:ILE:HG22	2.27	0.55
1:D:140:ALA:HB3	1:D:181:GLN:HE21	1.72	0.55
1:C:41:ASN:HB3	1:C:44:GLU:HB3	1.88	0.55
1:B:12:GLU:N	1:B:12:GLU:OE1	2.27	0.55
1:A:107:LEU:O	1:A:108:ASN:ND2	2.39	0.55
1:C:182:GLN:NE2	1:C:215:LYS:CB	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLY:HA2	1:D:118:PHE:CE1	2.42	0.55
1:D:301:ILE:CD1	1:D:301:ILE:C	2.70	0.55
1:D:109:ARG:HB3	1:D:113:GLU:OE1	2.06	0.55
1:D:140:ALA:O	1:D:171:SER:HA	2.06	0.55
1:C:230:LEU:HD23	1:C:235:ARG:HG2	1.89	0.55
1:B:90:LEU:HD13	1:B:90:LEU:C	2.27	0.55
1:B:4:PRO:O	1:B:5:LEU:HD12	2.07	0.54
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.42	0.54
1:D:55:ARG:NH2	1:D:281:THR:OG1	2.40	0.54
1:B:224:TYR:OH	1:B:239:THR:HG21	2.06	0.54
1:A:54:LYS:HG3	1:A:55:ARG:N	2.22	0.54
1:C:288:ILE:HB	1:C:289:PRO:CD	2.36	0.54
1:D:3:ILE:CG1	1:D:11:ILE:CD1	2.85	0.54
1:C:79:MET:HE3	4:C:508:HOH:O	2.07	0.54
1:C:138:ILE:HD12	1:C:153:ILE:HG12	1.89	0.54
1:A:258:CYS:HB2	1:A:261:ILE:HD11	1.89	0.54
1:B:140:ALA:O	1:B:171:SER:HA	2.08	0.54
1:A:200:LEU:HD23	1:A:219:ILE:HG22	1.90	0.54
1:B:282:LEU:C	1:B:282:LEU:HD13	2.28	0.54
1:B:49:ALA:O	1:B:53:VAL:HG23	2.08	0.54
1:A:196:LEU:CD2	1:A:196:LEU:C	2.76	0.54
1:D:140:ALA:HB3	1:D:181:GLN:NE2	2.22	0.54
1:B:300:VAL:O	1:B:303:THR:HB	2.08	0.54
1:B:228:LEU:CD2	1:B:274:LEU:O	2.56	0.53
1:A:273:LYS:O	1:A:274:LEU:HD12	2.08	0.53
1:B:163:THR:O	1:B:164:LYS:HD3	2.07	0.53
1:B:142:GLU:HB3	1:B:143:PRO:HD3	1.90	0.53
1:C:16:ILE:CD1	1:C:309:PRO:HB2	2.39	0.53
1:A:281:THR:O	1:A:281:THR:CG2	2.55	0.53
1:D:200:LEU:HD21	1:D:219:ILE:HA	1.89	0.53
1:C:98:ILE:HD12	1:C:98:ILE:C	2.29	0.53
1:D:288:ILE:HB	1:D:289:PRO:CD	2.37	0.53
1:A:21:ILE:O	1:A:65:VAL:HG23	2.07	0.53
1:B:138:ILE:HD11	1:B:169:THR:HB	1.91	0.53
1:A:57:MET:HG2	1:A:88:ILE:HD13	1.91	0.53
1:C:4:PRO:HB3	1:C:132:LYS:HB2	1.89	0.53
1:C:21:ILE:HA	1:C:65:VAL:HG12	1.90	0.53
1:D:102:LEU:HG	1:D:103:PRO:HD2	1.91	0.53
1:C:41:ASN:ND2	1:C:44:GLU:HB2	2.23	0.53
1:B:140:ALA:HB3	1:B:181:GLN:HE21	1.73	0.53
1:D:271:LYS:H	1:D:272:PRO:CD	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:HA	1:B:262:ASP:HB2	1.91	0.53
1:D:190:VAL:HG12	1:D:195:ILE:HD11	1.91	0.53
1:B:157:ALA:CB	1:B:188:GLU:HB3	2.39	0.53
1:A:70:MET:HE2	1:A:96:ILE:HG23	1.89	0.53
1:C:43:ASP:O	1:C:47:ARG:HG3	2.09	0.53
1:D:124:GLU:OE1	1:D:124:GLU:HA	2.08	0.53
1:D:271:LYS:H	1:D:272:PRO:HD2	1.72	0.53
1:B:206:ILE:HG13	1:B:210:LYS:HE3	1.91	0.53
1:B:44:GLU:HG3	1:B:47:ARG:NH2	2.24	0.53
1:D:98:ILE:HD13	1:D:102:LEU:HD13	1.91	0.52
1:D:3:ILE:HG13	1:D:11:ILE:HD12	1.90	0.52
1:C:177:THR:O	1:C:181:GLN:HG3	2.09	0.52
1:D:200:LEU:HD12	1:D:200:LEU:C	2.29	0.52
1:C:100:ILE:CG1	1:C:101:ASP:H	2.17	0.52
1:B:137:KCX:HG3	1:B:168:ILE:O	2.09	0.52
1:C:124:GLU:O	1:C:132:LYS:HE3	2.09	0.52
1:A:98:ILE:HD11	1:A:102:LEU:HD11	1.92	0.52
1:B:163:THR:OG1	1:B:165:VAL:HG22	2.09	0.52
1:D:6:VAL:HG21	1:D:90:LEU:HD12	1.91	0.52
1:D:267:LYS:HB2	1:D:270:TYR:HB2	1.90	0.52
1:D:283:ILE:CD1	1:D:284:PHE:CD2	2.93	0.52
1:A:240:LEU:O	1:A:241:ARG:HB2	2.10	0.52
1:A:3:ILE:HD11	1:A:313:PHE:CB	2.39	0.52
1:B:83:VAL:O	1:B:87:GLY:N	2.30	0.52
1:D:21:ILE:CA	1:D:65:VAL:HG11	2.37	0.52
1:C:228:LEU:HD22	1:C:228:LEU:H	1.75	0.52
1:A:89:ASN:HA	4:A:523:HOH:O	2.09	0.52
1:D:134:GLY:N	4:D:529:HOH:O	2.42	0.52
1:A:41:ASN:ND2	1:A:44:GLU:HB2	2.25	0.52
1:A:8:LYS:C	1:A:10:SER:H	2.14	0.52
1:B:137:KCX:HA	1:B:168:ILE:O	2.09	0.52
1:D:79:MET:HE1	4:D:517:HOH:O	2.09	0.52
1:B:19:THR:OG1	1:B:63:THR:HB	2.10	0.52
1:C:5:LEU:HG	4:C:513:HOH:O	2.09	0.52
1:C:230:LEU:HD11	1:C:234:LYS:CD	2.38	0.52
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.92	0.52
1:A:296:VAL:CG2	1:A:297:ASN:H	2.22	0.52
1:D:283:ILE:C	1:D:283:ILE:CD1	2.78	0.52
1:D:49:ALA:O	1:D:53:VAL:HG23	2.09	0.52
1:B:3:ILE:O	1:B:5:LEU:CD1	2.58	0.51
1:C:257:TYR:CE2	1:C:259:CYS:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:HD12	1:C:234:LYS:HD3	1.92	0.51
1:D:228:LEU:O	1:D:228:LEU:HD13	2.11	0.51
1:D:67:PRO:HB2	1:D:137:KCX:CE	2.41	0.51
1:B:301:ILE:C	1:B:301:ILE:CD1	2.71	0.51
1:A:86:THR:OG1	1:A:88:ILE:HG22	2.10	0.51
1:C:5:LEU:HD23	1:C:8:LYS:HB2	1.91	0.51
1:A:261:ILE:HD11	1:A:278:TRP:HH2	1.76	0.51
1:D:109:ARG:HB3	1:D:113:GLU:CD	2.31	0.51
1:A:52:GLU:HG3	1:A:280:ILE:CG2	2.41	0.51
1:C:79:MET:O	1:C:83:VAL:HG23	2.11	0.51
1:A:59:PHE:CZ	1:A:281:THR:HG21	2.45	0.51
1:D:236:ASN:HB3	1:D:290:PHE:CE2	2.46	0.51
1:D:157:ALA:CB	1:D:188:GLU:HG2	2.41	0.51
1:B:8:LYS:NZ	1:B:87:GLY:O	2.40	0.51
1:C:115:ALA:O	1:C:119:ILE:HG13	2.11	0.51
1:D:129:THR:HG22	1:D:130:LEU:N	2.26	0.51
1:A:206:ILE:HG13	1:A:210:LYS:HE3	1.92	0.51
1:A:108:ASN:O	1:A:108:ASN:ND2	2.34	0.51
1:D:174:HIS:O	1:D:175:ASN:CB	2.59	0.51
1:B:195:ILE:CG2	1:B:196:LEU:N	2.73	0.51
1:A:160:ASN:O	1:A:164:LYS:N	2.37	0.51
1:A:258:CYS:O	1:A:260:THR:N	2.44	0.50
1:D:137:KCX:HZ	1:D:170:HIS:HB2	1.76	0.50
1:A:255:HIS:CD2	1:A:283:ILE:HG23	2.45	0.50
1:A:31:ALA:HA	1:B:30:GLU:HG2	1.93	0.50
1:A:222:ASP:O	1:A:223:ARG:HG3	2.10	0.50
1:B:276:PRO:HA	4:B:528:HOH:O	2.10	0.50
1:C:65:VAL:HA	1:C:91:VAL:HB	1.93	0.50
1:C:224:TYR:CE1	1:C:236:ASN:ND2	2.79	0.50
1:D:11:ILE:C	1:D:11:ILE:CD1	2.79	0.50
1:B:286:ASP:O	1:B:289:PRO:HD2	2.11	0.50
1:C:35:GLN:HB3	1:D:74:ARG:HH21	1.75	0.50
1:A:65:VAL:HG23	1:A:65:VAL:O	2.10	0.50
1:C:141:ASP:CG	1:C:142:GLU:H	2.14	0.50
1:C:35:GLN:HG3	1:D:70:MET:HG3	1.93	0.50
1:D:166:PRO:HB2	1:D:312:PHE:CE2	2.47	0.50
1:B:97:TYR:CE1	1:B:99:TYR:HE1	2.30	0.50
1:A:8:LYS:O	1:A:10:SER:N	2.45	0.50
1:C:265:THR:HG23	1:C:266:ALA:H	1.75	0.50
1:B:229:PHE:O	1:B:230:LEU:HB2	2.11	0.50
1:A:55:ARG:CG	1:A:55:ARG:NH1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ILE:HG23	1:C:207:ASP:N	2.26	0.50
1:A:21:ILE:C	1:A:65:VAL:CG2	2.80	0.49
1:D:271:LYS:N	1:D:272:PRO:CD	2.76	0.49
1:A:141:ASP:OD1	1:A:142:GLU:N	2.41	0.49
1:B:63:THR:HG23	1:B:89:ASN:O	2.12	0.49
1:D:258:CYS:HB2	1:D:261:ILE:HB	1.94	0.49
1:B:216:GLY:HA2	1:B:250:LYS:NZ	2.27	0.49
1:D:26[A]:ARG:HG2	1:D:26[A]:ARG:NH1	2.15	0.49
1:A:104[B]:PHE:CD2	1:B:263:LEU:CD2	2.94	0.49
1:B:177:THR:O	1:B:181:GLN:HG3	2.12	0.49
1:B:76:ILE:HG23	1:B:77:ARG:N	2.27	0.49
1:A:296:VAL:CG2	1:A:297:ASN:N	2.75	0.49
1:D:129:THR:CG2	4:D:512:HOH:O	2.58	0.49
1:D:125:GLY:HA3	1:D:129:THR:O	2.12	0.49
1:B:1:MET:HB3	1:B:10:SER:HB3	1.92	0.49
1:C:130:LEU:HD22	1:C:130:LEU:N	2.28	0.49
1:A:261:ILE:HD11	1:A:278:TRP:CH2	2.47	0.49
1:B:206:ILE:HD12	1:B:242:LEU:HD21	1.94	0.49
1:B:233:ASP:OD1	1:B:234:LYS:N	2.45	0.49
1:C:3:ILE:HD11	1:C:313:PHE:CB	2.41	0.49
1:D:41:ASN:O	1:D:45:GLU:HG3	2.13	0.49
1:C:16:ILE:HG12	4:C:512:HOH:O	2.11	0.49
1:B:25:LEU:O	1:B:259:CYS:HB2	2.13	0.49
1:A:75:ASP:O	1:A:79:MET:HG3	2.13	0.49
1:D:65:VAL:O	1:D:65:VAL:HG13	2.13	0.49
1:C:228:LEU:N	1:C:228:LEU:HD22	2.28	0.49
1:B:118:PHE:O	1:B:122:ILE:HG13	2.13	0.49
1:D:3:ILE:CD1	1:D:11:ILE:HD11	2.42	0.49
1:A:162:GLU:OE1	1:A:162:GLU:O	2.30	0.49
1:C:52:GLU:CG	1:C:280:ILE:HG22	2.43	0.49
1:B:146:THR:OG1	1:B:149:VAL:CG2	2.54	0.49
1:D:288:ILE:CB	1:D:289:PRO:HD3	2.39	0.49
1:C:80:GLU:OE2	1:C:131:ASN:ND2	2.46	0.49
1:A:55:ARG:O	1:A:59:PHE:HD1	1.95	0.49
1:B:14:LYS:HG3	1:B:15:ASP:N	2.28	0.49
1:A:11:ILE:CD1	1:A:16:ILE:HG22	2.43	0.49
1:D:3:ILE:CG1	1:D:11:ILE:HD11	2.42	0.49
1:B:44:GLU:HG3	1:B:47:ARG:HH22	1.77	0.49
1:A:65:VAL:HG12	1:A:91:VAL:HB	1.94	0.49
1:A:196:LEU:C	1:A:196:LEU:HD23	2.33	0.49
1:A:292:LYS:HA	1:A:296:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:O	1:B:164:LYS:CD	2.61	0.48
1:D:16:ILE:CD1	1:D:309:PRO:HB2	2.43	0.48
1:A:5:LEU:HB2	1:A:8:LYS:HB2	1.95	0.48
1:D:4:PRO:O	1:D:5:LEU:HD12	2.13	0.48
1:C:29:SER:O	1:C:32:VAL:HG22	2.12	0.48
1:D:6:VAL:CG2	1:D:90:LEU:HD12	2.43	0.48
1:C:124:GLU:HA	1:C:124:GLU:OE1	2.13	0.48
1:C:147:LYS:HD2	1:C:147:LYS:N	2.28	0.48
1:C:3:ILE:HD11	1:C:313:PHE:HB3	1.96	0.48
1:A:126:ILE:O	1:A:129:THR:HB	2.13	0.48
1:C:269:GLU:HG2	1:C:270:TYR:CD2	2.49	0.48
1:A:129:THR:CG2	1:A:130:LEU:H	2.26	0.48
1:C:272:PRO:O	1:C:274:LEU:N	2.46	0.48
1:B:267:LYS:HD3	1:B:269:GLU:OE1	2.14	0.48
1:C:21:ILE:CA	1:C:65:VAL:CG1	2.90	0.48
1:A:142:GLU:N	1:A:143:PRO:CD	2.77	0.48
1:D:260:THR:O	1:D:260:THR:HG22	2.13	0.48
1:A:125:GLY:HA3	1:A:129:THR:O	2.14	0.48
1:D:255:HIS:NE2	1:D:283:ILE:HG13	2.28	0.48
1:C:64:ILE:HG13	1:C:88:ILE:HD11	1.96	0.48
1:A:169:THR:OG1	1:A:197:ILE:HA	2.14	0.48
1:A:177:THR:O	1:A:181:GLN:HG3	2.14	0.48
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.48	0.48
1:D:149:VAL:O	1:D:152:VAL:CG1	2.53	0.48
1:D:3:ILE:CG1	1:D:11:ILE:HD12	2.44	0.48
1:C:118:PHE:O	1:C:122:ILE:HG13	2.13	0.48
1:D:64:ILE:O	1:D:90:LEU:HD22	2.14	0.48
1:D:94:THR:O	1:D:137:KCX:N	2.47	0.48
1:C:22:HIS:HD2	1:C:256:ASP:HA	1.79	0.48
1:B:287:THR:O	1:B:290:PHE:HB3	2.13	0.48
1:B:142:GLU:N	1:B:143:PRO:CD	2.76	0.47
1:A:240:LEU:HD11	1:A:244:LYS:HE2	1.96	0.47
1:C:173:ALA:HB1	1:C:203:THR:CG2	2.44	0.47
1:A:281:THR:HG22	1:A:285:GLU:HG3	1.96	0.47
1:D:257:TYR:CD1	1:D:278:TRP:O	2.67	0.47
1:A:29:SER:HB2	1:A:32:VAL:CG2	2.42	0.47
1:D:224:TYR:OH	1:D:239:THR:HG21	2.14	0.47
1:D:219:ILE:CD1	1:D:251:ILE:HG12	2.32	0.47
1:A:126:ILE:HG13	1:A:131:ASN:O	2.15	0.47
1:C:224:TYR:HD1	1:C:232:VAL:HG13	1.80	0.47
1:A:204:ASP:OD2	4:A:515:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:OG1	1:A:149:VAL:HG23	2.15	0.47
1:B:70:MET:CE	1:B:96:ILE:HG23	2.44	0.47
1:D:99:TYR:HB3	1:D:143:PRO:HG3	1.95	0.47
1:B:275:ALA:N	1:B:276:PRO:HD3	2.30	0.47
1:B:224:TYR:HE1	1:B:236:ASN:ND2	2.13	0.47
1:C:100:ILE:CG1	1:C:101:ASP:N	2.75	0.47
1:B:310:LYS:N	4:B:530:HOH:O	2.47	0.47
1:B:3:ILE:CG2	1:B:11:ILE:CG1	2.93	0.47
1:D:103:PRO:HG2	1:D:106:PHE:CD2	2.50	0.47
1:A:64:ILE:O	1:A:90:LEU:HD23	2.15	0.47
1:D:70:MET:HE1	1:D:96:ILE:HG23	1.97	0.47
1:D:23:GLU:OE1	1:D:254:SER:OG	2.32	0.47
1:A:281:THR:O	1:A:285:GLU:HG3	2.14	0.47
1:C:228:LEU:HD11	1:C:274:LEU:HB3	1.96	0.47
1:C:63:THR:HA	1:C:89:ASN:HB2	1.97	0.47
1:B:23:GLU:O	1:B:66:ASP:HA	2.15	0.47
1:D:31:ALA:O	1:D:35:GLN:HG2	2.15	0.47
1:A:271:LYS:O	1:A:271:LYS:HD2	2.15	0.47
1:D:13:SER:CB	1:D:314:SER:HB3	2.45	0.47
1:A:240:LEU:O	1:A:241:ARG:CB	2.61	0.47
1:A:206:ILE:HD11	1:A:242:LEU:CG	2.41	0.46
1:D:301:ILE:HD12	1:D:302:ALA:CA	2.45	0.46
1:A:270:TYR:C	1:A:272:PRO:HD2	2.36	0.46
1:D:90:LEU:HD13	1:D:91:VAL:N	2.30	0.46
1:C:33:ARG:NH1	1:C:40:TYR:CD2	2.82	0.46
1:D:136:VAL:O	1:D:136:VAL:HG13	2.15	0.46
1:C:228:LEU:H	1:C:228:LEU:CD2	2.28	0.46
1:B:291:LEU:C	1:B:296:VAL:HG13	2.33	0.46
1:A:286:ASP:O	1:A:289:PRO:HD2	2.16	0.46
1:A:22:HIS:CE1	1:A:137:KCX:CX	2.99	0.46
1:C:83:VAL:O	1:C:87:GLY:N	2.45	0.46
1:A:98:ILE:HD12	1:A:102:LEU:HD12	1.85	0.46
1:C:94:THR:O	1:C:137:KCX:N	2.48	0.46
1:D:99:TYR:HD1	1:D:141:ASP:HB2	1.71	0.46
1:D:142:GLU:N	1:D:143:PRO:CD	2.76	0.46
1:A:53:VAL:HG11	1:A:88:ILE:HG21	1.97	0.46
1:D:3:ILE:HD11	1:D:11:ILE:HD11	1.96	0.46
1:A:3:ILE:CG2	1:A:4:PRO:HD2	2.46	0.46
1:D:130:LEU:N	1:D:130:LEU:HD22	2.30	0.46
1:B:292:LYS:HE3	1:B:298:GLU:OE1	2.15	0.46
1:B:3:ILE:CG2	1:B:3:ILE:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HG21	1:B:163:THR:HB	1.98	0.46
1:B:97:TYR:CE1	1:B:99:TYR:CE1	3.04	0.46
1:A:271:LYS:N	1:A:272:PRO:HD2	2.30	0.46
1:D:183:ARG:NH1	1:D:183:ARG:HB3	2.31	0.46
1:D:54:LYS:O	1:D:58:GLN:HG3	2.16	0.46
1:B:273:LYS:N	1:B:276:PRO:HG3	2.15	0.46
1:D:291:LEU:HB3	1:D:296:VAL:HG11	1.96	0.46
1:D:21:ILE:HG21	1:D:252:MET:HB3	1.98	0.46
1:C:146:THR:OG1	1:C:149:VAL:HG23	2.15	0.46
1:C:200:LEU:HD11	1:C:219:ILE:HB	1.98	0.46
1:D:67:PRO:HB2	1:D:137:KCX:HE2	1.98	0.46
1:D:219:ILE:HG13	1:D:219:ILE:O	2.15	0.45
1:B:224:TYR:CE1	1:B:236:ASN:ND2	2.84	0.45
1:A:19:THR:HA	1:A:63:THR:O	2.16	0.45
1:A:55:ARG:O	1:A:59:PHE:CD1	2.69	0.45
1:C:104[A]:PHE:HE1	1:D:99:TYR:HD2	1.62	0.45
1:D:146:THR:OG1	1:D:149:VAL:HG23	2.16	0.45
1:B:137:KCX:HE3	1:B:170:HIS:HB2	1.98	0.45
1:D:41:ASN:ND2	1:D:44:GLU:HB2	2.32	0.45
1:A:29:SER:O	1:A:30:GLU:C	2.54	0.45
1:C:16:ILE:HD11	1:C:309:PRO:HB2	1.97	0.45
1:C:239:THR:O	1:C:243:ILE:HG13	2.16	0.45
1:D:97:TYR:OH	1:D:99:TYR:OH	2.14	0.45
1:B:191:ASP:O	1:B:194:LYS:HB2	2.16	0.45
1:C:55:ARG:O	1:C:59:PHE:HD1	2.00	0.45
1:A:88:ILE:HG13	1:A:89:ASN:N	2.32	0.45
1:A:247:TYR:O	1:A:251:ILE:HG13	2.16	0.45
1:B:3:ILE:CG2	1:B:11:ILE:HG13	2.47	0.45
1:C:142:GLU:N	1:C:143:PRO:CD	2.80	0.45
1:C:88:ILE:CG1	1:C:89:ASN:N	2.79	0.45
1:C:271:LYS:N	1:C:272:PRO:CD	2.79	0.45
1:A:201:GLY:O	1:A:230:LEU:HD23	2.16	0.45
1:D:228:LEU:CD1	1:D:228:LEU:C	2.84	0.45
1:D:70:MET:HE2	1:D:96:ILE:HG23	1.98	0.45
1:D:118:PHE:O	1:D:122:ILE:HG13	2.16	0.45
1:A:258:CYS:C	1:A:260:THR:N	2.68	0.45
1:D:206:ILE:CD1	1:D:242:LEU:CD2	2.83	0.45
1:A:29:SER:HB3	4:A:521:HOH:O	2.16	0.45
1:B:176:ASN:HA	1:B:208:TYR:HH	1.74	0.45
1:D:21:ILE:CD1	1:D:65:VAL:HG11	2.37	0.45
1:C:258:CYS:O	1:C:259:CYS:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASN:HD22	1:D:190:VAL:HG13	1.77	0.45
1:A:2:ARG:HA	1:A:12:GLU:HA	1.97	0.45
1:A:70:MET:HE1	1:A:96:ILE:HG23	1.98	0.45
1:C:160:ASN:O	1:C:164:LYS:N	2.40	0.45
1:C:163:THR:O	1:C:164:LYS:HB2	2.17	0.45
1:C:202:ASP:HB3	1:C:229:PHE:HB3	1.98	0.45
1:C:17:GLY:N	4:C:512:HOH:O	2.44	0.44
1:D:292:LYS:CA	1:D:296:VAL:HG13	2.47	0.44
1:A:21:ILE:HG13	1:A:21:ILE:O	2.18	0.44
1:B:122:ILE:HD12	1:B:163:THR:HG21	1.98	0.44
1:B:198:GLY:O	1:B:199:HIS:HB2	2.17	0.44
1:D:206:ILE:HG23	1:D:207:ASP:N	2.32	0.44
1:C:105:TYR:CD2	1:D:262:ASP:OD1	2.62	0.44
1:B:180:GLU:OE1	1:B:183:ARG:NH1	2.40	0.44
1:C:261:ILE:CD1	1:C:271:LYS:CD	2.96	0.44
1:D:100:ILE:HG13	1:D:101:ASP:OD1	2.17	0.44
1:A:13:SER:CB	1:A:314:SER:HB3	2.46	0.44
1:B:257:TYR:HD1	1:B:278:TRP:CE2	2.36	0.44
1:B:176:ASN:HB2	4:B:542:HOH:O	2.17	0.44
1:B:309:PRO:HB2	4:B:530:HOH:O	2.16	0.44
1:C:293:ARG:C	1:C:294:ASN:HD22	2.21	0.44
1:A:93:GLY:HA3	1:A:135:PHE:CZ	2.52	0.44
1:C:205:ASN:ND2	1:C:208:TYR:HB2	2.32	0.44
1:A:130:LEU:CD2	1:A:130:LEU:N	2.78	0.44
1:C:282:LEU:C	1:C:282:LEU:CD2	2.86	0.44
1:A:270:TYR:O	1:A:271:LYS:C	2.56	0.44
1:A:180:GLU:OE2	1:A:183:ARG:NH1	2.51	0.44
1:B:27:VAL:CG1	1:B:261:ILE:HA	2.48	0.44
1:D:100:ILE:CG2	1:D:101:ASP:N	2.72	0.44
1:A:267:LYS:HB2	1:A:270:TYR:HD1	1.83	0.44
1:B:307:GLU:O	1:B:310:LYS:HB3	2.17	0.44
1:D:52:GLU:HG3	1:D:280:ILE:HG21	1.98	0.44
1:D:240:LEU:HD11	1:D:244:LYS:HE3	1.99	0.44
1:D:26[B]:ARG:HB2	1:D:260:THR:HB	2.00	0.44
1:C:283:ILE:HA	1:C:287:THR:HB	2.00	0.44
1:D:137:KCX:HA	1:D:168:ILE:O	2.17	0.44
1:B:183:ARG:HG2	1:B:183:ARG:O	2.18	0.44
1:D:160:ASN:HD22	1:D:190:VAL:HG22	1.84	0.43
1:D:269:GLU:OE2	1:D:269:GLU:N	2.50	0.43
1:D:196:LEU:O	1:D:196:LEU:CD2	2.65	0.43
1:A:95:GLY:HA2	1:A:118:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HG22	1:B:98:ILE:HG23	2.00	0.43
1:D:251:ILE:O	1:D:304:ILE:HG23	2.19	0.43
1:B:197:ILE:HG21	1:B:212:ILE:HD13	2.00	0.43
1:D:288:ILE:CB	1:D:289:PRO:CD	2.96	0.43
1:B:124:GLU:OE1	1:B:124:GLU:CA	2.64	0.43
1:A:223:ARG:HB2	4:A:504:HOH:O	2.19	0.43
1:C:269:GLU:OE2	1:C:269:GLU:N	2.40	0.43
1:B:2:ARG:HH21	1:B:13:SER:CB	2.08	0.43
1:B:27:VAL:HG23	1:B:72:LEU:O	2.18	0.43
1:C:79:MET:HE2	4:C:508:HOH:O	2.16	0.43
1:B:102:LEU:HD21	1:B:148:ASP:HB3	1.80	0.43
1:A:55:ARG:O	1:A:55:ARG:HD2	2.18	0.43
1:B:258:CYS:CB	1:B:261:ILE:HB	2.44	0.43
1:D:102:LEU:HB2	1:D:148:ASP:HB3	2.00	0.43
1:D:282:LEU:C	1:D:282:LEU:CD1	2.84	0.43
1:C:35:GLN:HA	1:C:35:GLN:OE1	2.18	0.43
1:C:308:ASN:N	1:C:309:PRO:CD	2.81	0.43
1:C:34:GLN:HG3	1:D:34:GLN:OE1	2.19	0.43
1:C:141:ASP:OD1	1:C:142:GLU:N	2.51	0.43
1:C:287:THR:O	1:C:290:PHE:HB3	2.17	0.43
1:A:23:GLU:OE1	1:A:254:SER:OG	2.35	0.43
1:A:136:VAL:CG1	1:A:167:ILE:HG12	2.49	0.43
1:B:3:ILE:HG23	1:B:11:ILE:HG12	2.01	0.43
1:C:149:VAL:O	1:C:153:ILE:HG13	2.18	0.43
1:A:3:ILE:CD1	1:A:313:PHE:HB3	2.49	0.43
1:D:183:ARG:HG2	1:D:187:GLU:OE1	2.19	0.43
1:D:177:THR:O	1:D:178:GLY:C	2.57	0.43
1:A:265:THR:OG1	1:B:108:ASN:ND2	2.52	0.43
1:D:21:ILE:CA	1:D:65:VAL:HG12	2.32	0.43
1:C:134:GLY:O	1:C:135:PHE:HB3	2.18	0.43
1:C:210:LYS:HB2	1:C:210:LYS:HE3	1.81	0.43
1:A:297:ASN:C	1:A:297:ASN:OD1	2.57	0.43
1:D:102:LEU:N	1:D:148:ASP:OD2	2.52	0.43
1:B:290:PHE:CE1	1:B:294:ASN:ND2	2.87	0.43
1:A:206:ILE:CG1	1:A:210:LYS:HE3	2.49	0.42
1:C:21:ILE:C	1:C:65:VAL:CG1	2.86	0.42
1:A:267:LYS:C	1:A:269:GLU:N	2.70	0.42
1:C:94:THR:O	1:C:136:VAL:HA	2.19	0.42
1:A:200:LEU:CD2	1:A:219:ILE:HG22	2.49	0.42
1:B:140:ALA:HB3	1:B:181:GLN:NE2	2.32	0.42
1:D:67:PRO:HB2	1:D:137:KCX:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LYS:HA	1:C:310:LYS:HE2	2.00	0.42
1:D:45:GLU:HG2	1:D:260:THR:HG21	2.01	0.42
1:B:191:ASP:HA	1:B:192:PRO:HD2	1.86	0.42
1:D:263:LEU:C	1:D:265:THR:H	2.22	0.42
1:C:230:LEU:HD12	1:C:231:PRO:HD2	2.00	0.42
1:C:19:THR:HA	1:C:63:THR:O	2.19	0.42
1:C:200:LEU:CD1	1:C:200:LEU:C	2.87	0.42
1:B:183:ARG:NH1	1:B:183:ARG:HB3	2.35	0.42
1:D:26[A]:ARG:HH22	1:D:75:ASP:HB2	1.80	0.42
1:A:255:HIS:CE1	1:A:283:ILE:HG12	2.55	0.42
1:C:175:ASN:HD21	1:C:177:THR:CG2	2.33	0.42
1:C:140:ALA:HB3	1:C:181:GLN:NE2	2.34	0.42
1:B:141:ASP:CG	1:B:142:GLU:N	2.72	0.42
1:A:296:VAL:CG2	4:A:566:HOH:O	2.52	0.42
1:D:296:VAL:O	1:D:296:VAL:HG13	2.19	0.42
1:A:224:TYR:HB3	1:A:282:LEU:HD12	2.01	0.42
1:C:97:TYR:OH	1:C:99:TYR:OH	2.25	0.42
1:B:103:PRO:O	1:B:105:TYR:N	2.53	0.42
1:A:98:ILE:HD11	1:A:102:LEU:CD1	2.41	0.42
1:D:16:ILE:HD11	1:D:310:LYS:N	2.35	0.42
1:C:173:ALA:HB1	1:C:203:THR:HG22	2.00	0.42
1:B:102:LEU:HD22	1:B:148:ASP:CB	2.20	0.42
1:D:221:LEU:HD12	1:D:251:ILE:HG23	2.02	0.42
1:A:25:LEU:HD11	1:A:90:LEU:CD1	2.31	0.42
1:C:225:GLY:HA3	1:C:278:TRP:HD1	1.84	0.42
1:B:28:PHE:HA	1:B:262:ASP:CB	2.50	0.42
1:B:136:VAL:HG13	1:B:167:ILE:HG12	1.99	0.42
1:B:195:ILE:HG22	1:B:196:LEU:H	1.85	0.42
1:A:240:LEU:CD2	1:A:294:ASN:OD1	2.68	0.42
1:B:3:ILE:CG2	1:B:11:ILE:HG12	2.49	0.42
1:D:160:ASN:HB2	1:D:167:ILE:HD11	2.02	0.42
1:A:52:GLU:HG3	1:A:280:ILE:HG22	2.01	0.42
1:C:142:GLU:N	1:C:143:PRO:HD2	2.35	0.42
1:D:17:GLY:HA3	1:D:62:LYS:HD3	2.01	0.42
1:B:169:THR:OG1	1:B:197:ILE:HA	2.20	0.42
1:A:8:LYS:C	1:A:10:SER:N	2.73	0.42
1:C:206:ILE:CG2	1:C:207:ASP:N	2.83	0.42
1:B:66:ASP:HA	1:B:67:PRO:HD3	1.89	0.42
1:A:271:LYS:N	1:A:272:PRO:CD	2.83	0.41
1:D:105:TYR:OH	1:D:109:ARG:NH1	2.53	0.41
1:D:157:ALA:HB1	1:D:188:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:HB2	1:A:312:PHE:CE2	2.55	0.41
1:A:124:GLU:O	1:A:132:LYS:NZ	2.54	0.41
1:C:76:ILE:HG23	1:C:77:ARG:N	2.35	0.41
1:D:200:LEU:CD1	1:D:200:LEU:C	2.88	0.41
1:A:267:LYS:O	1:A:269:GLU:N	2.54	0.41
1:A:240:LEU:HD21	1:A:294:ASN:OD1	2.21	0.41
1:D:141:ASP:C	1:D:143:PRO:HD2	2.41	0.41
1:A:21:ILE:CA	1:A:65:VAL:CG2	2.98	0.41
1:A:280:ILE:O	1:A:280:ILE:HG12	2.21	0.41
1:D:226:LEU:C	1:D:228:LEU:N	2.74	0.41
1:B:115:ALA:O	1:B:119:ILE:HG13	2.20	0.41
1:B:291:LEU:CA	1:B:296:VAL:HG11	2.49	0.41
1:A:228:LEU:CD1	1:A:228:LEU:C	2.88	0.41
1:B:57:MET:HE1	1:B:86:THR:O	2.20	0.41
1:A:21:ILE:CA	1:A:65:VAL:HG22	2.45	0.41
1:D:170:HIS:CG	1:D:199:HIS:CD2	3.04	0.41
1:C:13:SER:O	1:C:310:LYS:HG3	2.20	0.41
1:C:297:ASN:N	1:C:297:ASN:OD1	2.53	0.41
1:A:41:ASN:O	1:A:45:GLU:HG3	2.20	0.41
1:D:90:LEU:C	1:D:90:LEU:CD1	2.89	0.41
1:C:147:LYS:CD	1:C:147:LYS:H	2.32	0.41
1:D:134:GLY:O	1:D:166:PRO:HD2	2.21	0.41
1:A:79:MET:O	1:A:83:VAL:HG23	2.21	0.41
1:C:252:MET:HA	4:C:501:HOH:O	2.21	0.41
1:C:117:LEU:HD21	1:D:39:LEU:HD11	2.02	0.41
1:B:2:ARG:N	1:B:10:SER:OG	2.54	0.41
1:B:107:LEU:HD13	1:B:107:LEU:C	2.40	0.41
1:D:206:ILE:HD12	1:D:242:LEU:HD21	2.01	0.41
1:B:230:LEU:HD11	1:B:234:LYS:HD3	2.02	0.41
1:B:170:HIS:CE1	1:B:199:HIS:CD2	3.09	0.41
1:C:146:THR:O	1:C:147:LYS:C	2.59	0.41
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.54	0.41
1:C:222:ASP:HA	1:C:254:SER:H	1.86	0.41
1:C:301:ILE:HD12	1:C:302:ALA:CA	2.47	0.41
1:A:251:ILE:O	1:A:308:ASN:ND2	2.49	0.41
1:D:59:PHE:HB3	1:D:284:PHE:CD1	2.56	0.41
1:C:139:ALA:O	1:C:140:ALA:HB2	2.20	0.41
1:D:269:GLU:HG2	1:D:270:TYR:CD1	2.56	0.41
1:A:3:ILE:HG23	1:A:4:PRO:HD2	2.02	0.41
1:B:76:ILE:CG2	1:B:77:ARG:N	2.84	0.41
1:C:38:HIS:HB3	4:C:514:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE2	1:A:301:ILE:HD11	2.21	0.40
1:B:3:ILE:CD1	1:B:313:PHE:CD2	3.03	0.40
1:C:206:ILE:CD1	1:C:242:LEU:HD21	2.52	0.40
1:A:282:LEU:C	1:A:282:LEU:CD1	2.89	0.40
1:C:261:ILE:HD12	1:C:271:LYS:CE	2.51	0.40
1:A:286:ASP:OD1	1:A:286:ASP:C	2.60	0.40
1:D:185:LEU:O	1:D:190:VAL:HB	2.20	0.40
1:C:206:ILE:CD1	1:C:242:LEU:CD2	2.99	0.40
1:C:35:GLN:HG3	1:D:70:MET:CB	2.52	0.40
1:D:94:THR:O	1:D:136:VAL:HA	2.20	0.40
1:A:147:LYS:O	1:A:151:LYS:HG3	2.21	0.40
1:D:290:PHE:CZ	1:D:294:ASN:ND2	2.90	0.40
1:D:308:ASN:HA	1:D:311:LYS:NZ	2.36	0.40
1:A:94:THR:O	1:A:136:VAL:HA	2.21	0.40
1:A:71:GLY:O	1:B:104:PHE:HE2	2.03	0.40
1:D:301:ILE:CD1	1:D:302:ALA:N	2.70	0.40
1:A:293:ARG:CZ	1:C:277:ARG:HG2	2.52	0.40
1:D:140:ALA:CB	1:D:181:GLN:HE21	2.33	0.40
1:A:57:MET:SD	1:A:88:ILE:HB	2.61	0.40
1:A:70:MET:CB	1:B:35:GLN:HG3	2.51	0.40
1:A:221:LEU:HB3	4:A:539:HOH:O	2.20	0.40
1:A:160:ASN:ND2	1:A:190:VAL:HG13	2.37	0.40
1:A:92:ALA:O	1:A:133:ALA:HA	2.21	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:A:250:LYS:NZ	1:B:294:ASN:OD1[2_454]	2.17	0.03

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	312/314 (99%)	273 (88%)	31 (10%)	8 (3%)	7 14
1	B	311/314 (99%)	269 (86%)	37 (12%)	5 (2%)	12 26
1	C	312/314 (99%)	275 (88%)	31 (10%)	6 (2%)	10 22
1	D	312/314 (99%)	266 (85%)	37 (12%)	9 (3%)	6 12
All	All	1247/1256 (99%)	1083 (87%)	136 (11%)	28 (2%)	8 19

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	B	15	ASP
1	C	261	ILE
1	D	175	ASN
1	D	223	ARG
1	D	276	PRO
1	D	292	LYS
1	A	9	ASP
1	A	259	CYS
1	A	297	ASN
1	B	108	ASN
1	B	259	CYS
1	B	273	LYS
1	D	177	THR
1	D	296	VAL
1	A	276	PRO
1	C	268	PRO
1	C	287	THR
1	D	108	ASN
1	C	140	ALA
1	C	272	PRO
1	A	287	THR
1	B	287	THR
1	C	276	PRO
1	D	178	GLY
1	A	230	LEU
1	A	268	PRO
1	D	271	LYS

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	273/272 (100%)	264 (97%)	9 (3%)	45 73
1	B	272/272 (100%)	270 (99%)	2 (1%)	88 96
1	C	273/272 (100%)	270 (99%)	3 (1%)	80 93
1	D	273/272 (100%)	269 (98%)	4 (2%)	72 90
All	All	1091/1088 (100%)	1073 (98%)	18 (2%)	70 89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	52	GLU
1	A	55	ARG
1	A	108	ASN
1	A	196	LEU
1	A	271	LYS
1	A	294	ASN
1	A	301	ILE
1	A	310	LYS
1	B	52	GLU
1	B	301	ILE
1	C	147	LYS
1	C	200	LEU
1	C	294	ASN
1	D	26[A]	ARG
1	D	26[B]	ARG
1	D	200	LEU
1	D	297	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN

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Mol	Chain	Res	Type
1	A	58	GLN
1	A	160	ASN
1	B	34	GLN
1	B	108	ASN
1	B	176	ASN
1	B	236	ASN
1	B	294	ASN
1	C	34	GLN
1	C	160	ASN
1	C	182	GLN
1	C	236	ASN
1	C	294	ASN
1	D	58	GLN
1	D	182	GLN
1	D	236	ASN
1	D	297	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	A	137	1,3	7,11,12	0.49	0	7,12,14	0.78	0
1	KCX	B	137	1,3	7,11,12	0.48	0	7,12,14	0.76	0
1	KCX	C	137	1,3	7,11,12	0.48	0	7,12,14	0.79	0
1	KCX	D	137	1,3	7,11,12	0.53	0	7,12,14	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	137	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	137	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	137	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	137	1,3	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	137	KCX	2	0
1	B	137	KCX	3	0
1	C	137	KCX	2	0
1	D	137	KCX	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	313/314 (99%)	0.15	13 (4%) 40 38	25, 55, 137, 236	0
1	B	313/314 (99%)	0.27	20 (6%) 23 20	34, 71, 129, 205	0
1	C	313/314 (99%)	0.46	24 (7%) 16 14	32, 77, 152, 264	0
1	D	313/314 (99%)	0.81	40 (12%) 5 3	47, 88, 136, 236	0
All	All	1252/1256 (99%)	0.42	97 (7%) 16 14	25, 74, 137, 264	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	LEU	23.3
1	D	264	GLY	14.8
1	D	263	LEU	13.9
1	C	264	GLY	11.5
1	A	268	PRO	10.5
1	D	265	THR	9.6
1	C	265	THR	9.3
1	D	268	PRO	8.3
1	B	268	PRO	8.1
1	C	262	ASP	8.1
1	D	270	TYR	8.0
1	B	263	LEU	7.8
1	C	268	PRO	7.4
1	B	1	MET	7.2
1	C	274	LEU	7.1
1	A	267	LYS	6.4
1	A	260	THR	6.4
1	C	266	ALA	6.1
1	C	270	TYR	5.9
1	D	267	LYS	5.9
1	C	269	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	265	THR	5.5
1	D	259	CYS	5.5
1	D	200	LEU	5.2
1	D	275	ALA	5.0
1	D	262	ASP	4.9
1	A	261	ILE	4.9
1	C	267	LYS	4.8
1	D	260	THR	4.8
1	B	270	TYR	4.7
1	B	274	LEU	4.6
1	A	259	CYS	4.5
1	D	272	PRO	4.4
1	C	261	ILE	4.4
1	D	261	ILE	4.2
1	B	266	ALA	4.1
1	B	262	ASP	4.0
1	D	212	ILE	3.9
1	D	198	GLY	3.9
1	B	260	THR	3.9
1	D	271	LYS	3.8
1	D	277	ARG	3.8
1	D	273	LYS	3.7
1	B	271	LYS	3.6
1	C	275	ALA	3.6
1	D	1	MET	3.6
1	A	272	PRO	3.5
1	B	267	LYS	3.5
1	C	230	LEU	3.3
1	B	265	THR	3.3
1	D	228	LEU	3.3
1	B	261	ILE	3.2
1	D	208	TYR	3.2
1	D	274	LEU	3.2
1	D	209	ILE	3.1
1	C	140	ALA	3.1
1	D	222	ASP	3.1
1	D	197	ILE	3.0
1	C	278	TRP	3.0
1	D	266	ALA	3.0
1	D	177	THR	3.0
1	A	269	GLU	3.0
1	D	269	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	104[A]	PHE	2.9
1	A	270	TYR	2.9
1	B	272	PRO	2.9
1	A	263	LEU	2.9
1	A	277	ARG	2.8
1	A	262	ASP	2.8
1	B	264	GLY	2.7
1	B	273	LYS	2.7
1	B	117	LEU	2.6
1	B	269	GLU	2.6
1	C	271	LYS	2.5
1	D	202	ASP	2.5
1	D	258	CYS	2.5
1	C	260	THR	2.5
1	C	277	ARG	2.5
1	C	9	ASP	2.4
1	D	242	LEU	2.4
1	B	313	PHE	2.4
1	A	264	GLY	2.3
1	D	206	ILE	2.3
1	D	304	ILE	2.3
1	D	204	ASP	2.3
1	D	136	VAL	2.2
1	C	259	CYS	2.2
1	D	221	LEU	2.2
1	B	259	CYS	2.2
1	D	203	THR	2.2
1	D	171	SER	2.1
1	C	229	PHE	2.1
1	C	1	MET	2.1
1	D	215	LYS	2.1
1	C	272	PRO	2.1
1	B	90	LEU	2.1
1	D	174	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	C	137	12/13	0.97	0.14	-	35,40,44,64	0
1	KCX	A	137	12/13	0.95	0.15	-	27,31,33,39	0
1	KCX	D	137	12/13	0.96	0.15	-	60,63,67,67	0
1	KCX	B	137	12/13	0.97	0.16	-	30,45,55,56	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CO	C	402	1/1	0.88	0.08	-1.75	44,44,44,44	0
3	CO	D	402	1/1	0.72	0.08	-2.40	58,58,58,58	0
3	CO	A	402	1/1	0.92	0.07	-4.04	33,33,33,33	0
3	CO	B	402	1/1	0.95	0.07	-4.27	25,25,25,25	0
2	FE2	A	401	1/1	0.96	0.07	-	18,18,18,18	0
2	FE2	C	401	1/1	0.97	0.10	-	36,36,36,36	0
2	FE2	B	401	1/1	0.96	0.06	-	19,19,19,19	0
2	FE2	D	401	1/1	0.77	0.09	-	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.