Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 11:20 AM EST

PDB ID	:	2F7K
Title	:	Crystal Structure of Human Pyridoxal Kinase
Authors	:	Jiang, T.; Cao, P.; Gong, Y.; Tang, L.
Deposited on	:	2005-12-01
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

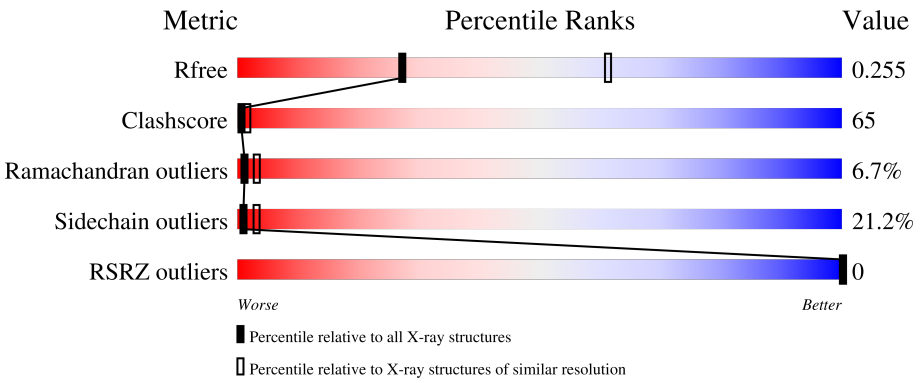
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	327	21% 59% 16% ••
1	B	327	26% 57% 15% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5327 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2560	1608	458	478	16	0	0	0
1	B	323	2560	1608	458	478	16	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	SER	-	cloning artifact	UNP O00764
A	-13	TYR	-	cloning artifact	UNP O00764
A	-12	TYR	-	cloning artifact	UNP O00764
A	-11	HIS	-	expression tag	UNP O00764
A	-10	HIS	-	expression tag	UNP O00764
A	-9	HIS	-	expression tag	UNP O00764
A	-8	HIS	-	expression tag	UNP O00764
A	-7	HIS	-	expression tag	UNP O00764
A	-6	HIS	-	expression tag	UNP O00764
A	-5	HIS	-	expression tag	UNP O00764
A	-4	GLU	-	cloning artifact	UNP O00764
A	-3	GLY	-	cloning artifact	UNP O00764
A	-2	VAL	-	cloning artifact	UNP O00764
A	-1	ARG	-	cloning artifact	UNP O00764
A	0	THR	-	cloning artifact	UNP O00764
B	-14	SER	-	cloning artifact	UNP O00764
B	-13	TYR	-	cloning artifact	UNP O00764
B	-12	TYR	-	cloning artifact	UNP O00764
B	-11	HIS	-	expression tag	UNP O00764
B	-10	HIS	-	expression tag	UNP O00764
B	-9	HIS	-	expression tag	UNP O00764
B	-8	HIS	-	expression tag	UNP O00764
B	-7	HIS	-	expression tag	UNP O00764
B	-6	HIS	-	expression tag	UNP O00764
B	-5	HIS	-	expression tag	UNP O00764

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLU	-	cloning artifact	UNP O00764
B	-3	GLY	-	cloning artifact	UNP O00764
B	-2	VAL	-	cloning artifact	UNP O00764
B	-1	ARG	-	cloning artifact	UNP O00764
B	0	THR	-	cloning artifact	UNP O00764

- Molecule 2 is water.

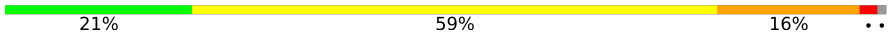
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	96	96	96	0	0
			Total	O		
2	B	111	111	111	0	0

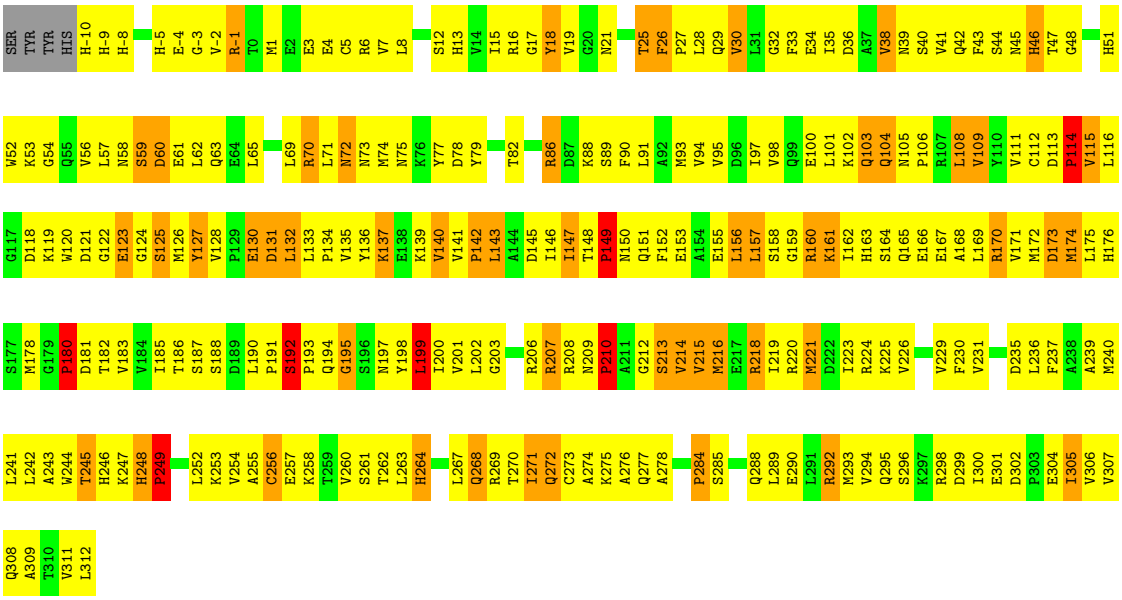
3 Residue-property plots (i)

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

- Molecule 1: Pyridoxal kinase

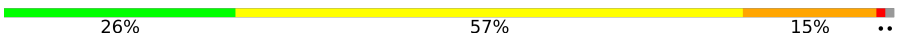
Chain A:

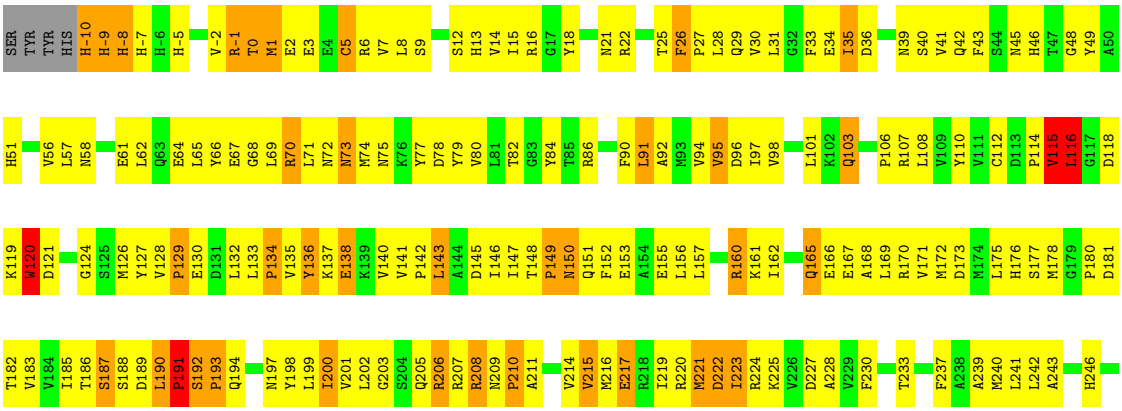




- Molecule 1: Pyridoxal kinase

Chain B:





P249
N250
N251
L252
K253
C256
E257
K258
T259
V260
S261
T262
L263
H264
H265
V266
L267
Q268
R269
T270
I271
Q272
C273
A274
A278
G279
E280
G281
V282
R283
P284
S285
P286
M287
Q288
L289
R292
M293
V294
Q295
S296
K297
R298
D299
I300
E301
D302
P303
E304
I305
V306
V307
Q308
A309
T310
V311
L312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	52.50Å 52.50Å 301.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 7.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.0 (8.00-2.80) 81.0 (7.99-2.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 2.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.271 0.213 , 0.255	Depositor DCC
R_{free} test set	709 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 71.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.190 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.46	0/2612	0.87	10/3540 (0.3%)
1	B	0.45	0/2612	0.83	3/3540 (0.1%)
All	All	0.45	0/5224	0.85	13/7080 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	PRO	CA-N-CD	-7.94	100.39	111.50
1	A	149	PRO	CA-N-CD	-7.75	100.66	111.50
1	B	120	TRP	CA-CB-CG	6.54	126.12	113.70
1	A	-3	GLY	N-CA-C	-6.51	96.83	113.10
1	A	192	SER	N-CA-C	-5.85	95.22	111.00
1	B	150	ASN	N-CA-C	-5.79	95.37	111.00
1	A	38	VAL	N-CA-C	-5.60	95.87	111.00
1	A	304	GLU	N-CA-C	-5.49	96.17	111.00
1	A	-4	GLU	N-CA-C	-5.20	96.96	111.00
1	A	150	ASN	N-CA-C	-5.19	96.99	111.00
1	B	116	LEU	N-CA-C	5.18	124.99	111.00
1	A	132	LEU	N-CA-C	5.11	124.81	111.00
1	A	199	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2551	354	0
1	B	2560	0	2551	334	0
2	A	96	0	0	0	0
2	B	111	0	0	3	0
All	All	5327	0	5102	660	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

All (660) 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:199:LEU:HB2	1:A:223:ILE:HB	1.38	1.05
1:A:72:ASN:HD21	1:A:74:MET:HG3	1.22	1.04
1:A:221:MET:HG2	1:A:309:ALA:HA	1.39	1.02
1:A:147:ILE:CD1	1:A:147:ILE:H	1.74	1.00
1:A:147:ILE:H	1:A:147:ILE:HD13	1.24	1.00
1:A:230:PHE:HE1	1:A:267:LEU:HB3	1.30	0.97
1:A:35:ILE:HD12	1:A:35:ILE:H	1.28	0.96
1:B:162:ILE:HD11	1:B:171:VAL:CG2	1.95	0.96
1:A:26:PHE:HB3	1:A:27:PRO:HD3	1.49	0.94
1:B:189:ASP:O	1:B:191:PRO:HD3	1.67	0.94
1:A:108:LEU:HG	1:A:109:VAL:H	1.33	0.93
1:A:181:ASP:HB2	1:A:207:ARG:NH2	1.84	0.93
1:A:263:LEU:O	1:A:267:LEU:HG	1.70	0.92
1:A:72:ASN:ND2	1:A:74:MET:HG3	1.85	0.90
1:B:84:TYR:HA	1:B:115:VAL:HB	1.52	0.89
1:B:253:LYS:O	1:B:257:GLU:HG3	1.71	0.89
1:B:311:VAL:HG21	2:B:396:HOH:O	1.73	0.88
1:A:254:VAL:HA	1:A:257:GLU:HB2	1.58	0.86
1:A:197:ASN:C	1:A:225:LYS:HD3	1.97	0.85
1:B:15:ILE:HD11	1:B:42:GLN:HE21	1.42	0.85
1:A:147:ILE:HD12	1:A:180:PRO:HB3	1.60	0.84
1:A:264:HIS:ND1	1:A:306:VAL:HG21	1.92	0.84
1:B:168:ALA:O	1:B:172:MET:HG3	1.77	0.83
1:A:170:ARG:CZ	1:A:170:ARG:HB2	2.07	0.83
1:B:160:ARG:HD2	1:B:161:LYS:H	1.44	0.83
1:B:165:GLN:HG3	1:B:220:ARG:NH1	1.93	0.83
1:A:152:PHE:CE1	1:A:156:LEU:HG	2.14	0.82
1:B:172:MET:HE1	1:B:202:LEU:HD22	1.61	0.82
1:A:4:GLU:HB3	1:A:6:ARG:HG3	1.61	0.82
1:A:8:LEU:HB2	1:A:77:TYR:CE2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HA	1:A:272:GLN:HB2	1.62	0.81
1:A:112:CYS:SG	1:A:114:PRO:HD3	2.22	0.80
1:B:210:PRO:HG2	1:B:215:VAL:CG1	2.11	0.80
1:B:278:ALA:HB2	1:B:288:GLN:NE2	1.97	0.79
1:A:147:ILE:CD1	1:A:147:ILE:N	2.45	0.79
1:A:181:ASP:HB2	1:A:207:ARG:HH21	1.44	0.79
1:A:230:PHE:CE1	1:A:267:LEU:HB3	2.18	0.79
1:A:220:ARG:C	1:A:221:MET:HG3	2.03	0.79
1:B:205:GLN:CB	1:B:252:LEU:HD11	2.13	0.79
1:B:26:PHE:O	1:B:30:VAL:HG12	1.83	0.78
1:B:90:PHE:O	1:B:94:VAL:HG23	1.83	0.78
1:A:254:VAL:HG12	1:A:258:LYS:HG3	1.64	0.78
1:A:140:VAL:O	1:A:143:LEU:HD12	1.83	0.78
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.66	0.77
1:A:173:ASP:HA	1:A:176:HIS:HB2	1.66	0.77
1:B:241:LEU:O	1:B:241:LEU:HD23	1.84	0.77
1:A:171:VAL:HA	1:A:174:MET:SD	2.24	0.77
1:B:-1:ARG:HG2	1:B:-1:ARG:O	1.85	0.76
1:B:162:ILE:HD11	1:B:171:VAL:HG21	1.65	0.76
1:A:192:SER:OG	1:A:200:ILE:HD11	1.85	0.76
1:B:91:LEU:HD12	1:B:91:LEU:O	1.84	0.76
1:B:124:GLY:HA3	1:B:152:PHE:CE2	2.21	0.76
1:B:207:ARG:NE	1:B:250:ASN:HD22	1.84	0.75
1:A:-5:HIS:O	1:A:-2:VAL:HG23	1.86	0.75
1:A:108:LEU:HG	1:A:109:VAL:N	2.01	0.75
1:A:28:LEU:CB	1:A:35:ILE:HD11	2.17	0.75
1:A:197:ASN:C	1:A:198:TYR:HD2	1.90	0.75
1:A:214:VAL:O	1:A:214:VAL:HG23	1.85	0.74
1:A:147:ILE:HD11	1:A:183:VAL:CG2	2.17	0.74
1:A:168:ALA:O	1:A:172:MET:HG3	1.86	0.74
1:A:78:ASP:C	1:A:108:LEU:HD12	2.08	0.74
1:A:230:PHE:CD1	1:A:267:LEU:HD22	2.23	0.74
1:A:147:ILE:HD11	1:A:183:VAL:HA	1.68	0.73
1:A:93:MET:O	1:A:97:ILE:HG13	1.88	0.73
1:A:147:ILE:CD1	1:A:183:VAL:HA	2.19	0.73
1:A:169:LEU:HD23	1:A:172:MET:HE2	1.69	0.73
1:B:296:SER:O	1:B:300:ILE:HG12	1.88	0.73
1:A:199:LEU:CB	1:A:223:ILE:HB	2.16	0.73
1:B:35:ILE:HD13	1:B:36:ASP:N	2.03	0.73
1:B:68:GLY:HA2	1:B:71:LEU:HD12	1.70	0.73
1:B:79:TYR:OH	1:B:246:HIS:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLN:HB2	1:B:188:SER:HA	1.71	0.73
1:A:135:VAL:HG13	1:A:139:LYS:HD2	1.69	0.73
1:B:206:ARG:HG3	1:B:207:ARG:N	2.03	0.73
1:A:28:LEU:O	1:A:33:PHE:HB2	1.88	0.73
1:A:12:SER:HB2	1:A:41:VAL:HG22	1.71	0.73
1:A:152:PHE:CZ	1:A:156:LEU:HG	2.23	0.73
1:A:244:TRP:CE3	1:A:258:LYS:HD2	2.24	0.72
1:B:112:CYS:O	1:B:147:ILE:HA	1.89	0.72
1:A:186:THR:HA	1:A:201:VAL:CG1	2.20	0.72
1:B:1:MET:O	1:B:1:MET:HG2	1.88	0.72
1:A:42:GLN:HE22	1:B:39:ASN:H	1.35	0.71
1:A:72:ASN:HD21	1:A:74:MET:CG	2.02	0.71
1:A:193:PRO:HD3	1:A:220:ARG:HH12	1.56	0.71
1:A:4:GLU:HG2	1:A:6:ARG:NH2	2.06	0.71
1:B:278:ALA:O	1:B:279:GLY:O	2.08	0.71
1:B:265:HIS:HD2	1:B:303:PRO:HB3	1.56	0.71
1:B:95:VAL:HG12	1:B:96:ASP:N	2.03	0.71
1:B:115:VAL:O	1:B:115:VAL:CG2	2.39	0.71
1:B:26:PHE:HB3	1:B:27:PRO:HD3	1.71	0.71
1:A:200:ILE:HD12	1:A:220:ARG:HD3	1.73	0.70
1:A:78:ASP:O	1:A:108:LEU:HD12	1.91	0.70
1:A:254:VAL:CA	1:A:257:GLU:HB2	2.21	0.70
1:B:311:VAL:O	1:B:312:LEU:HD23	1.91	0.70
1:A:72:ASN:OD1	1:A:74:MET:HB2	1.92	0.69
1:A:271:ILE:HD13	1:A:274:ALA:HB3	1.74	0.69
1:A:35:ILE:HD12	1:A:35:ILE:N	2.04	0.69
1:B:162:ILE:HD11	1:B:171:VAL:HG23	1.73	0.69
1:A:198:TYR:HA	1:A:223:ILE:O	1.93	0.69
1:A:128:VAL:HG13	1:A:132:LEU:HD13	1.73	0.69
1:A:29:GLN:O	1:B:294:VAL:HG13	1.92	0.69
1:B:239:ALA:O	1:B:242:LEU:HB3	1.92	0.69
1:B:200:ILE:HG22	1:B:201:VAL:H	1.58	0.69
1:B:172:MET:HA	1:B:175:LEU:HD12	1.72	0.69
1:A:27:PRO:HG3	1:A:300:ILE:HD13	1.76	0.68
1:B:115:VAL:CG1	1:B:136:TYR:HE1	2.07	0.68
1:B:141:VAL:HG21	1:B:157:LEU:HD22	1.75	0.68
1:A:186:THR:HA	1:A:201:VAL:HG13	1.74	0.68
1:B:120:TRP:HE3	1:B:120:TRP:C	1.97	0.68
1:B:273:CYS:SG	1:B:292:ARG:HG3	2.34	0.68
1:B:5:CYS:HA	1:B:78:ASP:OD2	1.93	0.68
1:A:264:HIS:CD2	1:A:268:GLN:HG3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:HG3	1:B:220:ARG:HH11	1.56	0.68
1:B:190:LEU:HD13	1:B:200:ILE:HG13	1.76	0.68
1:B:66:TYR:HA	1:B:69:LEU:HD12	1.76	0.68
1:B:197:ASN:HA	1:B:225:LYS:HD2	1.75	0.67
1:B:260:VAL:HA	1:B:263:LEU:HD23	1.74	0.67
1:A:36:ASP:HA	1:B:22:ARG:HH12	1.59	0.67
1:B:115:VAL:O	1:B:115:VAL:HG22	1.93	0.67
1:A:236:LEU:HD12	1:A:236:LEU:O	1.95	0.67
1:A:56:VAL:HG12	1:A:57:LEU:O	1.94	0.67
1:A:218:ARG:O	1:A:219:ILE:HG23	1.95	0.67
1:B:80:VAL:HG23	1:B:108:LEU:HD21	1.77	0.67
1:B:197:ASN:O	1:B:225:LYS:HB3	1.95	0.67
1:A:15:ILE:HG22	1:A:15:ILE:O	1.95	0.67
1:A:62:LEU:HD22	1:A:90:PHE:CZ	2.29	0.67
1:A:193:PRO:HD3	1:A:220:ARG:NH1	2.09	0.67
1:B:172:MET:HE2	1:B:185:ILE:HG13	1.77	0.67
1:A:4:GLU:HG2	1:A:6:ARG:CZ	2.25	0.66
1:A:39:ASN:H	1:B:42:GLN:HE22	1.42	0.66
1:A:16:ARG:HD2	1:B:74:MET:HB3	1.76	0.66
1:A:162:ILE:HG21	1:A:168:ALA:HB2	1.77	0.66
1:A:172:MET:O	1:A:175:LEU:HB2	1.94	0.66
1:A:28:LEU:HD22	1:A:33:PHE:CD1	2.30	0.66
1:A:155:GLU:CG	1:A:162:ILE:HG12	2.26	0.66
1:B:223:ILE:N	1:B:223:ILE:HD13	2.11	0.66
1:A:199:LEU:HB2	1:A:223:ILE:CB	2.20	0.65
1:B:205:GLN:HB3	1:B:252:LEU:HD11	1.79	0.65
1:A:15:ILE:HD12	1:A:43:PHE:O	1.97	0.65
1:B:12:SER:HB2	1:B:41:VAL:HG22	1.79	0.65
1:A:88:LYS:HG3	1:A:135:VAL:HG21	1.78	0.65
1:B:127:TYR:O	1:B:128:VAL:HG13	1.97	0.65
1:A:94:VAL:O	1:A:98:VAL:HG23	1.97	0.65
1:A:151:GLN:HB2	1:A:188:SER:HA	1.79	0.65
1:B:-8:HIS:NE2	1:B:-7:HIS:CE1	2.64	0.65
1:A:153:GLU:O	1:A:157:LEU:HD12	1.97	0.65
1:A:147:ILE:HD12	1:A:180:PRO:CB	2.27	0.64
1:B:120:TRP:C	1:B:120:TRP:CE3	2.70	0.64
1:B:142:PRO:HA	1:B:178:MET:O	1.97	0.64
1:B:242:LEU:HD23	1:B:242:LEU:C	2.18	0.64
1:A:45:ASN:HD21	1:B:72:ASN:HD22	1.45	0.64
1:B:115:VAL:CG1	1:B:136:TYR:CE1	2.80	0.64
1:B:7:VAL:HB	1:B:35:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:VAL:C	1:B:312:LEU:HD23	2.18	0.64
1:A:147:ILE:HD11	1:A:183:VAL:HG22	1.78	0.64
1:A:209:ASN:HB2	1:A:210:PRO:HD2	1.79	0.64
1:A:79:TYR:CD2	1:A:109:VAL:HB	2.33	0.64
1:B:265:HIS:CD2	1:B:303:PRO:HB3	2.33	0.63
1:B:252:LEU:HB3	1:B:256:CYS:SG	2.39	0.63
1:A:147:ILE:CD1	1:A:180:PRO:HB3	2.27	0.63
1:B:202:LEU:HD23	1:B:203:GLY:N	2.13	0.63
1:B:280:GLU:HG3	1:B:280:GLU:O	1.98	0.63
1:B:206:ARG:HD2	1:B:208:ARG:HD3	1.81	0.63
1:B:136:TYR:CE2	1:B:140:VAL:HG11	2.34	0.63
1:B:223:ILE:HG22	1:B:307:VAL:HG11	1.80	0.63
1:A:91:LEU:HA	1:A:94:VAL:HG23	1.80	0.62
1:A:155:GLU:HG3	1:A:162:ILE:HG12	1.80	0.62
1:A:230:PHE:HE1	1:A:267:LEU:CB	2.09	0.62
1:B:172:MET:CE	1:B:202:LEU:HD22	2.29	0.62
1:A:268:GLN:O	1:A:272:GLN:HB2	1.99	0.62
1:B:13:HIS:O	1:B:42:GLN:HA	2.00	0.62
1:A:28:LEU:HB3	1:A:35:ILE:HD11	1.82	0.62
1:A:38:VAL:HA	1:B:15:ILE:HD12	1.82	0.61
1:B:133:LEU:HD21	1:B:137:LYS:HE3	1.81	0.61
1:B:250:ASN:N	1:B:250:ASN:OD1	2.32	0.61
1:A:119:LYS:HG2	1:A:123:GLU:O	2.00	0.61
1:A:168:ALA:O	1:A:171:VAL:HG12	1.99	0.61
1:B:214:VAL:HG22	1:B:215:VAL:N	2.15	0.61
1:A:6:ARG:O	1:A:7:VAL:HG23	2.00	0.61
1:A:229:VAL:HG12	1:A:229:VAL:O	2.00	0.61
1:B:205:GLN:HB2	1:B:252:LEU:HD11	1.81	0.61
1:A:254:VAL:HA	1:A:257:GLU:CB	2.29	0.61
1:A:28:LEU:HD22	1:A:33:PHE:HD1	1.65	0.60
1:A:47:THR:HG22	1:A:52:TRP:CE2	2.36	0.60
1:A:16:ARG:HH11	1:B:74:MET:HG2	1.64	0.60
1:B:118:ASP:CG	1:B:119:LYS:H	2.05	0.60
1:B:8:LEU:HD13	1:B:77:TYR:CZ	2.36	0.60
1:B:26:PHE:C	1:B:26:PHE:HD1	2.03	0.60
1:A:28:LEU:C	1:A:35:ILE:HD11	2.21	0.60
1:A:12:SER:HB2	1:A:41:VAL:CG2	2.30	0.60
1:B:115:VAL:CG2	1:B:128:VAL:HG11	2.31	0.60
1:B:274:ALA:HA	1:B:288:GLN:O	2.01	0.60
1:B:49:TYR:CE1	1:B:286:PRO:HB2	2.37	0.59
1:B:133:LEU:CG	1:B:137:LYS:HE3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:THR:O	1:B:266:VAL:HG23	2.01	0.59
1:A:252:LEU:HD11	1:A:256:CYS:SG	2.42	0.59
1:B:198:TYR:HE1	1:B:224:ARG:HE	1.48	0.59
1:A:171:VAL:HG13	1:A:172:MET:N	2.18	0.59
1:A:206:ARG:HG3	1:A:216:MET:HG3	1.85	0.59
1:B:26:PHE:C	1:B:26:PHE:CD1	2.76	0.59
1:A:147:ILE:HD13	1:A:147:ILE:N	1.96	0.59
1:A:220:ARG:HG3	1:A:221:MET:N	2.18	0.58
1:B:-5:HIS:O	1:B:-2:VAL:HG23	2.03	0.58
1:B:84:TYR:CD2	1:B:115:VAL:HG23	2.38	0.58
1:A:136:TYR:HA	1:A:140:VAL:HB	1.85	0.58
1:A:264:HIS:HD2	1:A:268:GLN:HG3	1.67	0.58
1:B:70:ARG:HG3	1:B:75:ASN:ND2	2.18	0.58
1:B:208:ARG:HA	1:B:214:VAL:HA	1.84	0.58
1:A:261:SER:O	1:A:264:HIS:HB3	2.03	0.58
1:A:254:VAL:HG12	1:A:258:LYS:CG	2.30	0.58
1:B:98:VAL:HG11	1:B:110:TYR:CD1	2.39	0.58
1:B:133:LEU:CD2	1:B:137:LYS:HE3	2.34	0.58
1:B:0:THR:HG22	1:B:1:MET:N	2.19	0.57
1:B:57:LEU:HD11	1:B:65:LEU:HD22	1.86	0.57
1:A:45:ASN:HD22	1:B:74:MET:CE	2.18	0.57
1:B:69:LEU:HD23	1:B:74:MET:CE	2.35	0.57
1:A:53:LYS:HG2	1:B:64:GLU:OE1	2.05	0.57
1:A:242:LEU:C	1:A:242:LEU:HD23	2.25	0.57
1:B:214:VAL:HG22	1:B:215:VAL:O	2.04	0.57
1:A:181:ASP:HB2	1:A:207:ARG:CZ	2.35	0.57
1:A:26:PHE:HB3	1:A:27:PRO:CD	2.28	0.57
1:A:197:ASN:O	1:A:225:LYS:HD3	2.04	0.57
1:B:176:HIS:HD1	1:B:181:ASP:HA	1.70	0.57
1:A:151:GLN:CB	1:A:188:SER:HA	2.34	0.56
1:A:4:GLU:HB3	1:A:6:ARG:CG	2.32	0.56
1:A:139:LYS:O	1:A:143:LEU:HD11	2.06	0.56
1:A:169:LEU:HD23	1:A:172:MET:CE	2.33	0.56
1:B:84:TYR:HD2	1:B:115:VAL:HG23	1.70	0.56
1:B:115:VAL:HG22	1:B:128:VAL:HG11	1.88	0.56
1:B:210:PRO:HG2	1:B:215:VAL:HG13	1.88	0.56
1:B:287:MET:SD	1:B:287:MET:N	2.70	0.56
1:B:91:LEU:HD11	1:B:140:VAL:CG2	2.35	0.56
1:A:186:THR:CA	1:A:201:VAL:HG13	2.35	0.56
1:B:14:VAL:HA	1:B:43:PHE:O	2.05	0.56
1:B:128:VAL:HB	1:B:132:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:HD21	1:B:72:ASN:ND2	2.02	0.56
1:A:45:ASN:HD22	1:B:74:MET:HE1	1.71	0.56
1:B:57:LEU:CD2	1:B:62:LEU:HB2	2.36	0.56
1:A:12:SER:CB	1:A:41:VAL:HG22	2.36	0.55
1:A:153:GLU:O	1:A:157:LEU:HB2	2.06	0.55
1:A:165:GLN:HG3	1:A:166:GLU:N	2.20	0.55
1:B:120:TRP:HE3	1:B:120:TRP:O	1.87	0.55
1:A:16:ARG:NH1	1:B:74:MET:HG2	2.21	0.55
1:B:97:ILE:O	1:B:101:LEU:HG	2.06	0.55
1:B:133:LEU:HG	1:B:137:LYS:HE3	1.88	0.55
1:A:18:TYR:HD2	1:A:293:MET:HG3	1.72	0.54
1:A:257:GLU:OE1	1:A:305:ILE:HD12	2.08	0.54
1:B:115:VAL:HG12	1:B:136:TYR:CE1	2.42	0.54
1:B:26:PHE:CE2	1:B:294:VAL:HA	2.42	0.54
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.73	0.54
1:A:311:VAL:HG12	1:A:312:LEU:N	2.23	0.54
1:A:241:LEU:O	1:A:245:THR:HG23	2.07	0.54
1:B:71:LEU:C	1:B:73:ASN:H	2.11	0.54
1:A:45:ASN:ND2	1:B:72:ASN:HD22	2.05	0.54
1:A:220:ARG:O	1:A:221:MET:HG3	2.07	0.54
1:B:165:GLN:CG	1:B:220:ARG:NH1	2.69	0.54
1:A:270:THR:HA	1:A:292:ARG:HD2	1.90	0.54
1:B:273:CYS:HB2	1:B:292:ARG:NH2	2.23	0.54
1:B:46:HIS:CE1	1:B:48:GLY:HA3	2.42	0.54
1:B:162:ILE:HD12	1:B:167:GLU:C	2.28	0.54
1:A:248:HIS:N	1:A:248:HIS:CD2	2.75	0.54
1:B:0:THR:HG22	1:B:1:MET:H	1.72	0.54
1:A:18:TYR:N	1:A:18:TYR:CD1	2.75	0.54
1:A:256:CYS:O	1:A:260:VAL:HG23	2.08	0.54
1:A:6:ARG:CZ	1:B:16:ARG:HH21	2.22	0.53
1:A:32:GLY:HA2	1:B:294:VAL:HG11	1.89	0.53
1:A:254:VAL:C	1:A:257:GLU:HB2	2.28	0.53
1:B:147:ILE:HB	1:B:149:PRO:HD3	1.90	0.53
1:A:242:LEU:HD23	1:A:242:LEU:O	2.07	0.53
1:B:130:GLU:HG2	1:B:130:GLU:O	2.09	0.53
1:B:225:LYS:O	1:B:225:LYS:HG3	2.09	0.53
1:A:155:GLU:OE2	1:A:162:ILE:HG12	2.08	0.53
1:A:16:ARG:HH11	1:B:74:MET:CG	2.22	0.53
1:A:186:THR:HG23	1:A:237:PHE:CE1	2.44	0.53
1:B:67:GLU:O	1:B:68:GLY:C	2.46	0.53
1:B:200:ILE:N	1:B:200:ILE:HD13	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:O	1:B:223:ILE:HD13	2.09	0.53
1:A:248:HIS:N	1:A:249:PRO:CD	2.72	0.53
1:B:115:VAL:HG13	1:B:136:TYR:HE1	1.73	0.53
1:B:189:ASP:O	1:B:191:PRO:CD	2.48	0.53
1:A:237:PHE:HD1	1:A:263:LEU:HD12	1.74	0.53
1:A:118:ASP:CB	1:A:127:TYR:OH	2.57	0.52
1:A:165:GLN:HA	1:A:190:LEU:HD13	1.90	0.52
1:A:181:ASP:CB	1:A:207:ARG:NH2	2.67	0.52
1:A:208:ARG:HG2	1:A:213:SER:C	2.30	0.52
1:B:137:LYS:O	1:B:142:PRO:HD3	2.09	0.52
1:B:217:GLU:OE2	1:B:219:ILE:HG23	2.08	0.52
1:B:115:VAL:HG12	1:B:136:TYR:OH	2.09	0.52
1:A:28:LEU:HB2	1:A:35:ILE:HD11	1.91	0.52
1:A:32:GLY:HA2	1:B:294:VAL:CG1	2.40	0.52
1:A:244:TRP:C	1:A:246:HIS:H	2.13	0.52
1:B:-10:HIS:C	1:B:-8:HIS:H	2.12	0.52
1:B:28:LEU:O	1:B:33:PHE:HB2	2.10	0.52
1:A:19:VAL:HG12	1:A:231:VAL:HG12	1.91	0.52
1:B:9:SER:CB	1:B:35:ILE:HD11	2.40	0.52
1:A:247:LYS:O	1:A:247:LYS:HG3	2.08	0.52
1:A:311:VAL:HG12	1:A:312:LEU:H	1.75	0.52
1:B:172:MET:HE3	1:B:185:ILE:HD12	1.92	0.52
1:A:8:LEU:HB2	1:A:77:TYR:CD2	2.44	0.51
1:A:35:ILE:H	1:A:35:ILE:CD1	2.10	0.51
1:A:292:ARG:NH1	1:A:292:ARG:HG2	2.24	0.51
1:A:147:ILE:H	1:A:147:ILE:HD12	1.69	0.51
1:A:15:ILE:O	1:A:15:ILE:CG2	2.58	0.51
1:B:188:SER:HB2	1:B:190:LEU:HD12	1.91	0.51
1:A:44:SER:OG	1:A:45:ASN:ND2	2.43	0.51
1:A:114:PRO:O	1:A:116:LEU:HG	2.10	0.51
1:A:305:ILE:HG12	1:A:305:ILE:O	2.10	0.51
1:B:220:ARG:C	1:B:221:MET:HG3	2.30	0.51
1:A:148:THR:N	1:A:149:PRO:CD	2.74	0.51
1:A:162:ILE:CG2	1:A:168:ALA:HB2	2.39	0.51
1:B:12:SER:HB2	1:B:41:VAL:CG2	2.41	0.51
1:B:114:PRO:HG2	1:B:157:LEU:HD11	1.92	0.51
1:B:120:TRP:CE3	1:B:121:ASP:N	2.79	0.51
1:B:162:ILE:HD12	1:B:167:GLU:HB3	1.93	0.51
1:B:188:SER:HB2	1:B:190:LEU:CD1	2.40	0.51
1:A:298:ARG:HA	1:A:301:GLU:OE2	2.10	0.51
1:B:124:GLY:CA	1:B:152:PHE:CE2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HB3	1:B:134:PRO:CD	2.39	0.51
1:A:108:LEU:O	1:A:109:VAL:CG2	2.58	0.51
1:B:225:LYS:O	1:B:227:ASP:N	2.44	0.51
1:A:185:ILE:HG22	1:A:185:ILE:O	2.11	0.51
1:B:98:VAL:HG12	1:B:143:LEU:HD13	1.92	0.51
1:B:148:THR:N	1:B:149:PRO:HD3	2.25	0.51
1:B:206:ARG:HD3	1:B:214:VAL:HG21	1.93	0.51
1:A:118:ASP:HB3	1:A:127:TYR:OH	2.11	0.50
1:B:30:VAL:O	1:B:30:VAL:HG22	2.11	0.50
1:A:108:LEU:CG	1:A:109:VAL:H	2.17	0.50
1:B:124:GLY:HA3	1:B:152:PHE:HE2	1.71	0.50
1:A:18:TYR:N	1:A:18:TYR:HD1	2.10	0.50
1:A:36:ASP:OD1	1:B:16:ARG:HD3	2.10	0.50
1:A:152:PHE:O	1:A:155:GLU:N	2.44	0.50
1:B:206:ARG:HB2	1:B:206:ARG:NH1	2.26	0.50
1:A:75:ASN:O	1:A:101:LEU:CD2	2.60	0.50
1:A:135:VAL:O	1:A:139:LYS:HB2	2.12	0.50
1:A:194:GLN:O	1:A:195:GLY:O	2.30	0.50
1:A:277:GLN:C	1:A:288:GLN:HE22	2.14	0.50
1:B:115:VAL:HG13	1:B:136:TYR:CE1	2.47	0.50
1:A:71:LEU:HB3	1:B:51:HIS:CD2	2.46	0.50
1:A:90:PHE:O	1:A:93:MET:HB3	2.11	0.50
1:A:246:HIS:C	1:A:249:PRO:HD3	2.32	0.50
1:B:116:LEU:HD12	1:B:126:MET:CE	2.41	0.50
1:A:139:LYS:O	1:A:143:LEU:CD1	2.60	0.50
1:A:192:SER:O	1:A:193:PRO:C	2.47	0.50
1:B:220:ARG:HG2	1:B:221:MET:N	2.27	0.50
1:B:223:ILE:HD13	1:B:223:ILE:H	1.75	0.50
1:A:51:HIS:HB2	1:B:72:ASN:OD1	2.11	0.50
1:A:192:SER:C	1:A:194:GLN:N	2.63	0.50
1:B:223:ILE:O	1:B:224:ARG:C	2.46	0.50
1:B:91:LEU:HD11	1:B:140:VAL:HG21	1.93	0.49
1:B:210:PRO:HG2	1:B:215:VAL:HG11	1.91	0.49
1:A:111:VAL:HG22	1:A:146:ILE:HB	1.92	0.49
1:A:203:GLY:HA3	1:A:219:ILE:HD11	1.94	0.49
1:B:157:LEU:HB2	1:B:175:LEU:HD21	1.94	0.49
1:B:209:ASN:CG	1:B:210:PRO:HD3	2.33	0.49
1:A:26:PHE:CB	1:A:27:PRO:HD3	2.31	0.49
1:A:209:ASN:O	1:A:210:PRO:C	2.51	0.49
1:B:257:GLU:O	1:B:261:SER:HB2	2.12	0.49
1:A:253:LYS:O	1:A:257:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASN:OD1	1:B:61:GLU:N	2.43	0.49
1:B:80:VAL:CG2	1:B:108:LEU:HD21	2.42	0.49
1:B:192:SER:C	1:B:194:GLN:H	2.16	0.49
1:A:180:PRO:C	1:A:182:THR:H	2.15	0.49
1:A:273:CYS:C	1:A:275:LYS:N	2.64	0.49
1:B:182:THR:OG1	1:B:205:GLN:NE2	2.44	0.49
1:B:207:ARG:HE	1:B:250:ASN:HD22	1.59	0.49
1:A:148:THR:N	1:A:149:PRO:HD2	2.28	0.49
1:A:254:VAL:HG12	1:A:254:VAL:O	2.12	0.49
1:A:284:PRO:CB	1:A:289:LEU:HG	2.43	0.49
1:B:268:GLN:O	1:B:271:ILE:HG22	2.13	0.49
1:A:43:PHE:HA	1:A:54:GLY:HA3	1.94	0.48
1:B:66:TYR:CD2	1:B:97:ILE:HG13	2.48	0.48
1:A:79:TYR:OH	1:A:246:HIS:ND1	2.42	0.48
1:A:247:LYS:HB3	1:A:248:HIS:CD2	2.48	0.48
1:B:192:SER:O	1:B:194:GLN:N	2.46	0.48
1:B:271:ILE:HG23	1:B:272:GLN:N	2.29	0.48
1:A:51:HIS:CD2	1:B:71:LEU:HB3	2.48	0.48
1:B:82:THR:HB	1:B:110:TYR:HE2	1.78	0.48
1:A:269:ARG:NH1	1:A:299:ASP:OD1	2.44	0.48
1:B:197:ASN:O	1:B:199:LEU:HD12	2.13	0.48
1:A:58:ASN:O	1:A:59:SER:C	2.51	0.48
1:A:171:VAL:CG1	1:A:172:MET:N	2.77	0.48
1:A:-2:VAL:HG12	1:A:-2:VAL:O	2.12	0.48
1:A:268:GLN:O	1:A:272:GLN:N	2.46	0.48
1:B:185:ILE:O	1:B:187:SER:N	2.46	0.48
1:A:17:GLY:C	1:A:18:TYR:HD1	2.17	0.48
1:A:70:ARG:O	1:A:73:ASN:N	2.43	0.48
1:A:72:ASN:ND2	1:A:74:MET:CG	2.67	0.48
1:B:279:GLY:C	1:B:281:GLY:H	2.17	0.48
1:A:74:MET:HE1	2:B:363:HOH:O	2.13	0.48
1:B:9:SER:HB3	1:B:35:ILE:HD11	1.96	0.48
1:B:162:ILE:HD12	1:B:167:GLU:O	2.14	0.48
1:B:165:GLN:CG	1:B:220:ARG:HH11	2.24	0.48
1:A:102:LYS:C	1:A:104:GLN:N	2.67	0.48
1:A:193:PRO:CD	1:A:220:ARG:NH1	2.77	0.48
1:A:268:GLN:O	1:A:272:GLN:CB	2.61	0.48
1:A:207:ARG:O	1:A:215:VAL:HG13	2.13	0.48
1:A:252:LEU:CD1	1:A:256:CYS:SG	3.02	0.48
1:B:152:PHE:O	1:B:156:LEU:HG	2.14	0.48
1:B:192:SER:HB2	1:B:200:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:C	1:A:201:VAL:HG13	2.33	0.47
1:B:192:SER:HB2	1:B:220:ARG:HH21	1.79	0.47
1:A:-10:HIS:C	1:A:-8:HIS:H	2.17	0.47
1:A:124:GLY:O	1:A:125:SER:HB2	2.14	0.47
1:B:25:THR:HG23	1:B:35:ILE:HG21	1.96	0.47
1:A:62:LEU:HD23	1:A:93:MET:HB3	1.95	0.47
1:B:150:ASN:C	1:B:150:ASN:OD1	2.52	0.47
1:A:28:LEU:HB2	1:A:35:ILE:CD1	2.44	0.47
1:A:190:LEU:CD1	1:A:202:LEU:HD11	2.44	0.47
1:A:252:LEU:HG	1:A:252:LEU:O	2.13	0.47
1:B:80:VAL:HG11	1:B:98:VAL:HG22	1.96	0.47
1:A:17:GLY:C	1:A:18:TYR:CD1	2.88	0.47
1:A:102:LYS:NZ	1:A:143:LEU:O	2.47	0.47
1:A:133:LEU:O	1:A:137:LYS:HD3	2.15	0.47
1:A:165:GLN:O	1:A:168:ALA:HB3	2.14	0.47
1:A:165:GLN:OE1	1:A:220:ARG:NH2	2.48	0.47
1:A:269:ARG:NH2	1:A:299:ASP:OD1	2.46	0.47
1:B:136:TYR:O	1:B:141:VAL:HG23	2.14	0.47
1:A:102:LYS:HZ2	1:A:143:LEU:HB3	1.79	0.47
1:A:147:ILE:HD13	1:A:183:VAL:HA	1.94	0.47
1:B:190:LEU:HD12	1:B:190:LEU:N	2.30	0.47
1:B:240:MET:HA	1:B:240:MET:CE	2.45	0.47
1:B:269:ARG:O	1:B:269:ARG:HG2	2.15	0.47
1:A:60:ASP:HA	1:A:63:GLN:HB3	1.97	0.47
1:A:95:VAL:HG13	1:A:143:LEU:HD13	1.97	0.47
1:A:244:TRP:O	1:A:246:HIS:N	2.47	0.47
1:A:18:TYR:HD2	1:A:293:MET:CG	2.28	0.47
1:A:57:LEU:HD12	1:A:61:GLU:HB3	1.96	0.47
1:A:292:ARG:CG	1:A:292:ARG:HH11	2.28	0.46
1:B:82:THR:CB	1:B:110:TYR:HE2	2.28	0.46
1:B:86:ARG:HD2	1:B:129:PRO:HD3	1.97	0.46
1:B:165:GLN:O	1:B:165:GLN:OE1	2.32	0.46
1:B:67:GLU:O	1:B:70:ARG:N	2.49	0.46
1:B:268:GLN:C	1:B:270:THR:H	2.17	0.46
1:A:29:GLN:HG3	1:A:35:ILE:HD13	1.97	0.46
1:A:38:VAL:HG13	1:A:65:LEU:HD12	1.97	0.46
1:A:254:VAL:O	1:A:258:LYS:HG3	2.15	0.46
1:B:222:ASP:OD1	1:B:222:ASP:N	2.48	0.46
1:A:18:TYR:CD2	1:A:293:MET:CG	2.98	0.46
1:B:57:LEU:HD21	1:B:62:LEU:HB2	1.96	0.46
1:B:66:TYR:O	1:B:69:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:OH	1:B:246:HIS:CB	2.60	0.46
1:B:285:SER:O	1:B:289:LEU:HB2	2.16	0.46
1:A:112:CYS:O	1:A:114:PRO:HD2	2.15	0.46
1:B:42:GLN:O	1:B:42:GLN:CG	2.62	0.46
1:B:252:LEU:HD12	1:B:252:LEU:N	2.31	0.46
1:A:133:LEU:O	1:A:133:LEU:HD12	2.15	0.46
1:A:170:ARG:CZ	1:A:170:ARG:CB	2.88	0.46
1:A:-10:HIS:O	1:A:-8:HIS:N	2.48	0.46
1:A:27:PRO:O	1:A:30:VAL:HG22	2.15	0.46
1:A:240:MET:O	1:A:241:LEU:C	2.53	0.46
1:B:169:LEU:CD2	1:B:202:LEU:HD21	2.45	0.46
1:B:171:VAL:O	1:B:175:LEU:HD12	2.16	0.46
1:A:147:ILE:HD11	1:A:183:VAL:CA	2.41	0.46
1:A:199:LEU:HD23	1:A:225:LYS:HG2	1.97	0.46
1:A:278:ALA:N	1:A:288:GLN:HE22	2.14	0.46
1:B:41:VAL:HG12	1:B:56:VAL:HG13	1.98	0.46
1:B:252:LEU:O	1:B:256:CYS:CB	2.64	0.46
1:A:42:GLN:OE1	1:B:39:ASN:HB2	2.16	0.46
1:B:124:GLY:C	1:B:152:PHE:CE2	2.89	0.46
1:A:223:ILE:HG22	1:A:224:ARG:O	2.16	0.45
1:B:69:LEU:HD23	1:B:74:MET:HE3	1.98	0.45
1:B:282:VAL:HG22	1:B:283:ARG:N	2.31	0.45
1:A:220:ARG:CG	1:A:221:MET:N	2.78	0.45
1:B:283:ARG:O	1:B:283:ARG:HD3	2.16	0.45
1:A:214:VAL:O	1:A:214:VAL:CG2	2.58	0.45
1:A:216:MET:SD	1:A:218:ARG:HG3	2.57	0.45
1:B:7:VAL:CB	1:B:35:ILE:HG12	2.46	0.45
1:B:91:LEU:HD12	1:B:91:LEU:C	2.35	0.45
1:B:147:ILE:HD11	1:B:183:VAL:HG13	1.98	0.45
1:B:199:LEU:C	1:B:200:ILE:HD13	2.36	0.45
1:B:263:LEU:H	1:B:263:LEU:HD22	1.82	0.45
1:B:297:LYS:O	1:B:298:ARG:C	2.54	0.45
1:B:311:VAL:CG2	2:B:396:HOH:O	2.46	0.45
1:A:75:ASN:HD21	1:A:104:GLN:HG3	1.81	0.45
1:B:133:LEU:O	1:B:135:VAL:N	2.48	0.45
1:B:264:HIS:C	1:B:266:VAL:H	2.18	0.45
1:A:86:ARG:CG	1:A:86:ARG:O	2.64	0.45
1:B:29:GLN:C	1:B:31:LEU:H	2.19	0.45
1:A:91:LEU:HA	1:A:94:VAL:CG2	2.46	0.45
1:A:151:GLN:N	1:A:187:SER:O	2.50	0.45
1:B:126:MET:O	1:B:127:TYR:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:O	1:B:306:VAL:HG22	2.15	0.45
1:A:198:TYR:CE2	1:A:224:ARG:HD3	2.52	0.45
1:B:116:LEU:HD13	1:B:116:LEU:HA	1.65	0.45
1:B:279:GLY:O	1:B:281:GLY:N	2.49	0.45
1:A:25:THR:O	1:A:26:PHE:C	2.55	0.45
1:A:26:PHE:O	1:A:29:GLN:HB2	2.17	0.45
1:A:244:TRP:C	1:A:246:HIS:N	2.69	0.45
1:A:255:ALA:C	1:A:257:GLU:H	2.20	0.45
1:B:8:LEU:HB2	1:B:77:TYR:CD2	2.51	0.45
1:A:79:TYR:HH	1:A:246:HIS:CG	2.35	0.45
1:A:284:PRO:HB3	1:A:289:LEU:HG	1.99	0.45
1:B:103:GLN:HE21	1:B:103:GLN:HB3	1.65	0.45
1:B:166:GLU:HG2	1:B:166:GLU:O	2.17	0.45
1:A:103:GLN:O	1:A:103:GLN:NE2	2.50	0.44
1:A:105:ASN:HA	1:A:106:PRO:HD3	1.74	0.44
1:B:115:VAL:HG12	1:B:136:TYR:CZ	2.52	0.44
1:B:199:LEU:HD13	1:B:225:LYS:HB3	1.98	0.44
1:B:306:VAL:O	1:B:306:VAL:CG2	2.66	0.44
1:A:28:LEU:HB2	1:A:35:ILE:HG12	1.99	0.44
1:B:62:LEU:HB2	1:B:90:PHE:HE1	1.82	0.44
1:B:166:GLU:OE2	1:B:170:ARG:NH2	2.50	0.44
1:A:53:LYS:HB3	1:B:64:GLU:HG2	1.99	0.44
1:A:273:CYS:O	1:A:276:ALA:N	2.42	0.44
1:B:263:LEU:HD22	1:B:263:LEU:N	2.32	0.44
1:B:160:ARG:CD	1:B:161:LYS:H	2.21	0.44
1:A:5:CYS:SG	1:A:246:HIS:CD2	3.11	0.44
1:A:17:GLY:HA3	1:A:290:GLU:OE1	2.17	0.44
1:A:39:ASN:O	1:A:41:VAL:N	2.50	0.44
1:A:305:ILE:O	1:A:305:ILE:CG1	2.66	0.44
1:B:167:GLU:HA	1:B:170:ARG:HB2	2.00	0.44
1:A:47:THR:HA	1:A:52:TRP:CE3	2.52	0.44
1:A:273:CYS:O	1:A:274:ALA:C	2.55	0.44
1:B:5:CYS:HB3	1:B:33:PHE:CD2	2.53	0.44
1:B:283:ARG:HG2	1:B:283:ARG:HH11	1.81	0.44
1:A:5:CYS:HG	1:A:246:HIS:CD2	2.36	0.44
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.83	0.44
1:A:75:ASN:ND2	1:A:104:GLN:HG3	2.32	0.44
1:B:147:ILE:C	1:B:149:PRO:HD3	2.39	0.44
1:B:242:LEU:C	1:B:242:LEU:CD2	2.85	0.44
1:B:16:ARG:NH1	1:B:16:ARG:HG2	2.32	0.44
1:B:119:LYS:HE3	1:B:152:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:O	1:B:142:PRO:HG2	2.17	0.44
1:A:-2:VAL:O	1:B:272:GLN:NE2	2.51	0.44
1:A:82:THR:HG21	1:A:94:VAL:HG11	2.00	0.44
1:B:12:SER:CB	1:B:41:VAL:HG22	2.46	0.44
1:B:252:LEU:O	1:B:256:CYS:SG	2.75	0.44
1:A:198:TYR:HD2	1:A:198:TYR:N	2.16	0.43
1:A:223:ILE:O	1:A:224:ARG:C	2.56	0.43
1:A:161:LYS:HB3	1:A:161:LYS:HE3	1.66	0.43
1:B:7:VAL:CG1	1:B:35:ILE:HG12	2.49	0.43
1:B:157:LEU:HB2	1:B:175:LEU:CD2	2.48	0.43
1:B:92:ALA:O	1:B:95:VAL:HB	2.18	0.43
1:B:151:GLN:O	1:B:155:GLU:HG3	2.19	0.43
1:B:197:ASN:OD1	1:B:198:TYR:HD1	2.01	0.43
1:A:34:GLU:HG2	1:B:18:TYR:OH	2.18	0.43
1:B:133:LEU:C	1:B:135:VAL:N	2.72	0.43
1:B:190:LEU:HD13	1:B:200:ILE:CG1	2.48	0.43
1:A:115:VAL:HA	1:A:153:GLU:OE2	2.18	0.43
1:A:147:ILE:HD11	1:A:183:VAL:HG23	1.97	0.43
1:A:242:LEU:C	1:A:242:LEU:CD2	2.87	0.43
1:B:40:SER:O	1:B:57:LEU:N	2.47	0.43
1:A:79:TYR:CE2	1:A:109:VAL:HB	2.53	0.43
1:A:95:VAL:HG13	1:A:143:LEU:CD1	2.49	0.43
1:A:190:LEU:O	1:A:200:ILE:HG13	2.18	0.43
1:B:30:VAL:HG22	1:B:301:GLU:HG2	2.01	0.43
1:B:98:VAL:CG1	1:B:143:LEU:HD13	2.48	0.43
1:A:207:ARG:O	1:A:215:VAL:CG1	2.66	0.43
1:A:130:GLU:HG2	1:A:131:ASP:N	2.33	0.43
1:A:186:THR:O	1:A:201:VAL:HG13	2.19	0.43
1:A:219:ILE:CD1	1:A:256:CYS:SG	3.07	0.43
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.84	0.43
1:B:145:ASP:O	1:B:146:ILE:HG13	2.19	0.43
1:B:146:ILE:HG12	1:B:182:THR:HB	2.01	0.43
1:B:270:THR:HA	1:B:292:ARG:HG2	2.01	0.43
1:A:151:GLN:HB2	1:A:188:SER:CA	2.48	0.43
1:A:52:TRP:O	1:A:52:TRP:CD1	2.72	0.43
1:A:113:ASP:O	1:A:115:VAL:N	2.48	0.43
1:A:198:TYR:N	1:A:198:TYR:CD2	2.86	0.43
1:B:95:VAL:O	1:B:98:VAL:N	2.52	0.43
1:A:16:ARG:HG2	1:A:17:GLY:N	2.34	0.42
1:A:15:ILE:O	1:B:36:ASP:HB3	2.20	0.42
1:B:-8:HIS:CE1	1:B:-7:HIS:CE1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASN:OD1	1:B:198:TYR:N	2.52	0.42
1:A:15:ILE:HD11	1:B:65:LEU:HD11	2.01	0.42
1:A:140:VAL:HG12	1:A:141:VAL:N	2.33	0.42
1:A:285:SER:OG	1:A:288:GLN:HG3	2.20	0.42
1:B:141:VAL:O	1:B:180:PRO:HD3	2.19	0.42
1:B:176:HIS:ND1	1:B:180:PRO:O	2.52	0.42
1:B:287:MET:HG2	1:B:288:GLN:HG3	2.00	0.42
1:A:288:GLN:HE21	1:A:288:GLN:HB3	1.60	0.42
1:B:31:LEU:HD11	1:B:240:MET:HE1	2.02	0.42
1:B:214:VAL:HG22	1:B:215:VAL:H	1.82	0.42
1:B:252:LEU:O	1:B:256:CYS:HB2	2.19	0.42
1:A:240:MET:SD	1:A:262:THR:HG21	2.59	0.42
1:A:273:CYS:SG	1:A:292:ARG:NE	2.90	0.42
1:B:27:PRO:HA	1:B:30:VAL:CG1	2.50	0.42
1:B:160:ARG:HD2	1:B:161:LYS:N	2.22	0.42
1:B:162:ILE:CD1	1:B:171:VAL:HG21	2.43	0.42
1:B:205:GLN:OE1	1:B:252:LEU:CD1	2.67	0.42
1:B:278:ALA:CB	1:B:288:GLN:NE2	2.75	0.42
1:A:16:ARG:HG2	1:A:17:GLY:H	1.84	0.42
1:A:126:MET:HG2	1:A:128:VAL:H	1.85	0.42
1:A:248:HIS:CE1	1:A:258:LYS:HE3	2.55	0.42
1:B:251:ASN:OD1	1:B:251:ASN:O	2.38	0.42
1:B:268:GLN:O	1:B:270:THR:N	2.52	0.42
1:B:285:SER:HB2	1:B:287:MET:SD	2.60	0.42
1:A:171:VAL:O	1:A:175:LEU:HG	2.19	0.42
1:B:1:MET:O	1:B:1:MET:CG	2.64	0.42
1:B:46:HIS:CE1	1:B:48:GLY:CA	3.02	0.42
1:A:151:GLN:HB2	1:A:188:SER:CB	2.50	0.42
1:B:74:MET:HE3	1:B:74:MET:HB2	1.78	0.42
1:B:192:SER:HB2	1:B:220:ARG:NH2	2.34	0.42
1:B:214:VAL:CG2	1:B:215:VAL:N	2.82	0.42
1:A:28:LEU:HD21	1:A:239:ALA:O	2.20	0.42
1:A:60:ASP:OD1	1:A:60:ASP:N	2.53	0.42
1:A:294:VAL:C	1:A:296:SER:H	2.23	0.42
1:B:25:THR:O	1:B:26:PHE:C	2.58	0.42
1:B:162:ILE:HG23	1:B:167:GLU:HB2	2.01	0.42
1:B:175:LEU:O	1:B:178:MET:HB2	2.20	0.42
1:B:207:ARG:O	1:B:210:PRO:HD2	2.20	0.42
1:A:135:VAL:O	1:A:139:LYS:N	2.46	0.41
1:A:255:ALA:C	1:A:257:GLU:N	2.74	0.41
1:B:202:LEU:HD23	1:B:203:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLY:CA	1:A:290:GLU:CD	2.89	0.41
1:A:131:ASP:O	1:A:134:PRO:HD2	2.20	0.41
1:A:197:ASN:O	1:A:198:TYR:HD2	2.03	0.41
1:A:230:PHE:CE1	1:A:267:LEU:HD22	2.55	0.41
1:B:220:ARG:C	1:B:221:MET:CG	2.88	0.41
1:B:240:MET:HB3	1:B:240:MET:HE2	1.93	0.41
1:B:257:GLU:O	1:B:261:SER:CB	2.68	0.41
1:B:285:SER:OG	1:B:287:MET:SD	2.72	0.41
1:A:101:LEU:HA	1:A:101:LEU:HD23	1.78	0.41
1:A:146:ILE:CG2	1:A:241:LEU:HD23	2.50	0.41
1:A:209:ASN:CB	1:A:210:PRO:HD2	2.48	0.41
1:A:218:ARG:O	1:A:219:ILE:CG2	2.68	0.41
1:B:252:LEU:CD1	1:B:252:LEU:H	2.33	0.41
1:A:135:VAL:HG13	1:A:139:LYS:HB2	2.03	0.41
1:A:147:ILE:HB	1:A:149:PRO:HD2	2.03	0.41
1:A:155:GLU:O	1:A:159:GLY:N	2.43	0.41
1:A:235:ASP:O	1:A:239:ALA:HB2	2.20	0.41
1:B:6:ARG:HA	1:B:34:GLU:O	2.21	0.41
1:B:29:GLN:C	1:B:31:LEU:N	2.73	0.41
1:B:221:MET:HG2	1:B:309:ALA:HB2	2.03	0.41
1:B:294:VAL:O	1:B:296:SER:N	2.53	0.41
1:B:26:PHE:HE2	1:B:294:VAL:HA	1.84	0.41
1:A:116:LEU:HB2	1:A:153:GLU:HG2	2.03	0.41
1:A:164:SER:O	1:A:165:GLN:C	2.58	0.41
1:A:252:LEU:HD12	1:A:255:ALA:HB3	2.03	0.41
1:B:230:PHE:CD1	1:B:267:LEU:HD22	2.55	0.41
1:B:80:VAL:HG23	1:B:108:LEU:HD11	2.02	0.41
1:B:118:ASP:CG	1:B:119:LYS:N	2.73	0.41
1:B:175:LEU:HD13	1:B:183:VAL:HG11	2.02	0.41
1:B:206:ARG:HB2	1:B:206:ARG:HH11	1.85	0.41
1:A:-1:ARG:HE	1:A:-1:ARG:HB2	1.46	0.41
1:A:108:LEU:O	1:A:109:VAL:HG22	2.19	0.41
1:A:197:ASN:C	1:A:198:TYR:CD2	2.81	0.41
1:A:257:GLU:OE1	1:A:305:ILE:CD1	2.69	0.41
1:B:13:HIS:CE1	1:B:14:VAL:O	2.74	0.41
1:B:147:ILE:HG12	1:B:180:PRO:HB3	2.03	0.41
1:B:147:ILE:CD1	1:B:183:VAL:HG13	2.51	0.41
1:B:252:LEU:HD12	1:B:252:LEU:H	1.86	0.41
1:A:200:ILE:HD12	1:A:220:ARG:CD	2.48	0.41
1:A:219:ILE:HD11	1:A:252:LEU:HD21	2.02	0.41
1:A:86:ARG:O	1:A:86:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-10:HIS:CD2	1:B:-10:HIS:O	2.74	0.40
1:B:172:MET:HE1	1:B:202:LEU:CD2	2.41	0.40
1:B:237:PHE:CE2	1:B:241:LEU:HD12	2.56	0.40
1:B:283:ARG:HG2	1:B:283:ARG:NH1	2.36	0.40
1:A:13:HIS:HB2	1:A:39:ASN:HB3	2.02	0.40
1:A:128:VAL:HG11	1:A:132:LEU:HD22	2.02	0.40
1:B:268:GLN:C	1:B:270:THR:N	2.74	0.40
1:B:273:CYS:SG	1:B:292:ARG:NE	2.94	0.40
1:A:29:GLN:CG	1:A:35:ILE:HD13	2.51	0.40
1:B:274:ALA:CB	1:B:288:GLN:O	2.69	0.40
1:A:28:LEU:HB2	1:A:35:ILE:CG1	2.51	0.40
1:B:210:PRO:O	1:B:211:ALA:C	2.59	0.40
1:A:46:HIS:HE1	1:A:48:GLY:HA3	1.86	0.40
1:A:47:THR:HB	1:A:52:TRP:CH2	2.56	0.40
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	321/327 (98%)	229 (71%)	65 (20%)	27 (8%)	1 2
1	B	321/327 (98%)	240 (75%)	65 (20%)	16 (5%)	2 6
All	All	642/654 (98%)	469 (73%)	130 (20%)	43 (7%)	1 3

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	59	SER
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	195	GLY
1	A	210	PRO
1	A	249	PRO
1	B	186	THR
1	B	279	GLY
1	A	3	GLU
1	A	40	SER
1	A	161	LYS
1	A	214	VAL
1	A	243	ALA
1	A	264	HIS
1	B	228	ALA
1	B	243	ALA
1	B	280	GLU
1	B	295	GLN
1	A	25	THR
1	A	114	PRO
1	A	120	TRP
1	A	245	THR
1	B	193	PRO
1	B	269	ARG
1	A	26	PHE
1	A	69	LEU
1	A	108	LEU
1	A	125	SER
1	A	163	HIS
1	A	180	PRO
1	B	-9	HIS
1	B	253	LYS
1	B	305	ILE
1	A	295	GLN
1	B	259	THR
1	A	122	GLY
1	A	212	GLY
1	B	115	VAL
1	B	249	PRO
1	A	140	VAL
1	B	149	PRO
1	A	115	VAL
1	B	191	PRO

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	285/289 (99%)	226 (79%)	59 (21%)	1 3
1	B	285/289 (99%)	223 (78%)	62 (22%)	1 3
All	All	570/578 (99%)	449 (79%)	121 (21%)	1 3

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	1	MET
1	A	18	TYR
1	A	21	ASN
1	A	30	VAL
1	A	46	HIS
1	A	60	ASP
1	A	70	ARG
1	A	72	ASN
1	A	86	ARG
1	A	89	SER
1	A	100	GLU
1	A	103	GLN
1	A	104	GLN
1	A	114	PRO
1	A	121	ASP
1	A	123	GLU
1	A	127	TYR
1	A	130	GLU
1	A	131	ASP
1	A	137	LYS
1	A	142	PRO
1	A	143	LEU
1	A	145	ASP
1	A	147	ILE
1	A	149	PRO
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	158	SER
1	A	160	ARG
1	A	167	GLU
1	A	170	ARG
1	A	173	ASP
1	A	174	MET
1	A	178	MET
1	A	180	PRO
1	A	191	PRO
1	A	192	SER
1	A	199	LEU
1	A	207	ARG
1	A	210	PRO
1	A	213	SER
1	A	215	VAL
1	A	216	MET
1	A	218	ARG
1	A	221	MET
1	A	226	VAL
1	A	248	HIS
1	A	249	PRO
1	A	256	CYS
1	A	268	GLN
1	A	271	ILE
1	A	272	GLN
1	A	284	PRO
1	A	292	ARG
1	A	302	ASP
1	A	305	ILE
1	A	307	VAL
1	A	308	GLN
1	B	-10	HIS
1	B	-9	HIS
1	B	-8	HIS
1	B	-1	ARG
1	B	0	THR
1	B	1	MET
1	B	2	GLU
1	B	3	GLU
1	B	5	CYS
1	B	21	ASN

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Mol	Chain	Res	Type
1	B	26	PHE
1	B	35	ILE
1	B	45	ASN
1	B	70	ARG
1	B	73	ASN
1	B	91	LEU
1	B	95	VAL
1	B	103	GLN
1	B	106	PRO
1	B	107	ARG
1	B	115	VAL
1	B	116	LEU
1	B	120	TRP
1	B	129	PRO
1	B	134	PRO
1	B	136	TYR
1	B	138	GLU
1	B	143	LEU
1	B	153	GLU
1	B	160	ARG
1	B	165	GLN
1	B	173	ASP
1	B	177	SER
1	B	187	SER
1	B	190	LEU
1	B	191	PRO
1	B	192	SER
1	B	193	PRO
1	B	200	ILE
1	B	206	ARG
1	B	208	ARG
1	B	210	PRO
1	B	215	VAL
1	B	216	MET
1	B	217	GLU
1	B	221	MET
1	B	222	ASP
1	B	223	ILE
1	B	233	THR
1	B	249	PRO
1	B	250	ASN
1	B	260	VAL

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Mol	Chain	Res	Type
1	B	273	CYS
1	B	283	ARG
1	B	284	PRO
1	B	286	PRO
1	B	287	MET
1	B	293	MET
1	B	302	ASP
1	B	304	GLU
1	B	306	VAL
1	B	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	21	ASN
1	A	45	ASN
1	A	51	HIS
1	A	55	GLN
1	A	72	ASN
1	A	75	ASN
1	A	103	GLN
1	A	248	HIS
1	A	250	ASN
1	A	251	ASN
1	A	268	GLN
1	A	288	GLN
1	A	308	GLN
1	B	-10	HIS
1	B	-7	HIS
1	B	-5	HIS
1	B	21	ASN
1	B	29	GLN
1	B	42	GLN
1	B	51	HIS
1	B	63	GLN
1	B	73	ASN
1	B	103	GLN
1	B	209	ASN
1	B	248	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	323/327 (98%)	-0.28	0	100	100	36, 44, 50, 56	0
1	B	323/327 (98%)	-0.28	0	100	100	35, 44, 50, 55	0
All	All	646/654 (98%)	-0.28	0	100	100	35, 44, 50, 56	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.