Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:21 AM GMT

PDB ID	:	2QFI
Title	:	Structure of the zinc transporter YiiP
Authors	:	Lu, M.
Deposited on	:	2007-06-27
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

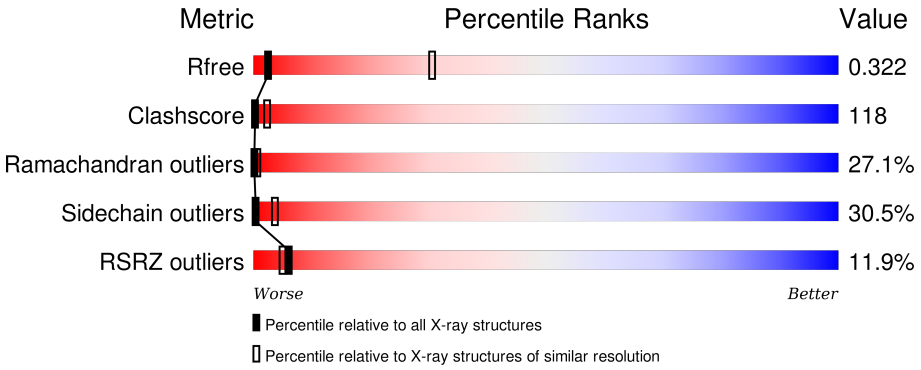
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	300	5% 12% 38% 33% 12% 5%
1	B	300	17% 15% 39% 29% 12% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4417 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 Ferrous-iron efflux pump fieF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			
1	B	286	Total	C	N	O	S	0	0	0
			2205	1419	378	397	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

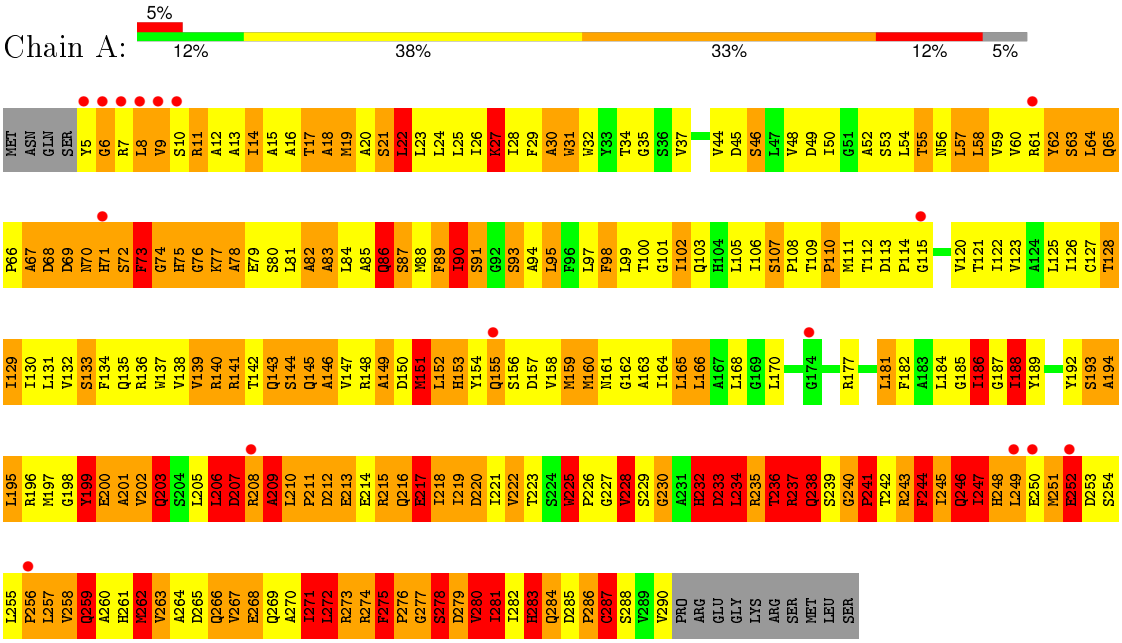
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	4	Total	Zn	0	0
			4	4		

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.

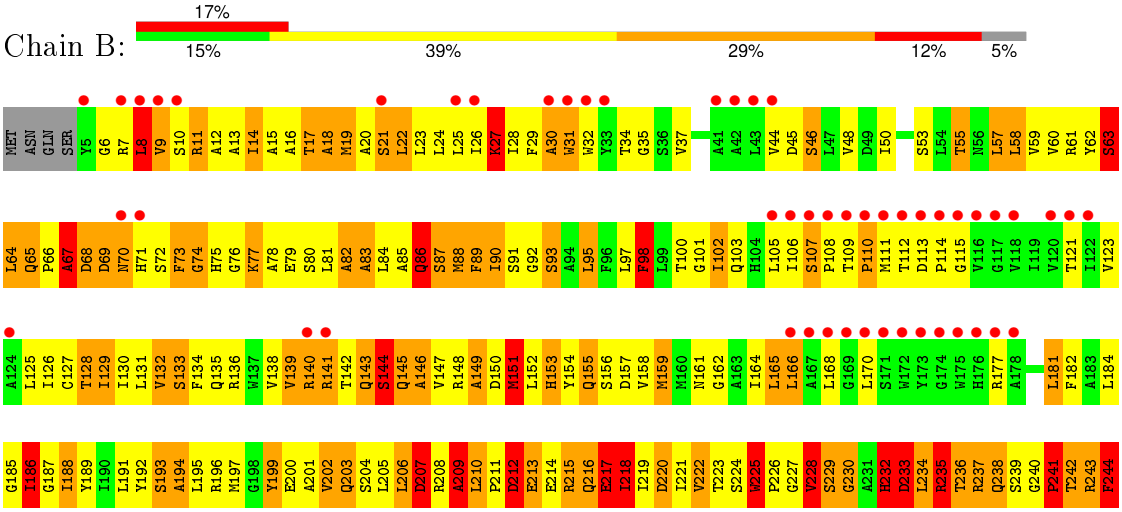
- Molecule 1: Ferrous-iron efflux pump fieF

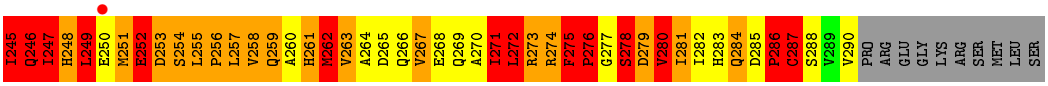
Chain A:



- Molecule 1: Ferrous-iron efflux pump fieF

Chain B:




I245
Q246
I247
H248
L249
E250
M251
E252
D253
S254
L255
P256
L257
V258
Q259
A260
H261
M262
V263
A264
D265
Q266
V267
E268
Q269
A270
I271
L272
R273
R274
F275
P276
G277
S278
D279
Y280
I281
I282
H283
Q284
D285
P286
C287
S288
V289
V290
PRO
ARG
GLU
GLY
LYS
ARG
SER
MET
LEU
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	106.66Å 110.84Å 130.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.80 39.29 – 3.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-3.80) 97.4 (39.29-3.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.322 , 0.329 0.328 , 0.322	Depositor DCC
R_{free} test set	742 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	118.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 155.7	EDS
Estimated twinning fraction	0.086 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	1 of 15522 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: ZN

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	1.41	25/2252 (1.1%)	1.39	37/3069 (1.2%)
1	B	1.07	9/2252 (0.4%)	1.22	18/3069 (0.6%)
All	All	1.25	34/4504 (0.8%)	1.31	55/6138 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24
1	B	0	23
All	All	0	47

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	ILE	CA-CB	8.52	1.74	1.54
1	A	279	ASP	CB-CG	7.99	1.68	1.51
1	A	247	ILE	CA-CB	7.64	1.72	1.54
1	B	247	ILE	CA-CB	7.59	1.72	1.54
1	A	268	GLU	CG-CD	7.35	1.62	1.51
1	A	275	PHE	CB-CG	7.32	1.63	1.51
1	A	238	GLN	N-CA	7.28	1.60	1.46
1	A	244	PHE	CB-CG	-7.00	1.39	1.51
1	A	266	GLN	CG-CD	6.83	1.66	1.51
1	B	286	PRO	N-CA	-6.76	1.35	1.47
1	A	244	PHE	CD2-CE2	-6.75	1.25	1.39
1	B	279	ASP	CB-CG	6.63	1.65	1.51
1	A	200	GLU	CB-CG	6.48	1.64	1.52
1	A	217	GLU	CG-CD	6.19	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ALA	CA-CB	6.17	1.65	1.52
1	A	275	PHE	CG-CD1	6.13	1.48	1.38
1	A	90	ILE	CA-CB	6.05	1.68	1.54
1	A	275	PHE	CG-CD2	5.98	1.47	1.38
1	B	275	PHE	CB-CG	5.98	1.61	1.51
1	A	225	TRP	CB-CG	-5.86	1.39	1.50
1	A	238	GLN	CB-CG	5.70	1.68	1.52
1	A	275	PHE	CD1-CE1	5.68	1.50	1.39
1	A	238	GLN	CG-CD	5.42	1.63	1.51
1	B	252	GLU	CB-CG	5.39	1.62	1.52
1	A	252	GLU	CG-CD	5.26	1.59	1.51
1	A	259	GLN	CG-CD	5.24	1.63	1.51
1	A	232	HIS	CA-CB	5.18	1.65	1.53
1	A	238	GLN	CA-C	5.16	1.66	1.52
1	B	238	GLN	N-CA	5.13	1.56	1.46
1	A	241	PRO	CG-CD	5.09	1.67	1.50
1	A	233	ASP	CA-C	5.08	1.66	1.52
1	B	217	GLU	CG-CD	5.03	1.59	1.51
1	A	237	ARG	N-CA	5.02	1.56	1.46
1	B	279	ASP	N-CA	5.00	1.56	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	N-CA-C	8.50	133.95	111.00
1	B	279	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	247	ILE	N-CA-CB	7.59	128.26	110.80
1	A	249	LEU	CA-CB-CG	7.50	132.56	115.30
1	B	233	ASP	N-CA-C	7.44	131.09	111.00
1	B	247	ILE	N-CA-CB	7.39	127.79	110.80
1	B	249	LEU	CA-CB-CG	7.36	132.23	115.30
1	A	281	ILE	CB-CA-C	-7.27	97.07	111.60
1	A	279	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	244	PHE	N-CA-C	7.01	129.93	111.00
1	A	280	VAL	N-CA-C	-6.98	92.17	111.00
1	A	238	GLN	N-CA-C	6.92	129.68	111.00
1	B	279	ASP	N-CA-C	-6.86	92.49	111.00
1	B	244	PHE	N-CA-C	6.70	129.10	111.00
1	A	232	HIS	CB-CA-C	6.48	123.36	110.40
1	A	283	HIS	N-CA-C	-6.45	93.58	111.00
1	A	252	GLU	C-N-CA	6.38	137.65	121.70
1	B	241	PRO	N-CA-C	6.38	128.68	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	252	GLU	C-N-CA	6.38	137.64	121.70
1	A	241	PRO	N-CA-C	6.32	128.54	112.10
1	A	83	ALA	N-CA-C	-6.29	94.02	111.00
1	B	232	HIS	CB-CA-C	6.21	122.82	110.40
1	A	152	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	58	LEU	CA-CB-CG	-5.89	101.74	115.30
1	A	75	HIS	N-CA-C	5.74	126.50	111.00
1	A	248	HIS	N-CA-C	5.74	126.50	111.00
1	A	225	TRP	CA-CB-CG	-5.72	102.83	113.70
1	A	207	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	206	LEU	N-CA-C	-5.67	95.69	111.00
1	A	199	TYR	CA-CB-CG	-5.63	102.71	113.40
1	A	208	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	279	ASP	N-CA-C	-5.59	95.90	111.00
1	A	287	CYS	N-CA-C	5.55	125.98	111.00
1	A	68	ASP	N-CA-C	-5.53	96.07	111.00
1	A	75	HIS	CB-CA-C	-5.53	99.34	110.40
1	A	91	SER	N-CA-C	-5.51	96.13	111.00
1	A	90	ILE	CB-CA-C	5.50	122.60	111.60
1	B	207	ASP	N-CA-C	-5.45	96.28	111.00
1	A	249	LEU	CB-CG-CD2	5.44	120.24	111.00
1	B	235	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	73	PHE	CB-CA-C	-5.42	99.56	110.40
1	B	232	HIS	C-N-CA	-5.36	108.31	121.70
1	A	287	CYS	CA-C-N	-5.33	105.47	117.20
1	B	68	ASP	N-CA-C	-5.33	96.62	111.00
1	A	207	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	254	SER	N-CA-C	-5.26	96.80	111.00
1	B	248	HIS	CB-CA-C	5.25	120.91	110.40
1	B	8	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	141	ARG	N-CA-C	-5.12	97.19	111.00
1	A	277	GLY	N-CA-C	-5.11	100.32	113.10
1	B	272	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	234	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	236	THR	N-CA-CB	-5.07	100.66	110.30
1	B	58	LEU	CA-CB-CG	-5.04	103.71	115.30
1	A	22	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Peptide
1	A	144	SER	Peptide
1	A	194	ALA	Peptide
1	A	195	LEU	Peptide
1	A	203	GLN	Peptide
1	A	209	ALA	Peptide
1	A	210	LEU	Peptide
1	A	225	TRP	Peptide
1	A	228	VAL	Peptide
1	A	234	LEU	Peptide
1	A	240	GLY	Peptide
1	A	243	ARG	Peptide
1	A	246	GLN	Peptide
1	A	258	VAL	Peptide
1	A	27	LYS	Peptide
1	A	271	ILE	Peptide
1	A	272	LEU	Peptide
1	A	278	SER	Peptide
1	A	280	VAL	Peptide
1	A	287	CYS	Peptide
1	A	6	GLY	Peptide
1	A	63	SER	Peptide
1	A	76	GLY	Peptide
1	A	97	LEU	Peptide
1	B	140	ARG	Peptide
1	B	141	ARG	Peptide
1	B	144	SER	Peptide
1	B	194	ALA	Peptide
1	B	203	GLN	Peptide
1	B	209	ALA	Peptide
1	B	210	LEU	Peptide
1	B	225	TRP	Peptide
1	B	228	VAL	Peptide
1	B	243	ARG	Peptide
1	B	246	GLN	Peptide
1	B	252	GLU	Peptide
1	B	258	VAL	Peptide
1	B	27	LYS	Peptide
1	B	271	ILE	Peptide
1	B	272	LEU	Peptide
1	B	276	PRO	Peptide
1	B	278	SER	Peptide
1	B	280	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	287	CYS	Peptide
1	B	63	SER	Peptide
1	B	67	ALA	Peptide
1	B	97	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2205	0	2239	542	4
1	B	2205	0	2239	514	0
2	A	4	0	0	0	2
2	B	3	0	0	0	0
All	All	4417	0	4478	1052	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 118.

All (1052) 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:232:HIS:CE1	1:B:245:ILE:HG21	1.36	1.61
1:B:245:ILE:CB	1:B:245:ILE:CA	1.74	1.56
1:B:232:HIS:CE1	1:B:245:ILE:CG2	1.96	1.49
1:B:232:HIS:NE2	1:B:245:ILE:CG2	1.79	1.41
1:B:232:HIS:NE2	1:B:245:ILE:HD12	1.47	1.30
1:A:67:ALA:HB1	1:A:72:SER:O	1.31	1.30
1:B:225:TRP:CZ3	1:B:266:GLN:HB3	1.70	1.27
1:A:6:GLY:O	1:A:12:ALA:HB3	1.34	1.26
1:A:225:TRP:CZ3	1:A:266:GLN:HB3	1.67	1.26
1:A:232:HIS:CE1	1:A:245:ILE:HG21	1.71	1.25
1:A:17:THR:N	1:A:148:ARG:HH22	1.34	1.23
1:B:67:ALA:HB1	1:B:72:SER:O	1.36	1.23
1:B:232:HIS:NE2	1:B:245:ILE:HG21	0.91	1.21
1:B:235:ARG:NH1	1:B:237:ARG:HD3	1.55	1.21
1:A:209:ALA:O	1:A:236:THR:HB	1.38	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HG2	1:B:277:GLY:O	1.40	1.18
1:A:202:VAL:O	1:A:205:LEU:HG	1.41	1.18
1:A:79:GLU:CB	1:A:147:VAL:HG21	1.75	1.17
1:A:87:SER:HB3	1:A:197:MET:HB2	1.24	1.16
1:B:87:SER:CB	1:B:197:MET:HB2	1.75	1.16
1:B:22:LEU:HD23	1:B:131:LEU:HB3	1.24	1.15
1:A:79:GLU:HB2	1:A:147:VAL:CG2	1.75	1.15
1:B:67:ALA:HB3	1:B:69:ASP:HA	1.19	1.15
1:A:252:GLU:HB3	1:A:256:PRO:HG3	1.26	1.15
1:A:232:HIS:NE2	1:A:245:ILE:HD12	1.61	1.14
1:B:87:SER:HB3	1:B:197:MET:CB	1.78	1.14
1:A:235:ARG:HH12	1:A:237:ARG:CD	1.63	1.11
1:B:230:GLY:HA2	1:B:249:LEU:HG	1.20	1.11
1:A:244:PHE:O	1:A:282:ILE:HG23	1.49	1.11
1:B:232:HIS:CE1	1:B:245:ILE:HG22	1.86	1.11
1:A:235:ARG:NH1	1:A:237:ARG:HD3	1.66	1.10
1:B:235:ARG:HH12	1:B:237:ARG:CD	1.64	1.10
1:A:240:GLY:CA	1:A:277:GLY:HA2	1.80	1.10
1:A:206:LEU:HD22	1:A:237:ARG:HE	0.95	1.10
1:A:67:ALA:HB3	1:A:69:ASP:HA	1.25	1.09
1:B:79:GLU:HB2	1:B:147:VAL:CG2	1.82	1.08
1:A:276:PRO:HG2	1:A:277:GLY:O	1.51	1.08
1:B:79:GLU:CB	1:B:147:VAL:HG21	1.81	1.08
1:A:22:LEU:HD23	1:A:131:LEU:HB3	1.24	1.07
1:B:206:LEU:HD22	1:B:237:ARG:HE	1.05	1.07
1:A:144:SER:CB	1:A:148:ARG:HG2	1.85	1.07
1:A:199:TYR:HA	1:A:202:VAL:CG2	1.85	1.07
1:A:230:GLY:HA2	1:A:249:LEU:HG	1.26	1.06
1:B:252:GLU:HB3	1:B:256:PRO:HG3	1.32	1.06
1:A:247:ILE:HG12	1:A:248:HIS:CD2	1.89	1.05
1:A:245:ILE:HG23	1:A:283:HIS:CD2	1.91	1.05
1:B:286:PRO:HG2	1:B:287:CYS:N	1.66	1.05
1:A:286:PRO:HG2	1:A:287:CYS:H	1.22	1.04
1:B:225:TRP:HZ3	1:B:266:GLN:CB	1.69	1.04
1:A:139:VAL:HG13	1:A:140:ARG:N	1.69	1.04
1:B:109:THR:HB	1:B:110:PRO:HD2	1.36	1.04
1:A:144:SER:HB3	1:A:148:ARG:HG2	1.36	1.04
1:B:232:HIS:NE2	1:B:245:ILE:CD1	2.20	1.04
1:B:17:THR:N	1:B:148:ARG:HH22	1.53	1.03
1:A:232:HIS:CE1	1:A:245:ILE:CG2	2.42	1.03
1:B:286:PRO:HG2	1:B:287:CYS:H	0.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:O	1:B:205:LEU:HG	1.57	1.03
1:A:87:SER:CB	1:A:197:MET:HB2	1.90	1.02
1:B:209:ALA:O	1:B:236:THR:HB	1.60	1.02
1:B:252:GLU:HB3	1:B:256:PRO:CG	1.88	1.02
1:B:272:LEU:HD13	1:B:273:ARG:HA	1.39	1.01
1:B:87:SER:HB3	1:B:197:MET:HB2	1.05	1.01
1:B:252:GLU:HA	1:B:256:PRO:HD3	1.39	1.01
1:A:209:ALA:HB1	1:A:236:THR:OG1	1.61	1.01
1:A:87:SER:HB3	1:A:197:MET:CB	1.91	1.01
1:B:199:TYR:HA	1:B:202:VAL:CG2	1.90	1.01
1:B:216:GLN:O	1:B:219:ILE:HG22	1.59	1.00
1:B:6:GLY:O	1:B:12:ALA:HB3	1.60	1.00
1:A:230:GLY:HA2	1:A:249:LEU:CG	1.90	1.00
1:A:225:TRP:HZ3	1:A:266:GLN:CB	1.74	1.00
1:A:235:ARG:HH12	1:A:237:ARG:HD3	0.84	1.00
1:A:225:TRP:CH2	1:A:266:GLN:HB3	1.96	0.99
1:A:262:MET:O	1:A:266:GLN:N	1.94	0.99
1:A:216:GLN:O	1:A:219:ILE:HG22	1.63	0.98
1:B:244:PHE:CD1	1:B:245:ILE:O	2.16	0.98
1:A:139:VAL:HG13	1:A:140:ARG:H	1.25	0.98
1:A:245:ILE:HA	1:A:283:HIS:O	1.61	0.98
1:A:244:PHE:CD1	1:A:245:ILE:O	2.16	0.98
1:A:240:GLY:HA3	1:A:277:GLY:HA2	1.46	0.98
1:A:109:THR:HB	1:A:110:PRO:HD2	1.42	0.98
1:A:73:PHE:C	1:A:73:PHE:CD2	2.36	0.97
1:B:159:MET:HG3	1:B:184:LEU:HD11	1.44	0.97
1:A:247:ILE:HG12	1:A:248:HIS:HD2	1.20	0.97
1:B:14:ILE:HD11	1:B:138:VAL:HA	1.43	0.97
1:B:234:LEU:H	1:B:234:LEU:CD1	1.78	0.96
1:A:199:TYR:HA	1:A:202:VAL:HG23	1.44	0.96
1:A:225:TRP:CZ3	1:A:266:GLN:CB	2.46	0.96
1:A:64:LEU:C	1:A:65:GLN:HE21	1.68	0.96
1:A:242:THR:H	1:A:280:VAL:HG12	1.31	0.95
1:A:240:GLY:HA2	1:A:277:GLY:HA2	1.48	0.95
1:A:63:SER:HA	1:A:76:GLY:HA2	1.49	0.95
1:A:272:LEU:HD13	1:A:273:ARG:HA	1.49	0.95
1:B:230:GLY:HA2	1:B:249:LEU:CG	1.96	0.95
1:A:17:THR:H	1:A:148:ARG:HH22	1.09	0.94
1:B:62:TYR:HA	1:B:65:GLN:HE22	1.29	0.94
1:A:85:ALA:O	1:A:89:PHE:O	1.86	0.94
1:B:256:PRO:C	1:B:257:LEU:HD23	1.88	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD22	1:A:237:ARG:NE	1.81	0.94
1:B:225:TRP:HZ3	1:B:266:GLN:HB3	1.13	0.94
1:A:251:MET:C	1:A:253:ASP:H	1.68	0.94
1:A:261:HIS:O	1:A:263:VAL:N	2.01	0.93
1:A:11:ARG:HH22	1:A:239:SER:HA	1.33	0.93
1:A:14:ILE:HD11	1:A:138:VAL:HA	1.48	0.93
1:A:138:VAL:O	1:A:139:VAL:O	1.84	0.93
1:B:240:GLY:CA	1:B:277:GLY:HA2	1.99	0.93
1:A:6:GLY:C	1:A:12:ALA:HB3	1.89	0.93
1:B:72:SER:HB3	1:B:75:HIS:HD2	1.33	0.92
1:B:261:HIS:O	1:B:263:VAL:N	2.03	0.92
1:A:21:SER:HA	1:A:24:LEU:HB2	1.53	0.91
1:B:240:GLY:HA2	1:B:277:GLY:HA2	1.52	0.91
1:B:11:ARG:HH22	1:B:239:SER:HA	1.34	0.91
1:B:225:TRP:CZ3	1:B:266:GLN:CB	2.49	0.91
1:A:17:THR:N	1:A:148:ARG:NH2	2.19	0.90
1:B:67:ALA:CB	1:B:69:ASP:HA	1.99	0.90
1:B:272:LEU:O	1:B:274:ARG:N	2.04	0.90
1:A:23:LEU:HD11	1:A:154:TYR:OH	1.72	0.90
1:A:256:PRO:C	1:A:257:LEU:HD23	1.92	0.89
1:A:159:MET:HG3	1:A:184:LEU:HD11	1.54	0.89
1:B:248:HIS:HB2	1:B:252:GLU:C	1.93	0.89
1:B:17:THR:H	1:B:148:ARG:HH22	1.13	0.89
1:B:262:MET:O	1:B:266:GLN:N	2.05	0.89
1:B:144:SER:CB	1:B:148:ARG:HG2	2.01	0.89
1:B:248:HIS:O	1:B:253:ASP:HB2	1.73	0.89
1:B:225:TRP:CH2	1:B:266:GLN:HB3	2.06	0.89
1:A:243:ARG:O	1:A:244:PHE:HD2	1.55	0.89
1:B:11:ARG:HA	1:B:142:THR:HG21	1.56	0.88
1:B:232:HIS:CD2	1:B:245:ILE:CB	2.56	0.88
1:B:235:ARG:HH12	1:B:237:ARG:HD3	0.74	0.88
1:B:234:LEU:H	1:B:234:LEU:HD12	1.35	0.88
1:A:143:GLN:H	1:A:143:GLN:CD	1.70	0.88
1:B:79:GLU:HB2	1:B:147:VAL:HG21	0.92	0.88
1:A:62:TYR:HA	1:A:65:GLN:HE22	1.38	0.88
1:A:264:ALA:O	1:A:267:VAL:HB	1.74	0.87
1:B:286:PRO:CG	1:B:287:CYS:H	1.79	0.87
1:A:57:LEU:HD23	1:A:58:LEU:HG	1.55	0.87
1:B:139:VAL:HG13	1:B:140:ARG:N	1.89	0.87
1:A:252:GLU:HA	1:A:256:PRO:HD3	1.57	0.86
1:B:139:VAL:HG13	1:B:140:ARG:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HB3	1:A:256:PRO:CG	2.04	0.86
1:A:144:SER:HB3	1:A:148:ARG:CG	2.04	0.86
1:B:144:SER:HB3	1:B:148:ARG:HG2	1.57	0.86
1:A:143:GLN:HB2	1:A:146:ALA:H	1.41	0.86
1:B:230:GLY:CA	1:B:249:LEU:HG	2.04	0.86
1:A:232:HIS:O	1:A:233:ASP:HB3	1.73	0.86
1:B:87:SER:HA	1:B:193:SER:HB3	1.56	0.86
1:B:232:HIS:O	1:B:233:ASP:HB3	1.76	0.86
1:B:143:GLN:HB2	1:B:146:ALA:H	1.40	0.85
1:B:242:THR:HB	1:B:280:VAL:HB	1.58	0.85
1:A:67:ALA:CB	1:A:69:ASP:HA	2.05	0.85
1:A:72:SER:HB3	1:A:75:HIS:HD2	1.40	0.85
1:B:262:MET:HA	1:B:265:ASP:HB3	1.58	0.85
1:A:230:GLY:CA	1:A:249:LEU:HG	2.05	0.85
1:A:278:SER:H	1:A:280:VAL:HG13	1.41	0.85
1:B:248:HIS:HB2	1:B:252:GLU:O	1.75	0.85
1:B:63:SER:HA	1:B:76:GLY:HA2	1.56	0.85
1:B:232:HIS:CD2	1:B:245:ILE:HG21	2.07	0.85
1:B:245:ILE:HA	1:B:283:HIS:O	1.77	0.84
1:A:243:ARG:O	1:A:244:PHE:CD2	2.30	0.84
1:A:247:ILE:CG2	1:A:248:HIS:N	2.41	0.84
1:B:199:TYR:HA	1:B:202:VAL:HG22	1.58	0.84
1:B:206:LEU:HD22	1:B:237:ARG:NE	1.91	0.84
1:A:242:THR:H	1:A:280:VAL:CG1	1.90	0.84
1:A:67:ALA:HB3	1:A:69:ASP:CA	2.08	0.84
1:A:278:SER:OG	1:A:280:VAL:CG1	2.25	0.84
1:B:242:THR:H	1:B:280:VAL:HG12	1.42	0.84
1:B:252:GLU:CA	1:B:256:PRO:HD3	2.07	0.84
1:A:232:HIS:O	1:A:233:ASP:CB	2.25	0.83
1:B:209:ALA:HB1	1:B:236:THR:OG1	1.77	0.83
1:B:232:HIS:CD2	1:B:245:ILE:CG2	2.61	0.83
1:B:245:ILE:CG2	1:B:285:ASP:OD2	2.26	0.83
1:B:256:PRO:HA	1:B:257:LEU:HD23	1.61	0.83
1:A:73:PHE:O	1:A:73:PHE:CD2	2.32	0.83
1:B:247:ILE:HG12	1:B:248:HIS:CD2	2.14	0.83
1:A:139:VAL:CG1	1:A:140:ARG:N	2.40	0.82
1:A:244:PHE:O	1:A:282:ILE:HD13	1.79	0.82
1:A:67:ALA:HA	1:A:75:HIS:NE2	1.94	0.82
1:A:232:HIS:NE2	1:A:245:ILE:HG21	1.93	0.82
1:B:21:SER:HA	1:B:24:LEU:HB2	1.60	0.82
1:A:259:GLN:O	1:A:261:HIS:N	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:HG12	1:A:142:THR:HG22	1.62	0.82
1:A:216:GLN:O	1:A:219:ILE:CG2	2.28	0.82
1:A:70:ASN:ND2	1:A:70:ASN:H	1.76	0.81
1:B:232:HIS:O	1:B:233:ASP:CB	2.27	0.81
1:A:242:THR:HB	1:A:280:VAL:HB	1.62	0.81
1:B:252:GLU:CB	1:B:256:PRO:CG	2.58	0.81
1:B:125:LEU:C	1:B:127:CYS:H	1.83	0.81
1:B:23:LEU:HD11	1:B:154:TYR:OH	1.81	0.81
1:A:87:SER:HA	1:A:193:SER:HB3	1.63	0.80
1:A:91:SER:O	1:A:93:SER:OG	1.99	0.80
1:A:225:TRP:HZ3	1:A:266:GLN:HB3	1.20	0.80
1:A:208:ARG:O	1:A:210:LEU:CA	2.30	0.79
1:A:247:ILE:CG2	1:A:248:HIS:H	1.95	0.79
1:B:252:GLU:HA	1:B:255:LEU:HB3	1.62	0.79
1:B:272:LEU:HD13	1:B:273:ARG:CA	2.13	0.79
1:A:145:GLN:HE22	1:A:239:SER:H	1.29	0.79
1:A:125:LEU:C	1:A:127:CYS:H	1.86	0.79
1:A:262:MET:HA	1:A:265:ASP:HB3	1.64	0.79
1:A:9:VAL:HB	1:A:141:ARG:HH21	1.47	0.78
1:B:6:GLY:C	1:B:12:ALA:HB3	2.03	0.78
1:A:144:SER:HG	1:A:148:ARG:H	1.31	0.78
1:B:247:ILE:HG23	1:B:248:HIS:CD2	2.18	0.78
1:A:203:GLN:HG3	1:A:205:LEU:HD12	1.65	0.78
1:B:218:ILE:O	1:B:222:VAL:HG23	1.84	0.78
1:B:245:ILE:HG23	1:B:285:ASP:OD2	1.83	0.78
1:B:143:GLN:CD	1:B:143:GLN:H	1.88	0.77
1:A:278:SER:N	1:A:280:VAL:HG13	2.00	0.77
1:A:245:ILE:HG22	1:A:285:ASP:HB2	1.66	0.77
1:A:230:GLY:HA2	1:A:249:LEU:CD1	2.14	0.77
1:B:245:ILE:CA	1:B:245:ILE:HB	2.10	0.77
1:B:268:GLU:OE2	1:B:282:ILE:N	2.18	0.77
1:B:203:GLN:HG2	1:B:208:ARG:HG2	1.67	0.77
1:A:203:GLN:HG2	1:A:208:ARG:HG2	1.67	0.76
1:A:248:HIS:HB2	1:A:252:GLU:O	1.85	0.76
1:A:62:TYR:C	1:A:64:LEU:H	1.88	0.76
1:B:73:PHE:C	1:B:73:PHE:CD2	2.58	0.76
1:A:107:SER:HB3	1:A:108:PRO:HD3	1.65	0.76
1:A:208:ARG:O	1:A:210:LEU:N	2.18	0.76
1:A:250:GLU:O	1:A:251:MET:HB2	1.85	0.76
1:A:261:HIS:C	1:A:263:VAL:H	1.84	0.76
1:A:18:ALA:O	1:A:22:LEU:N	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLN:HG3	1:B:205:LEU:HD12	1.66	0.76
1:B:107:SER:HB3	1:B:108:PRO:HD3	1.68	0.76
1:A:278:SER:OG	1:A:280:VAL:HG13	1.86	0.76
1:A:252:GLU:CB	1:A:256:PRO:HG3	2.10	0.76
1:B:247:ILE:CG2	1:B:248:HIS:N	2.49	0.76
1:B:18:ALA:O	1:B:22:LEU:N	2.14	0.75
1:A:14:ILE:HD13	1:A:141:ARG:HB3	1.67	0.75
1:A:228:VAL:H	1:A:248:HIS:HE1	1.35	0.75
1:B:67:ALA:HB3	1:B:69:ASP:CA	2.08	0.75
1:A:151:MET:O	1:A:154:TYR:N	2.19	0.75
1:B:222:VAL:HG13	1:B:267:VAL:HG11	1.69	0.75
1:B:67:ALA:CB	1:B:72:SER:O	2.27	0.75
1:B:144:SER:HB3	1:B:148:ARG:CG	2.17	0.75
1:B:232:HIS:NE2	1:B:245:ILE:CB	2.49	0.75
1:A:230:GLY:O	1:A:246:GLN:HA	1.86	0.74
1:B:91:SER:O	1:B:93:SER:OG	2.03	0.74
1:A:272:LEU:O	1:A:274:ARG:N	2.20	0.74
1:A:73:PHE:CE2	1:A:74:GLY:HA3	2.22	0.74
1:A:73:PHE:CG	1:A:74:GLY:N	2.55	0.74
1:B:232:HIS:CD2	1:B:245:ILE:HB	2.21	0.74
1:B:11:ARG:NH1	1:B:239:SER:OG	2.17	0.74
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.67	0.74
1:A:197:MET:O	1:A:201:ALA:HB2	1.88	0.74
1:A:244:PHE:HD1	1:A:245:ILE:O	1.69	0.74
1:A:247:ILE:HG23	1:A:248:HIS:N	2.02	0.74
1:A:263:VAL:HG12	1:A:264:ALA:H	1.52	0.74
1:B:136:ARG:O	1:B:139:VAL:HG12	1.88	0.74
1:A:67:ALA:CB	1:A:72:SER:O	2.25	0.74
1:A:208:ARG:O	1:A:210:LEU:HA	1.88	0.74
1:B:153:HIS:O	1:B:157:ASP:HB2	1.88	0.73
1:A:22:LEU:HD23	1:A:131:LEU:CB	2.12	0.73
1:A:248:HIS:HB2	1:A:252:GLU:C	2.09	0.73
1:B:232:HIS:CD2	1:B:245:ILE:HD12	2.23	0.73
1:A:230:GLY:O	1:A:246:GLN:CB	2.36	0.73
1:A:278:SER:OG	1:A:280:VAL:HG12	1.87	0.73
1:B:242:THR:HG22	1:B:243:ARG:H	1.53	0.73
1:B:64:LEU:C	1:B:65:GLN:HE21	1.91	0.73
1:A:269:GLN:HG3	1:B:269:GLN:HE22	1.52	0.73
1:B:85:ALA:O	1:B:89:PHE:O	2.04	0.73
1:B:72:SER:HB3	1:B:75:HIS:CD2	2.21	0.73
1:A:138:VAL:HG11	1:A:148:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD13	1:A:235:ARG:H	1.54	0.73
1:A:230:GLY:O	1:A:246:GLN:CA	2.36	0.73
1:A:273:ARG:HB3	1:A:274:ARG:NH2	2.04	0.72
1:B:230:GLY:HA3	1:B:247:ILE:O	1.89	0.72
1:A:145:GLN:HE22	1:A:239:SER:N	1.86	0.72
1:B:199:TYR:HA	1:B:202:VAL:HG23	1.70	0.72
1:B:261:HIS:C	1:B:263:VAL:H	1.90	0.72
1:B:222:VAL:HG13	1:B:267:VAL:CG1	2.19	0.72
1:A:232:HIS:NE2	1:A:245:ILE:CD1	2.47	0.72
1:A:245:ILE:HD13	1:A:283:HIS:HD2	1.53	0.72
1:A:274:ARG:HB2	1:A:274:ARG:HH11	1.53	0.72
1:A:252:GLU:CA	1:A:256:PRO:HD3	2.19	0.72
1:B:14:ILE:O	1:B:148:ARG:NH2	2.21	0.72
1:A:286:PRO:HG2	1:A:287:CYS:N	2.02	0.72
1:A:11:ARG:NH1	1:A:239:SER:OG	2.15	0.72
1:B:138:VAL:O	1:B:139:VAL:O	2.08	0.72
1:B:259:GLN:O	1:B:261:HIS:N	2.23	0.72
1:A:144:SER:O	1:A:147:VAL:HB	1.90	0.71
1:A:19:MET:HE3	1:A:135:GLN:HE22	1.54	0.71
1:A:283:HIS:CE1	1:A:285:ASP:OD1	2.44	0.71
1:B:233:ASP:O	1:B:244:PHE:HB3	1.89	0.71
1:A:240:GLY:CA	1:A:277:GLY:CA	2.67	0.71
1:A:148:ARG:O	1:A:150:ASP:N	2.23	0.71
1:B:228:VAL:O	1:B:229:SER:C	2.29	0.71
1:B:244:PHE:O	1:B:282:ILE:HD13	1.90	0.71
1:B:22:LEU:HD23	1:B:131:LEU:CB	2.13	0.71
1:B:208:ARG:O	1:B:210:LEU:HA	1.91	0.71
1:A:189:TYR:HA	1:A:192:TYR:HB3	1.74	0.70
1:A:144:SER:OG	1:A:148:ARG:N	2.18	0.70
1:A:17:THR:H	1:A:148:ARG:NH2	1.83	0.70
1:B:268:GLU:HG2	1:B:282:ILE:HG13	1.72	0.70
1:A:247:ILE:HG22	1:A:248:HIS:H	1.53	0.70
1:B:22:LEU:O	1:B:22:LEU:HD22	1.92	0.70
1:B:248:HIS:O	1:B:253:ASP:CB	2.39	0.70
1:A:272:LEU:HD13	1:A:273:ARG:CA	2.20	0.70
1:B:230:GLY:O	1:B:246:GLN:CB	2.39	0.70
1:B:252:GLU:OE1	1:B:255:LEU:HD23	1.90	0.70
1:A:245:ILE:CG2	1:A:285:ASP:OD2	2.40	0.70
1:A:207:ASP:C	1:A:209:ALA:N	2.44	0.70
1:B:270:ALA:C	1:B:272:LEU:H	1.96	0.70
1:B:84:LEU:HD12	1:B:201:ALA:HB1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLY:O	1:B:79:GLU:HG2	1.92	0.70
1:B:87:SER:HA	1:B:193:SER:CB	2.22	0.69
1:B:234:LEU:N	1:B:234:LEU:CD1	2.50	0.69
1:B:256:PRO:CA	1:B:257:LEU:HD23	2.22	0.69
1:B:234:LEU:O	1:B:235:ARG:O	2.10	0.69
1:B:245:ILE:HG22	1:B:285:ASP:HB2	1.75	0.69
1:B:247:ILE:HG22	1:B:248:HIS:H	1.56	0.69
1:A:268:GLU:OE2	1:A:282:ILE:N	2.26	0.69
1:B:219:ILE:HG23	1:B:220:ASP:OD1	1.92	0.69
1:A:240:GLY:HA2	1:A:277:GLY:CA	2.22	0.69
1:A:139:VAL:CG1	1:A:140:ARG:H	1.92	0.69
1:B:86:GLN:O	1:B:91:SER:HB3	1.92	0.69
1:B:14:ILE:HD13	1:B:141:ARG:HB3	1.75	0.69
1:B:243:ARG:O	1:B:244:PHE:HB3	1.91	0.69
1:A:196:ARG:HG2	1:A:197:MET:N	2.06	0.69
1:B:144:SER:OG	1:B:148:ARG:HG2	1.93	0.69
1:A:10:SER:O	1:A:12:ALA:N	2.26	0.68
1:B:9:VAL:HB	1:B:141:ARG:HH21	1.57	0.68
1:A:11:ARG:HA	1:A:142:THR:HG21	1.74	0.68
1:A:23:LEU:HB3	1:A:53:SER:HB2	1.76	0.68
1:A:67:ALA:HA	1:A:75:HIS:CE1	2.27	0.68
1:B:244:PHE:CE1	1:B:245:ILE:O	2.46	0.68
1:B:73:PHE:CG	1:B:74:GLY:N	2.61	0.68
1:A:153:HIS:O	1:A:157:ASP:HB2	1.93	0.68
1:A:84:LEU:HD12	1:A:201:ALA:HB1	1.73	0.68
1:A:286:PRO:CG	1:A:287:CYS:H	1.99	0.68
1:B:197:MET:O	1:B:201:ALA:HB2	1.94	0.68
1:B:57:LEU:HD23	1:B:58:LEU:HG	1.76	0.68
1:B:65:GLN:HB3	1:B:66:PRO:HD2	1.75	0.68
1:A:232:HIS:HE1	1:A:285:ASP:OD2	1.77	0.68
1:A:216:GLN:O	1:A:217:GLU:C	2.32	0.68
1:A:62:TYR:C	1:A:64:LEU:N	2.48	0.68
1:B:14:ILE:HG12	1:B:142:THR:HG22	1.75	0.68
1:B:264:ALA:O	1:B:267:VAL:HB	1.94	0.67
1:A:145:GLN:NE2	1:A:239:SER:H	1.92	0.67
1:B:250:GLU:HG2	1:B:251:MET:N	2.08	0.67
1:B:278:SER:N	1:B:280:VAL:HG13	2.09	0.67
1:A:263:VAL:CG1	1:A:264:ALA:N	2.58	0.67
1:B:189:TYR:HA	1:B:192:TYR:HB3	1.77	0.67
1:B:244:PHE:O	1:B:282:ILE:HG23	1.93	0.67
1:A:218:ILE:O	1:A:222:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:H	1:A:248:HIS:CE1	2.12	0.67
1:A:247:ILE:CG1	1:A:248:HIS:HD2	2.05	0.67
1:A:216:GLN:O	1:A:217:GLU:O	2.12	0.67
1:A:209:ALA:C	1:A:236:THR:HB	2.15	0.67
1:A:23:LEU:HB2	1:A:53:SER:OG	1.94	0.67
1:B:133:SER:HA	1:B:136:ARG:HB2	1.77	0.67
1:B:262:MET:O	1:B:266:GLN:HG3	1.93	0.67
1:B:218:ILE:HD12	1:B:242:THR:HG21	1.77	0.67
1:B:213:GLU:H	1:B:215:ARG:HB3	1.59	0.67
1:B:245:ILE:HD13	1:B:283:HIS:HD2	1.60	0.67
1:A:18:ALA:C	1:A:20:ALA:H	1.98	0.67
1:A:69:ASP:O	1:A:73:PHE:HA	1.95	0.67
1:B:159:MET:HB3	1:B:184:LEU:HD21	1.77	0.67
1:B:199:TYR:O	1:B:203:GLN:NE2	2.28	0.67
1:B:216:GLN:O	1:B:219:ILE:CG2	2.38	0.67
1:A:86:GLN:O	1:A:91:SER:HB3	1.94	0.67
1:B:261:HIS:CD2	1:B:265:ASP:HB2	2.29	0.67
1:B:27:LYS:HZ2	1:B:30:ALA:HB3	1.59	0.67
1:A:6:GLY:HA2	1:A:10:SER:H	1.60	0.66
1:A:19:MET:CE	1:A:135:GLN:HE22	2.06	0.66
1:A:232:HIS:CD2	1:A:245:ILE:HD12	2.31	0.66
1:B:27:LYS:NZ	1:B:30:ALA:HB3	2.10	0.66
1:A:14:ILE:O	1:A:148:ARG:NH2	2.27	0.66
1:B:209:ALA:O	1:B:210:LEU:HG	1.96	0.66
1:A:244:PHE:CE1	1:A:245:ILE:O	2.48	0.66
1:B:232:HIS:CD2	1:B:245:ILE:CG1	2.78	0.66
1:A:207:ASP:C	1:A:209:ALA:H	1.98	0.66
1:A:199:TYR:O	1:A:203:GLN:NE2	2.28	0.66
1:A:218:ILE:HD13	1:A:271:ILE:HG21	1.78	0.66
1:B:138:VAL:HG11	1:B:148:ARG:HG3	1.78	0.66
1:A:243:ARG:O	1:A:244:PHE:HB3	1.95	0.66
1:A:273:ARG:HB3	1:A:274:ARG:HH22	1.61	0.65
1:B:14:ILE:CD1	1:B:138:VAL:HA	2.22	0.65
1:A:144:SER:OG	1:A:148:ARG:HG2	1.96	0.65
1:B:278:SER:OG	1:B:280:VAL:CG1	2.45	0.65
1:B:286:PRO:CG	1:B:287:CYS:N	2.40	0.65
1:A:252:GLU:CB	1:A:256:PRO:CG	2.71	0.65
1:A:228:VAL:N	1:A:248:HIS:CE1	2.64	0.65
1:A:276:PRO:CG	1:A:277:GLY:O	2.39	0.65
1:B:243:ARG:O	1:B:244:PHE:CD2	2.50	0.65
1:B:242:THR:H	1:B:280:VAL:CG1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLY:O	1:B:246:GLN:CA	2.44	0.65
1:A:27:LYS:NZ	1:A:30:ALA:HB3	2.12	0.65
1:A:209:ALA:O	1:A:210:LEU:HG	1.96	0.65
1:A:73:PHE:CZ	1:A:74:GLY:O	2.50	0.65
1:B:245:ILE:HD13	1:B:283:HIS:CD2	2.31	0.65
1:B:208:ARG:O	1:B:210:LEU:CA	2.45	0.65
1:A:133:SER:HA	1:A:136:ARG:HB2	1.79	0.64
1:A:235:ARG:NH1	1:A:237:ARG:CD	2.41	0.64
1:B:151:MET:O	1:B:154:TYR:N	2.31	0.64
1:A:145:GLN:O	1:A:200:GLU:OE1	2.15	0.64
1:A:245:ILE:HG21	1:A:285:ASP:OD2	1.97	0.64
1:A:274:ARG:NH1	1:A:274:ARG:H	1.95	0.64
1:B:154:TYR:C	1:B:156:SER:H	2.00	0.64
1:B:149:ALA:CB	1:B:196:ARG:HH21	2.10	0.64
1:B:80:SER:O	1:B:83:ALA:HB3	1.97	0.64
1:A:136:ARG:O	1:A:139:VAL:HG12	1.97	0.64
1:A:14:ILE:CD1	1:A:138:VAL:HA	2.25	0.64
1:A:154:TYR:C	1:A:156:SER:H	2.01	0.64
1:B:216:GLN:O	1:B:217:GLU:C	2.34	0.64
1:A:192:TYR:CG	1:A:193:SER:N	2.66	0.63
1:A:199:TYR:HA	1:A:202:VAL:HG22	1.78	0.63
1:A:218:ILE:HD12	1:A:242:THR:HG21	1.78	0.63
1:A:203:GLN:HG3	1:A:205:LEU:CD1	2.28	0.63
1:B:233:ASP:O	1:B:244:PHE:CB	2.46	0.63
1:A:107:SER:HB3	1:A:108:PRO:CD	2.28	0.63
1:B:232:HIS:CE1	1:B:285:ASP:OD2	2.50	0.63
1:B:143:GLN:HB2	1:B:146:ALA:N	2.11	0.63
1:B:268:GLU:CG	1:B:282:ILE:HG13	2.28	0.63
1:A:144:SER:OG	1:A:144:SER:O	2.15	0.63
1:A:263:VAL:HG12	1:A:264:ALA:N	2.14	0.63
1:B:244:PHE:N	1:B:281:ILE:O	2.32	0.63
1:B:276:PRO:CG	1:B:277:GLY:O	2.31	0.63
1:B:230:GLY:O	1:B:246:GLN:HA	1.99	0.63
1:A:22:LEU:CD2	1:A:131:LEU:HB3	2.14	0.63
1:A:143:GLN:HB2	1:A:146:ALA:N	2.12	0.63
1:A:203:GLN:HG2	1:A:208:ARG:CG	2.29	0.62
1:B:70:ASN:H	1:B:70:ASN:ND2	1.95	0.62
1:A:166:LEU:HD13	1:A:168:LEU:HB3	1.81	0.62
1:A:186:ILE:HG22	1:A:187:GLY:H	1.65	0.62
1:A:248:HIS:HB2	1:A:252:GLU:HB2	1.80	0.62
1:A:65:GLN:HB3	1:A:66:PRO:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:H	1:B:148:ARG:NH2	1.93	0.62
1:B:247:ILE:HG23	1:B:248:HIS:HD2	1.65	0.62
1:B:268:GLU:HG2	1:B:282:ILE:CG1	2.29	0.62
1:B:243:ARG:O	1:B:244:PHE:HD2	1.81	0.62
1:A:9:VAL:HB	1:A:141:ARG:NH2	2.14	0.62
1:B:10:SER:O	1:B:12:ALA:N	2.32	0.62
1:A:259:GLN:C	1:A:261:HIS:H	2.03	0.62
1:A:79:GLU:HB2	1:A:147:VAL:HG21	0.81	0.62
1:B:251:MET:C	1:B:253:ASP:N	2.52	0.62
1:A:213:GLU:O	1:A:216:GLN:N	2.33	0.61
1:B:11:ARG:CA	1:B:142:THR:HG21	2.28	0.61
1:B:22:LEU:CD2	1:B:131:LEU:HB3	2.15	0.61
1:A:143:GLN:N	1:A:143:GLN:CD	2.49	0.61
1:A:212:ASP:O	1:A:213:GLU:HB2	1.99	0.61
1:B:23:LEU:HB3	1:B:53:SER:HB2	1.82	0.61
1:B:251:MET:C	1:B:253:ASP:H	1.92	0.61
1:A:198:GLY:O	1:A:199:TYR:CD1	2.52	0.61
1:A:67:ALA:C	1:A:69:ASP:H	2.01	0.61
1:A:235:ARG:HG2	1:A:236:THR:H	1.64	0.61
1:A:266:GLN:O	1:A:267:VAL:C	2.38	0.61
1:B:6:GLY:HA2	1:B:10:SER:H	1.66	0.61
1:B:107:SER:HB3	1:B:108:PRO:CD	2.31	0.61
1:A:138:VAL:O	1:A:139:VAL:C	2.38	0.61
1:B:221:ILE:O	1:B:224:SER:OG	2.19	0.61
1:A:18:ALA:H	1:A:148:ARG:NH2	1.98	0.61
1:A:199:TYR:N	1:A:201:ALA:HB3	2.15	0.61
1:A:76:GLY:O	1:A:79:GLU:HG2	2.01	0.61
1:B:252:GLU:HB3	1:B:256:PRO:CD	2.30	0.61
1:A:283:HIS:NE2	1:A:285:ASP:OD1	2.34	0.61
1:B:144:SER:O	1:B:147:VAL:HB	2.00	0.61
1:B:246:GLN:HE22	1:B:267:VAL:HG21	1.65	0.61
1:A:107:SER:HA	1:A:112:THR:HB	1.81	0.60
1:A:251:MET:O	1:A:253:ASP:N	2.29	0.60
1:A:81:LEU:O	1:A:83:ALA:N	2.32	0.60
1:A:109:THR:CB	1:A:110:PRO:HD2	2.25	0.60
1:B:107:SER:HA	1:B:112:THR:HB	1.82	0.60
1:A:251:MET:C	1:A:253:ASP:N	2.48	0.60
1:A:80:SER:O	1:A:83:ALA:HB3	2.01	0.60
1:B:217:GLU:O	1:B:218:ILE:C	2.40	0.60
1:B:73:PHE:CE1	1:B:74:GLY:O	2.54	0.60
1:B:278:SER:OG	1:B:280:VAL:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:HG2	1:A:282:ILE:HG13	1.83	0.60
1:B:18:ALA:H	1:B:148:ARG:NH2	1.99	0.60
1:B:63:SER:O	1:B:64:LEU:HD22	2.02	0.60
1:A:87:SER:HA	1:A:193:SER:CB	2.32	0.60
1:B:125:LEU:C	1:B:127:CYS:N	2.54	0.60
1:B:203:GLN:HG2	1:B:208:ARG:CG	2.31	0.60
1:B:69:ASP:O	1:B:73:PHE:HA	2.02	0.60
1:A:252:GLU:HA	1:A:255:LEU:HB3	1.82	0.60
1:A:72:SER:HB3	1:A:75:HIS:CD2	2.31	0.60
1:A:132:VAL:C	1:A:134:PHE:H	2.04	0.60
1:A:186:ILE:CG2	1:A:187:GLY:N	2.65	0.60
1:A:86:GLN:H	1:A:86:GLN:CD	2.05	0.60
1:A:14:ILE:CD1	1:A:141:ARG:HB3	2.30	0.60
1:A:159:MET:HB3	1:A:184:LEU:HD21	1.82	0.60
1:A:159:MET:CG	1:A:184:LEU:HD11	2.29	0.60
1:B:244:PHE:HD1	1:B:245:ILE:O	1.77	0.60
1:B:109:THR:HB	1:B:110:PRO:CD	2.22	0.60
1:A:186:ILE:HG22	1:A:187:GLY:N	2.17	0.60
1:A:252:GLU:OE1	1:A:255:LEU:HD23	2.02	0.60
1:B:30:ALA:H	1:B:31:TRP:HE3	1.49	0.60
1:A:199:TYR:O	1:A:202:VAL:N	2.35	0.59
1:B:19:MET:HE1	1:B:154:TYR:HE1	1.67	0.59
1:B:230:GLY:HA2	1:B:249:LEU:CD1	2.32	0.59
1:B:266:GLN:O	1:B:267:VAL:C	2.36	0.59
1:A:202:VAL:O	1:A:205:LEU:CG	2.34	0.59
1:A:270:ALA:C	1:A:272:LEU:H	2.05	0.59
1:B:29:PHE:HA	1:B:31:TRP:HZ3	1.67	0.59
1:A:13:ALA:O	1:A:16:ALA:N	2.34	0.59
1:A:67:ALA:C	1:A:69:ASP:N	2.56	0.59
1:B:262:MET:HA	1:B:265:ASP:CB	2.30	0.59
1:B:240:GLY:HA3	1:B:277:GLY:HA2	1.83	0.59
1:B:166:LEU:HD13	1:B:168:LEU:HB3	1.83	0.59
1:A:213:GLU:H	1:A:215:ARG:HB3	1.68	0.59
1:B:186:ILE:HG22	1:B:187:GLY:N	2.18	0.59
1:A:30:ALA:H	1:A:31:TRP:HE3	1.51	0.59
1:A:44:VAL:HG12	1:A:44:VAL:O	2.03	0.59
1:B:86:GLN:CD	1:B:86:GLN:H	2.06	0.59
1:A:230:GLY:HA3	1:A:247:ILE:O	2.03	0.58
1:B:186:ILE:CG2	1:B:187:GLY:N	2.66	0.58
1:A:10:SER:C	1:A:12:ALA:H	2.06	0.58
1:A:139:VAL:HG22	1:A:140:ARG:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:O	1:B:111:MET:N	2.36	0.58
1:A:18:ALA:O	1:A:20:ALA:N	2.29	0.58
1:A:242:THR:HG22	1:A:243:ARG:H	1.68	0.58
1:B:87:SER:HB2	1:B:197:MET:HB2	1.79	0.58
1:A:73:PHE:CD1	1:A:74:GLY:N	2.72	0.58
1:A:127:CYS:SG	1:A:128:THR:N	2.77	0.58
1:A:129:ILE:HG12	1:A:158:VAL:HG11	1.86	0.58
1:A:209:ALA:CB	1:A:236:THR:OG1	2.47	0.58
1:B:19:MET:CE	1:B:150:ASP:OD1	2.51	0.58
1:A:45:ASP:HA	1:A:48:VAL:HB	1.84	0.58
1:A:79:GLU:O	1:A:82:ALA:N	2.37	0.58
1:A:244:PHE:N	1:A:281:ILE:O	2.37	0.58
1:B:274:ARG:C	1:B:276:PRO:HA	2.24	0.58
1:B:153:HIS:O	1:B:157:ASP:N	2.37	0.58
1:B:232:HIS:HE1	1:B:285:ASP:OD2	1.86	0.58
1:B:232:HIS:NE2	1:B:245:ILE:CG1	2.67	0.58
1:A:139:VAL:HG22	1:A:140:ARG:N	2.18	0.58
1:A:247:ILE:CG1	1:A:248:HIS:CD2	2.79	0.58
1:A:85:ALA:O	1:A:87:SER:N	2.37	0.58
1:B:18:ALA:C	1:B:20:ALA:H	2.08	0.58
1:B:188:ILE:HG23	1:B:188:ILE:O	2.04	0.57
1:B:199:TYR:O	1:B:202:VAL:HG23	2.04	0.57
1:B:259:GLN:C	1:B:261:HIS:H	2.07	0.57
1:B:68:ASP:H	1:B:72:SER:HB2	1.68	0.57
1:A:25:LEU:O	1:A:28:ILE:HG22	2.04	0.57
1:A:11:ARG:HH12	1:A:239:SER:HG	1.49	0.57
1:A:261:HIS:CD2	1:A:265:ASP:HB2	2.39	0.57
1:B:278:SER:H	1:B:280:VAL:HG13	1.68	0.57
1:A:227:GLY:HA2	1:A:248:HIS:NE2	2.19	0.57
1:B:235:ARG:NH1	1:B:237:ARG:CD	2.39	0.57
1:A:278:SER:H	1:A:280:VAL:CG1	2.16	0.57
1:B:248:HIS:O	1:B:253:ASP:N	2.38	0.57
1:A:274:ARG:NH1	1:A:274:ARG:N	2.51	0.57
1:B:212:ASP:HA	1:B:215:ARG:CB	2.34	0.57
1:A:84:LEU:O	1:A:87:SER:OG	2.22	0.57
1:B:148:ARG:O	1:B:150:ASP:N	2.38	0.57
1:B:248:HIS:CB	1:B:252:GLU:C	2.71	0.57
1:B:218:ILE:HD13	1:B:271:ILE:HG21	1.87	0.57
1:A:248:HIS:O	1:A:253:ASP:HB2	2.05	0.56
1:A:214:GLU:HB3	1:A:274:ARG:HE	1.70	0.56
1:B:192:TYR:CG	1:B:193:SER:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:O	1:A:202:VAL:HG23	2.05	0.56
1:B:23:LEU:HB2	1:B:53:SER:OG	2.05	0.56
1:A:188:ILE:HG23	1:A:188:ILE:O	2.05	0.56
1:A:67:ALA:HB2	1:A:74:GLY:HA2	1.87	0.56
1:B:186:ILE:HG22	1:B:187:GLY:H	1.70	0.56
1:A:156:SER:HB3	1:A:189:TYR:CE1	2.40	0.56
1:A:217:GLU:O	1:A:218:ILE:C	2.43	0.56
1:B:252:GLU:CA	1:B:256:PRO:CD	2.82	0.56
1:B:256:PRO:HA	1:B:257:LEU:CD2	2.34	0.56
1:A:142:THR:O	1:A:142:THR:HG23	2.06	0.56
1:A:232:HIS:CE1	1:A:285:ASP:OD2	2.58	0.56
1:B:273:ARG:HB3	1:B:274:ARG:HH12	1.71	0.56
1:A:283:HIS:NE2	1:A:285:ASP:CG	2.59	0.56
1:B:87:SER:C	1:B:193:SER:HB2	2.27	0.56
1:A:243:ARG:C	1:A:244:PHE:HD2	2.08	0.56
1:B:136:ARG:O	1:B:139:VAL:CG1	2.54	0.56
1:B:109:THR:CB	1:B:110:PRO:HD2	2.20	0.56
1:A:109:THR:O	1:A:111:MET:N	2.38	0.56
1:B:85:ALA:O	1:B:87:SER:N	2.40	0.55
1:A:29:PHE:HA	1:A:31:TRP:HZ3	1.71	0.55
1:A:144:SER:HG	1:A:148:ARG:N	1.98	0.55
1:A:233:ASP:O	1:A:244:PHE:HB3	2.06	0.55
1:B:62:TYR:C	1:B:64:LEU:H	2.09	0.55
1:B:139:VAL:CG1	1:B:140:ARG:H	2.10	0.55
1:B:203:GLN:HG3	1:B:205:LEU:CD1	2.35	0.55
1:B:247:ILE:HG12	1:B:248:HIS:HD2	1.67	0.55
1:A:273:ARG:HB3	1:A:274:ARG:CZ	2.36	0.55
1:B:73:PHE:O	1:B:73:PHE:CD2	2.60	0.55
1:A:125:LEU:C	1:A:127:CYS:N	2.56	0.55
1:A:159:MET:HG3	1:A:161:ASN:HD22	1.72	0.55
1:B:225:TRP:HZ3	1:B:266:GLN:HB2	1.62	0.55
1:A:148:ARG:C	1:A:150:ASP:H	2.10	0.55
1:A:19:MET:CE	1:A:150:ASP:OD1	2.55	0.55
1:A:225:TRP:HZ3	1:A:266:GLN:HB2	1.67	0.55
1:A:132:VAL:O	1:A:136:ARG:N	2.36	0.55
1:B:153:HIS:HD2	1:B:157:ASP:HB2	1.72	0.55
1:B:252:GLU:CB	1:B:256:PRO:CD	2.84	0.55
1:B:227:GLY:HA2	1:B:248:HIS:NE2	2.22	0.54
1:B:245:ILE:CB	1:B:245:ILE:N	2.65	0.54
1:B:67:ALA:HB2	1:B:74:GLY:HA2	1.89	0.54
1:A:199:TYR:CA	1:A:202:VAL:HG23	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:O	1:A:229:SER:C	2.45	0.54
1:A:247:ILE:CG2	1:A:252:GLU:O	2.55	0.54
1:B:20:ALA:HB1	1:B:57:LEU:HD12	1.89	0.54
1:A:262:MET:HA	1:A:265:ASP:CB	2.35	0.54
1:B:142:THR:HG23	1:B:142:THR:O	2.08	0.54
1:B:256:PRO:C	1:B:257:LEU:CD2	2.72	0.54
1:B:60:VAL:C	1:B:62:TYR:H	2.10	0.54
1:B:25:LEU:O	1:B:28:ILE:HG22	2.07	0.54
1:B:263:VAL:HG12	1:B:264:ALA:H	1.73	0.54
1:B:234:LEU:N	1:B:234:LEU:HD13	2.23	0.54
1:A:188:ILE:O	1:A:189:TYR:CD1	2.61	0.54
1:B:159:MET:CG	1:B:184:LEU:HD11	2.28	0.54
1:A:73:PHE:CD2	1:A:74:GLY:N	2.74	0.54
1:B:213:GLU:O	1:B:216:GLN:N	2.41	0.54
1:B:261:HIS:O	1:B:264:ALA:N	2.40	0.54
1:B:263:VAL:CG1	1:B:264:ALA:N	2.71	0.54
1:B:279:ASP:O	1:B:281:ILE:HA	2.08	0.54
1:B:77:LYS:HZ2	1:B:206:LEU:HD21	1.72	0.53
1:B:85:ALA:HB3	1:B:86:GLN:NE2	2.24	0.53
1:A:205:LEU:HD12	1:A:205:LEU:O	2.09	0.53
1:A:87:SER:HB3	1:A:197:MET:HB3	1.86	0.53
1:B:243:ARG:O	1:B:244:PHE:CB	2.55	0.53
1:B:18:ALA:HB2	1:B:138:VAL:HG21	1.90	0.53
1:A:199:TYR:CA	1:A:202:VAL:CG2	2.74	0.53
1:A:243:ARG:CB	1:A:281:ILE:HD12	2.38	0.53
1:B:245:ILE:CA	1:B:245:ILE:CG2	2.78	0.53
1:A:143:GLN:N	1:A:143:GLN:OE1	2.33	0.53
1:B:152:LEU:HG	1:B:155:GLN:OE1	2.09	0.53
1:A:193:SER:C	1:A:195:LEU:H	2.12	0.53
1:A:196:ARG:CG	1:A:197:MET:N	2.70	0.53
1:A:243:ARG:O	1:A:244:PHE:CB	2.56	0.53
1:B:212:ASP:HA	1:B:215:ARG:HB3	1.91	0.53
1:B:216:GLN:HA	1:B:216:GLN:OE1	2.06	0.53
1:B:252:GLU:CB	1:B:256:PRO:HD3	2.39	0.53
1:B:264:ALA:O	1:B:267:VAL:N	2.42	0.53
1:B:202:VAL:HG23	1:B:203:GLN:HE22	1.72	0.53
1:B:272:LEU:HD13	1:B:273:ARG:N	2.24	0.53
1:A:244:PHE:O	1:A:282:ILE:CD1	2.55	0.53
1:A:6:GLY:C	1:A:12:ALA:CB	2.71	0.53
1:A:156:SER:HB3	1:A:189:TYR:HE1	1.73	0.52
1:B:9:VAL:HB	1:B:141:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:O	1:A:73:PHE:N	2.42	0.52
1:B:197:MET:O	1:B:201:ALA:CB	2.58	0.52
1:A:11:ARG:O	1:A:15:ALA:HB3	2.08	0.52
1:A:247:ILE:HG23	1:A:252:GLU:O	2.09	0.52
1:A:245:ILE:CG2	1:A:283:HIS:CD2	2.80	0.52
1:B:154:TYR:O	1:B:156:SER:N	2.42	0.52
1:B:77:LYS:HZ1	1:B:206:LEU:HG	1.74	0.52
1:B:273:ARG:HB3	1:B:274:ARG:NH1	2.24	0.52
1:A:237:ARG:HG3	1:A:241:PRO:HB2	1.92	0.52
1:A:87:SER:O	1:A:91:SER:O	2.27	0.52
1:A:269:GLN:CG	1:B:269:GLN:HE22	2.20	0.52
1:A:145:GLN:O	1:A:147:VAL:N	2.43	0.52
1:A:286:PRO:CG	1:A:287:CYS:N	2.64	0.52
1:A:66:PRO:O	1:A:69:ASP:OD1	2.27	0.52
1:B:247:ILE:CG2	1:B:252:GLU:O	2.58	0.52
1:B:223:THR:O	1:B:223:THR:HG22	2.09	0.52
1:B:22:LEU:HA	1:B:131:LEU:HD23	1.91	0.52
1:B:139:VAL:O	1:B:142:THR:C	2.48	0.52
1:B:18:ALA:N	1:B:148:ARG:NH2	2.58	0.52
1:B:219:ILE:HG23	1:B:220:ASP:H	1.73	0.52
1:A:209:ALA:HB1	1:A:236:THR:CB	2.40	0.51
1:A:65:GLN:HB2	1:A:75:HIS:HE1	1.75	0.51
1:A:154:TYR:O	1:A:156:SER:N	2.43	0.51
1:B:127:CYS:SG	1:B:128:THR:N	2.84	0.51
1:B:14:ILE:CD1	1:B:141:ARG:HB3	2.39	0.51
1:B:266:GLN:O	1:B:269:GLN:HB3	2.11	0.51
1:A:18:ALA:N	1:A:148:ARG:NH2	2.58	0.51
1:A:197:MET:O	1:A:201:ALA:CB	2.57	0.51
1:A:73:PHE:CZ	1:A:74:GLY:HA3	2.44	0.51
1:A:91:SER:HA	1:A:94:ALA:HB3	1.91	0.51
1:B:152:LEU:CB	1:B:192:TYR:CZ	2.94	0.51
1:B:22:LEU:HD13	1:B:23:LEU:CD2	2.40	0.51
1:B:245:ILE:HG23	1:B:283:HIS:CD2	2.46	0.51
1:B:144:SER:O	1:B:144:SER:OG	2.29	0.51
1:B:274:ARG:N	1:B:274:ARG:NH1	2.58	0.51
1:A:109:THR:HB	1:A:110:PRO:CD	2.27	0.51
1:B:162:GLY:HA3	1:B:181:LEU:HD12	1.93	0.51
1:A:150:ASP:OD1	1:A:151:MET:N	2.43	0.51
1:A:273:ARG:HB3	1:A:274:ARG:NH1	2.25	0.51
1:A:248:HIS:HB2	1:A:252:GLU:CB	2.41	0.51
1:B:132:VAL:O	1:B:136:ARG:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ARG:HB2	1:B:274:ARG:HH11	1.75	0.51
1:A:20:ALA:O	1:A:21:SER:CB	2.58	0.51
1:A:22:LEU:HA	1:A:131:LEU:HD23	1.92	0.51
1:A:65:GLN:HE21	1:A:65:GLN:N	2.06	0.51
1:A:139:VAL:CG2	1:A:140:ARG:H	2.23	0.51
1:A:150:ASP:OD1	1:A:150:ASP:C	2.49	0.51
1:B:132:VAL:C	1:B:134:PHE:H	2.14	0.51
1:A:189:TYR:CA	1:A:192:TYR:HB3	2.39	0.50
1:A:234:LEU:HD12	1:A:234:LEU:N	2.26	0.50
1:B:219:ILE:HG23	1:B:220:ASP:N	2.26	0.50
1:B:105:LEU:O	1:B:107:SER:N	2.43	0.50
1:A:156:SER:HB2	1:A:189:TYR:OH	2.11	0.50
1:A:269:GLN:CG	1:B:269:GLN:NE2	2.74	0.50
1:B:154:TYR:C	1:B:156:SER:N	2.64	0.50
1:B:234:LEU:HD13	1:B:235:ARG:H	1.76	0.50
1:B:248:HIS:HB3	1:B:252:GLU:H	1.76	0.50
1:B:252:GLU:CB	1:B:256:PRO:HG3	2.19	0.50
1:B:268:GLU:OE2	1:B:282:ILE:CB	2.59	0.50
1:B:278:SER:OG	1:B:280:VAL:HG12	2.09	0.50
1:A:64:LEU:O	1:A:65:GLN:NE2	2.44	0.50
1:A:143:GLN:CB	1:A:146:ALA:H	2.20	0.50
1:A:234:LEU:HD13	1:A:235:ARG:N	2.24	0.50
1:A:65:GLN:HB3	1:A:66:PRO:CD	2.41	0.50
1:B:281:ILE:HG22	1:B:282:ILE:N	2.27	0.50
1:A:105:LEU:O	1:A:107:SER:N	2.45	0.50
1:A:162:GLY:HA3	1:A:181:LEU:HD12	1.94	0.50
1:B:270:ALA:C	1:B:272:LEU:N	2.59	0.50
1:A:17:THR:O	1:A:21:SER:OG	2.27	0.50
1:B:229:SER:O	1:B:247:ILE:O	2.28	0.50
1:B:247:ILE:HG23	1:B:248:HIS:CG	2.46	0.50
1:B:65:GLN:HB3	1:B:66:PRO:CD	2.41	0.50
1:A:149:ALA:O	1:A:197:MET:SD	2.70	0.50
1:A:20:ALA:HB1	1:A:57:LEU:HD12	1.93	0.50
1:A:213:GLU:C	1:A:215:ARG:N	2.62	0.50
1:A:267:VAL:O	1:A:268:GLU:C	2.49	0.50
1:B:207:ASP:C	1:B:209:ALA:N	2.64	0.50
1:B:248:HIS:HB2	1:B:252:GLU:HB2	1.94	0.50
1:B:67:ALA:HA	1:B:75:HIS:NE2	2.26	0.50
1:A:283:HIS:NE2	1:A:285:ASP:OD2	2.45	0.50
1:B:270:ALA:O	1:B:272:LEU:N	2.44	0.50
1:A:154:TYR:C	1:A:156:SER:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASP:HA	1:B:48:VAL:HB	1.93	0.49
1:A:256:PRO:C	1:A:257:LEU:CD2	2.75	0.49
1:B:10:SER:C	1:B:12:ALA:H	2.14	0.49
1:B:17:THR:N	1:B:148:ARG:NH2	2.38	0.49
1:B:243:ARG:C	1:B:244:PHE:HD2	2.16	0.49
1:B:252:GLU:OE1	1:B:255:LEU:CD2	2.60	0.49
1:B:189:TYR:CA	1:B:192:TYR:HB3	2.42	0.49
1:B:248:HIS:O	1:B:253:ASP:CA	2.60	0.49
1:B:87:SER:CA	1:B:193:SER:CB	2.91	0.49
1:B:44:VAL:O	1:B:44:VAL:HG12	2.13	0.49
1:A:203:GLN:HA	1:A:205:LEU:O	2.12	0.49
1:A:63:SER:HA	1:A:76:GLY:CA	2.33	0.49
1:B:156:SER:HA	1:B:159:MET:HB2	1.95	0.49
1:B:18:ALA:O	1:B:20:ALA:N	2.42	0.49
1:B:62:TYR:C	1:B:64:LEU:N	2.66	0.49
1:A:19:MET:HE1	1:A:150:ASP:OD1	2.12	0.49
1:B:156:SER:HB3	1:B:189:TYR:HE1	1.78	0.49
1:B:156:SER:HB2	1:B:189:TYR:OH	2.12	0.49
1:B:205:LEU:HD12	1:B:205:LEU:O	2.12	0.49
1:A:22:LEU:HD13	1:A:23:LEU:CD2	2.43	0.49
1:A:85:ALA:HB3	1:A:86:GLN:NE2	2.27	0.49
1:B:209:ALA:HA	1:B:236:THR:O	2.13	0.49
1:B:22:LEU:HD13	1:B:23:LEU:HG	1.93	0.49
1:B:261:HIS:C	1:B:263:VAL:N	2.52	0.49
1:B:208:ARG:O	1:B:210:LEU:N	2.46	0.48
1:A:219:ILE:HG23	1:A:220:ASP:N	2.28	0.48
1:A:256:PRO:HA	1:A:257:LEU:HD23	1.94	0.48
1:A:11:ARG:HD3	1:A:145:GLN:H	1.79	0.48
1:B:23:LEU:CB	1:B:53:SER:HB2	2.41	0.48
1:A:57:LEU:O	1:A:60:VAL:HG22	2.14	0.48
1:A:73:PHE:CE1	1:A:74:GLY:O	2.66	0.48
1:B:214:GLU:HB3	1:B:274:ARG:HE	1.78	0.48
1:B:68:ASP:O	1:B:70:ASN:N	2.46	0.48
1:B:85:ALA:O	1:B:86:GLN:C	2.51	0.48
1:A:60:VAL:C	1:A:62:TYR:H	2.17	0.48
1:A:68:ASP:HB2	1:A:72:SER:HB2	1.95	0.48
1:B:247:ILE:HG23	1:B:248:HIS:CB	2.43	0.48
1:B:272:LEU:C	1:B:274:ARG:N	2.65	0.48
1:B:143:GLN:CB	1:B:146:ALA:H	2.20	0.48
1:B:263:VAL:O	1:B:266:GLN:HB2	2.13	0.48
1:A:198:GLY:O	1:A:199:TYR:HD1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:O	1:B:83:ALA:N	2.43	0.48
1:A:152:LEU:HG	1:A:155:GLN:OE1	2.13	0.48
1:A:270:ALA:C	1:A:272:LEU:N	2.66	0.48
1:A:85:ALA:C	1:A:87:SER:N	2.67	0.48
1:B:139:VAL:HG22	1:B:140:ARG:H	1.78	0.48
1:B:79:GLU:CA	1:B:147:VAL:HG21	2.40	0.48
1:B:145:GLN:O	1:B:200:GLU:OE1	2.30	0.48
1:A:49:ASP:O	1:A:52:ALA:HB3	2.14	0.48
1:B:152:LEU:HB2	1:B:192:TYR:CE1	2.48	0.48
1:B:250:GLU:O	1:B:251:MET:HB2	2.14	0.48
1:A:195:LEU:O	1:A:199:TYR:HB2	2.13	0.47
1:A:87:SER:HB2	1:A:197:MET:HB2	1.87	0.47
1:A:236:THR:C	1:A:237:ARG:HG2	2.34	0.47
1:B:143:GLN:C	1:B:145:GLN:N	2.67	0.47
1:B:247:ILE:HG23	1:B:248:HIS:N	2.27	0.47
1:A:6:GLY:HA3	1:A:12:ALA:HB2	1.96	0.47
1:A:18:ALA:C	1:A:20:ALA:N	2.67	0.47
1:A:238:GLN:O	1:A:239:SER:HB2	2.14	0.47
1:B:197:MET:C	1:B:199:TYR:H	2.18	0.47
1:A:235:ARG:HG2	1:A:236:THR:N	2.28	0.47
1:A:249:LEU:HA	1:A:253:ASP:OD2	2.15	0.47
1:A:274:ARG:CB	1:A:274:ARG:HH11	2.23	0.47
1:A:100:THR:HG22	1:A:101:GLY:N	2.30	0.47
1:A:27:LYS:HZ3	1:A:30:ALA:HB3	1.77	0.47
1:A:11:ARG:CA	1:A:142:THR:HG21	2.44	0.47
1:B:129:ILE:HG12	1:B:158:VAL:HG11	1.95	0.47
1:A:73:PHE:HD2	1:A:73:PHE:O	1.94	0.47
1:B:225:TRP:CG	1:B:226:PRO:HD2	2.50	0.47
1:A:156:SER:CB	1:A:189:TYR:OH	2.63	0.47
1:A:267:VAL:O	1:A:270:ALA:N	2.47	0.47
1:A:85:ALA:O	1:A:86:GLN:C	2.52	0.47
1:B:66:PRO:O	1:B:74:GLY:HA2	2.15	0.47
1:A:125:LEU:O	1:A:127:CYS:N	2.47	0.47
1:B:17:THR:O	1:B:21:SER:OG	2.29	0.47
1:B:91:SER:O	1:B:92:GLY:C	2.54	0.47
1:A:113:ASP:N	1:A:114:PRO:CD	2.78	0.47
1:A:229:SER:O	1:A:247:ILE:O	2.33	0.46
1:A:256:PRO:CA	1:A:257:LEU:HD23	2.45	0.46
1:A:262:MET:CA	1:A:265:ASP:HB3	2.41	0.46
1:A:234:LEU:O	1:A:235:ARG:O	2.33	0.46
1:A:60:VAL:O	1:A:64:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB3	1:A:69:ASP:OD1	2.15	0.46
1:B:19:MET:HE1	1:B:154:TYR:CE1	2.47	0.46
1:A:76:GLY:HA2	1:A:78:ALA:HB3	1.97	0.46
1:B:177:ARG:HB2	1:B:181:LEU:HD22	1.98	0.46
1:B:139:VAL:HG22	1:B:140:ARG:N	2.30	0.46
1:B:154:TYR:HA	1:B:157:ASP:HB3	1.98	0.46
1:B:19:MET:HE3	1:B:135:GLN:HE22	1.80	0.46
1:B:275:PHE:N	1:B:276:PRO:HA	2.31	0.46
1:B:79:GLU:O	1:B:80:SER:C	2.52	0.46
1:A:18:ALA:HB2	1:A:138:VAL:HG21	1.97	0.46
1:A:66:PRO:C	1:A:69:ASP:OD1	2.54	0.46
1:A:93:SER:C	1:A:95:LEU:N	2.67	0.46
1:B:139:VAL:CG1	1:B:140:ARG:N	2.60	0.46
1:B:11:ARG:NH2	1:B:239:SER:HA	2.16	0.46
1:B:245:ILE:CG1	1:B:245:ILE:CA	2.82	0.46
1:B:252:GLU:HB3	1:B:256:PRO:HD3	1.96	0.46
1:B:93:SER:C	1:B:95:LEU:N	2.68	0.46
1:A:245:ILE:CA	1:A:283:HIS:O	2.49	0.46
1:A:23:LEU:CB	1:A:53:SER:CB	2.94	0.46
1:A:78:ALA:O	1:A:81:LEU:HB3	2.16	0.46
1:B:225:TRP:O	1:B:228:VAL:HG22	2.16	0.46
1:B:238:GLN:O	1:B:239:SER:HB2	2.16	0.46
1:B:213:GLU:H	1:B:215:ARG:CB	2.26	0.46
1:A:244:PHE:O	1:A:282:ILE:CG2	2.42	0.46
1:A:267:VAL:HG12	1:A:268:GLU:N	2.30	0.46
1:A:243:ARG:HA	1:A:281:ILE:H	1.81	0.46
1:A:91:SER:HA	1:A:94:ALA:CB	2.44	0.46
1:B:201:ALA:O	1:B:204:SER:HB2	2.16	0.46
1:A:44:VAL:C	1:A:46:SER:H	2.19	0.46
1:A:230:GLY:O	1:A:246:GLN:HB3	2.13	0.45
1:A:23:LEU:HB3	1:A:53:SER:CB	2.46	0.45
1:B:154:TYR:O	1:B:158:VAL:N	2.47	0.45
1:B:236:THR:HA	1:B:241:PRO:O	2.16	0.45
1:B:87:SER:O	1:B:88:MET:C	2.54	0.45
1:A:136:ARG:O	1:A:139:VAL:CG1	2.63	0.45
1:A:139:VAL:O	1:A:142:THR:C	2.54	0.45
1:A:142:THR:O	1:A:142:THR:CG2	2.63	0.45
1:A:248:HIS:O	1:A:253:ASP:CB	2.63	0.45
1:A:66:PRO:O	1:A:67:ALA:CB	2.64	0.45
1:B:149:ALA:HB3	1:B:196:ARG:HH21	1.79	0.45
1:B:150:ASP:O	1:B:153:HIS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:HE1	1:B:150:ASP:OD1	2.17	0.45
1:B:18:ALA:HB1	1:B:135:GLN:HG2	1.97	0.45
1:A:219:ILE:HG23	1:A:220:ASP:H	1.81	0.45
1:A:245:ILE:HD13	1:A:283:HIS:CD2	2.42	0.45
1:B:156:SER:HB3	1:B:189:TYR:CE1	2.51	0.45
1:B:233:ASP:HB2	1:B:234:LEU:HD12	1.98	0.45
1:A:55:THR:O	1:A:59:VAL:HG23	2.16	0.45
1:A:152:LEU:CB	1:A:192:TYR:CZ	3.00	0.45
1:A:222:VAL:HG13	1:A:267:VAL:CG1	2.46	0.45
1:B:261:HIS:C	1:B:261:HIS:CD2	2.90	0.45
1:A:223:THR:O	1:A:223:THR:HG22	2.16	0.45
1:A:233:ASP:HB2	1:A:234:LEU:HD12	1.98	0.45
1:B:152:LEU:HA	1:B:155:GLN:HB2	1.99	0.45
1:B:203:GLN:HA	1:B:205:LEU:O	2.16	0.45
1:A:103:GLN:CA	1:A:108:PRO:HG3	2.47	0.45
1:A:153:HIS:HD2	1:A:157:ASP:HB2	1.81	0.45
1:A:215:ARG:HD2	1:A:234:LEU:HD23	1.98	0.45
1:A:73:PHE:CZ	1:A:74:GLY:CA	3.00	0.45
1:B:235:ARG:HG2	1:B:236:THR:H	1.81	0.45
1:B:268:GLU:OE2	1:B:282:ILE:HB	2.16	0.45
1:B:23:LEU:HB2	1:B:53:SER:CB	2.46	0.45
1:B:87:SER:HB3	1:B:197:MET:HB3	1.83	0.45
1:B:59:VAL:HG11	1:B:82:ALA:CB	2.46	0.45
1:A:253:ASP:HA	1:A:286:PRO:O	2.16	0.45
1:A:93:SER:C	1:A:95:LEU:H	2.19	0.45
1:B:150:ASP:O	1:B:151:MET:C	2.55	0.45
1:B:195:LEU:O	1:B:199:TYR:HB2	2.17	0.45
1:B:91:SER:C	1:B:93:SER:N	2.69	0.45
1:A:259:GLN:C	1:A:261:HIS:N	2.68	0.45
1:B:143:GLN:CD	1:B:143:GLN:N	2.66	0.45
1:B:11:ARG:HG2	1:B:144:SER:HA	1.99	0.45
1:B:233:ASP:N	1:B:244:PHE:CD1	2.85	0.45
1:A:185:GLY:O	1:A:189:TYR:HB2	2.17	0.45
1:A:238:GLN:HG3	1:A:238:GLN:O	2.17	0.45
1:A:23:LEU:CB	1:A:53:SER:OG	2.62	0.45
1:A:68:ASP:O	1:A:70:ASN:N	2.49	0.45
1:B:55:THR:O	1:B:59:VAL:HG23	2.16	0.45
1:A:184:LEU:O	1:A:188:ILE:HG22	2.17	0.44
1:B:125:LEU:O	1:B:127:CYS:N	2.47	0.44
1:B:154:TYR:HA	1:B:157:ASP:CB	2.46	0.44
1:B:152:LEU:HB3	1:B:192:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:267:VAL:HG23	2.17	0.44
1:B:143:GLN:O	1:B:145:GLN:N	2.51	0.44
1:B:213:GLU:C	1:B:215:ARG:N	2.69	0.44
1:B:244:PHE:O	1:B:282:ILE:CD1	2.62	0.44
1:A:154:TYR:O	1:A:158:VAL:N	2.49	0.44
1:A:149:ALA:CB	1:A:196:ARG:HH21	2.29	0.44
1:B:8:LEU:O	1:B:14:ILE:HG21	2.17	0.44
1:B:29:PHE:HA	1:B:31:TRP:CZ3	2.51	0.44
1:B:258:VAL:HG12	1:B:258:VAL:O	2.17	0.44
1:A:247:ILE:HG23	1:A:248:HIS:CD2	2.53	0.44
1:A:253:ASP:OD1	1:A:287:CYS:SG	2.66	0.44
1:B:222:VAL:HG13	1:B:267:VAL:HG13	1.94	0.44
1:B:64:LEU:HA	1:B:64:LEU:HD13	1.79	0.44
1:B:237:ARG:HG3	1:B:241:PRO:HB2	1.99	0.44
1:B:86:GLN:NE2	1:B:86:GLN:H	2.15	0.44
1:B:103:GLN:CA	1:B:108:PRO:HG3	2.47	0.44
1:A:152:LEU:HA	1:A:155:GLN:HB2	2.00	0.44
1:A:188:ILE:CG2	1:A:188:ILE:O	2.66	0.44
1:B:67:ALA:C	1:B:69:ASP:N	2.70	0.44
1:A:54:LEU:O	1:A:55:THR:C	2.56	0.44
1:A:81:LEU:O	1:A:84:LEU:N	2.50	0.44
1:B:144:SER:HG	1:B:148:ARG:H	1.61	0.44
1:B:150:ASP:OD1	1:B:150:ASP:C	2.56	0.44
1:B:153:HIS:CD2	1:B:153:HIS:C	2.91	0.44
1:B:236:THR:CG2	1:B:242:THR:HG23	2.47	0.44
1:A:54:LEU:O	1:A:55:THR:O	2.36	0.44
1:B:113:ASP:N	1:B:114:PRO:CD	2.80	0.44
1:B:138:VAL:O	1:B:139:VAL:C	2.55	0.44
1:A:146:ALA:HB1	1:A:196:ARG:NH2	2.33	0.44
1:A:268:GLU:O	1:A:269:GLN:C	2.56	0.44
1:A:66:PRO:O	1:A:67:ALA:HB2	2.18	0.44
1:B:142:THR:CG2	1:B:142:THR:O	2.66	0.44
1:B:263:VAL:HG12	1:B:264:ALA:N	2.31	0.44
1:B:44:VAL:C	1:B:46:SER:H	2.21	0.44
1:A:266:GLN:O	1:A:270:ALA:N	2.29	0.43
1:B:232:HIS:CD2	1:B:245:ILE:CD1	2.89	0.43
1:B:269:GLN:O	1:B:272:LEU:N	2.51	0.43
1:B:73:PHE:CZ	1:B:74:GLY:O	2.71	0.43
1:A:102:ILE:HG22	1:A:102:ILE:O	2.18	0.43
1:B:235:ARG:O	1:B:236:THR:HG23	2.17	0.43
1:B:245:ILE:CB	1:B:245:ILE:C	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:O	1:B:267:VAL:HG23	2.17	0.43
1:A:127:CYS:O	1:A:130:ILE:HG22	2.18	0.43
1:A:213:GLU:O	1:A:217:GLU:N	2.51	0.43
1:A:274:ARG:C	1:A:276:PRO:HA	2.39	0.43
1:A:23:LEU:CB	1:A:53:SER:HB2	2.45	0.43
1:A:156:SER:CB	1:A:189:TYR:CE1	3.01	0.43
1:A:216:GLN:OE1	1:A:216:GLN:HA	2.18	0.43
1:A:217:GLU:C	1:A:221:ILE:HD12	2.38	0.43
1:A:226:PRO:O	1:A:228:VAL:HG23	2.18	0.43
1:B:247:ILE:HG23	1:B:248:HIS:HB2	2.00	0.43
1:B:103:GLN:HA	1:B:108:PRO:HG3	2.00	0.43
1:A:18:ALA:HB3	1:A:148:ARG:NE	2.34	0.43
1:A:193:SER:O	1:A:195:LEU:N	2.52	0.43
1:A:234:LEU:CD1	1:A:234:LEU:N	2.81	0.43
1:B:20:ALA:O	1:B:21:SER:CB	2.66	0.43
1:B:267:VAL:O	1:B:270:ALA:N	2.52	0.43
1:A:148:ARG:C	1:A:150:ASP:N	2.71	0.43
1:A:213:GLU:O	1:A:216:GLN:CA	2.66	0.43
1:A:268:GLU:O	1:A:271:ILE:HG13	2.19	0.43
1:B:248:HIS:HB2	1:B:252:GLU:CA	2.49	0.43
1:B:87:SER:O	1:B:91:SER:O	2.36	0.43
1:B:45:ASP:O	1:B:45:ASP:CG	2.57	0.43
1:A:17:THR:O	1:A:18:ALA:O	2.37	0.43
1:B:188:ILE:CG2	1:B:188:ILE:O	2.66	0.43
1:B:65:GLN:CB	1:B:66:PRO:HD2	2.41	0.43
1:A:103:GLN:HA	1:A:108:PRO:HG3	1.99	0.43
1:A:150:ASP:O	1:A:151:MET:C	2.57	0.43
1:B:184:LEU:O	1:B:188:ILE:HG22	2.19	0.43
1:B:248:HIS:HB2	1:B:252:GLU:CB	2.49	0.43
1:B:245:ILE:CA	1:B:283:HIS:O	2.56	0.43
1:B:98:PHE:HD2	1:B:98:PHE:HA	1.71	0.43
1:A:137:TRP:CH2	1:A:141:ARG:CD	3.02	0.42
1:A:232:HIS:CE1	1:A:245:ILE:HG22	2.43	0.42
1:A:258:VAL:O	1:A:259:GLN:C	2.57	0.42
1:B:11:ARG:HD3	1:B:145:GLN:H	1.84	0.42
1:B:152:LEU:HB2	1:B:192:TYR:CZ	2.53	0.42
1:B:161:ASN:O	1:B:165:LEU:HB3	2.19	0.42
1:B:202:VAL:HG23	1:B:203:GLN:NE2	2.34	0.42
1:A:153:HIS:O	1:A:157:ASP:N	2.51	0.42
1:A:18:ALA:N	1:A:148:ARG:CZ	2.82	0.42
1:A:279:ASP:O	1:A:281:ILE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLY:O	1:B:189:TYR:HB2	2.20	0.42
1:B:246:GLN:O	1:B:284:GLN:HA	2.18	0.42
1:A:210:LEU:HA	1:A:211:PRO:HD2	1.63	0.42
1:A:242:THR:N	1:A:280:VAL:CG1	2.70	0.42
1:B:245:ILE:H	1:B:245:ILE:HG12	1.83	0.42
1:B:73:PHE:CD1	1:B:74:GLY:N	2.87	0.42
1:A:125:LEU:HG	1:A:128:THR:HB	2.01	0.42
1:B:27:LYS:HA	1:B:27:LYS:HD2	1.66	0.42
1:B:92:GLY:C	1:B:95:LEU:HD23	2.40	0.42
1:A:137:TRP:CH2	1:A:141:ARG:HD2	2.54	0.42
1:A:156:SER:HA	1:A:159:MET:HB2	2.01	0.42
1:A:193:SER:HA	1:A:197:MET:HG2	2.02	0.42
1:A:243:ARG:HB3	1:A:281:ILE:HD12	2.01	0.42
1:B:196:ARG:HG2	1:B:197:MET:N	2.33	0.42
1:A:161:ASN:O	1:A:165:LEU:HB3	2.20	0.42
1:A:193:SER:C	1:A:195:LEU:N	2.72	0.42
1:A:77:LYS:HZ1	1:A:206:LEU:HG	1.83	0.42
1:A:261:HIS:O	1:A:264:ALA:N	2.53	0.42
1:A:77:LYS:O	1:A:80:SER:N	2.52	0.42
1:B:11:ARG:O	1:B:15:ALA:HB3	2.19	0.42
1:B:145:GLN:OE1	1:B:238:GLN:OE1	2.38	0.42
1:A:264:ALA:O	1:A:268:GLU:N	2.42	0.42
1:A:77:LYS:O	1:A:78:ALA:C	2.58	0.42
1:B:252:GLU:HB2	1:B:256:PRO:HG2	2.02	0.42
1:A:78:ALA:O	1:A:79:GLU:C	2.56	0.42
1:B:130:ILE:HG13	1:B:131:LEU:HD12	2.02	0.42
1:B:252:GLU:CB	1:B:256:PRO:HG2	2.47	0.42
1:A:159:MET:HG3	1:A:161:ASN:ND2	2.33	0.41
1:A:216:GLN:O	1:A:219:ILE:HG23	2.17	0.41
1:B:11:ARG:N	1:B:142:THR:HG21	2.35	0.41
1:A:229:SER:O	1:A:248:HIS:HA	2.20	0.41
1:A:269:GLN:HG2	1:B:269:GLN:NE2	2.34	0.41
1:B:102:ILE:HG23	1:B:108:PRO:HD3	2.01	0.41
1:A:55:THR:HG22	1:A:56:ASN:N	2.35	0.41
1:A:222:VAL:HG13	1:A:267:VAL:HG11	2.02	0.41
1:A:272:LEU:HD13	1:A:273:ARG:N	2.35	0.41
1:B:285:ASP:HA	1:B:286:PRO:HD2	1.74	0.41
1:A:160:MET:HB3	1:A:163:ALA:HB3	2.00	0.41
1:A:237:ARG:N	1:A:241:PRO:O	2.53	0.41
1:A:248:HIS:C	1:A:250:GLU:H	2.24	0.41
1:B:242:THR:O	1:B:280:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HD13	1:A:129:ILE:HA	1.91	0.41
1:A:79:GLU:CA	1:A:147:VAL:HG21	2.46	0.41
1:B:209:ALA:C	1:B:236:THR:HB	2.34	0.41
1:B:13:ALA:O	1:B:16:ALA:N	2.49	0.41
1:B:144:SER:OG	1:B:148:ARG:N	2.31	0.41
1:B:84:LEU:HB2	1:B:201:ALA:HB1	2.01	0.41
1:A:284:GLN:CG	1:A:284:GLN:O	2.68	0.41
1:A:208:ARG:C	1:A:210:LEU:N	2.74	0.41
1:A:64:LEU:HD13	1:A:64:LEU:HA	1.81	0.41
1:B:213:GLU:O	1:B:217:GLU:N	2.54	0.41
1:B:279:ASP:O	1:B:280:VAL:C	2.57	0.41
1:A:144:SER:O	1:A:145:GLN:C	2.59	0.41
1:A:214:GLU:HA	1:A:217:GLU:HB2	2.03	0.41
1:A:250:GLU:HG2	1:A:251:MET:N	2.35	0.41
1:B:144:SER:HB3	1:B:148:ARG:HG3	1.99	0.41
1:A:285:ASP:HA	1:A:286:PRO:HD2	1.69	0.41
1:A:83:ALA:CA	1:A:86:GLN:HG2	2.50	0.41
1:B:23:LEU:CB	1:B:53:SER:CB	2.99	0.41
1:B:64:LEU:O	1:B:65:GLN:NE2	2.52	0.41
1:A:132:VAL:C	1:A:134:PHE:N	2.69	0.41
1:A:248:HIS:HB2	1:A:252:GLU:CA	2.51	0.41
1:A:67:ALA:HA	1:A:75:HIS:CD2	2.55	0.41
1:B:245:ILE:HG21	1:B:285:ASP:OD2	2.17	0.41
1:B:67:ALA:HB2	1:B:74:GLY:CA	2.51	0.41
1:A:6:GLY:HA2	1:A:10:SER:N	2.32	0.41
1:A:102:ILE:HG23	1:A:108:PRO:HD3	2.03	0.41
1:B:100:THR:HG22	1:B:101:GLY:N	2.36	0.41
1:A:212:ASP:HA	1:A:215:ARG:HB3	2.03	0.41
1:B:233:ASP:OD2	1:B:234:LEU:HD13	2.21	0.41
1:B:235:ARG:HH22	1:B:237:ARG:HD2	1.85	0.41
1:B:66:PRO:O	1:B:67:ALA:HB2	2.21	0.41
1:B:87:SER:CA	1:B:193:SER:HB2	2.51	0.41
1:A:177:ARG:HB2	1:A:181:LEU:HD22	2.03	0.41
1:A:229:SER:O	1:A:249:LEU:N	2.37	0.40
1:B:127:CYS:O	1:B:130:ILE:HG22	2.21	0.40
1:A:98:PHE:HA	1:A:98:PHE:HD2	1.72	0.40
1:A:185:GLY:O	1:A:186:ILE:C	2.60	0.40
1:B:159:MET:HG3	1:B:161:ASN:HD22	1.86	0.40
1:B:68:ASP:O	1:B:71:HIS:N	2.54	0.40
1:A:10:SER:C	1:A:12:ALA:N	2.71	0.40
1:A:120:VAL:O	1:A:120:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG13	1:A:122:ILE:HG12	2.04	0.40
1:A:215:ARG:HB3	1:A:216:GLN:H	1.75	0.40
1:A:217:GLU:O	1:A:219:ILE:N	2.54	0.40
1:B:228:VAL:O	1:B:229:SER:O	2.38	0.40
1:A:272:LEU:C	1:A:274:ARG:N	2.74	0.40
1:A:8:LEU:O	1:A:14:ILE:HG21	2.22	0.40
1:B:18:ALA:HB3	1:B:148:ARG:NE	2.37	0.40
1:A:212:ASP:HA	1:A:215:ARG:CB	2.51	0.40
1:A:212:ASP:O	1:A:213:GLU:CB	2.62	0.40
1:B:148:ARG:C	1:B:150:ASP:H	2.25	0.40
1:B:152:LEU:CB	1:B:192:TYR:CE1	3.05	0.40
1:B:243:ARG:HA	1:B:281:ILE:N	2.37	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:NE2	2:A:306:ZN:ZN[4_556]	1.49	0.71
1:A:68:ASP:N	2:A:303:ZN:ZN[4_556]	1.54	0.66
1:A:261:HIS:CE1	1:A:285:ASP:OD1[4_556]	1.56	0.64
1:A:261:HIS:ND1	1:A:285:ASP:OD1[4_556]	2.09	0.11

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/300 (95%)	133 (47%)	76 (27%)	75 (26%)	0	1
1	B	284/300 (95%)	129 (45%)	76 (27%)	79 (28%)	0	0
All	All	568/600 (95%)	262 (46%)	152 (27%)	154 (27%)	0	1

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	21	SER
1	A	55	THR
1	A	67	ALA
1	A	69	ASP
1	A	78	ALA
1	A	86	GLN
1	A	93	SER
1	A	102	ILE
1	A	110	PRO
1	A	126	ILE
1	A	139	VAL
1	A	151	MET
1	A	207	ASP
1	A	209	ALA
1	A	213	GLU
1	A	228	VAL
1	A	235	ARG
1	A	244	PHE
1	A	247	ILE
1	A	254	SER
1	A	260	ALA
1	A	273	ARG
1	A	276	PRO
1	B	18	ALA
1	B	21	SER
1	B	55	THR
1	B	67	ALA
1	B	69	ASP
1	B	78	ALA
1	B	86	GLN
1	B	102	ILE
1	B	110	PRO
1	B	126	ILE
1	B	139	VAL
1	B	149	ALA
1	B	151	MET
1	B	209	ALA
1	B	213	GLU
1	B	235	ARG
1	B	241	PRO
1	B	247	ILE
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	254	SER
1	B	255	LEU
1	B	260	ALA
1	B	273	ARG
1	B	276	PRO
1	B	278	SER
1	B	280	VAL
1	A	11	ARG
1	A	19	MET
1	A	34	THR
1	A	61	ARG
1	A	87	SER
1	A	90	ILE
1	A	106	ILE
1	A	129	ILE
1	A	145	GLN
1	A	149	ALA
1	A	181	LEU
1	A	186	ILE
1	A	194	ALA
1	A	201	ALA
1	A	217	GLU
1	A	218	ILE
1	A	225	TRP
1	A	241	PRO
1	A	251	MET
1	A	259	GLN
1	A	262	MET
1	A	267	VAL
1	A	271	ILE
1	A	286	PRO
1	B	11	ARG
1	B	19	MET
1	B	34	THR
1	B	61	ARG
1	B	87	SER
1	B	90	ILE
1	B	93	SER
1	B	106	ILE
1	B	128	THR
1	B	155	GLN
1	B	181	LEU

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Mol	Chain	Res	Type
1	B	186	ILE
1	B	194	ALA
1	B	207	ASP
1	B	216	GLN
1	B	217	GLU
1	B	225	TRP
1	B	228	VAL
1	B	230	GLY
1	B	244	PHE
1	B	245	ILE
1	B	251	MET
1	B	256	PRO
1	B	259	GLN
1	B	262	MET
1	B	271	ILE
1	B	286	PRO
1	A	72	SER
1	A	77	LYS
1	A	82	ALA
1	A	107	SER
1	A	128	THR
1	A	146	ALA
1	A	155	GLN
1	A	216	GLN
1	A	230	GLY
1	A	278	SER
1	B	82	ALA
1	B	88	MET
1	B	107	SER
1	B	115	GLY
1	B	145	GLN
1	B	211	PRO
1	A	30	ALA
1	A	71	HIS
1	A	88	MET
1	A	115	GLY
1	A	133	SER
1	A	211	PRO
1	A	215	ARG
1	B	30	ALA
1	B	77	LYS
1	B	144	SER

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Mol	Chain	Res	Type
1	B	212	ASP
1	B	215	ARG
1	B	261	HIS
1	A	62	TYR
1	A	74	GLY
1	A	272	LEU
1	A	275	PHE
1	B	63	SER
1	B	83	ALA
1	B	98	PHE
1	B	129	ILE
1	B	133	SER
1	B	146	ALA
1	B	249	LEU
1	A	37	VAL
1	A	252	GLU
1	B	37	VAL
1	B	218	ILE
1	B	275	PHE
1	A	35	GLY
1	A	188	ILE
1	B	35	GLY
1	A	164	ILE
1	A	256	PRO
1	B	74	GLY
1	B	164	ILE
1	B	267	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/249 (95%)	163 (69%)	73 (31%)	0 3
1	B	236/249 (95%)	165 (70%)	71 (30%)	0 4
All	All	472/498 (95%)	328 (70%)	144 (30%)	0 4

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	7	ARG
1	A	8	LEU
1	A	9	VAL
1	A	14	ILE
1	A	17	THR
1	A	22	LEU
1	A	26	ILE
1	A	27	LYS
1	A	31	TRP
1	A	32	TRP
1	A	46	SER
1	A	50	ILE
1	A	57	LEU
1	A	64	LEU
1	A	65	GLN
1	A	70	ASN
1	A	73	PHE
1	A	86	GLN
1	A	89	PHE
1	A	90	ILE
1	A	95	LEU
1	A	98	PHE
1	A	99	LEU
1	A	121	THR
1	A	123	VAL
1	A	143	GLN
1	A	151	MET
1	A	153	HIS
1	A	159	MET
1	A	160	MET
1	A	165	LEU
1	A	166	LEU
1	A	170	LEU
1	A	182	PHE
1	A	186	ILE
1	A	188	ILE
1	A	193	SER
1	A	199	TYR
1	A	202	VAL
1	A	203	GLN
1	A	206	LEU

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Mol	Chain	Res	Type
1	A	212	ASP
1	A	219	ILE
1	A	220	ASP
1	A	222	VAL
1	A	225	TRP
1	A	232	HIS
1	A	233	ASP
1	A	234	LEU
1	A	236	THR
1	A	237	ARG
1	A	238	GLN
1	A	241	PRO
1	A	245	ILE
1	A	246	GLN
1	A	247	ILE
1	A	252	GLU
1	A	257	LEU
1	A	262	MET
1	A	263	VAL
1	A	271	ILE
1	A	272	LEU
1	A	274	ARG
1	A	275	PHE
1	A	278	SER
1	A	280	VAL
1	A	281	ILE
1	A	283	HIS
1	A	284	GLN
1	A	287	CYS
1	A	288	SER
1	A	290	VAL
1	B	7	ARG
1	B	8	LEU
1	B	9	VAL
1	B	14	ILE
1	B	17	THR
1	B	22	LEU
1	B	26	ILE
1	B	27	LYS
1	B	31	TRP
1	B	32	TRP
1	B	46	SER

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Mol	Chain	Res	Type
1	B	50	ILE
1	B	57	LEU
1	B	64	LEU
1	B	65	GLN
1	B	70	ASN
1	B	73	PHE
1	B	86	GLN
1	B	89	PHE
1	B	90	ILE
1	B	95	LEU
1	B	98	PHE
1	B	121	THR
1	B	123	VAL
1	B	132	VAL
1	B	143	GLN
1	B	151	MET
1	B	153	HIS
1	B	159	MET
1	B	165	LEU
1	B	166	LEU
1	B	170	LEU
1	B	182	PHE
1	B	186	ILE
1	B	188	ILE
1	B	191	LEU
1	B	193	SER
1	B	199	TYR
1	B	202	VAL
1	B	206	LEU
1	B	212	ASP
1	B	218	ILE
1	B	220	ASP
1	B	222	VAL
1	B	225	TRP
1	B	229	SER
1	B	232	HIS
1	B	233	ASP
1	B	234	LEU
1	B	235	ARG
1	B	236	THR
1	B	237	ARG
1	B	241	PRO

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Mol	Chain	Res	Type
1	B	242	THR
1	B	245	ILE
1	B	246	GLN
1	B	247	ILE
1	B	252	GLU
1	B	257	LEU
1	B	262	MET
1	B	263	VAL
1	B	271	ILE
1	B	272	LEU
1	B	274	ARG
1	B	275	PHE
1	B	278	SER
1	B	281	ILE
1	B	284	GLN
1	B	287	CYS
1	B	288	SER
1	B	290	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	70	ASN
1	A	75	HIS
1	A	86	GLN
1	A	135	GLN
1	A	145	GLN
1	A	153	HIS
1	A	161	ASN
1	A	203	GLN
1	A	232	HIS
1	A	246	GLN
1	A	248	HIS
1	A	261	HIS
1	A	266	GLN
1	A	283	HIS
1	A	284	GLN
1	B	65	GLN
1	B	70	ASN
1	B	75	HIS
1	B	86	GLN

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Mol	Chain	Res	Type
1	B	135	GLN
1	B	145	GLN
1	B	153	HIS
1	B	161	ASN
1	B	203	GLN
1	B	246	GLN
1	B	261	HIS
1	B	266	GLN
1	B	269	GLN
1	B	284	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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	286/300 (95%)	0.10	16 (5%) 28 18	34, 112, 307, 364	0
1	B	286/300 (95%)	0.79	52 (18%) 2 1	48, 212, 575, 683	0
All	All	572/600 (95%)	0.45	68 (11%) 6 5	34, 151, 522, 683	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	15.8
1	B	43	LEU	12.7
1	B	169	GLY	10.2
1	B	167	ALA	9.8
1	B	168	LEU	9.7
1	B	118	VAL	6.7
1	B	41	ALA	6.5
1	B	71	HIS	6.4
1	B	178	ALA	6.3
1	B	106	ILE	6.2
1	B	110	PRO	6.1
1	B	115	GLY	6.1
1	B	44	VAL	6.1
1	A	8	LEU	6.0
1	A	9	VAL	5.9
1	B	117	GLY	5.5
1	A	10	SER	5.4
1	B	173	TYR	5.3
1	B	174	GLY	5.3
1	B	176	HIS	5.3
1	B	172	TRP	5.2
1	B	120	VAL	5.1
1	B	121	THR	5.1
1	B	32	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	250	GLU	4.8
1	B	30	ALA	4.7
1	A	5	TYR	4.3
1	B	141	ARG	4.3
1	B	108	PRO	4.2
1	B	107	SER	4.2
1	B	124	ALA	4.1
1	B	105	LEU	4.0
1	B	170	LEU	4.0
1	B	114	PRO	4.0
1	B	175	TRP	4.0
1	B	31	TRP	4.0
1	B	33	TYR	4.0
1	B	111	MET	4.0
1	B	112	THR	3.9
1	B	9	VAL	3.9
1	B	113	ASP	3.9
1	B	70	ASN	3.9
1	B	10	SER	3.8
1	B	8	LEU	3.7
1	B	166	LEU	3.7
1	B	7	ARG	3.7
1	B	122	ILE	3.3
1	A	155	GLN	3.2
1	B	25	LEU	3.1
1	B	109	THR	3.1
1	A	71	HIS	3.0
1	B	140	ARG	3.0
1	B	250	GLU	2.9
1	B	21	SER	2.7
1	B	171	SER	2.7
1	A	249	LEU	2.5
1	A	252	GLU	2.5
1	A	115	GLY	2.4
1	B	26	ILE	2.4
1	A	174	GLY	2.3
1	B	177	ARG	2.3
1	B	5	TYR	2.3
1	A	7	ARG	2.2
1	A	6	GLY	2.2
1	A	208	ARG	2.2
1	A	256	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	ARG	2.1
1	B	116	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
2	ZN	B	304	1/1	0.97	0.14	-0.84	8,8,8,8	0
2	ZN	B	305	1/1	0.96	0.09	-0.96	77,77,77,77	0
2	ZN	A	302	1/1	0.95	0.14	-1.62	28,28,28,28	0
2	ZN	A	303	1/1	0.98	0.02	-2.46	26,26,26,26	0
2	ZN	A	306	1/1	0.97	0.20	-	28,28,28,28	0
2	ZN	A	307	1/1	0.96	0.07	-	109,109,109,109	0
2	ZN	B	301	1/1	0.96	0.23	-	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.