Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2018 – 02:20 AM EST

PDB ID	:	1D6N
Title	:	TERNARY COMPLEX STRUCTURE OF HUMAN HGPRTASE, PRPP, MG2+, AND THE INHIBITOR HPP REVEALS THE INVOLVEMENT OF THE FLEXIBLE LOOP IN SUBSTRATE BINDING
Authors	:	Balendiran, G.K.
Deposited on	:	1999-10-14
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 2.70 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	Percentile Ranks	Value
Clashscore		97
Ramachandran outliers		14.9%
Sidechain outliers		20.3%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
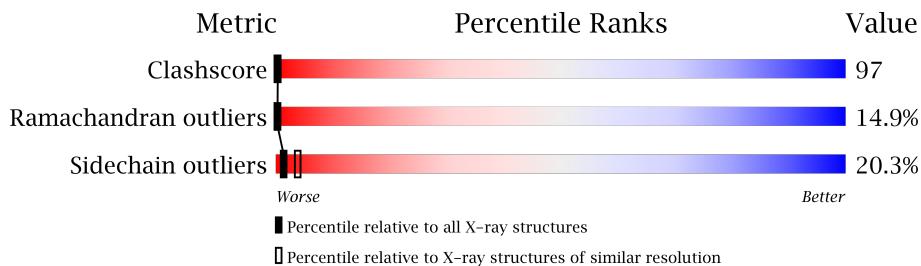
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	14% 55% 26% 5%
1	B	214	17% 57% 22% •
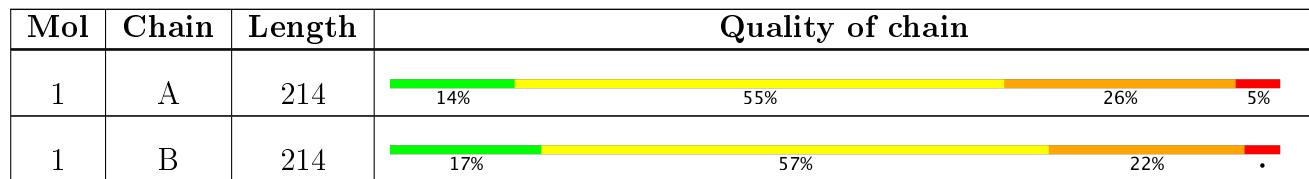
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PRP	A	312	-	-	X	-
4	PRP	B	314	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3490 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 PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBO SYLTRANSFERASE).

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1686	1076	282	318	10			
1	B	214	Total	C	N	O	S	0	0	0
			1686	1076	282	318	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	LYS	ENGINEERED	UNP P00492
A	102	GLY	LYS	CONFLICT	UNP P00492
B	68	ALA	LYS	ENGINEERED	UNP P00492
B	102	GLY	LYS	CONFLICT	UNP P00492

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3H-PYRAZOLO[4,3-D]PYRIMIDIN-7-OL (three-letter code: PPO) (formula: $C_5H_4N_4O$).

PPO
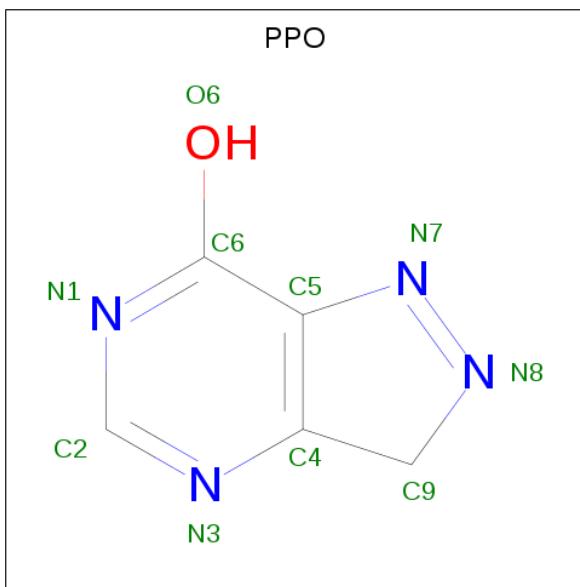
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	4	1		
3	B	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 4 is ALPHA-PHOSPHORIBOSYLPYROPHOSPHORIC ACID (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$).

PRP
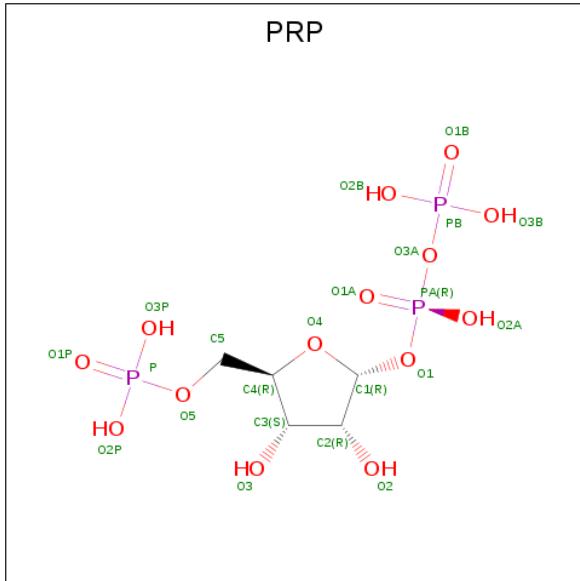
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			22	5	14	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	28	Total	O	0	0
			28	28		

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 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain A:

• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain B:
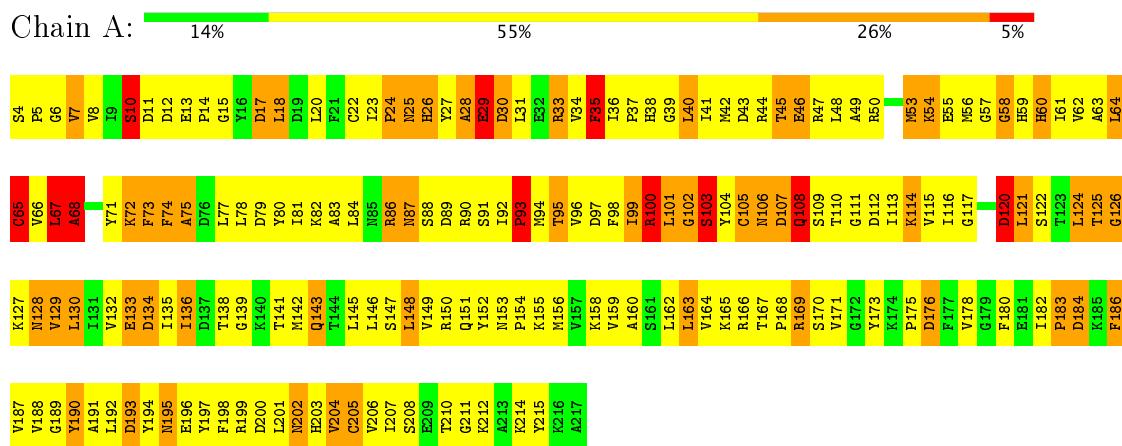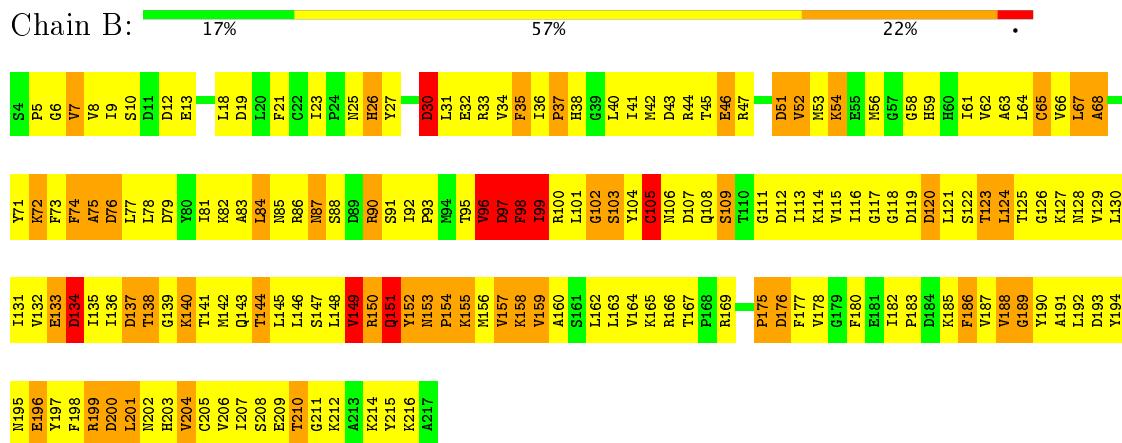
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	129.56Å 65.85Å 51.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.174 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3490	wwPDB-VP
Average B, all atoms (Å^2)	3.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PPO, PRP

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	0.60	1/1719 (0.1%)	1.05	19/2324 (0.8%)
1	B	0.92	6/1719 (0.3%)	1.43	19/2324 (0.8%)
All	All	0.77	7/3438 (0.2%)	1.25	38/4648 (0.8%)

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	7
1	B	0	5
All	All	0	12

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	CYS	CB-SG	-23.27	1.42	1.82
1	B	105	CYS	C-N	-13.68	1.02	1.34
1	B	109	SER	C-N	-8.09	1.15	1.34
1	B	151	GLN	CA-CB	-7.46	1.37	1.53
1	B	108	GLN	C-N	-6.47	1.19	1.34
1	A	105	CYS	C-N	6.03	1.48	1.34
1	B	133	GLU	C-N	-5.35	1.21	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	105	CYS	O-C-N	-28.23	77.53	122.70
1	B	97	ASP	CB-CG-OD2	17.88	134.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	ASP	CB-CG-OD1	-17.59	102.47	118.30
1	B	133	GLU	O-C-N	17.57	150.82	122.70
1	B	105	CYS	CA-C-N	14.19	148.41	117.20
1	B	133	GLU	CA-C-N	-13.95	86.50	117.20
1	B	133	GLU	C-N-CA	-13.26	88.56	121.70
1	B	109	SER	O-C-N	-12.99	101.92	122.70
1	B	105	CYS	C-N-CA	12.39	152.67	121.70
1	B	134	ASP	C-N-CA	11.23	149.77	121.70
1	A	108	GLN	C-N-CA	10.79	148.67	121.70
1	A	134	ASP	CA-CB-CG	10.41	136.30	113.40
1	B	134	ASP	CA-C-O	9.74	140.55	120.10
1	A	108	GLN	N-CA-CB	-9.53	93.45	110.60
1	A	103	SER	O-C-N	-8.44	109.19	122.70
1	B	134	ASP	O-C-N	-8.35	109.35	122.70
1	B	134	ASP	CB-CA-C	-8.10	94.20	110.40
1	A	67	LEU	CB-CA-C	8.05	125.50	110.20
1	A	108	GLN	CB-CA-C	8.02	126.44	110.40
1	A	106	ASN	CB-CA-C	7.47	125.34	110.40
1	A	100	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	150	ARG	N-CA-CB	-7.40	97.29	110.60
1	A	190	TYR	O-C-N	7.38	134.51	122.70
1	A	33	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	108	GLN	O-C-N	-7.23	111.12	122.70
1	B	109	SER	CA-C-N	6.87	132.31	117.20
1	B	109	SER	C-N-CA	6.67	138.38	121.70
1	A	65	CYS	CA-CB-SG	-6.35	102.58	114.00
1	A	190	TYR	CA-C-N	-5.79	104.47	117.20
1	A	109	SER	CB-CA-C	-5.66	99.35	110.10
1	A	103	SER	C-N-CA	5.48	135.41	121.70
1	B	151	GLN	N-CA-CB	5.48	120.47	110.60
1	A	67	LEU	O-C-N	-5.41	114.04	122.70
1	A	106	ASN	CA-CB-CG	5.34	125.14	113.40
1	A	190	TYR	C-N-CA	-5.30	108.44	121.70
1	A	100	ARG	CB-CA-C	5.30	120.99	110.40
1	B	109	SER	N-CA-CB	-5.17	102.74	110.50
1	B	98	PHE	CB-CG-CD2	-5.09	117.24	120.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	103	SER	Mainchain
1	A	108	GLN	Peptide
1	A	193	ASP	Mainchain
1	A	67	LEU	Peptide
1	A	68	ALA	Peptide
1	A	99	ILE	Mainchain
1	B	105	CYS	Mainchain,Peptide
1	B	109	SER	Mainchain,Peptide
1	B	149	VAL	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	1686	0	1687	350	0
1	B	1686	0	1684	333	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	3	1	0
3	B	10	0	3	1	0
4	A	22	0	6	14	0
4	B	22	0	7	7	0
5	A	24	0	0	4	0
5	B	28	0	0	8	0
All	All	3490	0	3390	663	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 97.

All (663) 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:64:LEU:CD2	1:A:124:LEU:HD21	1.50	1.41
1:A:65:CYS:SG	1:A:74:PHE:CD1	2.29	1.24
1:B:191:ALA:O	1:B:192:LEU:HD22	1.05	1.21
1:A:191:ALA:O	1:A:192:LEU:HD22	1.39	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:SG	1:A:132:VAL:HB	1.84	1.17
1:A:64:LEU:HD11	1:A:129:VAL:CG1	1.76	1.15
1:B:191:ALA:C	1:B:192:LEU:HD22	1.67	1.15
1:A:64:LEU:HD21	1:A:124:LEU:CD2	1.77	1.13
1:B:189:GLY:HA3	1:B:201:LEU:HD23	1.30	1.13
1:A:37:PRO:HD2	1:A:40:LEU:HD12	1.31	1.13
1:B:133:GLU:O	1:B:134:ASP:C	1.83	1.11
1:A:72:LYS:HZ2	1:B:82:LYS:HE2	1.16	1.11
1:A:64:LEU:HD22	1:A:124:LEU:HD21	1.33	1.11
1:A:129:VAL:HG12	1:A:130:LEU:H	1.16	1.10
1:B:191:ALA:O	1:B:192:LEU:CD2	1.99	1.09
1:A:64:LEU:HD21	1:A:124:LEU:HD21	1.13	1.09
1:A:63:ALA:HA	1:A:130:LEU:HB3	1.31	1.08
1:A:148:LEU:HA	1:A:151:GLN:HE21	1.10	1.08
1:B:160:ALA:HA	1:B:177:PHE:HB2	1.37	1.05
1:B:79:ASP:HA	1:B:82:LYS:HD3	1.35	1.04
1:B:67:LEU:HD23	1:B:68:ALA:H	1.15	1.04
1:B:64:LEU:CD1	1:B:97:ASP:HB3	1.89	1.03
1:A:27:TYR:CE2	1:A:198:PHE:HA	1.93	1.03
1:A:72:LYS:NZ	1:B:82:LYS:HE2	1.76	1.00
1:B:64:LEU:HD12	1:B:97:ASP:HB3	1.44	1.00
1:A:27:TYR:HE2	1:A:198:PHE:HA	1.26	0.97
1:B:142:MET:SD	1:B:145:LEU:HD23	2.04	0.97
1:B:207:ILE:HD12	1:B:212:LYS:HG2	1.46	0.97
1:B:85:ASN:ND2	1:B:92:ILE:HB	1.78	0.97
1:A:195:ASN:HD21	1:A:215:TYR:HB3	1.30	0.96
1:A:191:ALA:C	1:A:192:LEU:HD22	1.85	0.96
1:A:61:ILE:HG21	1:A:130:LEU:HD23	1.49	0.95
1:B:133:GLU:O	1:B:134:ASP:O	1.83	0.95
1:B:145:LEU:O	1:B:149:VAL:HG23	1.67	0.94
1:B:97:ASP:C	1:B:98:PHE:HD1	1.71	0.94
1:A:133:GLU:HG3	1:A:142:MET:CE	1.99	0.92
1:B:96:VAL:CG1	1:B:98:PHE:HE1	1.82	0.92
1:B:183:PRO:HB2	1:B:185:LYS:NZ	1.85	0.91
1:A:65:CYS:SG	1:A:74:PHE:CG	2.60	0.89
1:A:67:LEU:HG	1:A:99:ILE:O	1.73	0.89
1:A:68:ALA:O	4:A:312:PRP:PB	2.31	0.89
1:A:64:LEU:HD11	1:A:129:VAL:HG11	1.50	0.88
1:A:159:VAL:HB	1:A:176:ASP:H	1.37	0.88
1:A:65:CYS:O	1:A:99:ILE:HB	1.74	0.87
1:B:83:ALA:HA	1:B:86:ARG:NE	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TYR:HB2	5:B:912:HOH:O	1.74	0.87
1:B:38:HIS:H	1:B:203:HIS:HD2	1.21	0.86
1:A:65:CYS:SG	1:A:74:PHE:CE1	2.68	0.86
1:A:64:LEU:CD2	1:A:124:LEU:CD2	2.41	0.85
1:A:129:VAL:HG12	1:A:130:LEU:N	1.92	0.84
1:B:67:LEU:CD2	1:B:68:ALA:H	1.90	0.84
1:A:133:GLU:HG3	1:A:142:MET:HE2	1.59	0.84
1:B:126:GLY:O	1:B:127:LYS:HG3	1.78	0.84
1:A:100:ARG:HB3	1:A:117:GLY:O	1.78	0.84
1:B:100:ARG:HG3	1:B:102:GLY:H	1.43	0.83
1:A:67:LEU:HA	4:A:312:PRP:O3B	1.79	0.82
1:A:29:GLU:HB2	5:A:986:HOH:O	1.78	0.82
1:B:191:ALA:C	1:B:192:LEU:CD2	2.43	0.82
1:A:94:MET:O	1:B:196:GLU:HG3	1.79	0.82
1:B:35:PHE:HB3	1:B:36:ILE:HD12	1.59	0.82
1:B:96:VAL:HG11	1:B:98:PHE:HE1	1.42	0.81
1:B:183:PRO:HB2	1:B:185:LYS:HZ3	1.43	0.81
1:A:167:THR:OG1	1:A:168:PRO:HD2	1.80	0.81
1:B:149:VAL:HG12	1:B:149:VAL:O	1.79	0.81
1:A:125:THR:O	1:A:127:LYS:HG3	1.81	0.80
1:A:110:THR:HG22	1:A:111:GLY:N	1.96	0.80
1:A:198:PHE:HE1	1:A:207:ILE:HG23	1.47	0.79
1:A:110:THR:HG22	1:A:111:GLY:H	1.48	0.79
1:B:119:ASP:HB3	5:B:920:HOH:O	1.83	0.79
1:B:146:LEU:HA	1:B:149:VAL:HB	1.64	0.79
1:A:86:ARG:HD2	1:A:87:ASN:OD1	1.83	0.79
1:A:147:SER:HA	1:A:150:ARG:NH2	1.97	0.78
1:B:38:HIS:H	1:B:203:HIS:CD2	2.02	0.78
1:A:100:ARG:HD2	1:A:116:ILE:HB	1.66	0.78
1:A:127:LYS:N	1:A:155:LYS:H	1.81	0.78
1:B:199:ARG:NH1	1:B:199:ARG:HB3	1.99	0.78
1:A:82:LYS:NZ	1:B:72:LYS:HD3	1.99	0.78
1:B:100:ARG:HB3	1:B:117:GLY:C	2.05	0.77
1:B:199:ARG:HB3	1:B:199:ARG:HH11	1.47	0.77
1:B:23:ILE:O	1:B:23:ILE:HD12	1.84	0.77
1:B:97:ASP:C	1:B:98:PHE:CD1	2.58	0.77
1:A:6:GLY:HA3	1:A:44:ARG:NH2	2.00	0.77
1:A:64:LEU:HD11	1:A:129:VAL:HG12	1.66	0.76
1:A:6:GLY:O	1:A:8:VAL:HG13	1.84	0.76
1:B:18:LEU:CD1	1:B:31:LEU:HB3	2.16	0.76
1:A:128:ASN:N	1:A:128:ASN:HD22	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD13	1:B:97:ASP:HB3	1.66	0.76
1:B:146:LEU:O	1:B:150:ARG:HG3	1.86	0.76
1:A:148:LEU:HA	1:A:151:GLN:NE2	1.95	0.75
1:B:145:LEU:O	1:B:149:VAL:N	2.20	0.75
1:B:152:TYR:O	1:B:153:ASN:HB2	1.87	0.75
1:B:97:ASP:O	1:B:98:PHE:CD1	2.40	0.75
1:A:101:LEU:O	1:A:102:GLY:O	2.06	0.74
1:B:73:PHE:CE1	1:B:162:LEU:HB2	2.22	0.74
1:A:18:LEU:HD12	1:A:18:LEU:H	1.52	0.74
1:B:209:GLU:HA	1:B:212:LYS:HE3	1.68	0.74
1:A:100:ARG:HG2	1:A:102:GLY:H	1.53	0.74
1:B:96:VAL:HG11	1:B:98:PHE:CE1	2.22	0.74
1:A:129:VAL:CG1	1:A:130:LEU:H	1.98	0.74
1:B:123:THR:O	1:B:125:THR:N	2.20	0.73
1:A:202:ASN:H	1:A:202:ASN:ND2	1.86	0.73
1:B:72:LYS:HB3	1:B:191:ALA:HB2	1.69	0.73
1:B:147:SER:O	1:B:150:ARG:HB2	1.87	0.73
1:B:186:PHE:HD2	1:B:207:ILE:HD11	1.53	0.73
1:B:147:SER:HA	1:B:150:ARG:HD2	1.70	0.72
1:B:51:ASP:C	1:B:53:MET:H	1.93	0.72
1:B:96:VAL:CG1	1:B:98:PHE:CE1	2.69	0.72
1:A:63:ALA:HA	1:A:130:LEU:CB	2.16	0.72
1:B:188:VAL:HG21	1:B:198:PHE:CD2	2.24	0.72
1:A:196:GLU:OE1	1:B:95:THR:HA	1.89	0.72
1:B:34:VAL:HA	1:B:205:CYS:SG	2.29	0.72
1:B:190:TYR:O	1:B:192:LEU:HD23	1.90	0.72
1:B:36:ILE:HD12	1:B:36:ILE:N	2.05	0.72
1:B:85:ASN:HD21	1:B:92:ILE:HB	1.55	0.71
1:B:112:ASP:OD2	1:B:114:LYS:HG3	1.90	0.71
1:B:71:TYR:HE1	1:B:199:ARG:HH22	1.38	0.71
1:B:85:ASN:CG	1:B:92:ILE:HB	2.11	0.71
1:B:189:GLY:HA2	1:B:198:PHE:O	1.90	0.71
1:A:58:GLY:O	1:A:59:HIS:ND1	2.23	0.71
1:B:67:LEU:HD23	1:B:68:ALA:N	1.97	0.71
1:B:100:ARG:HG2	1:B:116:ILE:C	2.11	0.70
1:B:41:ILE:HG12	1:B:180:PHE:HE1	1.56	0.70
1:B:18:LEU:HD13	1:B:31:LEU:HB3	1.73	0.70
1:A:113:ILE:O	1:A:114:LYS:HD3	1.92	0.70
1:A:155:LYS:HD2	5:A:934:HOH:O	1.91	0.70
1:A:37:PRO:CD	1:A:40:LEU:HD12	2.18	0.70
1:B:142:MET:O	1:B:145:LEU:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HE2	1:B:71:TYR:OH	1.90	0.69
1:A:30:ASP:HB3	1:A:198:PHE:HZ	1.57	0.69
1:A:6:GLY:HA3	1:A:44:ARG:HH21	1.56	0.69
1:B:38:HIS:CD2	1:B:202:ASN:HB3	2.28	0.69
1:B:99:ILE:HG13	1:B:118:GLY:O	1.93	0.69
1:A:66:VAL:HB	5:A:989:HOH:O	1.92	0.69
1:B:31:LEU:HD11	1:B:201:LEU:CD1	2.23	0.69
1:A:61:ILE:HG13	1:A:128:ASN:HB2	1.75	0.69
1:A:159:VAL:HG12	1:A:160:ALA:H	1.55	0.69
1:A:167:THR:HB	1:A:184:ASP:OD1	1.93	0.69
1:B:189:GLY:HA3	1:B:201:LEU:CD2	2.17	0.69
1:B:18:LEU:HD23	1:B:34:VAL:HG23	1.73	0.69
1:B:85:ASN:OD1	1:B:92:ILE:HD12	1.92	0.69
1:A:113:ILE:C	1:A:114:LYS:HD3	2.13	0.69
1:A:13:GLU:OE2	1:A:14:PRO:HD2	1.93	0.69
1:B:62:VAL:HG22	1:B:95:THR:HG23	1.75	0.69
1:B:36:ILE:HG21	1:B:180:PHE:CE1	2.29	0.68
1:B:52:VAL:O	1:B:52:VAL:HG12	1.91	0.68
1:A:121:LEU:HD22	1:A:148:LEU:HD23	1.75	0.68
1:A:60:HIS:C	1:A:61:ILE:HD12	2.13	0.68
1:B:35:PHE:HB3	1:B:36:ILE:CD1	2.23	0.68
1:B:200:ASP:OD2	1:B:200:ASP:N	2.26	0.68
1:A:39:GLY:O	1:A:41:ILE:N	2.26	0.68
1:A:214:LYS:HG3	1:A:215:TYR:CE1	2.28	0.68
1:A:7:VAL:HB	1:A:180:PHE:CD2	2.28	0.68
1:B:135:ILE:HA	1:B:163:LEU:O	1.94	0.68
1:A:159:VAL:HG12	1:A:160:ALA:N	2.08	0.67
1:A:201:LEU:HD12	1:A:203:HIS:H	1.59	0.67
1:B:134:ASP:CG	1:B:135:ILE:N	2.45	0.67
1:B:71:TYR:O	1:B:74:PHE:HB3	1.94	0.67
1:B:100:ARG:H	1:B:118:GLY:HA3	1.60	0.67
1:A:45:THR:HA	1:A:48:LEU:HD13	1.77	0.67
1:A:63:ALA:HB2	5:A:952:HOH:O	1.94	0.66
1:B:7:VAL:HG23	1:B:44:ARG:HH11	1.60	0.66
1:A:186:PHE:HD2	1:A:207:ILE:CD1	2.06	0.66
1:A:53:MET:SD	1:A:92:ILE:HD11	2.35	0.66
1:B:131:ILE:HG22	1:B:132:VAL:N	2.11	0.66
1:A:196:GLU:HG3	1:B:95:THR:HB	1.76	0.66
1:B:214:LYS:HD3	1:B:215:TYR:CZ	2.30	0.66
1:B:62:VAL:HG22	1:B:95:THR:CG2	2.26	0.66
1:B:107:ASP:HA	1:B:186:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:314:PRP:O3B	4:B:314:PRP:O2A	2.14	0.66
1:B:74:PHE:CE1	1:B:78:LEU:HD22	2.31	0.65
1:A:126:GLY:C	1:A:155:LYS:HB2	2.15	0.65
1:A:162:LEU:HG	1:A:163:LEU:HD23	1.78	0.65
1:A:89:ASP:O	1:A:90:ARG:HD2	1.95	0.65
1:A:62:VAL:HA	1:A:95:THR:HG23	1.78	0.65
1:A:189:GLY:O	1:A:204:VAL:HG22	1.96	0.65
1:A:48:LEU:H	1:A:48:LEU:HD12	1.61	0.65
1:A:101:LEU:HA	1:A:115:VAL:HG22	1.78	0.65
1:B:7:VAL:HB	1:B:180:PHE:HA	1.79	0.65
1:B:41:ILE:HA	1:B:180:PHE:CZ	2.32	0.64
1:A:64:LEU:HD21	1:A:124:LEU:CG	2.27	0.64
1:A:124:LEU:O	1:A:154:PRO:HB3	1.97	0.64
1:A:74:PHE:CE1	1:A:78:LEU:HD11	2.33	0.64
1:B:121:LEU:HD23	1:B:124:LEU:HD22	1.78	0.64
1:B:113:ILE:HG21	1:B:144:THR:OG1	1.98	0.64
1:B:135:ILE:HG12	1:B:136:ILE:N	2.12	0.64
1:B:183:PRO:HB2	1:B:185:LYS:HZ1	1.62	0.64
1:A:190:TYR:O	1:A:191:ALA:HB3	1.96	0.64
1:B:77:LEU:O	1:B:81:ILE:HG13	1.96	0.63
1:A:110:THR:CG2	1:A:111:GLY:H	2.10	0.63
1:A:31:LEU:C	1:A:208:SER:HB3	2.18	0.63
1:B:188:VAL:HG23	1:B:201:LEU:HD22	1.80	0.63
1:A:104:TYR:CD2	1:A:105:CYS:N	2.67	0.63
1:A:98:PHE:CG	1:B:67:LEU:HD11	2.33	0.63
1:A:101:LEU:O	1:A:101:LEU:HG	1.99	0.63
1:B:41:ILE:HA	1:B:180:PHE:HZ	1.63	0.63
1:B:53:MET:SD	1:B:84:LEU:HD22	2.39	0.62
1:B:96:VAL:HG12	1:B:98:PHE:HE1	1.63	0.62
1:B:113:ILE:N	1:B:113:ILE:HD12	2.13	0.62
1:B:96:VAL:HG12	1:B:98:PHE:CE1	2.35	0.62
1:A:57:GLY:O	1:A:59:HIS:N	2.33	0.62
1:A:83:ALA:HB1	1:A:87:ASN:ND2	2.14	0.62
1:B:131:ILE:HD12	1:B:131:ILE:N	2.14	0.62
1:A:110:THR:CG2	1:A:111:GLY:N	2.62	0.62
1:A:103:SER:OG	4:A:312:PRP:O2A	2.16	0.62
1:B:113:ILE:HG21	1:B:144:THR:HG21	1.82	0.62
1:A:124:LEU:HD23	1:A:129:VAL:CG1	2.30	0.62
1:A:159:VAL:HG23	1:A:176:ASP:OD1	2.00	0.62
1:B:83:ALA:O	1:B:86:ARG:HG2	2.00	0.62
1:B:37:PRO:HB2	1:B:40:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:PHE:CD2	1:B:207:ILE:HD11	2.35	0.61
1:A:23:ILE:HD12	1:A:23:ILE:O	1.99	0.61
1:A:59:HIS:HB2	1:A:61:ILE:CD1	2.30	0.61
1:B:104:TYR:O	1:B:104:TYR:CD1	2.54	0.61
1:B:159:VAL:HG13	1:B:159:VAL:O	2.01	0.61
1:B:7:VAL:O	1:B:9:ILE:HG13	1.99	0.60
1:A:107:ASP:O	1:A:108:GLN:HB2	2.00	0.60
1:B:119:ASP:OD1	1:B:119:ASP:O	2.18	0.60
1:B:66:VAL:HB	1:B:133:GLU:HG3	1.83	0.60
1:A:40:LEU:O	1:A:44:ARG:HB2	2.01	0.60
1:A:67:LEU:CA	4:A:312:PRP:O3B	2.50	0.60
1:B:97:ASP:O	1:B:98:PHE:HD1	1.81	0.60
1:B:126:GLY:C	1:B:127:LYS:HG3	2.21	0.60
1:A:73:PHE:CE1	1:A:162:LEU:HD13	2.36	0.60
1:B:180:PHE:O	1:B:182:ILE:HG23	2.02	0.60
1:B:18:LEU:HD11	1:B:31:LEU:HB3	1.84	0.59
1:A:214:LYS:O	1:A:215:TYR:CD1	2.55	0.59
1:B:159:VAL:HG12	1:B:176:ASP:OD1	2.02	0.59
1:B:66:VAL:HB	1:B:133:GLU:CG	2.32	0.59
1:A:120:ASP:O	1:A:122:SER:N	2.32	0.59
1:A:7:VAL:O	1:A:180:PHE:HA	2.03	0.59
1:B:144:THR:O	1:B:148:LEU:HD12	2.03	0.59
1:A:29:GLU:N	1:A:29:GLU:OE2	2.36	0.59
1:B:103:SER:HB2	4:B:314:PRP:O1A	2.02	0.59
1:A:193:ASP:O	3:A:300:PPO:HC2	2.03	0.59
1:A:122:SER:HA	1:A:152:TYR:CE2	2.38	0.58
1:A:135:ILE:HG23	4:A:312:PRP:H2	1.84	0.58
1:A:191:ALA:C	1:A:192:LEU:CD2	2.68	0.58
1:A:54:LYS:O	1:A:55:GLU:C	2.42	0.58
1:B:112:ASP:C	1:B:113:ILE:HD12	2.24	0.58
1:A:18:LEU:CD2	1:A:31:LEU:HB2	2.34	0.58
1:B:188:VAL:O	1:B:204:VAL:HA	2.03	0.58
1:B:197:TYR:CE1	5:B:908:HOH:O	2.52	0.58
1:B:72:LYS:CB	1:B:191:ALA:HB2	2.34	0.58
1:A:100:ARG:HD2	1:A:116:ILE:CB	2.33	0.58
1:A:210:THR:OG1	1:A:211:GLY:N	2.37	0.58
1:A:41:ILE:O	1:A:42:MET:C	2.42	0.58
1:A:46:GLU:HA	1:A:80:TYR:CD2	2.39	0.58
1:B:18:LEU:HD11	1:B:31:LEU:C	2.24	0.57
1:A:83:ALA:O	1:A:86:ARG:HG3	2.03	0.57
1:A:67:LEU:CG	1:A:99:ILE:O	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:C	1:B:139:GLY:H	2.08	0.57
1:A:47:ARG:O	1:A:50:ARG:N	2.37	0.57
1:A:100:ARG:HD2	1:A:116:ILE:C	2.25	0.57
1:A:25:ASN:O	1:A:28:ALA:N	2.35	0.57
1:A:103:SER:HB3	4:A:312:PRP:O1A	2.04	0.57
1:A:133:GLU:OE2	4:A:312:PRP:H3	2.04	0.57
1:A:171:VAL:HG12	1:A:173:TYR:H	1.70	0.57
1:A:36:ILE:HD13	1:A:180:PHE:CE2	2.40	0.57
1:A:186:PHE:HB3	1:A:207:ILE:HD12	1.86	0.57
1:A:46:GLU:HB2	1:A:80:TYR:CZ	2.39	0.57
1:A:6:GLY:O	1:A:7:VAL:C	2.43	0.57
1:A:79:ASP:HA	1:A:82:LYS:HD2	1.85	0.57
1:A:100:ARG:HG2	1:A:102:GLY:N	2.19	0.57
1:A:126:GLY:O	1:A:155:LYS:HE3	2.04	0.57
1:A:198:PHE:CE1	1:A:207:ILE:HG23	2.36	0.57
1:A:195:ASN:ND2	1:A:215:TYR:HB3	2.12	0.57
1:A:86:ARG:CD	1:A:87:ASN:OD1	2.52	0.57
1:B:31:LEU:HD11	1:B:201:LEU:HD11	1.86	0.57
1:A:83:ALA:HB1	1:A:87:ASN:HD21	1.70	0.56
1:B:116:ILE:HG22	1:B:116:ILE:O	2.05	0.56
1:B:121:LEU:HD23	1:B:124:LEU:CD2	2.35	0.56
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.70	0.56
1:A:92:ILE:O	1:A:93:PRO:C	2.41	0.56
1:B:149:VAL:C	1:B:150:ARG:HG3	2.26	0.56
1:A:59:HIS:HB2	1:A:61:ILE:HD11	1.87	0.56
1:A:101:LEU:HD22	1:A:145:LEU:HB2	1.86	0.56
1:B:120:ASP:C	1:B:121:LEU:HD12	2.25	0.56
1:A:165:LYS:HG3	1:A:183:PRO:O	2.05	0.56
1:A:208:SER:O	1:A:212:LYS:HB2	2.05	0.56
1:A:67:LEU:C	1:A:67:LEU:HD12	2.26	0.56
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.71	0.56
1:A:124:LEU:HB3	1:A:129:VAL:HG22	1.88	0.56
1:B:192:LEU:CD2	1:B:192:LEU:N	2.68	0.56
1:B:36:ILE:HG22	1:B:41:ILE:HG13	1.87	0.56
1:B:144:THR:C	1:B:148:LEU:HD12	2.25	0.56
1:B:138:THR:N	4:B:314:PRP:O1P	2.38	0.56
1:A:100:ARG:CD	1:A:116:ILE:HB	2.35	0.56
1:B:25:ASN:C	1:B:27:TYR:H	2.09	0.56
1:A:39:GLY:C	1:A:41:ILE:N	2.58	0.56
1:B:100:ARG:HG2	1:B:116:ILE:O	2.06	0.56
1:A:29:GLU:OE2	1:A:30:ASP:OD1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:157:VAL:HA	2.06	0.56
1:A:82:LYS:HZ3	1:B:72:LYS:HD3	1.68	0.56
1:B:113:ILE:HG21	1:B:144:THR:CB	2.36	0.55
1:B:51:ASP:C	1:B:53:MET:N	2.60	0.55
1:A:18:LEU:HB3	1:A:23:ILE:HG12	1.88	0.55
1:B:131:ILE:HG22	1:B:132:VAL:H	1.71	0.55
1:B:67:LEU:O	1:B:68:ALA:HB3	2.05	0.55
1:A:105:CYS:O	1:A:106:ASN:ND2	2.38	0.55
1:A:124:LEU:HD23	1:A:129:VAL:HG11	1.88	0.55
1:B:35:PHE:C	1:B:36:ILE:HD12	2.27	0.55
1:A:100:ARG:CZ	1:A:116:ILE:O	2.54	0.55
1:A:162:LEU:HG	1:A:163:LEU:CD2	2.36	0.55
1:B:65:CYS:O	1:B:99:ILE:HG23	2.06	0.55
1:A:72:LYS:NZ	1:B:82:LYS:CE	2.61	0.55
1:B:38:HIS:N	1:B:203:HIS:HD2	1.97	0.55
1:B:41:ILE:HG21	1:B:190:TYR:CE2	2.41	0.55
1:B:86:ARG:HG2	1:B:87:ASN:H	1.72	0.55
1:A:204:VAL:O	1:A:204:VAL:HG12	2.07	0.55
1:A:178:VAL:CG1	1:A:180:PHE:O	2.55	0.55
1:B:187:VAL:HB	1:B:204:VAL:HG12	1.89	0.55
1:A:82:LYS:HZ2	1:B:72:LYS:HD3	1.69	0.55
1:A:147:SER:HA	1:A:150:ARG:HH22	1.71	0.54
1:B:32:GLU:HG3	1:B:33:ARG:HG3	1.89	0.54
1:B:103:SER:CB	4:B:314:PRP:O1A	2.56	0.54
1:A:167:THR:CG2	1:A:170:SER:HB3	2.37	0.54
1:B:164:VAL:HG21	1:B:178:VAL:CG2	2.37	0.54
1:A:159:VAL:HB	1:A:176:ASP:N	2.16	0.54
1:A:28:ALA:O	1:A:30:ASP:N	2.41	0.54
1:A:45:THR:O	1:A:48:LEU:N	2.40	0.54
1:B:148:LEU:C	1:B:150:ARG:H	2.10	0.54
1:B:71:TYR:CG	1:B:72:LYS:N	2.76	0.54
1:A:67:LEU:C	4:A:312:PRP:O3B	2.46	0.54
1:A:53:MET:O	1:A:56:MET:O	2.25	0.54
1:B:100:ARG:HG3	1:B:101:LEU:N	2.22	0.54
1:B:35:PHE:CD1	1:B:206:VAL:HG23	2.43	0.54
1:B:62:VAL:O	1:B:130:LEU:HD23	2.08	0.54
1:B:103:SER:C	1:B:105:CYS:H	2.11	0.53
1:B:199:ARG:CB	1:B:199:ARG:HH11	2.21	0.53
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.73	0.53
1:B:72:LYS:HB3	1:B:191:ALA:CB	2.37	0.53
1:A:168:PRO:HG2	1:A:169:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:O	1:A:81:ILE:HB	2.09	0.53
1:B:127:LYS:C	1:B:155:LYS:HB3	2.28	0.53
1:B:76:ASP:O	1:B:79:ASP:N	2.42	0.53
1:A:58:GLY:C	1:A:59:HIS:ND1	2.61	0.53
1:A:72:LYS:O	1:A:75:ALA:N	2.42	0.53
1:B:92:ILE:N	1:B:93:PRO:HD3	2.23	0.53
1:A:6:GLY:O	1:A:8:VAL:N	2.41	0.53
1:A:164:VAL:HG23	1:A:178:VAL:HG13	1.88	0.53
1:B:149:VAL:HG11	1:B:157:VAL:HG11	1.89	0.53
1:A:86:ARG:CZ	1:B:202:ASN:HD21	2.22	0.53
1:B:138:THR:OG1	1:B:140:LYS:HB2	2.09	0.53
1:A:125:THR:O	1:A:127:LYS:N	2.42	0.53
1:A:139:GLY:O	1:A:143:GLN:HB2	2.09	0.53
1:B:137:ASP:CG	1:B:138:THR:H	2.11	0.53
1:B:140:LYS:HE3	5:B:949:HOH:O	2.08	0.53
1:B:134:ASP:OD1	1:B:135:ILE:O	2.26	0.53
1:A:71:TYR:HB3	1:B:98:PHE:HZ	1.73	0.53
1:B:100:ARG:HD2	1:B:102:GLY:HA2	1.90	0.53
1:A:74:PHE:O	1:A:75:ALA:C	2.47	0.52
1:B:63:ALA:HA	1:B:130:LEU:CD2	2.39	0.52
1:B:127:LYS:O	1:B:155:LYS:HB3	2.09	0.52
1:A:201:LEU:HD11	1:A:203:HIS:HB2	1.90	0.52
1:B:36:ILE:CD1	1:B:36:ILE:N	2.72	0.52
1:A:72:LYS:O	1:A:73:PHE:C	2.47	0.52
1:A:74:PHE:O	1:A:77:LEU:N	2.43	0.52
1:A:73:PHE:CE2	1:A:162:LEU:HB2	2.45	0.52
1:A:67:LEU:HD12	1:A:68:ALA:N	2.24	0.52
1:B:124:LEU:HG	1:B:129:VAL:HG21	1.92	0.52
1:B:41:ILE:HD11	1:B:204:VAL:HG23	1.90	0.52
1:A:128:ASN:N	1:A:128:ASN:ND2	2.55	0.52
1:A:37:PRO:HD2	1:A:40:LEU:CD1	2.22	0.52
1:B:138:THR:HG22	1:B:169:ARG:HB2	1.92	0.52
1:B:63:ALA:HA	1:B:130:LEU:HD21	1.91	0.52
1:A:61:ILE:HG23	1:A:128:ASN:O	2.10	0.52
1:A:201:LEU:HD11	1:A:205:CYS:SG	2.50	0.52
1:A:39:GLY:C	1:A:41:ILE:H	2.12	0.52
1:A:188:VAL:CG2	1:A:207:ILE:HG12	2.39	0.52
1:B:75:ALA:O	1:B:78:LEU:N	2.43	0.52
1:B:45:THR:O	1:B:47:ARG:N	2.44	0.51
1:B:101:LEU:HD22	1:B:145:LEU:HD13	1.92	0.51
1:B:41:ILE:HD11	1:B:204:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE2	4:A:312:PRP:O3	2.28	0.51
1:A:188:VAL:HG13	1:A:207:ILE:HD11	1.91	0.51
1:A:24:PRO:HG3	1:B:86:ARG:CB	2.40	0.51
1:B:195:ASN:O	1:B:195:ASN:CG	2.49	0.51
1:B:175:PRO:O	1:B:176:ASP:CG	2.49	0.51
1:B:25:ASN:O	1:B:27:TYR:N	2.44	0.51
1:B:54:LYS:HD3	5:B:903:HOH:O	2.11	0.51
1:A:100:ARG:HD2	1:A:116:ILE:CA	2.41	0.51
1:B:122:SER:HA	1:B:152:TYR:CE1	2.46	0.51
1:B:134:ASP:OD1	1:B:135:ILE:N	2.44	0.51
1:B:158:LYS:O	1:B:159:VAL:HB	2.11	0.51
1:B:27:TYR:HA	1:B:30:ASP:OD2	2.10	0.51
1:A:133:GLU:CD	4:A:312:PRP:O3	2.49	0.51
1:A:146:LEU:HG	1:A:150:ARG:NH1	2.26	0.51
1:A:64:LEU:HB2	1:A:99:ILE:CD1	2.41	0.50
1:B:113:ILE:HG21	1:B:144:THR:CG2	2.41	0.50
1:B:127:LYS:O	1:B:155:LYS:N	2.43	0.50
1:B:140:LYS:O	1:B:143:GLN:HB2	2.11	0.50
3:B:301:PPO:C2	4:B:314:PRP:O2A	2.59	0.50
1:B:43:ASP:HA	1:B:46:GLU:HB3	1.93	0.50
1:A:45:THR:O	1:A:47:ARG:N	2.45	0.50
1:B:166:ARG:HH22	1:B:183:PRO:HG3	1.77	0.50
1:B:18:LEU:HD23	1:B:34:VAL:CG2	2.41	0.50
1:A:186:PHE:O	1:A:207:ILE:HG13	2.11	0.50
1:B:125:THR:HA	1:B:153:ASN:O	2.11	0.50
1:B:67:LEU:O	1:B:68:ALA:CB	2.59	0.50
1:A:126:GLY:O	1:A:155:LYS:HB2	2.12	0.50
1:A:71:TYR:CG	1:A:72:LYS:N	2.79	0.50
1:B:37:PRO:HD2	1:B:40:LEU:CD1	2.42	0.50
1:A:104:TYR:HD2	1:A:105:CYS:N	2.07	0.50
1:A:145:LEU:O	1:A:145:LEU:HD22	2.11	0.50
1:A:146:LEU:HD21	1:A:173:TYR:OH	2.11	0.50
1:A:190:TYR:CD2	1:A:190:TYR:O	2.65	0.50
1:B:130:LEU:HD23	1:B:130:LEU:H	1.77	0.50
1:B:135:ILE:HG12	1:B:136:ILE:H	1.77	0.50
1:B:75:ALA:O	1:B:76:ASP:C	2.50	0.50
1:B:144:THR:O	1:B:147:SER:HB3	2.12	0.49
1:B:166:ARG:NH2	1:B:183:PRO:HG3	2.27	0.49
1:B:23:ILE:HD12	1:B:23:ILE:C	2.31	0.49
1:A:27:TYR:CE2	1:A:198:PHE:HD2	2.30	0.49
1:A:63:ALA:O	1:A:96:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HB	1:B:129:VAL:HG22	1.94	0.49
1:A:29:GLU:OE2	1:A:30:ASP:N	2.44	0.49
1:B:131:ILE:CG2	1:B:132:VAL:N	2.76	0.49
1:B:41:ILE:HG21	1:B:190:TYR:HE2	1.78	0.49
1:A:82:LYS:HZ3	1:B:71:TYR:HE2	1.61	0.49
1:B:146:LEU:CA	1:B:149:VAL:HB	2.38	0.49
1:B:10:SER:C	1:B:12:ASP:H	2.15	0.49
1:B:18:LEU:HD23	1:B:34:VAL:N	2.27	0.49
1:A:186:PHE:HD2	1:A:207:ILE:HD12	1.74	0.49
1:B:100:ARG:CG	1:B:102:GLY:H	2.19	0.49
1:B:35:PHE:HB2	1:B:204:VAL:O	2.13	0.49
1:B:61:ILE:HG22	1:B:62:VAL:N	2.27	0.49
1:B:83:ALA:HA	1:B:86:ARG:CZ	2.43	0.49
1:A:167:THR:HG1	1:A:168:PRO:HD2	1.74	0.48
1:A:188:VAL:HG21	1:A:207:ILE:HG12	1.93	0.48
1:B:100:ARG:HB3	1:B:117:GLY:O	2.13	0.48
1:B:113:ILE:HD11	1:B:140:LYS:HG2	1.94	0.48
1:B:73:PHE:CD1	1:B:162:LEU:HB2	2.48	0.48
1:A:124:LEU:CD1	1:A:124:LEU:N	2.76	0.48
1:A:165:LYS:HA	1:A:182:ILE:O	2.13	0.48
1:A:133:GLU:OE2	4:A:312:PRP:C3	2.61	0.48
1:A:35:PHE:HE2	1:A:182:ILE:HB	1.77	0.48
1:B:132:VAL:O	1:B:133:GLU:HG3	2.13	0.48
1:B:137:ASP:O	1:B:139:GLY:N	2.46	0.48
1:B:164:VAL:HG21	1:B:178:VAL:HG21	1.93	0.48
1:A:192:LEU:HD22	1:A:192:LEU:N	2.27	0.48
1:A:92:ILE:O	1:A:93:PRO:O	2.30	0.48
1:B:208:SER:C	1:B:210:THR:N	2.66	0.48
1:B:138:THR:OG1	1:B:140:LYS:HE2	2.13	0.48
1:B:206:VAL:HG12	1:B:207:ILE:O	2.13	0.48
1:A:38:HIS:ND1	1:A:202:ASN:HB3	2.29	0.48
1:B:145:LEU:C	1:B:149:VAL:HG23	2.32	0.48
1:A:41:ILE:O	1:A:44:ARG:N	2.47	0.48
1:A:75:ALA:O	1:A:78:LEU:HB2	2.14	0.48
1:B:131:ILE:HG21	1:B:142:MET:CE	2.44	0.48
1:A:116:ILE:O	1:A:116:ILE:HG22	2.15	0.47
1:A:146:LEU:O	1:A:150:ARG:NH1	2.47	0.47
1:A:63:ALA:HB3	1:A:96:VAL:HG12	1.95	0.47
1:B:7:VAL:HG21	1:B:180:PHE:CD2	2.49	0.47
1:B:62:VAL:HG21	1:B:127:LYS:HE3	1.96	0.47
1:B:51:ASP:O	1:B:53:MET:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:CG1	1:A:160:ALA:H	2.25	0.47
1:A:195:ASN:HD21	1:A:215:TYR:CB	2.13	0.47
1:A:60:HIS:N	1:A:60:HIS:ND1	2.61	0.47
1:B:147:SER:O	1:B:150:ARG:N	2.46	0.47
1:A:166:ARG:HH11	1:A:166:ARG:HG3	1.79	0.47
1:A:210:THR:C	1:A:212:LYS:N	2.67	0.47
1:A:141:THR:O	1:A:142:MET:C	2.53	0.47
1:A:26:HIS:O	1:A:29:GLU:OE2	2.33	0.47
1:A:57:GLY:N	1:A:59:HIS:NE2	2.62	0.47
1:B:101:LEU:CD2	1:B:145:LEU:HB2	2.45	0.47
1:B:149:VAL:O	1:B:149:VAL:CG1	2.47	0.47
1:B:58:GLY:HA2	1:B:90:ARG:CZ	2.45	0.47
1:A:147:SER:HA	1:A:150:ARG:CZ	2.43	0.47
1:B:21:PHE:HD1	1:B:34:VAL:HG21	1.78	0.47
1:A:74:PHE:HD1	1:A:132:VAL:HG21	1.80	0.46
1:A:146:LEU:HG	1:A:150:ARG:HH11	1.79	0.46
1:B:134:ASP:OD1	1:B:135:ILE:C	2.54	0.46
1:A:40:LEU:O	1:A:44:ARG:CB	2.63	0.46
1:B:43:ASP:O	1:B:46:GLU:HB3	2.14	0.46
1:A:66:VAL:HG13	1:A:100:ARG:O	2.15	0.46
1:A:128:ASN:HD22	1:A:155:LYS:HB3	1.79	0.46
1:A:210:THR:C	1:A:212:LYS:H	2.19	0.46
1:A:18:LEU:O	1:A:23:ILE:HD11	2.16	0.46
1:A:11:ASP:C	1:A:13:GLU:H	2.18	0.46
1:A:159:VAL:CG1	1:A:160:ALA:N	2.78	0.46
1:A:199:ARG:HG3	1:A:200:ASP:N	2.29	0.46
1:B:208:SER:HB3	1:B:210:THR:HG23	1.96	0.46
1:A:68:ALA:O	4:A:312:PRP:O3A	2.34	0.46
1:B:165:LYS:C	1:B:167:THR:H	2.18	0.46
1:A:68:ALA:C	4:A:312:PRP:O3B	2.53	0.46
1:A:64:LEU:HB2	1:A:99:ILE:HD12	1.97	0.46
1:B:211:GLY:O	1:B:212:LYS:C	2.54	0.46
1:B:82:LYS:O	1:B:85:ASN:HB2	2.16	0.46
1:B:81:ILE:O	1:B:85:ASN:OD1	2.34	0.46
1:B:96:VAL:HG12	1:B:97:ASP:H	1.81	0.46
1:A:149:VAL:O	1:A:154:PRO:HD3	2.16	0.46
1:A:156:MET:CE	1:A:158:LYS:NZ	2.78	0.46
1:A:24:PRO:HG3	1:B:86:ARG:HB3	1.97	0.46
1:B:101:LEU:O	1:B:101:LEU:HG	2.16	0.46
1:A:44:ARG:O	1:A:47:ARG:HB3	2.16	0.46
1:A:45:THR:HG22	1:A:46:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:O	1:A:48:LEU:C	2.53	0.46
1:B:12:ASP:O	1:B:13:GLU:C	2.53	0.46
1:B:56:MET:HE2	1:B:61:ILE:HD12	1.98	0.46
1:A:156:MET:CG	1:A:158:LYS:HZ3	2.30	0.45
1:B:52:VAL:O	1:B:52:VAL:CG1	2.63	0.45
1:A:62:VAL:HG12	1:A:64:LEU:HD23	1.98	0.45
1:B:121:LEU:O	1:B:124:LEU:HB2	2.16	0.45
1:A:192:LEU:CD2	1:A:192:LEU:N	2.80	0.45
1:A:211:GLY:HA2	1:A:214:LYS:CB	2.47	0.45
1:A:41:ILE:O	1:A:43:ASP:N	2.50	0.45
1:B:140:LYS:HB3	4:B:314:PRP:O3P	2.16	0.45
1:A:30:ASP:HB3	1:A:198:PHE:CZ	2.45	0.45
1:B:45:THR:C	1:B:47:ARG:N	2.67	0.45
1:B:59:HIS:O	1:B:61:ILE:HG12	2.17	0.45
1:A:128:ASN:HA	1:A:156:MET:O	2.16	0.45
1:A:61:ILE:HG13	1:A:128:ASN:O	2.16	0.45
1:A:156:MET:CE	1:A:158:LYS:HZ3	2.28	0.45
1:A:194:TYR:O	1:A:195:ASN:C	2.55	0.45
1:A:79:ASP:HA	1:A:82:LYS:CD	2.47	0.45
1:A:82:LYS:NZ	1:B:72:LYS:CD	2.76	0.45
1:B:194:TYR:O	1:B:195:ASN:OD1	2.35	0.45
1:A:186:PHE:CD2	1:A:207:ILE:HD12	2.52	0.45
1:A:38:HIS:HB2	1:A:203:HIS:HD2	1.81	0.45
1:B:131:ILE:CD1	1:B:131:ILE:N	2.79	0.45
1:A:77:LEU:O	1:A:81:ILE:HG13	2.17	0.45
1:B:113:ILE:HA	1:B:141:THR:HG22	1.99	0.45
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.31	0.45
1:A:206:VAL:HG12	1:A:207:ILE:N	2.32	0.45
1:B:131:ILE:HD11	1:B:157:VAL:HG13	1.98	0.45
1:A:167:THR:OG1	1:A:168:PRO:CD	2.58	0.45
1:A:187:VAL:HB	1:A:204:VAL:HG12	1.98	0.45
1:A:26:HIS:CD2	1:A:27:TYR:HD1	2.35	0.45
1:B:137:ASP:C	1:B:139:GLY:N	2.69	0.45
1:B:197:TYR:O	1:B:198:PHE:HB2	2.17	0.45
1:A:10:SER:HB3	1:A:11:ASP:H	1.54	0.44
1:A:121:LEU:O	1:A:152:TYR:CD1	2.70	0.44
1:A:203:HIS:O	1:A:205:CYS:N	2.44	0.44
1:A:57:GLY:N	1:A:59:HIS:CD2	2.86	0.44
1:A:98:PHE:CD1	1:B:67:LEU:HD11	2.51	0.44
1:B:91:SER:C	1:B:92:ILE:HG13	2.37	0.44
1:A:176:ASP:N	1:A:176:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:O	1:B:157:VAL:HG12	2.17	0.44
1:A:201:LEU:HD21	1:A:205:CYS:SG	2.58	0.44
1:A:62:VAL:HG22	1:A:95:THR:HG21	1.98	0.44
1:B:37:PRO:O	1:B:40:LEU:HB3	2.17	0.44
1:B:6:GLY:O	1:B:8:VAL:N	2.50	0.44
1:A:44:ARG:O	1:A:45:THR:C	2.54	0.44
1:A:24:PRO:HB2	1:A:27:TYR:HB2	1.99	0.44
1:B:147:SER:O	1:B:150:ARG:CB	2.61	0.44
1:A:99:ILE:HG22	1:A:100:ARG:N	2.32	0.44
1:B:115:VAL:C	1:B:116:ILE:HG12	2.38	0.44
1:B:148:LEU:C	1:B:150:ARG:N	2.71	0.44
1:B:156:MET:CE	1:B:158:LYS:HE2	2.48	0.44
1:A:107:ASP:HB3	1:A:108:GLN:OE1	2.18	0.44
1:A:41:ILE:HG21	1:A:190:TYR:CE2	2.53	0.44
1:A:26:HIS:C	1:A:28:ALA:H	2.20	0.44
1:B:158:LYS:HB3	1:B:159:VAL:H	1.60	0.44
1:B:83:ALA:HA	1:B:86:ARG:CD	2.45	0.44
1:A:124:LEU:HD23	1:A:129:VAL:HG13	2.01	0.43
1:B:131:ILE:CG2	1:B:132:VAL:H	2.29	0.43
1:B:169:ARG:NH1	1:B:169:ARG:HG2	2.32	0.43
1:A:86:ARG:NH1	1:B:202:ASN:HD21	2.16	0.43
1:A:73:PHE:CD2	1:A:162:LEU:HB2	2.53	0.43
1:A:4:SER:OG	1:A:5:PRO:HD2	2.18	0.43
1:A:72:LYS:O	1:A:75:ALA:HB3	2.18	0.43
1:A:74:PHE:CD1	1:A:78:LEU:HD11	2.54	0.43
1:B:135:ILE:CG1	1:B:136:ILE:N	2.81	0.43
1:B:201:LEU:HD21	1:B:203:HIS:O	2.18	0.43
1:B:59:HIS:HE1	5:B:905:HOH:O	2.00	0.43
1:B:72:LYS:NZ	1:B:76:ASP:OD2	2.51	0.43
1:B:98:PHE:N	1:B:98:PHE:CD1	2.87	0.43
1:A:208:SER:C	1:A:210:THR:H	2.21	0.43
1:B:37:PRO:HD2	1:B:40:LEU:HD12	1.99	0.43
1:A:45:THR:O	1:A:46:GLU:C	2.57	0.43
1:B:137:ASP:HB3	4:B:314:PRP:O1P	2.18	0.43
1:A:138:THR:O	1:A:171:VAL:HG23	2.18	0.43
1:B:160:ALA:CA	1:B:177:PHE:HB2	2.26	0.43
1:B:61:ILE:CG2	1:B:62:VAL:N	2.81	0.43
1:B:189:GLY:O	1:B:190:TYR:HB3	2.19	0.43
1:A:46:GLU:HA	1:A:80:TYR:CG	2.54	0.43
1:B:210:THR:HA	5:B:911:HOH:O	2.18	0.43
1:A:136:ILE:HA	1:A:136:ILE:HD13	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HG23	1:B:167:THR:O	2.18	0.42
1:A:198:PHE:HE1	1:A:207:ILE:CG2	2.26	0.42
1:A:23:ILE:HA	1:A:24:PRO:HD3	1.93	0.42
1:A:124:LEU:HD12	1:A:124:LEU:N	2.35	0.42
1:A:78:LEU:O	1:A:82:LYS:HG3	2.18	0.42
1:A:7:VAL:HG11	1:A:180:PHE:HE2	1.85	0.42
1:A:67:LEU:O	1:A:68:ALA:CB	2.67	0.42
1:B:119:ASP:C	1:B:121:LEU:HD12	2.39	0.42
1:B:139:GLY:O	1:B:143:GLN:HG3	2.19	0.42
1:B:45:THR:C	1:B:47:ARG:H	2.22	0.42
1:A:73:PHE:CD1	1:A:162:LEU:HD13	2.55	0.42
1:A:159:VAL:CG1	1:A:175:PRO:HB3	2.50	0.42
1:B:72:LYS:HG2	1:B:190:TYR:CD1	2.55	0.42
1:B:72:LYS:O	1:B:74:PHE:N	2.52	0.42
1:A:134:ASP:OD2	4:A:312:PRP:O2B	2.38	0.42
1:A:202:ASN:HD22	1:A:202:ASN:H	1.61	0.42
1:A:7:VAL:HG23	1:A:44:ARG:NE	2.35	0.42
1:A:74:PHE:CD1	1:A:132:VAL:HG21	2.55	0.42
1:A:26:HIS:CD2	1:A:26:HIS:N	2.86	0.42
1:A:83:ALA:HA	1:A:86:ARG:CG	2.49	0.42
1:B:99:ILE:HA	1:B:118:GLY:HA3	2.01	0.42
1:A:182:ILE:O	1:A:183:PRO:O	2.37	0.42
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.91	0.42
1:A:45:THR:CA	1:A:48:LEU:HD13	2.45	0.42
1:A:64:LEU:HB3	1:A:97:ASP:HB2	2.02	0.42
1:B:164:VAL:CG1	1:B:165:LYS:N	2.83	0.42
1:B:107:ASP:CG	1:B:186:PHE:CE2	2.93	0.42
1:B:77:LEU:O	1:B:77:LEU:HD12	2.20	0.42
1:A:107:ASP:O	1:A:108:GLN:CB	2.65	0.42
1:A:190:TYR:HB2	1:A:202:ASN:O	2.20	0.42
1:A:26:HIS:CD2	1:A:27:TYR:CD1	3.08	0.42
1:A:27:TYR:CE2	1:A:198:PHE:CD2	3.08	0.42
1:A:46:GLU:O	1:A:49:ALA:HB3	2.20	0.42
1:B:64:LEU:HD12	1:B:97:ASP:CB	2.32	0.42
1:A:101:LEU:O	1:A:102:GLY:C	2.59	0.41
1:A:211:GLY:HA2	1:A:214:LYS:HB3	2.02	0.41
1:A:25:ASN:O	1:A:26:HIS:C	2.58	0.41
1:A:48:LEU:CD1	1:A:48:LEU:H	2.29	0.41
1:B:137:ASP:CG	1:B:138:THR:N	2.73	0.41
1:B:158:LYS:HB3	1:B:177:PHE:HE2	1.84	0.41
1:B:203:HIS:O	1:B:205:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASP:O	1:B:77:LEU:C	2.57	0.41
1:A:64:LEU:CD1	1:A:129:VAL:HG12	2.43	0.41
1:A:127:LYS:H	1:A:155:LYS:H	1.63	0.41
1:A:167:THR:OG1	1:A:169:ARG:NH1	2.54	0.41
1:A:199:ARG:C	1:A:201:LEU:H	2.24	0.41
1:A:61:ILE:CG2	1:A:130:LEU:HB2	2.50	0.41
1:A:168:PRO:HG2	1:A:169:ARG:N	2.36	0.41
1:A:7:VAL:HG11	1:A:180:PHE:CE2	2.55	0.41
1:A:17:ASP:OD2	1:A:17:ASP:N	2.52	0.41
1:B:59:HIS:HB3	1:B:128:ASN:ND2	2.36	0.41
1:A:186:PHE:HB2	1:A:212:LYS:NZ	2.36	0.41
1:A:93:PRO:HA	5:B:945:HOH:O	2.21	0.41
1:B:101:LEU:O	1:B:101:LEU:CG	2.68	0.41
1:B:104:TYR:O	1:B:106:ASN:N	2.54	0.41
1:B:36:ILE:HG22	1:B:41:ILE:CG1	2.50	0.41
1:B:37:PRO:O	1:B:40:LEU:CB	2.69	0.41
1:A:125:THR:O	1:A:126:GLY:C	2.59	0.41
1:B:146:LEU:O	1:B:149:VAL:C	2.59	0.41
1:A:15:GLY:CA	1:A:34:VAL:O	2.68	0.41
1:A:167:THR:HG22	1:A:170:SER:HB3	2.01	0.41
1:A:146:LEU:HD22	1:A:173:TYR:CE2	2.55	0.41
1:A:91:SER:C	1:A:92:ILE:HG13	2.41	0.41
1:B:104:TYR:O	1:B:104:TYR:HD1	2.02	0.41
1:B:146:LEU:HA	1:B:149:VAL:CB	2.43	0.41
1:B:36:ILE:HG21	1:B:41:ILE:HG12	2.03	0.41
1:A:190:TYR:HB3	1:A:204:VAL:HG22	2.03	0.41
1:A:26:HIS:CD2	1:A:27:TYR:H	2.39	0.41
1:B:134:ASP:OD2	1:B:134:ASP:N	2.54	0.41
1:B:21:PHE:HB3	1:B:203:HIS:CE1	2.56	0.41
1:A:72:LYS:CE	1:B:79:ASP:OD1	2.69	0.41
1:B:7:VAL:HG21	1:B:180:PHE:HD2	1.85	0.41
1:A:129:VAL:HG23	1:A:154:PRO:HB2	2.04	0.40
1:B:208:SER:C	1:B:210:THR:H	2.24	0.40
1:B:143:GLN:O	1:B:147:SER:N	2.42	0.40
1:B:7:VAL:O	1:B:7:VAL:HG12	2.19	0.40
1:A:200:ASP:HA	1:B:82:LYS:HB3	2.02	0.40
1:A:48:LEU:N	1:A:48:LEU:HD12	2.33	0.40
1:A:72:LYS:HZ3	1:B:82:LYS:CE	2.32	0.40
1:A:122:SER:HA	1:A:152:TYR:CD2	2.56	0.40
1:A:128:ASN:ND2	1:A:155:LYS:HB3	2.37	0.40
1:B:101:LEU:CD2	1:B:145:LEU:HD22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:N	1:B:163:LEU:O	2.54	0.40
1:B:183:PRO:CB	1:B:185:LYS:HZ1	2.32	0.40
1:B:90:ARG:NH1	1:B:90:ARG:HG2	2.36	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	212/214 (99%)	131 (62%)	53 (25%)	28 (13%)	0	0
1	B	212/214 (99%)	130 (61%)	47 (22%)	35 (16%)	0	0
All	All	424/428 (99%)	261 (62%)	100 (24%)	63 (15%)	0	0

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	10	SER
1	A	29	GLU
1	A	40	LEU
1	A	46	GLU
1	A	54	LYS
1	A	58	GLY
1	A	72	LYS
1	A	121	LEU
1	A	183	PRO
1	B	5	PRO
1	B	75	ALA
1	B	105	CYS
1	B	124	LEU
1	B	152	TYR

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Mol	Chain	Res	Type
1	B	158	LYS
1	B	159	VAL
1	B	175	PRO
1	A	35	PHE
1	A	120	ASP
1	A	126	GLY
1	A	204	VAL
1	B	26	HIS
1	B	52	VAL
1	B	72	LYS
1	B	76	ASP
1	B	87	ASN
1	B	134	ASP
1	B	137	ASP
1	B	138	THR
1	B	154	PRO
1	B	189	GLY
1	B	204	VAL
1	A	28	ALA
1	A	93	PRO
1	A	102	GLY
1	B	30	ASP
1	B	151	GLN
1	B	153	ASN
1	A	25	ASN
1	A	68	ALA
1	A	73	PHE
1	A	75	ALA
1	A	129	VAL
1	A	195	ASN
1	B	7	VAL
1	B	46	GLU
1	B	103	SER
1	A	24	PRO
1	A	45	THR
1	A	74	PHE
1	A	84	LEU
1	B	68	ALA
1	B	157	VAL
1	B	176	ASP
1	A	108	GLN
1	B	140	LYS

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Mol	Chain	Res	Type
1	B	149	VAL
1	B	188	VAL
1	B	96	VAL
1	B	99	ILE
1	B	111	GLY
1	B	102	GLY

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	187/187 (100%)	145 (78%)	42 (22%)	1	3
1	B	187/187 (100%)	153 (82%)	34 (18%)	2	5
All	All	374/374 (100%)	298 (80%)	76 (20%)	1	4

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	ASP
1	A	17	ASP
1	A	18	LEU
1	A	22	CYS
1	A	26	HIS
1	A	29	GLU
1	A	30	ASP
1	A	33	ARG
1	A	35	PHE
1	A	53	MET
1	A	60	HIS
1	A	64	LEU
1	A	65	CYS
1	A	67	LEU
1	A	86	ARG
1	A	87	ASN

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Mol	Chain	Res	Type
1	A	88	SER
1	A	93	PRO
1	A	95	THR
1	A	100	ARG
1	A	107	ASP
1	A	112	ASP
1	A	114	LYS
1	A	120	ASP
1	A	124	LEU
1	A	125	THR
1	A	128	ASN
1	A	130	LEU
1	A	133	GLU
1	A	136	ILE
1	A	143	GLN
1	A	148	LEU
1	A	153	ASN
1	A	163	LEU
1	A	169	ARG
1	A	176	ASP
1	A	184	ASP
1	A	186	PHE
1	A	197	TYR
1	A	202	ASN
1	A	205	CYS
1	B	19	ASP
1	B	26	HIS
1	B	30	ASP
1	B	35	PHE
1	B	37	PRO
1	B	42	MET
1	B	51	ASP
1	B	54	LYS
1	B	65	CYS
1	B	67	LEU
1	B	74	PHE
1	B	84	LEU
1	B	88	SER
1	B	90	ARG
1	B	96	VAL
1	B	97	ASP
1	B	98	PHE

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Mol	Chain	Res	Type
1	B	99	ILE
1	B	105	CYS
1	B	120	ASP
1	B	123	THR
1	B	134	ASP
1	B	144	THR
1	B	151	GLN
1	B	154	PRO
1	B	155	LYS
1	B	186	PHE
1	B	193	ASP
1	B	196	GLU
1	B	199	ARG
1	B	200	ASP
1	B	201	LEU
1	B	210	THR
1	B	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	106	ASN
1	A	128	ASN
1	A	151	GLN
1	A	195	ASN
1	B	26	HIS
1	B	38	HIS
1	B	59	HIS
1	B	128	ASN
1	B	202	ASN
1	B	203	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	PPO	A	300	-	9,11,11	3.82	5 (55%)	4,15,15	2.71	3 (75%)
4	PRP	A	312	2	20,22,22	2.43	9 (45%)	30,35,35	4.79	17 (56%)
3	PPO	B	301	-	9,11,11	4.08	6 (66%)	4,15,15	2.75	3 (75%)
4	PRP	B	314	2	20,22,22	2.26	10 (50%)	30,35,35	6.47	16 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PPO	A	300	-	-	0/0/6/6	0/1/2/2
4	PRP	A	312	2	-	0/16/33/33	0/1/1/1
3	PPO	B	301	-	-	0/0/6/6	0/1/2/2
4	PRP	B	314	2	-	0/16/33/33	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	PPO	C9-C4	-8.11	1.37	1.50
3	B	301	PPO	C9-C4	-7.98	1.37	1.50
4	A	312	PRP	PB-O3A	-5.72	1.50	1.60
3	A	300	PPO	C9-N8	-5.16	1.38	1.47
3	B	301	PPO	C9-N8	-4.70	1.38	1.47
4	B	314	PRP	C5-C4	-4.45	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	314	PRP	PB-O3A	-3.93	1.53	1.60
4	B	314	PRP	PB-O3B	-3.53	1.40	1.54
4	A	312	PRP	C5-C4	-3.49	1.40	1.51
4	A	312	PRP	C3-C4	-3.10	1.44	1.53
4	B	314	PRP	O5-C5	-2.74	1.33	1.44
4	B	314	PRP	C3-C4	-2.73	1.45	1.53
4	A	312	PRP	C1-C2	-2.48	1.49	1.52
4	A	312	PRP	P-O2P	-2.30	1.45	1.54
4	A	312	PRP	C3-C2	-2.21	1.47	1.53
4	B	314	PRP	C3-C2	-2.19	1.47	1.53
4	B	314	PRP	P-O2P	-2.13	1.46	1.54
4	A	312	PRP	O5-C5	-2.10	1.36	1.44
4	B	314	PRP	P-O5	2.03	1.66	1.60
4	B	314	PRP	PA-O1A	2.08	1.58	1.50
4	A	312	PRP	P-O5	2.34	1.67	1.60
3	B	301	PPO	C2-N3	2.38	1.38	1.33
4	B	314	PRP	PB-O1B	2.66	1.59	1.50
3	B	301	PPO	N7-N8	2.92	1.29	1.25
3	A	300	PPO	N7-N8	3.13	1.30	1.25
3	A	300	PPO	C2-N1	3.57	1.40	1.33
3	A	300	PPO	C4-N3	3.77	1.38	1.34
4	A	312	PRP	PA-O1	4.26	1.71	1.60
3	B	301	PPO	C2-N1	4.52	1.42	1.33
3	B	301	PPO	C4-N3	5.29	1.40	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	314	PRP	O1-PA-O1A	-7.28	80.83	109.46
4	B	314	PRP	O3B-PB-O1B	-7.24	82.19	110.50
4	B	314	PRP	O2A-PA-O1	-5.48	84.48	106.49
4	A	312	PRP	O3A-PB-O1B	-4.24	85.33	111.44
3	B	301	PPO	N1-C2-N3	-4.20	121.82	128.65
3	A	300	PPO	N1-C2-N3	-4.14	121.92	128.65
4	A	312	PRP	C5-C4-C3	-3.05	103.68	115.29
4	B	314	PRP	C5-C4-C3	-2.89	104.29	115.29
4	A	312	PRP	O2B-PB-O1B	-2.83	99.44	110.50
3	B	301	PPO	C2-N3-C4	-2.82	113.14	118.06
3	A	300	PPO	C2-N3-C4	-2.70	113.35	118.06
4	A	312	PRP	O1-PA-O1A	-2.57	99.36	109.46
4	A	312	PRP	O3B-PB-O2B	-2.50	97.54	107.61
4	B	314	PRP	O2B-PB-O1B	-2.42	101.03	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	312	PRP	O2A-PA-O1A	-2.27	100.54	112.28
4	A	312	PRP	O2P-P-O5	2.06	112.22	106.73
4	A	312	PRP	C1-C2-C3	2.07	104.96	102.29
3	B	301	PPO	C2-N1-C6	2.10	124.86	117.26
4	B	314	PRP	O2P-P-O5	2.14	112.42	106.73
4	A	312	PRP	P-O5-C5	2.15	124.23	118.30
3	A	300	PPO	C2-N1-C6	2.20	125.23	117.26
4	A	312	PRP	O4-C4-C3	2.23	109.60	105.17
4	B	314	PRP	O4-C4-C3	2.34	109.82	105.17
4	B	314	PRP	O5-C5-C4	2.38	117.44	109.00
4	B	314	PRP	C1-C2-C3	2.45	105.44	102.29
4	A	312	PRP	O3B-PB-O1B	2.58	120.61	110.50
4	A	312	PRP	O5-C5-C4	2.77	118.81	109.00
4	B	314	PRP	C2-C3-C4	2.77	108.01	102.62
4	A	312	PRP	C2-C3-C4	2.92	108.30	102.62
4	B	314	PRP	O4-C1-C2	3.43	109.48	104.97
4	A	312	PRP	O1-C1-C2	4.08	113.76	106.70
4	A	312	PRP	O4-C1-C2	4.09	110.35	104.97
4	A	312	PRP	PA-O1-C1	4.24	136.55	119.74
4	B	314	PRP	O1-C1-C2	4.84	115.08	106.70
4	B	314	PRP	O3B-PB-O2B	6.30	133.01	107.61
4	B	314	PRP	PA-O1-C1	6.34	144.87	119.74
4	B	314	PRP	O3A-PB-O1B	8.43	163.28	111.44
4	A	312	PRP	O3A-PA-O1	22.93	143.03	102.05
4	B	314	PRP	O3A-PA-O1	29.47	154.72	102.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	PPO	1	0
4	A	312	PRP	14	0
3	B	301	PPO	1	0
4	B	314	PRP	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	108:GLN	C	109:SER	N	1.19
1	B	109:SER	C	110:THR	N	1.15
1	B	105:CYS	C	106:ASN	N	1.02

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.