Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:00 AM GMT

PDB ID	:	2F55
Title	:	Two hepatitis c virus ns3 helicase domains complexed with the same strand of dna
Authors	:	Lu, J.Z.; Jordan, J.B.; Sakon, J.
Deposited on	:	2005-11-25
Resolution	:	3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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 3.30 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		56
Ramachandran outliers		8.3%
Sidechain outliers		9.7%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
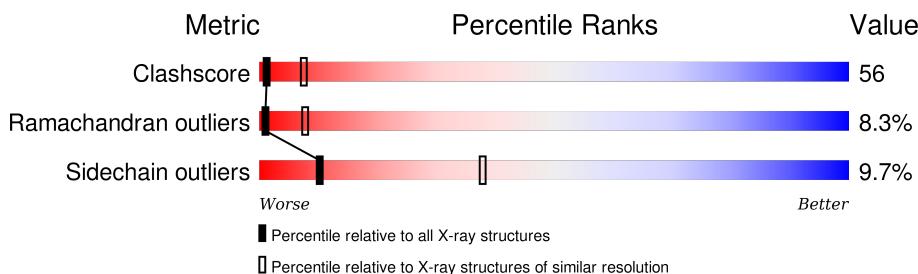
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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	D	13	23% 69% 8%
2	E	3	100%
3	A	435	38% 52% 9% ••
3	B	435	28% 57% 14% •
3	C	435	37% 51% 10% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10129 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 DNA chain called 5'-D(P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	D	13	247	117	26	91	13	0	0	0

- Molecule 2 is a DNA chain called 5'-D(P*(DU)P*(DU)P*(DU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	3	57	27	6	21	3	0	0	0

- Molecule 3 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	432	3251	2063	553	616	19	0	0	0
3	B	432	3251	2063	553	616	19	0	0	0
3	C	432	3251	2063	553	616	19	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
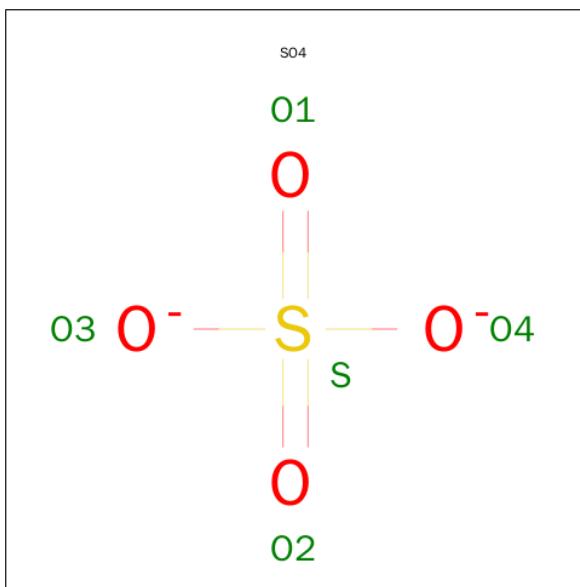
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	14	Total 14	O 14	0	0
5	C	25	Total 25	O 25	0	0
5	D	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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.

Note EDS was not executed.

• Molecule 1: 5'-D(P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU)P*(DU))-3'

Chain D:

• Molecule 2: 5'-D(P*(DU)P*(DU)P*(DU))-3'
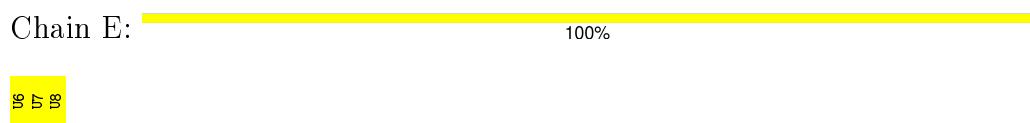
Chain E:

• Molecule 3: polyprotein
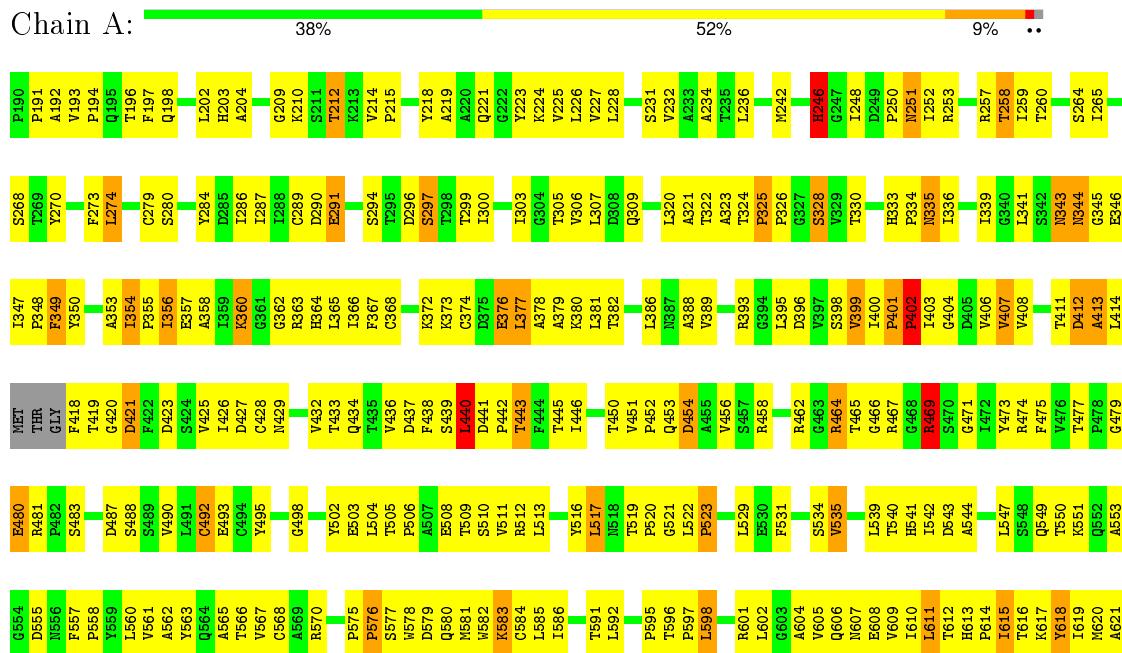
Chain A:

C622 M623 S624

• Molecule 3: polyprotein

Chain B:

28%   57%   14%
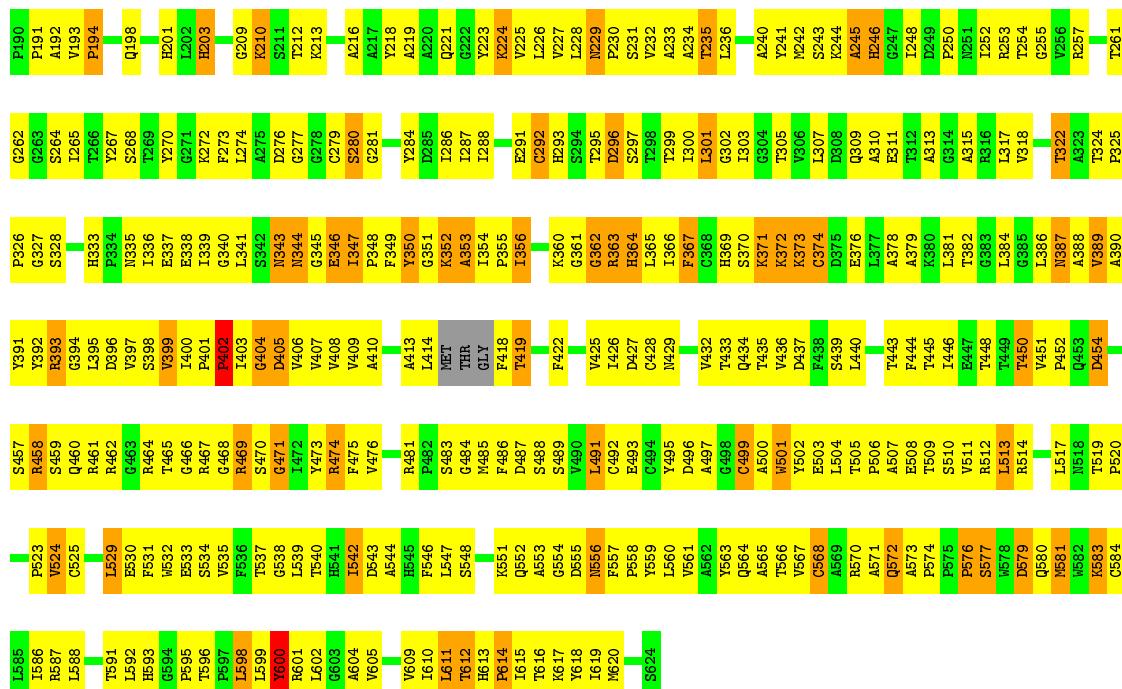
• Molecule 3: polyprotein

Chain C:

37%   51%   10%
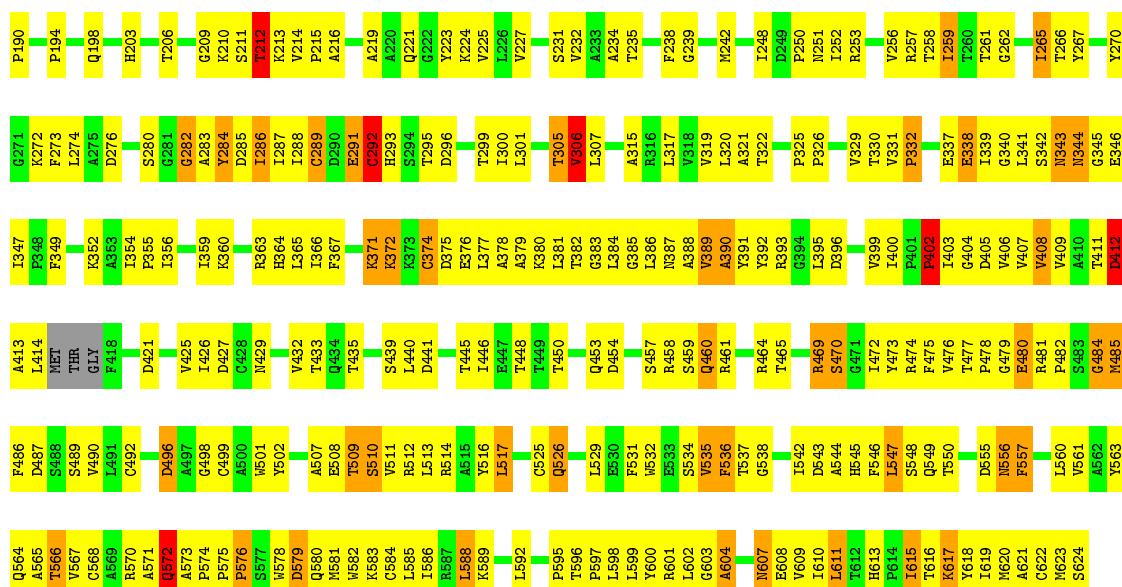
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.20Å 109.80Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30	Depositor
% Data completeness (in resolution range)	83.2 (50.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10129	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	D	0.70	0/272	0.98	1/412 (0.2%)
2	E	0.70	0/62	0.99	0/92
3	A	0.54	3/3331 (0.1%)	0.73	2/4548 (0.0%)
3	B	0.59	4/3331 (0.1%)	0.74	1/4548 (0.0%)
3	C	0.53	5/3331 (0.2%)	0.72	1/4548 (0.0%)
All	All	0.56	12/10327 (0.1%)	0.74	5/14148 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	469	ARG	NE-CZ	7.51	1.42	1.33
3	B	469	ARG	NE-CZ	7.47	1.42	1.33
3	A	469	ARG	NE-CZ	7.45	1.42	1.33
3	B	469	ARG	CZ-NH2	7.42	1.42	1.33
3	C	469	ARG	CZ-NH2	7.38	1.42	1.33
3	A	469	ARG	CZ-NH2	7.34	1.42	1.33
3	A	469	ARG	CZ-NH1	7.04	1.42	1.33
3	B	469	ARG	CZ-NH1	6.98	1.42	1.33
3	C	469	ARG	CZ-NH1	6.92	1.42	1.33
3	C	402	PRO	N-CD	5.50	1.55	1.47
3	B	402	PRO	N-CD	5.40	1.55	1.47
3	C	289	CYS	CB-SG	-5.35	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PRO	CA-N-CD	-12.76	93.64	111.50
3	B	402	PRO	CA-N-CD	-12.74	93.67	111.50
3	A	402	PRO	CA-N-CD	-11.23	95.78	111.50
3	A	401	PRO	C-N-CD	7.38	143.90	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	DU	O4'-C1'-C2'	5.03	109.92	105.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	247	0	131	18	0
2	E	57	0	31	6	0
3	A	3251	0	3216	332	0
3	B	3251	0	3215	434	0
3	C	3251	0	3215	354	0
4	A	5	0	0	0	0
4	C	5	0	0	1	0
5	A	20	0	0	2	0
5	B	14	0	0	0	0
5	C	25	0	0	3	0
5	D	3	0	0	0	0
All	All	10129	0	9808	1118	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 56.

All (1118) 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)
3:A:469:ARG:HB2	3:A:469:ARG:NH1	1.31	1.43
3:C:513:LEU:O	3:C:517:LEU:CD2	1.65	1.42
3:A:360:LYS:NZ	3:A:386:LEU:HD21	1.06	1.36
3:A:360:LYS:NZ	3:A:386:LEU:CD2	1.88	1.35
3:A:339:ILE:CG2	3:A:474:ARG:HG2	1.54	1.35
3:A:534:SER:HB2	3:A:622:CYS:SG	1.68	1.33
3:A:451:VAL:CG2	3:A:452:PRO:HD2	1.57	1.31
3:B:219:ALA:CB	3:B:265:ILE:HD11	1.57	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:513:LEU:O	3:B:517:LEU:HD23	1.17	1.31
3:B:451:VAL:CG2	3:B:452:PRO:HD2	1.60	1.30
3:B:346:GLU:OE2	3:B:356:ILE:HG22	1.27	1.29
3:A:534:SER:CB	3:A:622:CYS:SG	2.20	1.28
3:A:360:LYS:HZ3	3:A:386:LEU:CD2	1.45	1.23
3:B:346:GLU:CD	3:B:356:ILE:HG22	1.57	1.23
3:A:469:ARG:CB	3:A:469:ARG:HH11	1.50	1.23
3:B:513:LEU:O	3:B:517:LEU:CD2	1.87	1.23
3:C:531:PHE:O	3:C:534:SER:OG	1.54	1.21
3:B:451:VAL:HG22	3:B:452:PRO:CD	1.70	1.20
3:C:342:SER:CB	3:C:344:ASN:HD21	1.54	1.19
3:A:296:ASP:OD2	3:A:299:THR:CG2	1.89	1.18
3:A:209:GLY:HA2	3:A:212:THR:HG23	1.25	1.16
3:B:346:GLU:CD	3:B:356:ILE:CG2	2.16	1.14
3:C:342:SER:OG	3:C:344:ASN:ND2	1.78	1.14
3:B:344:ASN:ND2	3:B:355:PRO:HG2	1.61	1.14
3:B:379:ALA:HA	3:B:382:THR:HG23	1.26	1.14
3:A:534:SER:OG	3:A:622:CYS:SG	2.06	1.13
3:B:219:ALA:HB1	3:B:265:ILE:HD11	1.27	1.12
3:A:339:ILE:HG23	3:A:474:ARG:HG2	1.29	1.12
3:A:517:LEU:H	3:A:517:LEU:HD22	1.09	1.12
3:A:451:VAL:HG22	3:A:452:PRO:HD2	1.25	1.12
3:A:296:ASP:OD2	3:A:299:THR:HG22	1.45	1.11
3:A:382:THR:CG2	3:A:388:ALA:HB3	1.79	1.11
3:C:248:ILE:HD11	3:C:265:ILE:HG13	1.29	1.11
3:C:513:LEU:O	3:C:517:LEU:HD21	1.37	1.10
3:C:402:PRO:HD2	3:C:403:ILE:H	1.12	1.10
3:B:379:ALA:HA	3:B:382:THR:CG2	1.79	1.10
3:C:513:LEU:O	3:C:517:LEU:HD23	1.35	1.09
3:A:382:THR:HG22	3:A:388:ALA:HB3	1.15	1.09
3:B:403:ILE:HG12	3:B:404:GLY:H	1.13	1.09
3:B:346:GLU:OE1	3:B:356:ILE:CG2	2.01	1.09
3:B:219:ALA:HB2	3:B:265:ILE:HD11	1.33	1.07
3:C:342:SER:CB	3:C:344:ASN:ND2	2.16	1.07
3:A:339:ILE:CG2	3:A:474:ARG:CG	2.32	1.07
3:B:451:VAL:CG2	3:B:452:PRO:CD	2.28	1.06
3:B:286:ILE:HD13	3:B:317:LEU:HB3	1.34	1.06
3:B:346:GLU:OE2	3:B:356:ILE:CG2	2.03	1.06
3:A:360:LYS:CE	3:A:386:LEU:HD21	1.85	1.05
3:B:344:ASN:ND2	3:B:355:PRO:CG	2.20	1.04
3:A:451:VAL:HG23	3:A:452:PRO:HD2	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:339:ILE:HG21	3:A:474:ARG:HE	1.19	1.02
3:A:402:PRO:HD2	3:A:403:ILE:H	1.22	1.01
3:B:451:VAL:HG22	3:B:452:PRO:HD2	0.99	0.99
3:B:382:THR:HG22	3:B:386:LEU:O	1.63	0.98
3:C:343:ASN:H	3:C:343:ASN:HD22	1.01	0.98
3:C:360:LYS:NZ	3:C:386:LEU:HD21	1.78	0.97
3:A:248:ILE:HD11	3:A:265:ILE:HG12	1.46	0.97
3:A:451:VAL:HG22	3:A:452:PRO:CD	1.94	0.96
3:A:242:MET:HE3	3:A:248:ILE:HD13	1.46	0.96
3:C:517:LEU:HD22	3:C:517:LEU:N	1.81	0.95
3:A:343:ASN:HD22	3:A:344:ASN:HD22	1.14	0.95
3:C:378:ALA:O	3:C:382:THR:HG23	1.66	0.95
3:A:339:ILE:HG22	3:A:474:ARG:CG	1.94	0.95
3:C:402:PRO:CD	3:C:403:ILE:H	1.80	0.94
3:A:360:LYS:HZ1	3:A:386:LEU:CD2	1.76	0.94
3:A:242:MET:CE	3:A:248:ILE:HD13	1.98	0.94
3:C:342:SER:HB2	3:C:344:ASN:ND2	1.82	0.93
3:A:339:ILE:HG22	3:A:474:ARG:HG2	1.46	0.93
3:A:378:ALA:O	3:A:382:THR:HG23	1.69	0.92
1:D:15:DU:H5'	3:B:232:VAL:HG23	1.50	0.92
3:C:342:SER:HB2	3:C:344:ASN:HD21	1.35	0.91
3:A:517:LEU:N	3:A:517:LEU:HD22	1.84	0.91
3:B:379:ALA:CA	3:B:382:THR:HG23	2.00	0.91
2:E:7:DU:H5'	3:C:232:VAL:HG23	1.51	0.91
3:C:402:PRO:HD2	3:C:403:ILE:N	1.86	0.91
3:A:517:LEU:CD2	3:A:517:LEU:H	1.82	0.91
3:A:343:ASN:ND2	3:A:344:ASN:HD22	1.68	0.91
3:B:378:ALA:HB1	3:B:388:ALA:HA	1.53	0.90
3:A:429:ASN:ND2	3:A:453:GLN:HE22	1.70	0.90
3:B:248:ILE:HD11	3:B:265:ILE:HD13	1.52	0.90
3:B:344:ASN:H	3:B:344:ASN:HD22	1.13	0.90
3:B:403:ILE:HG12	3:B:404:GLY:N	1.83	0.90
3:B:378:ALA:O	3:B:382:THR:HG23	1.72	0.89
3:B:345:GLY:HA3	3:B:355:PRO:HA	1.53	0.89
3:B:393:ARG:HH12	3:B:413:ALA:CB	1.84	0.89
3:A:429:ASN:HD22	3:A:453:GLN:HE22	0.89	0.89
3:A:458:ARG:HD3	3:A:480:GLU:HB3	1.55	0.88
3:B:242:MET:HG3	3:B:248:ILE:CG2	2.03	0.88
3:C:344:ASN:H	3:C:344:ASN:HD22	1.18	0.88
3:B:454:ASP:HB2	3:B:483:SER:HB3	1.54	0.88
3:C:461:ARG:HA	3:C:464:ARG:HE	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:535:VAL:HG13	3:B:619:ILE:HD12	1.55	0.87
3:C:583:LYS:HA	3:C:586:ILE:HD12	1.54	0.87
3:B:402:PRO:HD2	3:B:403:ILE:H	1.40	0.87
3:A:601:ARG:HH11	3:A:601:ARG:HG3	1.38	0.87
3:A:225:VAL:HG23	3:A:265:ILE:HA	1.55	0.86
3:C:286:ILE:HD12	3:C:317:LEU:HB3	1.58	0.86
3:C:224:LYS:HB2	3:C:285:ASP:H	1.41	0.86
3:A:382:THR:HG22	3:A:388:ALA:CB	2.03	0.86
3:A:429:ASN:HD22	3:A:453:GLN:NE2	1.73	0.85
3:B:193:VAL:HG13	3:B:286:ILE:HD11	1.58	0.85
3:B:402:PRO:CD	3:B:403:ILE:H	1.89	0.85
3:C:343:ASN:HD22	3:C:343:ASN:N	1.74	0.85
3:A:402:PRO:HD2	3:A:403:ILE:N	1.89	0.85
3:B:242:MET:O	3:B:248:ILE:HG22	1.76	0.85
3:A:451:VAL:CG2	3:A:452:PRO:CD	2.49	0.84
3:B:397:VAL:O	3:B:400:ILE:HG12	1.78	0.84
3:B:403:ILE:CG1	3:B:404:GLY:H	1.90	0.84
3:A:426:ILE:HD13	3:A:474:ARG:HB2	1.59	0.84
3:B:393:ARG:HH12	3:B:413:ALA:HB3	1.41	0.84
3:B:346:GLU:OE1	3:B:356:ILE:HG22	1.69	0.84
3:A:403:ILE:CG2	3:A:404:GLY:N	2.41	0.83
3:B:468:GLY:O	3:B:469:ARG:HG2	1.78	0.83
3:A:296:ASP:OD2	3:A:299:THR:HG21	1.77	0.82
3:B:362:GLY:HA2	3:B:405:ASP:HB2	1.60	0.82
3:C:343:ASN:H	3:C:343:ASN:ND2	1.74	0.82
3:C:363:ARG:HD2	3:C:406:VAL:HG12	1.61	0.82
3:B:381:LEU:HB3	3:B:386:LEU:HD22	1.61	0.81
3:B:543:ASP:HB3	3:B:546:PHE:HD2	1.44	0.81
3:B:296:ASP:O	3:B:300:ILE:HD13	1.80	0.81
3:A:236:LEU:HD23	3:A:252:ILE:HG21	1.62	0.81
3:A:364:HIS:HB2	3:A:407:VAL:HG12	1.62	0.81
3:B:201:HIS:HB3	3:B:203:HIS:CE1	2.16	0.81
3:A:432:VAL:HG22	3:A:450:THR:HG22	1.63	0.81
3:B:451:VAL:HG23	3:B:452:PRO:HD2	1.62	0.81
3:A:403:ILE:HG22	3:A:404:GLY:N	1.96	0.80
3:C:360:LYS:HZ2	3:C:386:LEU:HD21	1.45	0.80
3:A:517:LEU:HD21	3:A:529:LEU:HD11	1.63	0.80
3:B:402:PRO:HD2	3:B:403:ILE:N	1.97	0.80
3:C:556:ASN:HB3	3:C:557:PHE:HD1	1.47	0.79
3:B:219:ALA:CB	3:B:265:ILE:CD1	2.51	0.79
3:A:248:ILE:HD11	3:A:265:ILE:CG1	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:402:PRO:CD	3:C:403:ILE:N	2.42	0.79
3:B:491:LEU:HD23	3:B:525:CYS:SG	2.23	0.79
3:B:286:ILE:CD1	3:B:317:LEU:HB3	2.12	0.79
3:C:359:ILE:HA	3:C:364:HIS:ND1	1.97	0.79
3:C:296:ASP:OD1	3:C:299:THR:HG21	1.83	0.79
3:A:265:ILE:H	3:A:265:ILE:HD12	1.48	0.79
3:B:386:LEU:HD12	3:B:386:LEU:N	1.98	0.79
3:B:371:LYS:HE3	3:B:371:LYS:H	1.47	0.79
3:B:203:HIS:CD2	3:B:325:PRO:HG3	2.17	0.78
3:C:344:ASN:N	3:C:344:ASN:HD22	1.81	0.78
3:C:382:THR:CG2	3:C:388:ALA:O	2.31	0.78
3:C:251:ASN:HD21	3:C:262:GLY:N	1.82	0.78
3:A:469:ARG:NH1	3:A:469:ARG:CB	2.24	0.78
3:B:346:GLU:CD	3:B:356:ILE:HG21	2.02	0.78
3:B:402:PRO:CG	3:B:403:ILE:H	1.95	0.78
3:A:445:THR:HA	3:A:601:ARG:O	1.82	0.78
3:A:339:ILE:HG21	3:A:474:ARG:NE	1.97	0.78
3:B:378:ALA:O	3:B:382:THR:CG2	2.31	0.78
3:A:402:PRO:CD	3:A:403:ILE:H	1.95	0.78
3:A:347:ILE:HD12	3:A:354:ILE:HD12	1.64	0.78
3:B:452:PRO:HG2	3:C:331:VAL:HG11	1.66	0.78
3:C:219:ALA:HB2	3:C:265:ILE:HD11	1.66	0.77
3:A:347:ILE:HD11	3:A:354:ILE:HB	1.67	0.77
3:B:219:ALA:HB1	3:B:265:ILE:CD1	2.13	0.77
3:C:242:MET:HB3	3:C:248:ILE:CG2	2.14	0.77
3:A:402:PRO:CD	3:A:403:ILE:N	2.48	0.76
3:A:192:ALA:O	3:A:194:PRO:HD3	1.86	0.76
3:A:613:HIS:CE1	3:A:615:ILE:HD13	2.20	0.76
3:C:190:PRO:HB3	3:C:214:VAL:HG13	1.67	0.75
3:B:344:ASN:N	3:B:344:ASN:HD22	1.84	0.75
3:B:402:PRO:CD	3:B:403:ILE:N	2.47	0.75
3:A:242:MET:HB3	3:A:248:ILE:HG23	1.66	0.75
3:C:224:LYS:H	3:C:285:ASP:HB2	1.51	0.75
3:C:360:LYS:HZ1	3:C:386:LEU:HD21	1.47	0.75
1:D:14:DU:H5	3:B:393:ARG:CZ	2.17	0.75
3:B:242:MET:HG3	3:B:248:ILE:HG22	1.68	0.75
3:C:248:ILE:HD11	3:C:265:ILE:CG1	2.15	0.75
3:C:224:LYS:N	3:C:285:ASP:HB2	2.02	0.75
3:B:344:ASN:ND2	3:B:344:ASN:H	1.85	0.74
3:B:203:HIS:HD2	3:B:325:PRO:HG3	1.51	0.74
3:B:434:GLN:HA	3:B:448:THR:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:ASP:OD1	3:C:299:THR:CG2	2.36	0.74
3:C:253:ARG:HH11	3:C:272:LYS:NZ	1.86	0.74
3:A:343:ASN:C	3:A:343:ASN:ND2	2.41	0.73
3:C:300:ILE:HD12	3:C:490:VAL:HG11	1.69	0.73
3:B:352:LYS:HG2	3:B:476:VAL:HG13	1.71	0.73
3:B:344:ASN:HD21	3:B:355:PRO:HG2	1.51	0.73
3:B:535:VAL:HG13	3:B:619:ILE:CD1	2.18	0.73
1:D:14:DU:H6	3:B:413:ALA:HB2	1.69	0.73
3:A:436:VAL:HG11	3:A:488:SER:HB3	1.71	0.73
3:A:429:ASN:HA	3:A:453:GLN:NE2	2.04	0.73
3:C:296:ASP:CG	3:C:299:THR:HG22	2.10	0.73
3:A:607:ASN:ND2	3:A:608:GLU:HG2	2.04	0.73
3:A:339:ILE:HG22	3:A:474:ARG:HG3	1.69	0.73
3:C:382:THR:HG22	3:C:388:ALA:O	1.89	0.73
3:C:517:LEU:N	3:C:517:LEU:CD2	2.52	0.72
3:B:344:ASN:CG	3:B:355:PRO:HG2	2.09	0.72
3:B:219:ALA:HB2	3:B:265:ILE:CD1	2.15	0.72
3:A:403:ILE:CG2	3:A:404:GLY:H	2.02	0.72
3:A:566:THR:O	3:A:570:ARG:HB2	1.89	0.72
3:A:477:THR:HG23	3:B:544:ALA:HB1	1.71	0.72
3:B:347:ILE:HB	3:B:354:ILE:HG13	1.70	0.72
3:B:485:MET:HA	3:B:524:VAL:O	1.89	0.72
3:B:451:VAL:HG23	3:B:452:PRO:CD	2.17	0.72
3:C:440:LEU:HD12	3:C:440:LEU:N	2.04	0.72
3:B:538:GLY:O	3:B:540:THR:N	2.23	0.71
3:A:280:SER:HB3	3:A:309:GLN:NE2	2.05	0.71
1:D:20:DU:C2'	1:D:21:DU:H5"	2.20	0.71
3:C:390:ALA:HA	3:C:409:VAL:O	1.90	0.71
3:B:400:ILE:HG21	3:B:419:THR:H	1.55	0.71
3:B:349:PHE:O	3:B:351:GLY:N	2.24	0.71
3:A:348:PRO:O	3:A:349:PHE:HB2	1.89	0.71
3:B:264:SER:C	3:B:265:ILE:HD12	2.12	0.70
3:B:402:PRO:CG	3:B:403:ILE:N	2.53	0.70
3:A:193:VAL:HG21	3:A:223:TYR:CE1	2.26	0.70
3:A:343:ASN:HD22	3:A:344:ASN:N	1.89	0.70
3:A:297:SER:HB3	3:A:493:GLU:HG2	1.73	0.70
3:B:402:PRO:HG2	3:B:403:ILE:H	1.55	0.70
3:A:477:THR:HG23	3:B:544:ALA:CB	2.22	0.70
3:B:349:PHE:C	3:B:351:GLY:H	1.95	0.70
3:A:547:LEU:HD13	3:A:551:LYS:HG3	1.73	0.70
3:B:387:ASN:HD22	3:B:387:ASN:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:248:ILE:CD1	3:A:265:ILE:HG12	2.22	0.70
3:C:239:GLY:HA3	3:C:252:ILE:HD11	1.73	0.70
3:B:236:LEU:HD12	3:B:252:ILE:HG21	1.72	0.69
3:A:400:ILE:HD11	3:A:408:VAL:HG13	1.73	0.69
3:C:556:ASN:HB3	3:C:557:PHE:CD1	2.27	0.69
3:B:394:GLY:O	3:B:395:LEU:HD23	1.92	0.69
3:B:473:TYR:HE2	3:B:475:PHE:HB3	1.58	0.69
3:B:252:ILE:HD13	3:B:267:TYR:HB2	1.74	0.69
3:B:551:LYS:HG3	3:B:552:GLN:N	2.08	0.69
3:A:343:ASN:HD22	3:A:344:ASN:ND2	1.89	0.69
3:A:360:LYS:NZ	3:A:360:LYS:HA	2.08	0.69
3:A:531:PHE:O	3:A:534:SER:OG	2.08	0.69
3:A:209:GLY:O	3:A:214:VAL:HG23	1.92	0.69
3:A:595:PRO:HB3	3:A:608:GLU:HG3	1.73	0.69
3:C:253:ARG:NH1	3:C:272:LYS:NZ	2.41	0.68
3:B:226:LEU:HD12	3:B:284:TYR:CD2	2.28	0.68
1:D:20:DU:H2"	1:D:21:DU:H5"	1.75	0.68
3:C:581:MET:HG3	3:C:582:TRP:NE1	2.07	0.68
3:B:210:LYS:N	3:B:210:LYS:HD2	2.09	0.68
3:A:360:LYS:CE	3:A:386:LEU:CD2	2.58	0.68
3:C:378:ALA:HB2	3:C:390:ALA:HB2	1.75	0.68
3:A:607:ASN:HD21	3:A:608:GLU:HG2	1.57	0.68
3:C:564:GLN:HE22	3:C:598:LEU:HD12	1.59	0.68
3:C:542:ILE:HA	3:C:566:THR:HG21	1.76	0.68
3:A:333:HIS:HB3	3:A:336:ILE:HB	1.75	0.68
1:D:14:DU:H5	3:B:393:ARG:NH1	2.09	0.68
1:D:16:DU:H5'	3:B:272:LYS:N	2.08	0.68
3:C:460:GLN:HE21	3:C:460:GLN:HA	1.57	0.68
3:B:361:GLY:HA2	3:B:407:VAL:HG23	1.76	0.68
3:B:393:ARG:HH22	3:B:413:ALA:H	1.40	0.67
3:C:446:ILE:HG21	3:C:557:PHE:CZ	2.29	0.67
3:A:194:PRO:HG2	3:A:198:GLN:OE1	1.93	0.67
3:B:574:PRO:O	3:B:596:THR:HG23	1.94	0.67
3:A:253:ARG:HB2	3:A:268:SER:HB2	1.76	0.67
3:B:386:LEU:HD12	3:B:386:LEU:H	1.60	0.67
3:B:458:ARG:HG2	3:B:458:ARG:HH11	1.59	0.67
3:C:209:GLY:O	3:C:214:VAL:HG23	1.94	0.67
3:C:253:ARG:HH11	3:C:272:LYS:HZ3	1.40	0.67
3:A:403:ILE:HG23	3:A:404:GLY:H	1.60	0.67
3:C:285:ASP:O	3:C:286:ILE:HD13	1.95	0.67
3:B:542:ILE:HD13	3:B:543:ASP:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:HG22	3:C:306:VAL:N	2.08	0.67
3:A:360:LYS:HZ1	3:A:386:LEU:HD22	1.59	0.67
3:C:619:ILE:HD12	3:C:619:ILE:H	1.59	0.67
3:B:229:ASN:ND2	3:B:230:PRO:HD2	2.10	0.67
3:B:566:THR:O	3:B:570:ARG:HG3	1.94	0.67
3:A:433:THR:HG22	3:A:434:GLN:N	2.09	0.67
3:B:346:GLU:OE1	3:B:356:ILE:HG21	1.93	0.66
3:B:252:ILE:CD1	3:B:267:TYR:HB2	2.25	0.66
3:C:411:THR:C	3:C:413:ALA:H	1.98	0.66
3:B:371:LYS:CE	3:B:371:LYS:H	2.08	0.66
3:C:253:ARG:NH1	3:C:272:LYS:HZ3	1.92	0.66
3:C:194:PRO:HG2	3:C:317:LEU:HD13	1.77	0.66
3:B:501:TRP:CZ3	3:B:551:LYS:HD3	2.31	0.66
3:B:426:ILE:HD13	3:B:474:ARG:CG	2.25	0.66
3:A:344:ASN:O	3:A:355:PRO:HG3	1.95	0.66
3:B:542:ILE:HD12	3:B:547:LEU:HB2	1.78	0.66
3:B:495:TYR:O	3:B:499:CYS:HB2	1.96	0.66
3:C:564:GLN:NE2	3:C:598:LEU:HD12	2.11	0.66
3:C:396:ASP:HB2	3:C:399:VAL:HG13	1.78	0.66
3:B:565:ALA:HA	3:B:568:CYS:HB2	1.77	0.66
3:C:514:ARG:HG3	3:C:514:ARG:HH11	1.60	0.66
3:C:411:THR:O	3:C:413:ALA:N	2.29	0.65
3:A:224:LYS:HE2	3:A:264:SER:HA	1.78	0.65
3:A:305:THR:HA	3:A:512:ARG:HD2	1.77	0.65
3:C:396:ASP:O	3:C:399:VAL:HG22	1.95	0.65
3:B:457:SER:O	3:B:461:ARG:HG3	1.97	0.65
3:A:265:ILE:N	3:A:265:ILE:HD12	2.11	0.65
3:B:378:ALA:HB1	3:B:388:ALA:CA	2.26	0.65
3:B:611:LEU:HD23	3:B:611:LEU:N	2.11	0.65
3:A:252:ILE:HD12	3:A:259:ILE:HD12	1.76	0.65
3:B:393:ARG:HH12	3:B:413:ALA:HB2	1.62	0.65
3:C:615:ILE:O	3:C:619:ILE:HD12	1.95	0.65
3:B:513:LEU:O	3:B:517:LEU:HD21	1.95	0.65
3:C:377:LEU:HB3	3:C:409:VAL:HG11	1.79	0.65
3:C:565:ALA:HB1	3:C:585:LEU:HD21	1.79	0.65
3:A:607:ASN:ND2	3:A:608:GLU:N	2.45	0.64
3:B:372:LYS:HG2	3:B:376:GLU:OE2	1.96	0.64
3:A:443:THR:HA	3:A:623:MET:HE1	1.78	0.64
3:B:381:LEU:CB	3:B:386:LEU:HD22	2.26	0.64
3:C:425:VAL:HG23	3:C:465:THR:HG22	1.80	0.64
3:A:246:HIS:HB3	3:A:248:ILE:HG22	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:291:GLU:O	3:B:293:HIS:N	2.30	0.64
3:B:243:SER:HA	3:B:248:ILE:O	1.97	0.64
3:B:286:ILE:HG22	3:B:288:ILE:HD11	1.79	0.64
3:C:440:LEU:HD12	3:C:440:LEU:H	1.61	0.64
3:C:615:ILE:HG22	3:C:619:ILE:HD11	1.79	0.64
3:A:620:MET:O	3:A:623:MET:HB2	1.97	0.64
3:A:458:ARG:CD	3:A:480:GLU:HB3	2.27	0.64
3:A:498:GLY:O	3:A:504:LEU:N	2.31	0.64
3:A:333:HIS:ND1	3:A:334:PRO:HD2	2.13	0.64
3:B:212:THR:HG23	3:B:213:LYS:N	2.13	0.63
3:C:225:VAL:HG21	3:C:265:ILE:HD13	1.79	0.63
3:C:214:VAL:N	3:C:215:PRO:HD2	2.13	0.63
3:B:451:VAL:HG22	3:B:452:PRO:N	2.13	0.63
3:C:363:ARG:HD2	3:C:406:VAL:CG1	2.28	0.63
1:D:18:DU:O4	3:B:551:LYS:HD2	1.99	0.63
3:A:343:ASN:HD22	3:A:343:ASN:C	2.00	0.63
3:C:272:LYS:HG3	3:C:276:ASP:OD2	1.98	0.63
3:A:505:THR:HG23	3:A:508:GLU:OE2	1.98	0.63
3:C:347:ILE:HD11	3:C:356:ILE:HG12	1.81	0.63
3:C:282:GLY:O	3:C:284:TYR:N	2.32	0.63
3:B:371:LYS:CD	3:B:371:LYS:H	2.12	0.63
3:C:251:ASN:ND2	3:C:261:THR:H	1.96	0.63
3:C:299:THR:HG23	3:C:300:ILE:N	2.13	0.63
3:C:441:ASP:CG	3:C:601:ARG:HE	2.02	0.63
3:C:616:THR:HA	3:C:619:ILE:HD13	1.81	0.62
3:B:509:THR:O	3:B:513:LEU:HB2	1.99	0.62
3:C:224:LYS:H	3:C:285:ASP:CB	2.11	0.62
3:A:543:ASP:HB2	3:A:566:THR:HG23	1.80	0.62
3:B:576:PRO:O	3:B:577:SER:HB3	1.99	0.62
3:C:286:ILE:HD12	3:C:317:LEU:CB	2.28	0.62
3:A:373:LYS:HD3	3:A:373:LYS:O	2.00	0.62
3:B:616:THR:O	3:B:620:MET:HG3	2.00	0.62
3:C:607:ASN:O	3:C:609:VAL:HG13	1.99	0.62
3:C:273:PHE:CZ	3:C:306:VAL:HG12	2.35	0.62
3:B:402:PRO:HG2	3:B:403:ILE:N	2.14	0.62
3:A:358:ALA:HB1	3:A:474:ARG:NH1	2.14	0.62
3:B:347:ILE:HD11	3:B:356:ILE:HB	1.80	0.62
3:C:557:PHE:CD1	3:C:557:PHE:N	2.68	0.62
3:B:572:GLN:C	3:B:592:LEU:HD23	2.20	0.62
3:C:538:GLY:HA3	3:C:618:TYR:CE2	2.34	0.62
3:B:467:ARG:HH11	3:B:467:ARG:HB2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:473:TYR:CE2	3:B:475:PHE:HB3	2.35	0.62
3:A:242:MET:HE1	3:A:248:ILE:HG21	1.82	0.62
3:C:337:GLU:OE1	3:C:339:ILE:HD11	1.99	0.62
3:C:517:LEU:H	3:C:517:LEU:HD22	1.60	0.61
3:B:517:LEU:HD22	3:B:517:LEU:N	2.15	0.61
3:C:248:ILE:CD1	3:C:265:ILE:HG13	2.17	0.61
3:B:193:VAL:N	3:B:194:PRO:HD3	2.15	0.61
3:B:254:THR:HG22	3:B:255:GLY:N	2.15	0.61
3:C:546:PHE:HD1	3:C:584:CYS:HB2	1.65	0.61
3:A:462:ARG:HG3	3:A:473:TYR:CG	2.34	0.61
3:B:324:THR:HG21	3:B:459:SER:HB2	1.83	0.61
3:B:287:ILE:N	3:B:287:ILE:HD12	2.15	0.61
3:C:287:ILE:HD13	3:C:315:ALA:HB1	1.83	0.61
3:C:378:ALA:O	3:C:382:THR:CG2	2.45	0.61
3:A:242:MET:CE	3:A:248:ILE:HG21	2.31	0.61
1:D:18:DU:O4'	3:A:350:TYR:HA	2.00	0.61
3:A:454:ASP:OD1	3:A:456:VAL:N	2.28	0.61
3:A:513:LEU:O	3:A:517:LEU:CD2	2.49	0.60
3:A:613:HIS:HE1	3:A:615:ILE:HD13	1.64	0.60
3:A:553:ALA:HB3	3:A:555:ASP:OD2	2.01	0.60
3:A:300:ILE:HD12	3:A:490:VAL:HG11	1.83	0.60
3:C:242:MET:HB3	3:C:248:ILE:HG23	1.84	0.60
3:B:344:ASN:C	3:B:355:PRO:HG3	2.22	0.60
3:B:542:ILE:CD1	3:B:547:LEU:HB2	2.31	0.60
3:C:596:THR:H	3:C:609:VAL:HG12	1.66	0.60
3:C:288:ILE:H	3:C:288:ILE:HD12	1.67	0.60
3:A:601:ARG:NH1	3:A:601:ARG:HG3	2.09	0.60
3:B:335:ASN:C	3:B:336:ILE:HG13	2.22	0.60
3:B:242:MET:HG3	3:B:248:ILE:HG21	1.80	0.60
3:C:344:ASN:N	3:C:344:ASN:ND2	2.50	0.60
3:C:602:LEU:O	3:C:602:LEU:HD23	2.01	0.60
3:A:481:ARG:HH21	3:B:588:LEU:HD11	1.66	0.60
3:C:305:THR:OG1	3:C:512:ARG:HD3	2.02	0.60
3:A:346:GLU:CD	3:A:346:GLU:H	2.04	0.60
3:C:287:ILE:HD12	3:C:287:ILE:N	2.16	0.59
3:A:466:GLY:HA2	3:A:471:GLY:H	1.65	0.59
3:B:244:LYS:O	3:B:245:ALA:HB2	2.02	0.59
3:A:210:LYS:NZ	3:A:210:LYS:HB2	2.17	0.59
3:B:288:ILE:HD12	3:B:288:ILE:N	2.17	0.59
3:A:400:ILE:HD12	3:A:408:VAL:HG22	1.83	0.59
3:C:613:HIS:CE1	3:C:615:ILE:HG12	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:446:ILE:HG22	3:A:446:ILE:O	2.01	0.59
3:B:261:THR:HG22	3:B:262:GLY:N	2.16	0.59
3:A:579:ASP:O	3:A:581:MET:N	2.35	0.59
3:C:382:THR:HG21	3:C:388:ALA:O	2.01	0.59
3:B:485:MET:HG2	3:B:524:VAL:C	2.23	0.59
3:A:582:TRP:O	3:A:584:CYS:N	2.35	0.59
3:B:300:ILE:H	3:B:300:ILE:HD12	1.68	0.59
3:A:193:VAL:HG11	3:A:286:ILE:HD11	1.84	0.59
3:A:481:ARG:NH2	3:B:588:LEU:HD11	2.17	0.59
3:C:583:LYS:HA	3:C:586:ILE:CD1	2.31	0.59
3:B:586:ILE:HG23	3:B:587:ARG:N	2.18	0.59
3:A:579:ASP:C	3:A:581:MET:H	2.05	0.59
3:B:226:LEU:HD12	3:B:284:TYR:CE2	2.38	0.59
3:C:472:ILE:HG21	3:C:474:ARG:CZ	2.33	0.59
3:A:193:VAL:HG23	3:A:193:VAL:O	2.02	0.59
3:B:564:GLN:HE22	3:B:599:LEU:H	1.50	0.59
3:B:363:ARG:HA	3:B:363:ARG:NE	2.18	0.59
3:C:588:LEU:CD1	3:C:592:LEU:HD21	2.32	0.59
3:C:365:LEU:C	3:C:366:ILE:HD12	2.23	0.58
3:B:236:LEU:HD12	3:B:252:ILE:CG2	2.33	0.58
3:A:607:ASN:ND2	3:A:608:GLU:H	2.01	0.58
3:B:343:ASN:HD22	3:B:343:ASN:H	1.50	0.58
3:C:365:LEU:HD12	3:C:408:VAL:O	2.03	0.58
3:B:194:PRO:HG2	3:B:198:GLN:OE1	2.04	0.58
1:D:15:DU:H5'	3:B:232:VAL:CG2	2.29	0.58
3:A:343:ASN:ND2	3:A:344:ASN:ND2	2.47	0.58
3:B:344:ASN:ND2	3:B:355:PRO:HG3	2.12	0.58
3:A:363:ARG:HG2	3:A:406:VAL:HG12	1.86	0.58
3:C:402:PRO:CG	3:C:403:ILE:N	2.66	0.58
3:C:615:ILE:HG22	3:C:619:ILE:CD1	2.33	0.58
3:A:381:LEU:O	3:A:386:LEU:HB2	2.04	0.58
3:B:351:GLY:O	3:B:353:ALA:N	2.34	0.58
3:C:596:THR:HB	3:C:609:VAL:CG1	2.33	0.58
3:C:382:THR:HA	3:C:386:LEU:O	2.04	0.58
3:A:495:TYR:CE1	3:A:509:THR:HB	2.39	0.58
3:C:487:ASP:C	3:C:489:SER:H	2.07	0.57
3:B:347:ILE:HG21	3:B:354:ILE:HD11	1.84	0.57
3:A:547:LEU:C	3:A:547:LEU:HD13	2.23	0.57
3:C:566:THR:O	3:C:570:ARG:HG2	2.03	0.57
3:B:216:ALA:HB2	3:B:242:MET:HE1	1.84	0.57
3:B:387:ASN:H	3:B:387:ASN:HD22	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:372:LYS:HE2	3:B:376:GLU:OE2	2.04	0.57
3:C:224:LYS:N	3:C:285:ASP:OD2	2.35	0.57
3:C:498:GLY:HA2	3:C:502:TYR:HD2	1.70	0.57
3:B:379:ALA:HA	3:B:382:THR:HG21	1.79	0.57
3:B:226:LEU:HB2	3:B:284:TYR:CD1	2.40	0.57
3:A:258:THR:O	3:A:259:ILE:HG13	2.05	0.57
3:B:426:ILE:HD13	3:B:474:ARG:HG2	1.86	0.57
3:A:248:ILE:O	3:A:250:PRO:HD3	2.04	0.57
3:C:231:SER:HB3	3:C:234:ALA:HB3	1.85	0.57
3:C:425:VAL:HG11	3:C:461:ARG:O	2.05	0.57
3:C:582:TRP:O	3:C:586:ILE:HG13	2.04	0.57
3:C:509:THR:O	3:C:510:SER:C	2.42	0.57
3:B:248:ILE:HG23	3:B:250:PRO:HD3	1.86	0.57
3:B:244:LYS:O	3:B:245:ALA:CB	2.52	0.57
3:C:511:VAL:O	3:C:514:ARG:HB3	2.05	0.56
3:C:547:LEU:O	3:C:549:GLN:N	2.38	0.56
3:B:350:TYR:CE1	3:B:428:CYS:HB2	2.40	0.56
3:A:202:LEU:O	3:A:203:HIS:ND1	2.38	0.56
3:C:441:ASP:O	3:C:601:ARG:NE	2.38	0.56
3:A:303:ILE:HA	3:A:306:VAL:HG12	1.87	0.56
3:A:265:ILE:CD1	3:A:265:ILE:H	2.18	0.56
3:B:392:TYR:H	3:B:395:LEU:HD12	1.70	0.56
3:B:504:LEU:HA	3:B:508:GLU:OE2	2.05	0.56
3:B:484:GLY:O	3:B:523:PRO:HA	2.05	0.56
3:C:376:GLU:O	3:C:379:ALA:HB3	2.06	0.56
3:B:386:LEU:H	3:B:386:LEU:CD1	2.18	0.56
3:B:367:PHE:O	3:B:428:CYS:HB3	2.05	0.56
3:B:386:LEU:N	3:B:386:LEU:CD1	2.68	0.56
3:B:300:ILE:H	3:B:300:ILE:CD1	2.18	0.56
3:B:349:PHE:C	3:B:351:GLY:N	2.57	0.56
3:A:467:ARG:HG3	3:A:467:ARG:HH11	1.71	0.56
3:A:287:ILE:HG21	3:A:306:VAL:HG21	1.87	0.56
3:A:214:VAL:N	3:A:215:PRO:HD2	2.19	0.56
3:C:611:LEU:N	3:C:611:LEU:HD23	2.21	0.56
3:B:279:CYS:O	3:B:281:GLY:N	2.39	0.56
3:C:568:CYS:HB3	3:C:573:ALA:O	2.05	0.56
3:B:212:THR:HG23	3:B:213:LYS:H	1.69	0.56
3:B:226:LEU:C	3:B:226:LEU:HD23	2.26	0.56
3:C:285:ASP:C	3:C:286:ILE:HD13	2.26	0.56
3:B:373:LYS:HA	3:B:376:GLU:CD	2.26	0.56
3:B:432:VAL:HA	3:B:450:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:226:LEU:HD21	3:B:228:LEU:HD21	1.88	0.55
3:B:487:ASP:OD1	3:B:488:SER:N	2.39	0.55
3:C:253:ARG:HH22	3:C:276:ASP:CG	2.10	0.55
3:A:466:GLY:HA2	3:A:471:GLY:N	2.22	0.55
3:C:371:LYS:HA	3:C:374:CYS:HB2	1.88	0.55
3:B:571:ALA:O	3:B:573:ALA:N	2.40	0.55
3:C:557:PHE:N	3:C:557:PHE:HD1	2.04	0.55
3:A:563:TYR:O	3:A:567:VAL:HG12	2.07	0.55
3:A:364:HIS:O	3:A:407:VAL:HA	2.07	0.55
3:B:297:SER:HB3	3:B:493:GLU:HB3	1.89	0.55
3:B:517:LEU:N	3:B:517:LEU:CD2	2.71	0.54
2:E:7:DU:H5'	3:C:232:VAL:CG2	2.31	0.54
3:C:427:ASP:OD1	3:C:461:ARG:HD3	2.07	0.54
3:B:365:LEU:HD22	3:B:422:PHE:CE1	2.42	0.54
3:B:404:GLY:O	3:B:406:VAL:N	2.41	0.54
3:A:363:ARG:HA	3:A:406:VAL:O	2.07	0.54
3:C:446:ILE:HG22	3:C:446:ILE:O	2.06	0.54
3:A:433:THR:HG22	3:A:434:GLN:H	1.71	0.54
3:B:253:ARG:HB2	3:B:268:SER:HB2	1.88	0.54
3:C:535:VAL:O	3:C:537:THR:N	2.40	0.54
3:C:356:ILE:HD11	3:C:384:LEU:HD13	1.89	0.54
3:B:543:ASP:HB3	3:B:546:PHE:CD2	2.34	0.54
3:C:543:ASP:OD2	3:C:545:HIS:HB3	2.07	0.54
3:A:341:LEU:HD22	3:A:353:ALA:O	2.08	0.54
3:C:475:PHE:CE2	3:C:478:PRO:HA	2.43	0.54
3:A:602:LEU:HD23	3:A:602:LEU:O	2.07	0.54
3:C:366:ILE:HG13	3:C:426:ILE:HB	1.90	0.54
3:A:439:SER:O	3:A:440:LEU:C	2.46	0.54
1:D:14:DU:H6	3:B:413:ALA:CB	2.36	0.54
3:C:425:VAL:HG23	3:C:465:THR:CG2	2.38	0.54
3:A:356:ILE:CG2	3:A:357:GLU:N	2.71	0.54
3:B:295:THR:HA	3:B:300:ILE:HD11	1.90	0.54
3:C:563:TYR:O	3:C:567:VAL:HG23	2.08	0.54
3:C:525:CYS:SG	3:C:526:GLN:N	2.80	0.54
3:B:409:VAL:HG12	3:B:410:ALA:N	2.23	0.54
3:B:232:VAL:HG13	3:B:254:THR:HG21	1.88	0.54
3:C:224:LYS:HB2	3:C:285:ASP:N	2.18	0.54
3:B:274:LEU:HD21	3:B:302:GLY:HA2	1.90	0.54
3:A:320:LEU:HD23	3:A:320:LEU:N	2.22	0.54
3:A:610:ILE:HG22	3:A:612:THR:H	1.73	0.54
3:A:570:ARG:HG3	3:A:570:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:ILE:O	3:A:307:LEU:HB2	2.07	0.54
1:D:17:DU:N3	1:D:19:DU:C2	2.71	0.54
3:C:509:THR:O	3:C:512:ARG:N	2.41	0.53
3:C:517:LEU:H	3:C:517:LEU:CD2	2.19	0.53
3:C:224:LYS:H	3:C:285:ASP:CG	2.11	0.53
3:A:289:CYS:SG	3:A:306:VAL:HG11	2.48	0.53
3:C:341:LEU:CD2	3:C:354:ILE:HD13	2.39	0.53
3:B:346:GLU:OE2	3:B:347:ILE:HG13	2.08	0.53
3:C:615:ILE:CG2	3:C:619:ILE:HD11	2.38	0.53
3:C:288:ILE:N	3:C:288:ILE:HD12	2.24	0.53
3:C:258:THR:O	3:C:259:ILE:HG13	2.08	0.53
3:C:572:GLN:HA	3:C:572:GLN:HE21	1.72	0.53
3:A:535:VAL:HG12	3:A:535:VAL:O	2.09	0.53
3:B:224:LYS:HA	3:B:264:SER:HB2	1.90	0.53
3:C:360:LYS:HZ1	3:C:386:LEU:CD2	2.18	0.53
3:B:296:ASP:OD2	3:B:296:ASP:C	2.46	0.53
3:A:300:ILE:CD1	3:A:490:VAL:HG11	2.38	0.53
3:C:400:ILE:N	3:C:400:ILE:HD12	2.23	0.53
3:C:440:LEU:CD1	3:C:440:LEU:N	2.69	0.53
3:B:364:HIS:HB2	3:B:407:VAL:HG22	1.91	0.53
3:B:426:ILE:HD13	3:B:474:ARG:CB	2.39	0.53
3:B:509:THR:O	3:B:509:THR:HG22	2.07	0.53
3:B:225:VAL:HG12	3:B:226:LEU:N	2.24	0.53
3:A:442:PRO:HB3	3:A:611:LEU:HD22	1.89	0.53
3:A:303:ILE:HG22	3:A:307:LEU:HD12	1.90	0.53
3:B:615:ILE:O	3:B:616:THR:C	2.46	0.53
3:B:567:VAL:HG11	3:B:599:LEU:HD11	1.89	0.53
3:A:418:PHE:CG	3:A:419:THR:N	2.77	0.53
3:B:501:TRP:O	3:B:503:GLU:N	2.41	0.52
3:B:598:LEU:HD12	3:B:609:VAL:HG11	1.90	0.52
3:A:226:LEU:HB2	3:A:284:TYR:CD1	2.44	0.52
3:B:346:GLU:O	3:B:348:PRO:HD3	2.09	0.52
3:A:210:LYS:HB2	3:A:210:LYS:HZ2	1.75	0.52
3:C:514:ARG:CZ	3:C:514:ARG:HB2	2.39	0.52
3:A:344:ASN:N	3:A:344:ASN:ND2	2.58	0.52
3:A:615:ILE:N	3:A:615:ILE:CD1	2.73	0.52
3:B:365:LEU:HD22	3:B:422:PHE:CD1	2.44	0.52
3:B:393:ARG:N	3:B:393:ARG:HD2	2.23	0.52
3:A:396:ASP:O	3:A:399:VAL:HG22	2.09	0.52
3:C:402:PRO:CG	3:C:403:ILE:H	2.21	0.52
3:C:557:PHE:O	3:C:561:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:610:ILE:C	3:A:611:LEU:HG	2.30	0.52
3:A:336:ILE:HD11	3:A:466:GLY:HA3	1.92	0.52
3:B:372:LYS:C	3:B:374:CYS:H	2.13	0.52
3:A:373:LYS:HD3	3:A:373:LYS:C	2.29	0.52
3:C:454:ASP:HA	3:C:481:ARG:O	2.10	0.52
3:A:360:LYS:HE2	3:A:386:LEU:HD21	1.88	0.52
3:C:209:GLY:HA2	3:C:212:THR:HG23	1.92	0.52
3:C:232:VAL:O	3:C:235:THR:HB	2.10	0.52
3:B:387:ASN:ND2	3:B:387:ASN:H	2.07	0.52
3:B:579:ASP:OD1	3:B:581:MET:N	2.39	0.52
3:B:400:ILE:CG2	3:B:419:THR:H	2.23	0.52
3:C:565:ALA:O	3:C:567:VAL:N	2.42	0.52
3:C:366:ILE:HD13	3:C:407:VAL:HG12	1.91	0.52
3:C:588:LEU:HD12	3:C:592:LEU:HD21	1.91	0.52
3:B:389:VAL:CG2	3:B:408:VAL:HG22	2.40	0.52
3:A:516:TYR:CE2	3:A:522:LEU:HD13	2.45	0.52
3:A:367:PHE:O	3:A:428:CYS:HB3	2.10	0.52
3:C:429:ASN:HA	3:C:453:GLN:CD	2.31	0.52
3:B:235:THR:HG22	3:B:236:LEU:N	2.24	0.51
3:B:609:VAL:O	3:B:609:VAL:HG23	2.10	0.51
3:C:549:GLN:HE22	3:C:584:CYS:HA	1.74	0.51
3:B:402:PRO:HG2	3:B:403:ILE:HG22	1.92	0.51
3:C:565:ALA:C	3:C:567:VAL:N	2.63	0.51
3:A:374:CYS:SG	3:A:411:THR:HG23	2.50	0.51
3:C:492:CYS:HB2	3:C:532:TRP:CH2	2.45	0.51
3:C:382:THR:HG22	3:C:388:ALA:HB3	1.92	0.51
3:C:578:TRP:CE3	3:C:586:ILE:HG12	2.45	0.51
3:C:224:LYS:CB	3:C:285:ASP:H	2.18	0.51
3:C:296:ASP:CG	3:C:299:THR:CG2	2.76	0.51
3:B:387:ASN:ND2	3:B:387:ASN:N	2.57	0.51
3:C:543:ASP:O	3:C:545:HIS:N	2.42	0.51
3:A:196:THR:HG22	3:A:197:PHE:H	1.76	0.51
3:A:218:TYR:O	3:A:223:TYR:HB2	2.09	0.51
3:A:398:SER:O	3:A:399:VAL:C	2.48	0.51
3:A:400:ILE:HD11	3:A:408:VAL:CG1	2.40	0.51
3:A:251:ASN:HB3	3:A:260:THR:HA	1.93	0.51
3:B:300:ILE:N	3:B:300:ILE:HD12	2.25	0.51
3:C:272:LYS:HE2	3:C:276:ASP:OD1	2.10	0.51
3:A:360:LYS:HA	3:A:360:LYS:HZ1	1.76	0.51
3:C:330:THR:O	3:C:331:VAL:HG23	2.09	0.51
3:C:426:ILE:N	3:C:426:ILE:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:454:ASP:O	3:B:458:ARG:HB2	2.10	0.51
3:A:356:ILE:HD11	3:A:386:LEU:HD11	1.93	0.51
3:C:214:VAL:N	3:C:215:PRO:CD	2.74	0.51
3:A:508:GLU:O	3:A:511:VAL:HB	2.10	0.51
3:A:231:SER:HB3	3:A:234:ALA:HB3	1.93	0.51
3:B:344:ASN:N	3:B:344:ASN:ND2	2.53	0.51
3:B:193:VAL:HG22	3:B:218:TYR:HE1	1.76	0.51
3:B:488:SER:O	3:B:491:LEU:HB2	2.11	0.51
3:B:360:LYS:HG3	3:B:361:GLY:N	2.26	0.51
2:E:8:DU:OP1	3:C:232:VAL:HG22	2.10	0.51
3:A:618:TYR:O	3:A:621:ALA:N	2.44	0.51
3:B:564:GLN:O	3:B:564:GLN:HG3	2.11	0.51
3:C:392:TYR:CE1	3:C:395:LEU:HG	2.46	0.51
3:B:379:ALA:C	3:B:381:LEU:H	2.14	0.50
3:B:277:GLY:O	3:B:280:SER:HB2	2.11	0.50
3:C:344:ASN:CG	3:C:345:GLY:H	2.14	0.50
3:C:295:THR:CG2	3:C:486:PHE:HD2	2.25	0.50
3:A:605:VAL:O	3:A:605:VAL:HG13	2.10	0.50
3:A:296:ASP:O	3:A:299:THR:HG22	2.12	0.50
3:C:223:TYR:HA	3:C:285:ASP:OD2	2.10	0.50
3:C:224:LYS:HE2	3:C:284:TYR:HA	1.93	0.50
3:C:292:CYS:SG	3:C:321:ALA:O	2.69	0.50
3:B:192:ALA:CB	3:B:194:PRO:HD3	2.42	0.50
3:B:226:LEU:HD23	3:B:227:VAL:N	2.25	0.50
3:B:193:VAL:N	3:B:194:PRO:CD	2.74	0.50
3:B:191:PRO:HD2	3:B:218:TYR:OH	2.11	0.50
3:A:549:GLN:HG2	3:A:584:CYS:HB3	1.93	0.50
3:B:389:VAL:HG23	3:B:408:VAL:HG13	1.93	0.50
3:A:503:GLU:O	3:A:504:LEU:HD23	2.10	0.50
3:B:379:ALA:C	3:B:381:LEU:N	2.65	0.50
3:C:581:MET:HG3	3:C:582:TRP:CD1	2.47	0.50
3:B:491:LEU:O	3:B:495:TYR:HD2	1.94	0.50
3:A:583:LYS:O	3:A:586:ILE:HG12	2.12	0.50
3:C:251:ASN:O	3:C:266:THR:HA	2.11	0.50
3:B:382:THR:C	3:B:384:LEU:H	2.15	0.50
3:C:366:ILE:N	3:C:366:ILE:HD12	2.26	0.50
3:C:514:ARG:CG	3:C:514:ARG:HH11	2.25	0.50
3:C:543:ASP:C	3:C:545:HIS:N	2.65	0.50
3:A:376:GLU:O	3:A:379:ALA:N	2.45	0.49
3:B:369:HIS:HB2	3:B:432:VAL:CG2	2.42	0.49
3:C:366:ILE:HD13	3:C:407:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:467:ARG:NH1	3:B:467:ARG:HB2	2.27	0.49
3:B:373:LYS:HA	3:B:376:GLU:OE2	2.11	0.49
3:B:496:ASP:OD2	3:B:557:PHE:HA	2.11	0.49
3:B:485:MET:CA	3:B:524:VAL:O	2.58	0.49
3:A:273:PHE:CZ	3:A:279:CYS:N	2.80	0.49
3:A:280:SER:HB3	3:A:309:GLN:HE22	1.75	0.49
3:A:399:VAL:HG23	3:A:400:ILE:N	2.27	0.49
3:A:465:THR:C	3:A:467:ARG:H	2.15	0.49
3:A:368:CYS:SG	3:A:373:LYS:HD2	2.52	0.49
3:C:486:PHE:CE1	3:C:525:CYS:HB2	2.46	0.49
3:B:496:ASP:OD2	3:B:558:PRO:HD2	2.12	0.49
3:A:212:THR:O	3:A:215:PRO:HG2	2.12	0.49
3:C:619:ILE:HA	3:C:622:CYS:HB3	1.94	0.49
3:C:291:GLU:C	3:C:293:HIS:H	2.15	0.49
3:B:510:SER:O	3:B:514:ARG:N	2.45	0.49
3:B:468:GLY:C	3:B:469:ARG:HG2	2.31	0.49
3:C:615:ILE:O	3:C:616:THR:C	2.51	0.49
3:A:433:THR:CG2	3:A:434:GLN:N	2.75	0.49
3:B:339:ILE:HG21	3:B:474:ARG:NH1	2.28	0.49
3:A:458:ARG:HD3	3:A:480:GLU:CB	2.37	0.49
3:C:507:ALA:O	3:C:511:VAL:HG23	2.11	0.49
3:B:309:GLN:O	3:B:310:ALA:C	2.50	0.49
3:C:380:LYS:O	3:C:384:LEU:HG	2.12	0.49
3:C:364:HIS:O	3:C:407:VAL:HA	2.12	0.49
3:A:257:ARG:HG3	3:A:258:THR:H	1.77	0.49
3:B:399:VAL:O	3:B:399:VAL:HG12	2.12	0.49
3:A:591:THR:O	3:A:592:LEU:HG	2.13	0.49
3:B:397:VAL:CG2	3:B:400:ILE:HG13	2.43	0.49
3:B:571:ALA:O	3:B:572:GLN:C	2.51	0.49
3:C:477:THR:HG22	3:C:479:GLY:O	2.11	0.49
3:B:434:GLN:HE21	3:B:489:SER:HB2	1.77	0.49
3:B:614:PRO:O	3:B:617:LYS:HB2	2.11	0.49
3:B:378:ALA:C	3:B:382:THR:HG23	2.32	0.49
3:B:347:ILE:CD1	3:B:356:ILE:HB	2.43	0.49
3:C:378:ALA:HB2	3:C:389:VAL:O	2.12	0.49
3:B:210:LYS:N	3:B:210:LYS:CD	2.74	0.49
3:C:411:THR:C	3:C:413:ALA:N	2.64	0.49
3:A:296:ASP:H	3:A:299:THR:CG2	2.26	0.48
3:A:610:ILE:HG22	3:A:611:LEU:N	2.28	0.48
3:A:279:CYS:HB3	3:A:309:GLN:HB2	1.95	0.48
3:B:576:PRO:HB3	3:B:605:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:465:THR:OG1	3:B:466:GLY:N	2.45	0.48
3:A:613:HIS:ND1	3:A:614:PRO:HD2	2.27	0.48
3:A:598:LEU:HD22	3:A:605:VAL:HG21	1.95	0.48
3:B:225:VAL:CG1	3:B:226:LEU:N	2.76	0.48
3:B:564:GLN:HB2	3:B:600:TYR:CE1	2.48	0.48
3:A:270:TYR:OH	3:A:289:CYS:HB3	2.12	0.48
3:B:530:GLU:O	3:B:534:SER:HB3	2.13	0.48
3:B:583:LYS:HD2	3:B:584:CYS:N	2.28	0.48
3:A:356:ILE:HG23	3:A:357:GLU:N	2.27	0.48
3:A:204:ALA:HB3	3:A:210:LYS:HG3	1.94	0.48
3:C:238:PHE:O	3:C:242:MET:HG2	2.12	0.48
3:C:215:PRO:HG2	3:C:216:ALA:H	1.79	0.48
3:B:496:ASP:OD1	3:B:559:TYR:HB3	2.12	0.48
3:A:540:THR:HG23	3:A:541:HIS:CD2	2.48	0.48
3:C:381:LEU:C	3:C:383:GLY:N	2.65	0.48
3:B:201:HIS:HB3	3:B:203:HIS:HE1	1.74	0.48
3:A:509:THR:O	3:A:510:SER:C	2.50	0.48
3:B:555:ASP:O	3:B:556:ASN:C	2.52	0.48
3:C:389:VAL:HG23	3:C:408:VAL:HA	1.95	0.48
3:C:407:VAL:O	3:C:409:VAL:HG23	2.14	0.48
3:C:253:ARG:NH1	3:C:276:ASP:OD1	2.46	0.48
3:C:413:ALA:C	3:C:414:LEU:HD12	2.34	0.48
3:C:448:THR:HG23	3:C:448:THR:O	2.14	0.48
3:C:211:SER:HB2	3:C:227:VAL:HG11	1.96	0.48
3:C:343:ASN:ND2	3:C:343:ASN:N	2.43	0.48
3:A:429:ASN:CA	3:A:453:GLN:NE2	2.75	0.48
3:C:253:ARG:HH12	3:C:276:ASP:CG	2.17	0.48
1:D:24:DU:H5	3:A:393:ARG:NE	2.29	0.48
3:A:376:GLU:O	3:A:378:ALA:N	2.47	0.48
3:B:254:THR:HG22	3:B:255:GLY:H	1.77	0.48
3:C:487:ASP:C	3:C:489:SER:N	2.67	0.48
3:A:513:LEU:O	3:A:517:LEU:HD22	2.13	0.48
3:B:371:LYS:N	3:B:371:LYS:HE3	2.22	0.48
3:B:253:ARG:HB2	3:B:268:SER:CB	2.44	0.48
3:A:437:ASP:O	3:A:438:PHE:C	2.51	0.48
3:C:516:TYR:HB3	3:C:517:LEU:HD22	1.94	0.47
3:C:286:ILE:CD1	3:C:317:LEU:HB3	2.39	0.47
3:B:272:LYS:HE3	3:B:276:ASP:OD2	2.14	0.47
3:C:509:THR:O	3:C:511:VAL:N	2.47	0.47
3:B:389:VAL:O	3:B:390:ALA:HB2	2.14	0.47
3:A:596:THR:HG23	3:A:597:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:492:CYS:SG	3:A:560:LEU:HD11	2.54	0.47
3:A:601:ARG:NH1	3:A:601:ARG:CG	2.74	0.47
3:B:573:ALA:C	3:B:592:LEU:HD22	2.34	0.47
3:B:389:VAL:HG23	3:B:408:VAL:HG22	1.96	0.47
3:C:496:ASP:OD1	3:C:496:ASP:C	2.52	0.47
3:B:345:GLY:HA3	3:B:355:PRO:CA	2.37	0.47
3:B:286:ILE:HD13	3:B:317:LEU:CB	2.25	0.47
3:B:551:LYS:CG	3:B:552:GLN:N	2.77	0.47
3:C:615:ILE:O	3:C:618:TYR:HB3	2.14	0.47
3:C:565:ALA:O	3:C:568:CYS:N	2.47	0.47
3:C:404:GLY:O	3:C:405:ASP:C	2.53	0.47
3:B:612:THR:O	3:B:613:HIS:C	2.52	0.47
3:A:382:THR:HA	3:A:386:LEU:O	2.14	0.47
3:B:485:MET:HG2	3:B:524:VAL:O	2.14	0.47
3:B:617:LYS:O	3:B:618:TYR:C	2.53	0.47
3:C:270:TYR:O	3:C:274:LEU:HD12	2.14	0.47
3:B:458:ARG:HG2	3:B:458:ARG:NH1	2.27	0.47
3:B:397:VAL:O	3:B:400:ILE:CG1	2.56	0.47
3:B:561:VAL:O	3:B:561:VAL:HG12	2.15	0.47
3:A:469:ARG:O	3:A:469:ARG:HG3	2.14	0.47
3:A:617:LYS:O	3:A:620:MET:HB3	2.15	0.47
3:A:621:ALA:C	3:A:623:MET:N	2.67	0.47
3:B:393:ARG:NH1	3:B:413:ALA:HB3	2.20	0.47
3:B:564:GLN:NE2	3:B:599:LEU:H	2.13	0.47
3:B:372:LYS:C	3:B:374:CYS:N	2.68	0.47
3:C:392:TYR:CZ	3:C:395:LEU:HD11	2.49	0.47
3:C:623:MET:O	3:C:624:SER:OG	2.30	0.47
1:D:25:DU:H5"	3:A:232:VAL:HG23	1.96	0.47
3:B:514:ARG:O	3:B:517:LEU:N	2.43	0.47
3:C:390:ALA:HB3	5:C:38:HOH:O	2.14	0.47
3:A:595:PRO:CB	3:A:608:GLU:HG3	2.42	0.47
3:C:239:GLY:HA2	3:C:250:PRO:HG3	1.95	0.47
3:C:547:LEU:C	3:C:549:GLN:N	2.68	0.47
3:C:453:GLN:HB2	3:C:457:SER:HB3	1.95	0.47
3:B:381:LEU:HD13	3:B:386:LEU:HD22	1.95	0.47
3:B:391:TYR:HD2	3:B:413:ALA:O	1.97	0.47
3:C:299:THR:HG23	3:C:300:ILE:H	1.78	0.47
3:A:436:VAL:HG12	3:A:487:ASP:OD2	2.15	0.47
3:B:462:ARG:HG2	3:B:462:ARG:O	2.14	0.47
3:B:366:ILE:HA	3:B:426:ILE:HB	1.96	0.47
3:C:588:LEU:HD11	3:C:592:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:492:CYS:SG	3:C:560:LEU:HD11	2.53	0.47
3:C:286:ILE:C	3:C:287:ILE:HD12	2.34	0.47
3:B:485:MET:HG3	3:B:524:VAL:HG23	1.95	0.47
3:B:213:LYS:HB2	3:B:213:LYS:NZ	2.29	0.47
3:C:325:PRO:HA	3:C:326:PRO:HD3	1.83	0.47
3:C:342:SER:C	3:C:344:ASN:H	2.18	0.46
3:C:425:VAL:CG2	3:C:465:THR:HG22	2.44	0.46
3:A:400:ILE:HG22	3:A:401:PRO:O	2.14	0.46
3:B:336:ILE:O	3:B:338:GLU:N	2.49	0.46
3:B:512:ARG:HH11	3:B:512:ARG:HG3	1.79	0.46
3:A:412:ASP:O	3:A:413:ALA:HB2	2.15	0.46
3:B:563:TYR:C	3:B:565:ALA:H	2.19	0.46
3:A:398:SER:O	3:A:400:ILE:N	2.48	0.46
3:A:290:ASP:O	3:A:291:GLU:C	2.54	0.46
3:C:439:SER:O	3:C:440:LEU:C	2.53	0.46
3:A:336:ILE:CD1	3:A:466:GLY:HA3	2.43	0.46
3:B:496:ASP:OD2	3:B:557:PHE:CA	2.64	0.46
3:B:445:THR:HA	3:B:601:ARG:O	2.14	0.46
3:A:377:LEU:O	3:A:381:LEU:HG	2.16	0.46
3:A:339:ILE:O	3:A:474:ARG:HA	2.16	0.46
3:C:598:LEU:HD11	3:C:600:TYR:O	2.15	0.46
3:B:600:TYR:O	3:B:600:TYR:HD1	1.98	0.46
3:B:253:ARG:CB	3:B:268:SER:HB2	2.44	0.46
3:B:408:VAL:HG12	3:B:409:VAL:N	2.30	0.46
3:B:409:VAL:O	3:B:410:ALA:HB2	2.16	0.46
3:B:451:VAL:HG23	3:B:452:PRO:HD3	1.97	0.46
3:C:421:ASP:HA	3:C:464:ARG:O	2.16	0.46
3:B:572:GLN:CD	3:B:572:GLN:N	2.68	0.46
3:B:462:ARG:HG3	3:B:473:TYR:CD1	2.51	0.46
3:C:596:THR:O	3:C:609:VAL:HB	2.15	0.46
3:B:365:LEU:HG	3:B:365:LEU:O	2.15	0.46
3:A:274:LEU:HB3	3:A:502:TYR:CD1	2.51	0.46
3:C:432:VAL:HG12	3:C:450:THR:HG22	1.98	0.46
3:B:452:PRO:HG2	3:C:331:VAL:CG1	2.41	0.46
3:A:477:THR:HG23	3:B:544:ALA:HB3	1.97	0.46
3:B:301:LEU:CD2	3:B:512:ARG:HD3	2.46	0.46
3:A:618:TYR:O	3:A:619:ILE:C	2.52	0.46
3:C:300:ILE:CD1	3:C:490:VAL:HG11	2.40	0.46
3:C:190:PRO:CB	3:C:214:VAL:HG13	2.39	0.46
3:A:305:THR:OG1	3:A:512:ARG:NH1	2.49	0.46
3:B:192:ALA:O	3:B:317:LEU:HD22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:427:ASP:OD2	3:B:461:ARG:HD2	2.16	0.46
3:A:226:LEU:HD12	3:A:227:VAL:N	2.30	0.46
2:E:6:DU:O5'	3:C:393:ARG:NH1	2.48	0.46
3:C:367:PHE:HE1	3:C:412:ASP:HA	1.79	0.46
3:B:486:PHE:N	3:B:524:VAL:O	2.46	0.46
3:C:564:GLN:OE1	3:C:564:GLN:O	2.32	0.46
3:C:435:THR:HB	3:C:487:ASP:OD1	2.16	0.46
3:B:303:ILE:O	3:B:307:LEU:HG	2.15	0.46
3:B:497:ALA:O	3:B:500:ALA:N	2.49	0.46
3:B:563:TYR:C	3:B:565:ALA:N	2.69	0.46
3:B:408:VAL:CG1	3:B:409:VAL:N	2.79	0.46
3:C:372:LYS:C	3:C:372:LYS:HD3	2.36	0.46
3:C:382:THR:CG2	3:C:388:ALA:HB3	2.45	0.45
3:A:578:TRP:CZ3	3:A:585:LEU:O	2.70	0.45
3:B:392:TYR:HB2	3:B:395:LEU:HD11	1.98	0.45
3:C:535:VAL:HG12	3:C:536:PHE:N	2.32	0.45
3:A:469:ARG:HB2	3:A:469:ARG:HH11	0.57	0.45
3:B:450:THR:OG1	3:B:451:VAL:N	2.49	0.45
3:C:615:ILE:O	3:C:618:TYR:N	2.50	0.45
3:B:361:GLY:HA2	3:B:407:VAL:CG2	2.44	0.45
3:B:599:LEU:HD22	3:B:615:ILE:HG22	1.98	0.45
3:B:373:LYS:HA	3:B:376:GLU:CG	2.46	0.45
3:C:543:ASP:C	3:C:545:HIS:H	2.20	0.45
3:A:362:GLY:HA3	3:A:423:ASP:OD2	2.15	0.45
3:C:595:PRO:HB2	3:C:609:VAL:HA	1.98	0.45
3:A:495:TYR:CD1	3:A:509:THR:HB	2.52	0.45
3:B:466:GLY:HA2	3:B:471:GLY:HA3	1.99	0.45
3:C:349:PHE:CE2	3:C:426:ILE:HG22	2.51	0.45
3:A:442:PRO:HB3	3:A:611:LEU:CD2	2.46	0.45
3:A:611:LEU:HD12	5:A:56:HOH:O	2.16	0.45
3:C:616:THR:O	3:C:617:LYS:C	2.55	0.45
3:C:381:LEU:C	3:C:383:GLY:H	2.19	0.45
3:A:429:ASN:ND2	3:A:453:GLN:NE2	2.46	0.45
3:C:425:VAL:HB	3:C:473:TYR:HD1	1.81	0.45
3:B:586:ILE:CG2	3:B:587:ARG:N	2.77	0.45
3:A:429:ASN:HA	3:A:453:GLN:HE22	1.77	0.45
3:B:400:ILE:HD11	3:B:418:PHE:HD2	1.82	0.45
3:B:371:LYS:HB3	3:B:392:TYR:HD2	1.81	0.45
3:C:508:GLU:O	3:C:511:VAL:HB	2.16	0.45
3:B:292:CYS:SG	3:B:322:THR:CG2	3.05	0.45
3:B:327:GLY:O	3:B:328:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:578:TRP:O	3:C:579:ASP:O	2.34	0.45
3:C:299:THR:CG2	3:C:300:ILE:N	2.78	0.45
3:B:485:MET:CG	3:B:524:VAL:HG23	2.46	0.45
3:B:591:THR:O	3:B:592:LEU:HG	2.17	0.45
3:C:575:PRO:O	3:C:576:PRO:O	2.34	0.45
3:C:547:LEU:C	3:C:549:GLN:H	2.20	0.45
3:B:561:VAL:O	3:B:561:VAL:CG1	2.65	0.45
3:A:323:ALA:O	3:A:324:THR:HG23	2.16	0.45
3:A:296:ASP:O	3:A:297:SER:C	2.54	0.45
3:B:492:CYS:O	3:B:495:TYR:HB2	2.17	0.45
3:C:546:PHE:CD1	3:C:584:CYS:HB2	2.47	0.45
3:A:557:PHE:O	3:A:561:VAL:HG23	2.17	0.45
3:B:520:PRO:HA	3:C:213:LYS:NZ	2.32	0.45
3:A:406:VAL:HG22	3:A:407:VAL:N	2.32	0.45
3:C:460:GLN:CA	3:C:460:GLN:HE21	2.23	0.45
3:B:426:ILE:HD13	3:B:474:ARG:HB2	1.99	0.45
3:A:555:ASP:O	3:A:558:PRO:HD3	2.16	0.45
3:A:604:ALA:O	3:A:606:GLN:HG3	2.16	0.45
3:A:350:TYR:CE1	3:A:428:CYS:HB2	2.52	0.44
3:B:299:THR:HG22	3:B:303:ILE:CD1	2.47	0.44
3:A:577:SER:HB3	3:A:606:GLN:HG3	1.99	0.44
3:B:436:VAL:HG22	3:B:437:ASP:N	2.32	0.44
3:C:469:ARG:O	3:C:470:SER:O	2.35	0.44
3:B:346:GLU:O	3:B:348:PRO:CD	2.65	0.44
3:B:286:ILE:HG22	3:B:288:ILE:CD1	2.45	0.44
3:C:545:HIS:O	3:C:546:PHE:C	2.55	0.44
3:B:433:THR:O	3:B:435:THR:HG23	2.17	0.44
3:C:603:GLY:O	3:C:604:ALA:C	2.55	0.44
3:B:513:LEU:HD13	3:B:517:LEU:HD21	1.99	0.44
3:C:407:VAL:HG12	3:C:407:VAL:O	2.18	0.44
3:A:433:THR:CG2	3:A:434:GLN:H	2.30	0.44
3:A:579:ASP:C	3:A:581:MET:N	2.69	0.44
3:C:517:LEU:HG	3:C:529:LEU:HD11	1.99	0.44
3:B:369:HIS:HB2	3:B:432:VAL:HG23	1.98	0.44
3:B:382:THR:CG2	3:B:386:LEU:O	2.52	0.44
3:C:305:THR:O	3:C:307:LEU:N	2.51	0.44
3:B:579:ASP:OD1	3:B:580:GLN:N	2.51	0.44
3:B:497:ALA:O	3:B:499:CYS:N	2.50	0.44
3:B:339:ILE:HG21	3:B:474:ARG:HH11	1.82	0.44
3:C:288:ILE:HA	3:C:319:VAL:HB	1.98	0.44
3:A:598:LEU:CD2	3:A:605:VAL:HG21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:379:ALA:O	3:B:381:LEU:N	2.51	0.44
3:A:226:LEU:HD11	3:A:228:LEU:CD2	2.48	0.44
3:A:226:LEU:HD11	3:A:228:LEU:HD21	1.98	0.44
3:C:445:THR:OG1	3:C:601:ARG:HB2	2.18	0.44
3:C:257:ARG:HH11	3:C:257:ARG:HG2	1.83	0.44
3:B:270:TYR:O	3:B:273:PHE:HB3	2.18	0.44
3:B:341:LEU:HD23	3:B:476:VAL:HG22	2.00	0.44
3:A:595:PRO:HG2	3:A:610:ILE:HD11	1.99	0.44
3:B:372:LYS:O	3:B:374:CYS:N	2.51	0.44
3:A:389:VAL:HG23	3:A:389:VAL:O	2.18	0.44
3:A:214:VAL:HB	3:A:215:PRO:CD	2.47	0.43
3:B:226:LEU:CD2	3:B:228:LEU:HG	2.48	0.43
3:A:257:ARG:CG	3:A:258:THR:H	2.29	0.43
3:B:291:GLU:C	3:B:293:HIS:H	2.20	0.43
3:C:301:LEU:HD12	3:C:301:LEU:O	2.18	0.43
3:A:219:ALA:C	3:A:221:GLN:H	2.21	0.43
3:B:381:LEU:CD1	3:B:386:LEU:HD22	2.49	0.43
3:C:300:ILE:HD12	3:C:490:VAL:CG1	2.45	0.43
3:A:542:ILE:HD11	3:A:562:ALA:HB3	2.00	0.43
3:B:221:GLN:HB2	3:B:223:TYR:CD2	2.53	0.43
3:B:514:ARG:HD3	3:B:529:LEU:CD1	2.49	0.43
3:C:356:ILE:O	3:C:356:ILE:HG22	2.18	0.43
3:A:464:ARG:NH2	3:A:467:ARG:NH2	2.66	0.43
3:B:212:THR:CG2	3:B:213:LYS:N	2.80	0.43
3:C:346:GLU:OE1	3:C:346:GLU:N	2.52	0.43
3:B:414:LEU:HD23	3:B:464:ARG:HG3	2.00	0.43
3:A:325:PRO:O	3:A:328:SER:HB2	2.18	0.43
3:A:330:THR:OG1	3:A:480:GLU:HG2	2.18	0.43
3:A:615:ILE:O	3:A:616:THR:C	2.56	0.43
3:B:434:GLN:NE2	3:B:489:SER:HB2	2.33	0.43
3:A:607:ASN:O	3:A:609:VAL:HG13	2.19	0.43
3:C:621:ALA:C	3:C:623:MET:H	2.21	0.43
3:B:532:TRP:O	3:B:533:GLU:C	2.54	0.43
3:C:214:VAL:H	3:C:215:PRO:HD2	1.83	0.43
3:C:596:THR:N	3:C:609:VAL:HG12	2.32	0.43
3:C:429:ASN:HD21	3:C:475:PHE:HB2	1.83	0.43
3:C:381:LEU:HD13	3:C:407:VAL:HG11	2.01	0.43
3:B:454:ASP:HA	3:B:481:ARG:HB3	1.99	0.43
3:C:565:ALA:CB	3:C:585:LEU:HD11	2.48	0.43
3:C:256:VAL:O	3:C:257:ARG:HG3	2.19	0.43
3:A:248:ILE:HG23	3:A:248:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:258:THR:C	3:A:259:ILE:HG13	2.38	0.43
3:B:564:GLN:HA	3:B:599:LEU:HD12	2.01	0.43
3:B:426:ILE:HA	3:B:474:ARG:HB2	1.99	0.43
3:C:396:ASP:HA	5:C:49:HOH:O	2.19	0.43
3:C:565:ALA:C	3:C:567:VAL:H	2.22	0.43
3:A:379:ALA:O	3:A:380:LYS:C	2.57	0.43
3:B:403:ILE:CG1	3:B:404:GLY:N	2.55	0.43
3:B:491:LEU:CD2	3:B:525:CYS:SG	3.03	0.43
3:B:540:THR:O	3:B:563:TYR:OH	2.29	0.43
3:B:501:TRP:CE3	3:B:551:LYS:HD3	2.53	0.43
3:C:618:TYR:O	3:C:622:CYS:HB2	2.17	0.43
1:D:17:DU:O2	1:D:17:DU:C2'	2.67	0.43
3:C:359:ILE:HG13	3:C:360:LYS:N	2.34	0.43
3:B:467:ARG:C	3:B:469:ARG:H	2.22	0.43
3:A:257:ARG:HG2	3:A:257:ARG:HH11	1.84	0.43
3:B:203:HIS:CD2	3:B:325:PRO:CG	2.98	0.43
3:C:596:THR:HB	3:C:609:VAL:HG11	1.99	0.43
3:B:279:CYS:C	3:B:281:GLY:N	2.72	0.43
3:C:291:GLU:O	3:C:293:HIS:N	2.50	0.43
3:A:360:LYS:HZ3	3:A:386:LEU:HD21	0.59	0.43
3:B:450:THR:O	3:B:451:VAL:HB	2.18	0.43
3:B:226:LEU:HD21	3:B:228:LEU:CD2	2.49	0.43
3:B:286:ILE:C	3:B:287:ILE:HD12	2.38	0.43
3:B:317:LEU:HG	3:B:318:VAL:N	2.34	0.43
3:B:429:ASN:ND2	3:B:476:VAL:H	2.17	0.43
3:A:305:THR:O	3:A:309:GLN:HG3	2.19	0.43
3:C:588:LEU:O	3:C:588:LEU:HD12	2.19	0.43
3:B:279:CYS:C	3:B:281:GLY:H	2.21	0.43
3:B:409:VAL:CG1	3:B:410:ALA:N	2.82	0.43
3:A:419:THR:HG22	3:A:419:THR:O	2.19	0.43
3:C:458:ARG:O	3:C:459:SER:C	2.57	0.43
3:A:622:CYS:O	3:A:624:SER:N	2.52	0.42
3:C:383:GLY:C	3:C:385:GLY:H	2.22	0.42
3:B:254:THR:HB	3:B:257:ARG:O	2.18	0.42
3:C:232:VAL:O	3:C:235:THR:N	2.52	0.42
3:B:497:ALA:C	3:B:499:CYS:N	2.72	0.42
3:C:253:ARG:HB3	3:C:253:ARG:NH1	2.34	0.42
3:A:465:THR:OG1	3:A:466:GLY:N	2.52	0.42
3:B:360:LYS:HG3	3:B:361:GLY:H	1.84	0.42
3:C:526:GLN:NE2	3:C:526:GLN:H	2.16	0.42
3:B:396:ASP:C	3:B:398:SER:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:297:SER:CB	3:A:493:GLU:HG2	2.46	0.42
3:B:287:ILE:HD11	3:B:315:ALA:HB2	2.01	0.42
3:A:225:VAL:CG2	3:A:265:ILE:HA	2.38	0.42
3:C:461:ARG:O	3:C:464:ARG:HG2	2.19	0.42
3:A:366:ILE:HG22	3:A:367:PHE:N	2.34	0.42
3:A:226:LEU:HD12	3:A:227:VAL:H	1.83	0.42
3:B:241:TYR:CD1	3:B:241:TYR:C	2.93	0.42
3:C:516:TYR:C	3:C:517:LEU:HD22	2.37	0.42
3:A:210:LYS:HA	3:A:214:VAL:CG2	2.49	0.42
3:C:381:LEU:O	3:C:384:LEU:N	2.52	0.42
3:B:232:VAL:O	3:B:235:THR:N	2.52	0.42
3:C:251:ASN:ND2	3:C:261:THR:OG1	2.51	0.42
3:C:616:THR:O	3:C:619:ILE:N	2.52	0.42
3:C:571:ALA:O	3:C:573:ALA:N	2.51	0.42
3:B:372:LYS:O	3:B:376:GLU:HG3	2.20	0.42
3:C:331:VAL:HG12	3:C:331:VAL:O	2.19	0.42
3:B:576:PRO:CD	3:B:596:THR:HG21	2.49	0.42
3:C:514:ARG:CG	3:C:514:ARG:NH1	2.81	0.42
3:B:566:THR:HG22	3:B:570:ARG:HD2	2.01	0.42
3:C:337:GLU:CD	3:C:339:ILE:HD11	2.40	0.42
3:C:492:CYS:HB2	3:C:532:TRP:CZ2	2.55	0.42
3:A:322:THR:OG1	3:A:323:ALA:N	2.53	0.42
3:B:519:THR:HG23	3:B:520:PRO:HD2	2.01	0.42
3:B:439:SER:O	3:B:440:LEU:C	2.57	0.42
3:A:441:ASP:CG	3:A:441:ASP:O	2.58	0.42
3:A:475:PHE:CD1	3:A:475:PHE:N	2.86	0.42
3:B:560:LEU:HA	3:B:560:LEU:HD12	1.77	0.42
3:A:512:ARG:HH11	3:A:512:ARG:HG3	1.84	0.42
3:C:239:GLY:HA3	3:C:252:ILE:CD1	2.48	0.42
3:A:366:ILE:CG2	3:A:367:PHE:N	2.82	0.42
3:A:333:HIS:CD2	3:A:336:ILE:HD12	2.55	0.42
3:B:599:LEU:HD22	3:B:615:ILE:CG2	2.49	0.42
3:B:229:ASN:HD22	3:B:231:SER:H	1.67	0.42
3:C:441:ASP:OD2	3:C:601:ARG:NE	2.52	0.42
3:C:547:LEU:O	3:C:550:THR:N	2.52	0.42
3:A:531:PHE:CE1	3:A:535:VAL:CG2	3.03	0.42
3:B:226:LEU:C	3:B:226:LEU:CD2	2.88	0.42
1:D:20:DU:O5'	1:D:20:DU:H6	2.19	0.42
3:C:258:THR:C	3:C:259:ILE:HD12	2.39	0.42
3:C:203:HIS:CD2	3:C:322:THR:HG22	2.55	0.42
3:A:395:LEU:HD23	3:A:395:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:265:ILE:HD12	3:B:265:ILE:N	2.35	0.42
3:C:402:PRO:HG2	3:C:403:ILE:N	2.34	0.42
1:D:20:DU:H3	3:A:372:LYS:HG2	1.84	0.42
3:C:599:LEU:HD22	3:C:615:ILE:CG2	2.49	0.42
3:C:339:ILE:O	3:C:474:ARG:HG3	2.20	0.42
3:B:425:VAL:HG23	3:B:465:THR:HB	2.01	0.42
3:C:484:GLY:O	3:C:485:MET:HB2	2.19	0.42
3:B:506:PRO:HG2	3:B:537:THR:HA	2.02	0.42
3:A:297:SER:HB3	3:A:493:GLU:CG	2.47	0.42
3:C:578:TRP:NE1	3:C:589:LYS:NZ	2.67	0.42
3:A:615:ILE:N	3:A:615:ILE:HD12	2.34	0.42
3:B:326:PRO:HG3	3:B:523:PRO:HG3	2.01	0.42
3:B:389:VAL:HG12	3:B:399:VAL:HG12	2.02	0.42
3:A:557:PHE:HB3	3:A:560:LEU:HB2	2.02	0.42
3:C:338:GLU:HG2	3:C:338:GLU:H	1.52	0.42
3:A:443:THR:CA	3:A:623:MET:HE1	2.49	0.42
3:C:578:TRP:CE2	3:C:589:LYS:NZ	2.88	0.42
3:A:477:THR:CG2	3:B:544:ALA:HB3	2.50	0.42
3:B:563:TYR:O	3:B:565:ALA:N	2.53	0.42
3:A:345:GLY:HA3	3:A:353:ALA:HB1	2.02	0.42
3:C:480:GLU:HG2	3:C:481:ARG:N	2.35	0.42
3:A:202:LEU:HD23	3:A:202:LEU:HA	1.81	0.42
3:B:505:THR:C	3:B:507:ALA:N	2.71	0.42
3:C:341:LEU:HD11	3:C:354:ILE:HD11	2.02	0.41
3:B:519:THR:HG23	3:B:520:PRO:CD	2.50	0.41
3:A:420:GLY:O	3:A:421:ASP:C	2.57	0.41
2:E:8:DU:H3'	2:E:8:DU:H6	2.02	0.41
3:C:412:ASP:OD1	3:C:461:ARG:NH2	2.52	0.41
3:B:543:ASP:CB	3:B:546:PHE:HD2	2.23	0.41
3:C:617:LYS:O	3:C:620:MET:HB3	2.20	0.41
3:B:333:HIS:HB3	3:B:336:ILE:HD12	2.02	0.41
3:B:225:VAL:HG22	3:B:286:ILE:HB	2.01	0.41
3:C:381:LEU:O	3:C:383:GLY:N	2.54	0.41
3:B:341:LEU:O	3:B:352:LYS:HG3	2.20	0.41
3:A:279:CYS:O	3:A:280:SER:C	2.58	0.41
3:B:209:GLY:HA2	3:B:212:THR:CG2	2.50	0.41
3:C:608:GLU:O	3:C:609:VAL:HG13	2.20	0.41
3:B:504:LEU:HD21	3:B:512:ARG:NH2	2.36	0.41
3:A:425:VAL:HG12	3:A:425:VAL:O	2.21	0.41
3:C:210:LYS:HG3	4:C:102:SO4:O3	2.21	0.41
3:A:458:ARG:O	3:A:458:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:564:GLN:HE22	3:B:598:LEU:HA	1.85	0.41
3:A:519:THR:HA	3:A:520:PRO:HD3	1.70	0.41
3:B:240:ALA:C	3:B:242:MET:N	2.73	0.41
3:B:467:ARG:O	3:B:469:ARG:N	2.48	0.41
3:C:190:PRO:HG2	5:C:4:HOH:O	2.20	0.41
3:A:193:VAL:HG21	3:A:223:TYR:CZ	2.55	0.41
3:C:391:TYR:CG	3:C:392:TYR:N	2.88	0.41
3:B:519:THR:HA	3:B:520:PRO:HD3	1.76	0.41
3:C:597:PRO:HA	3:C:610:ILE:O	2.19	0.41
3:C:407:VAL:O	3:C:408:VAL:C	2.58	0.41
3:B:397:VAL:HG23	3:B:400:ILE:HG13	2.02	0.41
3:B:210:LYS:H	3:B:210:LYS:CD	2.31	0.41
3:C:596:THR:HB	3:C:609:VAL:HG12	2.01	0.41
3:B:511:VAL:HG13	3:B:512:ARG:N	2.36	0.41
1:D:17:DU:H3	1:D:19:DU:C2	2.32	0.41
3:C:270:TYR:OH	3:C:289:CYS:HB3	2.20	0.41
3:A:321:ALA:O	3:A:322:THR:HB	2.20	0.41
3:A:535:VAL:O	3:A:539:LEU:HG	2.20	0.41
3:B:393:ARG:HG3	3:B:393:ARG:NH1	2.35	0.41
3:A:547:LEU:C	3:A:547:LEU:CD1	2.88	0.41
3:C:619:ILE:O	3:C:622:CYS:N	2.54	0.41
3:B:229:ASN:ND2	3:B:230:PRO:CD	2.82	0.41
3:C:341:LEU:HB3	3:C:352:LYS:HB3	2.03	0.41
2:E:6:DU:H5"	3:C:393:ARG:NH2	2.36	0.41
3:A:421:ASP:HA	5:A:5:HOH:O	2.19	0.41
3:A:621:ALA:C	3:A:623:MET:H	2.24	0.41
3:B:378:ALA:O	3:B:382:THR:HG22	2.17	0.41
3:C:378:ALA:CB	3:C:389:VAL:O	2.69	0.41
3:B:443:THR:HG21	3:B:619:ILE:CG2	2.50	0.41
3:C:341:LEU:HD22	3:C:354:ILE:HD13	2.02	0.41
3:C:454:ASP:OD2	3:C:454:ASP:N	2.51	0.41
3:A:365:LEU:HD22	3:A:414:LEU:HD23	2.01	0.41
3:B:254:THR:CG2	3:B:255:GLY:N	2.82	0.41
3:B:393:ARG:HG3	3:B:393:ARG:HH11	1.85	0.41
3:B:458:ARG:CG	3:B:458:ARG:NH1	2.83	0.41
3:A:610:ILE:HG22	3:A:611:LEU:H	1.85	0.41
3:B:596:THR:O	3:B:598:LEU:N	2.50	0.41
3:C:508:GLU:O	3:C:509:THR:C	2.58	0.41
3:A:505:THR:O	3:A:506:PRO:C	2.59	0.41
3:C:346:GLU:OE1	3:C:355:PRO:HA	2.21	0.41
3:B:595:PRO:HB2	3:B:610:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:ASN:ND2	3:C:344:ASN:H	1.98	0.41
3:A:335:ASN:O	3:A:336:ILE:HG12	2.21	0.41
3:B:396:ASP:C	3:B:398:SER:N	2.74	0.41
3:B:602:LEU:HD12	3:B:602:LEU:HA	1.85	0.41
3:A:355:PRO:O	3:A:356:ILE:C	2.59	0.40
3:A:360:LYS:HZ2	3:A:360:LYS:HA	1.86	0.40
3:B:219:ALA:HB2	3:B:265:ILE:CG1	2.51	0.40
3:B:264:SER:O	3:B:265:ILE:HD12	2.22	0.40
3:B:347:ILE:HB	3:B:354:ILE:O	2.21	0.40
3:B:381:LEU:HD13	3:B:386:LEU:CD2	2.51	0.40
3:B:192:ALA:C	3:B:194:PRO:HD3	2.41	0.40
3:A:427:ASP:OD2	3:A:428:CYS:N	2.54	0.40
3:C:319:VAL:C	3:C:320:LEU:HD12	2.42	0.40
3:C:242:MET:HG3	3:C:267:TYR:CE2	2.56	0.40
3:A:592:LEU:HA	3:A:592:LEU:HD23	1.92	0.40
3:A:562:ALA:O	3:A:565:ALA:HB3	2.20	0.40
3:C:203:HIS:CD2	3:C:322:THR:CG2	3.04	0.40
3:B:505:THR:OG1	3:B:507:ALA:HB3	2.22	0.40
3:A:210:LYS:HA	3:A:214:VAL:HG21	2.04	0.40
3:B:568:CYS:O	3:B:573:ALA:O	2.39	0.40
3:A:550:THR:O	3:A:551:LYS:C	2.59	0.40
3:B:209:GLY:HA2	3:B:212:THR:HG22	2.02	0.40
3:B:209:GLY:O	3:B:213:LYS:N	2.50	0.40
3:B:212:THR:CG2	3:B:213:LYS:H	2.34	0.40
3:A:307:LEU:HD13	3:A:519:THR:HG21	2.03	0.40
3:A:575:PRO:O	3:A:576:PRO:C	2.59	0.40
3:A:326:PRO:HG2	3:A:521:GLY:O	2.22	0.40
3:A:344:ASN:N	3:A:344:ASN:HD22	2.19	0.40
3:C:253:ARG:NH2	3:C:276:ASP:CG	2.72	0.40
3:A:512:ARG:NH1	3:A:512:ARG:HG3	2.36	0.40
3:C:598:LEU:HD12	3:C:599:LEU:H	1.87	0.40
3:B:229:ASN:CG	3:B:230:PRO:HD2	2.40	0.40
3:C:575:PRO:HB3	3:C:585:LEU:HD12	2.02	0.40
3:C:258:THR:HG22	3:C:259:ILE:N	2.36	0.40
3:A:619:ILE:O	3:A:622:CYS:N	2.55	0.40
3:B:232:VAL:O	3:B:234:ALA:N	2.54	0.40
3:C:578:TRP:CZ3	3:C:586:ILE:HA	2.55	0.40
3:C:363:ARG:NH1	3:C:406:VAL:HG11	2.36	0.40
3:C:555:ASP:HB3	3:C:561:VAL:HG21	2.03	0.40
3:B:370:SER:HA	3:B:371:LYS:HE3	2.02	0.40
3:B:371:LYS:HB3	3:B:392:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:347:ILE:CD1	3:A:354:ILE:HD12	2.42	0.40
3:C:453:GLN:HG3	3:C:453:GLN:O	2.22	0.40
3:B:309:GLN:O	3:B:313:ALA:N	2.54	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	
3	A	428/435 (98%)	318 (74%)	86 (20%)	24 (6%)	2	16
3	B	428/435 (98%)	282 (66%)	104 (24%)	42 (10%)	1	5
3	C	428/435 (98%)	296 (69%)	92 (22%)	40 (9%)	1	6
All	All	1284/1305 (98%)	896 (70%)	282 (22%)	106 (8%)	1	8

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	246	HIS
3	A	349	PHE
3	A	413	ALA
3	A	583	LYS
3	B	245	ALA
3	B	280	SER
3	B	292	CYS
3	B	340	GLY
3	B	350	TYR
3	B	364	HIS
3	B	402	PRO
3	B	470	SER
3	B	502	TYR
3	B	539	LEU

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Mol	Chain	Res	Type
3	B	572	GLN
3	C	221	GLN
3	C	283	ALA
3	C	408	VAL
3	C	412	ASP
3	C	470	SER
3	C	535	VAL
3	C	536	PHE
3	C	576	PRO
3	C	579	ASP
3	A	258	THR
3	A	377	LEU
3	A	399	VAL
3	A	479	GLY
3	A	580	GLN
3	A	618	TYR
3	B	246	HIS
3	B	337	GLU
3	B	352	LYS
3	B	353	ALA
3	B	405	ASP
3	B	444	PHE
3	B	454	ASP
3	B	471	GLY
3	B	556	ASN
3	B	604	ALA
3	C	280	SER
3	C	484	GLY
3	C	548	SER
3	C	556	ASN
3	C	604	ALA
3	C	607	ASN
3	A	297	SER
3	A	376	GLU
3	A	402	PRO
3	A	421	ASP
3	A	440	LEU
3	A	523	PRO
3	B	233	ALA
3	B	374	CYS
3	B	389	VAL
3	B	401	PRO

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Mol	Chain	Res	Type
3	C	284	TYR
3	C	292	CYS
3	C	305	THR
3	C	306	VAL
3	C	332	PRO
3	C	340	GLY
3	C	390	ALA
3	C	476	VAL
3	C	509	THR
3	C	510	SER
3	C	544	ALA
3	B	311	GLU
3	B	372	LYS
3	B	529	LEU
3	B	576	PRO
3	B	577	SER
3	C	291	GLU
3	C	389	VAL
3	C	501	TRP
3	C	547	LEU
3	C	566	THR
3	A	191	PRO
3	A	291	GLU
3	A	544	ALA
3	A	576	PRO
3	A	623	MET
3	B	235	THR
3	B	399	VAL
3	B	553	ALA
3	B	600	TYR
3	C	485	MET
3	B	373	LYS
3	C	212	THR
3	C	259	ILE
3	C	572	GLN
3	A	356	ILE
3	A	535	VAL
3	B	404	GLY
3	B	446	ILE
3	B	614	PRO
3	C	282	GLY
3	C	482	PRO

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Mol	Chain	Res	Type
3	A	325	PRO
3	C	402	PRO
3	B	194	PRO
3	B	347	ILE
3	B	554	GLY
3	C	615	ILE
3	B	362	GLY
3	C	329	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	352/354 (99%)	323 (92%)	29 (8%)	14	48
3	B	352/354 (99%)	311 (88%)	41 (12%)	7	29
3	C	352/354 (99%)	320 (91%)	32 (9%)	12	41
All	All	1056/1062 (99%)	954 (90%)	102 (10%)	10	38

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	212	THR
3	A	246	HIS
3	A	251	ASN
3	A	274	LEU
3	A	294	SER
3	A	328	SER
3	A	335	ASN
3	A	343	ASN
3	A	344	ASN
3	A	354	ILE
3	A	360	LYS
3	A	402	PRO
3	A	407	VAL
3	A	412	ASP

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Mol	Chain	Res	Type
3	A	440	LEU
3	A	443	THR
3	A	454	ASP
3	A	464	ARG
3	A	469	ARG
3	A	480	GLU
3	A	483	SER
3	A	492	CYS
3	A	517	LEU
3	A	523	PRO
3	A	568	CYS
3	A	598	LEU
3	A	611	LEU
3	A	615	ILE
3	A	623	MET
3	B	203	HIS
3	B	210	LYS
3	B	224	LYS
3	B	229	ASN
3	B	246	HIS
3	B	296	ASP
3	B	301	LEU
3	B	305	THR
3	B	322	THR
3	B	343	ASN
3	B	344	ASN
3	B	346	GLU
3	B	356	ILE
3	B	363	ARG
3	B	367	PHE
3	B	371	LYS
3	B	387	ASN
3	B	393	ARG
3	B	402	PRO
3	B	419	THR
3	B	450	THR
3	B	458	ARG
3	B	460	GLN
3	B	474	ARG
3	B	491	LEU
3	B	499	CYS
3	B	501	TRP

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Mol	Chain	Res	Type
3	B	513	LEU
3	B	524	VAL
3	B	531	PHE
3	B	542	ILE
3	B	548	SER
3	B	568	CYS
3	B	579	ASP
3	B	581	MET
3	B	583	LYS
3	B	593	HIS
3	B	598	LEU
3	B	600	TYR
3	B	611	LEU
3	B	612	THR
3	C	198	GLN
3	C	206	THR
3	C	212	THR
3	C	265	ILE
3	C	286	ILE
3	C	292	CYS
3	C	306	VAL
3	C	332	PRO
3	C	338	GLU
3	C	343	ASN
3	C	344	ASN
3	C	371	LYS
3	C	372	LYS
3	C	374	CYS
3	C	375	ASP
3	C	387	ASN
3	C	402	PRO
3	C	412	ASP
3	C	433	THR
3	C	460	GLN
3	C	480	GLU
3	C	496	ASP
3	C	499	CYS
3	C	517	LEU
3	C	526	GLN
3	C	557	PHE
3	C	572	GLN
3	C	574	PRO

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Mol	Chain	Res	Type
3	C	580	GLN
3	C	588	LEU
3	C	611	LEU
3	C	617	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	251	ASN
3	A	343	ASN
3	A	453	GLN
3	A	541	HIS
3	A	607	ASN
3	B	203	HIS
3	B	229	ASN
3	B	333	HIS
3	B	343	ASN
3	B	344	ASN
3	B	387	ASN
3	B	429	ASN
3	B	434	GLN
3	B	460	GLN
3	B	564	GLN
3	B	580	GLN
3	B	606	GLN
3	C	198	GLN
3	C	201	HIS
3	C	203	HIS
3	C	251	ASN
3	C	335	ASN
3	C	343	ASN
3	C	344	ASN
3	C	387	ASN
3	C	460	GLN
3	C	526	GLN
3	C	549	GLN
3	C	564	GLN
3	C	572	GLN
3	C	580	GLN

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	SO4	A	101	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	C	102	-	4,4,4	0.17	0	6,6,6	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	101	-	-	0/0/0/0	0/0/0/0
4	SO4	C	102	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	102	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.