Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:54 am BST

PDB ID	:	4V5I
Title	:	Structure of the Phage P2 Baseplate in its Activated Conformation with Ca
Authors	:	Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; van Heel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on	:	2010-02-05
Resolution	:	5.46 Å(reported)

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

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

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

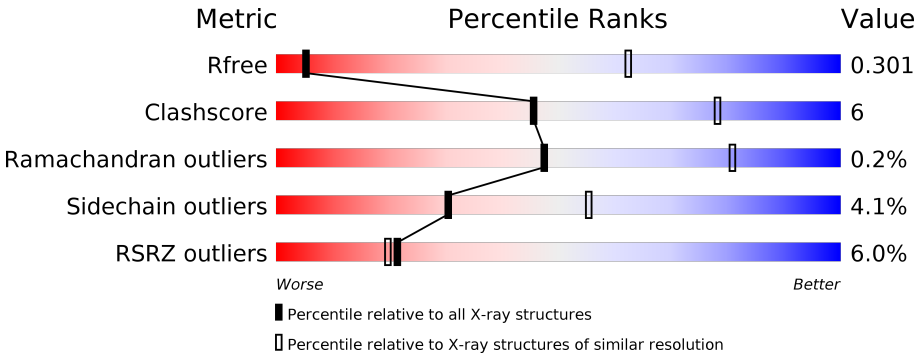
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 5.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1018 (7.08-3.82)
Clashscore	141614	1005 (7.02-3.90)
Ramachandran outliers	138981	1013 (7.10-3.82)
Sidechain outliers	138945	1190 (7.12-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	372	11% 84% 14%
1	AY	372	10% 86% 12%
1	AZ	372	10% 83% 16%
1	B0	372	8% 85% 14%
1	BY	372	4% 86% 12%
1	BZ	372	8% 85% 14%

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Mol	Chain	Length	Quality of chain
2	AA	263	2% 89% 11%
2	AB	263	6% 92% 8%
2	AC	263	5% 92% 8%
2	AD	263	6% 87% 13%
2	AE	263	3% 90% 10%
2	AF	263	6% 90% 10%
2	AG	263	9% 89% 10%
2	AH	263	3% 92% 7%
2	AI	263	8% 92% 8%
2	AJ	263	5% 91% 9%
2	AK	263	4% 89% 11%
2	AL	263	8% 92% 8%
2	AM	263	8% 90% 10%
2	AN	263	5% 85% 15%
2	AO	263	5% 91% 9%
2	AP	263	7% 87% 12%
2	AQ	263	10% 90% 10%
2	AR	263	6% 89% 11%
2	BA	263	4% 89% 11%
2	BB	263	5% 91% 9%
2	BC	263	5% 92% 8%
2	BD	263	6% 88% 12%
2	BE	263	4% 90% 10%
2	BF	263	8% 90% 10%
2	BG	263	8% 89% 10%

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Mol	Chain	Length	Quality of chain
2	BH	263	8% 92% 7%
2	BI	263	4% 92% 8%
2	BJ	263	3% 91% 9%
2	BK	263	8% 91% 9%
2	BL	263	8% 92% 8%
2	BM	263	9% 88% 11%
2	BN	263	6% 87% 13%
2	BO	263	6% 91% 9%
2	BP	263	12% 88% 11%
2	BQ	263	8% 89% 10%
2	BR	263	10% 89% 11%
3	AS	298	5% 74% 22%
3	AT	298	5% 72% 24%
3	AU	298	2% 73% 23%
3	AV	298	5% 76% 20%
3	AW	298	3% 79% 19%
3	AX	298	4% 74% 23%
3	BS	298	4% 76% 21%
3	BT	298	3% 73% 23%
3	BU	298	3% 73% 24%
3	BV	298	5% 77% 19%
3	BW	298	2% 80% 17%
3	BX	298	4% 75% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 119484 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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	B0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AI	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AJ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AK	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AL	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AM	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AN	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AO	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AP	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AQ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AR	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BI	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BJ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BK	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BL	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BM	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BN	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BO	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BP	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BQ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BR	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AT	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AU	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AV	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AW	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AX	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BS	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BT	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BU	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BV	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BW	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BX	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

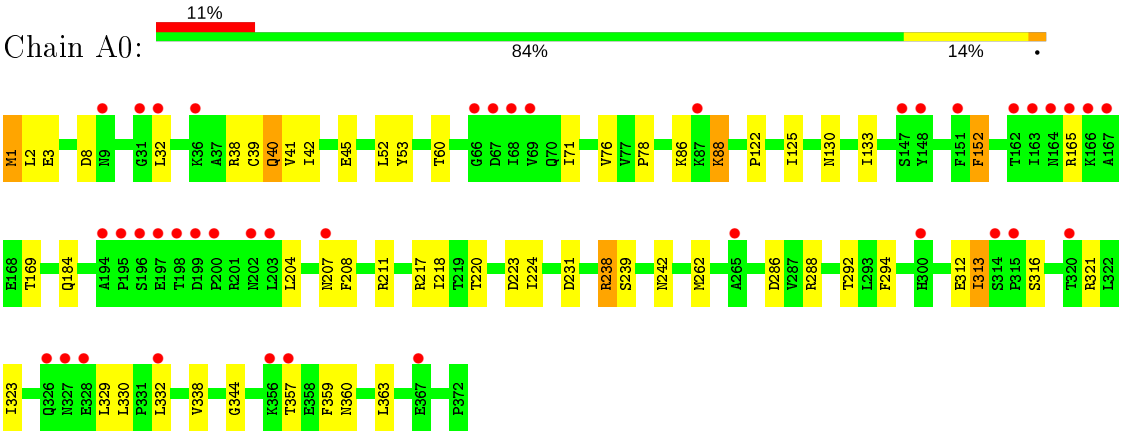
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BU	1	Total Ca 1 1	0	0
4	BT	1	Total Ca 1 1	0	0
4	AV	1	Total Ca 1 1	0	0
4	BV	1	Total Ca 1 1	0	0
4	AW	1	Total Ca 1 1	0	0
4	AT	1	Total Ca 1 1	0	0
4	BS	1	Total Ca 1 1	0	0
4	AU	1	Total Ca 1 1	0	0
4	AX	1	Total Ca 1 1	0	0
4	BW	1	Total Ca 1 1	0	0
4	BX	1	Total Ca 1 1	0	0
4	AS	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

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

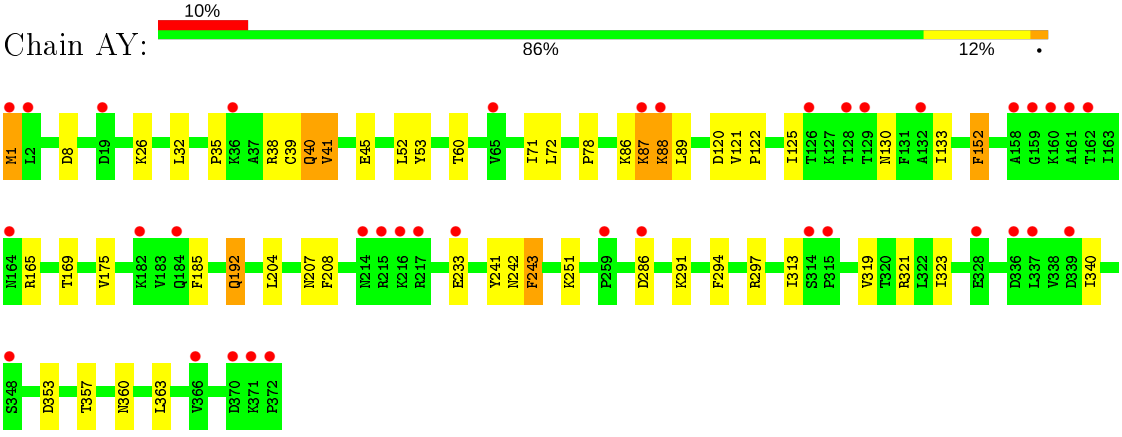
- Molecule 1: ORF16

Chain A0:



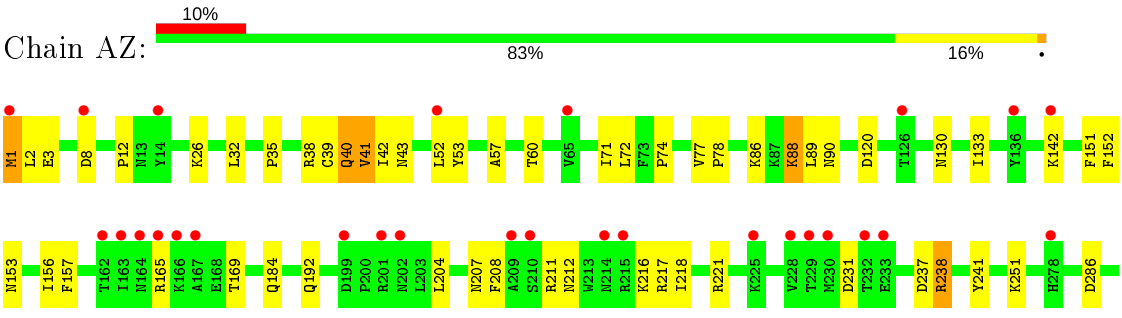
- Molecule 1: ORF16

Chain AY:



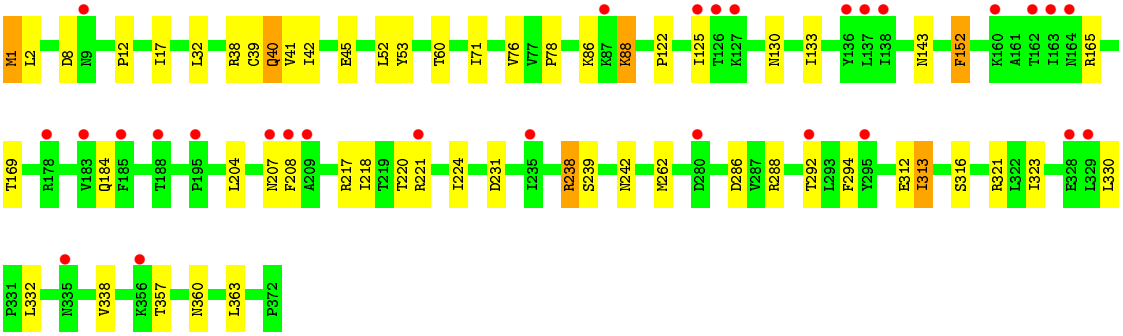
- Molecule 1: ORF16

Chain AZ:



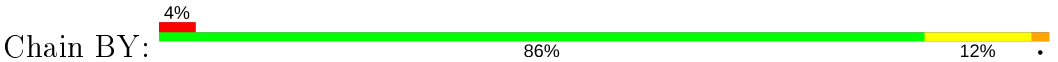
• Molecule 1: ORF16

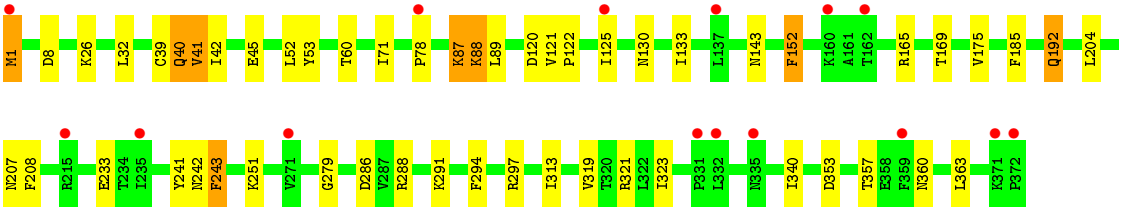
Chain B0:



• Molecule 1: ORF16

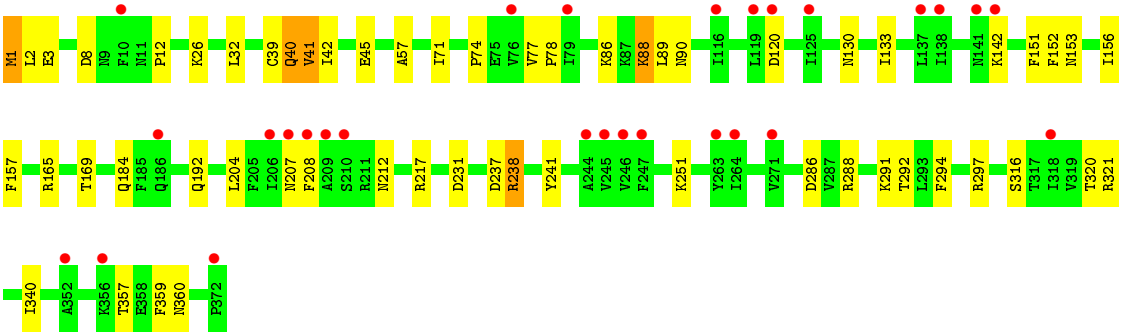
Chain BY:





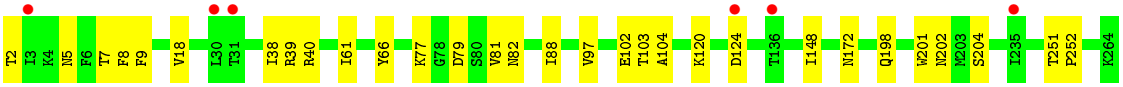
• Molecule 1: ORF16

Chain BZ:



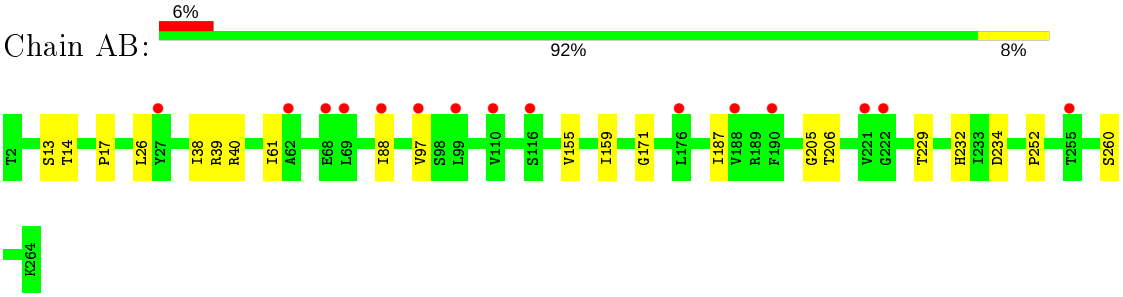
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AA:



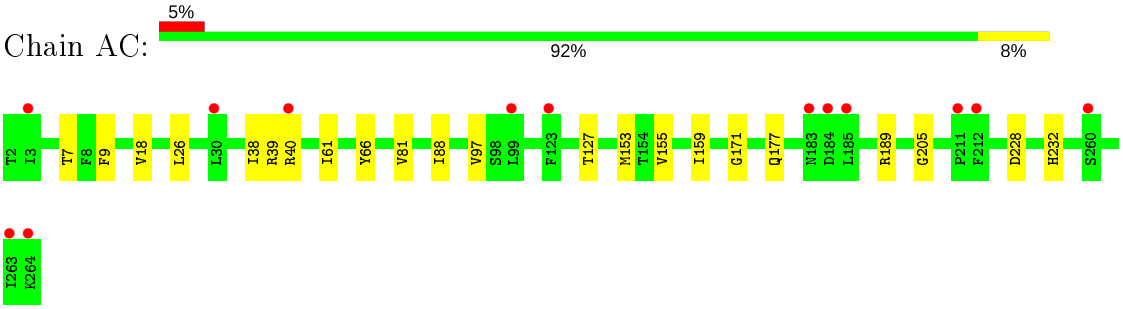
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AB:



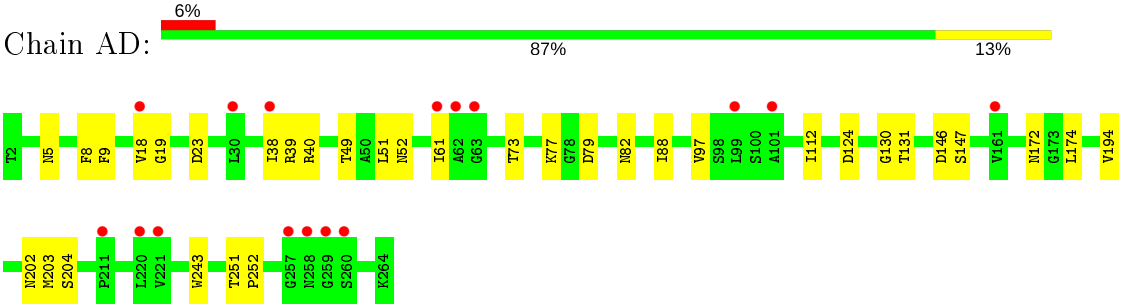
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AC:



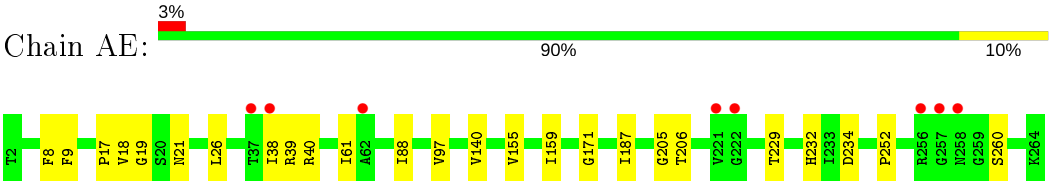
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AD:



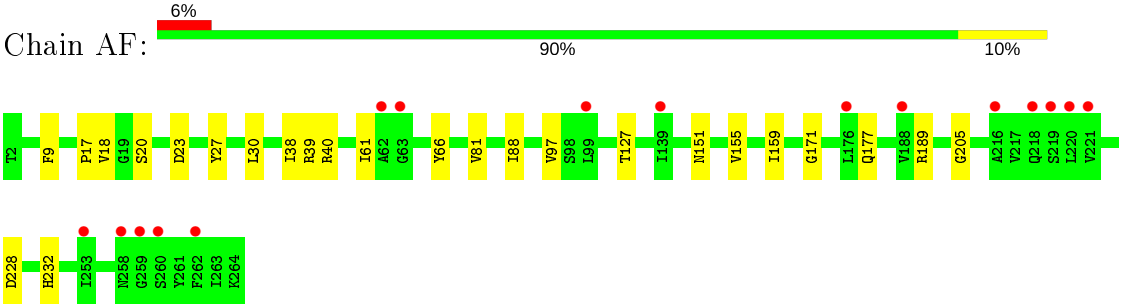
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AE:



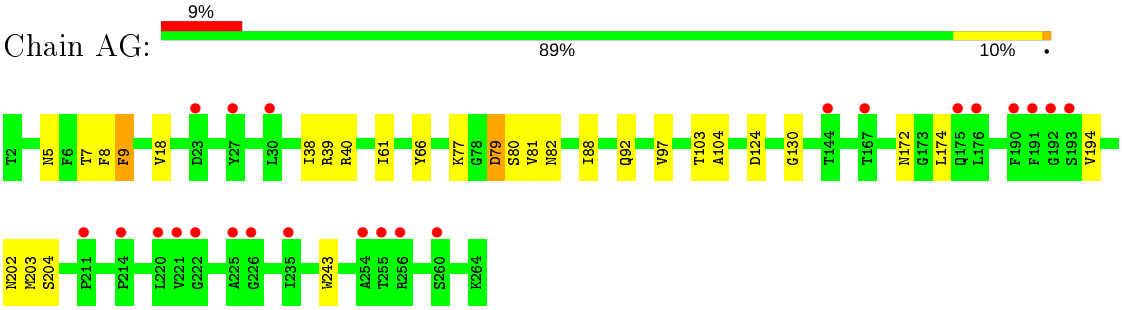
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AF:



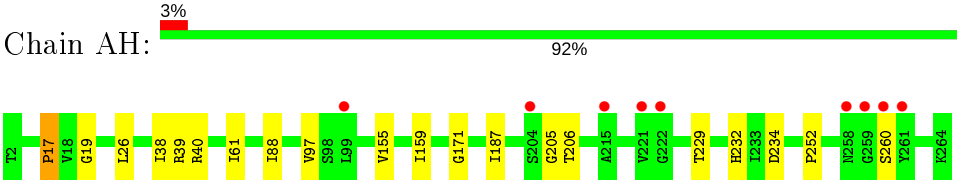
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AG:



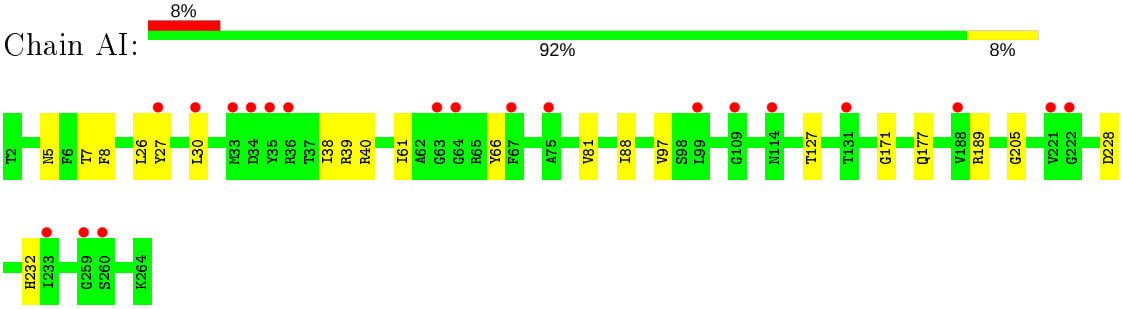
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AH:



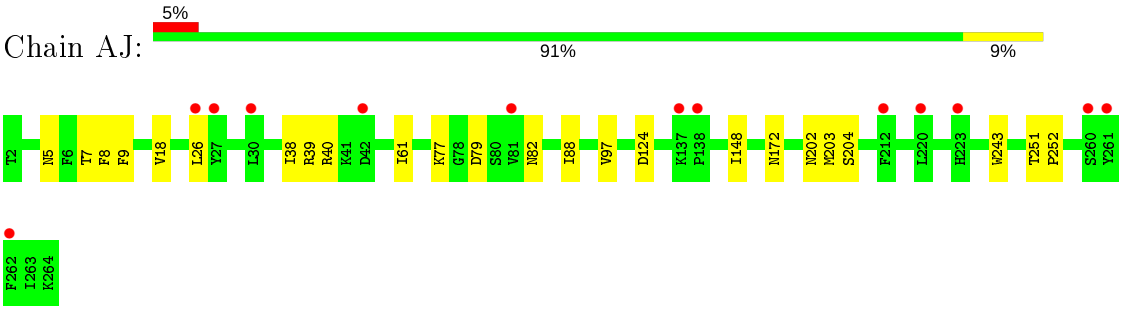
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AI:



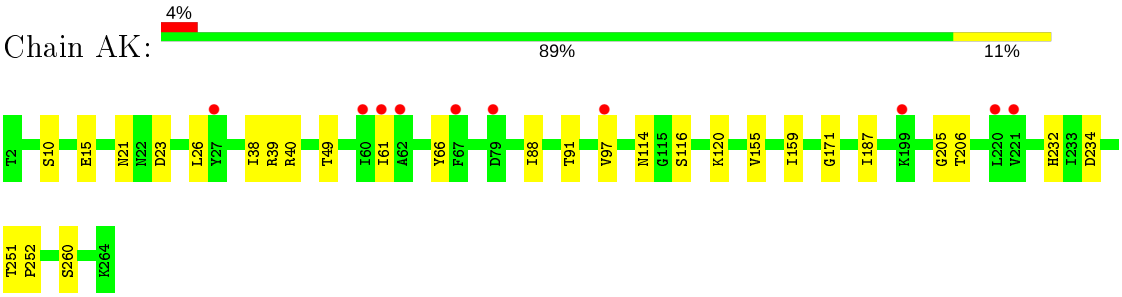
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AJ:



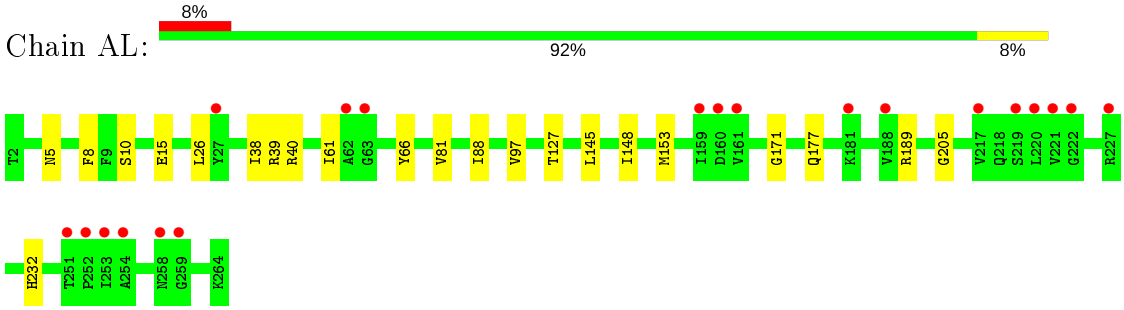
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AK:



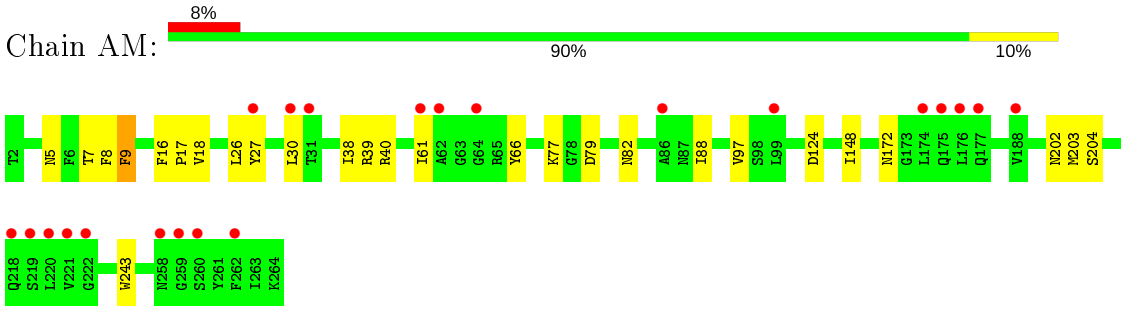
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AL:



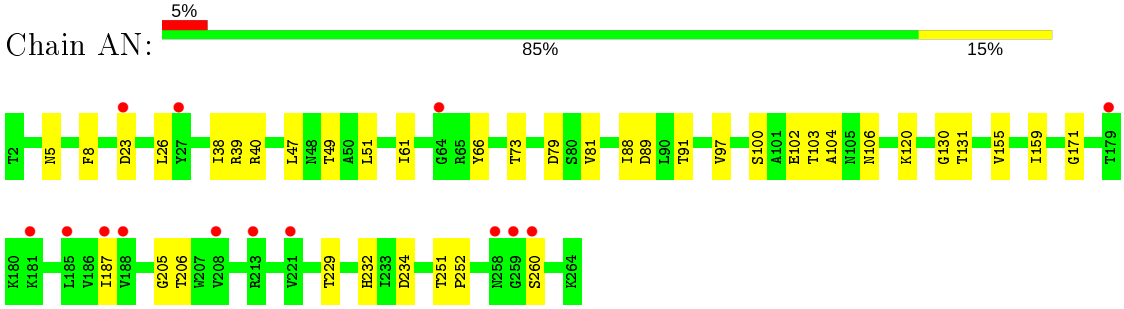
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AM:



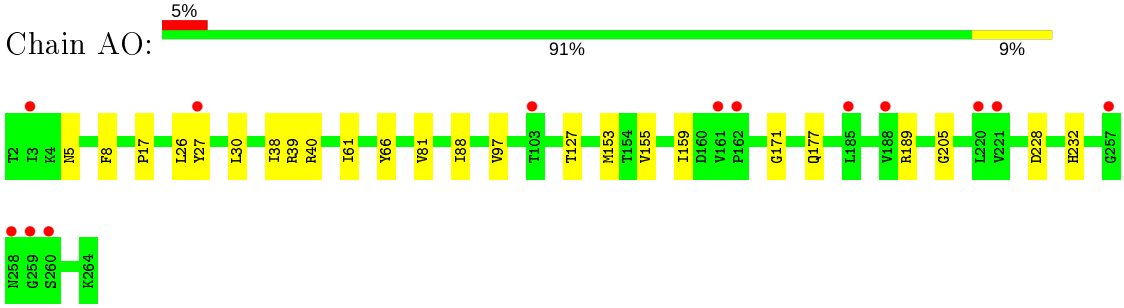
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AN:



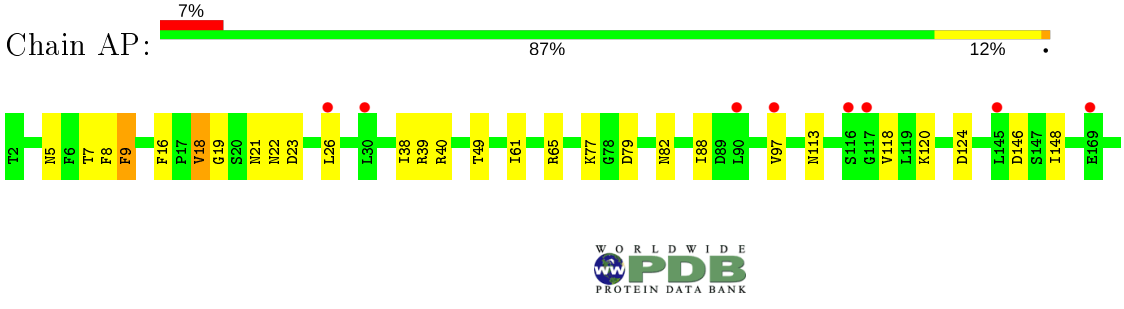
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

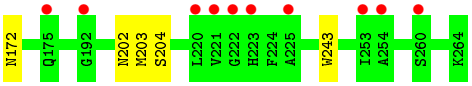
Chain AO:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

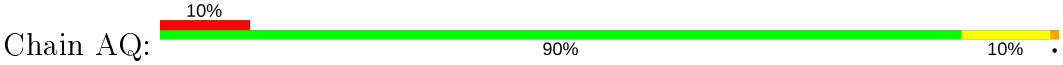
Chain AP:

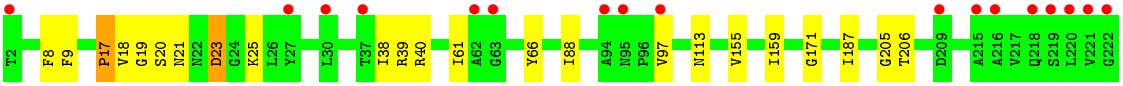


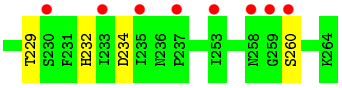


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AQ:

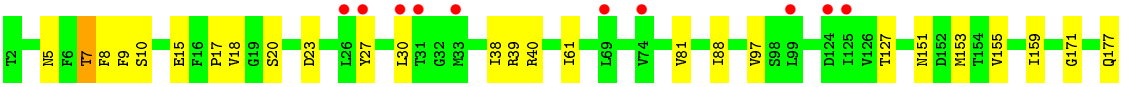


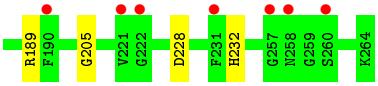




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

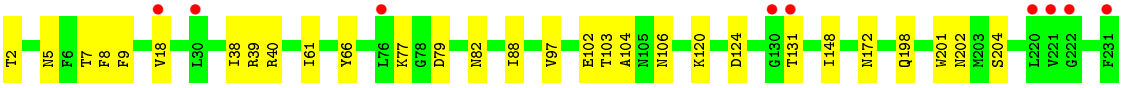
Chain AR:





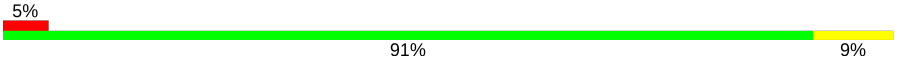
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

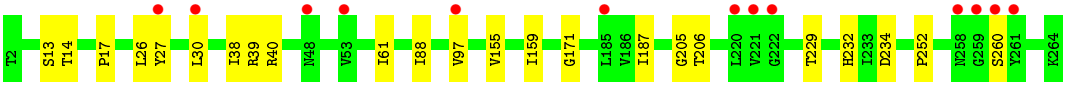
Chain BA:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

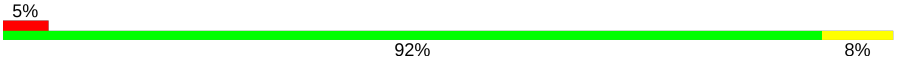
Chain BB:

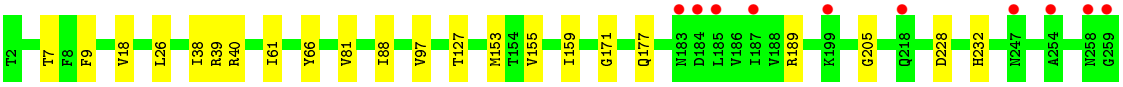




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

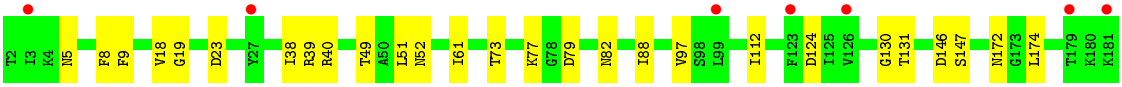
Chain BC:

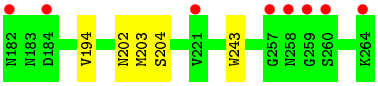




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BD:



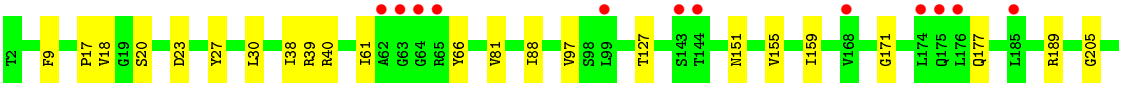


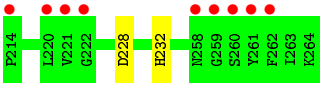
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BE:

• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

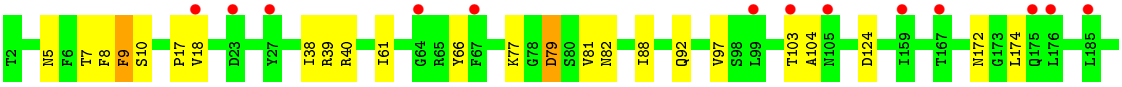
Chain BF:

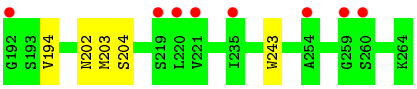




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

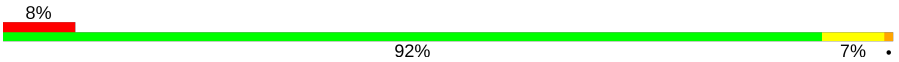
Chain BG:

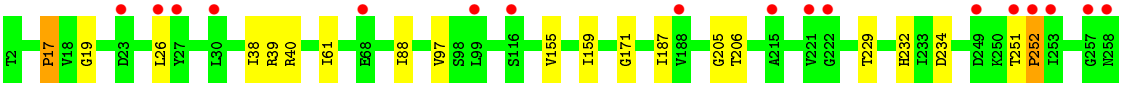




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

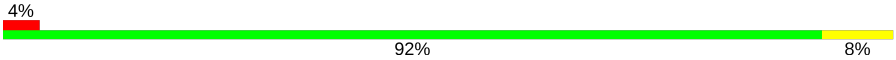
Chain BH:

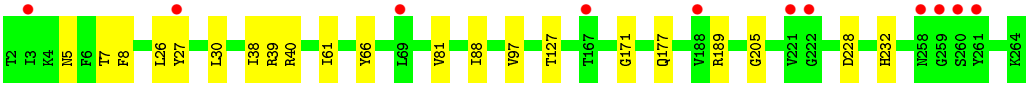




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

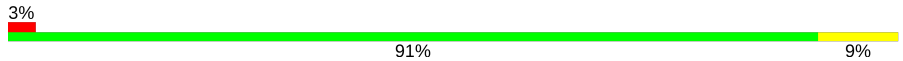
Chain BI:

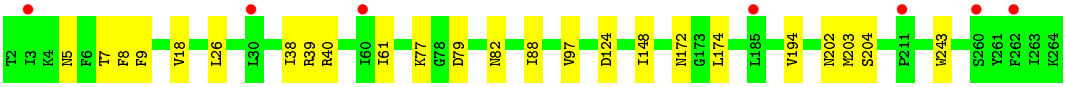




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

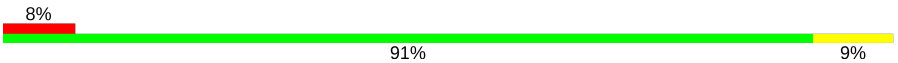
Chain BJ:

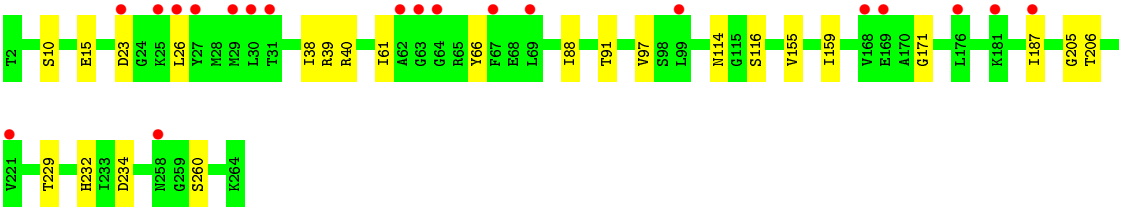




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

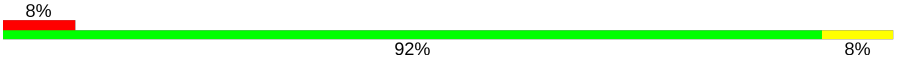
Chain BK:

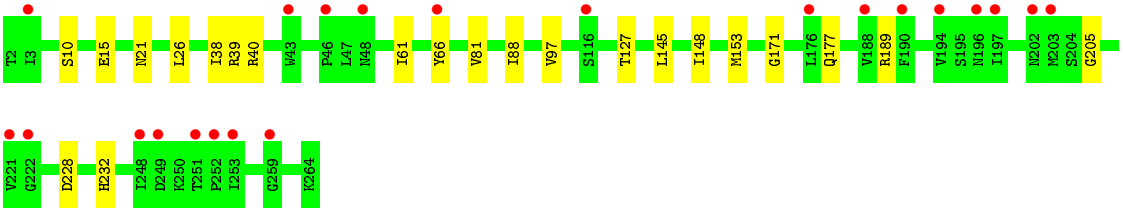




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

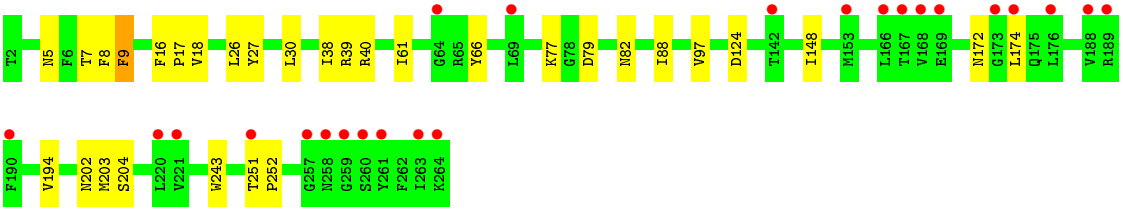
Chain BL:





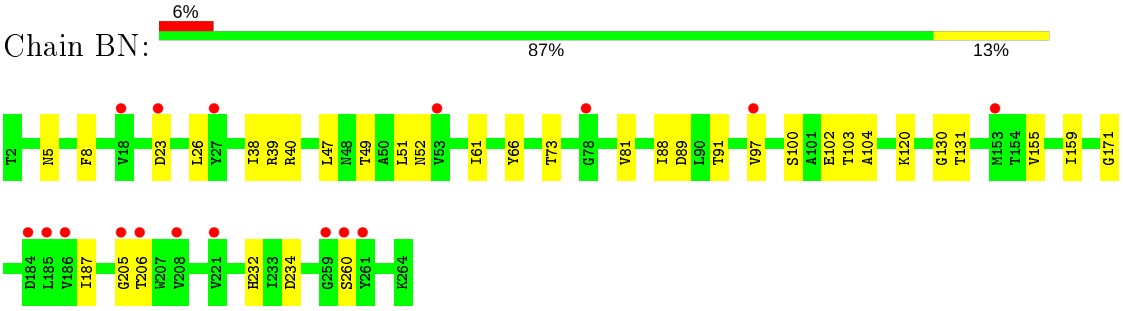
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BM:



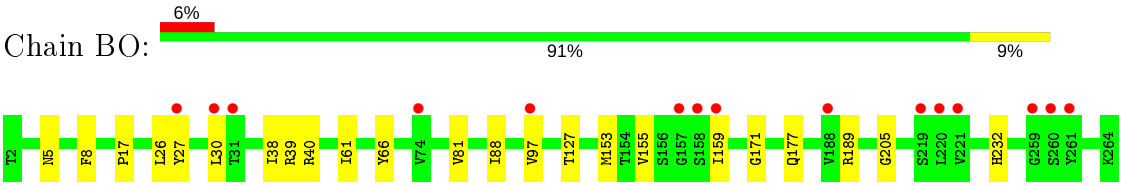
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BN:



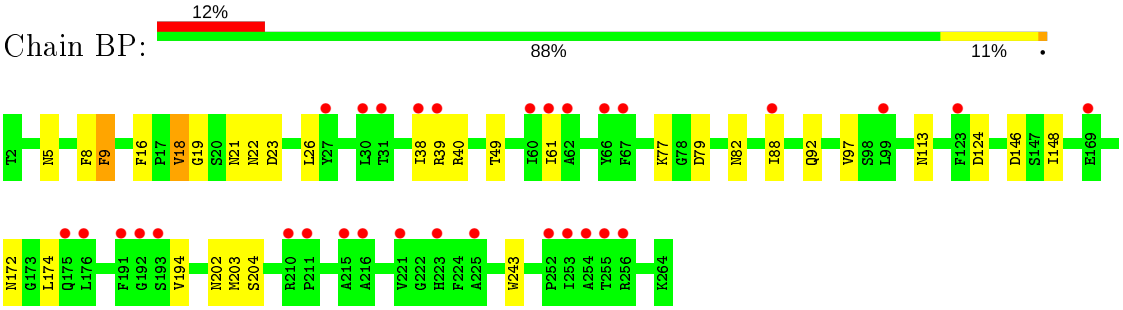
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BO:



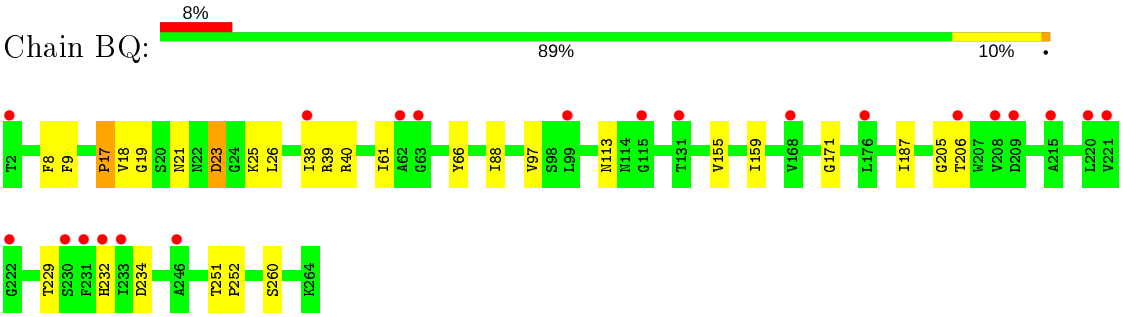
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BP:



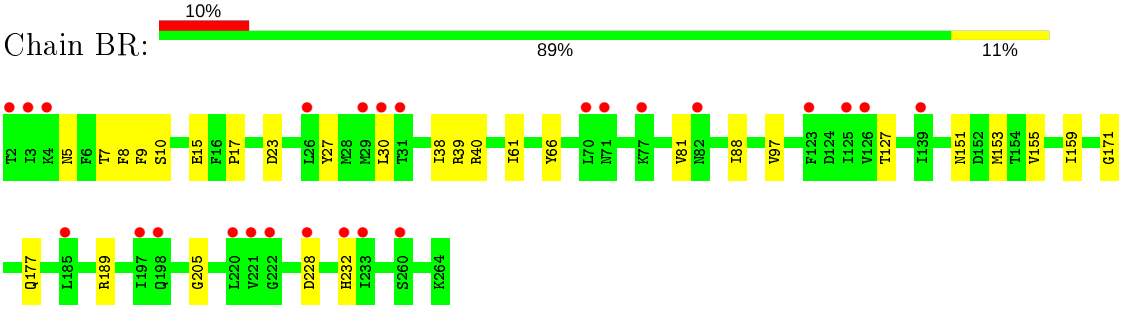
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BQ:



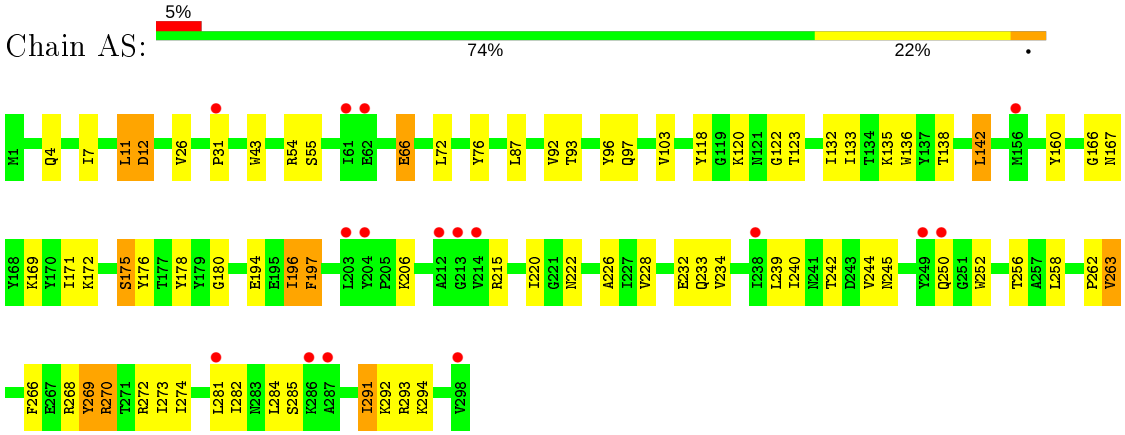
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BR:



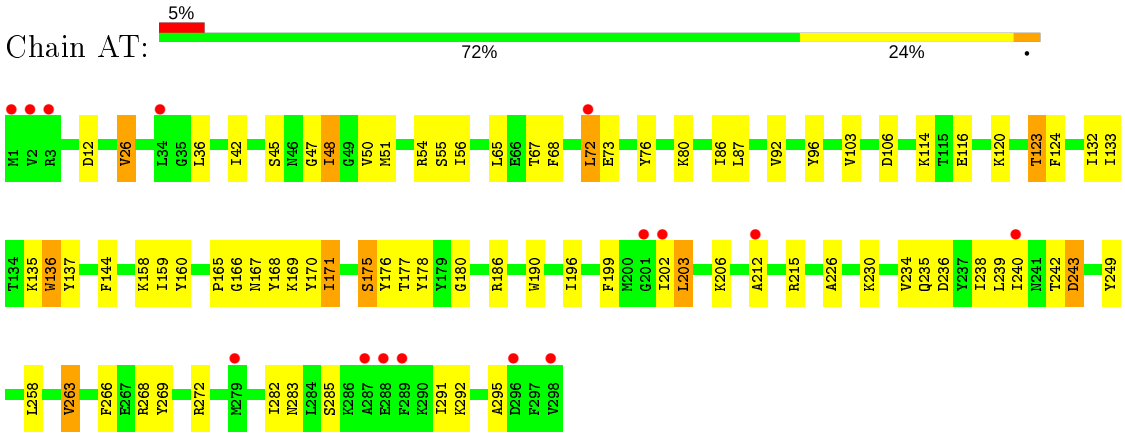
• Molecule 3: ORF15

Chain AS:



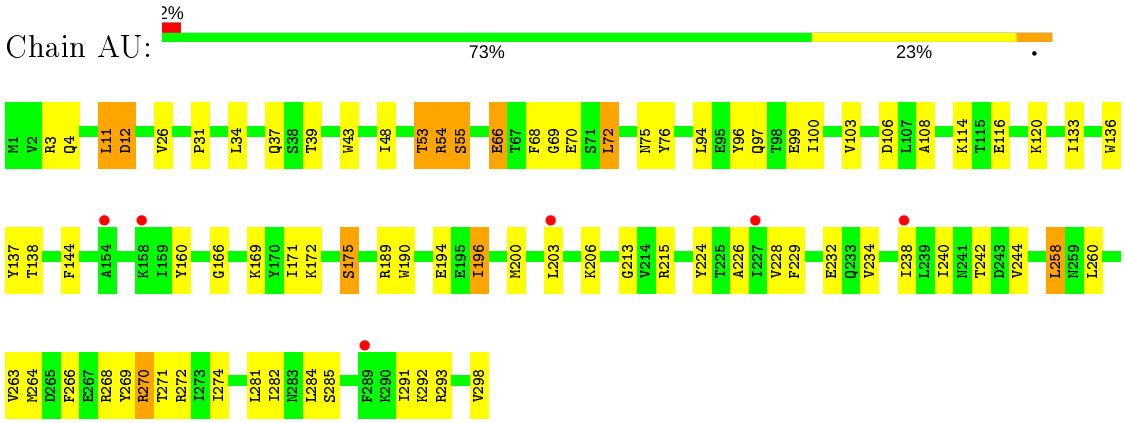
• Molecule 3: ORF15

Chain AT:



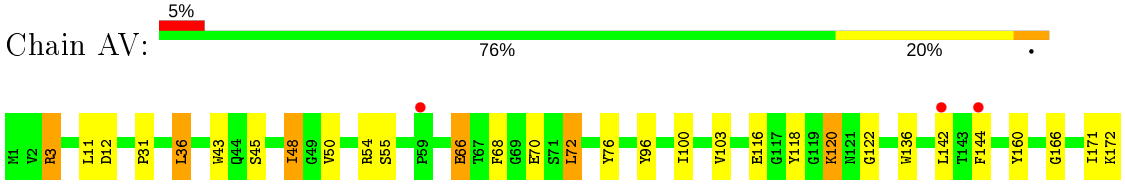
• Molecule 3: ORF15

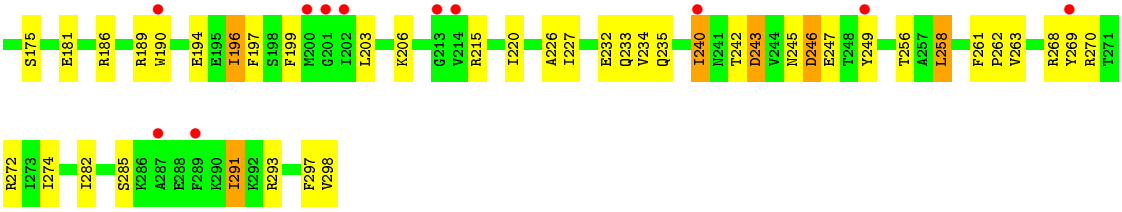
Chain AU:



• Molecule 3: ORF15

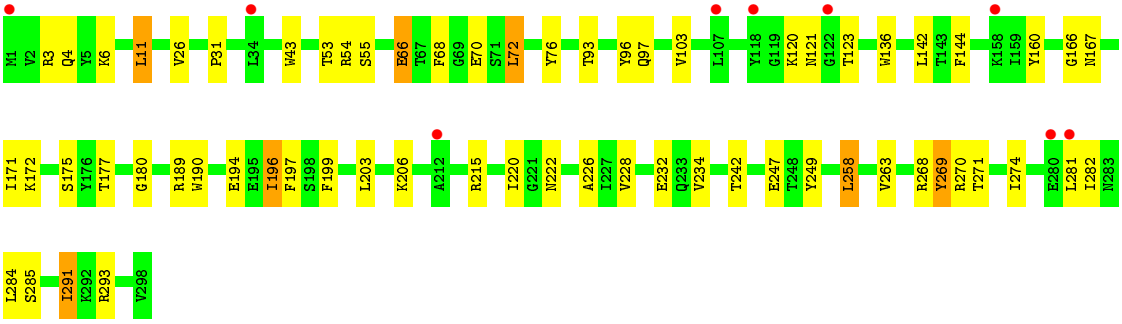
Chain AV:





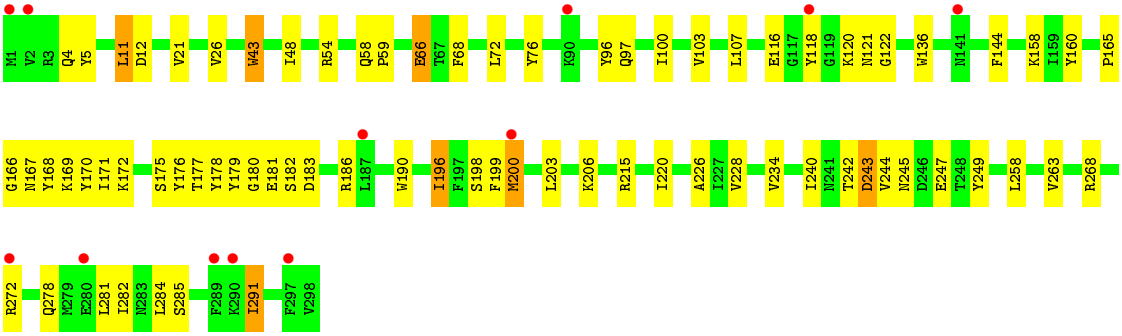
• Molecule 3: ORF15

Chain AW:



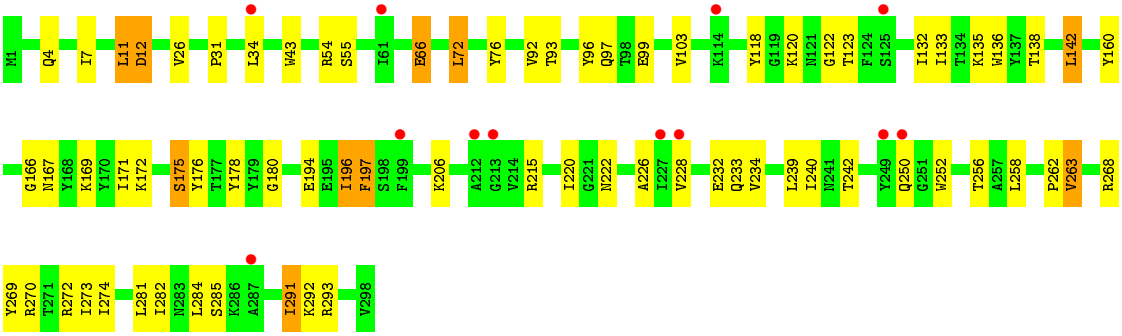
• Molecule 3: ORF15

Chain AX:



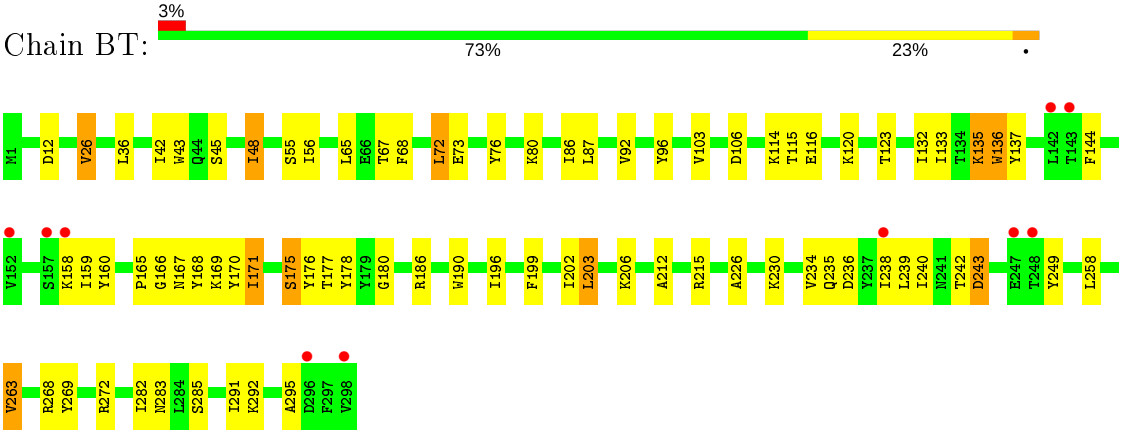
• Molecule 3: ORF15

Chain BS:



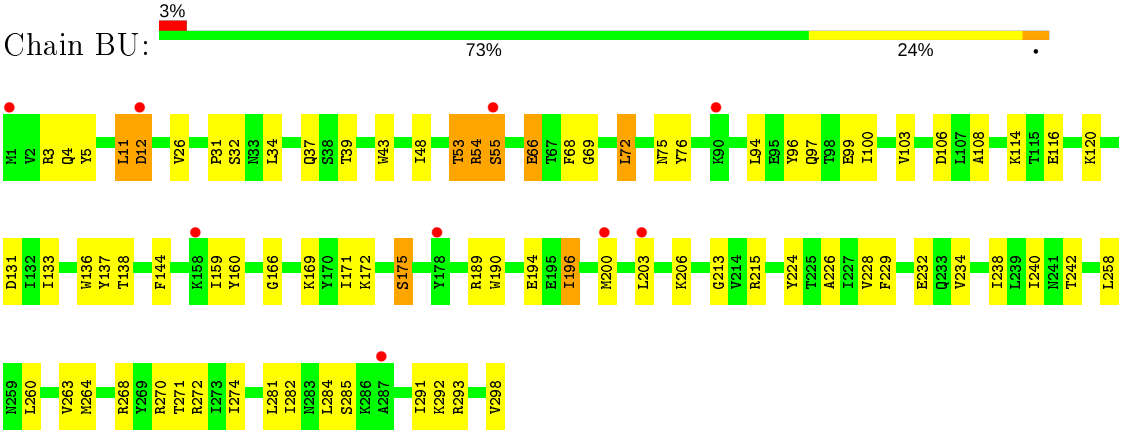
• Molecule 3: ORF15

Chain BT:



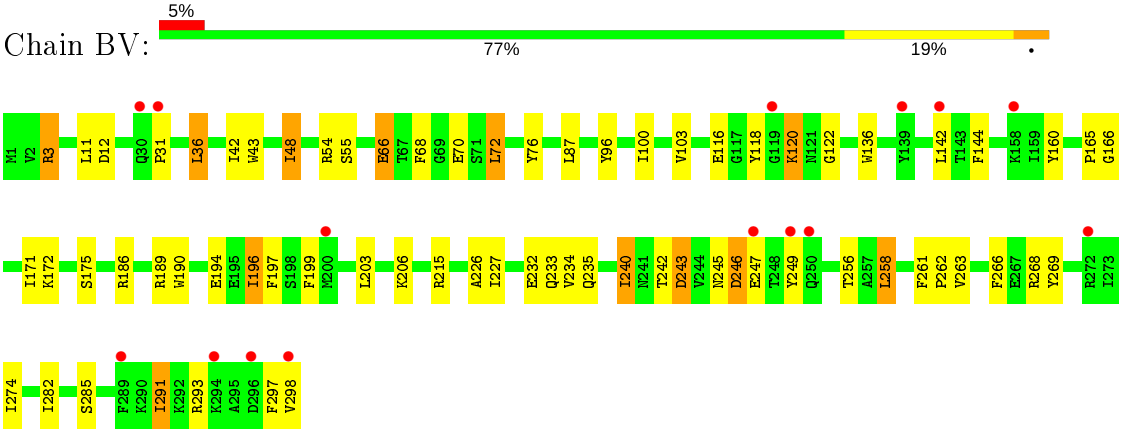
- Molecule 3: ORF15

Chain BU:



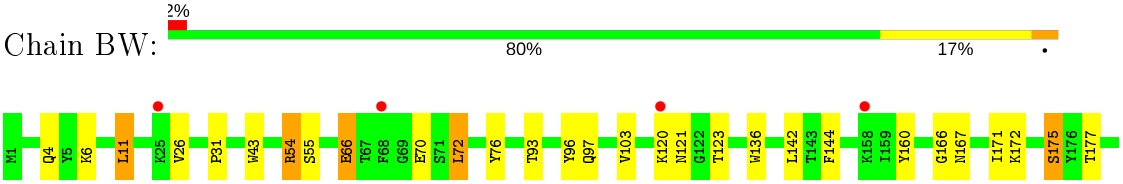
- Molecule 3: ORF15

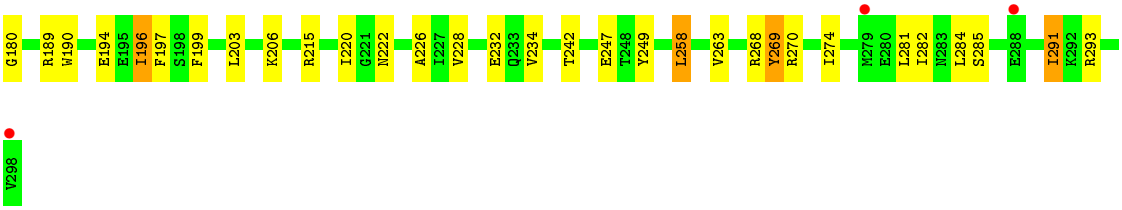
Chain BV:



- Molecule 3: ORF15

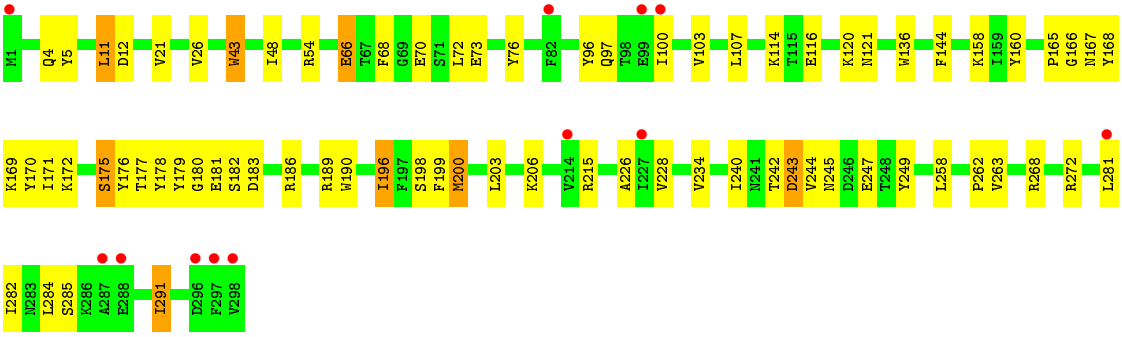
Chain BW:





• Molecule 3: ORF15

Chain BX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	219.52Å 219.34Å 392.43Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	44.56 – 5.46 44.56 – 5.46	Depositor EDS
% Data completeness (in resolution range)	91.0 (44.56-5.46) 90.9 (44.56-5.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 5.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.291 , 0.297 0.298 , 0.301	Depositor DCC
R_{free} test set	5621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	205.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 403.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.409 for k,h,-l 0.399 for -k,-h,-l 0.408 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	119484	wwPDB-VP
Average B, all atoms (Å^2)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	A0	0.38	0/3069	0.64	0/4175
1	AY	0.38	0/3069	0.65	0/4175
1	AZ	0.37	0/3069	0.63	0/4175
1	B0	0.38	0/3069	0.64	0/4175
1	BY	0.38	0/3069	0.65	0/4175
1	BZ	0.37	0/3069	0.63	0/4175
2	AA	0.32	0/2048	0.63	0/2791
2	AB	0.36	0/2048	0.58	0/2791
2	AC	0.35	0/2048	0.59	0/2791
2	AD	0.32	0/2048	0.61	0/2791
2	AE	0.36	0/2048	0.58	0/2791
2	AF	0.36	0/2048	0.58	0/2791
2	AG	0.32	0/2048	0.62	0/2791
2	AH	0.37	0/2048	0.58	0/2791
2	AI	0.37	0/2048	0.58	0/2791
2	AJ	0.34	0/2048	0.63	0/2791
2	AK	0.36	0/2048	0.59	0/2791
2	AL	0.36	0/2048	0.58	0/2791
2	AM	0.34	0/2048	0.63	0/2791
2	AN	0.36	0/2048	0.58	0/2791
2	AO	0.36	0/2048	0.58	0/2791
2	AP	0.34	0/2048	0.63	0/2791
2	AQ	0.37	0/2048	0.58	0/2791
2	AR	0.37	0/2048	0.59	0/2791
2	BA	0.32	0/2048	0.63	0/2791
2	BB	0.36	0/2048	0.58	0/2791
2	BC	0.35	0/2048	0.59	0/2791
2	BD	0.32	0/2048	0.61	0/2791
2	BE	0.36	0/2048	0.58	0/2791
2	BF	0.36	0/2048	0.58	0/2791
2	BG	0.32	0/2048	0.62	0/2791
2	BH	0.37	0/2048	0.58	0/2791

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
2	BI	0.37	0/2048	0.58	0/2791
2	BJ	0.34	0/2048	0.63	0/2791
2	BK	0.35	0/2048	0.59	0/2791
2	BL	0.36	0/2048	0.58	0/2791
2	BM	0.34	0/2048	0.63	0/2791
2	BN	0.36	0/2048	0.58	0/2791
2	BO	0.36	0/2048	0.58	0/2791
2	BP	0.34	0/2048	0.63	0/2791
2	BQ	0.37	0/2048	0.58	0/2791
2	BR	0.37	0/2048	0.59	0/2791
3	AS	0.36	0/2485	0.69	0/3356
3	AT	0.36	0/2485	0.69	0/3356
3	AU	0.35	0/2485	0.67	0/3356
3	AV	0.36	0/2485	0.67	0/3356
3	AW	0.35	0/2485	0.66	0/3356
3	AX	0.36	0/2485	0.67	0/3356
3	BS	0.36	0/2485	0.69	0/3356
3	BT	0.36	0/2485	0.69	0/3356
3	BU	0.35	0/2485	0.67	0/3356
3	BV	0.36	0/2485	0.67	0/3356
3	BW	0.35	0/2485	0.66	0/3356
3	BX	0.36	0/2485	0.67	0/3356
All	All	0.36	0/121962	0.62	0/165798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	A0	3000	0	2956	55	0
1	AY	3000	0	2956	37	0
1	AZ	3000	0	2956	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	3000	0	2956	45	0
1	BY	3000	0	2956	36	0
1	BZ	3000	0	2956	53	0
2	AA	2008	0	1971	22	0
2	AB	2008	0	1971	16	0
2	AC	2008	0	1971	15	0
2	AD	2008	0	1971	57	0
2	AE	2008	0	1971	34	0
2	AF	2008	0	1971	20	0
2	AG	2008	0	1971	34	0
2	AH	2008	0	1971	9	0
2	AI	2008	0	1971	10	0
2	AJ	2008	0	1971	11	0
2	AK	2008	0	1971	15	0
2	AL	2008	0	1971	10	0
2	AM	2008	0	1971	15	0
2	AN	2008	0	1971	38	0
2	AO	2008	0	1971	13	0
2	AP	2008	0	1971	35	0
2	AQ	2008	0	1971	42	0
2	AR	2008	0	1971	32	0
2	BA	2008	0	1971	18	0
2	BB	2008	0	1971	17	0
2	BC	2008	0	1971	15	0
2	BD	2008	0	1971	46	0
2	BE	2008	0	1971	35	0
2	BF	2008	0	1971	21	0
2	BG	2008	0	1971	25	0
2	BH	2008	0	1971	11	0
2	BI	2008	0	1971	10	0
2	BJ	2008	0	1971	10	0
2	BK	2008	0	1971	12	0
2	BL	2008	0	1971	11	0
2	BM	2008	0	1971	16	0
2	BN	2008	0	1971	37	0
2	BO	2008	0	1971	12	0
2	BP	2008	0	1971	23	0
2	BQ	2008	0	1971	31	0
2	BR	2008	0	1971	23	0
3	AS	2432	0	2392	117	0
3	AT	2432	0	2392	107	0
3	AU	2432	0	2392	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AV	2432	0	2392	98	0
3	AW	2432	0	2392	74	0
3	AX	2432	0	2392	141	0
3	BS	2432	0	2392	96	0
3	BT	2432	0	2392	102	0
3	BU	2432	0	2392	92	0
3	BV	2432	0	2392	95	0
3	BW	2432	0	2392	74	0
3	BX	2432	0	2392	112	0
4	AS	1	0	0	0	0
4	AT	1	0	0	0	0
4	AU	1	0	0	0	0
4	AV	1	0	0	0	0
4	AW	1	0	0	0	0
4	AX	1	0	0	0	0
4	BS	1	0	0	0	0
4	BT	1	0	0	0	0
4	BU	1	0	0	0	0
4	BV	1	0	0	0	0
4	BW	1	0	0	0	0
4	BX	1	0	0	0	0
All	All	119484	0	117396	1507	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 6.

All (1507) 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:AW:120:LYS:HD3	3:BV:68:PHE:CE1	1.26	1.65
3:AV:68:PHE:CD1	3:BW:120:LYS:HD3	1.30	1.61
3:AV:68:PHE:CE1	3:BW:120:LYS:HD3	1.28	1.58
3:AU:68:PHE:CE1	3:BX:120:LYS:HD3	1.37	1.54
3:AW:120:LYS:HD3	3:BV:68:PHE:CD1	1.42	1.54
3:AX:120:LYS:HD3	3:BU:68:PHE:CE1	1.40	1.51
2:AD:52:ASN:CG	3:AS:258:LEU:CD2	1.81	1.49
2:AD:52:ASN:CG	3:AS:258:LEU:HD22	1.30	1.47
3:AV:68:PHE:CE1	3:BW:120:LYS:CD	2.01	1.43
2:AD:52:ASN:ND2	3:AS:258:LEU:HD22	1.28	1.43
1:A0:42:ILE:HB	3:AX:43:TRP:CZ2	1.51	1.41
3:AW:120:LYS:CD	3:BV:68:PHE:CE1	2.04	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:130:GLY:O	3:AS:262:PRO:CB	1.70	1.36
3:AV:68:PHE:CD1	3:BW:120:LYS:CD	2.08	1.36
2:AG:103:THR:CB	1:AZ:78:PRO:HG3	1.53	1.36
3:AV:120:LYS:HZ2	3:BW:66:GLU:CG	1.42	1.32
1:B0:42:ILE:HB	3:BX:43:TRP:CZ2	1.66	1.30
2:AG:103:THR:HB	1:AZ:78:PRO:CG	1.62	1.30
2:BD:52:ASN:CG	3:BS:258:LEU:HD22	1.51	1.28
3:AV:120:LYS:NZ	3:BW:66:GLU:CG	1.99	1.24
2:AD:73:THR:CB	3:AS:256:THR:HG21	1.68	1.22
2:AD:131:THR:HG22	3:AS:262:PRO:O	1.38	1.21
2:BD:52:ASN:ND2	3:BS:258:LEU:HD22	1.54	1.21
3:AW:66:GLU:CG	3:BV:120:LYS:HZ2	1.54	1.20
1:A0:42:ILE:CB	3:AX:43:TRP:HZ2	1.55	1.20
2:BD:52:ASN:CG	3:BS:258:LEU:CD2	2.10	1.20
3:AW:120:LYS:CD	3:BV:68:PHE:CD1	2.21	1.19
2:BD:130:GLY:O	3:BS:262:PRO:HB3	1.39	1.19
3:AU:68:PHE:CE1	3:BX:120:LYS:CD	2.25	1.19
2:BD:131:THR:HG22	3:BS:262:PRO:O	1.42	1.18
2:AB:13:SER:O	3:AS:169:LYS:HD2	1.44	1.16
2:BB:13:SER:O	3:BS:169:LYS:HD2	1.46	1.15
2:BD:130:GLY:O	3:BS:262:PRO:CB	1.93	1.15
3:AW:66:GLU:CG	3:BV:120:LYS:NZ	2.10	1.15
2:AD:130:GLY:O	3:AS:262:PRO:HB3	1.34	1.15
1:A0:88:LYS:NZ	2:AN:104:ALA:HB3	1.62	1.14
2:AD:130:GLY:O	3:AS:262:PRO:HB2	1.42	1.12
3:AX:120:LYS:CD	3:BU:68:PHE:CE1	2.29	1.12
2:AD:52:ASN:ND2	3:AS:258:LEU:CD2	2.03	1.11
2:BD:73:THR:CB	3:BS:256:THR:HG21	1.81	1.10
2:AQ:18:VAL:HG12	3:AX:168:TYR:O	1.50	1.10
2:AQ:17:PRO:HB3	3:AX:167:ASN:HD22	1.11	1.09
3:AV:68:PHE:CE1	3:BW:120:LYS:CG	2.35	1.08
2:AQ:17:PRO:HB3	3:AX:169:LYS:HE3	1.35	1.08
2:BG:103:THR:CB	1:BZ:78:PRO:HG3	1.83	1.07
2:BN:131:THR:HG22	3:BV:262:PRO:O	1.52	1.07
2:BB:13:SER:C	3:BS:169:LYS:HD2	1.74	1.07
2:BB:13:SER:O	3:BS:169:LYS:CD	2.04	1.06
2:BB:13:SER:O	3:BS:169:LYS:CE	2.03	1.06
3:AW:66:GLU:HG2	3:BV:120:LYS:HZ2	1.09	1.06
3:AV:120:LYS:NZ	3:BW:66:GLU:HG3	1.69	1.06
2:AB:13:SER:O	3:AS:169:LYS:CD	2.03	1.05
2:AD:52:ASN:CB	3:AS:258:LEU:HD22	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:86:LYS:NZ	2:AN:81:VAL:HB	1.70	1.05
2:AB:13:SER:O	3:AS:169:LYS:CE	2.05	1.04
2:AQ:18:VAL:O	3:AX:167:ASN:HA	1.57	1.04
3:AS:197:PHE:CD1	3:AT:48:ILE:HG22	1.93	1.03
1:B0:42:ILE:CB	3:BX:43:TRP:HZ2	1.71	1.03
2:AB:13:SER:C	3:AS:169:LYS:HD2	1.78	1.03
2:AD:52:ASN:CG	3:AS:258:LEU:HD23	1.72	1.02
2:BG:103:THR:HB	1:BZ:78:PRO:HG3	1.03	1.02
2:BN:130:GLY:O	3:BV:262:PRO:HB3	1.60	1.02
3:BS:242:THR:CG2	3:BS:272:ARG:HG3	1.90	1.02
3:AV:120:LYS:HZ2	3:BW:66:GLU:HG2	0.85	1.01
3:AS:242:THR:CG2	3:AS:272:ARG:HG3	1.90	1.01
2:AD:52:ASN:CB	3:AS:258:LEU:CD2	2.38	1.00
3:AU:120:LYS:HZ1	3:BX:66:GLU:HG3	1.22	1.00
3:AW:120:LYS:CG	3:BV:68:PHE:CE1	2.44	0.99
3:AW:120:LYS:CD	3:BV:68:PHE:HE1	1.59	0.99
2:BG:103:THR:HB	1:BZ:78:PRO:CG	1.91	0.99
3:AW:120:LYS:CG	3:BV:68:PHE:HE1	1.75	0.98
2:AD:73:THR:HB	3:AS:256:THR:CG2	1.94	0.97
3:AS:66:GLU:HG3	3:BT:120:LYS:NZ	1.78	0.97
2:AQ:19:GLY:HA2	3:AX:166:GLY:O	1.65	0.97
3:AV:68:PHE:HE1	3:BW:120:LYS:CG	1.71	0.97
2:AD:73:THR:HB	3:AS:256:THR:HG21	1.47	0.97
1:B0:42:ILE:HB	3:BX:43:TRP:HZ2	0.80	0.96
3:AU:53:THR:CG2	1:AZ:359:PHE:HB3	1.95	0.96
2:BQ:17:PRO:HB3	3:BX:167:ASN:HD22	1.29	0.96
3:BT:116:GLU:HB2	3:BU:31:PRO:HD2	1.48	0.96
1:BY:169:THR:HG21	1:BZ:294:PHE:CE2	2.00	0.96
3:AX:66:GLU:HG3	3:BU:120:LYS:HZ1	1.31	0.95
2:BN:51:LEU:HD12	3:BV:262:PRO:HG2	1.46	0.95
2:BA:103:THR:HB	1:BY:78:PRO:HG3	1.46	0.95
3:AV:68:PHE:CD1	3:BW:120:LYS:HB3	2.03	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:HG2	1.30	0.94
2:AN:131:THR:HG22	3:AV:262:PRO:O	1.65	0.94
2:BE:17:PRO:CB	3:BT:167:ASN:HD22	1.79	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:CD	1.64	0.93
2:BB:13:SER:O	3:BS:169:LYS:NZ	2.02	0.93
2:AD:73:THR:CG2	3:AS:256:THR:HG21	1.99	0.92
2:AP:18:VAL:HG13	3:AX:158:LYS:O	1.70	0.92
2:BD:52:ASN:CB	3:BS:258:LEU:HD22	2.01	0.91
3:AW:66:GLU:HG3	3:BV:120:LYS:NZ	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:52:ASN:OD1	3:AS:258:LEU:HD23	1.70	0.91
2:AE:17:PRO:CB	3:AT:167:ASN:HD22	1.81	0.91
3:AV:68:PHE:CE1	3:BW:120:LYS:HG2	2.02	0.91
2:BE:17:PRO:HB3	3:BT:167:ASN:HD22	1.36	0.91
3:AV:68:PHE:HD1	3:BW:120:LYS:CD	1.77	0.90
3:AV:43:TRP:CD1	1:AZ:42:ILE:HD13	2.07	0.90
2:AE:17:PRO:HB3	3:AT:167:ASN:HD22	1.37	0.89
3:AT:116:GLU:HB2	3:AU:31:PRO:HD2	1.53	0.89
2:AA:103:THR:HB	1:AY:78:PRO:HG3	1.53	0.89
2:BD:73:THR:HB	3:BS:256:THR:HG21	1.52	0.89
2:AG:103:THR:CG2	1:AZ:78:PRO:HG3	2.01	0.89
3:AW:120:LYS:HB3	3:BV:68:PHE:CD1	2.08	0.88
3:AV:120:LYS:NZ	3:BW:66:GLU:HG2	1.72	0.88
2:AQ:17:PRO:HG3	3:AX:169:LYS:HE2	1.55	0.88
2:AQ:19:GLY:CA	3:AX:166:GLY:O	2.21	0.88
3:AU:68:PHE:CD1	3:BX:120:LYS:HD3	2.09	0.87
1:A0:88:LYS:HZ1	2:AN:104:ALA:HB3	1.36	0.87
2:BD:130:GLY:O	3:BS:262:PRO:HB2	1.75	0.86
2:BE:18:VAL:HG12	3:BT:168:TYR:O	1.75	0.85
2:AQ:17:PRO:HB3	3:AX:167:ASN:ND2	1.91	0.85
2:BD:73:THR:HB	3:BS:256:THR:CG2	2.05	0.85
3:AU:53:THR:HG21	1:AZ:359:PHE:HB3	1.58	0.85
2:BD:52:ASN:ND2	3:BS:258:LEU:CD2	2.33	0.85
3:AW:66:GLU:HG2	3:BV:120:LYS:NZ	1.80	0.85
1:A0:86:LYS:HZ2	2:AN:81:VAL:HB	1.40	0.85
2:AA:104:ALA:HB2	1:AY:88:LYS:NZ	1.91	0.85
3:AS:133:ILE:HA	3:AT:42:ILE:HG21	1.59	0.85
2:BQ:17:PRO:HB3	3:BX:169:LYS:HE3	1.59	0.85
2:AQ:17:PRO:CB	3:AX:167:ASN:HD22	1.89	0.84
2:BE:19:GLY:HA2	3:BT:166:GLY:O	1.76	0.84
3:AW:120:LYS:HG2	3:BV:68:PHE:HE1	1.41	0.84
2:AE:17:PRO:CB	3:AT:167:ASN:HB2	2.08	0.84
2:BN:73:THR:OG1	3:BV:256:THR:HG21	1.76	0.84
3:AU:68:PHE:CZ	3:BX:120:LYS:HD3	2.11	0.84
2:AB:13:SER:O	3:AS:169:LYS:NZ	2.10	0.84
3:AU:66:GLU:HG2	3:BX:120:LYS:HE2	1.60	0.83
2:AQ:18:VAL:CG1	3:AX:168:TYR:O	2.25	0.83
3:AU:120:LYS:NZ	3:BX:66:GLU:HG3	1.92	0.83
3:AX:120:LYS:HD3	3:BU:68:PHE:CD1	2.13	0.83
1:A0:86:LYS:HZ1	2:AN:81:VAL:HB	1.42	0.83
3:AS:197:PHE:CD1	3:AT:48:ILE:CG2	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:294:PHE:CE2	1:AZ:169:THR:HG21	2.13	0.83
2:AN:51:LEU:HD12	3:AV:262:PRO:HG2	1.59	0.82
2:AQ:21:ASN:OD1	3:AX:165:PRO:HG2	1.78	0.82
3:AU:120:LYS:NZ	3:BX:66:GLU:CG	2.42	0.82
2:BE:17:PRO:CB	3:BT:167:ASN:HB2	2.10	0.82
2:AE:18:VAL:HG12	3:AT:168:TYR:O	1.79	0.82
2:BE:9:PHE:HA	3:BT:170:TYR:O	1.79	0.82
2:AE:19:GLY:HA2	3:AT:166:GLY:O	1.80	0.81
3:AU:120:LYS:HZ1	3:BX:66:GLU:CG	1.93	0.81
3:AW:120:LYS:NZ	3:BV:66:GLU:HG3	1.94	0.81
2:AE:17:PRO:HB2	3:AT:167:ASN:HB2	1.62	0.81
2:AE:9:PHE:HA	3:AT:170:TYR:O	1.80	0.81
3:AX:120:LYS:HE2	3:BU:66:GLU:HG2	1.63	0.81
3:AW:120:LYS:HE2	3:BV:66:GLU:HG2	1.61	0.81
2:BQ:18:VAL:HG12	3:BX:168:TYR:O	1.79	0.81
2:AD:73:THR:CB	3:AS:256:THR:CG2	2.49	0.81
2:AD:52:ASN:HD22	3:AS:258:LEU:HD22	1.46	0.81
1:B0:239:SER:HB2	1:B0:312:GLU:O	1.81	0.81
2:BE:17:PRO:HB3	3:BT:167:ASN:ND2	1.96	0.80
2:AG:103:THR:HB	1:AZ:78:PRO:HG3	0.82	0.80
3:AT:73:GLU:HG3	3:AU:100:ILE:HG23	1.61	0.80
2:AG:79:ASP:O	1:AZ:212:ASN:ND2	2.14	0.80
2:BE:17:PRO:HB2	3:BT:167:ASN:HB2	1.64	0.80
2:AC:9:PHE:HA	3:AS:178:TYR:HB2	1.62	0.80
3:BS:242:THR:HG22	3:BS:272:ARG:HG3	1.64	0.80
2:BE:17:PRO:HB3	3:BT:169:LYS:HE3	1.64	0.79
1:A0:239:SER:HB2	1:A0:312:GLU:O	1.81	0.79
3:AW:120:LYS:HG2	3:BV:68:PHE:CE1	2.15	0.79
3:AV:68:PHE:CD1	3:BW:120:LYS:CG	2.62	0.79
2:BQ:18:VAL:O	3:BX:167:ASN:HA	1.81	0.79
2:AE:17:PRO:HB3	3:AT:167:ASN:ND2	1.97	0.79
1:A0:42:ILE:HD13	3:AX:43:TRP:NE1	1.97	0.79
2:BD:52:ASN:CG	3:BS:258:LEU:HD23	2.01	0.79
2:AN:130:GLY:O	3:AV:262:PRO:HB3	1.81	0.79
3:AV:66:GLU:HG2	3:BW:120:LYS:HE2	1.65	0.79
2:BB:14:THR:HA	3:BS:169:LYS:HE2	1.63	0.79
3:AW:120:LYS:CD	3:BV:68:PHE:HD1	1.91	0.79
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ1	1.42	0.78
3:AS:142:LEU:HD12	3:AS:291:ILE:HD12	1.65	0.78
2:AF:17:PRO:HA	3:AT:177:THR:HG22	1.65	0.78
3:AS:273:ILE:HD11	3:AT:48:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:66:GLU:CG	3:BT:120:LYS:NZ	2.45	0.78
2:BF:17:PRO:HA	3:BT:177:THR:HG22	1.66	0.78
1:AY:169:THR:HG21	1:AZ:294:PHE:CE2	2.19	0.78
3:BS:142:LEU:HD12	3:BS:291:ILE:HD12	1.65	0.78
1:A0:330:LEU:HB2	3:AV:261:PHE:CE2	2.19	0.78
2:AN:49:THR:HB	3:AV:258:LEU:HD21	1.64	0.78
3:AT:120:LYS:NZ	3:BS:66:GLU:HG3	1.98	0.77
3:AW:120:LYS:HZ1	3:BV:66:GLU:HG3	1.46	0.77
3:AX:120:LYS:HD3	3:BU:68:PHE:CZ	2.16	0.77
2:AN:73:THR:OG1	3:AV:256:THR:HG21	1.85	0.77
2:BE:21:ASN:OD1	3:BT:165:PRO:HG2	1.84	0.77
3:AS:242:THR:HG22	3:AS:272:ARG:HG3	1.64	0.77
2:BN:49:THR:O	3:BV:258:LEU:HD21	1.85	0.77
2:AD:73:THR:HG21	3:AS:256:THR:HG21	1.65	0.77
2:BD:52:ASN:CB	3:BS:258:LEU:CD2	2.61	0.77
3:AX:66:GLU:HG3	3:BU:120:LYS:NZ	2.00	0.76
2:AG:79:ASP:C	1:AZ:212:ASN:HD21	1.89	0.76
3:AU:242:THR:CG2	3:AU:272:ARG:HG3	2.16	0.76
3:AV:68:PHE:HD1	3:BW:120:LYS:HB3	1.45	0.76
2:AQ:19:GLY:HA2	3:AX:166:GLY:C	2.05	0.76
3:BU:242:THR:CG2	3:BU:272:ARG:HG3	2.16	0.76
2:BQ:19:GLY:HA2	3:BX:166:GLY:O	1.85	0.76
3:AW:66:GLU:CB	3:BV:120:LYS:HZ2	1.98	0.76
3:AS:66:GLU:HG2	3:BT:120:LYS:HE2	1.69	0.75
3:AX:120:LYS:HD3	3:BU:68:PHE:HE1	1.37	0.75
3:AX:66:GLU:CG	3:BU:120:LYS:NZ	2.49	0.75
2:BR:9:PHE:CE2	3:BX:181:GLU:HG3	2.21	0.75
2:AD:73:THR:OG1	3:AS:256:THR:HG21	1.86	0.75
1:B0:88:LYS:NZ	2:BN:104:ALA:HB3	2.01	0.75
2:AE:21:ASN:OD1	3:AT:165:PRO:HG2	1.87	0.75
2:AE:17:PRO:HB3	3:AT:169:LYS:HE3	1.68	0.75
3:AU:53:THR:HG23	1:AZ:359:PHE:HB3	1.69	0.74
2:AP:65:ARG:NH2	3:AX:181:GLU:OE2	2.19	0.74
2:BC:9:PHE:HA	3:BS:178:TYR:HB2	1.68	0.74
3:AV:68:PHE:CD1	3:BW:120:LYS:CB	2.70	0.74
3:AW:120:LYS:NZ	3:BV:66:GLU:CG	2.50	0.74
3:BU:53:THR:CG2	1:BZ:359:PHE:HB3	2.17	0.74
3:BS:197:PHE:CD1	3:BT:48:ILE:HG22	2.22	0.74
2:AQ:18:VAL:C	3:AX:167:ASN:HA	2.06	0.74
2:BR:9:PHE:CZ	3:BX:181:GLU:HG3	2.23	0.74
2:BD:73:THR:OG1	3:BS:256:THR:HG21	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:9:PHE:CD1	3:AS:180:GLY:HA2	2.23	0.73
2:AR:23:ASP:OD2	3:AX:176:TYR:OH	2.06	0.73
3:AW:120:LYS:HB3	3:BV:68:PHE:HD1	1.52	0.73
1:A0:38:ARG:NH2	3:AW:269:TYR:O	2.21	0.73
2:AR:9:PHE:CE1	3:AX:180:GLY:CA	2.72	0.73
3:BS:31:PRO:HD2	3:BX:116:GLU:HB2	1.70	0.73
2:AD:131:THR:HB	3:AS:263:VAL:HG23	1.71	0.72
2:AD:131:THR:CG2	3:AS:262:PRO:O	2.31	0.72
3:AV:66:GLU:HG3	3:BW:120:LYS:NZ	2.04	0.72
1:A0:1:MET:SD	3:AX:48:ILE:HD13	2.30	0.72
3:AV:48:ILE:HD13	1:AZ:1:MET:SD	2.30	0.72
2:AG:81:VAL:HB	1:AZ:86:LYS:NZ	2.05	0.72
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ3	1.53	0.72
3:AU:68:PHE:HE1	3:BX:120:LYS:HD3	1.40	0.71
3:AS:244:VAL:HG21	3:AT:50:VAL:HG22	1.72	0.71
1:B0:294:PHE:CE2	1:BZ:169:THR:HG21	2.25	0.71
2:AC:18:VAL:HG13	3:AS:176:TYR:CZ	2.26	0.71
2:AQ:9:PHE:HA	3:AX:170:TYR:O	1.91	0.71
2:AQ:17:PRO:CB	3:AX:169:LYS:HE3	2.17	0.71
2:AR:9:PHE:CE1	3:AX:180:GLY:HA2	2.26	0.71
1:B0:42:ILE:HD13	3:BX:43:TRP:NE1	2.06	0.70
1:A0:211:ARG:NH2	2:AN:79:ASP:HB2	2.06	0.70
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ3	1.56	0.70
2:BC:9:PHE:CD1	3:BS:180:GLY:HA2	2.27	0.70
3:AU:68:PHE:HE1	3:BX:120:LYS:CG	2.05	0.70
2:AP:113:ASN:O	3:AX:186:ARG:NH2	2.24	0.70
3:AX:66:GLU:CG	3:BU:120:LYS:HZ1	2.00	0.70
2:AA:77:LYS:H	2:AA:82:ASN:HD21	1.39	0.70
2:AQ:18:VAL:O	3:AX:167:ASN:CA	2.38	0.70
2:AD:73:THR:HB	3:AS:256:THR:HG23	1.72	0.70
2:BE:17:PRO:HG3	3:BT:169:LYS:HE2	1.74	0.70
2:AP:22:ASN:HD21	3:AX:182:SER:CB	2.04	0.69
3:AS:242:THR:HG22	3:AS:272:ARG:CG	2.21	0.69
3:BT:80:LYS:HE3	3:BU:298:VAL:HG22	1.74	0.69
3:AW:121:ASN:HD21	3:BV:68:PHE:HB3	1.57	0.69
2:BP:18:VAL:HG13	3:BX:158:LYS:O	1.91	0.69
2:AB:14:THR:HA	3:AS:169:LYS:HE2	1.73	0.69
2:BE:18:VAL:O	3:BT:167:ASN:HA	1.93	0.69
3:BS:242:THR:HG22	3:BS:272:ARG:CG	2.22	0.69
3:AV:120:LYS:NZ	3:BW:66:GLU:CB	2.55	0.69
2:BE:19:GLY:CA	3:BT:166:GLY:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:120:LYS:HG2	3:BT:68:PHE:CE1	2.28	0.69
3:AS:197:PHE:HD1	3:AT:48:ILE:CG2	2.06	0.69
1:A0:294:PHE:HE2	1:AZ:169:THR:HG21	1.57	0.69
2:BA:77:LYS:H	2:BA:82:ASN:HD21	1.39	0.69
3:AV:70:GLU:HG2	3:BW:70:GLU:HG2	1.74	0.69
3:BT:45:SER:OG	1:BY:1:MET:HB3	1.94	0.68
2:AD:73:THR:HG21	3:AS:256:THR:CG2	2.23	0.68
3:AS:250:GLN:HE21	3:AS:252:TRP:HE1	1.42	0.68
1:B0:88:LYS:HZ1	2:BN:104:ALA:HB3	1.59	0.68
2:AR:17:PRO:HA	3:AX:177:THR:HG22	1.74	0.68
2:AD:52:ASN:HB2	3:AS:258:LEU:HD22	1.71	0.68
3:AW:120:LYS:CE	3:BV:66:GLU:HG2	2.23	0.68
3:BS:250:GLN:HE21	3:BS:252:TRP:HE1	1.42	0.68
2:AD:77:LYS:H	2:AD:82:ASN:HD21	1.42	0.68
3:AU:68:PHE:CD1	3:BX:120:LYS:CD	2.72	0.68
3:AT:80:LYS:HE3	3:AU:298:VAL:HG22	1.75	0.68
3:AU:66:GLU:HB3	3:BX:120:LYS:HZ3	1.58	0.68
3:BV:43:TRP:CD1	1:BZ:42:ILE:HD13	2.28	0.68
2:AP:77:LYS:H	2:AP:82:ASN:HD21	1.41	0.68
2:BP:77:LYS:H	2:BP:82:ASN:HD21	1.41	0.68
3:AV:120:LYS:HZ1	3:BW:66:GLU:CG	2.05	0.67
2:AQ:23:ASP:OD2	3:AX:168:TYR:HE2	1.78	0.67
2:AM:77:LYS:H	2:AM:82:ASN:HD21	1.42	0.67
2:AF:18:VAL:O	3:AT:175:SER:OG	2.10	0.67
2:AD:73:THR:CG2	3:AS:256:THR:CG2	2.72	0.67
3:AS:31:PRO:HD2	3:AX:116:GLU:HB2	1.75	0.67
2:AG:103:THR:HB	1:AZ:78:PRO:CB	2.25	0.67
3:BW:142:LEU:HG	3:BW:291:ILE:HD12	1.77	0.67
2:AP:19:GLY:HA3	3:AX:180:GLY:O	1.95	0.67
3:AT:120:LYS:HZ3	3:BS:66:GLU:HG3	1.59	0.67
3:AU:68:PHE:CE1	3:BX:120:LYS:CG	2.77	0.67
2:BN:130:GLY:O	3:BV:262:PRO:CB	2.41	0.66
2:BJ:77:LYS:H	2:BJ:82:ASN:HD21	1.41	0.66
3:AW:70:GLU:HG2	3:BV:70:GLU:HG2	1.75	0.66
3:AX:120:LYS:HZ3	3:BU:66:GLU:HB3	1.59	0.66
2:BN:49:THR:HB	3:BV:258:LEU:HD21	1.75	0.66
2:BN:49:THR:HG21	3:BV:235:GLN:NE2	2.10	0.66
2:BD:23:ASP:OD2	3:BT:178:TYR:HE1	1.77	0.66
2:AJ:77:LYS:H	2:AJ:82:ASN:HD21	1.41	0.66
2:BD:77:LYS:H	2:BD:82:ASN:HD21	1.42	0.66
3:AU:271:THR:HA	1:AZ:3:GLU:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BM:77:LYS:H	2:BM:82:ASN:HD21	1.42	0.66
3:AS:66:GLU:CG	3:BT:120:LYS:HZ3	2.07	0.66
2:BC:18:VAL:HG13	3:BS:176:TYR:CZ	2.31	0.66
3:AV:120:LYS:HZ3	3:BW:66:GLU:HG3	1.61	0.66
2:AD:52:ASN:ND2	3:AS:258:LEU:HB3	2.10	0.66
3:BT:73:GLU:HG3	3:BU:100:ILE:HG23	1.77	0.66
1:BZ:238:ARG:HG3	1:BZ:316:SER:HA	1.78	0.66
2:AG:77:LYS:H	2:AG:82:ASN:HD21	1.42	0.66
3:AS:133:ILE:HG13	3:AT:42:ILE:HD13	1.78	0.66
3:AU:269:TYR:O	1:AZ:38:ARG:NH2	2.27	0.66
2:BG:77:LYS:H	2:BG:82:ASN:HD21	1.42	0.66
2:AE:18:VAL:O	3:AT:167:ASN:HA	1.96	0.66
3:AW:142:LEU:HG	3:AW:291:ILE:HD12	1.77	0.66
2:BQ:17:PRO:HG3	3:BX:169:LYS:HE2	1.78	0.66
2:AE:17:PRO:HB2	3:AT:167:ASN:CB	2.25	0.65
3:AW:120:LYS:CB	3:BV:68:PHE:CD1	2.80	0.65
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ2	1.60	0.65
2:AD:51:LEU:CD1	3:AS:262:PRO:HG2	2.26	0.65
2:AP:22:ASN:ND2	3:AX:182:SER:OG	2.30	0.65
3:BU:76:TYR:HB3	3:BV:100:ILE:HD11	1.78	0.65
2:BD:52:ASN:OD1	3:BS:258:LEU:HD23	1.95	0.65
2:AN:49:THR:HB	3:AV:258:LEU:CD2	2.26	0.65
3:AS:244:VAL:CG2	3:AT:50:VAL:HG22	2.27	0.65
1:AZ:238:ARG:HG3	1:AZ:316:SER:HA	1.78	0.65
1:BZ:89:LEU:HD22	1:BZ:192:GLN:HG3	1.79	0.65
2:AE:17:PRO:HG3	3:AT:169:LYS:HE2	1.77	0.65
3:AV:120:LYS:HZ1	3:BW:66:GLU:CB	2.09	0.65
2:BN:49:THR:HG21	3:BV:235:GLN:HE22	1.62	0.65
3:BU:53:THR:HG21	1:BZ:359:PHE:HB3	1.79	0.65
3:AW:66:GLU:CB	3:BV:120:LYS:NZ	2.58	0.65
2:BD:131:THR:HA	3:BS:262:PRO:HB2	1.78	0.65
2:BA:120:LYS:HE2	3:BS:222:ASN:ND2	2.12	0.64
1:AY:152:PHE:HB2	1:AY:208:PHE:HB2	1.80	0.64
1:AY:243:PHE:HA	1:AY:313:ILE:HD11	1.79	0.64
3:BS:250:GLN:NE2	3:BS:252:TRP:HE1	1.96	0.64
3:AX:120:LYS:CG	3:BU:68:PHE:HE1	2.11	0.64
2:AQ:23:ASP:OD2	3:AX:168:TYR:CE2	2.50	0.64
2:AQ:17:PRO:HB3	3:AX:169:LYS:CE	2.20	0.64
3:AX:120:LYS:HZ3	3:BU:66:GLU:CB	2.10	0.64
1:AZ:89:LEU:HD22	1:AZ:192:GLN:HG3	1.79	0.64
3:AS:250:GLN:NE2	3:AS:252:TRP:HE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:68:PHE:CD1	3:BX:120:LYS:HB3	2.33	0.64
2:AE:19:GLY:CA	3:AT:166:GLY:O	2.44	0.64
2:AG:79:ASP:CA	1:AZ:212:ASN:HD21	2.11	0.63
1:BY:152:PHE:HB2	1:BY:208:PHE:HB2	1.80	0.63
3:AV:66:GLU:CG	3:BW:120:LYS:NZ	2.62	0.63
3:BV:116:GLU:HB2	3:BW:31:PRO:HD2	1.79	0.63
2:BE:17:PRO:HB2	3:BT:167:ASN:CB	2.26	0.63
2:BD:73:THR:CG2	3:BS:256:THR:HG21	2.28	0.63
2:AD:23:ASP:OD2	3:AT:178:TYR:HE1	1.82	0.63
3:BV:247:GLU:OE1	3:BV:249:TYR:HE2	1.82	0.63
3:AV:247:GLU:OE1	3:AV:249:TYR:HE2	1.82	0.63
3:AU:68:PHE:HD1	3:BX:120:LYS:HB3	1.63	0.63
2:AD:51:LEU:HD11	3:AS:262:PRO:HG2	1.81	0.63
3:AX:11:LEU:HD23	3:AX:12:ASP:H	1.64	0.63
3:AT:120:LYS:HE2	3:BS:66:GLU:HG2	1.80	0.63
3:AW:66:GLU:HG3	3:BV:120:LYS:HZ3	1.64	0.63
3:BX:11:LEU:HD23	3:BX:12:ASP:H	1.63	0.63
1:BY:243:PHE:HA	1:BY:313:ILE:HD11	1.79	0.63
1:A0:152:PHE:HB2	1:A0:208:PHE:HB2	1.81	0.62
2:AQ:17:PRO:HG3	3:AX:169:LYS:CE	2.27	0.62
3:AU:224:TYR:HB2	1:AZ:74:PRO:HB2	1.81	0.62
2:AD:52:ASN:CB	3:AS:258:LEU:HD21	2.27	0.62
3:AV:45:SER:CB	1:AZ:42:ILE:HG22	2.29	0.62
1:A0:330:LEU:HB2	3:AV:261:PHE:HE2	1.64	0.62
2:BD:73:THR:CB	3:BS:256:THR:CG2	2.63	0.62
3:AV:66:GLU:HG3	3:BW:120:LYS:HZ1	1.63	0.62
1:BY:241:TYR:HB2	1:BY:291:LYS:HD2	1.81	0.62
2:AP:9:PHE:HA	3:AX:160:TYR:O	1.99	0.62
2:BR:23:ASP:OD2	3:BX:176:TYR:OH	2.17	0.62
2:BB:17:PRO:HB3	3:BS:167:ASN:HB2	1.81	0.62
3:AX:120:LYS:CD	3:BU:68:PHE:CD1	2.77	0.62
1:A0:88:LYS:HE2	2:AN:106:ASN:OD1	1.99	0.62
3:AU:271:THR:HA	1:AZ:3:GLU:CG	2.30	0.62
2:AF:23:ASP:OD2	3:AT:176:TYR:OH	2.17	0.62
3:AV:68:PHE:HD1	3:BW:120:LYS:CB	2.09	0.62
3:AU:120:LYS:HE2	3:BX:66:GLU:HG2	1.82	0.62
3:AS:245:ASN:OD1	3:AT:51:MET:N	2.26	0.61
1:B0:152:PHE:HB2	1:B0:208:PHE:HB2	1.81	0.61
3:AV:66:GLU:HG2	3:BW:120:LYS:CE	2.30	0.61
1:A0:88:LYS:HZ2	2:AN:104:ALA:HB3	1.62	0.61
3:AW:215:ARG:HB3	3:AW:282:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:66:GLU:CB	3:BX:120:LYS:HZ3	2.13	0.61
3:BX:199:PHE:N	3:BX:242:THR:OG1	2.33	0.61
1:A0:88:LYS:NZ	2:AN:104:ALA:CB	2.52	0.61
3:BW:215:ARG:HB3	3:BW:282:ILE:HD11	1.83	0.61
3:AS:215:ARG:HB3	3:AS:282:ILE:HD11	1.82	0.61
1:A0:3:GLU:HG3	3:AW:271:THR:HA	1.83	0.61
3:AX:247:GLU:OE1	3:AX:249:TYR:HE2	1.83	0.61
2:AQ:19:GLY:HA3	3:AX:166:GLY:O	2.01	0.61
3:AT:120:LYS:HZ3	3:BS:66:GLU:CG	2.14	0.61
1:AY:241:TYR:HB2	1:AY:291:LYS:HD2	1.81	0.61
1:BZ:90:ASN:HD22	1:BZ:192:GLN:NE2	1.99	0.61
2:AD:131:THR:O	3:AS:263:VAL:HG23	2.01	0.60
3:AS:269:TYR:O	1:AY:38:ARG:NH2	2.29	0.60
2:BD:51:LEU:CD1	3:BS:262:PRO:HG2	2.31	0.60
3:AT:235:GLN:HE22	3:AT:258:LEU:HD12	1.66	0.60
2:AA:104:ALA:CB	1:AY:88:LYS:NZ	2.63	0.60
1:AZ:90:ASN:HD22	1:AZ:192:GLN:NE2	1.99	0.60
3:BT:235:GLN:HE22	3:BT:258:LEU:HD12	1.66	0.60
3:BX:247:GLU:OE1	3:BX:249:TYR:HE2	1.83	0.60
1:B0:294:PHE:HE2	1:BZ:169:THR:HG21	1.66	0.60
3:BU:53:THR:HG23	1:BZ:359:PHE:HB3	1.84	0.60
2:BG:81:VAL:HB	1:BZ:86:LYS:NZ	2.16	0.60
3:AV:68:PHE:CE1	3:BW:120:LYS:CE	2.83	0.60
3:AX:120:LYS:CG	3:BU:68:PHE:CE1	2.84	0.60
2:AE:17:PRO:CB	3:AT:167:ASN:ND2	2.58	0.60
2:AA:104:ALA:HB3	1:AY:88:LYS:HD2	1.84	0.60
3:AU:53:THR:HG21	1:AZ:359:PHE:CB	2.29	0.60
3:AV:50:VAL:HG11	1:AZ:60:THR:HG22	1.84	0.60
2:AP:23:ASP:OD2	3:AX:178:TYR:HE1	1.85	0.60
3:BU:137:TYR:HD1	3:BU:292:LYS:HB2	1.66	0.60
3:AU:66:GLU:CG	3:BX:120:LYS:NZ	2.64	0.60
2:BE:17:PRO:CB	3:BT:167:ASN:ND2	2.56	0.60
3:AW:121:ASN:ND2	3:BV:68:PHE:HB3	2.16	0.60
3:BX:12:ASP:HB2	3:BX:200:MET:HG3	1.84	0.60
3:AS:206:LYS:HG3	3:AS:285:SER:HB3	1.84	0.60
3:BS:215:ARG:HB3	3:BS:282:ILE:HD11	1.82	0.60
3:BX:199:PHE:CE1	3:BX:242:THR:HG21	2.37	0.60
2:AR:18:VAL:HG12	3:AX:176:TYR:O	2.02	0.60
1:A0:42:ILE:HD13	3:AX:43:TRP:HE1	1.65	0.60
2:BF:23:ASP:OD2	3:BT:176:TYR:OH	2.18	0.60
3:AX:12:ASP:HB2	3:AX:200:MET:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:9:PHE:CZ	3:AX:181:GLU:HG3	2.37	0.59
2:BD:52:ASN:HB2	3:BS:258:LEU:HD22	1.82	0.59
2:AG:92:GLN:NE2	3:AU:189:ARG:CZ	2.65	0.59
2:AD:49:THR:CG2	3:AS:233:GLN:HB2	2.32	0.59
3:AV:171:ILE:HG22	3:AV:172:LYS:H	1.68	0.59
3:AU:66:GLU:HG3	3:BX:120:LYS:HZ1	1.66	0.59
3:BS:206:LYS:HG3	3:BS:285:SER:HB3	1.84	0.59
2:AG:79:ASP:O	1:AZ:212:ASN:CG	2.40	0.59
3:AU:137:TYR:HD1	3:AU:292:LYS:HB2	1.66	0.59
3:AX:199:PHE:CE1	3:AX:242:THR:HG21	2.37	0.59
2:BN:49:THR:HB	3:BV:258:LEU:CD2	2.32	0.59
3:BX:215:ARG:HB3	3:BX:282:ILE:HD11	1.84	0.59
3:AV:68:PHE:HB3	3:BW:121:ASN:HD21	1.66	0.59
2:BA:104:ALA:HB2	1:BY:88:LYS:NZ	2.17	0.59
3:AX:199:PHE:N	3:AX:242:THR:OG1	2.33	0.59
3:BU:215:ARG:HB3	3:BU:282:ILE:HD11	1.83	0.59
3:AU:120:LYS:CE	3:BX:66:GLU:HG2	2.33	0.59
3:AU:215:ARG:HB3	3:AU:282:ILE:HD11	1.83	0.59
2:BQ:19:GLY:CA	3:BX:166:GLY:O	2.49	0.59
2:AD:131:THR:HA	3:AS:262:PRO:HB2	1.84	0.59
3:BV:247:GLU:OE1	3:BV:249:TYR:CE2	2.56	0.59
3:AX:215:ARG:HB3	3:AX:282:ILE:HD11	1.84	0.58
3:BS:273:ILE:HD11	3:BT:48:ILE:HD12	1.83	0.58
3:AT:73:GLU:CG	3:AU:100:ILE:HG23	2.31	0.58
2:BG:79:ASP:O	1:BZ:212:ASN:ND2	2.37	0.58
1:BZ:41:VAL:HG23	1:BZ:57:ALA:HB1	1.85	0.58
2:AP:21:ASN:HB3	3:AX:181:GLU:CD	2.23	0.58
1:AZ:41:VAL:HG23	1:AZ:57:ALA:HB1	1.85	0.58
2:AN:120:LYS:HE2	3:AW:222:ASN:ND2	2.18	0.58
2:AN:51:LEU:HD12	3:AV:262:PRO:CG	2.33	0.58
2:AR:88:ILE:HG12	2:AR:97:VAL:HG22	1.85	0.58
3:AU:238:ILE:HG22	3:AU:240:ILE:HG23	1.85	0.58
3:AV:116:GLU:HB2	3:AW:31:PRO:HD2	1.84	0.58
3:AV:226:ALA:HB3	3:AV:268:ARG:HB3	1.85	0.58
3:AX:120:LYS:NZ	3:BU:66:GLU:CG	2.66	0.58
2:AR:9:PHE:CE2	3:AX:181:GLU:HG3	2.38	0.58
3:AT:45:SER:OG	1:AY:1:MET:HB3	2.04	0.58
2:AF:88:ILE:HG12	2:AF:97:VAL:HG22	1.86	0.58
3:BU:238:ILE:HG22	3:BU:240:ILE:HG23	1.85	0.58
1:BZ:153:ASN:HB3	1:BZ:156:ILE:HG12	1.85	0.58
2:AC:88:ILE:HG12	2:AC:97:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BS:196:ILE:HG13	3:BS:274:ILE:HB	1.85	0.58
2:BQ:21:ASN:OD1	3:BX:165:PRO:HG2	2.03	0.58
2:BO:88:ILE:HG12	2:BO:97:VAL:HG22	1.85	0.58
3:BV:171:ILE:HG22	3:BV:172:LYS:H	1.68	0.58
2:AD:49:THR:HG22	3:AS:233:GLN:HB2	1.85	0.57
2:AE:18:VAL:HG13	3:AT:168:TYR:CD2	2.38	0.57
3:AU:68:PHE:HB3	3:BX:121:ASN:HD21	1.68	0.57
3:AV:247:GLU:OE1	3:AV:249:TYR:CE2	2.56	0.57
2:AI:88:ILE:HG12	2:AI:97:VAL:HG22	1.85	0.57
1:A0:330:LEU:HB2	3:AV:261:PHE:CD2	2.39	0.57
3:AW:120:LYS:CG	3:BV:68:PHE:CD1	2.78	0.57
1:AZ:153:ASN:HB3	1:AZ:156:ILE:HG12	1.85	0.57
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ1	1.69	0.57
3:AS:66:GLU:HG2	3:BT:120:LYS:CE	2.34	0.57
3:AU:66:GLU:HG2	3:BX:120:LYS:CE	2.30	0.57
3:BV:226:ALA:HB3	3:BV:268:ARG:HB3	1.85	0.57
2:AO:88:ILE:HG12	2:AO:97:VAL:HG22	1.85	0.57
3:AX:206:LYS:HG3	3:AX:285:SER:HB3	1.86	0.57
3:BU:114:LYS:NZ	3:BV:298:VAL:O	2.37	0.57
2:BF:18:VAL:O	3:BT:175:SER:OG	2.07	0.57
2:BF:88:ILE:HG12	2:BF:97:VAL:HG22	1.86	0.57
2:BN:51:LEU:HD12	3:BV:262:PRO:CG	2.26	0.57
2:BE:18:VAL:HG13	3:BT:168:TYR:CD2	2.39	0.57
2:AQ:21:ASN:CG	3:AX:165:PRO:HG2	2.24	0.57
2:AR:20:SER:HA	3:AX:170:TYR:CD1	2.40	0.57
3:AS:196:ILE:HG13	3:AS:274:ILE:HB	1.85	0.57
1:B0:86:LYS:NZ	2:BN:81:VAL:HB	2.19	0.57
2:BR:88:ILE:HG12	2:BR:97:VAL:HG22	1.85	0.57
2:BR:9:PHE:CE1	3:BX:180:GLY:CA	2.87	0.57
2:AA:120:LYS:HE2	3:AS:222:ASN:ND2	2.19	0.57
2:AR:9:PHE:CZ	3:AX:180:GLY:C	2.78	0.57
1:A0:78:PRO:HG3	2:AN:103:THR:HB	1.87	0.57
3:AU:196:ILE:HG22	3:AU:293:ARG:HD3	1.87	0.57
2:AP:21:ASN:CB	3:AX:181:GLU:HG2	2.35	0.57
2:BI:88:ILE:HG12	2:BI:97:VAL:HG22	1.85	0.57
3:AV:68:PHE:HB3	3:BW:121:ASN:ND2	2.20	0.56
2:BC:88:ILE:HG12	2:BC:97:VAL:HG22	1.85	0.56
2:BR:17:PRO:HA	3:BX:177:THR:HG22	1.87	0.56
3:BT:73:GLU:HB2	3:BU:99:GLU:CD	2.25	0.56
2:AD:131:THR:HG22	3:AS:262:PRO:C	2.18	0.56
3:BU:240:ILE:HD12	3:BU:240:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AW:206:LYS:HG3	3:AW:285:SER:HB3	1.87	0.56
3:AT:266:PHE:CD1	1:AZ:221:ARG:HB2	2.40	0.56
3:AV:206:LYS:HG3	3:AV:285:SER:HB3	1.87	0.56
3:AT:240:ILE:HD12	3:AT:240:ILE:O	2.06	0.56
2:AR:23:ASP:OD2	3:AX:176:TYR:CE2	2.58	0.56
3:BX:206:LYS:HG3	3:BX:285:SER:HB3	1.86	0.56
1:A0:41:VAL:HG11	1:A0:71:ILE:HG12	1.87	0.56
2:AL:88:ILE:HG12	2:AL:97:VAL:HG22	1.86	0.56
2:AM:26:LEU:HD13	2:AN:66:TYR:HB2	1.88	0.56
3:AU:76:TYR:HB3	3:AV:100:ILE:HD11	1.86	0.56
2:BD:19:GLY:HA2	3:BT:180:GLY:O	2.05	0.56
3:BW:206:LYS:HG3	3:BW:285:SER:HB3	1.87	0.56
2:AC:18:VAL:HG13	3:AS:176:TYR:CE2	2.41	0.56
2:AE:187:ILE:HG12	2:AE:260:SER:HB3	1.88	0.56
2:AK:10:SER:HA	2:AK:15:GLU:HB2	1.88	0.56
2:AN:187:ILE:HG12	2:AN:260:SER:HB3	1.88	0.56
3:AS:270:ARG:NH1	1:AY:72:LEU:HD22	2.21	0.56
3:BW:76:TYR:HB3	3:BX:100:ILE:HD11	1.87	0.56
3:AX:120:LYS:CD	3:BU:68:PHE:HE1	2.01	0.56
2:BQ:18:VAL:CG1	3:BX:168:TYR:O	2.52	0.56
2:AB:17:PRO:HB3	3:AS:167:ASN:HB2	1.88	0.56
2:BE:187:ILE:HG12	2:BE:260:SER:HB3	1.88	0.56
2:BL:88:ILE:HG12	2:BL:97:VAL:HG22	1.86	0.56
3:BU:196:ILE:HG22	3:BU:293:ARG:HD3	1.87	0.56
2:BN:51:LEU:CD1	3:BV:262:PRO:HG2	2.28	0.56
3:AX:120:LYS:HB3	3:BU:68:PHE:HD1	1.71	0.55
3:AX:247:GLU:OE1	3:AX:249:TYR:CE2	2.59	0.55
2:BB:88:ILE:HG12	2:BB:97:VAL:HG22	1.88	0.55
2:BM:26:LEU:HD13	2:BN:66:TYR:HB2	1.88	0.55
3:BV:206:LYS:HG3	3:BV:285:SER:HB3	1.87	0.55
2:BN:120:LYS:NZ	3:BW:220:ILE:O	2.34	0.55
3:BU:224:TYR:HB2	1:BZ:74:PRO:HB2	1.88	0.55
3:BX:240:ILE:O	3:BX:240:ILE:HD12	2.07	0.55
3:BX:247:GLU:OE1	3:BX:249:TYR:CE2	2.59	0.55
3:AS:197:PHE:HB2	3:AT:48:ILE:HG21	1.88	0.55
3:AU:66:GLU:HG3	3:BX:120:LYS:NZ	2.22	0.55
3:AX:120:LYS:CE	3:BU:66:GLU:HG2	2.33	0.55
2:AQ:18:VAL:O	3:AX:168:TYR:N	2.39	0.55
1:B0:42:ILE:HD13	3:BX:43:TRP:HE1	1.69	0.55
1:A0:88:LYS:CE	2:AN:106:ASN:OD1	2.54	0.55
2:AB:155:VAL:HG21	2:AB:159:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:120:LYS:NZ	3:BS:66:GLU:CG	2.66	0.55
3:BT:240:ILE:HD12	3:BT:240:ILE:O	2.06	0.55
2:BG:103:THR:CG2	1:BZ:78:PRO:HG3	2.35	0.55
2:AN:47:LEU:HD22	3:AV:233:GLN:CD	2.26	0.55
3:AX:120:LYS:HB3	3:BU:68:PHE:CD1	2.41	0.55
3:BT:160:TYR:HB3	3:BT:166:GLY:HA3	1.89	0.55
3:AU:108:ALA:HB2	3:AU:133:ILE:HD11	1.89	0.55
3:AU:240:ILE:O	3:AU:240:ILE:HD12	2.05	0.55
1:AZ:41:VAL:HG11	1:AZ:71:ILE:HG12	1.88	0.55
3:AU:120:LYS:NZ	3:BX:66:GLU:HG2	2.22	0.55
2:AD:131:THR:HB	3:AS:263:VAL:CG2	2.37	0.55
2:BF:23:ASP:OD2	3:BT:176:TYR:CE2	2.60	0.55
2:BN:187:ILE:HG12	2:BN:260:SER:HB3	1.88	0.55
2:AQ:187:ILE:HG12	2:AQ:260:SER:HB3	1.88	0.55
3:AX:240:ILE:O	3:AX:240:ILE:HD12	2.07	0.55
2:BH:187:ILE:HG12	2:BH:260:SER:HB3	1.88	0.55
2:AK:88:ILE:HG12	2:AK:97:VAL:HG22	1.89	0.55
3:BU:160:TYR:HB3	3:BU:166:GLY:HA3	1.89	0.55
2:AD:52:ASN:ND2	3:AS:258:LEU:CB	2.70	0.55
3:AS:87:LEU:O	3:AT:54:ARG:NH1	2.40	0.55
1:B0:41:VAL:HG11	1:B0:71:ILE:HG12	1.88	0.55
2:AB:88:ILE:HG12	2:AB:97:VAL:HG22	1.88	0.54
2:AN:89:ASP:OD2	3:AW:189:ARG:NH1	2.33	0.54
3:AT:123:THR:HG21	3:BS:120:LYS:HD2	1.89	0.54
2:AG:92:GLN:HE21	3:AU:189:ARG:NE	2.05	0.54
3:AX:120:LYS:NZ	3:BU:66:GLU:HG3	2.23	0.54
2:BK:10:SER:HA	2:BK:15:GLU:HB2	1.87	0.54
2:BK:187:ILE:HG12	2:BK:260:SER:HB3	1.88	0.54
1:BY:243:PHE:CD1	1:BY:243:PHE:C	2.80	0.54
2:AG:80:SER:OG	1:AZ:211:ARG:HD2	2.07	0.54
2:AB:187:ILE:HG12	2:AB:260:SER:HB3	1.88	0.54
2:BQ:187:ILE:HG12	2:BQ:260:SER:HB3	1.88	0.54
2:AE:88:ILE:HG12	2:AE:97:VAL:HG22	1.89	0.54
2:AH:187:ILE:HG12	2:AH:260:SER:HB3	1.88	0.54
2:AH:88:ILE:HG12	2:AH:97:VAL:HG22	1.89	0.54
2:AK:187:ILE:HG12	2:AK:260:SER:HB3	1.88	0.54
2:AP:5:ASN:HB3	2:AP:8:PHE:CD1	2.42	0.54
2:AC:18:VAL:CG1	3:AS:176:TYR:CZ	2.90	0.54
3:AU:160:TYR:HB3	3:AU:166:GLY:HA3	1.89	0.54
1:AY:243:PHE:C	1:AY:243:PHE:CD1	2.80	0.54
3:BT:106:ASP:O	3:BT:133:ILE:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:66:GLU:HG2	3:BU:120:LYS:HE2	1.89	0.54
3:AS:160:TYR:HB3	3:AS:166:GLY:HA3	1.89	0.54
2:BQ:88:ILE:HG12	2:BQ:97:VAL:HG22	1.89	0.54
3:BT:215:ARG:HB3	3:BT:282:ILE:HD11	1.89	0.54
2:BD:73:THR:HB	3:BS:256:THR:HG23	1.87	0.54
1:BZ:41:VAL:HG11	1:BZ:71:ILE:HG12	1.88	0.54
2:AM:88:ILE:HG12	2:AM:97:VAL:HG22	1.90	0.54
3:AX:226:ALA:HB3	3:AX:268:ARG:HB3	1.89	0.54
2:BA:104:ALA:HB2	1:BY:88:LYS:HZ2	1.72	0.54
2:BQ:17:PRO:HB3	3:BX:167:ASN:ND2	2.12	0.54
3:BX:167:ASN:ND2	3:BX:169:LYS:HE3	2.23	0.54
2:AN:49:THR:O	3:AV:258:LEU:HD21	2.08	0.54
3:AT:160:TYR:HB3	3:AT:166:GLY:HA3	1.89	0.54
3:AT:215:ARG:HB3	3:AT:282:ILE:HD11	1.89	0.54
2:BK:88:ILE:HG12	2:BK:97:VAL:HG22	1.89	0.54
2:BP:5:ASN:HB3	2:BP:8:PHE:CD1	2.42	0.54
1:A0:294:PHE:CE2	1:AZ:169:THR:CG2	2.88	0.53
2:AQ:8:PHE:O	3:AX:170:TYR:HB2	2.07	0.53
2:AQ:88:ILE:HG12	2:AQ:97:VAL:HG22	1.89	0.53
3:AU:242:THR:HG23	3:AU:272:ARG:HG3	1.87	0.53
1:A0:344:GLY:HA3	3:AV:270:ARG:HH11	1.73	0.53
2:BB:187:ILE:HG12	2:BB:260:SER:HB3	1.88	0.53
3:BU:242:THR:HG23	3:BU:272:ARG:HG3	1.87	0.53
3:BU:55:SER:HB3	1:BZ:359:PHE:CE1	2.44	0.53
3:AT:106:ASP:O	3:AT:133:ILE:HB	2.08	0.53
3:BS:160:TYR:HB3	3:BS:166:GLY:HA3	1.89	0.53
2:AN:47:LEU:HD22	3:AV:233:GLN:NE2	2.23	0.53
2:AP:21:ASN:H	3:AX:181:GLU:HG2	1.73	0.53
2:BB:155:VAL:HG21	2:BB:159:ILE:HD11	1.88	0.53
2:BF:17:PRO:HA	3:BT:177:THR:CG2	2.37	0.53
2:BN:131:THR:CG2	3:BV:262:PRO:O	2.42	0.53
3:AW:120:LYS:HZ3	3:BV:66:GLU:CG	2.21	0.53
1:B0:238:ARG:HG3	1:B0:316:SER:HA	1.89	0.53
3:BT:114:LYS:HB3	3:BU:34:LEU:HB2	1.90	0.53
3:AX:121:ASN:HD21	3:BU:68:PHE:HB3	1.73	0.53
1:B0:169:THR:HG21	1:BY:294:PHE:CE2	2.42	0.53
2:AD:19:GLY:HA2	3:AT:180:GLY:O	2.08	0.53
3:AX:167:ASN:ND2	3:AX:169:LYS:HE3	2.23	0.53
2:BE:88:ILE:HG12	2:BE:97:VAL:HG22	1.89	0.53
1:A0:45:GLU:HA	1:A0:357:THR:HG22	1.91	0.53
2:AG:88:ILE:HG12	2:AG:97:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AJ:88:ILE:HG12	2:AJ:97:VAL:HG22	1.90	0.53
2:AN:47:LEU:HB3	3:AV:233:GLN:OE1	2.09	0.53
2:BH:88:ILE:HG12	2:BH:97:VAL:HG22	1.89	0.53
3:BU:108:ALA:HB2	3:BU:133:ILE:HD11	1.89	0.53
2:AA:5:ASN:HB3	2:AA:8:PHE:CD1	2.44	0.53
2:AN:88:ILE:HG12	2:AN:97:VAL:HG22	1.89	0.53
2:AP:26:LEU:HD13	2:AQ:66:TYR:HB2	1.91	0.53
2:BN:47:LEU:HB3	3:BV:233:GLN:OE1	2.09	0.53
3:BS:133:ILE:HA	3:BT:42:ILE:HG21	1.91	0.53
2:BA:120:LYS:HE2	3:BS:222:ASN:HD21	1.74	0.53
3:BX:226:ALA:HB3	3:BX:268:ARG:HB3	1.89	0.53
3:AT:206:LYS:HG3	3:AT:285:SER:HB3	1.91	0.53
2:BF:18:VAL:HG12	3:BT:176:TYR:O	2.10	0.53
1:A0:238:ARG:HG3	1:A0:316:SER:HA	1.90	0.52
3:AX:160:TYR:HB3	3:AX:166:GLY:HA3	1.91	0.52
2:BD:5:ASN:HB3	2:BD:8:PHE:CD1	2.44	0.52
2:BP:88:ILE:HG12	2:BP:97:VAL:HG22	1.91	0.52
3:AW:68:PHE:CE1	3:BV:120:LYS:HD2	2.44	0.52
2:AD:5:ASN:HB3	2:AD:8:PHE:CD1	2.44	0.52
3:AW:196:ILE:HG13	3:AW:274:ILE:HB	1.90	0.52
3:AX:183:ASP:O	3:AX:186:ARG:HG3	2.09	0.52
1:B0:45:GLU:HA	1:B0:357:THR:HG22	1.91	0.52
2:AP:88:ILE:HG12	2:AP:97:VAL:HG22	1.91	0.52
2:AF:17:PRO:CA	3:AT:177:THR:HG22	2.36	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:NZ	2.24	0.52
2:BN:88:ILE:HG12	2:BN:97:VAL:HG22	1.89	0.52
2:BP:26:LEU:HD13	2:BQ:66:TYR:HB2	1.91	0.52
2:BQ:25:LYS:HE2	2:BQ:113:ASN:HB3	1.91	0.52
3:BT:206:LYS:HG3	3:BT:285:SER:HB3	1.91	0.52
3:BU:55:SER:HB3	1:BZ:359:PHE:HE1	1.74	0.52
2:BA:5:ASN:HB3	2:BA:8:PHE:CD1	2.44	0.52
2:BJ:88:ILE:HG12	2:BJ:97:VAL:HG22	1.91	0.52
2:AP:21:ASN:HB3	3:AX:181:GLU:HG2	1.92	0.52
1:AZ:241:TYR:HB2	1:AZ:291:LYS:HD2	1.91	0.52
2:BG:88:ILE:HG12	2:BG:97:VAL:HG22	1.90	0.52
2:BR:9:PHE:CE1	3:BX:180:GLY:HA2	2.44	0.52
2:AF:23:ASP:OD2	3:AT:176:TYR:CE2	2.63	0.52
3:BW:196:ILE:HG13	3:BW:274:ILE:HB	1.90	0.52
3:AT:230:LYS:HG3	3:AT:263:VAL:HG22	1.91	0.52
3:AV:142:LEU:HG	3:AV:291:ILE:HD12	1.90	0.52
3:BX:183:ASP:O	3:BX:186:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:116:GLU:HB2	3:AV:31:PRO:HD2	1.91	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:HZ2	1.70	0.52
2:AA:148:ILE:HB	2:AC:153:MET:HG3	1.92	0.52
2:BE:17:PRO:HB2	3:BT:167:ASN:HD22	1.72	0.52
3:BV:142:LEU:HG	3:BV:291:ILE:HD12	1.90	0.52
1:BY:89:LEU:HD22	1:BY:192:GLN:HG3	1.92	0.52
3:AU:281:LEU:HB3	3:AU:284:LEU:HD12	1.92	0.52
3:AW:160:TYR:HB3	3:AW:166:GLY:HA3	1.92	0.52
3:AW:66:GLU:CG	3:BV:120:LYS:HZ3	2.15	0.52
2:AQ:20:SER:OG	3:AX:165:PRO:O	2.18	0.52
2:AQ:18:VAL:HG13	3:AX:168:TYR:CD2	2.45	0.52
3:AV:43:TRP:CZ2	1:AZ:43:ASN:HB2	2.45	0.52
2:BL:145:LEU:HD13	2:BL:148:ILE:HD11	1.91	0.52
3:BT:230:LYS:HG3	3:BT:263:VAL:HG22	1.91	0.52
1:B0:12:PRO:HB2	1:BY:288:ARG:NH2	2.25	0.52
1:BZ:241:TYR:HB2	1:BZ:291:LYS:HD2	1.91	0.52
2:BR:9:PHE:HE2	3:BX:181:GLU:HG3	1.72	0.51
3:BT:132:ILE:HD13	3:BT:135:LYS:HG3	1.92	0.51
3:BW:226:ALA:HB3	3:BW:268:ARG:HB3	1.92	0.51
2:BP:5:ASN:O	2:BP:16:PHE:HB3	2.10	0.51
2:AA:88:ILE:HG12	2:AA:97:VAL:HG22	1.92	0.51
1:A0:42:ILE:HD13	3:AX:43:TRP:CE2	2.44	0.51
2:AP:5:ASN:O	2:AP:16:PHE:HB3	2.11	0.51
2:AQ:25:LYS:HE2	2:AQ:113:ASN:HB3	1.92	0.51
2:BM:88:ILE:HG12	2:BM:97:VAL:HG22	1.90	0.51
3:BS:242:THR:HG23	3:BS:272:ARG:HG3	1.89	0.51
3:BX:160:TYR:HB3	3:BX:166:GLY:HA3	1.91	0.51
1:BY:32:LEU:HD11	1:BY:204:LEU:HB2	1.92	0.51
2:AD:52:ASN:HD21	3:AS:258:LEU:HB3	1.75	0.51
3:AS:266:PHE:CG	1:AY:35:PRO:HD2	2.46	0.51
3:AT:87:LEU:HA	3:AU:54:ARG:NH1	2.25	0.51
3:AT:132:ILE:HD13	3:AT:135:LYS:HG3	1.92	0.51
2:BA:88:ILE:HG12	2:BA:97:VAL:HG22	1.92	0.51
2:AI:177:GLN:HB3	2:AI:189:ARG:HB2	1.93	0.51
2:AN:100:SER:HB3	3:AW:220:ILE:HG21	1.92	0.51
3:AT:199:PHE:N	3:AT:242:THR:OG1	2.39	0.51
2:BA:148:ILE:HB	2:BC:153:MET:HG3	1.92	0.51
2:AQ:17:PRO:CB	3:AX:169:LYS:CE	2.84	0.51
2:BI:177:GLN:HB3	2:BI:189:ARG:HB2	1.93	0.51
3:BW:160:TYR:HB3	3:BW:166:GLY:HA3	1.92	0.51
2:AC:177:GLN:HB3	2:AC:189:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:145:LEU:HD13	2:AL:148:ILE:HD11	1.91	0.51
3:AS:270:ARG:HG3	1:AY:72:LEU:HB3	1.93	0.51
2:BF:177:GLN:HB3	2:BF:189:ARG:HB2	1.93	0.51
2:BO:177:GLN:HB3	2:BO:189:ARG:HB2	1.93	0.51
3:BX:144:PHE:HB3	3:BX:190:TRP:CE2	2.45	0.51
3:AX:167:ASN:HD22	3:AX:169:LYS:HE3	1.76	0.51
1:AY:89:LEU:HD22	1:AY:192:GLN:HG3	1.92	0.51
1:AZ:157:PHE:HE2	1:AZ:208:PHE:HB3	1.76	0.51
2:BC:177:GLN:HB3	2:BC:189:ARG:HB2	1.93	0.51
2:BQ:9:PHE:HA	3:BX:170:TYR:O	2.11	0.51
3:AX:66:GLU:HG2	3:BU:120:LYS:NZ	2.26	0.51
2:BG:10:SER:N	3:BU:160:TYR:O	2.30	0.51
3:BX:167:ASN:HD22	3:BX:169:LYS:HE3	1.76	0.51
2:AB:13:SER:O	3:AS:169:LYS:HE2	2.05	0.50
3:AS:244:VAL:HG21	3:AT:50:VAL:CG2	2.40	0.50
1:AY:32:LEU:HD11	1:AY:204:LEU:HB2	1.92	0.50
2:BN:89:ASP:OD2	3:BW:189:ARG:NH1	2.37	0.50
3:BS:171:ILE:HG22	3:BS:172:LYS:H	1.76	0.50
3:AW:120:LYS:CB	3:BV:68:PHE:HD1	2.21	0.50
1:BY:120:ASP:HB2	1:BZ:292:THR:HB	1.93	0.50
1:A0:32:LEU:HD11	1:A0:204:LEU:HB2	1.93	0.50
2:AO:177:GLN:HB3	2:AO:189:ARG:HB2	1.93	0.50
3:AT:73:GLU:HB2	3:AU:99:GLU:CD	2.30	0.50
3:AX:144:PHE:HB3	3:AX:190:TRP:CE2	2.45	0.50
3:AX:66:GLU:HG2	3:BU:120:LYS:CE	2.40	0.50
2:BN:102:GLU:OE1	3:BW:222:ASN:ND2	2.40	0.50
2:AF:17:PRO:HA	3:AT:177:THR:CG2	2.38	0.50
2:AQ:20:SER:HA	3:AX:160:TYR:CD1	2.46	0.50
1:A0:42:ILE:HB	3:AX:43:TRP:HZ2	0.61	0.50
3:BS:197:PHE:HD1	3:BT:48:ILE:HG22	1.76	0.50
2:AP:120:LYS:NZ	3:AX:220:ILE:O	2.37	0.50
3:AV:45:SER:HB2	1:AZ:42:ILE:HG22	1.92	0.50
2:BP:113:ASN:O	3:BX:186:ARG:NH2	2.44	0.50
3:AT:124:PHE:O	3:BS:120:LYS:NZ	2.43	0.50
3:BT:238:ILE:HG22	3:BT:240:ILE:HG23	1.94	0.50
3:BU:138:THR:O	3:BU:292:LYS:HA	2.11	0.50
1:BZ:157:PHE:HE2	1:BZ:208:PHE:HB3	1.76	0.50
2:AD:88:ILE:HG12	2:AD:97:VAL:HG22	1.93	0.50
3:AV:120:LYS:HZ1	3:BW:66:GLU:HB3	1.75	0.50
3:AU:116:GLU:OE2	3:AV:3:ARG:HG3	2.11	0.50
1:B0:122:PRO:HD2	1:B0:125:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BM:9:PHE:HB2	3:BW:180:GLY:HA2	1.92	0.50
3:BT:243:ASP:OD1	3:BT:243:ASP:C	2.50	0.50
3:BU:281:LEU:HB3	3:BU:284:LEU:HD12	1.92	0.50
3:BT:87:LEU:HA	3:BU:54:ARG:NH1	2.26	0.50
1:A0:288:ARG:NH2	1:AZ:12:PRO:HB2	2.27	0.50
2:BA:102:GLU:OE2	3:BS:220:ILE:HD12	2.12	0.50
3:BU:196:ILE:HG13	3:BU:274:ILE:HB	1.94	0.50
3:AS:4:GLN:HB2	3:AS:97:GLN:HB3	1.93	0.50
3:AW:226:ALA:HB3	3:AW:268:ARG:HB3	1.92	0.50
2:AA:81:VAL:HB	1:AY:86:LYS:NZ	2.27	0.50
3:AU:266:PHE:CG	1:AZ:35:PRO:HD2	2.47	0.50
1:B0:32:LEU:HD11	1:B0:204:LEU:HB2	1.93	0.50
2:BB:13:SER:C	3:BS:169:LYS:CD	2.59	0.50
2:AO:171:GLY:HA3	2:AO:205:GLY:H	1.77	0.50
3:AT:36:LEU:HD22	3:AT:56:ILE:HD11	1.93	0.50
3:AV:196:ILE:HG13	3:AV:274:ILE:HB	1.94	0.50
2:AP:21:ASN:HB3	3:AX:181:GLU:CG	2.42	0.50
2:BD:88:ILE:HG12	2:BD:97:VAL:HG22	1.93	0.50
2:BL:177:GLN:HB3	2:BL:189:ARG:HB2	1.93	0.50
2:AJ:5:ASN:HB3	2:AJ:8:PHE:CD1	2.47	0.50
1:AY:39:CYS:HB2	1:AY:60:THR:OG1	2.12	0.50
2:BK:116:SER:OG	3:BV:186:ARG:O	2.29	0.50
3:BV:240:ILE:C	3:BV:240:ILE:HD12	2.32	0.50
3:BV:96:TYR:HB3	3:BV:103:VAL:HG23	1.94	0.50
2:AA:172:ASN:HD21	2:AA:204:SER:H	1.60	0.49
2:AL:177:GLN:HB3	2:AL:189:ARG:HB2	1.93	0.49
2:AR:177:GLN:HB3	2:AR:189:ARG:HB2	1.93	0.49
2:AR:9:PHE:CE1	3:AX:180:GLY:N	2.80	0.49
3:AU:171:ILE:HG22	3:AU:172:LYS:H	1.77	0.49
3:AU:68:PHE:HE1	3:BX:120:LYS:HG2	1.76	0.49
1:B0:76:VAL:HG11	1:B0:88:LYS:HD2	1.94	0.49
2:BA:172:ASN:HD21	2:BA:204:SER:H	1.60	0.49
2:BO:171:GLY:HA3	2:BO:205:GLY:H	1.77	0.49
2:BR:177:GLN:HB3	2:BR:189:ARG:HB2	1.93	0.49
3:BV:48:ILE:HG21	1:BZ:1:MET:HE1	1.92	0.49
1:A0:218:ILE:HB	1:A0:338:VAL:HG12	1.95	0.49
2:AF:177:GLN:HB3	2:AF:189:ARG:HB2	1.93	0.49
2:AP:22:ASN:HD21	3:AX:182:SER:HB3	1.77	0.49
3:AS:171:ILE:HG22	3:AS:172:LYS:H	1.76	0.49
3:AT:199:PHE:H	3:AT:242:THR:HG1	1.57	0.49
3:AX:199:PHE:CZ	3:AX:242:THR:HG21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B0:86:LYS:HZ2	2:BN:81:VAL:HB	1.75	0.49
2:BN:120:LYS:HE2	3:BW:222:ASN:ND2	2.27	0.49
3:BS:4:GLN:HB2	3:BS:97:GLN:HB3	1.93	0.49
2:BF:17:PRO:CA	3:BT:177:THR:HG22	2.37	0.49
3:AU:138:THR:O	3:AU:292:LYS:HA	2.11	0.49
1:AZ:152:PHE:CB	1:AZ:208:PHE:HB2	2.42	0.49
3:AV:43:TRP:HE1	1:AZ:42:ILE:HB	1.77	0.49
3:BX:199:PHE:CZ	3:BX:242:THR:HG21	2.47	0.49
1:A0:122:PRO:HD2	1:A0:125:ILE:HD12	1.94	0.49
1:A0:242:ASN:O	1:A0:313:ILE:HD12	2.12	0.49
2:AQ:39:ARG:HB2	2:AQ:61:ILE:HB	1.94	0.49
3:AW:76:TYR:HB3	3:AX:100:ILE:HD11	1.94	0.49
3:BS:11:LEU:O	3:BS:12:ASP:CG	2.51	0.49
3:BS:197:PHE:CD1	3:BT:48:ILE:CG2	2.94	0.49
3:AX:120:LYS:HZ1	3:BU:66:GLU:HG3	1.77	0.49
3:AW:120:LYS:CE	3:BV:68:PHE:CE1	2.90	0.49
3:BW:4:GLN:HB2	3:BW:97:GLN:HB3	1.94	0.49
2:AI:171:GLY:HA3	2:AI:205:GLY:H	1.77	0.49
3:AT:243:ASP:C	3:AT:243:ASP:OD1	2.50	0.49
3:AU:270:ARG:NH1	1:AZ:72:LEU:HD22	2.28	0.49
3:AX:171:ILE:HG22	3:AX:172:LYS:H	1.77	0.49
3:BS:196:ILE:HG22	3:BS:293:ARG:HD3	1.95	0.49
3:BT:36:LEU:HD22	3:BT:56:ILE:HD11	1.93	0.49
3:BX:171:ILE:HG22	3:BX:172:LYS:H	1.77	0.49
1:BY:45:GLU:HA	1:BY:357:THR:HG22	1.95	0.49
2:AK:39:ARG:HB2	2:AK:61:ILE:HB	1.94	0.49
2:AN:39:ARG:HB2	2:AN:61:ILE:HB	1.94	0.49
2:AR:7:THR:HA	3:AX:178:TYR:CE2	2.47	0.49
3:AW:4:GLN:HB2	3:AW:97:GLN:HB3	1.94	0.49
3:BV:196:ILE:HG13	3:BV:274:ILE:HB	1.94	0.49
1:BZ:152:PHE:CB	1:BZ:208:PHE:HB2	2.42	0.49
1:A0:76:VAL:HG11	1:A0:88:LYS:HD2	1.94	0.49
2:AF:171:GLY:HA3	2:AF:205:GLY:H	1.77	0.49
2:AF:18:VAL:HG12	3:AT:176:TYR:O	2.12	0.49
3:AU:196:ILE:HG13	3:AU:274:ILE:HB	1.94	0.49
2:AP:118:VAL:HG23	3:AX:278:GLN:NE2	2.27	0.49
2:BC:18:VAL:HG13	3:BS:176:TYR:CE2	2.47	0.49
2:BQ:39:ARG:HB2	2:BQ:61:ILE:HB	1.94	0.49
3:BU:171:ILE:HG22	3:BU:172:LYS:H	1.77	0.49
2:AG:79:ASP:CB	1:AZ:212:ASN:HD21	2.25	0.49
3:AS:11:LEU:O	3:AS:12:ASP:CG	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:52:ASN:HB2	3:AS:258:LEU:CD2	2.30	0.49
3:AU:53:THR:HG21	1:AZ:359:PHE:CA	2.43	0.49
2:AK:91:THR:HG21	3:AV:189:ARG:HB2	1.93	0.49
1:B0:218:ILE:HB	1:B0:338:VAL:HG12	1.95	0.49
2:BC:18:VAL:CG1	3:BS:176:TYR:CZ	2.96	0.49
2:BF:171:GLY:HA3	2:BF:205:GLY:H	1.77	0.49
2:BG:79:ASP:C	1:BZ:212:ASN:HD21	2.16	0.49
2:BP:22:ASN:HD21	3:BX:182:SER:CB	2.25	0.49
2:BM:17:PRO:HA	3:BW:177:THR:HG22	1.95	0.49
2:BN:100:SER:HB3	3:BW:220:ILE:HG21	1.95	0.49
2:AJ:26:LEU:HD13	2:AK:66:TYR:HB2	1.94	0.49
2:AR:171:GLY:HA3	2:AR:205:GLY:H	1.77	0.49
3:AS:133:ILE:HA	3:AT:42:ILE:CG2	2.39	0.49
3:AU:229:PHE:CD1	3:AU:264:MET:HB3	2.48	0.49
3:AV:240:ILE:C	3:AV:240:ILE:HD12	2.32	0.49
1:AY:233:GLU:HB2	1:AY:321:ARG:HH21	1.78	0.49
2:BC:171:GLY:HA3	2:BC:205:GLY:H	1.77	0.49
2:BJ:5:ASN:HB3	2:BJ:8:PHE:CD1	2.47	0.49
2:BJ:26:LEU:HD13	2:BK:66:TYR:HB2	1.94	0.49
3:BT:199:PHE:CE1	3:BT:242:THR:HG21	2.48	0.49
3:BU:229:PHE:CD1	3:BU:264:MET:HB3	2.48	0.49
1:BY:169:THR:HG21	1:BZ:294:PHE:CZ	2.47	0.49
1:BY:39:CYS:HB2	1:BY:60:THR:OG1	2.12	0.49
3:AT:199:PHE:CE1	3:AT:242:THR:HG21	2.48	0.49
2:BG:92:GLN:HE21	3:BU:189:ARG:NE	2.11	0.49
1:B0:242:ASN:O	1:B0:313:ILE:HD12	2.12	0.48
2:BH:19:GLY:HA2	3:BU:166:GLY:O	2.13	0.48
2:BH:39:ARG:HB2	2:BH:61:ILE:HB	1.95	0.48
2:BL:171:GLY:HA3	2:BL:205:GLY:H	1.77	0.48
2:BN:39:ARG:HB2	2:BN:61:ILE:HB	1.93	0.48
2:BQ:8:PHE:O	3:BX:170:TYR:HB2	2.12	0.48
3:BT:199:PHE:N	3:BT:242:THR:OG1	2.39	0.48
3:BV:87:LEU:HA	3:BW:54:ARG:NH1	2.28	0.48
1:A0:184:GLN:HE22	1:A0:217:ARG:HH22	1.61	0.48
3:AT:238:ILE:HG22	3:AT:240:ILE:HG23	1.94	0.48
2:BI:171:GLY:HA3	2:BI:205:GLY:H	1.77	0.48
3:BT:76:TYR:HE1	3:BU:96:TYR:OH	1.96	0.48
3:BX:242:THR:O	3:BX:272:ARG:HD3	2.13	0.48
1:BY:233:GLU:HB2	1:BY:321:ARG:HH21	1.77	0.48
2:AE:39:ARG:HB2	2:AE:61:ILE:HB	1.94	0.48
2:AR:17:PRO:HA	3:AX:177:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:212:ALA:HB2	3:AT:283:ASN:HD22	1.79	0.48
3:AU:114:LYS:NZ	3:AV:298:VAL:O	2.45	0.48
2:BQ:17:PRO:HB3	3:BX:169:LYS:CE	2.38	0.48
2:BH:17:PRO:HB3	3:BU:169:LYS:HE3	1.94	0.48
3:BV:215:ARG:HB3	3:BV:282:ILE:HD11	1.95	0.48
2:AH:39:ARG:HB2	2:AH:61:ILE:HB	1.94	0.48
1:B0:288:ARG:NH2	1:BZ:12:PRO:HB2	2.28	0.48
3:BV:36:LEU:HD21	3:BV:297:PHE:HB2	1.96	0.48
3:AU:272:ARG:NH1	1:AZ:40:GLN:OE1	2.46	0.48
1:B0:184:GLN:HE22	1:B0:217:ARG:HH22	1.61	0.48
1:B0:294:PHE:CE2	1:BZ:169:THR:CG2	2.96	0.48
2:BE:39:ARG:HB2	2:BE:61:ILE:HB	1.95	0.48
2:BD:52:ASN:ND2	3:BS:258:LEU:HB3	2.29	0.48
2:BR:9:PHE:CZ	3:BX:180:GLY:C	2.87	0.48
2:BG:104:ALA:HB3	1:BZ:88:LYS:HD2	1.94	0.48
1:A0:231:ASP:OD2	1:A0:321:ARG:NH1	2.47	0.48
2:AC:171:GLY:HA3	2:AC:205:GLY:H	1.77	0.48
2:AN:49:THR:HG21	3:AV:235:GLN:NE2	2.29	0.48
3:AS:196:ILE:HG22	3:AS:293:ARG:HD3	1.95	0.48
3:AT:120:LYS:HZ1	3:BS:66:GLU:HG3	1.75	0.48
3:AV:243:ASP:OD1	3:AV:243:ASP:C	2.52	0.48
1:AY:45:GLU:HA	1:AY:357:THR:HG22	1.95	0.48
3:BS:96:TYR:HH	3:BX:76:TYR:HE1	1.62	0.48
3:BX:281:LEU:HB3	3:BX:284:LEU:HD12	1.96	0.48
2:AR:10:SER:HA	2:AR:15:GLU:HB2	1.96	0.48
3:AV:36:LEU:HD21	3:AV:297:PHE:HB2	1.96	0.48
1:AZ:237:ASP:C	1:AZ:238:ARG:HG2	2.33	0.48
2:BG:92:GLN:NE2	3:BU:189:ARG:CZ	2.77	0.48
2:BK:39:ARG:HB2	2:BK:61:ILE:HB	1.94	0.48
2:BN:47:LEU:HD22	3:BV:233:GLN:CD	2.34	0.48
2:BE:18:VAL:CG1	3:BT:168:TYR:O	2.54	0.48
2:BD:23:ASP:OD2	3:BT:178:TYR:CE1	2.62	0.48
3:BV:144:PHE:HB3	3:BV:190:TRP:CE2	2.49	0.48
2:BR:9:PHE:HZ	3:BX:181:GLU:HG3	1.76	0.48
1:BY:122:PRO:HD2	1:BY:125:ILE:HD12	1.96	0.48
3:AS:239:LEU:C	3:AS:239:LEU:HD23	2.34	0.48
3:AS:242:THR:O	3:AS:272:ARG:HD3	2.14	0.48
3:AT:26:VAL:HG23	3:AT:67:THR:HG22	1.96	0.48
1:B0:231:ASP:OD2	1:B0:321:ARG:NH1	2.47	0.48
2:BR:10:SER:HA	2:BR:15:GLU:HB2	1.96	0.48
3:BT:26:VAL:HG23	3:BT:67:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:9:PHE:CZ	3:AX:181:GLU:N	2.82	0.48
1:AY:122:PRO:HD2	1:AY:125:ILE:HD12	1.96	0.48
2:BR:171:GLY:HA3	2:BR:205:GLY:H	1.77	0.48
3:BS:239:LEU:HD23	3:BS:239:LEU:C	2.35	0.48
1:BZ:237:ASP:C	1:BZ:238:ARG:HG2	2.33	0.48
3:AU:106:ASP:O	3:AU:133:ILE:HB	2.14	0.48
2:AK:116:SER:OG	3:AV:186:ARG:O	2.32	0.48
3:AX:68:PHE:CE1	3:BU:120:LYS:HD3	2.48	0.48
2:BB:39:ARG:HB2	2:BB:61:ILE:HB	1.95	0.48
2:BD:131:THR:O	3:BS:263:VAL:HG23	2.13	0.48
3:BS:242:THR:O	3:BS:272:ARG:HD3	2.14	0.48
3:BU:116:GLU:HB2	3:BV:31:PRO:HD2	1.95	0.48
3:BW:11:LEU:HD12	3:BW:93:THR:HG21	1.96	0.48
3:AU:194:GLU:HB2	3:AU:293:ARG:HD2	1.96	0.47
3:AV:96:TYR:HB3	3:AV:103:VAL:HG23	1.94	0.47
2:BI:27:TYR:HA	2:BI:30:LEU:HD12	1.96	0.47
2:BR:27:TYR:HA	2:BR:30:LEU:HD12	1.96	0.47
3:BT:226:ALA:HB3	3:BT:268:ARG:HB3	1.95	0.47
2:BP:9:PHE:HA	3:BX:160:TYR:O	2.13	0.47
2:AP:148:ILE:HB	2:AR:153:MET:HG3	1.96	0.47
2:AR:23:ASP:OD2	3:AX:176:TYR:CZ	2.67	0.47
3:AV:215:ARG:HB3	3:AV:282:ILE:HD11	1.95	0.47
3:AW:11:LEU:HD12	3:AW:93:THR:HG21	1.96	0.47
3:AW:171:ILE:HG22	3:AW:172:LYS:H	1.79	0.47
2:AP:19:GLY:CA	3:AX:180:GLY:O	2.62	0.47
3:AX:242:THR:O	3:AX:272:ARG:HD3	2.13	0.47
1:A0:169:THR:HG21	1:AY:294:PHE:CE2	2.49	0.47
3:BT:212:ALA:HB2	3:BT:283:ASN:HD22	1.79	0.47
3:BV:243:ASP:C	3:BV:243:ASP:OD1	2.52	0.47
3:AU:120:LYS:HD3	3:BX:68:PHE:CE1	2.49	0.47
2:AB:39:ARG:HB2	2:AB:61:ILE:HB	1.95	0.47
2:AR:27:TYR:HA	2:AR:30:LEU:HD12	1.96	0.47
3:AT:226:ALA:HB3	3:AT:268:ARG:HB3	1.95	0.47
2:AQ:17:PRO:CG	3:AX:169:LYS:CE	2.93	0.47
3:BT:199:PHE:H	3:BT:242:THR:HG1	1.57	0.47
3:AU:66:GLU:CG	3:BX:120:LYS:CE	2.92	0.47
1:BZ:231:ASP:OD2	1:BZ:321:ARG:NH1	2.47	0.47
2:BN:73:THR:CB	3:BV:256:THR:HG21	2.44	0.47
3:BW:171:ILE:HG22	3:BW:172:LYS:H	1.79	0.47
2:AB:13:SER:C	3:AS:169:LYS:CD	2.62	0.47
2:AL:171:GLY:HA3	2:AL:205:GLY:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:281:LEU:HB3	3:AS:284:LEU:HD12	1.96	0.47
3:AU:11:LEU:O	3:AU:12:ASP:CG	2.52	0.47
3:AX:281:LEU:HB3	3:AX:284:LEU:HD12	1.96	0.47
2:BD:73:THR:HG21	3:BS:256:THR:HG21	1.94	0.47
3:BU:106:ASP:O	3:BU:133:ILE:HB	2.14	0.47
3:BU:194:GLU:HB2	3:BU:293:ARG:HD2	1.96	0.47
2:AD:77:LYS:H	2:AD:82:ASN:ND2	2.12	0.47
3:AV:160:TYR:HB3	3:AV:166:GLY:HA3	1.95	0.47
3:AV:144:PHE:HB3	3:AV:190:TRP:CE2	2.49	0.47
3:AV:66:GLU:CG	3:BW:120:LYS:HZ3	2.26	0.47
1:AZ:231:ASP:OD2	1:AZ:321:ARG:NH1	2.47	0.47
3:BU:11:LEU:O	3:BU:12:ASP:CG	2.52	0.47
3:BV:160:TYR:HB3	3:BV:166:GLY:HA3	1.95	0.47
2:AD:23:ASP:OD2	3:AT:178:TYR:CE1	2.67	0.47
3:AU:244:VAL:HG11	1:AZ:1:MET:HE1	1.96	0.47
3:BS:281:LEU:HB3	3:BS:284:LEU:HD12	1.96	0.47
2:BE:18:VAL:C	3:BT:167:ASN:HA	2.35	0.47
1:A0:359:PHE:O	3:AW:53:THR:HG21	2.14	0.47
2:BD:51:LEU:HD12	3:BS:262:PRO:HG2	1.95	0.47
3:BS:72:LEU:HD22	3:BS:76:TYR:CE2	2.50	0.47
3:BX:4:GLN:HB2	3:BX:97:GLN:HB3	1.96	0.47
2:AI:27:TYR:HA	2:AI:30:LEU:HD12	1.96	0.47
3:AV:196:ILE:HD13	3:AV:291:ILE:HG12	1.97	0.47
2:BF:23:ASP:OD2	3:BT:176:TYR:HE2	1.97	0.47
2:AP:172:ASN:HD21	2:AP:204:SER:H	1.63	0.47
2:BD:19:GLY:CA	3:BT:180:GLY:O	2.63	0.47
3:BV:196:ILE:HD13	3:BV:291:ILE:HG12	1.97	0.47
3:AX:196:ILE:HD13	3:AX:291:ILE:HG13	1.97	0.47
3:BV:243:ASP:OD1	3:BV:245:ASN:N	2.48	0.47
3:BX:72:LEU:HD22	3:BX:76:TYR:CE2	2.50	0.47
2:AM:5:ASN:HB3	2:AM:8:PHE:CD1	2.50	0.46
2:AH:17:PRO:HB3	3:AU:169:LYS:HE3	1.97	0.46
3:AV:43:TRP:NE1	1:AZ:42:ILE:HB	2.30	0.46
2:BG:172:ASN:HD21	2:BG:204:SER:H	1.63	0.46
2:BP:148:ILE:HB	2:BR:153:MET:HG3	1.96	0.46
2:BE:9:PHE:HD2	3:BT:170:TYR:C	2.18	0.46
2:AA:102:GLU:OE2	3:AS:220:ILE:HD12	2.15	0.46
2:BM:5:ASN:HB3	2:BM:8:PHE:CD1	2.51	0.46
2:BP:172:ASN:HD21	2:BP:204:SER:H	1.63	0.46
3:BW:72:LEU:HD22	3:BW:76:TYR:CE2	2.50	0.46
3:BX:196:ILE:HD13	3:BX:291:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AG:172:ASN:HD21	2:AG:204:SER:H	1.63	0.46
2:AG:79:ASP:O	1:AZ:212:ASN:OD1	2.32	0.46
3:AS:194:GLU:HB2	3:AS:293:ARG:HD2	1.97	0.46
3:AS:72:LEU:HD22	3:AS:76:TYR:CE2	2.50	0.46
3:AX:96:TYR:HB3	3:AX:103:VAL:HG23	1.98	0.46
3:BT:242:THR:O	3:BT:272:ARG:HD3	2.16	0.46
3:BU:72:LEU:HD22	3:BU:76:TYR:CE2	2.51	0.46
3:BV:196:ILE:HG22	3:BV:293:ARG:HD3	1.98	0.46
1:A0:292:THR:HB	1:AZ:120:ASP:HB2	1.97	0.46
2:AQ:17:PRO:CA	3:AX:169:LYS:HD3	2.46	0.46
3:AT:242:THR:O	3:AT:272:ARG:HD3	2.16	0.46
2:BA:77:LYS:H	2:BA:82:ASN:ND2	2.11	0.46
2:BG:81:VAL:HB	1:BZ:86:LYS:HZ1	1.79	0.46
1:A0:130:ASN:HA	1:A0:133:ILE:HD12	1.98	0.46
2:AM:172:ASN:HD21	2:AM:204:SER:H	1.62	0.46
2:AE:9:PHE:HD2	3:AT:170:TYR:C	2.18	0.46
3:AV:68:PHE:HD1	3:BW:120:LYS:HD2	1.72	0.46
3:AW:72:LEU:HD22	3:AW:76:TYR:CE2	2.50	0.46
2:BE:19:GLY:HA2	3:BT:166:GLY:C	2.35	0.46
2:BQ:19:GLY:HA2	3:BX:166:GLY:C	2.35	0.46
2:BQ:17:PRO:CB	3:BX:167:ASN:HD22	2.13	0.46
2:BA:131:THR:HG22	3:BX:262:PRO:O	2.16	0.46
2:AD:112:ILE:O	3:AT:186:ARG:NH1	2.46	0.46
2:AR:9:PHE:CD1	3:AX:180:GLY:HA2	2.51	0.46
1:AZ:130:ASN:HA	1:AZ:133:ILE:HD12	1.98	0.46
2:BB:13:SER:O	3:BS:169:LYS:HE2	2.07	0.46
2:BE:171:GLY:HA3	2:BE:205:GLY:H	1.81	0.46
3:BV:72:LEU:HD22	3:BV:76:TYR:CE2	2.50	0.46
3:AT:96:TYR:HB3	3:AT:103:VAL:HG23	1.98	0.46
3:AU:206:LYS:HG3	3:AU:285:SER:HB3	1.98	0.46
3:AV:243:ASP:OD1	3:AV:245:ASN:N	2.48	0.46
2:AA:81:VAL:HB	1:AY:86:LYS:HZ1	1.81	0.46
2:BD:172:ASN:HD21	2:BD:204:SER:H	1.64	0.46
2:BM:148:ILE:HB	2:BO:153:MET:HG3	1.98	0.46
2:BP:77:LYS:H	2:BP:82:ASN:ND2	2.12	0.46
3:BU:69:GLY:H	3:BU:75:ASN:HD21	1.64	0.46
3:AV:196:ILE:HG22	3:AV:293:ARG:HD3	1.98	0.46
2:AE:171:GLY:HA3	2:AE:205:GLY:H	1.81	0.46
2:AE:26:LEU:HD13	2:AF:66:TYR:HB2	1.98	0.46
2:AR:5:ASN:HB3	2:AR:8:PHE:CD1	2.51	0.46
3:AV:72:LEU:HD22	3:AV:76:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:72:LEU:HD22	3:AX:76:TYR:CE2	2.51	0.46
2:BH:171:GLY:HA3	2:BH:205:GLY:H	1.81	0.46
2:BK:171:GLY:HA3	2:BK:205:GLY:H	1.81	0.46
3:BS:194:GLU:HB2	3:BS:293:ARG:HD2	1.97	0.46
3:BT:76:TYR:CE1	3:BU:96:TYR:OH	2.68	0.46
3:BT:96:TYR:HB3	3:BT:103:VAL:HG23	1.98	0.46
3:AU:72:LEU:HD22	3:AU:76:TYR:CE2	2.51	0.45
1:B0:130:ASN:HA	1:B0:133:ILE:HD12	1.98	0.45
2:BE:26:LEU:HD13	2:BF:66:TYR:HB2	1.98	0.45
3:BU:229:PHE:CD1	3:BU:260:LEU:HB3	2.52	0.45
3:BW:144:PHE:HB3	3:BW:190:TRP:CE2	2.52	0.45
2:AE:18:VAL:HG13	3:AT:168:TYR:CE2	2.51	0.45
3:AU:229:PHE:CD1	3:AU:260:LEU:HB3	2.52	0.45
3:AX:4:GLN:HB2	3:AX:97:GLN:HB3	1.96	0.45
1:AY:130:ASN:HA	1:AY:133:ILE:HD12	1.99	0.45
1:AY:251:LYS:HG2	1:AY:297:ARG:HD3	1.97	0.45
2:BG:17:PRO:HA	3:BU:159:ILE:HG22	1.98	0.45
2:BQ:17:PRO:HG3	3:BX:169:LYS:CE	2.45	0.45
2:BR:5:ASN:HB3	2:BR:8:PHE:CD1	2.51	0.45
3:BU:242:THR:CG2	3:BU:272:ARG:CG	2.93	0.45
1:BZ:130:ASN:HA	1:BZ:133:ILE:HD12	1.98	0.45
2:AD:172:ASN:HD21	2:AD:204:SER:H	1.64	0.45
2:AE:8:PHE:O	3:AT:170:TYR:HB2	2.15	0.45
1:A0:42:ILE:CB	3:AX:43:TRP:CZ2	2.47	0.45
2:BG:77:LYS:H	2:BG:82:ASN:ND2	2.12	0.45
3:BU:206:LYS:HG3	3:BU:285:SER:HB3	1.97	0.45
2:BO:17:PRO:CB	3:BW:167:ASN:HB2	2.47	0.45
2:AB:26:LEU:HD13	2:AC:66:TYR:HB2	1.98	0.45
2:AJ:172:ASN:HD21	2:AJ:204:SER:H	1.63	0.45
3:AT:72:LEU:HD22	3:AT:76:TYR:CE2	2.51	0.45
3:AU:96:TYR:HB3	3:AU:103:VAL:HG23	1.99	0.45
3:AW:120:LYS:CE	3:BV:66:GLU:CG	2.92	0.45
2:AP:113:ASN:C	3:AX:186:ARG:NH2	2.68	0.45
2:BE:8:PHE:O	3:BT:170:TYR:HB2	2.16	0.45
3:BU:4:GLN:HB2	3:BU:97:GLN:HB3	1.97	0.45
3:BX:96:TYR:HB3	3:BX:103:VAL:HG23	1.98	0.45
1:BY:169:THR:HG21	1:BZ:294:PHE:HE2	1.71	0.45
3:AU:229:PHE:CE1	3:AU:264:MET:HB3	2.52	0.45
3:AU:4:GLN:HB2	3:AU:97:GLN:HB3	1.97	0.45
3:AU:69:GLY:H	3:AU:75:ASN:HD21	1.64	0.45
3:AV:120:LYS:NZ	3:BW:66:GLU:HB3	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:329:LEU:HB3	3:AV:261:PHE:CG	2.52	0.45
1:B0:78:PRO:HG3	2:BN:103:THR:HB	1.98	0.45
2:BJ:172:ASN:HD21	2:BJ:204:SER:H	1.63	0.45
2:BJ:148:ILE:HB	2:BL:153:MET:HG3	1.99	0.45
3:BT:144:PHE:HB3	3:BT:190:TRP:CE2	2.52	0.45
1:B0:1:MET:SD	3:BX:48:ILE:HD13	2.57	0.45
2:AM:27:TYR:HA	2:AM:30:LEU:HD12	1.99	0.45
2:AP:39:ARG:HB2	2:AP:61:ILE:HB	1.99	0.45
3:AT:240:ILE:HG22	3:AT:249:TYR:HD1	1.82	0.45
2:BQ:171:GLY:HA3	2:BQ:205:GLY:H	1.81	0.45
3:BS:11:LEU:HD12	3:BS:93:THR:HG21	1.99	0.45
3:BT:72:LEU:HD22	3:BT:76:TYR:CE2	2.51	0.45
2:BN:52:ASN:ND2	3:BV:258:LEU:HG	2.32	0.45
1:BY:130:ASN:HA	1:BY:133:ILE:HD12	1.99	0.45
2:AG:77:LYS:H	2:AG:82:ASN:ND2	2.12	0.45
2:AJ:148:ILE:HB	2:AL:153:MET:HG3	1.99	0.45
2:BA:106:ASN:OD1	1:BY:88:LYS:HD2	2.17	0.45
2:BM:27:TYR:HA	2:BM:30:LEU:HD12	1.99	0.45
3:BU:144:PHE:HB3	3:BU:190:TRP:CE2	2.52	0.45
2:AM:17:PRO:HA	3:AW:177:THR:HG22	1.98	0.45
3:AW:144:PHE:HB3	3:AW:190:TRP:CE2	2.52	0.45
2:BP:22:ASN:ND2	3:BX:182:SER:OG	2.43	0.45
2:AD:146:ASP:O	2:AF:151:ASN:HB2	2.17	0.45
2:AR:81:VAL:HG22	2:AR:127:THR:HG23	1.99	0.45
3:AT:76:TYR:HE1	3:AU:96:TYR:OH	2.00	0.45
2:AG:9:PHE:HA	3:AU:160:TYR:HB2	1.98	0.45
3:AU:144:PHE:HB3	3:AU:190:TRP:CE2	2.52	0.45
2:BD:77:LYS:H	2:BD:82:ASN:ND2	2.12	0.45
2:BM:172:ASN:HD21	2:BM:204:SER:H	1.62	0.45
3:BU:116:GLU:OE2	3:BV:3:ARG:HG3	2.16	0.45
1:BY:251:LYS:HG2	1:BY:297:ARG:HD3	1.97	0.45
2:AB:171:GLY:HA3	2:AB:205:GLY:H	1.81	0.45
3:AT:136:TRP:HB2	3:AT:295:ALA:O	2.17	0.45
2:BB:171:GLY:HA3	2:BB:205:GLY:H	1.81	0.45
2:BD:51:LEU:HD11	3:BS:262:PRO:HG2	1.97	0.45
2:BR:81:VAL:HG22	2:BR:127:THR:HG23	1.99	0.45
2:AH:171:GLY:HA3	2:AH:205:GLY:H	1.81	0.44
2:AJ:39:ARG:HB2	2:AJ:61:ILE:HB	1.99	0.44
2:AR:23:ASP:OD2	3:AX:176:TYR:HE2	1.99	0.44
3:AU:266:PHE:CD2	1:AZ:35:PRO:HD2	2.52	0.44
2:BC:81:VAL:HG22	2:BC:127:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BN:171:GLY:HA3	2:BN:205:GLY:H	1.81	0.44
3:BW:194:GLU:HB2	3:BW:293:ARG:HD2	1.99	0.44
2:BP:19:GLY:HA3	3:BX:180:GLY:O	2.17	0.44
2:AA:77:LYS:H	2:AA:82:ASN:ND2	2.11	0.44
2:AM:148:ILE:HB	2:AO:153:MET:HG3	1.98	0.44
2:AQ:171:GLY:HA3	2:AQ:205:GLY:H	1.81	0.44
2:BD:146:ASP:O	2:BF:151:ASN:HB2	2.17	0.44
2:BP:39:ARG:HB2	2:BP:61:ILE:HB	1.99	0.44
2:BQ:251:THR:HA	2:BQ:252:PRO:HD3	1.86	0.44
1:A0:220:THR:HG21	1:A0:332:LEU:HD21	2.00	0.44
2:AG:104:ALA:HB3	1:AZ:88:LYS:HD2	1.98	0.44
3:AS:239:LEU:HD23	3:AS:240:ILE:N	2.32	0.44
3:BT:240:ILE:HG22	3:BT:249:TYR:HD1	1.82	0.44
3:BS:197:PHE:HD1	3:BT:48:ILE:CG2	2.30	0.44
2:AA:39:ARG:HB2	2:AA:61:ILE:HB	2.00	0.44
2:AC:81:VAL:HG22	2:AC:127:THR:HG23	1.99	0.44
2:AO:81:VAL:HG22	2:AO:127:THR:HG23	1.99	0.44
3:AT:144:PHE:HB3	3:AT:190:TRP:CE2	2.52	0.44
2:BH:26:LEU:HD13	2:BI:66:TYR:HB2	1.99	0.44
3:BU:96:TYR:HB3	3:BU:103:VAL:HG23	1.99	0.44
1:BY:1:MET:HG3	1:BY:40:GLN:HB2	2.00	0.44
2:AA:172:ASN:ND2	2:AA:204:SER:H	2.16	0.44
3:AU:70:GLU:HG2	3:BX:70:GLU:HG2	1.99	0.44
3:AW:247:GLU:OE1	3:AW:249:TYR:HE2	2.01	0.44
1:AZ:184:GLN:HE22	1:AZ:217:ARG:HH22	1.66	0.44
3:BU:229:PHE:CE1	3:BU:264:MET:HB3	2.52	0.44
3:BU:271:THR:HA	1:BZ:3:GLU:HG3	1.99	0.44
3:AX:120:LYS:CE	3:BU:66:GLU:CG	2.96	0.44
3:BV:76:TYR:HE1	3:BW:96:TYR:HH	1.63	0.44
2:AF:81:VAL:HG22	2:AF:127:THR:HG23	1.99	0.44
2:AK:171:GLY:HA3	2:AK:205:GLY:H	1.81	0.44
2:AN:171:GLY:HA3	2:AN:205:GLY:H	1.81	0.44
3:AS:11:LEU:HD12	3:AS:93:THR:HG21	1.99	0.44
3:AS:138:THR:O	3:AS:292:LYS:HA	2.17	0.44
3:AU:242:THR:CG2	3:AU:272:ARG:CG	2.93	0.44
3:AV:194:GLU:HB2	3:AV:293:ARG:HD2	1.99	0.44
3:AX:5:TYR:HB3	3:AX:21:VAL:HG23	2.00	0.44
3:AU:55:SER:HB3	1:AZ:359:PHE:CE1	2.53	0.44
1:B0:220:THR:HG21	1:B0:332:LEU:HD21	2.00	0.44
1:B0:262:MET:SD	1:BZ:142:LYS:HG2	2.57	0.44
2:BA:39:ARG:HB2	2:BA:61:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:26:LEU:HD13	2:BC:66:TYR:HB2	1.99	0.44
2:BG:39:ARG:HB2	2:BG:61:ILE:HB	2.00	0.44
2:BI:81:VAL:HG22	2:BI:127:THR:HG23	1.99	0.44
2:BK:26:LEU:HD13	2:BL:66:TYR:HB2	2.00	0.44
3:BS:239:LEU:HD23	3:BS:240:ILE:N	2.33	0.44
2:BF:20:SER:HA	3:BT:170:TYR:CD1	2.53	0.44
1:BZ:251:LYS:HG2	1:BZ:297:ARG:HD3	1.98	0.44
2:BG:9:PHE:HA	3:BU:160:TYR:HB2	1.98	0.44
3:BT:136:TRP:HB2	3:BT:295:ALA:O	2.17	0.44
2:AG:39:ARG:HB2	2:AG:61:ILE:HB	2.00	0.44
2:AL:39:ARG:HB2	2:AL:61:ILE:HB	2.00	0.44
3:AT:76:TYR:CE1	3:AU:96:TYR:OH	2.70	0.44
1:AZ:251:LYS:HG2	1:AZ:297:ARG:HD3	1.98	0.44
2:BL:39:ARG:HB2	2:BL:61:ILE:HB	2.00	0.44
2:BM:66:TYR:HB2	2:BO:26:LEU:HD13	1.99	0.44
2:BQ:18:VAL:C	3:BX:167:ASN:HA	2.36	0.44
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ2	1.82	0.44
3:AW:194:GLU:HB2	3:AW:293:ARG:HD2	1.99	0.44
1:B0:39:CYS:HB2	1:B0:60:THR:OG1	2.18	0.44
2:BC:39:ARG:HB2	2:BC:61:ILE:HB	2.00	0.44
2:BD:112:ILE:O	3:BT:186:ARG:NH1	2.45	0.44
2:BH:17:PRO:HB3	3:BU:169:LYS:CE	2.48	0.44
3:BS:138:THR:O	3:BS:292:LYS:HA	2.17	0.44
1:BZ:32:LEU:HD11	1:BZ:204:LEU:HB2	1.99	0.44
1:A0:1:MET:HG3	1:A0:40:GLN:HB2	2.00	0.43
2:AH:26:LEU:HD13	2:AI:66:TYR:HB2	1.99	0.43
2:AM:39:ARG:HB2	2:AM:61:ILE:HB	2.00	0.43
2:AR:9:PHE:CZ	3:AX:180:GLY:HA2	2.53	0.43
1:AZ:1:MET:HG3	1:AZ:40:GLN:HB2	2.00	0.43
1:B0:1:MET:HG3	1:B0:40:GLN:HB2	2.00	0.43
2:BL:81:VAL:HG22	2:BL:127:THR:HG23	2.00	0.43
2:BO:81:VAL:HG22	2:BO:127:THR:HG23	1.99	0.43
1:A0:262:MET:SD	1:AZ:142:LYS:HG2	2.57	0.43
2:AK:114:ASN:O	3:AV:186:ARG:CD	2.66	0.43
2:AK:49:THR:HB	3:AU:258:LEU:HD21	2.00	0.43
2:AM:66:TYR:HB2	2:AO:26:LEU:HD13	1.99	0.43
2:BD:39:ARG:HB2	2:BD:61:ILE:HB	2.00	0.43
2:BE:155:VAL:HG21	2:BE:159:ILE:HD11	2.00	0.43
2:BF:81:VAL:HG22	2:BF:127:THR:HG23	1.99	0.43
2:BO:27:TYR:HA	2:BO:30:LEU:HD12	2.00	0.43
2:BO:39:ARG:HB2	2:BO:61:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:49:THR:CG2	3:BS:233:GLN:HB2	2.49	0.43
3:BV:194:GLU:HB2	3:BV:293:ARG:HD2	1.99	0.43
1:BY:41:VAL:HG11	1:BY:71:ILE:HG12	2.00	0.43
2:AD:39:ARG:HB2	2:AD:61:ILE:HB	2.00	0.43
2:AD:51:LEU:HD12	3:AS:262:PRO:HG2	2.00	0.43
1:B0:12:PRO:HB2	1:BY:288:ARG:CZ	2.47	0.43
3:BX:5:TYR:HB3	3:BX:21:VAL:HG23	2.00	0.43
1:A0:39:CYS:HB2	1:A0:60:THR:OG1	2.18	0.43
2:AA:66:TYR:HB2	2:AC:26:LEU:HD13	1.99	0.43
2:AF:9:PHE:CB	3:AT:180:GLY:HA2	2.48	0.43
2:AH:155:VAL:HG21	2:AH:159:ILE:HD11	2.00	0.43
2:AL:81:VAL:HG22	2:AL:127:THR:HG23	2.00	0.43
2:AO:39:ARG:HB2	2:AO:61:ILE:HB	2.00	0.43
2:AQ:20:SER:HA	3:AX:160:TYR:CE1	2.53	0.43
2:AE:18:VAL:C	3:AT:167:ASN:HA	2.39	0.43
2:AM:9:PHE:HB2	3:AW:180:GLY:HA2	2.01	0.43
3:AV:66:GLU:CG	3:BW:120:LYS:CE	2.95	0.43
2:AQ:155:VAL:HG21	2:AQ:159:ILE:HD11	2.01	0.43
2:AH:19:GLY:HA2	3:AU:166:GLY:O	2.19	0.43
2:AG:92:GLN:HE21	3:AU:189:ARG:CZ	2.31	0.43
1:AY:1:MET:HG3	1:AY:40:GLN:HB2	1.99	0.43
1:AY:41:VAL:HG11	1:AY:71:ILE:HG12	2.00	0.43
2:BF:155:VAL:HG21	2:BF:159:ILE:HD11	2.01	0.43
2:AE:155:VAL:HG21	2:AE:159:ILE:HD11	2.00	0.43
2:AI:81:VAL:HG22	2:AI:127:THR:HG23	1.99	0.43
2:AP:49:THR:HB	3:AW:258:LEU:HD21	2.00	0.43
2:AK:21:ASN:H	3:AV:181:GLU:HG2	1.83	0.43
1:AZ:32:LEU:HD11	1:AZ:204:LEU:HB2	1.99	0.43
1:B0:17:ILE:HD13	1:BY:279:GLY:O	2.18	0.43
2:BF:39:ARG:HB2	2:BF:61:ILE:HB	2.00	0.43
2:BJ:39:ARG:HB2	2:BJ:61:ILE:HB	1.99	0.43
3:BS:96:TYR:HB3	3:BS:103:VAL:HG23	1.99	0.43
1:BZ:184:GLN:HE22	1:BZ:217:ARG:HH22	1.66	0.43
2:AK:26:LEU:HD13	2:AL:66:TYR:HB2	2.00	0.43
3:AS:96:TYR:HB3	3:AS:103:VAL:HG23	1.99	0.43
3:AT:171:ILE:H	3:AT:175:SER:HA	1.84	0.43
3:AW:196:ILE:HD11	3:AW:199:PHE:HD1	1.83	0.43
2:AG:79:ASP:OD1	1:AZ:216:LYS:HB2	2.18	0.43
2:BA:66:TYR:HB2	2:BC:26:LEU:HD13	1.99	0.43
2:BI:39:ARG:HB2	2:BI:61:ILE:HB	2.00	0.43
2:BM:77:LYS:H	2:BM:82:ASN:ND2	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BT:137:TYR:CE1	3:BT:292:LYS:HD2	2.54	0.43
3:BU:271:THR:HA	1:BZ:3:GLU:CG	2.49	0.43
3:BV:48:ILE:HD13	1:BZ:1:MET:SD	2.59	0.43
2:BP:92:GLN:HE21	3:BX:189:ARG:NE	2.17	0.43
1:BY:121:VAL:HG11	1:BY:175:VAL:HG21	2.01	0.43
3:BT:43:TRP:HD1	1:BY:42:ILE:HB	1.84	0.43
2:AC:39:ARG:HB2	2:AC:61:ILE:HB	2.00	0.43
2:AE:17:PRO:CB	3:AT:167:ASN:CB	2.86	0.43
2:AE:17:PRO:HG3	3:AT:169:LYS:CE	2.48	0.43
2:AI:39:ARG:HB2	2:AI:61:ILE:HB	2.00	0.43
3:AS:118:TYR:HB3	3:AS:122:GLY:HA2	1.99	0.43
1:B0:143:ASN:O	1:BY:288:ARG:NH1	2.51	0.43
1:B0:221:ARG:HB2	3:BV:266:PHE:HB3	2.00	0.43
2:BE:18:VAL:HG13	3:BT:168:TYR:CE2	2.54	0.43
2:BG:172:ASN:ND2	2:BG:204:SER:H	2.17	0.43
2:BL:21:ASN:OD1	3:BV:165:PRO:HG2	2.19	0.43
3:BW:196:ILE:HD11	3:BW:199:PHE:HD1	1.83	0.43
3:BW:247:GLU:OE1	3:BW:249:TYR:HE2	2.01	0.43
2:AD:52:ASN:ND2	3:AS:258:LEU:CG	2.77	0.43
2:AJ:251:THR:HA	2:AJ:252:PRO:HD3	1.87	0.43
2:AO:155:VAL:HG21	2:AO:159:ILE:HD11	2.01	0.43
2:BA:172:ASN:ND2	2:BA:204:SER:H	2.16	0.43
2:BO:155:VAL:HG21	2:BO:159:ILE:HD11	2.01	0.43
2:AA:120:LYS:HE2	3:AS:222:ASN:HD21	1.84	0.43
2:AG:172:ASN:ND2	2:AG:204:SER:H	2.17	0.43
2:AP:7:THR:HG23	3:AX:160:TYR:CE2	2.54	0.43
3:AU:66:GLU:CB	3:BX:120:LYS:NZ	2.82	0.43
2:BR:39:ARG:HB2	2:BR:61:ILE:HB	2.00	0.43
2:BN:91:THR:HG21	3:BW:189:ARG:HB2	2.01	0.43
3:BX:196:ILE:HD11	3:BX:199:PHE:HD1	1.84	0.43
3:BX:198:SER:HA	3:BX:242:THR:OG1	2.19	0.43
2:AF:23:ASP:OD2	3:AT:176:TYR:HE2	2.01	0.42
2:AJ:77:LYS:H	2:AJ:82:ASN:ND2	2.12	0.42
2:AN:26:LEU:HD13	2:AO:66:TYR:HB2	2.01	0.42
2:BK:91:THR:HG21	3:BV:189:ARG:HB2	2.01	0.42
3:BS:118:TYR:HB3	3:BS:122:GLY:HA2	2.00	0.42
3:BU:203:LEU:HB2	3:BU:238:ILE:HB	2.01	0.42
2:AF:27:TYR:HA	2:AF:30:LEU:HD12	2.01	0.42
2:AG:174:LEU:HB2	2:AG:194:VAL:HG22	2.01	0.42
2:AO:27:TYR:HA	2:AO:30:LEU:HD12	2.00	0.42
3:BT:171:ILE:H	3:BT:175:SER:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BU:203:LEU:HD13	3:BU:213:GLY:HA2	2.01	0.42
3:BW:96:TYR:HB3	3:BW:103:VAL:HG23	2.01	0.42
3:BX:243:ASP:OD1	3:BX:245:ASN:N	2.52	0.42
2:AN:155:VAL:HG21	2:AN:159:ILE:HD11	2.01	0.42
2:AO:5:ASN:HB3	2:AO:8:PHE:CD1	2.54	0.42
3:AW:96:TYR:HB3	3:AW:103:VAL:HG23	2.01	0.42
3:AX:243:ASP:OD1	3:AX:245:ASN:N	2.52	0.42
2:BH:155:VAL:HG21	2:BH:159:ILE:HD11	2.01	0.42
2:BN:155:VAL:HG21	2:BN:159:ILE:HD11	2.01	0.42
2:BO:5:ASN:HB3	2:BO:8:PHE:CD1	2.54	0.42
2:BQ:155:VAL:HG21	2:BQ:159:ILE:HD11	2.00	0.42
2:AG:203:MET:SD	2:AG:243:TRP:HB2	2.59	0.42
2:AR:9:PHE:CZ	3:AX:180:GLY:CA	3.03	0.42
2:AD:19:GLY:CA	3:AT:180:GLY:O	2.67	0.42
3:BT:43:TRP:CD1	1:BY:42:ILE:HB	2.54	0.42
3:BV:118:TYR:HB3	3:BV:122:GLY:HA2	2.02	0.42
3:BS:34:LEU:HB2	3:BX:114:LYS:HB3	2.00	0.42
3:AU:120:LYS:HZ3	3:BX:66:GLU:CG	2.29	0.42
2:AD:147:SER:HB2	2:AE:140:VAL:HG22	2.02	0.42
2:AR:39:ARG:HB2	2:AR:61:ILE:HB	2.00	0.42
3:AS:66:GLU:CG	3:BT:120:LYS:CE	2.96	0.42
2:AG:92:GLN:NE2	3:AU:189:ARG:NE	2.67	0.42
3:AU:203:LEU:HD13	3:AU:213:GLY:HA2	2.01	0.42
2:BG:203:MET:SD	2:BG:243:TRP:HB2	2.59	0.42
2:BM:39:ARG:HB2	2:BM:61:ILE:HB	2.00	0.42
2:BR:155:VAL:HG21	2:BR:159:ILE:HD11	2.02	0.42
3:BU:226:ALA:HB3	3:BU:268:ARG:HB3	2.01	0.42
3:BW:247:GLU:OE1	3:BW:249:TYR:CE2	2.73	0.42
2:BQ:9:PHE:CE1	3:BX:172:LYS:HB2	2.54	0.42
2:AF:39:ARG:HB2	2:AF:61:ILE:HB	2.00	0.42
2:AM:77:LYS:H	2:AM:82:ASN:ND2	2.13	0.42
2:AF:20:SER:HA	3:AT:170:TYR:CD1	2.54	0.42
3:AT:137:TYR:CE1	3:AT:292:LYS:HD2	2.54	0.42
3:AV:118:TYR:HB3	3:AV:122:GLY:HA2	2.02	0.42
2:BC:155:VAL:HG21	2:BC:159:ILE:HD11	2.02	0.42
2:BF:27:TYR:HA	2:BF:30:LEU:HD12	2.01	0.42
2:BQ:18:VAL:HG13	3:BX:168:TYR:CD2	2.54	0.42
3:BW:199:PHE:CE1	3:BW:242:THR:HG21	2.55	0.42
3:BW:196:ILE:HD13	3:BW:291:ILE:HG12	2.02	0.42
1:BZ:1:MET:HG3	1:BZ:40:GLN:HB2	2.00	0.42
1:A0:76:VAL:HG21	1:A0:88:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:155:VAL:HG21	2:AC:159:ILE:HD11	2.02	0.42
3:AW:199:PHE:CE1	3:AW:242:THR:HG21	2.55	0.42
3:AX:196:ILE:HD11	3:AX:199:PHE:HD1	1.84	0.42
1:AZ:241:TYR:CD2	1:AZ:241:TYR:N	2.88	0.42
2:BJ:77:LYS:H	2:BJ:82:ASN:ND2	2.12	0.42
2:BN:26:LEU:HD13	2:BO:66:TYR:HB2	2.01	0.42
2:BK:114:ASN:O	3:BV:186:ARG:CD	2.68	0.42
1:B0:38:ARG:NH2	3:BW:269:TYR:O	2.48	0.42
2:AK:155:VAL:HG21	2:AK:159:ILE:HD11	2.02	0.42
2:AM:5:ASN:O	2:AM:16:PHE:HB3	2.20	0.42
2:AQ:20:SER:N	3:AX:160:TYR:CD1	2.88	0.42
2:AR:18:VAL:CG1	3:AX:176:TYR:O	2.65	0.42
3:AS:132:ILE:HG21	3:AS:135:LYS:HB2	2.00	0.42
3:AT:114:LYS:HB3	3:AU:34:LEU:HB2	2.02	0.42
3:AU:203:LEU:HB2	3:AU:238:ILE:HB	2.01	0.42
2:AN:91:THR:HG21	3:AW:189:ARG:HB2	2.01	0.42
2:AP:21:ASN:N	3:AX:181:GLU:HG2	2.34	0.42
2:AR:155:VAL:HG21	2:AR:159:ILE:HD11	2.02	0.42
3:AT:86:ILE:HA	3:AT:92:VAL:HG21	2.01	0.42
3:AW:196:ILE:HD13	3:AW:291:ILE:HG12	2.02	0.42
3:AX:198:SER:HA	3:AX:242:THR:OG1	2.19	0.42
2:BE:17:PRO:CB	3:BT:167:ASN:CB	2.87	0.42
2:BP:23:ASP:OD2	3:BX:178:TYR:HE1	2.03	0.42
2:BQ:23:ASP:OD2	3:BX:168:TYR:HE2	2.03	0.42
1:BY:52:LEU:HD23	1:BY:53:TYR:CE2	2.55	0.42
1:BZ:77:VAL:O	1:BZ:89:LEU:HB3	2.20	0.42
2:AI:5:ASN:HB3	2:AI:8:PHE:CD1	2.55	0.42
2:BP:49:THR:HB	3:BW:258:LEU:HD21	2.01	0.42
3:BT:86:ILE:HA	3:BT:92:VAL:HG21	2.01	0.42
2:AE:18:VAL:CG1	3:AT:168:TYR:O	2.59	0.41
3:AS:294:LYS:HD2	3:AT:47:GLY:O	2.19	0.41
3:AV:199:PHE:CZ	3:AV:242:THR:HG21	2.55	0.41
3:AS:266:PHE:CD2	1:AY:35:PRO:HD2	2.55	0.41
1:AZ:77:VAL:O	1:AZ:89:LEU:HB3	2.20	0.41
2:BD:147:SER:HB2	2:BE:140:VAL:HG22	2.02	0.41
3:BS:132:ILE:HG21	3:BS:135:LYS:HB2	2.00	0.41
3:BU:131:ASP:HB3	3:BV:42:ILE:HD12	2.01	0.41
3:BS:99:GLU:OE2	3:BX:73:GLU:HB2	2.19	0.41
2:AF:155:VAL:HG21	2:AF:159:ILE:HD11	2.01	0.41
2:AK:251:THR:HA	2:AK:252:PRO:HD3	1.90	0.41
2:AP:77:LYS:H	2:AP:82:ASN:ND2	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:53:THR:HG21	1:AZ:359:PHE:C	2.41	0.41
2:BD:203:MET:SD	2:BD:243:TRP:HB2	2.60	0.41
3:BT:202:ILE:HG12	3:BT:239:LEU:HD12	2.01	0.41
3:BT:87:LEU:HA	3:BU:54:ARG:HH11	1.85	0.41
2:BR:9:PHE:CZ	3:BX:181:GLU:N	2.88	0.41
3:AW:247:GLU:OE1	3:AW:249:TYR:CE2	2.73	0.41
2:BD:73:THR:CG2	3:BS:256:THR:CG2	2.98	0.41
2:BG:66:TYR:HB2	2:BI:26:LEU:HD13	2.02	0.41
2:BI:5:ASN:HB3	2:BI:8:PHE:CD1	2.55	0.41
3:BV:199:PHE:CZ	3:BV:242:THR:HG21	2.55	0.41
3:BW:281:LEU:HB3	3:BW:284:LEU:HD12	2.03	0.41
1:A0:323:ILE:HA	1:A0:363:LEU:O	2.20	0.41
1:A0:52:LEU:HD23	1:A0:53:TYR:CE2	2.55	0.41
2:AD:203:MET:SD	2:AD:243:TRP:HB2	2.60	0.41
2:AJ:203:MET:SD	2:AJ:243:TRP:HB2	2.61	0.41
2:AQ:229:THR:HB	2:AR:228:ASP:HB2	2.03	0.41
3:AT:202:ILE:HG12	3:AT:239:LEU:HD12	2.00	0.41
1:AY:121:VAL:HG11	1:AY:175:VAL:HG21	2.01	0.41
1:AY:323:ILE:HA	1:AY:363:LEU:O	2.20	0.41
2:BG:5:ASN:HB3	2:BG:8:PHE:CD1	2.56	0.41
2:BK:155:VAL:HG21	2:BK:159:ILE:HD11	2.02	0.41
2:BE:21:ASN:CG	3:BT:165:PRO:HG2	2.40	0.41
3:BT:199:PHE:HB3	3:BT:291:ILE:HD13	2.02	0.41
2:AD:251:THR:HA	2:AD:252:PRO:HD3	1.96	0.41
3:AT:203:LEU:HD21	3:AT:240:ILE:HG13	2.03	0.41
1:B0:323:ILE:HA	1:B0:363:LEU:O	2.20	0.41
1:B0:76:VAL:HG21	1:B0:88:LYS:HE3	2.02	0.41
2:BM:251:THR:HA	2:BM:252:PRO:HD3	1.90	0.41
2:BN:100:SER:CB	3:BW:220:ILE:HG21	2.51	0.41
2:BQ:23:ASP:OD2	3:BX:168:TYR:CE2	2.74	0.41
2:BQ:229:THR:HB	2:BR:228:ASP:HB2	2.03	0.41
2:BP:21:ASN:HB3	3:BX:181:GLU:CD	2.41	0.41
3:BS:99:GLU:CD	3:BX:73:GLU:HB2	2.41	0.41
1:B0:288:ARG:CZ	1:BZ:12:PRO:HB2	2.50	0.41
2:AA:251:THR:HA	2:AA:252:PRO:HD3	1.95	0.41
2:AE:19:GLY:HA2	3:AT:166:GLY:C	2.39	0.41
2:AG:5:ASN:HB3	2:AG:8:PHE:CD1	2.56	0.41
2:AP:5:ASN:HD21	2:AQ:97:VAL:HB	1.85	0.41
1:A0:223:ASP:CG	3:AV:272:ARG:HH12	2.24	0.41
1:B0:330:LEU:HB2	3:BV:261:PHE:CE2	2.55	0.41
2:BD:172:ASN:ND2	2:BD:204:SER:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BG:174:LEU:HB2	2:BG:194:VAL:HG22	2.02	0.41
2:BJ:203:MET:SD	2:BJ:243:TRP:HB2	2.60	0.41
1:BZ:241:TYR:CD2	1:BZ:241:TYR:N	2.88	0.41
2:AG:66:TYR:HB2	2:AI:26:LEU:HD13	2.02	0.41
3:AS:171:ILE:H	3:AS:175:SER:HA	1.86	0.41
3:AS:7:ILE:HG23	3:AS:92:VAL:CG1	2.51	0.41
3:AT:199:PHE:HB3	3:AT:291:ILE:HD13	2.02	0.41
2:AK:120:LYS:NZ	3:AV:220:ILE:O	2.48	0.41
3:AV:76:TYR:HE1	3:AW:96:TYR:HH	1.63	0.41
2:AP:21:ASN:CG	3:AX:181:GLU:HG2	2.41	0.41
1:AY:52:LEU:HD23	1:AY:53:TYR:CE2	2.55	0.41
2:BM:5:ASN:O	2:BM:16:PHE:HB3	2.20	0.41
2:BQ:26:LEU:HD13	2:BR:66:TYR:HB2	2.03	0.41
2:BE:9:PHE:CA	3:BT:170:TYR:O	2.61	0.41
3:BU:171:ILE:H	3:BU:175:SER:HA	1.86	0.41
3:BT:115:THR:HG22	3:BU:32:SER:O	2.21	0.41
3:BV:246:ASP:O	3:BV:246:ASP:CG	2.59	0.41
1:BY:323:ILE:HA	1:BY:363:LEU:O	2.20	0.41
1:BZ:89:LEU:CD2	1:BZ:192:GLN:HG3	2.49	0.41
2:AN:102:GLU:OE1	3:AW:222:ASN:ND2	2.46	0.41
2:AP:172:ASN:ND2	2:AP:204:SER:H	2.19	0.41
3:AU:226:ALA:HB3	3:AU:268:ARG:HB3	2.01	0.41
3:AX:58:GLN:HA	3:AX:59:PRO:HD3	1.99	0.41
1:AY:120:ASP:HB2	1:AZ:292:THR:HB	2.03	0.41
2:BB:229:THR:HB	2:BC:228:ASP:HB2	2.03	0.41
2:BM:203:MET:SD	2:BM:243:TRP:HB2	2.61	0.41
2:BP:174:LEU:HB2	2:BP:194:VAL:HG22	2.03	0.41
2:BD:73:THR:HG21	3:BS:256:THR:CG2	2.51	0.41
3:BU:272:ARG:NH1	1:BZ:3:GLU:OE1	2.54	0.41
1:BY:143:ASN:O	1:BZ:288:ARG:NH1	2.53	0.41
2:AH:229:THR:HB	2:AI:228:ASP:HB2	2.03	0.41
2:AM:203:MET:SD	2:AM:243:TRP:HB2	2.61	0.41
3:AT:158:LYS:HD2	3:AT:176:TYR:CE1	2.56	0.41
3:AU:271:THR:HA	1:AZ:3:GLU:HG2	2.02	0.41
3:AV:246:ASP:O	3:AV:246:ASP:CG	2.59	0.41
1:AZ:52:LEU:HD23	1:AZ:53:TYR:CE2	2.56	0.41
2:BP:146:ASP:O	2:BR:151:ASN:HB2	2.21	0.41
2:AE:17:PRO:HB2	3:AT:167:ASN:HD22	1.76	0.41
3:AW:281:LEU:HB3	3:AW:284:LEU:HD12	2.03	0.41
1:AY:185:PHE:CE2	1:AY:208:PHE:HA	2.56	0.41
1:AY:87:LYS:HZ1	1:AY:89:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BF:23:ASP:OD2	3:BT:176:TYR:CZ	2.74	0.41
2:BH:251:THR:HA	2:BH:252:PRO:HD3	1.89	0.41
2:BM:174:LEU:HB2	2:BM:194:VAL:HG22	2.03	0.41
3:BV:240:ILE:CD1	3:BV:242:THR:HG23	2.51	0.41
2:AA:198:GLN:HB2	2:AA:201:TRP:CD1	2.56	0.41
2:AB:229:THR:HB	2:AC:228:ASP:HB2	2.03	0.41
2:AJ:172:ASN:ND2	2:AJ:204:SER:H	2.19	0.41
2:AN:251:THR:HA	2:AN:252:PRO:HD3	1.90	0.41
2:AN:229:THR:HB	2:AO:228:ASP:HB2	2.03	0.41
3:AS:242:THR:HG23	3:AS:272:ARG:HG3	1.89	0.41
2:AE:9:PHE:CA	3:AT:170:TYR:O	2.61	0.41
3:AT:87:LEU:HA	3:AU:54:ARG:HH11	1.84	0.41
2:BL:10:SER:HA	2:BL:15:GLU:HB2	2.03	0.41
2:BP:172:ASN:ND2	2:BP:204:SER:H	2.19	0.41
3:BS:171:ILE:H	3:BS:175:SER:HA	1.86	0.41
3:BT:158:LYS:HD2	3:BT:176:TYR:CE1	2.56	0.41
3:BT:203:LEU:HD21	3:BT:240:ILE:HG13	2.02	0.41
2:AE:229:THR:HB	2:AF:228:ASP:HB2	2.03	0.40
2:AM:172:ASN:ND2	2:AM:204:SER:H	2.19	0.40
3:AS:226:ALA:HB3	3:AS:268:ARG:HB3	2.03	0.40
2:AG:130:GLY:HA3	1:AZ:218:ILE:HG23	2.02	0.40
2:BA:198:GLN:HB2	2:BA:201:TRP:CD1	2.56	0.40
2:BD:174:LEU:HB2	2:BD:194:VAL:HG22	2.03	0.40
3:AT:68:PHE:CE1	3:BS:120:LYS:HG2	2.56	0.40
3:BX:171:ILE:H	3:BX:175:SER:HA	1.86	0.40
1:BY:87:LYS:HZ1	1:BY:89:LEU:HD23	1.86	0.40
2:AL:10:SER:HA	2:AL:15:GLU:HB2	2.03	0.40
2:AL:5:ASN:HB3	2:AL:8:PHE:CD1	2.56	0.40
2:AO:17:PRO:CB	3:AW:167:ASN:HB2	2.51	0.40
2:AP:146:ASP:O	2:AR:151:ASN:HB2	2.21	0.40
2:AG:79:ASP:CB	1:AZ:212:ASN:ND2	2.85	0.40
1:B0:52:LEU:HD23	1:B0:53:TYR:CE2	2.56	0.40
2:BB:27:TYR:HA	2:BB:30:LEU:HD12	2.03	0.40
2:BJ:174:LEU:HB2	2:BJ:194:VAL:HG22	2.04	0.40
3:BS:7:ILE:HG23	3:BS:92:VAL:CG1	2.51	0.40
1:BZ:45:GLU:HA	1:BZ:357:THR:HG22	2.03	0.40
2:AP:203:MET:SD	2:AP:243:TRP:HB2	2.61	0.40
3:AV:240:ILE:CD1	3:AV:242:THR:HG23	2.51	0.40
1:A0:3:GLU:CG	3:AW:271:THR:HA	2.51	0.40
3:AX:118:TYR:HB3	3:AX:122:GLY:HA2	2.04	0.40
2:BE:17:PRO:HG3	3:BT:169:LYS:CE	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BS:226:ALA:HB3	3:BS:268:ARG:HB3	2.03	0.40
2:AD:174:LEU:HB2	2:AD:194:VAL:HG22	2.02	0.40
3:AU:171:ILE:H	3:AU:175:SER:HA	1.86	0.40
2:BE:229:THR:HB	2:BF:228:ASP:HB2	2.03	0.40
2:BH:229:THR:HB	2:BI:228:ASP:HB2	2.03	0.40
2:AN:5:ASN:HB3	2:AN:8:PHE:CD1	2.57	0.40
2:AQ:17:PRO:N	3:AX:169:LYS:HD3	2.36	0.40
3:AT:132:ILE:HG21	3:AT:135:LYS:HB2	2.04	0.40
3:AW:3:ARG:HD2	3:AW:3:ARG:C	2.42	0.40
3:AS:270:ARG:CZ	1:AY:72:LEU:HD22	2.51	0.40
2:BF:9:PHE:CB	3:BT:180:GLY:HA2	2.52	0.40
2:BG:9:PHE:HB2	3:BU:166:GLY:CA	2.51	0.40
2:BK:229:THR:HB	2:BL:228:ASP:HB2	2.03	0.40
2:BN:5:ASN:HB3	2:BN:8:PHE:CD1	2.57	0.40
2:BP:203:MET:SD	2:BP:243:TRP:HB2	2.61	0.40
3:BT:116:GLU:OE2	3:BU:5:TYR:CE2	2.74	0.40
3:BW:171:ILE:H	3:BW:175:SER:HA	1.86	0.40
1:BY:185:PHE:CE2	1:BY:208:PHE:HA	2.56	0.40
1:B0:292:THR:HB	1:BZ:120:ASP:HB2	2.03	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	A0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	AY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	AZ	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	B0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	BY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BZ	370/372 (100%)	357 (96%)	13 (4%)	0	100	100
2	AA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AG	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AP	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BG	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BP	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
3	AS	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
3	AT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	22	62
3	AU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	22	62
3	AV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	22	62
3	AW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	22	62
3	AX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
3	BS	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	22	62
3	BT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	22	62
3	BU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	22	62
3	BV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	22	62
3	BW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	22	62
3	BX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
All	All	15168/15276 (99%)	14418 (95%)	726 (5%)	24 (0%)	47	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AS	175	SER
3	AT	175	SER
3	AU	175	SER
3	AV	175	SER
3	AW	175	SER
3	AX	175	SER
3	BS	175	SER
3	BT	175	SER
3	BU	175	SER
3	BV	175	SER
3	BW	175	SER
3	BX	175	SER
3	AS	136	TRP

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Mol	Chain	Res	Type
3	AU	136	TRP
3	AV	136	TRP
3	AW	136	TRP
3	AX	136	TRP
3	BS	136	TRP
3	BU	136	TRP
3	BV	136	TRP
3	BW	136	TRP
3	BX	136	TRP
3	AT	136	TRP
3	BT	136	TRP

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	A0	337/337 (100%)	324 (96%)	13 (4%)	32	57
1	AY	337/337 (100%)	319 (95%)	18 (5%)	22	49
1	AZ	337/337 (100%)	321 (95%)	16 (5%)	26	52
1	B0	337/337 (100%)	324 (96%)	13 (4%)	32	57
1	BY	337/337 (100%)	319 (95%)	18 (5%)	22	49
1	BZ	337/337 (100%)	321 (95%)	16 (5%)	26	52
2	AA	227/227 (100%)	218 (96%)	9 (4%)	31	56
2	AB	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AC	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	AD	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AE	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AF	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	AG	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AH	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AI	227/227 (100%)	223 (98%)	4 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AJ	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AK	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AL	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	AM	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AN	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AO	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	AP	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AQ	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AR	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BA	227/227 (100%)	218 (96%)	9 (4%)	31	56
2	BB	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BC	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BD	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BE	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BF	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	BG	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BH	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BI	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BJ	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BK	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BL	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BM	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BN	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BO	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	BP	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BQ	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BR	227/227 (100%)	223 (98%)	4 (2%)	59	77
3	AS	264/265 (100%)	246 (93%)	18 (7%)	16	42
3	AT	264/265 (100%)	248 (94%)	16 (6%)	18	45
3	AU	264/265 (100%)	241 (91%)	23 (9%)	10	33
3	AV	264/265 (100%)	241 (91%)	23 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AW	264/265 (100%)	244 (92%)	20 (8%)	13 39
3	AX	264/265 (100%)	247 (94%)	17 (6%)	17 44
3	BS	264/265 (100%)	245 (93%)	19 (7%)	14 41
3	BT	264/265 (100%)	247 (94%)	17 (6%)	17 44
3	BU	264/265 (100%)	241 (91%)	23 (9%)	10 33
3	BV	264/265 (100%)	241 (91%)	23 (9%)	10 33
3	BW	264/265 (100%)	244 (92%)	20 (8%)	13 39
3	BX	264/265 (100%)	247 (94%)	17 (6%)	17 44
All	All	13362/13374 (100%)	12818 (96%)	544 (4%)	30 55

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	1	MET
1	A0	2	LEU
1	A0	8	ASP
1	A0	40	GLN
1	A0	88	LYS
1	A0	152	PHE
1	A0	165	ARG
1	A0	207	ASN
1	A0	224	ILE
1	A0	238	ARG
1	A0	286	ASP
1	A0	313	ILE
1	A0	360	ASN
2	AA	2	THR
2	AA	7	THR
2	AA	9	PHE
2	AA	18	VAL
2	AA	38	ILE
2	AA	40	ARG
2	AA	79	ASP
2	AA	124	ASP
2	AA	202	ASN
2	AB	38	ILE
2	AB	40	ARG
2	AB	206	THR
2	AB	232	HIS

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Mol	Chain	Res	Type
2	AB	234	ASP
2	AB	252	PRO
2	AC	7	THR
2	AC	38	ILE
2	AC	40	ARG
2	AC	232	HIS
2	AD	9	PHE
2	AD	18	VAL
2	AD	38	ILE
2	AD	40	ARG
2	AD	79	ASP
2	AD	124	ASP
2	AD	202	ASN
2	AE	38	ILE
2	AE	40	ARG
2	AE	206	THR
2	AE	232	HIS
2	AE	234	ASP
2	AE	252	PRO
2	AF	38	ILE
2	AF	40	ARG
2	AF	232	HIS
2	AG	7	THR
2	AG	9	PHE
2	AG	18	VAL
2	AG	38	ILE
2	AG	40	ARG
2	AG	79	ASP
2	AG	124	ASP
2	AG	202	ASN
2	AH	17	PRO
2	AH	38	ILE
2	AH	40	ARG
2	AH	206	THR
2	AH	232	HIS
2	AH	234	ASP
2	AH	252	PRO
2	AI	7	THR
2	AI	38	ILE
2	AI	40	ARG
2	AI	232	HIS
2	AJ	7	THR

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Mol	Chain	Res	Type
2	AJ	9	PHE
2	AJ	18	VAL
2	AJ	38	ILE
2	AJ	40	ARG
2	AJ	79	ASP
2	AJ	124	ASP
2	AJ	202	ASN
2	AK	23	ASP
2	AK	38	ILE
2	AK	40	ARG
2	AK	206	THR
2	AK	232	HIS
2	AK	234	ASP
2	AL	26	LEU
2	AL	38	ILE
2	AL	40	ARG
2	AL	232	HIS
2	AM	7	THR
2	AM	9	PHE
2	AM	18	VAL
2	AM	38	ILE
2	AM	40	ARG
2	AM	79	ASP
2	AM	124	ASP
2	AM	202	ASN
2	AN	23	ASP
2	AN	38	ILE
2	AN	40	ARG
2	AN	206	THR
2	AN	232	HIS
2	AN	234	ASP
2	AO	38	ILE
2	AO	40	ARG
2	AO	232	HIS
2	AP	9	PHE
2	AP	18	VAL
2	AP	38	ILE
2	AP	40	ARG
2	AP	79	ASP
2	AP	124	ASP
2	AP	202	ASN
2	AQ	17	PRO

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Mol	Chain	Res	Type
2	AQ	23	ASP
2	AQ	38	ILE
2	AQ	40	ARG
2	AQ	206	THR
2	AQ	232	HIS
2	AQ	234	ASP
2	AR	7	THR
2	AR	38	ILE
2	AR	40	ARG
2	AR	232	HIS
3	AS	11	LEU
3	AS	12	ASP
3	AS	26	VAL
3	AS	43	TRP
3	AS	54	ARG
3	AS	55	SER
3	AS	66	GLU
3	AS	123	THR
3	AS	142	LEU
3	AS	196	ILE
3	AS	197	PHE
3	AS	228	VAL
3	AS	232	GLU
3	AS	234	VAL
3	AS	263	VAL
3	AS	269	TYR
3	AS	270	ARG
3	AS	291	ILE
3	AT	12	ASP
3	AT	26	VAL
3	AT	48	ILE
3	AT	55	SER
3	AT	65	LEU
3	AT	72	LEU
3	AT	123	THR
3	AT	159	ILE
3	AT	171	ILE
3	AT	196	ILE
3	AT	203	LEU
3	AT	234	VAL
3	AT	236	ASP
3	AT	243	ASP

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Mol	Chain	Res	Type
3	AT	263	VAL
3	AT	269	TYR
3	AU	3	ARG
3	AU	11	LEU
3	AU	12	ASP
3	AU	26	VAL
3	AU	37	GLN
3	AU	39	THR
3	AU	43	TRP
3	AU	48	ILE
3	AU	53	THR
3	AU	54	ARG
3	AU	55	SER
3	AU	66	GLU
3	AU	72	LEU
3	AU	94	LEU
3	AU	196	ILE
3	AU	200	MET
3	AU	228	VAL
3	AU	232	GLU
3	AU	234	VAL
3	AU	258	LEU
3	AU	263	VAL
3	AU	270	ARG
3	AU	291	ILE
3	AV	3	ARG
3	AV	11	LEU
3	AV	12	ASP
3	AV	36	LEU
3	AV	48	ILE
3	AV	54	ARG
3	AV	55	SER
3	AV	66	GLU
3	AV	72	LEU
3	AV	120	LYS
3	AV	196	ILE
3	AV	197	PHE
3	AV	203	LEU
3	AV	227	ILE
3	AV	232	GLU
3	AV	234	VAL
3	AV	240	ILE

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Mol	Chain	Res	Type
3	AV	243	ASP
3	AV	246	ASP
3	AV	258	LEU
3	AV	263	VAL
3	AV	269	TYR
3	AV	291	ILE
3	AW	6	LYS
3	AW	11	LEU
3	AW	26	VAL
3	AW	43	TRP
3	AW	54	ARG
3	AW	55	SER
3	AW	66	GLU
3	AW	72	LEU
3	AW	123	THR
3	AW	196	ILE
3	AW	197	PHE
3	AW	203	LEU
3	AW	228	VAL
3	AW	232	GLU
3	AW	234	VAL
3	AW	258	LEU
3	AW	263	VAL
3	AW	269	TYR
3	AW	270	ARG
3	AW	291	ILE
3	AX	11	LEU
3	AX	26	VAL
3	AX	43	TRP
3	AX	54	ARG
3	AX	66	GLU
3	AX	107	LEU
3	AX	179	TYR
3	AX	196	ILE
3	AX	200	MET
3	AX	203	LEU
3	AX	228	VAL
3	AX	234	VAL
3	AX	243	ASP
3	AX	244	VAL
3	AX	258	LEU
3	AX	263	VAL

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Mol	Chain	Res	Type
3	AX	291	ILE
1	AY	1	MET
1	AY	8	ASP
1	AY	26	LYS
1	AY	40	GLN
1	AY	41	VAL
1	AY	87	LYS
1	AY	88	LYS
1	AY	152	PHE
1	AY	165	ARG
1	AY	192	GLN
1	AY	207	ASN
1	AY	242	ASN
1	AY	243	PHE
1	AY	286	ASP
1	AY	319	VAL
1	AY	340	ILE
1	AY	353	ASP
1	AY	360	ASN
1	AZ	1	MET
1	AZ	2	LEU
1	AZ	8	ASP
1	AZ	26	LYS
1	AZ	39	CYS
1	AZ	40	GLN
1	AZ	41	VAL
1	AZ	88	LYS
1	AZ	151	PHE
1	AZ	165	ARG
1	AZ	207	ASN
1	AZ	238	ARG
1	AZ	286	ASP
1	AZ	320	THR
1	AZ	340	ILE
1	AZ	360	ASN
1	B0	1	MET
1	B0	2	LEU
1	B0	8	ASP
1	B0	40	GLN
1	B0	88	LYS
1	B0	152	PHE
1	B0	165	ARG

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Mol	Chain	Res	Type
1	B0	207	ASN
1	B0	224	ILE
1	B0	238	ARG
1	B0	286	ASP
1	B0	313	ILE
1	B0	360	ASN
2	BA	2	THR
2	BA	7	THR
2	BA	9	PHE
2	BA	18	VAL
2	BA	38	ILE
2	BA	40	ARG
2	BA	79	ASP
2	BA	124	ASP
2	BA	202	ASN
2	BB	38	ILE
2	BB	40	ARG
2	BB	206	THR
2	BB	232	HIS
2	BB	234	ASP
2	BB	252	PRO
2	BC	7	THR
2	BC	38	ILE
2	BC	40	ARG
2	BC	232	HIS
2	BD	9	PHE
2	BD	18	VAL
2	BD	38	ILE
2	BD	40	ARG
2	BD	79	ASP
2	BD	124	ASP
2	BD	202	ASN
2	BE	38	ILE
2	BE	40	ARG
2	BE	206	THR
2	BE	232	HIS
2	BE	234	ASP
2	BE	252	PRO
2	BF	38	ILE
2	BF	40	ARG
2	BF	232	HIS
2	BG	7	THR

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Mol	Chain	Res	Type
2	BG	9	PHE
2	BG	18	VAL
2	BG	38	ILE
2	BG	40	ARG
2	BG	79	ASP
2	BG	124	ASP
2	BG	202	ASN
2	BH	17	PRO
2	BH	38	ILE
2	BH	40	ARG
2	BH	206	THR
2	BH	232	HIS
2	BH	234	ASP
2	BH	252	PRO
2	BI	7	THR
2	BI	38	ILE
2	BI	40	ARG
2	BI	232	HIS
2	BJ	7	THR
2	BJ	9	PHE
2	BJ	18	VAL
2	BJ	38	ILE
2	BJ	40	ARG
2	BJ	79	ASP
2	BJ	124	ASP
2	BJ	202	ASN
2	BK	23	ASP
2	BK	38	ILE
2	BK	40	ARG
2	BK	206	THR
2	BK	232	HIS
2	BK	234	ASP
2	BL	26	LEU
2	BL	38	ILE
2	BL	40	ARG
2	BL	232	HIS
2	BM	7	THR
2	BM	9	PHE
2	BM	18	VAL
2	BM	38	ILE
2	BM	40	ARG
2	BM	79	ASP

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Mol	Chain	Res	Type
2	BM	124	ASP
2	BM	202	ASN
2	BN	23	ASP
2	BN	38	ILE
2	BN	40	ARG
2	BN	206	THR
2	BN	232	HIS
2	BN	234	ASP
2	BO	38	ILE
2	BO	40	ARG
2	BO	232	HIS
2	BP	9	PHE
2	BP	18	VAL
2	BP	38	ILE
2	BP	40	ARG
2	BP	79	ASP
2	BP	124	ASP
2	BP	202	ASN
2	BQ	17	PRO
2	BQ	23	ASP
2	BQ	38	ILE
2	BQ	40	ARG
2	BQ	206	THR
2	BQ	232	HIS
2	BQ	234	ASP
2	BR	7	THR
2	BR	38	ILE
2	BR	40	ARG
2	BR	232	HIS
3	BS	11	LEU
3	BS	12	ASP
3	BS	26	VAL
3	BS	43	TRP
3	BS	54	ARG
3	BS	55	SER
3	BS	66	GLU
3	BS	72	LEU
3	BS	123	THR
3	BS	142	LEU
3	BS	196	ILE
3	BS	197	PHE
3	BS	228	VAL

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Mol	Chain	Res	Type
3	BS	232	GLU
3	BS	234	VAL
3	BS	263	VAL
3	BS	269	TYR
3	BS	270	ARG
3	BS	291	ILE
3	BT	12	ASP
3	BT	26	VAL
3	BT	48	ILE
3	BT	55	SER
3	BT	65	LEU
3	BT	72	LEU
3	BT	123	THR
3	BT	135	LYS
3	BT	159	ILE
3	BT	171	ILE
3	BT	196	ILE
3	BT	203	LEU
3	BT	234	VAL
3	BT	236	ASP
3	BT	243	ASP
3	BT	263	VAL
3	BT	269	TYR
3	BU	3	ARG
3	BU	11	LEU
3	BU	12	ASP
3	BU	26	VAL
3	BU	37	GLN
3	BU	39	THR
3	BU	43	TRP
3	BU	48	ILE
3	BU	53	THR
3	BU	54	ARG
3	BU	55	SER
3	BU	66	GLU
3	BU	72	LEU
3	BU	94	LEU
3	BU	196	ILE
3	BU	200	MET
3	BU	228	VAL
3	BU	232	GLU
3	BU	234	VAL

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Mol	Chain	Res	Type
3	BU	258	LEU
3	BU	263	VAL
3	BU	270	ARG
3	BU	291	ILE
3	BV	3	ARG
3	BV	11	LEU
3	BV	12	ASP
3	BV	36	LEU
3	BV	48	ILE
3	BV	54	ARG
3	BV	55	SER
3	BV	66	GLU
3	BV	72	LEU
3	BV	120	LYS
3	BV	196	ILE
3	BV	197	PHE
3	BV	203	LEU
3	BV	227	ILE
3	BV	232	GLU
3	BV	234	VAL
3	BV	240	ILE
3	BV	243	ASP
3	BV	246	ASP
3	BV	258	LEU
3	BV	263	VAL
3	BV	269	TYR
3	BV	291	ILE
3	BW	6	LYS
3	BW	11	LEU
3	BW	26	VAL
3	BW	43	TRP
3	BW	54	ARG
3	BW	55	SER
3	BW	66	GLU
3	BW	72	LEU
3	BW	123	THR
3	BW	196	ILE
3	BW	197	PHE
3	BW	203	LEU
3	BW	228	VAL
3	BW	232	GLU
3	BW	234	VAL

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Mol	Chain	Res	Type
3	BW	258	LEU
3	BW	263	VAL
3	BW	269	TYR
3	BW	270	ARG
3	BW	291	ILE
3	BX	11	LEU
3	BX	26	VAL
3	BX	43	TRP
3	BX	54	ARG
3	BX	66	GLU
3	BX	107	LEU
3	BX	179	TYR
3	BX	196	ILE
3	BX	200	MET
3	BX	203	LEU
3	BX	228	VAL
3	BX	234	VAL
3	BX	243	ASP
3	BX	244	VAL
3	BX	258	LEU
3	BX	263	VAL
3	BX	291	ILE
1	BY	1	MET
1	BY	8	ASP
1	BY	26	LYS
1	BY	40	GLN
1	BY	41	VAL
1	BY	87	LYS
1	BY	88	LYS
1	BY	152	PHE
1	BY	165	ARG
1	BY	192	GLN
1	BY	207	ASN
1	BY	242	ASN
1	BY	243	PHE
1	BY	286	ASP
1	BY	319	VAL
1	BY	340	ILE
1	BY	353	ASP
1	BY	360	ASN
1	BZ	1	MET
1	BZ	2	LEU

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Mol	Chain	Res	Type
1	BZ	8	ASP
1	BZ	26	LYS
1	BZ	39	CYS
1	BZ	40	GLN
1	BZ	41	VAL
1	BZ	88	LYS
1	BZ	151	PHE
1	BZ	165	ARG
1	BZ	207	ASN
1	BZ	238	ARG
1	BZ	286	ASP
1	BZ	320	THR
1	BZ	340	ILE
1	BZ	360	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	184	GLN
1	A0	267	ASN
2	AA	5	ASN
2	AA	71	ASN
2	AA	82	ASN
2	AA	172	ASN
2	AA	175	GLN
2	AB	71	ASN
2	AC	172	ASN
2	AD	5	ASN
2	AD	52	ASN
2	AD	71	ASN
2	AD	82	ASN
2	AD	92	GLN
2	AD	172	ASN
2	AD	175	GLN
2	AD	196	ASN
2	AE	54	GLN
2	AE	71	ASN
2	AF	172	ASN
2	AG	71	ASN
2	AG	82	ASN
2	AG	92	GLN
2	AG	172	ASN

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Mol	Chain	Res	Type
2	AG	175	GLN
2	AG	196	ASN
2	AH	71	ASN
2	AI	151	ASN
2	AI	172	ASN
2	AJ	71	ASN
2	AJ	82	ASN
2	AJ	172	ASN
2	AJ	175	GLN
2	AJ	196	ASN
2	AK	54	GLN
2	AK	71	ASN
2	AL	151	ASN
2	AL	172	ASN
2	AM	71	ASN
2	AM	82	ASN
2	AM	172	ASN
2	AM	175	GLN
2	AM	196	ASN
2	AN	54	GLN
2	AN	71	ASN
2	AO	172	ASN
2	AP	5	ASN
2	AP	22	ASN
2	AP	71	ASN
2	AP	82	ASN
2	AP	92	GLN
2	AP	172	ASN
2	AP	175	GLN
2	AP	196	ASN
2	AQ	71	ASN
2	AR	151	ASN
2	AR	172	ASN
3	AS	102	GLN
3	AS	222	ASN
3	AS	250	GLN
3	AT	102	GLN
3	AT	167	ASN
3	AT	235	GLN
3	AU	23	ASN
3	AU	75	ASN
3	AU	250	GLN

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Mol	Chain	Res	Type
3	AV	23	ASN
3	AV	102	GLN
3	AV	121	ASN
3	AV	235	GLN
3	AV	250	GLN
3	AW	102	GLN
3	AW	121	ASN
3	AX	102	GLN
3	AX	121	ASN
3	AX	167	ASN
3	AX	250	GLN
3	AX	278	GLN
1	AY	11	ASN
1	AY	90	ASN
1	AY	143	ASN
1	AZ	143	ASN
1	AZ	184	GLN
1	AZ	192	GLN
1	AZ	212	ASN
1	B0	184	GLN
1	B0	267	ASN
2	BA	5	ASN
2	BA	71	ASN
2	BA	82	ASN
2	BA	172	ASN
2	BA	175	GLN
2	BB	71	ASN
2	BC	172	ASN
2	BD	5	ASN
2	BD	52	ASN
2	BD	71	ASN
2	BD	82	ASN
2	BD	92	GLN
2	BD	172	ASN
2	BD	175	GLN
2	BD	196	ASN
2	BE	54	GLN
2	BE	71	ASN
2	BF	172	ASN
2	BG	71	ASN
2	BG	82	ASN
2	BG	92	GLN

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Mol	Chain	Res	Type
2	BG	172	ASN
2	BG	175	GLN
2	BG	196	ASN
2	BH	71	ASN
2	BI	151	ASN
2	BI	172	ASN
2	BJ	71	ASN
2	BJ	82	ASN
2	BJ	172	ASN
2	BJ	175	GLN
2	BJ	196	ASN
2	BK	71	ASN
2	BL	151	ASN
2	BL	172	ASN
2	BM	71	ASN
2	BM	82	ASN
2	BM	172	ASN
2	BM	175	GLN
2	BM	196	ASN
2	BN	54	GLN
2	BN	71	ASN
2	BO	172	ASN
2	BP	5	ASN
2	BP	22	ASN
2	BP	71	ASN
2	BP	82	ASN
2	BP	92	GLN
2	BP	172	ASN
2	BP	175	GLN
2	BP	196	ASN
2	BQ	54	GLN
2	BQ	71	ASN
2	BR	151	ASN
2	BR	172	ASN
3	BS	102	GLN
3	BS	222	ASN
3	BS	250	GLN
3	BT	102	GLN
3	BT	167	ASN
3	BT	222	ASN
3	BT	235	GLN
3	BU	23	ASN

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Mol	Chain	Res	Type
3	BU	75	ASN
3	BU	250	GLN
3	BV	23	ASN
3	BV	102	GLN
3	BV	121	ASN
3	BV	235	GLN
3	BV	250	GLN
3	BW	102	GLN
3	BW	121	ASN
3	BX	102	GLN
3	BX	121	ASN
3	BX	167	ASN
3	BX	250	GLN
1	BY	90	ASN
1	BY	143	ASN
1	BZ	143	ASN
1	BZ	184	GLN
1	BZ	192	GLN
1	BZ	212	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A0	372/372 (100%)	0.53	40 (10%) 5 8	351, 388, 435, 523	0
1	AY	372/372 (100%)	0.36	37 (9%) 7 9	359, 396, 449, 555	0
1	AZ	372/372 (100%)	0.42	38 (10%) 6 9	364, 394, 445, 557	0
1	B0	372/372 (100%)	0.41	29 (7%) 13 13	337, 377, 425, 485	0
1	BY	372/372 (100%)	0.14	15 (4%) 38 32	331, 361, 429, 557	0
1	BZ	372/372 (100%)	0.31	28 (7%) 14 14	332, 360, 422, 502	0
2	AA	263/263 (100%)	0.06	6 (2%) 60 52	248, 312, 407, 435	0
2	AB	263/263 (100%)	0.13	15 (5%) 23 22	284, 350, 440, 481	0
2	AC	263/263 (100%)	-0.11	13 (4%) 29 27	257, 345, 417, 473	0
2	AD	263/263 (100%)	0.21	16 (6%) 21 19	258, 320, 441, 485	0
2	AE	263/263 (100%)	-0.05	8 (3%) 50 41	277, 344, 466, 480	0
2	AF	263/263 (100%)	0.11	16 (6%) 21 19	265, 367, 471, 497	0
2	AG	263/263 (100%)	0.26	23 (8%) 10 11	265, 348, 500, 556	0
2	AH	263/263 (100%)	-0.08	9 (3%) 45 38	315, 402, 524, 572	0
2	AI	263/263 (100%)	0.14	20 (7%) 13 14	282, 416, 532, 576	0
2	AJ	263/263 (100%)	0.01	13 (4%) 29 27	264, 342, 429, 539	0
2	AK	263/263 (100%)	0.00	10 (3%) 40 34	255, 301, 456, 521	0
2	AL	263/263 (100%)	0.17	20 (7%) 13 14	277, 345, 485, 575	0
2	AM	263/263 (100%)	0.17	22 (8%) 11 12	266, 358, 425, 467	0
2	AN	263/263 (100%)	0.20	14 (5%) 26 25	252, 313, 386, 420	0
2	AO	263/263 (100%)	0.13	13 (4%) 29 27	276, 347, 419, 449	0
2	AP	263/263 (100%)	0.20	18 (6%) 17 16	267, 341, 556, 576	0
2	AQ	263/263 (100%)	0.30	25 (9%) 8 9	295, 397, 566, 605	0
2	AR	263/263 (100%)	0.20	17 (6%) 18 17	298, 417, 541, 571	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	BA	263/263 (100%)	0.08	11 (4%) 36 31	259, 312, 430, 466	0
2	BB	263/263 (100%)	0.05	13 (4%) 29 27	282, 346, 455, 506	0
2	BC	263/263 (100%)	-0.03	13 (4%) 29 27	273, 344, 419, 481	0
2	BD	263/263 (100%)	0.17	15 (5%) 23 22	252, 316, 445, 484	0
2	BE	263/263 (100%)	-0.01	11 (4%) 36 31	274, 342, 448, 477	0
2	BF	263/263 (100%)	0.34	21 (7%) 12 13	258, 361, 457, 487	0
2	BG	263/263 (100%)	0.27	21 (7%) 12 13	252, 346, 496, 557	0
2	BH	263/263 (100%)	0.15	20 (7%) 13 14	314, 408, 514, 559	0
2	BI	263/263 (100%)	0.00	11 (4%) 36 31	276, 420, 541, 584	0
2	BJ	263/263 (100%)	-0.17	7 (2%) 54 46	268, 345, 419, 521	0
2	BK	263/263 (100%)	0.10	20 (7%) 13 14	256, 305, 435, 496	0
2	BL	263/263 (100%)	0.19	22 (8%) 11 12	283, 341, 452, 534	0
2	BM	263/263 (100%)	0.37	24 (9%) 9 10	264, 357, 438, 484	0
2	BN	263/263 (100%)	0.18	17 (6%) 18 17	255, 316, 388, 433	0
2	BO	263/263 (100%)	0.07	15 (5%) 23 22	276, 348, 418, 453	0
2	BP	263/263 (100%)	0.31	31 (11%) 4 7	261, 365, 541, 549	0
2	BQ	263/263 (100%)	0.18	21 (7%) 12 13	312, 413, 547, 559	0
2	BR	263/263 (100%)	0.29	25 (9%) 8 9	308, 418, 537, 556	0
3	AS	298/298 (100%)	0.29	16 (5%) 25 24	219, 262, 346, 379	0
3	AT	298/298 (100%)	0.26	15 (5%) 28 26	230, 260, 318, 344	0
3	AU	298/298 (100%)	0.16	6 (2%) 65 57	228, 269, 334, 364	0
3	AV	298/298 (100%)	0.21	14 (4%) 31 28	229, 264, 317, 332	0
3	AW	298/298 (100%)	0.17	9 (3%) 50 41	213, 254, 317, 347	0
3	AX	298/298 (100%)	0.10	12 (4%) 38 32	216, 255, 347, 401	0
3	BS	298/298 (100%)	0.21	12 (4%) 38 32	222, 256, 339, 388	0
3	BT	298/298 (100%)	0.19	10 (3%) 45 38	218, 265, 316, 343	0
3	BU	298/298 (100%)	0.09	9 (3%) 50 41	228, 262, 338, 382	0
3	BV	298/298 (100%)	0.28	15 (5%) 28 26	218, 260, 305, 324	0
3	BW	298/298 (100%)	0.08	7 (2%) 60 52	215, 256, 341, 403	0
3	BX	298/298 (100%)	0.09	12 (4%) 38 32	228, 272, 370, 407	0
All	All	15276/15276 (100%)	0.17	920 (6%) 21 20	213, 344, 468, 605	0

All (920) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AQ	221	VAL	16.4
2	AQ	220	LEU	15.4
2	BN	260	SER	9.5
2	BO	260	SER	9.4
2	BF	260	SER	9.3
2	BM	259	GLY	9.1
1	A0	32	LEU	9.1
2	BF	259	GLY	8.8
1	A0	198	THR	8.8
2	BB	260	SER	8.7
2	BH	260	SER	8.6
2	BH	259	GLY	8.6
1	B0	164	ASN	8.5
2	BP	192	GLY	8.4
2	BO	259	GLY	8.3
2	BR	30	LEU	8.2
2	BI	259	GLY	8.1
2	BC	260	SER	8.1
2	AF	260	SER	8.1
2	BR	221	VAL	8.1
2	AO	260	SER	7.9
1	BZ	209	ALA	7.8
2	BM	258	ASN	7.6
2	AR	222	GLY	7.6
1	BY	1	MET	7.5
1	AZ	367	GLU	7.5
1	A0	202	ASN	7.5
2	AM	176	LEU	7.5
1	A0	164	ASN	7.4
2	AR	221	VAL	7.4
2	AD	258	ASN	7.4
2	BE	258	ASN	7.3
1	A0	195	PRO	7.1
2	BG	254	ALA	7.0
3	AS	298	VAL	7.0
2	BM	174	LEU	7.0
2	AQ	222	GLY	7.0
2	BQ	221	VAL	7.0
2	BQ	230	SER	7.0
2	BG	221	VAL	6.9
1	AZ	164	ASN	6.8
2	AL	221	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
2	BM	257	GLY	6.6
2	AO	259	GLY	6.5
2	AF	259	GLY	6.5
1	BZ	208	PHE	6.5
2	AG	192	GLY	6.4
2	BP	193	SER	6.4
2	BB	221	VAL	6.4
2	AM	221	VAL	6.3
2	BN	259	GLY	6.3
2	BQ	222	GLY	6.3
2	BL	252	PRO	6.3
1	AZ	215	ARG	6.2
2	BI	260	SER	6.2
1	AY	217	ARG	6.1
2	BR	3	ILE	6.1
2	AF	62	ALA	6.0
2	AR	31	THR	6.0
1	AY	128	THR	6.0
1	A0	196	SER	6.0
2	BA	221	VAL	5.9
2	AP	222	GLY	5.9
2	AM	260	SER	5.9
2	BF	221	VAL	5.8
1	BY	215	ARG	5.8
3	BX	298	VAL	5.7
2	AM	175	GLN	5.7
2	BQ	231	PHE	5.7
1	A0	197	GLU	5.7
1	B0	162	THR	5.6
1	AY	164	ASN	5.6
2	BQ	233	ILE	5.6
2	AG	225	ALA	5.6
2	AE	221	VAL	5.5
1	B0	195	PRO	5.5
2	AR	258	ASN	5.5
1	BZ	207	ASN	5.4
2	AP	117	GLY	5.4
2	AD	221	VAL	5.4
2	BM	188	VAL	5.4
2	BR	31	THR	5.3
2	BM	260	SER	5.3
1	A0	327	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
2	AQ	260	SER	5.3
2	AG	211	PRO	5.3
2	AI	36	ARG	5.2
1	A0	326	GLN	5.2
2	AQ	219	SER	5.2
2	BH	261	TYR	5.2
2	BF	63	GLY	5.1
2	AK	221	VAL	5.1
2	BA	260	SER	5.1
2	BA	130	GLY	5.1
2	BA	222	GLY	5.1
2	BO	157	GLY	5.0
2	AH	260	SER	5.0
2	AD	260	SER	5.0
1	AY	129	THR	5.0
2	AG	254	ALA	5.0
2	AM	174	LEU	4.9
3	BV	296	ASP	4.9
2	BH	222	GLY	4.9
2	AI	35	TYR	4.9
1	A0	68	ILE	4.9
2	BM	176	LEU	4.9
2	AO	221	VAL	4.9
2	BK	30	LEU	4.8
2	BO	219	SER	4.8
1	AY	372	PRO	4.8
1	B0	209	ALA	4.7
2	AQ	63	GLY	4.7
2	AG	221	VAL	4.7
2	AD	161	VAL	4.7
1	AY	1	MET	4.7
1	AZ	1	MET	4.6
2	AN	260	SER	4.6
2	BR	126	VAL	4.6
2	AN	258	ASN	4.6
2	BM	168	VAL	4.6
1	BY	372	PRO	4.6
2	BG	260	SER	4.6
2	AP	254	ALA	4.5
2	BQ	2	THR	4.5
2	AN	259	GLY	4.5
1	AZ	210	SER	4.5

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Mol	Chain	Res	Type	RSRZ
3	AT	288	GLU	4.5
2	AE	257	GLY	4.5
3	AT	298	VAL	4.5
2	AF	220	LEU	4.5
2	BM	167	THR	4.5
2	BI	188	VAL	4.4
2	BB	259	GLY	4.4
2	BD	264	LYS	4.4
1	A0	356	LYS	4.4
3	BS	212	ALA	4.4
2	BD	260	SER	4.3
2	AQ	259	GLY	4.3
2	BC	247	ASN	4.3
2	AA	31	THR	4.3
3	AU	158	LYS	4.3
2	BE	259	GLY	4.3
3	AT	240	ILE	4.3
2	BK	64	GLY	4.3
2	BR	228	ASP	4.3
2	BE	257	GLY	4.3
2	BG	220	LEU	4.2
2	BH	221	VAL	4.2
1	BY	162	THR	4.2
2	BP	211	PRO	4.2
2	BM	190	PHE	4.2
2	BR	29	MET	4.2
2	AG	256	ARG	4.2
2	AB	222	GLY	4.2
2	BR	260	SER	4.2
3	AT	287	ALA	4.2
3	BX	99	GLU	4.2
2	BN	185	LEU	4.2
2	AQ	94	ALA	4.2
2	BP	176	LEU	4.2
2	BB	222	GLY	4.2
2	AE	258	ASN	4.1
1	A0	151	PHE	4.1
1	AY	315	PRO	4.1
2	AM	62	ALA	4.1
1	AZ	233	GLU	4.1
2	AF	63	GLY	4.1
1	A0	31	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	AH	258	ASN	4.1
2	AD	38	ILE	4.1
2	AL	254	ALA	4.1
3	BV	247	GLU	4.1
2	AL	63	GLY	4.1
1	AY	158	ALA	4.1
2	BP	61	ILE	4.0
2	BQ	62	ALA	4.0
2	BF	220	LEU	4.0
1	A0	332	LEU	4.0
2	BP	254	ALA	4.0
3	BT	247	GLU	4.0
2	AM	258	ASN	4.0
2	AR	99	LEU	4.0
3	BT	158	LYS	4.0
2	AL	62	ALA	4.0
1	B0	292	THR	4.0
2	AL	222	GLY	4.0
2	BK	168	VAL	4.0
2	BQ	215	ALA	4.0
2	BO	30	LEU	4.0
2	BM	221	VAL	4.0
1	AZ	52	LEU	4.0
2	AQ	95	ASN	4.0
2	BF	174	LEU	4.0
2	BP	175	GLN	4.0
2	BI	221	VAL	4.0
1	B0	280	ASP	4.0
2	BK	27	TYR	3.9
2	AP	221	VAL	3.9
2	BE	260	SER	3.9
2	AP	223	HIS	3.9
3	BV	298	VAL	3.9
1	A0	199	ASP	3.9
2	BD	257	GLY	3.9
3	BU	158	LYS	3.9
2	BH	258	ASN	3.9
2	AI	188	VAL	3.9
1	A0	265	ALA	3.9
2	BH	116	SER	3.9
2	BJ	260	SER	3.9
1	AZ	299	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	AM	188	VAL	3.9
2	BN	221	VAL	3.9
1	A0	162	THR	3.9
2	AC	184	ASP	3.8
2	BH	253	ILE	3.8
1	AZ	166	LYS	3.8
2	BO	221	VAL	3.8
1	AY	162	THR	3.8
2	BD	181	LYS	3.8
2	AD	18	VAL	3.8
2	AN	221	VAL	3.8
2	BF	99	LEU	3.8
1	B0	125	ILE	3.8
3	AT	202	ILE	3.8
3	AT	34	LEU	3.8
1	A0	200	PRO	3.8
2	AF	219	SER	3.8
2	BP	253	ILE	3.8
2	AC	183	ASN	3.8
2	AG	190	PHE	3.8
2	BO	159	ILE	3.8
2	BD	221	VAL	3.8
2	AA	30	LEU	3.7
2	AM	259	GLY	3.7
2	BQ	38	ILE	3.7
2	BP	252	PRO	3.7
2	BM	153	MET	3.7
2	AQ	253	ILE	3.7
1	BZ	264	ILE	3.7
2	BR	197	ILE	3.7
3	AV	287	ALA	3.7
2	AL	188	VAL	3.7
2	AJ	26	LEU	3.7
2	BE	221	VAL	3.7
2	AH	222	GLY	3.7
2	AQ	27	TYR	3.7
2	AG	23	ASP	3.7
3	AU	203	LEU	3.7
2	AN	181	LYS	3.7
2	BA	259	GLY	3.7
2	BM	261	TYR	3.7
2	BP	62	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
3	AT	2	VAL	3.7
2	BL	43	TRP	3.7
2	AC	260	SER	3.6
2	AG	226	GLY	3.6
2	BN	186	VAL	3.6
1	BY	271	VAL	3.6
2	BL	194	VAL	3.6
2	BH	252	PRO	3.6
1	BZ	142	LYS	3.6
2	AJ	261	TYR	3.6
2	AJ	260	SER	3.6
2	AL	219	SER	3.6
2	BC	258	ASN	3.6
2	BG	175	GLN	3.6
1	B0	328	GLU	3.6
2	AQ	30	LEU	3.6
1	AZ	136	TYR	3.6
1	AZ	368	SER	3.6
2	AG	167	THR	3.6
2	AD	259	GLY	3.6
2	AR	30	LEU	3.5
2	AD	211	PRO	3.5
2	BL	221	VAL	3.5
2	AL	258	ASN	3.5
2	BL	197	ILE	3.5
2	BF	262	PHE	3.5
3	BX	296	ASP	3.5
2	AB	69	LEU	3.5
1	AY	126	THR	3.5
1	A0	66	GLY	3.5
1	BZ	76	VAL	3.5
2	BF	222	GLY	3.5
2	AG	175	GLN	3.5
3	AV	289	PHE	3.5
2	BP	38	ILE	3.5
1	AY	233	GLU	3.5
2	BF	64	GLY	3.5
2	AD	99	LEU	3.4
1	AZ	209	ALA	3.4
2	AE	222	GLY	3.4
2	BO	158	SER	3.4
2	BQ	220	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	BV	249	TYR	3.4
1	AY	36	LYS	3.4
2	AQ	62	ALA	3.4
2	AN	23	ASP	3.4
1	AY	314	SER	3.4
2	BM	220	LEU	3.4
2	BF	144	THR	3.4
2	BL	202	ASN	3.4
1	A0	314	SER	3.4
1	A0	315	PRO	3.4
2	AN	213	ARG	3.4
2	AP	30	LEU	3.4
2	BP	216	ALA	3.4
3	BS	34	LEU	3.4
1	AY	159	GLY	3.4
2	BP	31	THR	3.4
2	BC	259	GLY	3.4
2	BL	188	VAL	3.4
1	B0	127	LYS	3.3
3	BS	213	GLY	3.3
2	BF	176	LEU	3.3
2	BB	48	ASN	3.3
2	AG	27	TYR	3.3
2	BG	27	TYR	3.3
2	BK	31	THR	3.3
1	A0	9	ASN	3.3
1	BY	335	ASN	3.3
1	B0	163	ILE	3.3
1	AZ	201	ARG	3.3
1	AZ	315	PRO	3.3
2	BH	257	GLY	3.3
2	AD	220	LEU	3.3
2	AM	177	GLN	3.3
3	AW	158	LYS	3.3
2	BG	192	GLY	3.3
1	AZ	230	MET	3.3
2	BR	222	GLY	3.3
1	AY	337	LEU	3.3
2	BB	30	LEU	3.3
3	AX	200	MET	3.3
1	BZ	372	PRO	3.3
1	AY	371	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	AT	212	ALA	3.2
1	AY	87	LYS	3.2
3	BW	279	MET	3.2
2	AQ	215	ALA	3.2
1	BZ	356	LYS	3.2
3	AU	238	ILE	3.2
2	BR	220	LEU	3.2
2	AI	75	ALA	3.2
3	AS	287	ALA	3.2
3	AW	281	LEU	3.2
2	AG	191	PHE	3.2
2	BD	258	ASN	3.2
2	AQ	233	ILE	3.2
1	AZ	319	VAL	3.2
2	AM	27	TYR	3.2
1	AZ	278	HIS	3.2
2	BA	220	LEU	3.2
2	BL	251	THR	3.2
2	BB	261	TYR	3.2
2	AG	220	LEU	3.2
2	AF	258	ASN	3.2
1	A0	194	ALA	3.2
2	AK	62	ALA	3.2
2	BR	4	LYS	3.2
2	AI	259	GLY	3.1
2	AA	3	ILE	3.1
3	BX	100	ILE	3.1
3	BU	1	MET	3.1
2	AO	220	LEU	3.1
2	AM	61	ILE	3.1
2	AL	227	ARG	3.1
2	AH	221	VAL	3.1
1	AY	88	LYS	3.1
2	AF	221	VAL	3.1
3	AV	201	GLY	3.1
3	AT	72	LEU	3.1
3	BU	287	ALA	3.1
2	BH	188	VAL	3.1
3	AT	296	ASP	3.1
3	BX	281	LEU	3.1
1	AZ	126	THR	3.1
3	AT	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
3	BU	203	LEU	3.1
2	AI	64	GLY	3.1
2	BK	69	LEU	3.1
2	BM	189	ARG	3.1
2	BM	166	LEU	3.1
2	BH	99	LEU	3.1
3	BV	139	TYR	3.1
2	AP	116	SER	3.1
3	AU	154	ALA	3.1
2	BP	223	HIS	3.1
3	AS	212	ALA	3.1
2	AJ	27	TYR	3.0
2	AL	220	LEU	3.0
2	BN	261	TYR	3.0
3	AV	213	GLY	3.0
2	BI	27	TYR	3.0
2	BR	233	ILE	3.0
2	BO	188	VAL	3.0
3	BU	12	ASP	3.0
1	B0	126	THR	3.0
2	AI	260	SER	3.0
2	AN	27	TYR	3.0
2	BD	27	TYR	3.0
2	AI	114	ASN	3.0
2	AL	161	VAL	3.0
2	BG	235	ILE	3.0
2	BB	220	LEU	3.0
2	BK	26	LEU	3.0
2	BD	184	ASP	3.0
2	BG	99	LEU	3.0
1	BY	371	LYS	3.0
2	BB	97	VAL	3.0
2	BF	261	TYR	3.0
1	A0	163	ILE	3.0
2	AN	187	ILE	3.0
2	BK	221	VAL	3.0
1	A0	207	ASN	3.0
2	AN	208	VAL	2.9
1	AY	182	LYS	2.9
1	AZ	165	ARG	2.9
2	BP	256	ARG	2.9
1	B0	208	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	BB	258	ASN	2.9
3	BS	249	TYR	2.9
3	AV	200	MET	2.9
1	AZ	320	THR	2.9
1	A0	67	ASP	2.9
2	BN	206	THR	2.9
1	AZ	65	VAL	2.9
2	BP	66	TYR	2.9
3	AU	289	PHE	2.9
3	AV	190	TRP	2.9
2	AR	125	ILE	2.9
2	BP	67	PHE	2.9
1	AY	132	ALA	2.9
2	AK	27	TYR	2.9
2	AJ	262	PHE	2.9
1	B0	160	LYS	2.9
2	AI	63	GLY	2.9
2	BN	97	VAL	2.9
2	AO	27	TYR	2.9
1	BY	160	LYS	2.9
2	BM	142	THR	2.9
2	BO	220	LEU	2.9
1	BZ	244	ALA	2.8
2	BB	53	VAL	2.8
1	AY	184	GLN	2.8
2	BE	99	LEU	2.8
2	AJ	212	PHE	2.8
2	BH	215	ALA	2.8
1	BZ	210	SER	2.8
3	AX	272	ARG	2.8
2	AH	259	GLY	2.8
2	BM	263	ILE	2.8
3	BW	158	LYS	2.8
1	AZ	232	THR	2.8
1	AY	348	SER	2.8
3	AV	214	VAL	2.8
2	AF	262	PHE	2.8
1	A0	203	LEU	2.8
1	BZ	263	TYR	2.8
2	BL	196	ASN	2.8
2	BG	259	GLY	2.8
2	BL	222	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	AX	1	MET	2.8
2	BH	251	THR	2.8
2	BJ	185	LEU	2.8
2	BE	222	GLY	2.8
1	AY	370	ASP	2.8
2	BF	62	ALA	2.8
2	BP	215	ALA	2.8
2	AL	160	ASP	2.8
1	B0	329	LEU	2.8
2	BG	176	LEU	2.8
2	BD	259	GLY	2.8
2	AR	257	GLY	2.8
2	BF	143	SER	2.8
2	BL	176	LEU	2.8
1	BY	78	PRO	2.8
2	AC	99	LEU	2.8
1	AZ	162	THR	2.8
2	AK	67	PHE	2.8
2	BG	167	THR	2.8
3	BS	227	ILE	2.8
2	BQ	63	GLY	2.8
2	AH	99	LEU	2.8
2	AK	97	VAL	2.8
2	BL	66	TYR	2.8
2	BQ	232	HIS	2.8
2	AQ	97	VAL	2.8
2	BK	99	LEU	2.8
2	BP	30	LEU	2.8
3	BV	142	LEU	2.8
3	AX	187	LEU	2.7
2	AC	264	LYS	2.7
2	AG	193	SER	2.7
2	AQ	237	PRO	2.7
1	B0	235	ILE	2.7
2	BD	99	LEU	2.7
2	BK	67	PHE	2.7
3	AV	269	TYR	2.7
3	AW	122	GLY	2.7
2	BC	185	LEU	2.7
2	AB	88	ILE	2.7
2	BQ	246	ALA	2.7
1	B0	87	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	AQ	216	ALA	2.7
2	BD	182	ASN	2.7
1	AY	339	ASP	2.7
2	BF	258	ASN	2.7
2	AR	231	PHE	2.7
2	BP	221	VAL	2.7
3	AS	204	TYR	2.7
3	BT	143	THR	2.7
2	AO	103	THR	2.7
2	AO	185	LEU	2.7
2	BQ	208	VAL	2.7
2	BI	258	ASN	2.7
2	BR	232	HIS	2.7
3	BT	248	THR	2.7
2	BQ	168	VAL	2.7
3	BU	90	LYS	2.7
1	B0	183	VAL	2.7
2	AP	26	LEU	2.7
2	BA	18	VAL	2.7
2	AQ	258	ASN	2.7
2	AG	30	LEU	2.7
2	AI	99	LEU	2.7
2	BC	218	GLN	2.7
2	BO	97	VAL	2.7
2	AG	214	PRO	2.7
1	B0	207	ASN	2.7
2	AD	62	ALA	2.7
3	BX	288	GLU	2.7
2	AM	86	ALA	2.6
2	AR	27	TYR	2.6
2	AB	27	TYR	2.6
2	AR	124	ASP	2.6
2	BB	27	TYR	2.6
2	AP	145	LEU	2.6
2	BK	62	ALA	2.6
2	BO	27	TYR	2.6
1	BZ	120	ASP	2.6
2	AI	34	ASP	2.6
2	AJ	220	LEU	2.6
2	BQ	99	LEU	2.6
2	AI	27	TYR	2.6
2	AM	30	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	AZ	228	VAL	2.6
2	AN	185	LEU	2.6
1	A0	87	LYS	2.6
1	AY	2	LEU	2.6
3	AS	213	GLY	2.6
3	AW	1	MET	2.6
2	AL	253	ILE	2.6
2	AO	258	ASN	2.6
2	AJ	81	VAL	2.6
3	BS	125	SER	2.6
2	AK	199	LYS	2.6
2	BL	259	GLY	2.6
2	BJ	262	PHE	2.6
2	BR	139	ILE	2.6
2	AM	99	LEU	2.6
1	BZ	271	VAL	2.6
2	AA	124	ASP	2.6
2	BC	262	PHE	2.6
1	B0	335	ASN	2.6
3	AX	118	TYR	2.6
2	AE	256	ARG	2.6
2	AL	259	GLY	2.6
3	AT	201	GLY	2.6
2	AG	255	THR	2.6
2	AF	176	LEU	2.6
2	AB	110	VAL	2.6
2	BL	253	ILE	2.6
2	AF	188	VAL	2.6
2	BN	153	MET	2.6
3	BV	294	LYS	2.6
2	AF	218	GLN	2.6
2	BG	185	LEU	2.6
3	AX	280	GLU	2.6
1	A0	148	TYR	2.6
2	AB	190	PHE	2.6
3	AS	250	GLN	2.6
3	AT	289	PHE	2.6
1	A0	328	GLU	2.6
2	BP	255	THR	2.6
2	BA	30	LEU	2.6
2	BL	203	MET	2.6
3	BS	114	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	AM	218	GLN	2.5
2	BQ	115	GLY	2.5
1	AY	19	ASP	2.5
2	BJ	3	ILE	2.5
2	AB	68	GLU	2.5
1	AZ	163	ILE	2.5
1	BY	332	LEU	2.5
2	BC	184	ASP	2.5
1	BZ	186	GLN	2.5
1	B0	9	ASN	2.5
2	AC	40	ARG	2.5
2	BK	63	GLY	2.5
3	BV	119	GLY	2.5
2	AC	211	PRO	2.5
2	BM	169	GLU	2.5
1	B0	138	ILE	2.5
1	BZ	137	LEU	2.5
2	BG	159	ILE	2.5
3	AX	90	LYS	2.5
2	BL	116	SER	2.5
2	AQ	218	GLN	2.5
2	BN	53	VAL	2.5
2	BP	39	ARG	2.5
2	BC	183	ASN	2.5
2	AP	260	SER	2.5
2	BO	31	THR	2.5
2	BG	105	ASN	2.5
2	BK	187	ILE	2.5
3	AV	142	LEU	2.5
3	AV	144	PHE	2.5
2	BI	167	THR	2.5
2	AP	225	ALA	2.5
1	BY	331	PRO	2.5
1	B0	136	TYR	2.5
2	BL	248	ILE	2.5
1	A0	357	THR	2.5
2	AC	185	LEU	2.5
2	BK	25	LYS	2.5
2	BR	77	LYS	2.5
2	AE	37	THR	2.5
1	AZ	199	ASP	2.5
1	BY	125	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	BP	191	PHE	2.5
2	AI	109	GLY	2.5
2	BF	175	GLN	2.5
1	A0	300	HIS	2.5
2	AJ	138	PRO	2.5
3	BW	298	VAL	2.5
2	BI	69	LEU	2.5
2	AP	253	ILE	2.4
2	BM	64	GLY	2.4
2	AM	220	LEU	2.4
2	AG	235	ILE	2.4
2	BQ	206	THR	2.4
3	AS	203	LEU	2.4
2	BC	261	TYR	2.4
3	AS	61	ILE	2.4
3	AX	290	LYS	2.4
2	BM	264	LYS	2.4
1	BZ	116	ILE	2.4
1	AY	160	LYS	2.4
2	BI	222	GLY	2.4
3	AS	214	VAL	2.4
2	BK	176	LEU	2.4
3	BX	1	MET	2.4
2	BE	146	ASP	2.4
2	BK	169	GLU	2.4
1	A0	69	VAL	2.4
1	AY	216	LYS	2.4
1	AY	65	VAL	2.4
2	BG	23	ASP	2.4
2	AD	63	GLY	2.4
3	BX	287	ALA	2.4
2	BP	60	ILE	2.4
1	BZ	138	ILE	2.4
2	AF	99	LEU	2.4
2	AF	253	ILE	2.4
2	AM	31	THR	2.4
2	BI	261	TYR	2.4
3	AS	238	ILE	2.4
3	AS	281	LEU	2.4
2	AO	3	ILE	2.4
3	BS	250	GLN	2.4
3	BU	55	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	BP	225	ALA	2.4
3	BW	68	PHE	2.4
2	AP	97	VAL	2.4
2	AI	30	LEU	2.4
3	AT	3	ARG	2.4
3	AW	280	GLU	2.4
2	AN	188	VAL	2.4
2	BK	258	ASN	2.4
2	AR	190	PHE	2.4
2	BA	76	LEU	2.4
2	BH	26	LEU	2.4
1	A0	36	LYS	2.4
2	AC	123	PHE	2.4
3	AS	156	MET	2.4
3	AV	240	ILE	2.4
3	BW	288	GLU	2.4
2	AJ	137	LYS	2.3
1	AY	366	VAL	2.3
2	AL	217	VAL	2.3
2	AB	176	LEU	2.3
2	AD	61	ILE	2.3
2	BR	198	GLN	2.3
3	AS	249	TYR	2.3
1	AZ	316	SER	2.3
2	BL	48	ASN	2.3
2	AK	220	LEU	2.3
3	BX	82	PHE	2.3
2	AC	30	LEU	2.3
2	AC	212	PHE	2.3
2	AM	262	PHE	2.3
2	BH	27	TYR	2.3
3	AV	202	ILE	2.3
2	AL	251	THR	2.3
2	AD	30	LEU	2.3
2	AR	69	LEU	2.3
2	BC	254	ALA	2.3
1	A0	147	SER	2.3
2	AG	260	SER	2.3
3	AS	31	PRO	2.3
3	BT	157	SER	2.3
1	B0	356	LYS	2.3
2	AP	220	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	BH	30	LEU	2.3
2	AQ	37	THR	2.3
3	AX	297	PHE	2.3
3	BV	289	PHE	2.3
1	A0	320	THR	2.3
1	BZ	318	ILE	2.3
2	AC	263	ILE	2.3
2	BE	62	ALA	2.3
3	BS	287	ALA	2.3
3	AW	107	LEU	2.3
2	AK	60	ILE	2.3
2	BG	103	THR	2.3
2	BM	251	THR	2.3
2	BP	27	TYR	2.3
3	AX	141	ASN	2.3
3	BV	30	GLN	2.3
2	AO	161	VAL	2.3
2	BM	173	GLY	2.3
3	AV	249	TYR	2.3
1	B0	185	PHE	2.3
2	BA	231	PHE	2.3
1	AZ	229	THR	2.3
2	BD	123	PHE	2.3
1	AZ	167	ALA	2.3
2	BG	67	PHE	2.3
1	A0	167	ALA	2.3
3	BV	158	LYS	2.3
2	AL	27	TYR	2.3
3	BT	152	VAL	2.3
2	AP	90	LEU	2.3
2	AB	97	VAL	2.3
2	AL	181	LYS	2.3
2	BO	74	VAL	2.3
2	BL	190	PHE	2.3
1	B0	137	LEU	2.3
1	BZ	119	LEU	2.3
2	BD	3	ILE	2.3
3	AW	34	LEU	2.3
1	AY	215	ARG	2.2
2	AC	3	ILE	2.2
2	AH	204	SER	2.2
2	BD	179	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	BT	142	LEU	2.2
2	AD	101	ALA	2.2
2	AI	221	VAL	2.2
1	AZ	14	TYR	2.2
2	BA	131	THR	2.2
2	BL	46	PRO	2.2
2	BN	184	ASP	2.2
1	AZ	202	ASN	2.2
2	AO	162	PRO	2.2
2	BL	249	ASP	2.2
1	AZ	300	HIS	2.2
2	AL	159	ILE	2.2
2	BJ	60	ILE	2.2
1	BY	359	PHE	2.2
2	BR	2	THR	2.2
3	AV	59	PRO	2.2
1	BZ	141	ASN	2.2
1	AZ	369	GLY	2.2
2	AB	188	VAL	2.2
2	AE	62	ALA	2.2
2	BN	208	VAL	2.2
1	AY	328	GLU	2.2
1	BZ	247	PHE	2.2
3	BU	200	MET	2.2
2	BG	219	SER	2.2
2	BD	126	VAL	2.2
2	BR	82	ASN	2.2
2	AM	219	SER	2.2
1	B0	178	ARG	2.2
2	BK	29	MET	2.2
2	AO	257	GLY	2.2
2	BR	185	LEU	2.2
1	BZ	246	VAL	2.2
3	AS	286	LYS	2.2
1	AY	214	ASN	2.2
1	AZ	304	PRO	2.2
2	AG	222	GLY	2.2
2	BJ	30	LEU	2.2
1	AZ	8	ASP	2.2
1	AZ	142	LYS	2.2
2	AQ	209	ASP	2.2
2	AR	26	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	AY	259	PRO	2.2
2	AP	192	GLY	2.2
2	BF	214	PRO	2.2
2	AF	139	ILE	2.2
2	AJ	223	HIS	2.2
2	BL	3	ILE	2.2
2	BN	18	VAL	2.2
2	BP	88	ILE	2.2
3	BX	214	VAL	2.2
1	AY	161	ALA	2.2
2	AG	176	LEU	2.2
2	BR	123	PHE	2.2
3	AX	289	PHE	2.2
2	AO	188	VAL	2.2
2	AP	169	GLU	2.2
2	BN	205	GLY	2.2
2	AF	216	ALA	2.2
2	AN	64	GLY	2.1
2	BE	159	ILE	2.1
1	A0	166	LYS	2.1
2	AI	67	PHE	2.1
2	BP	169	GLU	2.1
1	BY	137	LEU	2.1
2	BN	78	GLY	2.1
2	BN	27	TYR	2.1
2	AG	144	THR	2.1
2	AQ	2	THR	2.1
2	BN	23	ASP	2.1
3	AX	2	VAL	2.1
2	AH	261	TYR	2.1
2	BC	199	LYS	2.1
2	BF	168	VAL	2.1
2	AR	74	VAL	2.1
3	BW	25	LYS	2.1
2	AH	215	ALA	2.1
1	A0	367	GLU	2.1
2	AM	64	GLY	2.1
2	BQ	131	THR	2.1
2	BF	185	LEU	2.1
2	BC	187	ILE	2.1
2	BP	99	LEU	2.1
2	BK	23	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	AQ	235	ILE	2.1
2	BE	27	TYR	2.1
3	AT	279	MET	2.1
3	BX	297	PHE	2.1
2	BH	249	ASP	2.1
2	AK	61	ILE	2.1
2	BH	23	ASP	2.1
2	BI	3	ILE	2.1
2	BM	69	LEU	2.1
3	BV	272	ARG	2.1
1	AY	336	ASP	2.1
3	BS	199	PHE	2.1
1	B0	188	THR	2.1
2	BR	70	LEU	2.1
2	AR	260	SER	2.1
3	AW	212	ALA	2.1
3	BS	228	VAL	2.1
2	AB	116	SER	2.1
3	BS	61	ILE	2.1
1	B0	295	TYR	2.1
1	BZ	79	ILE	2.1
3	BV	250	GLN	2.1
2	AI	222	GLY	2.1
2	AA	235	ILE	2.1
2	BP	210	ARG	2.1
1	BZ	352	ALA	2.1
2	AB	99	LEU	2.1
2	AQ	230	SER	2.1
2	BB	185	LEU	2.1
2	BK	181	LYS	2.1
1	BZ	206	ILE	2.1
3	BV	200	MET	2.1
2	AL	252	PRO	2.1
2	BJ	211	PRO	2.1
2	AB	62	ALA	2.1
1	A0	165	ARG	2.0
1	AY	286	ASP	2.0
2	AK	79	ASP	2.0
3	BT	296	ASP	2.0
3	BV	31	PRO	2.0
3	BW	120	LYS	2.0
2	AI	233	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	BZ	125	ILE	2.0
2	AD	257	GLY	2.0
2	BG	64	GLY	2.0
3	AU	227	ILE	2.0
1	AZ	214	ASN	2.0
1	B0	221	ARG	2.0
2	AB	221	VAL	2.0
2	BQ	176	LEU	2.0
2	AE	38	ILE	2.0
2	BR	125	ILE	2.0
2	AI	33	MET	2.0
2	AR	33	MET	2.0
2	BH	68	GLU	2.0
3	BT	298	VAL	2.0
2	AN	179	THR	2.0
1	BZ	10	PHE	2.0
3	BT	238	ILE	2.0
2	AB	255	THR	2.0
2	AJ	42	ASP	2.0
2	BF	65	ARG	2.0
2	BR	26	LEU	2.0
2	BR	71	ASN	2.0
1	BY	235	ILE	2.0
2	BP	123	PHE	2.0
1	BZ	245	VAL	2.0
3	AS	62	GLU	2.0
1	AZ	225	LYS	2.0
2	AA	136	THR	2.0
2	AI	131	THR	2.0
2	AJ	30	LEU	2.0
2	AP	175	GLN	2.0
3	BX	227	ILE	2.0
3	AW	118	TYR	2.0
2	AM	222	GLY	2.0
2	BO	261	TYR	2.0
2	BQ	209	ASP	2.0
2	BG	18	VAL	2.0
3	BU	178	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	BX	301	1/1	0.79	0.26	287,287,287,287	0
4	CA	AW	301	1/1	0.80	0.29	266,266,266,266	0
4	CA	BS	301	1/1	0.80	0.34	267,267,267,267	0
4	CA	BV	301	1/1	0.80	0.26	272,272,272,272	0
4	CA	BW	301	1/1	0.81	0.26	268,268,268,268	0
4	CA	AS	301	1/1	0.82	0.33	281,281,281,281	0
4	CA	BU	301	1/1	0.83	0.32	269,269,269,269	0
4	CA	BT	301	1/1	0.85	0.35	279,279,279,279	0
4	CA	AU	301	1/1	0.88	0.35	275,275,275,275	0
4	CA	AV	301	1/1	0.89	0.36	276,276,276,276	0
4	CA	AX	301	1/1	0.92	0.29	275,275,275,275	0
4	CA	AT	301	1/1	0.94	0.25	275,275,275,275	0

6.5 Other polymers (i)

There are no such residues in this entry.