



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:51 PM UTC

PDB ID : 4V5I / pdb_00004v5i
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

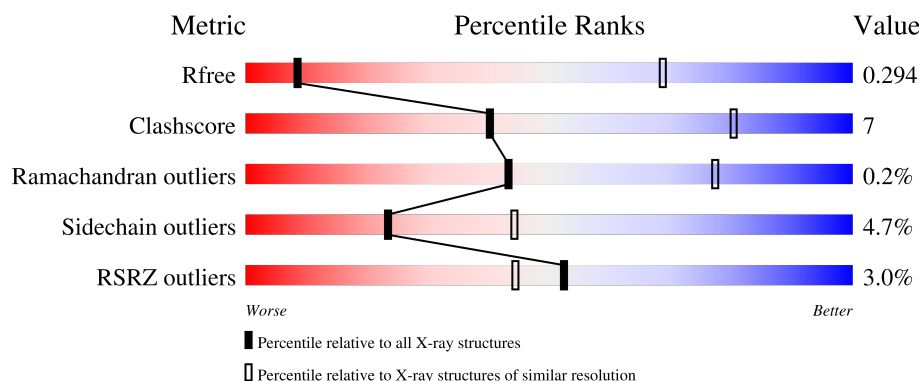
1 Overall quality at a glance

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}	180053	1066 (6.92-4.00)
Clashscore	190562	1123 (6.92-4.00)
Ramachandran outliers	187476	1026 (6.92-3.96)
Sidechain outliers	187428	1000 (6.92-3.96)
RSRZ outliers	180081	1059 (6.92-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 83% 15% .
1	AY	372	3% 84% 14% ..
1	AZ	372	5% 80% 18% .
1	B0	372	2% 84% 14% .
1	BY	372	2% 84% 14% ..

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Mol	Chain	Length	Quality of chain
1	BZ	372	
2	AA	263	
2	AB	263	
2	AC	263	
2	AD	263	
2	AE	263	
2	AF	263	
2	AG	263	
2	AH	263	
2	AI	263	
2	AJ	263	
2	AK	263	
2	AL	263	
2	AM	263	
2	AN	263	
2	AO	263	
2	AP	263	
2	AQ	263	
2	AR	263	
2	BA	263	
2	BB	263	
2	BC	263	
2	BD	263	
2	BE	263	
2	BF	263	

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Mol	Chain	Length	Quality of chain
2	BG	263	
2	BH	263	
2	BI	263	
2	BJ	263	
2	BK	263	
2	BL	263	
2	BM	263	
2	BN	263	
2	BO	263	
2	BP	263	
2	BQ	263	
2	BR	263	
3	AS	298	
3	AT	298	
3	AU	298	
3	AV	298	
3	AW	298	
3	AX	298	
3	BS	298	
3	BT	298	
3	BU	298	
3	BV	298	
3	BW	298	
3	BX	298	

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

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

- Molecule 3 is a protein called ORF15.

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

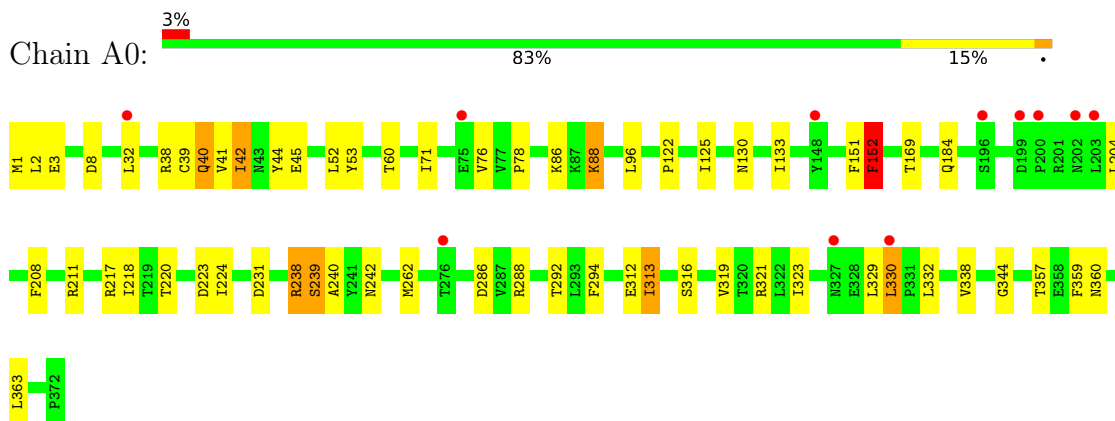
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

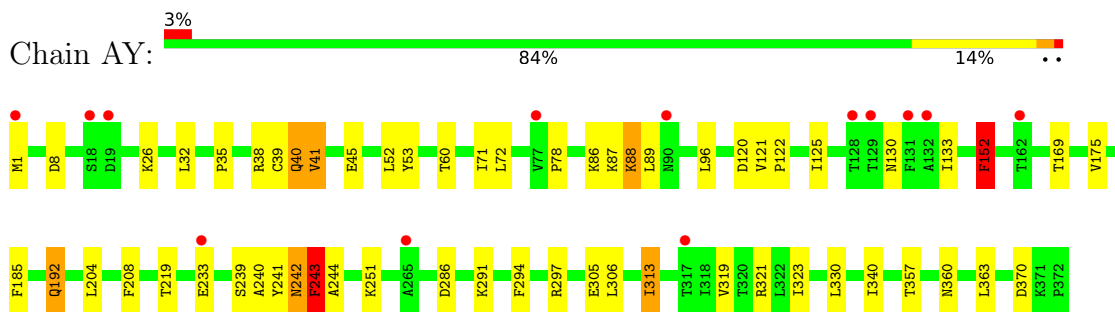
3 Residue-property plots [i](#)

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

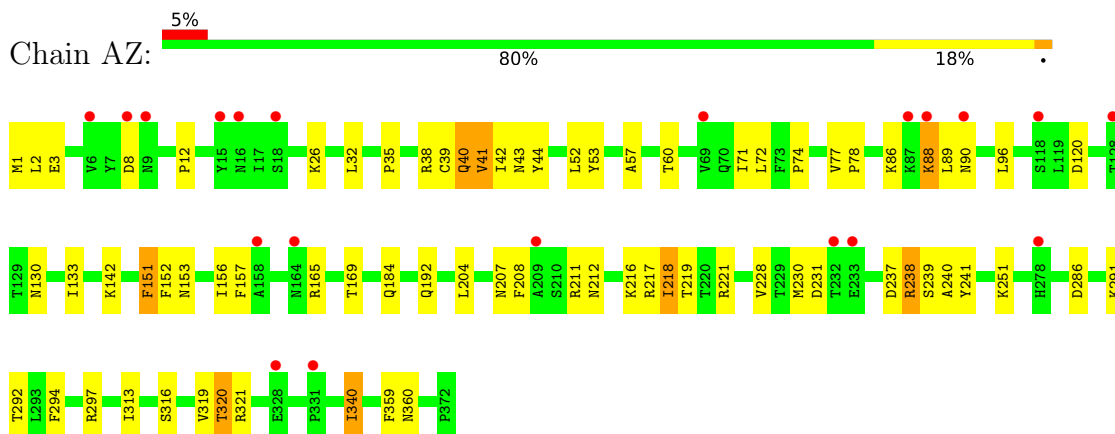
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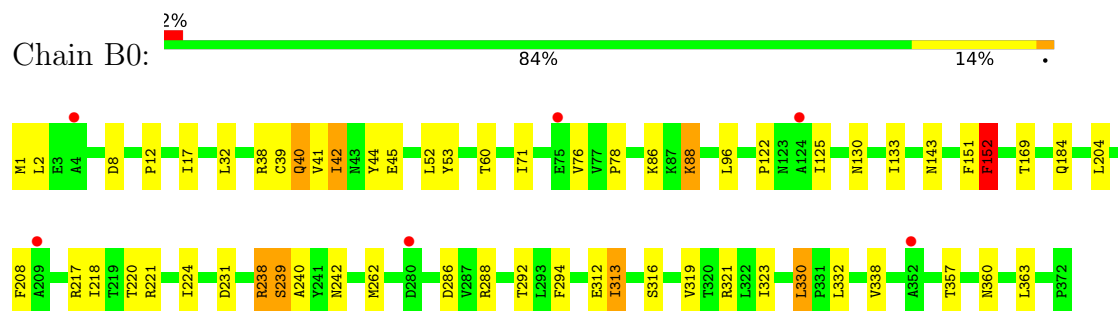
- Molecule 1: ORF16



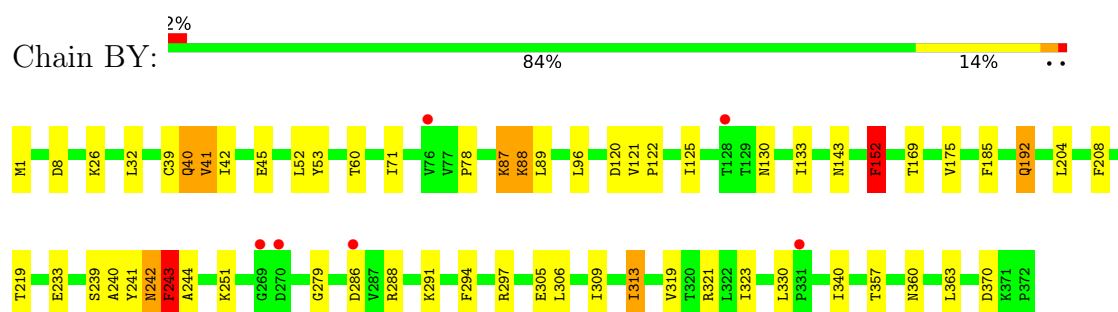
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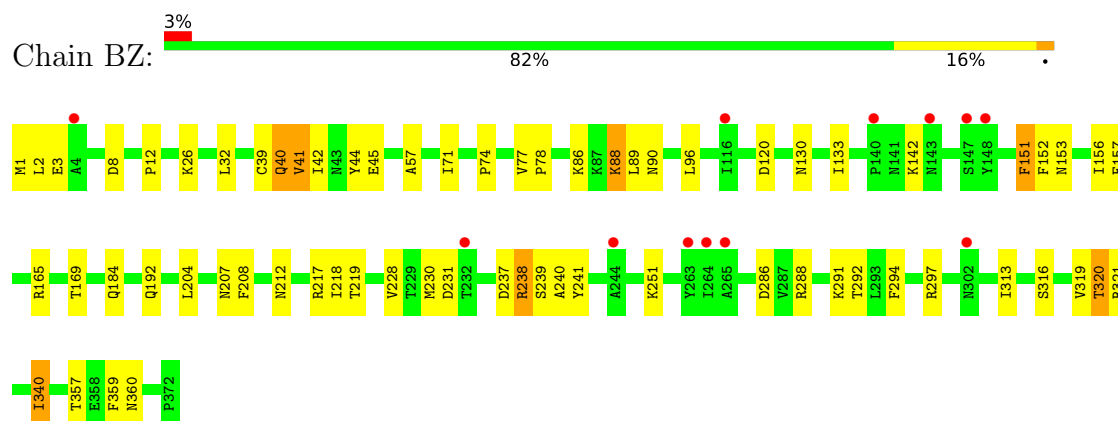
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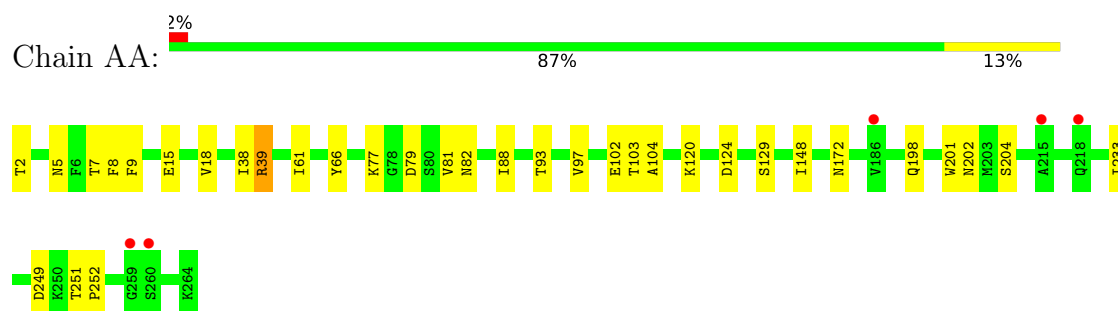
- Molecule 1: ORF16



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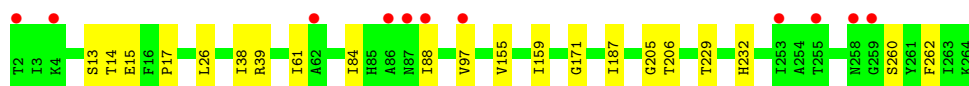


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

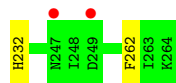
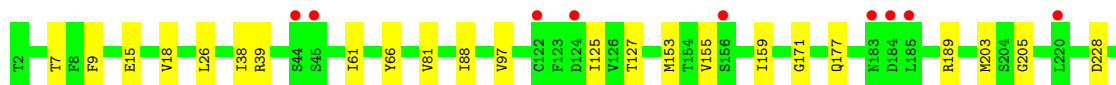


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN





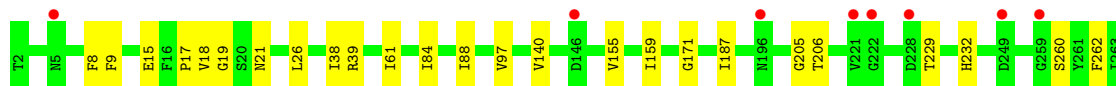
● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



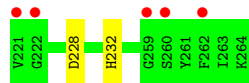
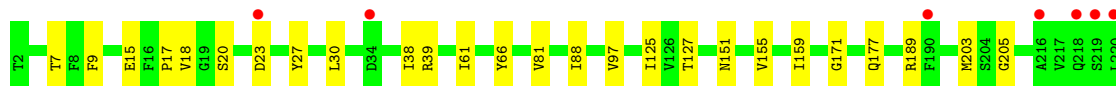
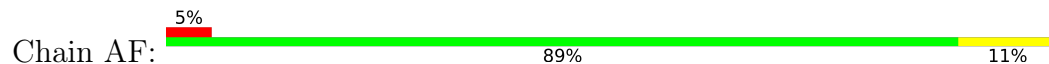
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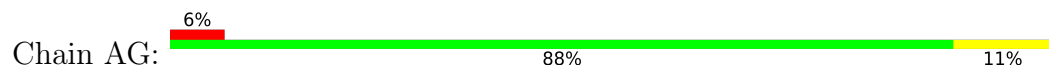
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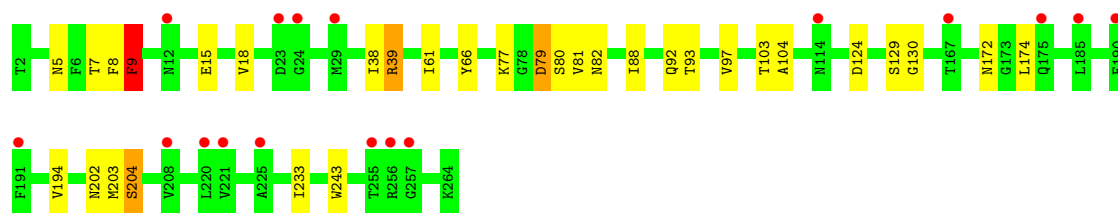


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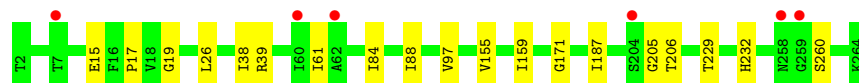


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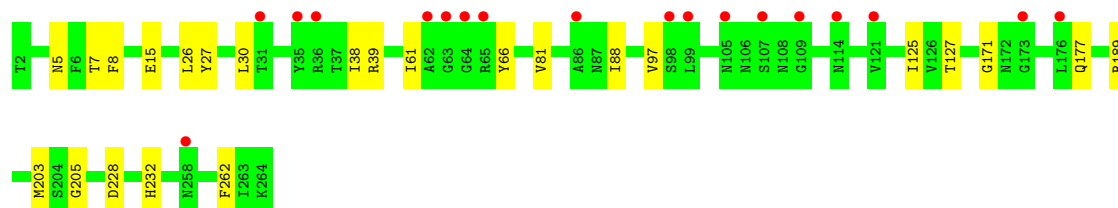




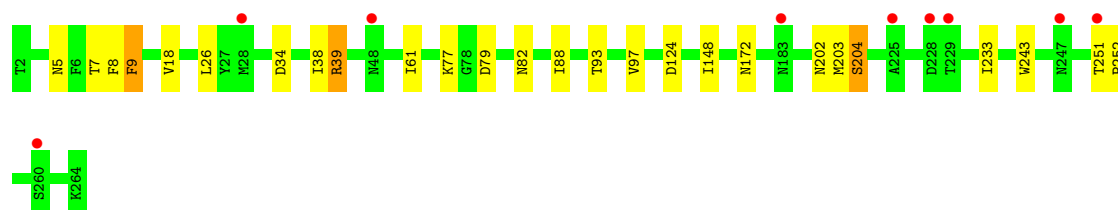
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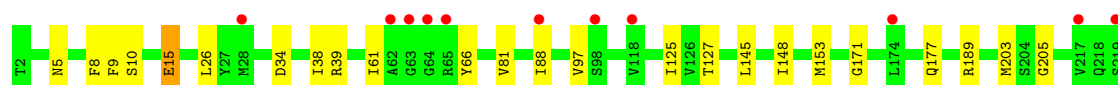
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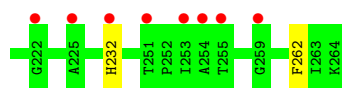


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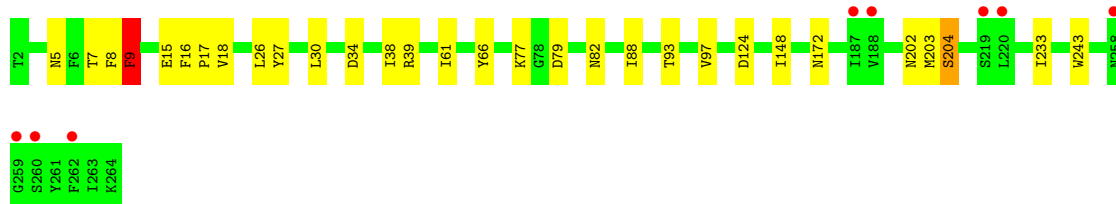
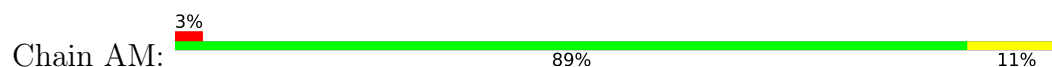


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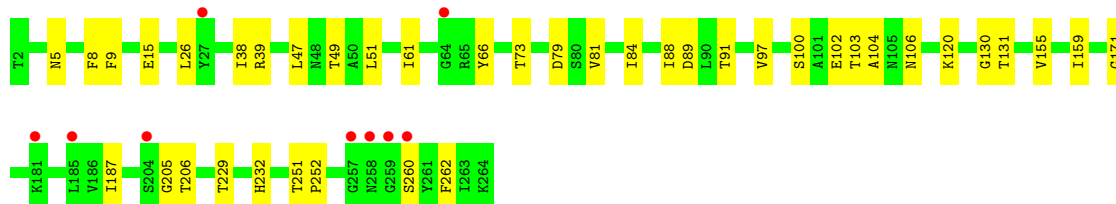
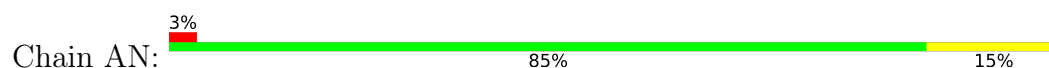




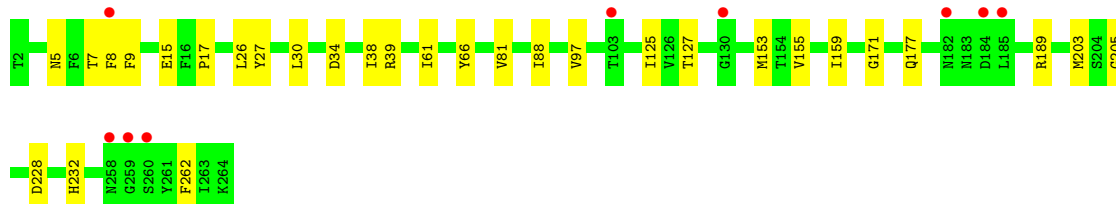
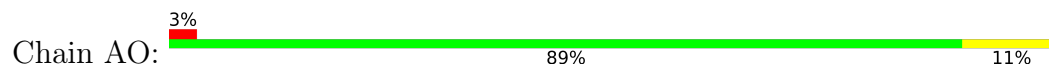
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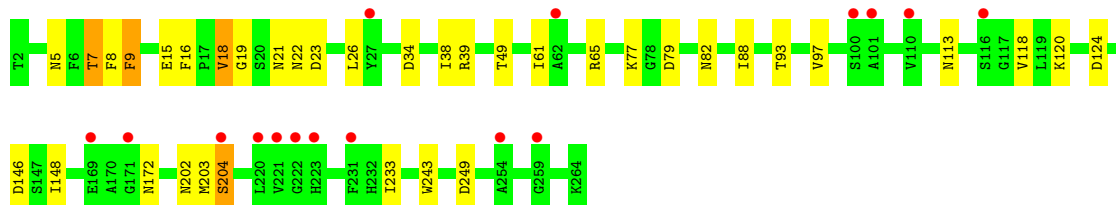
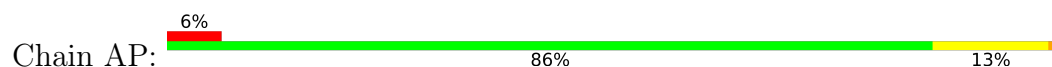
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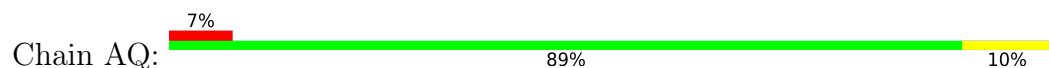
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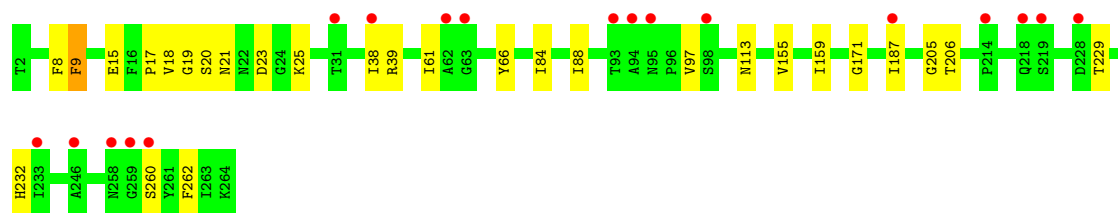


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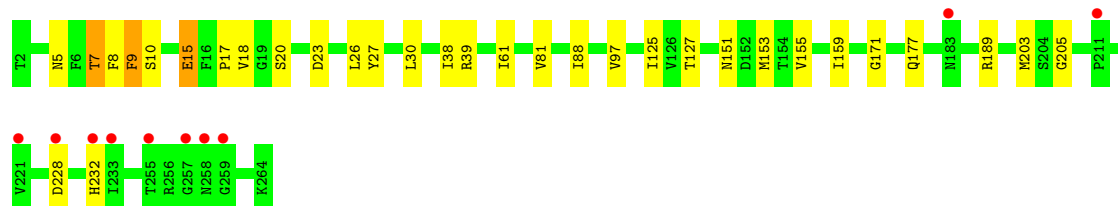


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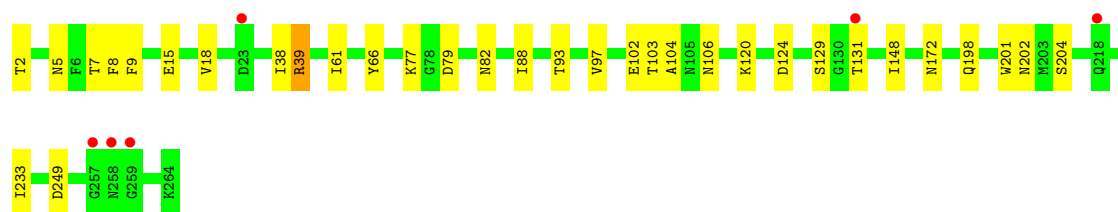
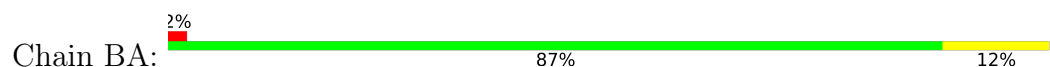




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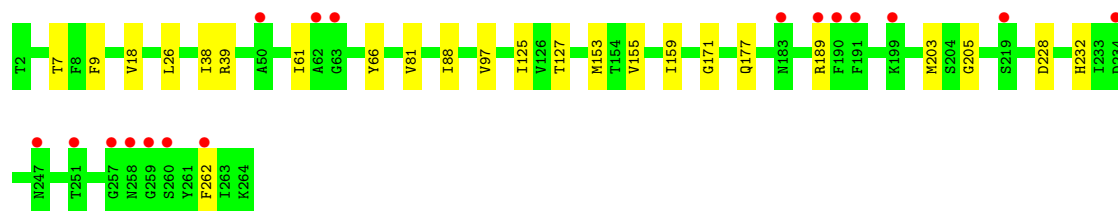
● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



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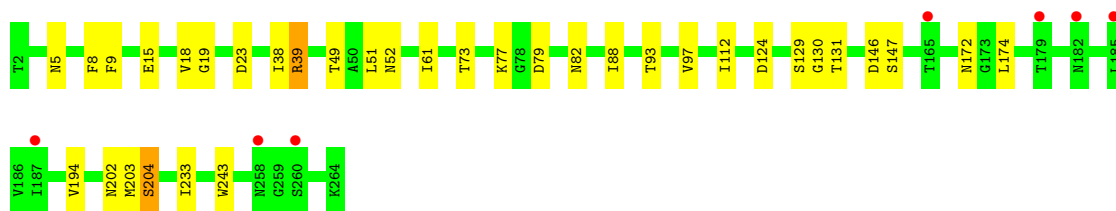


● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



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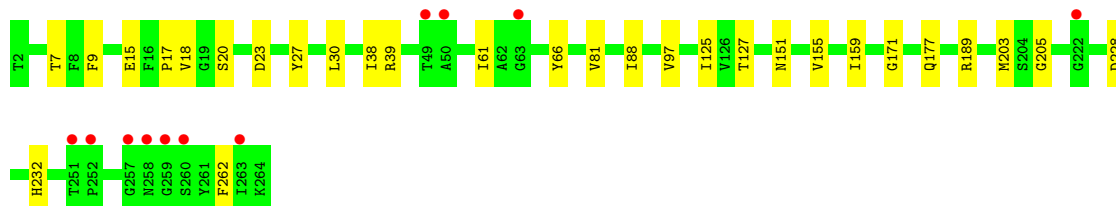
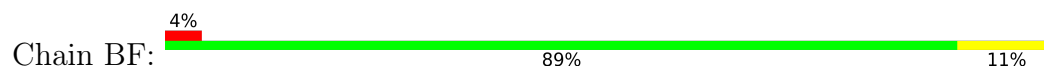




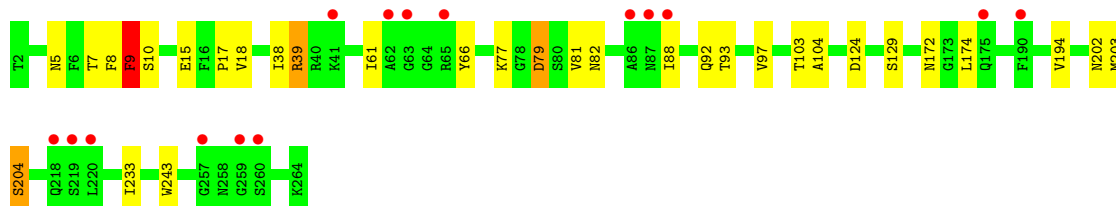
● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



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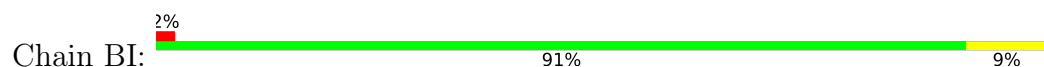
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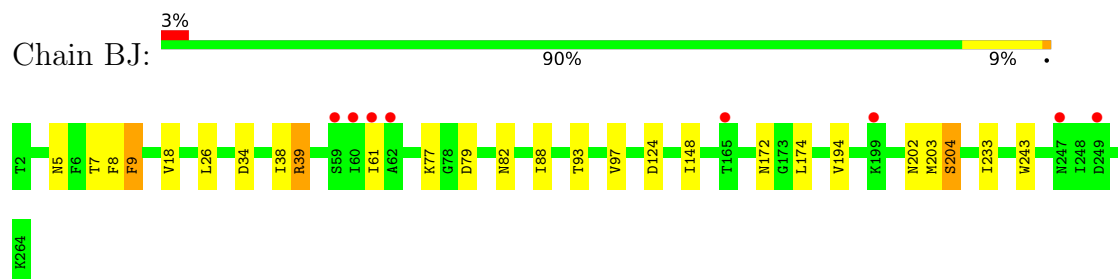
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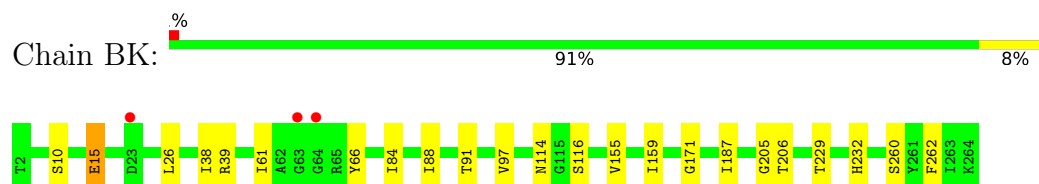
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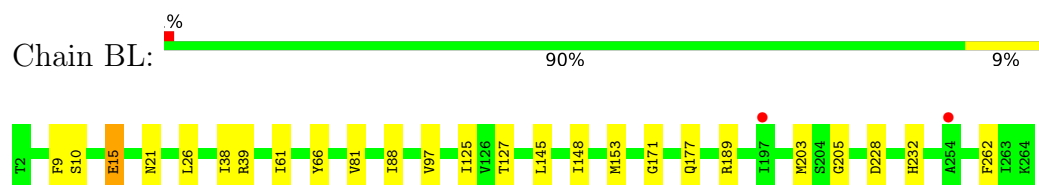
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



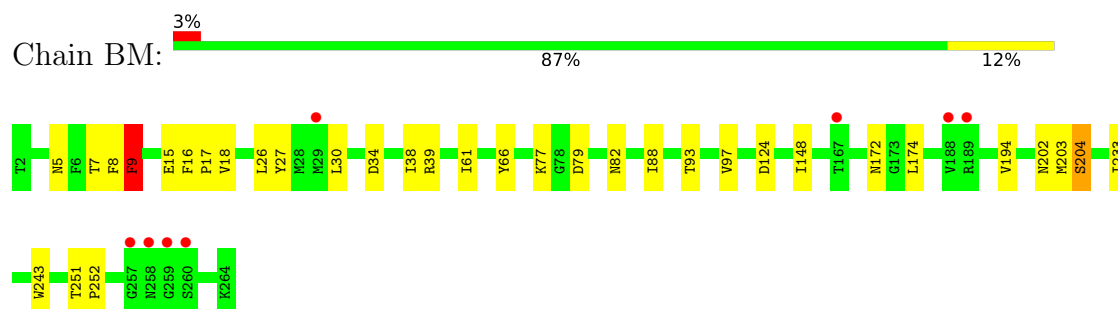
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



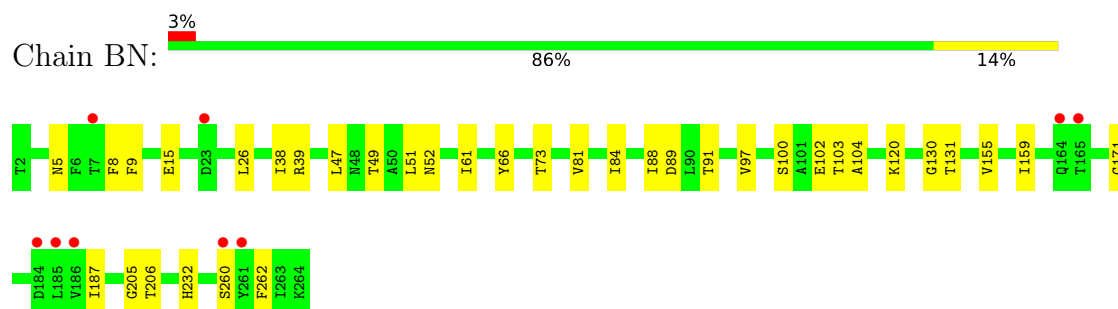
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



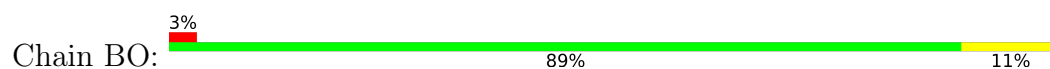
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

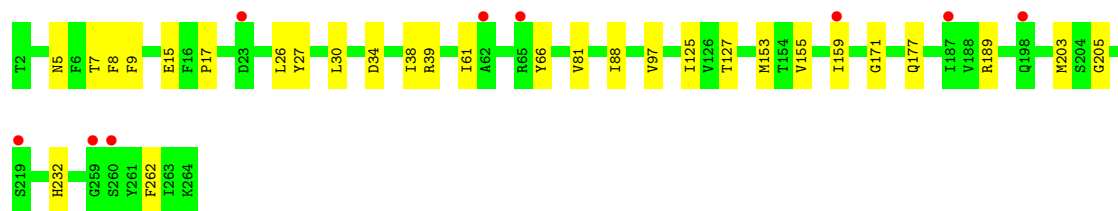


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

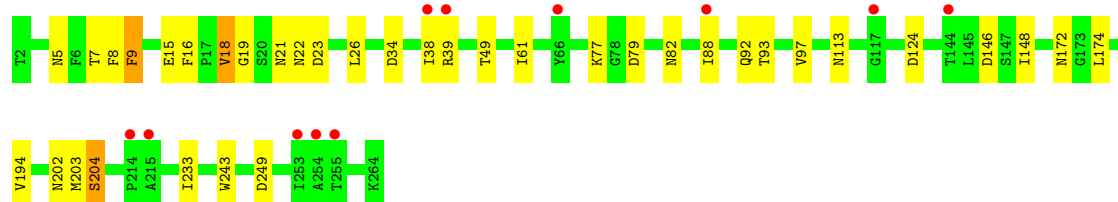
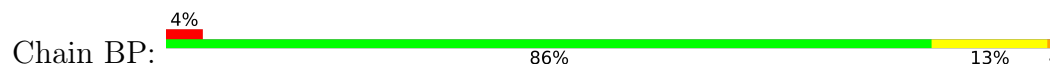


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

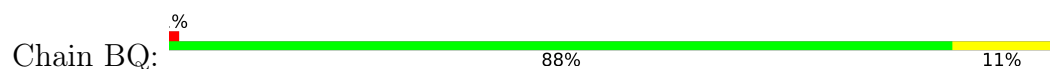




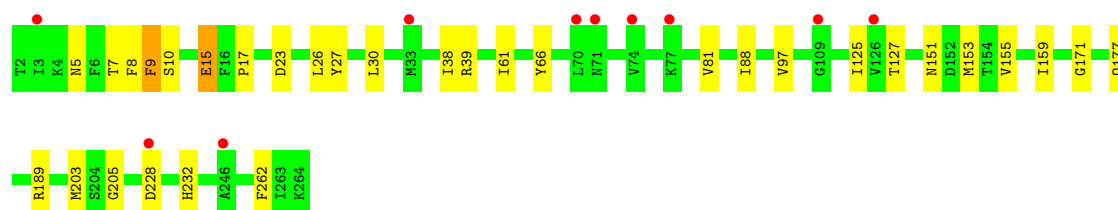
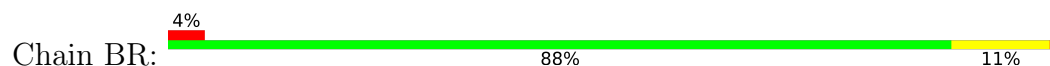
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



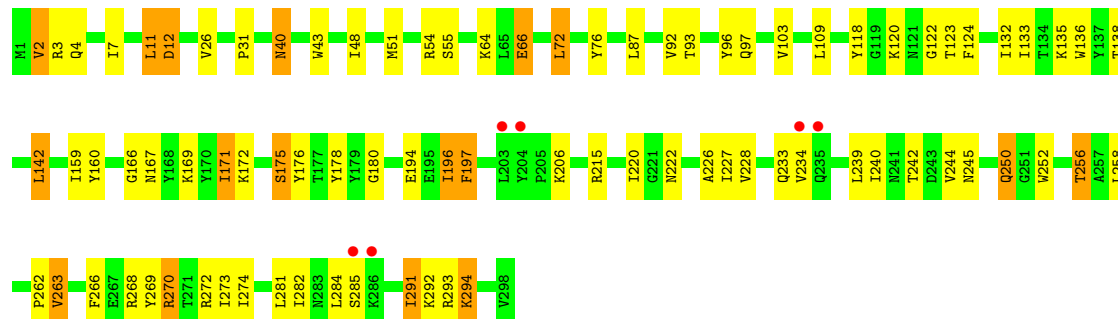
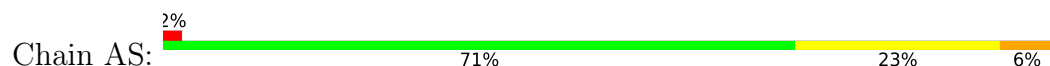
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



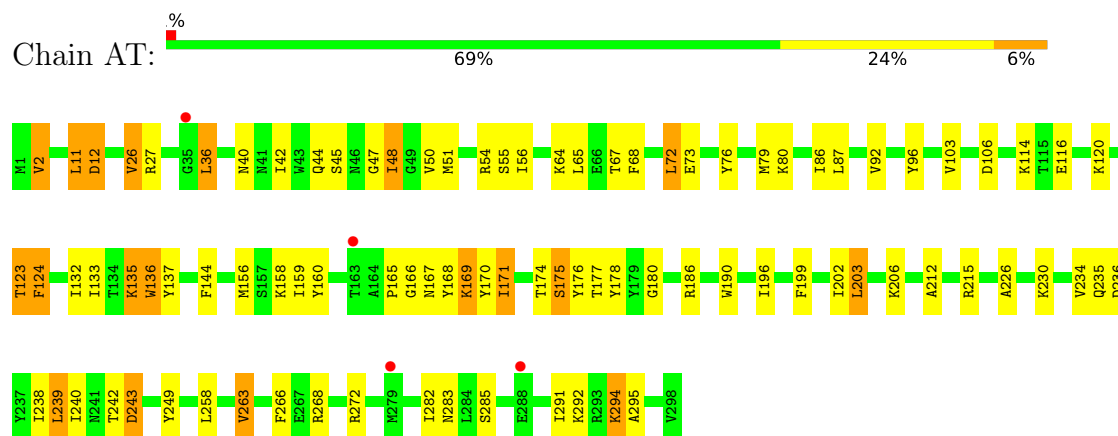
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



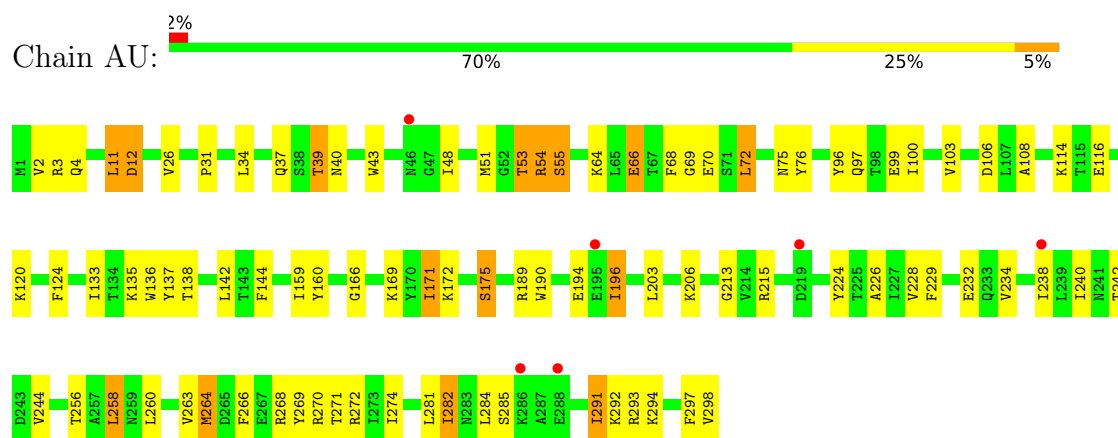
• Molecule 3: ORF15



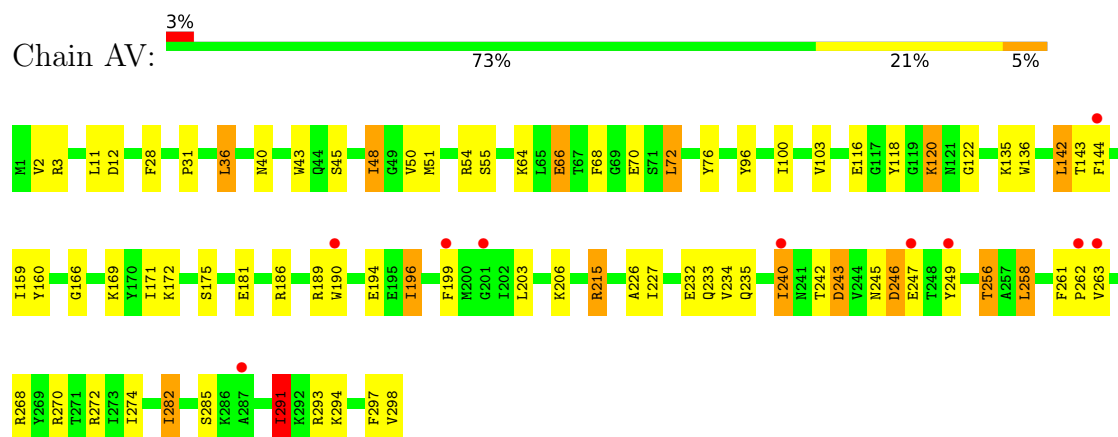
- Molecule 3: ORF15



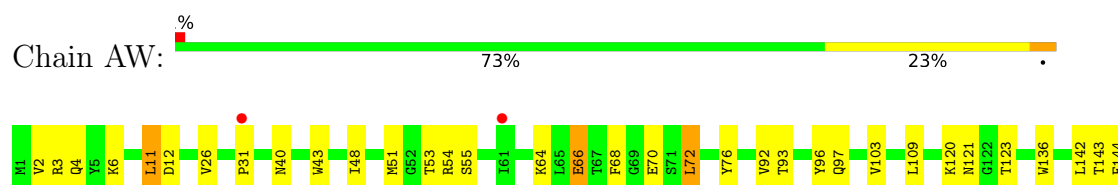
- Molecule 3: ORF15

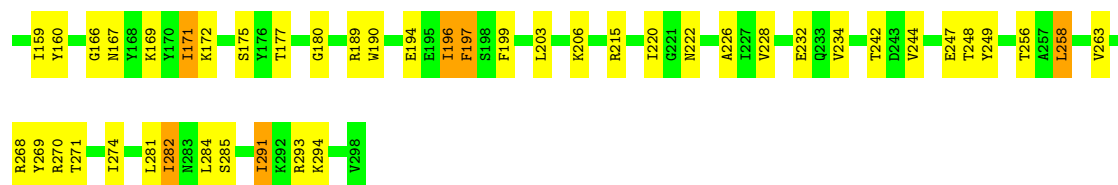


- Molecule 3: ORF15

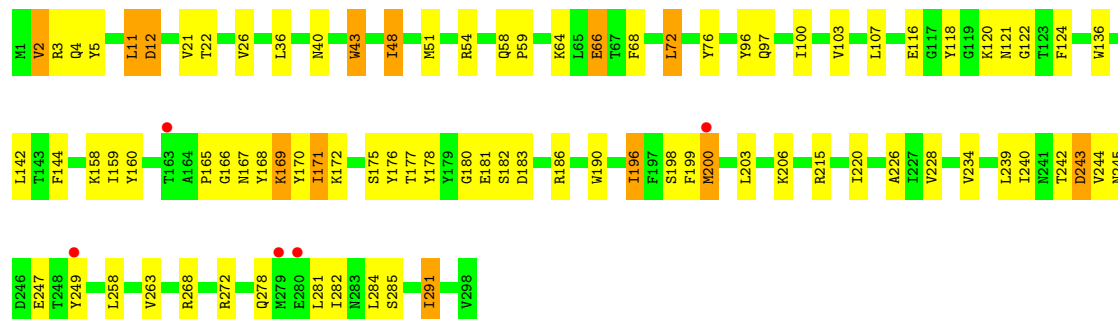
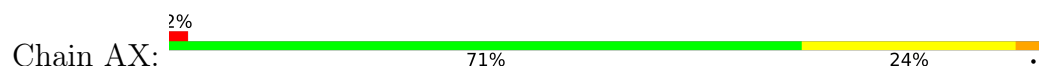


- Molecule 3: ORF15

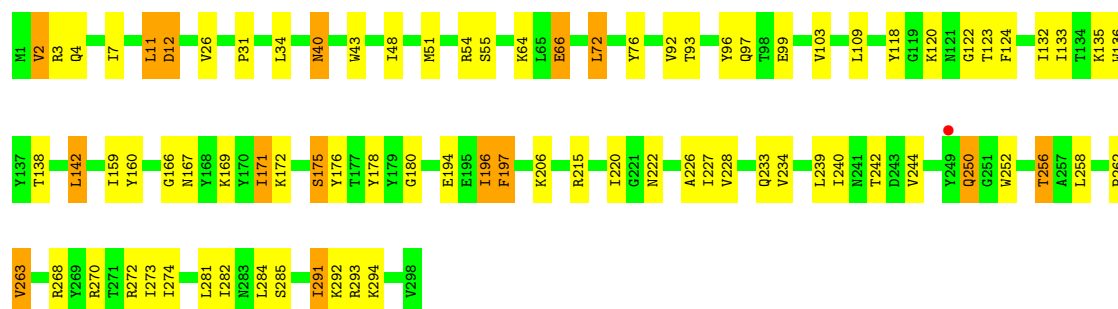




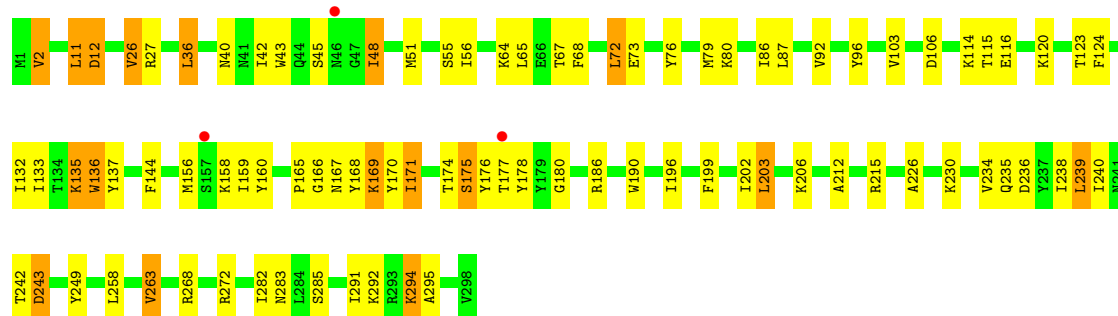
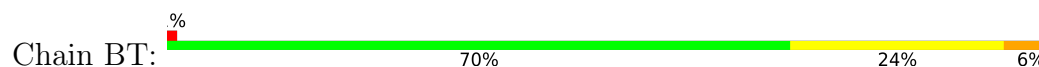
• Molecule 3: ORF15



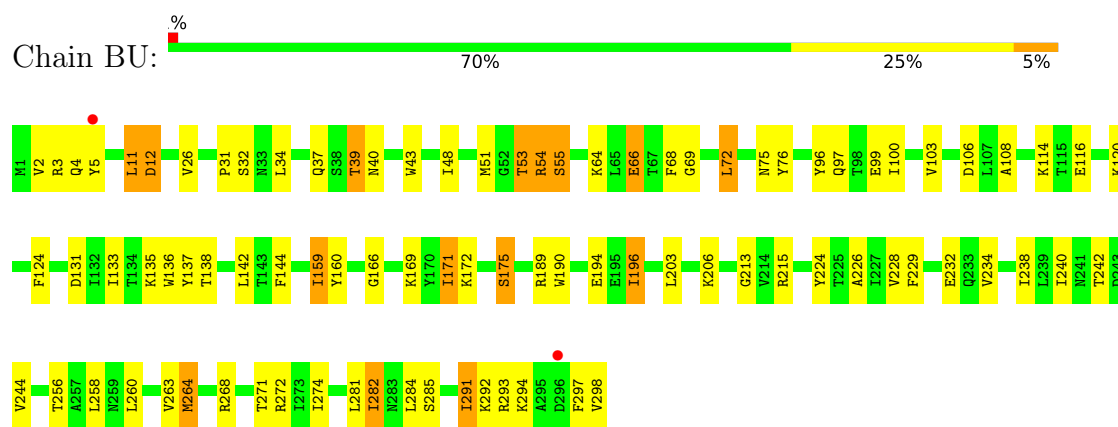
• Molecule 3: ORF15



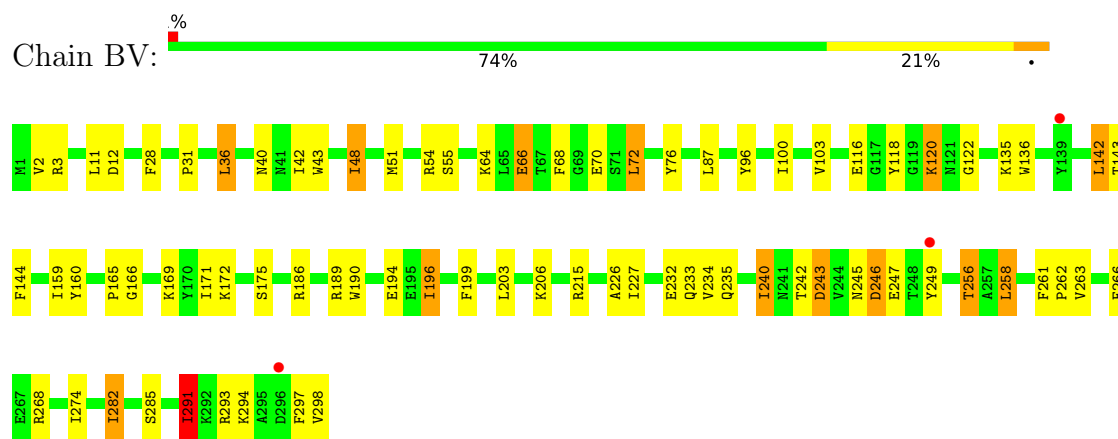
• Molecule 3: ORF15



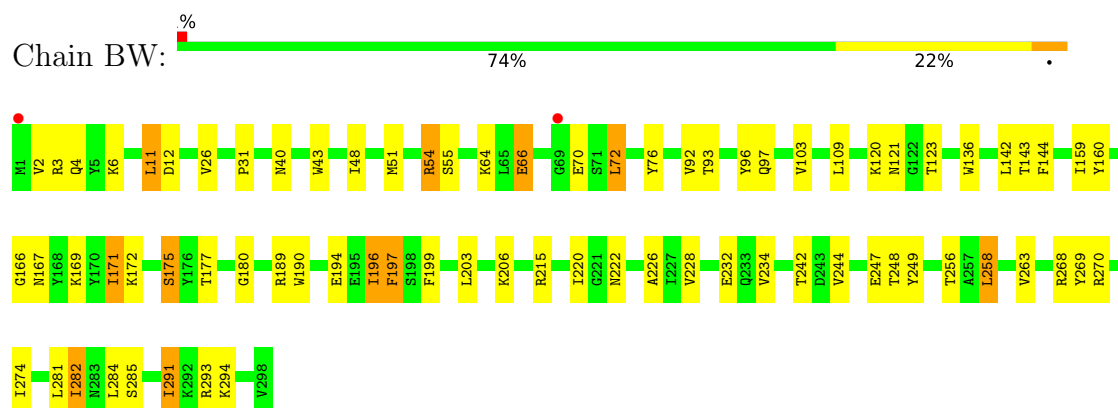
• Molecule 3: ORF15



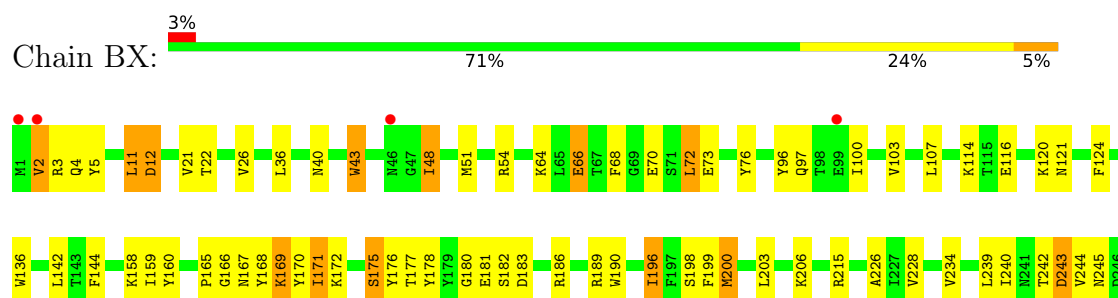
• Molecule 3: ORF15



• Molecule 3: ORF15



• Molecule 3: ORF15





4 Data and refinement statistics

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) 91.0 (44.56-5.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 5.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.291 , 0.297 0.292 , 0.294	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)	0.26 , 547.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.72	0/3069	1.26	5/4175 (0.1%)
1	AY	0.72	0/3069	1.26	12/4175 (0.3%)
1	AZ	0.71	0/3069	1.23	7/4175 (0.2%)
1	B0	0.72	0/3069	1.26	5/4175 (0.1%)
1	BY	0.72	0/3069	1.26	14/4175 (0.3%)
1	BZ	0.71	0/3069	1.23	7/4175 (0.2%)
2	AA	0.58	0/2048	1.07	4/2791 (0.1%)
2	AB	0.69	0/2048	1.14	2/2791 (0.1%)
2	AC	0.70	0/2048	1.16	4/2791 (0.1%)
2	AD	0.57	0/2048	1.05	4/2791 (0.1%)
2	AE	0.71	0/2048	1.15	2/2791 (0.1%)
2	AF	0.72	0/2048	1.16	3/2791 (0.1%)
2	AG	0.58	0/2048	1.05	5/2791 (0.2%)
2	AH	0.71	0/2048	1.14	1/2791 (0.0%)
2	AI	0.72	0/2048	1.16	4/2791 (0.1%)
2	AJ	0.61	0/2048	1.10	4/2791 (0.1%)
2	AK	0.69	0/2048	1.15	2/2791 (0.1%)
2	AL	0.71	0/2048	1.16	6/2791 (0.2%)
2	AM	0.62	0/2048	1.11	4/2791 (0.1%)
2	AN	0.70	0/2048	1.15	3/2791 (0.1%)
2	AO	0.71	0/2048	1.16	6/2791 (0.2%)
2	AP	0.62	0/2048	1.11	5/2791 (0.2%)
2	AQ	0.71	0/2048	1.14	3/2791 (0.1%)
2	AR	0.73	0/2048	1.16	4/2791 (0.1%)
2	BA	0.58	0/2048	1.07	4/2791 (0.1%)
2	BB	0.69	0/2048	1.14	2/2791 (0.1%)
2	BC	0.70	0/2048	1.16	3/2791 (0.1%)
2	BD	0.57	0/2048	1.05	4/2791 (0.1%)
2	BE	0.71	0/2048	1.15	1/2791 (0.0%)
2	BF	0.72	0/2048	1.16	4/2791 (0.1%)
2	BG	0.58	0/2048	1.05	5/2791 (0.2%)
2	BH	0.71	0/2048	1.14	2/2791 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BI	0.72	0/2048	1.16	4/2791 (0.1%)
2	BJ	0.62	0/2048	1.10	4/2791 (0.1%)
2	BK	0.69	0/2048	1.15	2/2791 (0.1%)
2	BL	0.71	0/2048	1.16	5/2791 (0.2%)
2	BM	0.62	0/2048	1.11	4/2791 (0.1%)
2	BN	0.70	0/2048	1.15	3/2791 (0.1%)
2	BO	0.71	0/2048	1.16	6/2791 (0.2%)
2	BP	0.62	0/2048	1.11	5/2791 (0.2%)
2	BQ	0.71	0/2048	1.14	3/2791 (0.1%)
2	BR	0.73	0/2048	1.16	5/2791 (0.2%)
3	AS	0.62	0/2485	1.17	7/3356 (0.2%)
3	AT	0.63	0/2485	1.20	8/3356 (0.2%)
3	AU	0.63	0/2485	1.17	5/3356 (0.1%)
3	AV	0.65	0/2485	1.17	3/3356 (0.1%)
3	AW	0.63	0/2485	1.16	2/3356 (0.1%)
3	AX	0.65	1/2485 (0.0%)	1.18	6/3356 (0.2%)
3	BS	0.62	0/2485	1.17	7/3356 (0.2%)
3	BT	0.63	0/2485	1.20	8/3356 (0.2%)
3	BU	0.63	0/2485	1.17	5/3356 (0.1%)
3	BV	0.65	0/2485	1.17	3/3356 (0.1%)
3	BW	0.63	0/2485	1.16	2/3356 (0.1%)
3	BX	0.65	1/2485 (0.0%)	1.18	6/3356 (0.2%)
All	All	0.67	2/121962 (0.0%)	1.16	244/165798 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AX	22	THR	CA-C	6.82	1.61	1.53
3	BX	22	THR	CA-C	6.77	1.61	1.53

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AY	152	PHE	CA-CB-CG	11.97	125.77	113.80
1	BY	152	PHE	CA-CB-CG	11.97	125.77	113.80
1	B0	152	PHE	CA-CB-CG	11.56	125.36	113.80
1	A0	152	PHE	CA-CB-CG	11.53	125.33	113.80
2	BK	15	GLU	N-CA-C	7.50	119.14	110.97
2	AK	15	GLU	N-CA-C	7.47	119.12	110.97
3	BW	12	ASP	CA-CB-CG	7.46	120.06	112.60
3	AW	12	ASP	CA-CB-CG	7.41	120.01	112.60
1	B0	240	ALA	N-CA-C	6.96	121.94	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A0	240	ALA	N-CA-C	6.91	121.88	113.17
3	BU	124	PHE	CA-CB-CG	6.81	120.61	113.80
3	AU	124	PHE	CA-CB-CG	6.81	120.61	113.80
3	AT	294	LYS	N-CA-C	6.71	118.66	110.41
3	BT	294	LYS	N-CA-C	6.70	118.65	110.41
3	AX	12	ASP	CA-CB-CG	6.59	119.19	112.60
3	BX	12	ASP	CA-CB-CG	6.57	119.17	112.60
3	AV	12	ASP	CA-CB-CG	6.56	119.16	112.60
3	BV	12	ASP	CA-CB-CG	6.56	119.16	112.60
2	BR	9	PHE	N-CA-C	6.52	120.45	109.76
2	AR	9	PHE	N-CA-C	6.51	120.44	109.76
3	AT	12	ASP	CA-CB-CG	6.48	119.08	112.60
3	BT	12	ASP	CA-CB-CG	6.47	119.07	112.60
3	BS	12	ASP	CA-CB-CG	6.45	119.05	112.60
3	AS	12	ASP	CA-CB-CG	6.45	119.05	112.60
1	B0	239	SER	N-CA-C	6.38	119.49	110.50
1	A0	239	SER	N-CA-C	6.37	119.48	110.50
3	AU	12	ASP	CA-CB-CG	6.25	118.85	112.60
3	BU	12	ASP	CA-CB-CG	6.22	118.82	112.60
1	BY	242	ASN	N-CA-C	6.07	118.69	111.71
2	BP	249	ASP	CA-C-N	6.05	128.67	120.38
2	BP	249	ASP	C-N-CA	6.05	128.67	120.38
1	AY	242	ASN	N-CA-C	6.02	118.63	111.71
2	AP	249	ASP	CA-C-N	6.00	128.60	120.38
2	AP	249	ASP	C-N-CA	6.00	128.60	120.38
2	BD	15	GLU	N-CA-C	5.95	117.44	111.07
2	AD	15	GLU	N-CA-C	5.92	117.40	111.07
2	BN	15	GLU	N-CA-C	5.91	117.42	110.97
2	BP	15	GLU	N-CA-C	5.87	117.35	111.07
1	BY	240	ALA	N-CA-C	5.87	120.56	113.17
1	AY	240	ALA	N-CA-C	5.85	120.55	113.17
2	AP	15	GLU	N-CA-C	5.85	117.33	111.07
1	BY	243	PHE	CA-CB-CG	5.84	119.64	113.80
1	AZ	151	PHE	CA-CB-CG	5.83	119.63	113.80
2	BC	203	MET	CA-C-N	5.83	129.56	120.82
2	BC	203	MET	C-N-CA	5.83	129.56	120.82
2	BO	203	MET	CA-C-N	5.82	129.56	120.82
2	BO	203	MET	C-N-CA	5.82	129.56	120.82
2	AF	203	MET	CA-C-N	5.82	129.55	120.82
2	AF	203	MET	C-N-CA	5.82	129.55	120.82
3	AT	2	VAL	CA-C-N	5.82	129.13	120.87
3	AT	2	VAL	C-N-CA	5.82	129.13	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AR	203	MET	CA-C-N	5.82	129.54	120.82
2	AR	203	MET	C-N-CA	5.82	129.54	120.82
1	AY	243	PHE	CA-CB-CG	5.81	119.61	113.80
2	BI	203	MET	CA-C-N	5.81	129.53	120.82
2	BI	203	MET	C-N-CA	5.81	129.53	120.82
2	AI	203	MET	CA-C-N	5.80	129.53	120.82
2	AI	203	MET	C-N-CA	5.80	129.53	120.82
2	BR	203	MET	CA-C-N	5.80	129.52	120.82
2	BR	203	MET	C-N-CA	5.80	129.52	120.82
2	AO	203	MET	CA-C-N	5.80	129.52	120.82
2	AO	203	MET	C-N-CA	5.80	129.52	120.82
1	BY	219	THR	CB-CA-C	5.79	119.78	110.16
2	AC	203	MET	CA-C-N	5.78	129.50	120.82
2	AC	203	MET	C-N-CA	5.78	129.50	120.82
3	AS	197	PHE	CA-CB-CG	5.78	119.58	113.80
3	BS	197	PHE	CA-CB-CG	5.78	119.58	113.80
2	AO	15	GLU	N-CA-C	5.77	118.06	111.02
2	BL	203	MET	CA-C-N	5.77	129.48	120.82
2	BL	203	MET	C-N-CA	5.77	129.48	120.82
2	BF	203	MET	CA-C-N	5.77	129.48	120.82
2	BF	203	MET	C-N-CA	5.77	129.48	120.82
1	AZ	240	ALA	N-CA-C	5.77	120.44	113.17
2	AL	203	MET	CA-C-N	5.77	129.47	120.82
2	AL	203	MET	C-N-CA	5.77	129.47	120.82
1	AY	219	THR	CB-CA-C	5.76	119.72	110.16
1	BZ	151	PHE	CA-CB-CG	5.76	119.56	113.80
3	BT	2	VAL	CA-C-N	5.75	129.03	120.87
3	BT	2	VAL	C-N-CA	5.75	129.03	120.87
3	BS	2	VAL	CA-C-N	5.73	129.00	120.87
3	BS	2	VAL	C-N-CA	5.73	129.00	120.87
2	BJ	204	SER	N-CA-C	5.71	119.99	113.19
2	BO	15	GLU	N-CA-C	5.71	117.99	111.02
3	AS	2	VAL	CA-C-N	5.70	128.97	120.87
3	AS	2	VAL	C-N-CA	5.70	128.97	120.87
1	BZ	240	ALA	N-CA-C	5.69	120.34	113.17
2	AL	15	GLU	N-CA-C	5.68	117.95	111.02
2	BL	15	GLU	N-CA-C	5.68	117.95	111.02
3	BX	2	VAL	CA-C-N	5.67	128.92	120.87
3	BX	2	VAL	C-N-CA	5.67	128.92	120.87
1	BY	244	ALA	N-CA-C	5.66	118.18	109.07
1	AY	244	ALA	N-CA-C	5.66	118.18	109.07
2	BL	9	PHE	N-CA-C	5.66	119.04	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AX	2	VAL	CA-C-N	5.65	128.90	120.87
3	AX	2	VAL	C-N-CA	5.65	128.90	120.87
2	BM	204	SER	N-CA-C	5.64	119.90	113.19
2	AL	9	PHE	N-CA-C	5.64	119.01	109.76
2	BP	204	SER	N-CA-C	5.64	119.90	113.19
2	AP	204	SER	N-CA-C	5.63	119.90	113.19
2	BG	9	PHE	CA-CB-CG	5.63	119.43	113.80
2	AJ	9	PHE	CA-CB-CG	5.62	119.42	113.80
2	AG	9	PHE	CA-CB-CG	5.62	119.42	113.80
2	AJ	204	SER	N-CA-C	5.61	119.86	113.19
3	BU	39	THR	N-CA-C	-5.60	100.06	109.07
2	AQ	15	GLU	N-CA-C	5.59	117.84	111.02
2	AM	204	SER	N-CA-C	5.58	119.83	113.19
2	BH	15	GLU	N-CA-C	5.58	117.83	111.02
3	AU	39	THR	N-CA-C	-5.57	100.09	109.07
2	AB	15	GLU	N-CA-C	5.57	117.81	111.02
2	AG	204	SER	N-CA-C	5.56	119.81	113.19
3	AU	264	MET	N-CA-C	5.56	117.72	110.43
2	BQ	15	GLU	N-CA-C	5.55	117.79	111.02
1	A0	151	PHE	CA-CB-CG	5.55	119.35	113.80
2	BG	204	SER	N-CA-C	5.55	119.79	113.19
2	AD	204	SER	N-CA-C	5.54	119.78	113.19
1	B0	151	PHE	CA-CB-CG	5.54	119.34	113.80
2	BG	15	GLU	N-CA-C	5.53	117.77	111.02
2	BB	15	GLU	N-CA-C	5.53	117.76	111.02
2	BJ	9	PHE	CA-CB-CG	5.52	119.32	113.80
3	BU	264	MET	N-CA-C	5.52	117.66	110.43
2	AM	15	GLU	N-CA-C	5.51	117.72	111.11
2	BM	15	GLU	N-CA-C	5.51	117.72	111.11
2	AM	34	ASP	CA-CB-CG	5.51	118.11	112.60
1	AZ	219	THR	CB-CA-C	5.50	119.60	110.74
1	BZ	219	THR	CB-CA-C	5.49	119.58	110.74
2	AH	15	GLU	N-CA-C	5.48	117.71	111.02
2	AG	15	GLU	N-CA-C	5.48	117.70	111.02
2	BD	204	SER	N-CA-C	5.47	119.70	113.19
1	AY	239	SER	N-CA-C	5.46	117.94	110.24
2	AA	15	GLU	N-CA-C	5.45	117.65	111.11
3	BS	124	PHE	CA-CB-CG	5.43	119.23	113.80
1	BY	239	SER	N-CA-C	5.43	117.90	110.24
2	BM	34	ASP	CA-CB-CG	5.42	118.02	112.60
3	BX	72	LEU	CA-C-N	5.40	127.47	120.44
3	BX	72	LEU	C-N-CA	5.40	127.47	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AX	72	LEU	CA-C-N	5.39	127.45	120.44
3	AX	72	LEU	C-N-CA	5.39	127.45	120.44
2	BA	15	GLU	N-CA-C	5.39	117.58	111.11
1	AZ	228	VAL	N-CA-C	5.36	116.00	109.30
1	BZ	228	VAL	N-CA-C	5.36	116.00	109.30
3	BT	124	PHE	CA-CB-CG	5.34	119.14	113.80
3	AT	124	PHE	CA-CB-CG	5.33	119.14	113.80
2	AE	15	GLU	N-CA-C	5.33	117.53	111.02
3	AS	124	PHE	CA-CB-CG	5.33	119.12	113.80
1	A0	44	TYR	N-CA-C	5.32	118.41	109.95
2	BE	15	GLU	N-CA-C	5.31	117.50	111.02
3	AT	27	ARG	N-CA-C	5.29	118.03	109.40
1	B0	44	TYR	N-CA-C	5.29	118.35	109.95
3	BT	27	ARG	N-CA-C	5.27	117.99	109.40
2	BD	39	ARG	N-CA-C	-5.27	100.31	108.90
2	AR	15	GLU	N-CA-C	5.26	117.44	111.02
2	BR	15	GLU	N-CA-C	5.26	117.44	111.02
2	AD	39	ARG	N-CA-C	-5.24	100.36	108.90
2	AA	249	ASP	CA-CB-CG	5.23	117.83	112.60
1	AZ	44	TYR	N-CA-C	5.23	118.11	109.85
1	BZ	44	TYR	N-CA-C	5.23	118.11	109.85
2	BA	249	ASP	CA-CB-CG	5.22	117.82	112.60
2	AO	9	PHE	N-CA-C	5.22	118.73	109.96
2	AN	15	GLU	N-CA-C	5.21	117.38	111.02
2	AC	262	PHE	CA-CB-CG	5.21	119.01	113.80
2	AG	39	ARG	N-CA-C	-5.21	100.42	108.90
3	BS	40	ASN	N-CA-C	5.20	119.47	113.18
1	BY	152	PHE	N-CA-C	5.20	117.90	109.06
2	BG	39	ARG	N-CA-C	-5.20	100.43	108.90
2	BO	9	PHE	N-CA-C	5.20	118.69	109.96
3	AS	40	ASN	N-CA-C	5.19	119.46	113.18
2	BQ	9	PHE	CA-CB-CG	5.19	118.99	113.80
2	BC	262	PHE	CA-CB-CG	5.19	118.99	113.80
2	AF	15	GLU	N-CA-C	5.18	117.34	111.02
2	BA	39	ARG	N-CA-C	-5.18	100.45	108.90
2	AA	39	ARG	N-CA-C	-5.18	100.46	108.90
1	AY	305	GLU	CA-C-N	5.18	127.22	120.28
1	AY	305	GLU	C-N-CA	5.18	127.22	120.28
2	BF	15	GLU	N-CA-C	5.18	117.34	111.02
1	BZ	239	SER	N-CA-C	5.17	117.73	110.23
1	AY	152	PHE	N-CA-C	5.16	117.84	109.06
2	AM	9	PHE	CA-CB-CG	5.16	118.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AG	129	SER	N-CA-C	-5.16	101.03	109.80
2	BG	129	SER	N-CA-C	-5.16	101.03	109.80
3	AT	294	LYS	CA-C-N	5.15	129.23	121.40
3	AT	294	LYS	C-N-CA	5.15	129.23	121.40
2	BO	262	PHE	CA-CB-CG	5.15	118.95	113.80
3	BT	294	LYS	CA-C-N	5.15	129.22	121.40
3	BT	294	LYS	C-N-CA	5.15	129.22	121.40
2	BM	9	PHE	CA-CB-CG	5.15	118.95	113.80
2	AA	129	SER	N-CA-C	-5.14	101.06	109.80
3	AX	124	PHE	CA-CB-CG	5.14	118.94	113.80
2	AQ	9	PHE	CA-CB-CG	5.14	118.94	113.80
2	AI	262	PHE	CA-CB-CG	5.13	118.93	113.80
1	AZ	239	SER	N-CA-C	5.13	117.67	110.23
3	BX	124	PHE	CA-CB-CG	5.13	118.93	113.80
1	AY	370	ASP	CA-C-N	5.12	126.13	119.78
1	AY	370	ASP	C-N-CA	5.12	126.13	119.78
3	BV	28	PHE	CA-CB-CG	5.12	118.92	113.80
3	BS	250	GLN	N-CA-C	5.12	117.24	108.90
2	AN	262	PHE	CA-CB-CG	5.12	118.92	113.80
3	AV	28	PHE	CA-CB-CG	5.12	118.92	113.80
2	AO	262	PHE	CA-CB-CG	5.11	118.91	113.80
2	BI	15	GLU	N-CA-C	5.11	117.25	111.02
1	BY	305	GLU	CA-C-N	5.11	127.12	120.28
1	BY	305	GLU	C-N-CA	5.11	127.12	120.28
2	BK	262	PHE	CA-CB-CG	5.11	118.91	113.80
3	BU	291	ILE	N-CA-C	5.11	115.66	108.36
2	AJ	34	ASP	CA-CB-CG	5.10	117.70	112.60
3	AV	291	ILE	N-CA-C	5.10	115.66	108.36
2	BI	262	PHE	CA-CB-CG	5.10	118.90	113.80
2	BP	34	ASP	CA-CB-CG	5.10	117.70	112.60
2	AK	262	PHE	CA-CB-CG	5.10	118.90	113.80
3	AU	291	ILE	N-CA-C	5.09	115.64	108.36
2	BJ	34	ASP	CA-CB-CG	5.09	117.69	112.60
2	AB	262	PHE	CA-CB-CG	5.09	118.89	113.80
3	BV	291	ILE	N-CA-C	5.08	115.63	108.36
2	AN	9	PHE	CA-CB-CG	5.08	118.88	113.80
3	AS	250	GLN	N-CA-C	5.08	117.25	109.07
1	BZ	340	ILE	N-CA-C	5.08	115.62	108.36
2	AD	129	SER	N-CA-C	-5.08	101.17	109.80
2	BA	129	SER	N-CA-C	-5.08	101.17	109.80
2	BB	262	PHE	CA-CB-CG	5.07	118.87	113.80
2	AI	15	GLU	N-CA-C	5.07	117.20	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BD	129	SER	N-CA-C	-5.07	101.19	109.80
2	AL	34	ASP	CA-CB-CG	5.06	117.66	112.60
3	BW	197	PHE	CA-CB-CG	5.06	118.86	113.80
1	AZ	340	ILE	N-CA-C	5.06	115.59	108.36
1	BY	370	ASP	CA-C-N	5.06	126.05	119.78
1	BY	370	ASP	C-N-CA	5.06	126.05	119.78
2	BL	262	PHE	CA-CB-CG	5.05	118.85	113.80
2	AP	34	ASP	CA-CB-CG	5.05	117.65	112.60
2	BO	34	ASP	CA-CB-CG	5.05	117.65	112.60
2	AQ	262	PHE	CA-CB-CG	5.05	118.85	113.80
2	BN	9	PHE	CA-CB-CG	5.04	118.84	113.80
2	AC	15	GLU	N-CA-C	5.04	117.17	111.02
3	AW	197	PHE	CA-CB-CG	5.04	118.83	113.80
2	AJ	39	ARG	N-CA-C	-5.03	100.70	108.90
2	AO	34	ASP	CA-CB-CG	5.03	117.63	112.60
2	BJ	39	ARG	N-CA-C	-5.03	100.70	108.90
2	BN	262	PHE	CA-CB-CG	5.03	118.83	113.80
1	BY	309	ILE	CA-C-N	5.03	127.33	120.54
1	BY	309	ILE	C-N-CA	5.03	127.33	120.54
2	AE	262	PHE	CA-CB-CG	5.02	118.82	113.80
2	AL	262	PHE	CA-CB-CG	5.02	118.82	113.80
2	BQ	262	PHE	CA-CB-CG	5.01	118.81	113.80
2	BF	262	PHE	CA-CB-CG	5.01	118.81	113.80
2	BH	262	PHE	CA-CB-CG	5.01	118.81	113.80
2	BR	262	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	57	0
1	AY	3000	0	2956	38	0
1	AZ	3000	0	2956	75	0
1	B0	3000	0	2956	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BY	3000	0	2956	38	0
1	BZ	3000	0	2956	54	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	35	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	14	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	36	0
2	AQ	2008	0	1971	43	0
2	AR	2008	0	1971	34	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	32	0
2	BR	2008	0	1971	23	0
3	AS	2432	0	2392	122	0
3	AT	2432	0	2392	111	0
3	AU	2432	0	2392	100	0
3	AV	2432	0	2392	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AW	2432	0	2392	75	0
3	AX	2432	0	2392	151	0
3	BS	2432	0	2392	99	0
3	BT	2432	0	2392	106	0
3	BU	2432	0	2392	96	0
3	BV	2432	0	2392	94	0
3	BW	2432	0	2392	76	0
3	BX	2432	0	2392	117	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	1553	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 7.

All (1553) 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
2:AD:52:ASN:CG	3:AS:258:LEU:CD2	1.81	1.53
2:AD:52:ASN:CG	3:AS:258:LEU:HD22	1.30	1.52
3:AX:120:LYS:HD3	3:BU:68:PHE:CE1	1.40	1.51
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
2:AD:130:GLY:O	3:AS:262:PRO:CB	1.70	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:BD:52:ASN:CG	3:BS:258:LEU:HD22	1.51	1.33
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
3:AV:120:LYS:HZ2	3:BW:66:GLU:CG	1.45	1.27
3:AV:120:LYS:NZ	3:BW:66:GLU:CG	1.99	1.24
2:BD:52:ASN:CG	3:BS:258:LEU:CD2	2.10	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	1.52	1.20
1:A0:42:ILE:CB	3:AX:43:TRP:HZ2	1.55	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:BB:13:SER:C	3:BS:169:LYS:HD2	1.74	1.11
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
3:AW:66:GLU:HG2	3:BV:120:LYS:HZ2	0.99	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:AB:13:SER:C	3:AS:169:LYS:HD2	1.78	1.07
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
3:AV:120:LYS:HZ2	3:BW:66:GLU:HG2	1.12	1.06
3:AV:120:LYS:NZ	3:BW:66:GLU:HG3	1.69	1.06
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
2:AB:13:SER:O	3:AS:169:LYS:CD	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:52:ASN:CB	3:AS:258:LEU:HD22	1.86	1.05
1:A0:86:LYS:NZ	2:AN:81:VAL:HB	1.70	1.05
2:AD:52:ASN:CG	3:AS:258:LEU:HD23	1.72	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:AV:120:LYS:NZ	3:BW:66:GLU:HG2	1.72	0.90
2:AE:17:PRO:HB3	3:AT:167:ASN:HD22	1.37	0.89
3:AV:120:LYS:HZ2	3:BW:66:GLU:CB	1.84	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
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
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
3:AW:66:GLU:HG2	3:BV:120:LYS:NZ	1.80	0.85
2:BD:52:ASN:ND2	3:BS:258:LEU:CD2	2.33	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:BD:52:ASN:CG	3:BS:258:LEU:HD23	2.01	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
1:A0:294:PHE:CE2	1:AZ:169:THR:HG21	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:PHE:HA	3:AT:170:TYR:O	1.80	0.81
2:AE:17:PRO:HB2	3:AT:167:ASN:HB2	1.62	0.81
3:AX:120:LYS:HE2	3:BU:66:GLU:HG2	1.63	0.81
2:AG:79:ASP:C	1:AZ:212:ASN:HD21	1.89	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
3:AX:66:GLU:HG3	3:BU:120:LYS:HZ1	1.45	0.81
1:A0:88:LYS:HZ1	2:AN:104:ALA:HB3	1.40	0.81
2:AQ:19:GLY:HA2	3:AX:166:GLY:C	2.05	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
1:A0:42:ILE:HD13	3:AX:43:TRP:NE1	1.97	0.79
2:AE:17:PRO:HB3	3:AT:167:ASN:ND2	1.97	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
2:AQ:18:VAL:C	3:AX:167:ASN:HA	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AF:17:PRO:HA	3:AT:177:THR:HG22	1.65	0.78
3:AS:142:LEU:HD12	3:AS:291:ILE:HD12	1.65	0.78
3:AS:66:GLU:CG	3:BT:120:LYS:NZ	2.45	0.78
3:AS:273:ILE:HD11	3:AT:48:ILE:HD12	1.65	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
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
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:AS:66:GLU:HG2	3:BT:120:LYS:HE2	1.69	0.75
3:AX:66:GLU:CG	3:BU:120:LYS:NZ	2.49	0.75
3:AX:120:LYS:HD3	3:BU:68:PHE:HE1	1.37	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:17:PRO:HB3	3:AT:169:LYS:HE3	1.68	0.75
2:AE:21:ASN:OD1	3:AT:165:PRO:HG2	1.87	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: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
2:AC:9:PHE:CD1	3:AS:180:GLY:HA2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:AV:48:ILE:HD13	1:AZ:1:MET:SD	2.30	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
2:AP:113:ASN:O	3:AX:186:ARG:NH2	2.24	0.70
3:AU:68:PHE:HE1	3:BX:120:LYS:CG	2.05	0.70
3:AV:120:LYS:HZ3	3:BW:66:GLU:CG	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:AW:121:ASN:HD21	3:BV:68:PHE:HB3	1.57	0.69
3:BT:80:LYS:HE3	3:BU:298:VAL:HG22	1.74	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
2:BE:19:GLY:CA	3:BT:166:GLY:O	2.40	0.69
3:AS:120:LYS:HG2	3:BT:68:PHE:CE1	2.28	0.69
1:A0:294:PHE:HE2	1:AZ:169:THR:HG21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:197:PHE:HD1	3:AT:48:ILE:CG2	2.06	0.69
3:AV:70:GLU:HG2	3:BW:70:GLU:HG2	1.74	0.69
2:BA:77:LYS:H	2:BA:82:ASN:HD21	1.39	0.69
3:BT:45:SER:OG	1:BY:1:MET:HB3	1.94	0.68
2:BF:18:VAL:O	3:BT:175:SER:OG	2.07	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
3:AV:120:LYS:HZ3	3:BW:66:GLU:HG3	1.54	0.68
2:AD:52:ASN:HB2	3:AS:258:LEU:HD22	1.71	0.68
2:AR:17:PRO:HA	3:AX:177:THR:HG22	1.74	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
2:AD:131:THR:HG22	3:AS:262:PRO:C	2.18	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
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: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
3:AW:66:GLU:CB	3:BV:120:LYS:NZ	2.58	0.66
2:BN:130:GLY:O	3:BV:262:PRO:CB	2.41	0.66
3:AW:70:GLU:HG2	3:BV:70:GLU:HG2	1.75	0.66
2:BJ:77:LYS:H	2:BJ:82:ASN:HD21	1.41	0.66
3:AV:120:LYS:HZ2	3:BW:66:GLU:HB3	1.59	0.66
1:A0:88:LYS:HZ2	2:AN:104:ALA:HB3	1.55	0.66
2:BD:23:ASP:OD2	3:BT:178:TYR:HE1	1.77	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: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:AS:66:GLU:CG	3:BT:120:LYS:HZ3	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:271:THR:HA	1:AZ:3:GLU:HG3	1.76	0.66
2:BM:77:LYS:H	2:BM:82:ASN:HD21	1.42	0.66
2:BC:18:VAL:HG13	3:BS:176:TYR:CZ	2.31	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
3:BS:244:VAL:HG11	1:BY:1:MET:HE1	1.78	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
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
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:AX:120:LYS:CG	3:BU:68:PHE:HE1	2.11	0.64
3:BS:250:GLN:NE2	3:BS:252:TRP:HE1	1.96	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
2:AG:79:ASP:O	1:AZ:212:ASN:CG	2.40	0.64
1:AZ:89:LEU:HD22	1:AZ:192:GLN:HG3	1.79	0.64
3:AV:66:GLU:HG3	3:BW:120:LYS:HZ1	1.62	0.64
3:AS:250:GLN:NE2	3:AS:252:TRP:HE1	1.96	0.64
3:AU:68:PHE:CD1	3:BX:120:LYS:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:AX:120:LYS:HZ1	3:BU:66:GLU:HG3	1.62	0.63
2:BD:73:THR:CG2	3:BS:256:THR:HG21	2.28	0.63
2:BE:17:PRO:HB2	3:BT:167:ASN:CB	2.26	0.63
2:AD:23:ASP:OD2	3:AT:178:TYR:HE1	1.82	0.63
3:AW:66:GLU:CB	3:BV:120:LYS:HZ2	2.11	0.63
2:AP:21:ASN:HB3	3:AX:181:GLU:CD	2.23	0.63
3:BV:247:GLU:OE1	3:BV:249:TYR:HE2	1.82	0.63
3:AU:68:PHE:HD1	3:BX:120:LYS:HB3	1.63	0.63
3:AV:247:GLU:OE1	3:AV:249:TYR:HE2	1.82	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: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
1:BY:241:TYR:HB2	1:BY:291:LYS:HD2	1.81	0.62
2:AB:13:SER:C	3:AS:169:LYS:CD	2.62	0.62
2:AP:9:PHE:HA	3:AX:160:TYR:O	1.99	0.62
2:BB:17:PRO:HB3	3:BS:167:ASN:HB2	1.81	0.62
2:BR:23:ASP:OD2	3:BX:176:TYR:OH	2.17	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
2:AQ:21:ASN:CG	3:AX:165:PRO:HG2	2.24	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
2:AF:18:VAL:O	3:AT:175:SER:OG	2.10	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AV:66:GLU:HG2	3:BW:120:LYS:CE	2.30	0.61
3:BT:73:GLU:HB2	3:BU:99:GLU:CD	2.25	0.61
3:AU:66:GLU:CB	3:BX:120:LYS:HZ3	2.13	0.61
3:AW:215:ARG:HB3	3:AW:282:ILE:HD11	1.83	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:AX:120:LYS:HZ3	3:BU:66:GLU:HB3	1.65	0.61
3:BW:215:ARG:HB3	3:BW:282:ILE:HD11	1.83	0.61
1:A0:3:GLU:HG3	3:AW:271:THR:HA	1.83	0.61
3:AS:215:ARG:HB3	3:AS:282:ILE:HD11	1.82	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
2:AR:9:PHE:CZ	3:AX:180:GLY:C	2.78	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
2:AA:104:ALA:CB	1:AY:88:LYS:NZ	2.63	0.60
3:AT:235:GLN:HE22	3:AT:258:LEU:HD12	1.66	0.60
1:AZ:90:ASN:HD22	1:AZ:192:GLN:NE2	1.99	0.60
1:B0:294:PHE:HE2	1:BZ:169:THR:HG21	1.66	0.60
2:BG:81:VAL:HB	1:BZ:86:LYS:NZ	2.16	0.60
3:BT:235:GLN:HE22	3:BT:258:LEU:HD12	1.66	0.60
3:BU:53:THR:HG23	1:BZ:359:PHE:HB3	1.84	0.60
3:BX:247:GLU:OE1	3:BX:249:TYR:HE2	1.83	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:AA:104:ALA:HB3	1:AY:88:LYS:HD2	1.84	0.60
2:AE:17:PRO:CB	3:AT:167:ASN:ND2	2.58	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
3:AW:121:ASN:ND2	3:BV:68:PHE:HB3	2.16	0.60
2:BE:17:PRO:CB	3:BT:167:ASN:ND2	2.56	0.60
3:BX:12:ASP:HB2	3:BX:200:MET:HG3	1.84	0.60
2:AN:47:LEU:HD22	3:AV:233:GLN:CD	2.26	0.60
3:AS:206:LYS:HG3	3:AS:285:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A0:42:ILE:HD13	3:AX:43:TRP:HE1	1.65	0.60
2:AR:18:VAL:HG12	3:AX:176:TYR:O	2.02	0.60
2:BF:23:ASP:OD2	3:BT:176:TYR:OH	2.18	0.60
2:AR:9:PHE:CZ	3:AX:181:GLU:HG3	2.37	0.59
3:AX:12:ASP:HB2	3:AX:200:MET:HG3	1.84	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:AU:66:GLU:HG3	3:BX:120:LYS:HZ1	1.66	0.59
3:AV:171:ILE:HG22	3:AV:172:LYS:H	1.68	0.59
3:BS:206:LYS:HG3	3:BS:285:SER:HB3	1.84	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
1:BY:243:PHE:CD1	1:BY:243:PHE:C	2.80	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
3:AV:48:ILE:HG21	1:AZ:1:MET:HE1	1.84	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
1:AY:243:PHE:CD1	1:AY:243:PHE:C	2.80	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
3:AT:79:MET:HE3	3:AU:297:PHE:HZ	1.68	0.58
1:AZ:41:VAL:HG23	1:AZ:57:ALA:HB1	1.85	0.58
2:AN:51:LEU:HD12	3:AV:262:PRO:CG	2.33	0.58
2:AN:120:LYS:HE2	3:AW:222:ASN:ND2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B0:88:LYS:HZ1	2:BN:104:ALA:HB3	1.68	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
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
2:AG:79:ASP:C	1:AZ:212:ASN:ND2	2.61	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
1:A0:330:LEU:HB2	3:AV:261:PHE:CD2	2.39	0.57
2:AI:88:ILE:HG12	2:AI:97:VAL:HG22	1.85	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:AX:66:GLU:CG	3:BU:120:LYS:HZ3	2.16	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:BE:18:VAL:HG13	3:BT:168:TYR:CD2	2.39	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: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:9:PHE:CE1	3:BX:180:GLY:CA	2.87	0.57
2:BR:88:ILE:HG12	2:BR:97:VAL:HG22	1.85	0.57
2:AA:120:LYS:HE2	3:AS:222:ASN:ND2	2.19	0.57
1:A0:78:PRO:HG3	2:AN:103:THR:HB	1.87	0.57
2:AP:21:ASN:CB	3:AX:181:GLU:HG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:196:ILE:HG22	3:AU:293:ARG:HD3	1.87	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:BU:240:ILE:O	3:BU:240:ILE:HD12	2.05	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:AW:206:LYS:HG3	3:AW: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
2:BN:51:LEU:CD1	3:BV:262:PRO:HG2	2.28	0.56
3:BU:196:ILE:HG22	3:BU:293:ARG:HD3	1.87	0.56
3:AS:244:VAL:HG11	1:AY:1:MET:HE1	1.87	0.55
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:BU:224:TYR:HB2	1:BZ:74:PRO:HB2	1.88	0.55
3:BV:206:LYS:HG3	3:BV:285:SER:HB3	1.87	0.55
3:BX:240:ILE:HD12	3:BX:240:ILE:O	2.07	0.55
3:BX:247:GLU:OE1	3:BX:249:TYR:CE2	2.59	0.55
2:AQ:18:VAL:O	3:AX:168:TYR:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:AT:120:LYS:NZ	3:BS:66:GLU:CG	2.66	0.55
2:BG:103:THR:CG2	1:BZ:78:PRO:HG3	2.35	0.55
3:BT:240:ILE:HD12	3:BT:240:ILE:O	2.06	0.55
3:AT:73:GLU:HB2	3:AU:99:GLU:CD	2.30	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:120:LYS:NZ	3:BX:66:GLU:HG2	2.22	0.55
3:AU:240:ILE:HD12	3:AU:240:ILE:O	2.05	0.55
1:AZ:41:VAL:HG11	1:AZ:71:ILE:HG12	1.88	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:HD12	3:AX:240:ILE:O	2.07	0.55
2:BH:187:ILE:HG12	2:BH:260:SER:HB3	1.88	0.55
3:BT:243:ASP:OD1	3:BT:243:ASP:C	2.50	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:AG:92:GLN:HE21	3:AU:189:ARG:NE	2.05	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
3:AV:120:LYS:NZ	3:BW:66:GLU:CB	2.55	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
3:BV:240:ILE:C	3:BV:240:ILE:HD12	2.32	0.54
2:AG:80:SER:OG	1:AZ:211:ARG:HD2	2.07	0.54
3:AX:40:ASN:HB3	3:AX:51:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:18:VAL:CG1	3:AS:176:TYR:CZ	2.90	0.54
2:AE:88:ILE:HG12	2:AE:97:VAL:HG22	1.89	0.54
2:AH:88:ILE:HG12	2:AH:97:VAL:HG22	1.89	0.54
2:AH:187:ILE:HG12	2:AH:260:SER:HB3	1.88	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
3:AU:160:TYR:HB3	3:AU:166:GLY:HA3	1.89	0.54
3:AX:66:GLU:HG2	3:BU:120:LYS:HE2	1.89	0.54
3:BS:11:LEU:O	3:BS:12:ASP:CG	2.51	0.54
3:BT:106:ASP:O	3:BT:133:ILE:HB	2.07	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:AS:11:LEU:O	3:AS:12:ASP:CG	2.51	0.54
3:AT:160:TYR:HB3	3:AT:166:GLY:HA3	1.89	0.54
3:AT:199:PHE:H	3:AT:242:THR:HG1	1.55	0.54
3:AT:215:ARG:HB3	3:AT:282:ILE:HD11	1.89	0.54
3:AT:243:ASP:C	3:AT:243:ASP:OD1	2.50	0.54
2:BG:79:ASP:C	1:BZ:212:ASN:HD21	2.16	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
1:A0:344:GLY:HA3	3:AV:270:ARG:HH11	1.73	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
3:AV:240:ILE:C	3:AV:240:ILE:HD12	2.32	0.53
2:BB:187:ILE:HG12	2:BB:260:SER:HB3	1.88	0.53
3:BU:55:SER:HB3	1:BZ:359:PHE:CE1	2.44	0.53
3:BU:242:THR:HG23	3:BU:272:ARG:HG3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B0:238:ARG:HG3	1:B0:316:SER:HA	1.89	0.53
2:BB:13:SER:C	3:BS:169:LYS:CD	2.59	0.53
3:BT:114:LYS:HB3	3:BU:34:LEU:HB2	1.90	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
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
1:B0:86:LYS:HZ1	2:BN:81:VAL:HB	1.72	0.53
2:BH:88:ILE:HG12	2:BH:97:VAL:HG22	1.89	0.53
2:BR:9:PHE:CZ	3:BX:180:GLY:C	2.87	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
3:AX:66:GLU:CG	3:BU:120:LYS:HZ1	2.17	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
3:AV:243:ASP:OD1	3:AV:243:ASP:C	2.52	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
1:AZ:237:ASP:C	1:AZ:238:ARG:HG2	2.33	0.53
2:BN:47:LEU:HD22	3:BV:233:GLN:CD	2.34	0.53
3:AS:239:LEU:C	3:AS:239:LEU:HD23	2.34	0.53
3:AX:120:LYS:HZ3	3:BU:66:GLU:CB	2.22	0.53
2:BF:18:VAL:HG12	3:BT:176:TYR:O	2.10	0.53
3:BT:79:MET:HE3	3:BU:297:PHE:HZ	1.73	0.53
3:BX:40:ASN:HB3	3:BX:51:MET:HE3	1.89	0.53
1:A0:238:ARG:HG3	1:A0:316:SER:HA	1.90	0.52
3:AW:68:PHE:CE1	3:BV:120:LYS:HD2	2.44	0.52
3:AX:160:TYR:HB3	3:AX:166:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:BS:239:LEU:HD23	3:BS:239:LEU:C	2.35	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:AF:17:PRO:CA	3:AT:177:THR:HG22	2.36	0.52
2:AP:88:ILE:HG12	2:AP:97:VAL:HG22	1.91	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
3:BV:243:ASP:C	3:BV:243:ASP:OD1	2.52	0.52
2:AP:21:ASN:HB3	3:AX:181:GLU:HG2	1.92	0.52
3:AW:66:GLU:HG3	3:BV:120:LYS:HZ3	1.67	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
3:AU:11:LEU:O	3:AU:12:ASP:CG	2.52	0.52
3:AU:116:GLU:HB2	3:AV:31:PRO:HD2	1.91	0.52
2:BE:18:VAL:C	3:BT:167:ASN:HA	2.35	0.52
3:BU:11:LEU:O	3:BU:12:ASP:CG	2.52	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
2:AQ:18:VAL:HG13	3:AX:168:TYR:CD2	2.45	0.52
3:AU:281:LEU:HB3	3:AU:284:LEU:HD12	1.92	0.52
3:AV:43:TRP:CZ2	1:AZ:43:ASN:HB2	2.45	0.52
3:AW:160:TYR:HB3	3:AW:166:GLY:HA3	1.92	0.52
1:B0:12:PRO:HB2	1:BY:288:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:BZ:237:ASP:C	1:BZ:238:ARG:HG2	2.33	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
2:BE:9:PHE:HD2	3:BT:170:TYR:C	2.18	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:BQ:19:GLY:HA2	3:BX:166:GLY:C	2.35	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:BE:19:GLY:HA2	3:BT:166:GLY:C	2.35	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
2:AE:9:PHE:HD2	3:AT:170:TYR:C	2.18	0.51
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:66:GLU:HG2	3:BU:120:LYS:NZ	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:BG:10:SER:N	3:BU:160:TYR:O	2.30	0.51
2:BQ:9:PHE:HA	3:BX:170:TYR:O	2.11	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
3:AW:120:LYS:CB	3:BV:68:PHE:HD1	2.21	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
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:AX:66:GLU:HG2	3:BU:120:LYS:CE	2.40	0.50
3:AX:144:PHE:HB3	3:AX:190:TRP:CE2	2.45	0.50
2:BN:102:GLU:OE1	3:BW:222:ASN:ND2	2.40	0.50
1:A0:42:ILE:HB	3:AX:43:TRP:HZ2	0.61	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
2:BQ:18:VAL:C	3:BX:167:ASN:HA	2.36	0.50
3:BS:197:PHE:HD1	3:BT:48:ILE:HG22	1.76	0.50
3:BT:156:MET:HE3	3:BT:174:THR:HG22	1.94	0.50
3:AT:124:PHE:O	3:BS:120:LYS:NZ	2.43	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: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:AU:116:GLU:OE2	3:AV:3:ARG:HG3	2.11	0.50
3:AV:76:TYR:HE1	3:AW:96:TYR:HH	1.60	0.50
1:B0:122:PRO:HD2	1:B0:125:ILE:HD12	1.94	0.50
2:BM:9:PHE:HB2	3:BW:180:GLY:HA2	1.92	0.50
3:BT:87:LEU:HA	3:BU:54:ARG:NH1	2.26	0.50
3:BU:281:LEU:HB3	3:BU:284:LEU:HD12	1.92	0.50
1:A0:288:ARG:NH2	1:AZ:12:PRO:HB2	2.27	0.50
3:AT:156:MET:HE3	3:AT:174:THR:HG22	1.94	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
2:AA:81:VAL:HB	1:AY:86:LYS:NZ	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:4:GLN:HB2	3:AS:97:GLN:HB3	1.93	0.50
3:AU:266:PHE:CG	1:AZ:35:PRO:HD2	2.47	0.50
3:AW:226:ALA:HB3	3:AW:268:ARG:HB3	1.92	0.50
1:B0:32:LEU:HD11	1:B0:204:LEU:HB2	1.93	0.50
2:AO:171:GLY:HA3	2:AO:205:GLY:H	1.77	0.50
2:AP:21:ASN:HB3	3:AX:181:GLU:CG	2.42	0.50
2:AP:113:ASN:C	3:AX:186:ARG:NH2	2.68	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: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:BN:120:LYS:NZ	3:BW:220:ILE:O	2.34	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: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:9:PHE:CE1	3:AX:180:GLY:N	2.80	0.49
2:AR:177:GLN:HB3	2:AR:189:ARG:HB2	1.93	0.49
3:AU:68:PHE:HE1	3:BX:120:LYS:HG2	1.76	0.49
3:AU:171:ILE:HG22	3:AU:172:LYS:H	1.77	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
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:AX:199:PHE:CZ	3:AX:242:THR:HG21	2.47	0.49
2:BF:17:PRO:CA	3:BT:177:THR:HG22	2.37	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
3:AU:138:THR:O	3:AU:292:LYS:HA	2.11	0.49
3:AV:43:TRP:HE1	1:AZ:42:ILE:HB	1.77	0.49
1:AZ:152:PHE:CB	1:AZ:208:PHE:HB2	2.42	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:20:SER:OG	3:AX:165:PRO:O	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AW:120:LYS:CE	3:BV:68:PHE:CE1	2.90	0.49
3:BS:197:PHE:CD1	3:BT:48:ILE:CG2	2.94	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: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:18:VAL:HG12	3:AT:176:TYR:O	2.12	0.49
2:AF:171:GLY:HA3	2:AF:205:GLY:H	1.77	0.49
2:AP:118:VAL:HG23	3:AX:278:GLN:NE2	2.27	0.49
3:AU:196:ILE:HG13	3:AU:274:ILE:HB	1.94	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:AD:52:ASN:HB2	3:AS:258:LEU:CD2	2.30	0.49
2:AG:79:ASP:CB	1:AZ:212:ASN:HD21	2.25	0.49
2:AK:91:THR:HG21	3:AV:189:ARG:HB2	1.93	0.49
3:AU:53:THR:HG21	1:AZ:359:PHE:CA	2.43	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: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:BP:22:ASN:HD21	3:BX:182:SER:CB	2.25	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
1:AY:233:GLU:HB2	1:AY:321:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:CYS:HB2	1:BY:60:THR:OG1	2.12	0.49
1:BY:169:THR:HG21	1:BZ:294:PHE:CZ	2.47	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
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:BH:17:PRO:HB3	3:BU:169:LYS:HE3	1.94	0.48
2:BQ:17:PRO:HB3	3:BX:169:LYS:CE	2.38	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
3:AX:200:MET:HE1	3:AX:239:LEU:HD21	1.95	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:BD:52:ASN:ND2	3:BS:258:LEU:HB3	2.29	0.48
2:BE:39:ARG:HB2	2:BE:61:ILE:HB	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AY:45:GLU:HA	1:AY:357:THR:HG22	1.95	0.48
3:BX:281:LEU:HB3	3:BX:284:LEU:HD12	1.96	0.48
2:AE:18:VAL:C	3:AT:167:ASN:HA	2.39	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
2:BD:23:ASP:OD2	3:BT:178:TYR:CE1	2.62	0.48
2:BE:18:VAL:CG1	3:BT:168:TYR:O	2.54	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:BR:9:PHE:HZ	3:BX:181:GLU:HG3	1.76	0.48
3:BV:144:PHE:HB3	3:BV:190:TRP:CE2	2.49	0.48
3:BX:200:MET:HE1	3:BX:239:LEU:HD21	1.95	0.48
1:BY:122:PRO:HD2	1:BY:125:ILE:HD12	1.96	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
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
2:AK:116:SER:OG	3:AV:186:ARG:O	2.32	0.48
3:AU:106:ASP:O	3:AU:133:ILE:HB	2.14	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:BP:9:PHE:HA	3:BX:160:TYR:O	2.13	0.47
2:BR:27:TYR:HA	2:BR:30:LEU:HD12	1.96	0.47
3:BT:199:PHE:H	3:BT:242:THR:HG1	1.57	0.47
3:BT:226:ALA:HB3	3:BT:268:ARG:HB3	1.95	0.47
1:A0:169:THR:HG21	1:AY:294:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AP:19:GLY:CA	3:AX:180:GLY:O	2.62	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:AU:120:LYS:HD3	3:BX:68:PHE:CE1	2.49	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
3:AX:242:THR:O	3:AX:272:ARG:HD3	2.13	0.47
2:BG:81:VAL:HB	1:BZ:86:LYS:HZ1	1.78	0.47
3:BT:212:ALA:HB2	3:BT:283:ASN:HD22	1.79	0.47
2:AB:39:ARG:HB2	2:AB:61:ILE:HB	1.95	0.47
2:AQ:17:PRO:CG	3:AX:169:LYS:CE	2.93	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
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:AL:171:GLY:HA3	2:AL:205:GLY:H	1.77	0.47
3:AS:281:LEU:HB3	3:AS:284:LEU:HD12	1.96	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:144:PHE:HB3	3:AV:190:TRP:CE2	2.49	0.47
3:AV:160:TYR:HB3	3:AV:166:GLY:HA3	1.95	0.47
1:AZ:231:ASP:OD2	1:AZ:321:ARG:NH1	2.47	0.47
3:BV:160:TYR:HB3	3:BV:166:GLY:HA3	1.95	0.47
1:A0:359:PHE:O	3:AW:53:THR:HG21	2.14	0.47
2:AD:23:ASP:OD2	3:AT:178:TYR:CE1	2.67	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:BS:281:LEU:HB3	3:BS:284:LEU:HD12	1.96	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:120:LYS:NZ	3:AX:220:ILE:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AH:17:PRO:HB3	3:AU:169:LYS:HE3	1.97	0.46
2:AM:5:ASN:HB3	2:AM:8:PHE:CD1	2.50	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: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
2:AG:79:ASP:O	1:AZ:212:ASN:OD1	2.32	0.46
2:AG:172:ASN:HD21	2:AG:204:SER:H	1.63	0.46
3:AS:72:LEU:HD22	3:AS:76:TYR:CE2	2.50	0.46
3:AS:194:GLU:HB2	3:AS:293:ARG:HD2	1.97	0.46
3:AU:53:THR:HG21	1:AZ:359:PHE:C	2.41	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
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
3:AV:68:PHE:HD1	3:BW:120:LYS:HD2	1.72	0.46
3:AW:66:GLU:CB	3:BV:120:LYS:HZ1	2.28	0.46
3:AW:72:LEU:HD22	3:AW:76:TYR:CE2	2.50	0.46
2:BA:131:THR:HG22	3:BX:262:PRO:O	2.16	0.46
2:BE:21:ASN:CG	3:BT:165:PRO:HG2	2.40	0.46
2:BQ:17:PRO:CB	3:BX:167:ASN:HD22	2.13	0.46
3:BS:99:GLU:CD	3:BX:73:GLU:HB2	2.41	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
2:AR:23:ASP:CG	3:AX:176:TYR:HH	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BE:171:GLY:HA3	2:BE:205:GLY:H	1.81	0.46
2:BP:21:ASN:HB3	3:BX:181:GLU:CD	2.41	0.46
3:BV:72:LEU:HD22	3:BV:76:TYR:CE2	2.50	0.46
1:A0:223:ASP:CG	3:AV:272:ARG:HH12	2.24	0.46
2:AA:81:VAL:HB	1:AY:86:LYS:HZ1	1.81	0.46
2:AE:19:GLY:HA2	3:AT:166:GLY:C	2.39	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: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
2:AP:21:ASN:CG	3:AX:181:GLU:HG2	2.41	0.46
3:AV:66:GLU:CG	3:BW:120:LYS:HZ3	2.28	0.46
3:AV:196:ILE:HG22	3:AV:293:ARG:HD3	1.98	0.46
3:BV:246:ASP:CG	3:BV:246:ASP:O	2.59	0.46
2:AE:26:LEU:HD13	2:AF:66:TYR:HB2	1.98	0.46
2:AE:171:GLY:HA3	2:AE:205:GLY:H	1.81	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
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
3:AV:246:ASP:CG	3:AV:246:ASP:O	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A0:42:ILE:CB	3:AX:43:TRP:CZ2	2.47	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
2:BG:77:LYS:H	2:BG:82:ASN:ND2	2.12	0.45
2:BO:17:PRO:CB	3:BW:167:ASN:HB2	2.47	0.45
3:BU:206:LYS:HG3	3:BU:285:SER:HB3	1.97	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
1:AZ:230:MET:HE3	1:AZ:320:THR:HG21	1.99	0.45
2:BE:8:PHE:O	3:BT:170:TYR:HB2	2.16	0.45
3:BT:40:ASN:HB3	3:BT:51:MET:HE3	1.99	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
1:A0:329:LEU:HB3	3:AV:261:PHE:CG	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:AU:229:PHE:CE1	3:AU:264:MET:HB3	2.52	0.45
1:B0:1:MET:SD	3:BX:48:ILE:HD13	2.57	0.45
1:B0:78:PRO:HG3	2:BN:103:THR:HB	1.98	0.45
2:BJ:148:ILE:HB	2:BL:153:MET:HG3	1.99	0.45
2:BJ:172:ASN:HD21	2:BJ:204:SER:H	1.63	0.45
3:BT:144:PHE:HB3	3:BT:190:TRP:CE2	2.52	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:BN:52:ASN:ND2	3:BV:258:LEU:HG	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AG:9:PHE:HA	3:AU:160:TYR:HB2	1.98	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
3:AU:144:PHE:HB3	3:AU:190:TRP:CE2	2.52	0.45
3:AW:3:ARG:C	3:AW:3:ARG:HD2	2.42	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
3:BW:40:ASN:HB3	3:BW:51:MET:HE3	1.99	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
3:BX:243:ASP:OD1	3:BX:243:ASP:C	2.60	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
2:BN:171:GLY:HA3	2:BN:205:GLY:H	1.81	0.44
2:BP:19:GLY:HA3	3:BX:180:GLY:O	2.17	0.44
3:BW:194:GLU:HB2	3:BW:293:ARG:HD2	1.99	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
3:AT:40:ASN:HB3	3:AT:51:MET:HE3	1.99	0.44
3:AX:243:ASP:OD1	3:AX:243:ASP:C	2.60	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:BS:197:PHE:HD1	3:BT:48:ILE:CG2	2.30	0.44
3:BT:240:ILE:HG22	3:BT:249:TYR:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:AS:40:ASN:HB3	3:AS:51:MET:HE3	2.00	0.44
3:AU:70:GLU:HG2	3:BX:70:GLU:HG2	1.99	0.44
3:AV:120:LYS:HZ1	3:BW:66:GLU:HG3	1.73	0.44
3:AW:247:GLU:OE1	3:AW:249:TYR:HE2	2.01	0.44
3:AX:120:LYS:CE	3:BU:66:GLU:CG	2.96	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
1:BZ:230:MET:HE3	1:BZ:320:THR:HG21	1.99	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:55:SER:HB3	1:AZ:359:PHE:CE1	2.53	0.44
3:AU:242:THR:CG2	3:AU:272:ARG:CG	2.93	0.44
3:AV:40:ASN:HB3	3:AV:51:MET:HE3	2.00	0.44
3:AV:194:GLU:HB2	3:AV:293:ARG:HD2	1.99	0.44
3:AW:40:ASN:HB3	3:AW:51:MET:HE3	2.00	0.44
3:AX:5:TYR:HB3	3:AX:21:VAL:HG23	2.00	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
2:BB:26:LEU:HD13	2:BC:66:TYR:HB2	1.99	0.44
2:BF:20:SER:HA	3:BT:170:TYR:CD1	2.53	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
3:BV:40:ASN:HB3	3:BV:51:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BX:199:PHE:H	3:BX:242:THR:HG1	1.62	0.44
1:A0:152:PHE:C	1:A0:152:PHE:CD2	2.96	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:AU:40:ASN:HB3	3:AU:51:MET:HE3	2.00	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: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
2:BQ:20:SER:OG	3:BX:165:PRO:O	2.32	0.44
3:BS:40:ASN:HB3	3:BS:51:MET:HE3	2.00	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:49:THR:HB	3:AU:258:LEU:HD21	2.00	0.43
2:AK:114:ASN:O	3:AV:186:ARG:CD	2.66	0.43
2:AM:66:TYR:HB2	2:AO:26:LEU:HD13	1.99	0.43
3:AV:120:LYS:NZ	3:BW:66:GLU:HB3	2.28	0.43
2:BD:39:ARG:HB2	2:BD:61:ILE:HB	2.00	0.43
2:BD:49:THR:CG2	3:BS:233:GLN:HB2	2.49	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
3:BV:48:ILE:HG21	1:BZ:1:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B0:152:PHE:C	1:B0:152:PHE:CD2	2.96	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:AM:9:PHE:HB2	3:AW:180:GLY:HA2	2.01	0.43
2:AO:39:ARG:HB2	2:AO:61:ILE:HB	2.00	0.43
2:AP:65:ARG:HH22	3:AX:181:GLU:CD	2.20	0.43
2:AQ:20:SER:HA	3:AX:160:TYR:CE1	2.53	0.43
3:AV:66:GLU:CG	3:BW:120:LYS:CE	2.95	0.43
2:AG:92:GLN:HE21	3:AU:189:ARG:CZ	2.31	0.43
2:AH:19:GLY:HA2	3:AU:166:GLY:O	2.19	0.43
2:AQ:155:VAL:HG21	2:AQ:159:ILE:HD11	2.01	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
1:AY:152:PHE:C	1:AY:152:PHE:CD2	2.96	0.43
2:BF:155:VAL:HG21	2:BF:159:ILE:HD11	2.01	0.43
3:BU:40:ASN:HB3	3:BU:51:MET:HE3	2.00	0.43
3:BW:3:ARG:HD2	3:BW:3:ARG:C	2.43	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:AK:21:ASN:H	3:AV:181:GLU:HG2	1.83	0.43
2:AP:49:THR:HB	3:AW:258:LEU:HD21	2.00	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:AG:79:ASP:OD1	1:AZ:216:LYS:HB2	2.18	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: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)
2:BP:92:GLN:HE21	3:BX:189:ARG:NE	2.17	0.43
3:BT:43:TRP:HD1	1:BY:42:ILE:HB	1.84	0.43
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
1:BY:121:VAL:HG11	1:BY:175:VAL:HG21	2.01	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:BN:91:THR:HG21	3:BW:189:ARG:HB2	2.01	0.43
2:BR:39:ARG:HB2	2:BR:61:ILE:HB	2.00	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
1:BY:152:PHE:C	1:BY:152:PHE:CD2	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AX:3:ARG:HD2	3:AX:3:ARG:C	2.44	0.42
3:BT:171:ILE:H	3:BT:175:SER:HA	1.84	0.42
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:AD:19:GLY:CA	3:AT:180:GLY:O	2.67	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
3:AU:120:LYS:HZ3	3:BX:66:GLU:CG	2.29	0.42
3:AX:66:GLU:CB	3:BU:120:LYS:HZ3	2.32	0.42
3:BS:34:LEU:HB2	3:BX:114:LYS:HB3	2.00	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
2:AD:147:SER:HB2	2:AE:140:VAL:HG22	2.02	0.42
2:AG:92:GLN:NE2	3:AU:189:ARG:NE	2.67	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
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:BQ:9:PHE:CE1	3:BX:172:LYS:HB2	2.54	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
3:BX:3:ARG:HD2	3:BX:3:ARG:C	2.44	0.42
2:AF:20:SER:HA	3:AT:170:TYR:CD1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BW:196:ILE:HD13	3:BW:291:ILE:HG12	2.02	0.42
3:BW:199:PHE:CE1	3:BW:242:THR:HG21	2.55	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
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
1:B0:38:ARG:NH2	3:BW:269:TYR:O	2.48	0.42
2:BJ:77:LYS:H	2:BJ:82:ASN:ND2	2.12	0.42
2:BK:114:ASN:O	3:BV:186:ARG:CD	2.68	0.42
2:BN:26:LEU:HD13	2:BO:66:TYR:HB2	2.01	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: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: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: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:AV:48:ILE:CG2	1:AZ:1:MET:HE1	2.48	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:266:PHE:CD2	1:AY:35:PRO:HD2	2.55	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
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:99:GLU:OE2	3:BX:73:GLU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:BD:203:MET:SD	2:BD:243:TRP:HB2	2.60	0.41
2:BR:9:PHE:CZ	3:BX:181:GLU:N	2.88	0.41
3:BT:87:LEU:HA	3:BU:54:ARG:HH11	1.85	0.41
3:BT:202:ILE:HG12	3:BT:239:LEU:HD12	2.01	0.41
3:AW:199:PHE:H	3:AW:242:THR:HG1	1.66	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:A0:52:LEU:HD23	1:A0:53:TYR:CE2	2.55	0.41
1:A0:323:ILE:HA	1:A0:363:LEU:O	2.20	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
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:B0:76:VAL:HG21	1:B0:88:LYS:HE3	2.02	0.41
1:B0:288:ARG:CZ	1:BZ:12:PRO:HB2	2.50	0.41
1:B0:323:ILE:HA	1:B0:363:LEU:O	2.20	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:AA:251:THR:HA	2:AA:252:PRO:HD3	1.95	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:B0:152:PHE:C	1:B0:152:PHE:HD2	2.29	0.41
1:B0:330:LEU:HB2	3:BV:261:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:172:ASN:ND2	2:BD:204:SER:H	2.19	0.41
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
2:AR:9:PHE:CE1	3:AX:180:GLY:C	2.99	0.41
3:AS:7:ILE:HG23	3:AS:92:VAL:CG1	2.51	0.41
3:AS:171:ILE:H	3:AS:175:SER:HA	1.86	0.41
3:AT:199:PHE:HB3	3:AT:291:ILE:HD13	2.02	0.41
1:AY:52:LEU:HD23	1:AY:53:TYR:CE2	2.55	0.41
2:BE:9:PHE:CA	3:BT:170:TYR:O	2.61	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
3:BS:3:ARG:HD2	3:BS:3:ARG:C	2.46	0.41
3:BT:115:THR:HG22	3:BU:32:SER:O	2.21	0.41
3:BU:171:ILE:H	3:BU:175:SER:HA	1.86	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:BD:73:THR:HG21	3:BS:256:THR:CG2	2.51	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
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:AE:17:PRO:HB2	3:AT:167:ASN:HD22	1.76	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:11:LEU:O	3:AT:12:ASP:CG	2.64	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: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:AZ:52:LEU:HD23	1:AZ:53:TYR:CE2	2.56	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BP:146:ASP:O	2:BR:151:ASN:HB2	2.21	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:AE:9:PHE:CA	3:AT:170:TYR:O	2.61	0.41
2:AJ:172:ASN:ND2	2:AJ:204:SER:H	2.19	0.41
2:AN:229:THR:HB	2:AO:228:ASP:HB2	2.03	0.41
2:AN:251:THR:HA	2:AN:252:PRO:HD3	1.90	0.41
3:AS:239:LEU:C	3:AS:239:LEU:CD2	2.94	0.41
3:AS:242:THR:HG23	3:AS:272:ARG:HG3	1.89	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:11:LEU:O	3:BT:12:ASP:CG	2.64	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:AG:130:GLY:HA3	1:AZ:218:ILE:HG23	2.02	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
3:AT:68:PHE:CE1	3:BS:120:LYS:HG2	2.56	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:BS:239:LEU:C	3:BS:239:LEU:CD2	2.94	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
1:A0:152:PHE:C	1:A0:152:PHE:HD2	2.29	0.40
2:AG:79:ASP:CB	1:AZ:212:ASN:ND2	2.85	0.40
2:AL:5:ASN:HB3	2:AL:8:PHE:CD1	2.56	0.40
2:AL:10:SER:HA	2:AL:15:GLU:HB2	2.03	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
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
1:A0:3:GLU:CG	3:AW:271:THR:HA	2.51	0.40
2:AP:203:MET:SD	2:AP:243:TRP:HB2	2.61	0.40
2:AQ:19:GLY:C	3:AX:160:TYR:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:3:ARG:C	3:AS:3:ARG:HD2	2.46	0.40
3:AV:240:ILE:CD1	3:AV:242:THR:HG23	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
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:AS:133:ILE:O	3:AT:44:GLN:CD	2.64	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:AS:270:ARG:CZ	1:AY:72:LEU:HD22	2.51	0.40
3:AT:132:ILE:HG21	3:AT:135:LYS:HB2	2.04	0.40
1:B0:292:THR:HB	1:BZ:120:ASP:HB2	2.03	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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	18	55
3	AT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	18	55
3	AU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	18	55
3	AV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	18	55
3	AW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	18	55
3	AX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	18	55
3	BS	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	18	55
3	BT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	18	55
3	BU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	18	55
3	BV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	18	55
3	BW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	18	55
3	BX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	18	55
All	All	15168/15276 (99%)	14418 (95%)	726 (5%)	24 (0%)	43	77

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

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Mol	Chain	Res	Type
3	BV	175	SER
3	BW	175	SER
3	BX	175	SER
3	AS	136	TRP
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 ⓘ

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%)	323 (96%)	14 (4%)	26	48	
1	AY	337/337 (100%)	319 (95%)	18 (5%)	20	40	
1	AZ	337/337 (100%)	318 (94%)	19 (6%)	19	39	
1	B0	337/337 (100%)	323 (96%)	14 (4%)	26	48	
1	BY	337/337 (100%)	319 (95%)	18 (5%)	20	40	
1	BZ	337/337 (100%)	318 (94%)	19 (6%)	19	39	
2	AA	227/227 (100%)	217 (96%)	10 (4%)	25	46	
2	AB	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AC	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AD	227/227 (100%)	219 (96%)	8 (4%)	32	53	
2	AE	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AF	227/227 (100%)	223 (98%)	4 (2%)	51	66	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	AG	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	AH	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AI	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AJ	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	AK	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AL	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AM	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	AN	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AO	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AP	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	AQ	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	AR	227/227 (100%)	222 (98%)	5 (2%)	45	63	
2	BA	227/227 (100%)	217 (96%)	10 (4%)	25	46	
2	BB	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BC	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BD	227/227 (100%)	219 (96%)	8 (4%)	32	53	
2	BE	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BF	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BG	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	BH	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BI	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BJ	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	BK	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BL	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BM	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	BN	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BO	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BP	227/227 (100%)	218 (96%)	9 (4%)	28	48	
2	BQ	227/227 (100%)	223 (98%)	4 (2%)	51	66	
2	BR	227/227 (100%)	222 (98%)	5 (2%)	45	63	
3	AS	264/265 (100%)	240 (91%)	24 (9%)	9	27	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AT	264/265 (100%)	242 (92%)	22 (8%)	10	30
3	AU	264/265 (100%)	235 (89%)	29 (11%)	6	20
3	AV	264/265 (100%)	234 (89%)	30 (11%)	5	19
3	AW	264/265 (100%)	231 (88%)	33 (12%)	4	16
3	AX	264/265 (100%)	240 (91%)	24 (9%)	9	27
3	BS	264/265 (100%)	240 (91%)	24 (9%)	9	27
3	BT	264/265 (100%)	242 (92%)	22 (8%)	10	30
3	BU	264/265 (100%)	235 (89%)	29 (11%)	6	20
3	BV	264/265 (100%)	235 (89%)	29 (11%)	6	20
3	BW	264/265 (100%)	231 (88%)	33 (12%)	4	16
3	BX	264/265 (100%)	240 (91%)	24 (9%)	9	27
All	All	13362/13374 (100%)	12731 (95%)	631 (5%)	23	44

All (631) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	2	LEU
1	A0	8	ASP
1	A0	40	GLN
1	A0	42	ILE
1	A0	88	LYS
1	A0	96	LEU
1	A0	152	PHE
1	A0	224	ILE
1	A0	238	ARG
1	A0	286	ASP
1	A0	313	ILE
1	A0	319	VAL
1	A0	330	LEU
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	79	ASP
2	AA	93	THR
2	AA	124	ASP

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Mol	Chain	Res	Type
2	AA	202	ASN
2	AA	233	ILE
2	AB	38	ILE
2	AB	84	ILE
2	AB	206	THR
2	AB	232	HIS
2	AC	7	THR
2	AC	38	ILE
2	AC	125	ILE
2	AC	232	HIS
2	AD	9	PHE
2	AD	18	VAL
2	AD	38	ILE
2	AD	79	ASP
2	AD	93	THR
2	AD	124	ASP
2	AD	202	ASN
2	AD	233	ILE
2	AE	38	ILE
2	AE	84	ILE
2	AE	206	THR
2	AE	232	HIS
2	AF	7	THR
2	AF	38	ILE
2	AF	125	ILE
2	AF	232	HIS
2	AG	7	THR
2	AG	9	PHE
2	AG	18	VAL
2	AG	38	ILE
2	AG	79	ASP
2	AG	93	THR
2	AG	124	ASP
2	AG	202	ASN
2	AG	233	ILE
2	AH	38	ILE
2	AH	84	ILE
2	AH	206	THR
2	AH	232	HIS
2	AI	7	THR
2	AI	38	ILE
2	AI	125	ILE

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Mol	Chain	Res	Type
2	AI	232	HIS
2	AJ	7	THR
2	AJ	9	PHE
2	AJ	18	VAL
2	AJ	38	ILE
2	AJ	79	ASP
2	AJ	93	THR
2	AJ	124	ASP
2	AJ	202	ASN
2	AJ	233	ILE
2	AK	38	ILE
2	AK	84	ILE
2	AK	206	THR
2	AK	232	HIS
2	AL	26	LEU
2	AL	38	ILE
2	AL	125	ILE
2	AL	232	HIS
2	AM	7	THR
2	AM	9	PHE
2	AM	18	VAL
2	AM	38	ILE
2	AM	79	ASP
2	AM	93	THR
2	AM	124	ASP
2	AM	202	ASN
2	AM	233	ILE
2	AN	38	ILE
2	AN	84	ILE
2	AN	206	THR
2	AN	232	HIS
2	AO	7	THR
2	AO	38	ILE
2	AO	125	ILE
2	AO	232	HIS
2	AP	7	THR
2	AP	9	PHE
2	AP	18	VAL
2	AP	38	ILE
2	AP	79	ASP
2	AP	93	THR
2	AP	124	ASP

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Mol	Chain	Res	Type
2	AP	202	ASN
2	AP	233	ILE
2	AQ	38	ILE
2	AQ	84	ILE
2	AQ	206	THR
2	AQ	232	HIS
2	AR	7	THR
2	AR	26	LEU
2	AR	38	ILE
2	AR	125	ILE
2	AR	232	HIS
3	AS	2	VAL
3	AS	11	LEU
3	AS	26	VAL
3	AS	43	TRP
3	AS	48	ILE
3	AS	54	ARG
3	AS	55	SER
3	AS	64	LYS
3	AS	66	GLU
3	AS	72	LEU
3	AS	109	LEU
3	AS	123	THR
3	AS	142	LEU
3	AS	159	ILE
3	AS	171	ILE
3	AS	196	ILE
3	AS	227	ILE
3	AS	228	VAL
3	AS	234	VAL
3	AS	256	THR
3	AS	263	VAL
3	AS	270	ARG
3	AS	291	ILE
3	AS	294	LYS
3	AT	2	VAL
3	AT	11	LEU
3	AT	26	VAL
3	AT	36	LEU
3	AT	48	ILE
3	AT	55	SER
3	AT	64	LYS

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Mol	Chain	Res	Type
3	AT	65	LEU
3	AT	72	LEU
3	AT	123	THR
3	AT	135	LYS
3	AT	159	ILE
3	AT	169	LYS
3	AT	171	ILE
3	AT	196	ILE
3	AT	203	LEU
3	AT	234	VAL
3	AT	236	ASP
3	AT	239	LEU
3	AT	243	ASP
3	AT	263	VAL
3	AT	294	LYS
3	AU	2	VAL
3	AU	3	ARG
3	AU	11	LEU
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	64	LYS
3	AU	66	GLU
3	AU	72	LEU
3	AU	135	LYS
3	AU	142	LEU
3	AU	159	ILE
3	AU	171	ILE
3	AU	196	ILE
3	AU	228	VAL
3	AU	232	GLU
3	AU	234	VAL
3	AU	244	VAL
3	AU	256	THR
3	AU	258	LEU
3	AU	263	VAL
3	AU	282	ILE

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Mol	Chain	Res	Type
3	AU	291	ILE
3	AU	294	LYS
3	AV	2	VAL
3	AV	11	LEU
3	AV	36	LEU
3	AV	48	ILE
3	AV	54	ARG
3	AV	55	SER
3	AV	64	LYS
3	AV	66	GLU
3	AV	72	LEU
3	AV	120	LYS
3	AV	135	LYS
3	AV	142	LEU
3	AV	143	THR
3	AV	159	ILE
3	AV	169	LYS
3	AV	196	ILE
3	AV	203	LEU
3	AV	215	ARG
3	AV	227	ILE
3	AV	232	GLU
3	AV	234	VAL
3	AV	240	ILE
3	AV	243	ASP
3	AV	246	ASP
3	AV	256	THR
3	AV	258	LEU
3	AV	263	VAL
3	AV	282	ILE
3	AV	291	ILE
3	AV	294	LYS
3	AW	2	VAL
3	AW	6	LYS
3	AW	11	LEU
3	AW	26	VAL
3	AW	43	TRP
3	AW	48	ILE
3	AW	54	ARG
3	AW	55	SER
3	AW	64	LYS
3	AW	66	GLU

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Mol	Chain	Res	Type
3	AW	72	LEU
3	AW	92	VAL
3	AW	109	LEU
3	AW	123	THR
3	AW	143	THR
3	AW	159	ILE
3	AW	169	LYS
3	AW	171	ILE
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	244	VAL
3	AW	248	THR
3	AW	256	THR
3	AW	258	LEU
3	AW	263	VAL
3	AW	270	ARG
3	AW	282	ILE
3	AW	291	ILE
3	AW	294	LYS
3	AX	2	VAL
3	AX	11	LEU
3	AX	26	VAL
3	AX	36	LEU
3	AX	43	TRP
3	AX	48	ILE
3	AX	54	ARG
3	AX	64	LYS
3	AX	66	GLU
3	AX	107	LEU
3	AX	142	LEU
3	AX	159	ILE
3	AX	169	LYS
3	AX	171	ILE
3	AX	196	ILE
3	AX	200	MET
3	AX	203	LEU
3	AX	228	VAL
3	AX	234	VAL

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Mol	Chain	Res	Type
3	AX	243	ASP
3	AX	244	VAL
3	AX	258	LEU
3	AX	263	VAL
3	AX	291	ILE
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	96	LEU
1	AY	152	PHE
1	AY	192	GLN
1	AY	242	ASN
1	AY	243	PHE
1	AY	286	ASP
1	AY	306	LEU
1	AY	313	ILE
1	AY	319	VAL
1	AY	330	LEU
1	AY	340	ILE
1	AY	360	ASN
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	96	LEU
1	AZ	151	PHE
1	AZ	165	ARG
1	AZ	207	ASN
1	AZ	218	ILE
1	AZ	238	ARG
1	AZ	286	ASP
1	AZ	313	ILE
1	AZ	319	VAL
1	AZ	320	THR
1	AZ	340	ILE
1	AZ	360	ASN

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Mol	Chain	Res	Type
1	B0	2	LEU
1	B0	8	ASP
1	B0	40	GLN
1	B0	42	ILE
1	B0	88	LYS
1	B0	96	LEU
1	B0	152	PHE
1	B0	224	ILE
1	B0	238	ARG
1	B0	286	ASP
1	B0	313	ILE
1	B0	319	VAL
1	B0	330	LEU
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	79	ASP
2	BA	93	THR
2	BA	124	ASP
2	BA	202	ASN
2	BA	233	ILE
2	BB	38	ILE
2	BB	84	ILE
2	BB	206	THR
2	BB	232	HIS
2	BC	7	THR
2	BC	38	ILE
2	BC	125	ILE
2	BC	232	HIS
2	BD	9	PHE
2	BD	18	VAL
2	BD	38	ILE
2	BD	79	ASP
2	BD	93	THR
2	BD	124	ASP
2	BD	202	ASN
2	BD	233	ILE
2	BE	38	ILE
2	BE	84	ILE

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Mol	Chain	Res	Type
2	BE	206	THR
2	BE	232	HIS
2	BF	7	THR
2	BF	38	ILE
2	BF	125	ILE
2	BF	232	HIS
2	BG	7	THR
2	BG	9	PHE
2	BG	18	VAL
2	BG	38	ILE
2	BG	79	ASP
2	BG	93	THR
2	BG	124	ASP
2	BG	202	ASN
2	BG	233	ILE
2	BH	38	ILE
2	BH	84	ILE
2	BH	206	THR
2	BH	232	HIS
2	BI	7	THR
2	BI	38	ILE
2	BI	125	ILE
2	BI	232	HIS
2	BJ	7	THR
2	BJ	9	PHE
2	BJ	18	VAL
2	BJ	38	ILE
2	BJ	79	ASP
2	BJ	93	THR
2	BJ	124	ASP
2	BJ	202	ASN
2	BJ	233	ILE
2	BK	38	ILE
2	BK	84	ILE
2	BK	206	THR
2	BK	232	HIS
2	BL	26	LEU
2	BL	38	ILE
2	BL	125	ILE
2	BL	232	HIS
2	BM	7	THR
2	BM	9	PHE

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Mol	Chain	Res	Type
2	BM	18	VAL
2	BM	38	ILE
2	BM	79	ASP
2	BM	93	THR
2	BM	124	ASP
2	BM	202	ASN
2	BM	233	ILE
2	BN	38	ILE
2	BN	84	ILE
2	BN	206	THR
2	BN	232	HIS
2	BO	7	THR
2	BO	38	ILE
2	BO	125	ILE
2	BO	232	HIS
2	BP	7	THR
2	BP	9	PHE
2	BP	18	VAL
2	BP	38	ILE
2	BP	79	ASP
2	BP	93	THR
2	BP	124	ASP
2	BP	202	ASN
2	BP	233	ILE
2	BQ	38	ILE
2	BQ	84	ILE
2	BQ	206	THR
2	BQ	232	HIS
2	BR	7	THR
2	BR	26	LEU
2	BR	38	ILE
2	BR	125	ILE
2	BR	232	HIS
3	BS	2	VAL
3	BS	11	LEU
3	BS	26	VAL
3	BS	43	TRP
3	BS	48	ILE
3	BS	54	ARG
3	BS	55	SER
3	BS	64	LYS
3	BS	66	GLU

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Mol	Chain	Res	Type
3	BS	72	LEU
3	BS	109	LEU
3	BS	123	THR
3	BS	142	LEU
3	BS	159	ILE
3	BS	171	ILE
3	BS	196	ILE
3	BS	227	ILE
3	BS	228	VAL
3	BS	234	VAL
3	BS	256	THR
3	BS	263	VAL
3	BS	270	ARG
3	BS	291	ILE
3	BS	294	LYS
3	BT	2	VAL
3	BT	11	LEU
3	BT	26	VAL
3	BT	36	LEU
3	BT	48	ILE
3	BT	55	SER
3	BT	64	LYS
3	BT	65	LEU
3	BT	72	LEU
3	BT	123	THR
3	BT	135	LYS
3	BT	159	ILE
3	BT	169	LYS
3	BT	171	ILE
3	BT	196	ILE
3	BT	203	LEU
3	BT	234	VAL
3	BT	236	ASP
3	BT	239	LEU
3	BT	243	ASP
3	BT	263	VAL
3	BT	294	LYS
3	BU	2	VAL
3	BU	3	ARG
3	BU	11	LEU
3	BU	26	VAL
3	BU	37	GLN

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Mol	Chain	Res	Type
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	64	LYS
3	BU	66	GLU
3	BU	72	LEU
3	BU	135	LYS
3	BU	142	LEU
3	BU	159	ILE
3	BU	171	ILE
3	BU	196	ILE
3	BU	228	VAL
3	BU	232	GLU
3	BU	234	VAL
3	BU	244	VAL
3	BU	256	THR
3	BU	258	LEU
3	BU	263	VAL
3	BU	282	ILE
3	BU	291	ILE
3	BU	294	LYS
3	BV	2	VAL
3	BV	11	LEU
3	BV	36	LEU
3	BV	48	ILE
3	BV	54	ARG
3	BV	55	SER
3	BV	64	LYS
3	BV	66	GLU
3	BV	72	LEU
3	BV	120	LYS
3	BV	135	LYS
3	BV	142	LEU
3	BV	143	THR
3	BV	159	ILE
3	BV	169	LYS
3	BV	196	ILE
3	BV	203	LEU
3	BV	227	ILE

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Mol	Chain	Res	Type
3	BV	232	GLU
3	BV	234	VAL
3	BV	240	ILE
3	BV	243	ASP
3	BV	246	ASP
3	BV	256	THR
3	BV	258	LEU
3	BV	263	VAL
3	BV	282	ILE
3	BV	291	ILE
3	BV	294	LYS
3	BW	2	VAL
3	BW	6	LYS
3	BW	11	LEU
3	BW	26	VAL
3	BW	43	TRP
3	BW	48	ILE
3	BW	54	ARG
3	BW	55	SER
3	BW	64	LYS
3	BW	66	GLU
3	BW	72	LEU
3	BW	92	VAL
3	BW	109	LEU
3	BW	123	THR
3	BW	143	THR
3	BW	159	ILE
3	BW	169	LYS
3	BW	171	ILE
3	BW	196	ILE
3	BW	197	PHE
3	BW	203	LEU
3	BW	228	VAL
3	BW	232	GLU
3	BW	234	VAL
3	BW	244	VAL
3	BW	248	THR
3	BW	256	THR
3	BW	258	LEU
3	BW	263	VAL
3	BW	270	ARG
3	BW	282	ILE

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Mol	Chain	Res	Type
3	BW	291	ILE
3	BW	294	LYS
3	BX	2	VAL
3	BX	11	LEU
3	BX	26	VAL
3	BX	36	LEU
3	BX	43	TRP
3	BX	48	ILE
3	BX	54	ARG
3	BX	64	LYS
3	BX	66	GLU
3	BX	107	LEU
3	BX	142	LEU
3	BX	159	ILE
3	BX	169	LYS
3	BX	171	ILE
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	8	ASP
1	BY	26	LYS
1	BY	40	GLN
1	BY	41	VAL
1	BY	87	LYS
1	BY	88	LYS
1	BY	96	LEU
1	BY	152	PHE
1	BY	192	GLN
1	BY	242	ASN
1	BY	243	PHE
1	BY	286	ASP
1	BY	306	LEU
1	BY	313	ILE
1	BY	319	VAL
1	BY	330	LEU

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Mol	Chain	Res	Type
1	BY	340	ILE
1	BY	360	ASN
1	BZ	2	LEU
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	96	LEU
1	BZ	151	PHE
1	BZ	165	ARG
1	BZ	207	ASN
1	BZ	218	ILE
1	BZ	238	ARG
1	BZ	286	ASP
1	BZ	313	ILE
1	BZ	319	VAL
1	BZ	320	THR
1	BZ	340	ILE
1	BZ	360	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (318) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	11	ASN
1	A0	43	ASN
1	A0	184	GLN
1	A0	193	HIS
1	A0	214	ASN
1	A0	267	ASN
2	AA	48	ASN
2	AA	71	ASN
2	AA	82	ASN
2	AA	172	ASN
2	AA	196	ASN
2	AA	236	ASN
2	AB	48	ASN
2	AB	57	ASN
2	AB	164	GLN
2	AB	177	GLN
2	AB	183	ASN

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Mol	Chain	Res	Type
2	AC	54	GLN
2	AC	57	ASN
2	AC	71	ASN
2	AC	172	ASN
2	AC	236	ASN
2	AD	48	ASN
2	AD	52	ASN
2	AD	57	ASN
2	AD	71	ASN
2	AD	82	ASN
2	AD	92	GLN
2	AD	172	ASN
2	AD	196	ASN
2	AD	236	ASN
2	AE	57	ASN
2	AE	164	GLN
2	AE	177	GLN
2	AF	54	GLN
2	AF	57	ASN
2	AF	71	ASN
2	AF	172	ASN
2	AF	236	ASN
2	AG	48	ASN
2	AG	57	ASN
2	AG	71	ASN
2	AG	82	ASN
2	AG	92	GLN
2	AG	172	ASN
2	AG	196	ASN
2	AG	236	ASN
2	AH	48	ASN
2	AH	57	ASN
2	AH	164	GLN
2	AH	177	GLN
2	AH	218	GLN
2	AI	57	ASN
2	AI	172	ASN
2	AI	258	ASN
2	AJ	48	ASN
2	AJ	57	ASN
2	AJ	71	ASN
2	AJ	82	ASN

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Mol	Chain	Res	Type
2	AJ	172	ASN
2	AJ	196	ASN
2	AJ	236	ASN
2	AK	57	ASN
2	AK	164	GLN
2	AK	177	GLN
2	AL	54	GLN
2	AL	71	ASN
2	AL	172	ASN
2	AL	236	ASN
2	AM	48	ASN
2	AM	57	ASN
2	AM	71	ASN
2	AM	82	ASN
2	AM	172	ASN
2	AM	196	ASN
2	AM	236	ASN
2	AN	48	ASN
2	AN	57	ASN
2	AN	92	GLN
2	AN	164	GLN
2	AN	177	GLN
2	AN	218	GLN
2	AO	54	GLN
2	AO	57	ASN
2	AO	71	ASN
2	AO	172	ASN
2	AO	236	ASN
2	AO	258	ASN
2	AP	5	ASN
2	AP	22	ASN
2	AP	48	ASN
2	AP	57	ASN
2	AP	71	ASN
2	AP	82	ASN
2	AP	92	GLN
2	AP	172	ASN
2	AP	196	ASN
2	AP	236	ASN
2	AQ	48	ASN
2	AQ	57	ASN
2	AQ	164	GLN

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Mol	Chain	Res	Type
2	AQ	177	GLN
2	AR	54	GLN
2	AR	57	ASN
2	AR	71	ASN
2	AR	172	ASN
2	AR	236	ASN
3	AS	102	GLN
3	AS	233	GLN
3	AS	250	GLN
3	AS	259	ASN
3	AT	4	GLN
3	AT	23	ASN
3	AT	77	GLN
3	AT	141	ASN
3	AT	167	ASN
3	AT	235	GLN
3	AT	259	ASN
3	AU	23	ASN
3	AU	75	ASN
3	AU	97	GLN
3	AU	141	ASN
3	AU	250	GLN
3	AU	259	ASN
3	AV	23	ASN
3	AV	77	GLN
3	AV	97	GLN
3	AV	121	ASN
3	AV	141	ASN
3	AV	235	GLN
3	AV	250	GLN
3	AV	259	ASN
3	AW	77	GLN
3	AW	121	ASN
3	AW	235	GLN
3	AW	245	ASN
3	AW	259	ASN
3	AX	121	ASN
3	AX	141	ASN
3	AX	167	ASN
3	AX	233	GLN
3	AX	235	GLN
3	AX	250	GLN

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Mol	Chain	Res	Type
3	AX	259	ASN
3	AX	278	GLN
1	AY	11	ASN
1	AY	24	ASN
1	AY	90	ASN
1	AY	123	ASN
1	AY	164	ASN
1	AY	186	GLN
1	AY	214	ASN
1	AY	267	ASN
1	AZ	11	ASN
1	AZ	16	ASN
1	AZ	24	ASN
1	AZ	90	ASN
1	AZ	130	ASN
1	AZ	164	ASN
1	AZ	184	GLN
1	AZ	192	GLN
1	AZ	193	HIS
1	AZ	212	ASN
1	AZ	214	ASN
1	AZ	267	ASN
1	B0	11	ASN
1	B0	43	ASN
1	B0	143	ASN
1	B0	184	GLN
1	B0	193	HIS
1	B0	214	ASN
1	B0	267	ASN
2	BA	48	ASN
2	BA	71	ASN
2	BA	82	ASN
2	BA	172	ASN
2	BA	236	ASN
2	BB	48	ASN
2	BB	57	ASN
2	BB	164	GLN
2	BB	177	GLN
2	BC	54	GLN
2	BC	57	ASN
2	BC	71	ASN
2	BC	172	ASN

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Mol	Chain	Res	Type
2	BC	236	ASN
2	BD	48	ASN
2	BD	52	ASN
2	BD	57	ASN
2	BD	71	ASN
2	BD	82	ASN
2	BD	172	ASN
2	BD	196	ASN
2	BD	236	ASN
2	BE	57	ASN
2	BE	164	GLN
2	BE	177	GLN
2	BF	54	GLN
2	BF	57	ASN
2	BF	71	ASN
2	BF	172	ASN
2	BF	236	ASN
2	BG	48	ASN
2	BG	57	ASN
2	BG	71	ASN
2	BG	82	ASN
2	BG	92	GLN
2	BG	172	ASN
2	BG	196	ASN
2	BG	236	ASN
2	BH	48	ASN
2	BH	57	ASN
2	BH	177	GLN
2	BH	218	GLN
2	BI	57	ASN
2	BI	172	ASN
2	BI	258	ASN
2	BJ	48	ASN
2	BJ	57	ASN
2	BJ	71	ASN
2	BJ	82	ASN
2	BJ	172	ASN
2	BJ	196	ASN
2	BJ	236	ASN
2	BK	48	ASN
2	BK	57	ASN
2	BK	164	GLN

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Mol	Chain	Res	Type
2	BL	57	ASN
2	BL	172	ASN
2	BM	48	ASN
2	BM	57	ASN
2	BM	71	ASN
2	BM	82	ASN
2	BM	172	ASN
2	BM	196	ASN
2	BM	236	ASN
2	BN	48	ASN
2	BN	57	ASN
2	BN	92	GLN
2	BN	164	GLN
2	BN	218	GLN
2	BO	57	ASN
2	BO	172	ASN
2	BO	236	ASN
2	BO	258	ASN
2	BP	22	ASN
2	BP	48	ASN
2	BP	57	ASN
2	BP	71	ASN
2	BP	82	ASN
2	BP	92	GLN
2	BP	172	ASN
2	BP	196	ASN
2	BP	236	ASN
2	BP	258	ASN
2	BQ	57	ASN
2	BQ	164	GLN
2	BQ	177	GLN
2	BR	54	GLN
2	BR	57	ASN
2	BR	71	ASN
2	BR	172	ASN
2	BR	236	ASN
3	BS	102	GLN
3	BS	141	ASN
3	BS	250	GLN
3	BS	259	ASN
3	BT	4	GLN
3	BT	23	ASN

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Mol	Chain	Res	Type
3	BT	141	ASN
3	BT	167	ASN
3	BT	235	GLN
3	BT	259	ASN
3	BU	23	ASN
3	BU	37	GLN
3	BU	75	ASN
3	BU	97	GLN
3	BU	141	ASN
3	BU	250	GLN
3	BU	259	ASN
3	BV	23	ASN
3	BV	77	GLN
3	BV	97	GLN
3	BV	121	ASN
3	BV	141	ASN
3	BV	235	GLN
3	BV	250	GLN
3	BV	259	ASN
3	BW	77	GLN
3	BW	121	ASN
3	BW	235	GLN
3	BW	245	ASN
3	BX	121	ASN
3	BX	141	ASN
3	BX	167	ASN
3	BX	233	GLN
3	BX	235	GLN
3	BX	250	GLN
3	BX	259	ASN
1	BY	11	ASN
1	BY	24	ASN
1	BY	90	ASN
1	BY	123	ASN
1	BY	164	ASN
1	BY	186	GLN
1	BY	214	ASN
1	BY	267	ASN
1	BZ	11	ASN
1	BZ	16	ASN
1	BZ	24	ASN
1	BZ	90	ASN

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Mol	Chain	Res	Type
1	BZ	130	ASN
1	BZ	164	ASN
1	BZ	184	GLN
1	BZ	192	GLN
1	BZ	212	ASN
1	BZ	214	ASN
1	BZ	267	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A0	372/372 (100%)	0.00	11 (2%)	52	44	351, 388, 435, 523	0
1	AY	372/372 (100%)	0.06	13 (3%)	47	42	359, 396, 449, 555	0
1	AZ	372/372 (100%)	0.08	20 (5%)	31	32	364, 394, 444, 557	0
1	B0	372/372 (100%)	0.03	6 (1%)	70	58	337, 377, 425, 485	0
1	BY	372/372 (100%)	-0.08	6 (1%)	70	58	331, 361, 429, 557	0
1	BZ	372/372 (100%)	-0.04	12 (3%)	50	43	332, 360, 422, 502	0
2	AA	263/263 (100%)	-0.13	5 (1%)	66	55	248, 312, 407, 435	0
2	AB	263/263 (100%)	-0.05	11 (4%)	40	38	284, 350, 440, 481	0
2	AC	263/263 (100%)	-0.02	11 (4%)	40	38	257, 345, 417, 473	0
2	AD	263/263 (100%)	0.02	8 (3%)	52	44	258, 320, 441, 485	0
2	AE	263/263 (100%)	-0.07	8 (3%)	52	44	277, 344, 466, 480	0
2	AF	263/263 (100%)	-0.02	12 (4%)	37	36	265, 367, 471, 497	0
2	AG	263/263 (100%)	0.11	17 (6%)	25	28	265, 348, 500, 556	0
2	AH	263/263 (100%)	-0.09	6 (2%)	61	51	315, 402, 524, 572	0
2	AI	263/263 (100%)	0.17	18 (6%)	23	27	282, 416, 532, 576	0
2	AJ	263/263 (100%)	-0.05	9 (3%)	48	42	264, 342, 429, 539	0
2	AK	263/263 (100%)	-0.20	4 (1%)	72	59	255, 301, 456, 521	0
2	AL	263/263 (100%)	-0.03	19 (7%)	21	25	277, 345, 485, 575	0
2	AM	263/263 (100%)	-0.05	8 (3%)	52	44	266, 358, 425, 467	0
2	AN	263/263 (100%)	-0.03	9 (3%)	48	42	252, 313, 386, 420	0
2	AO	263/263 (100%)	0.03	9 (3%)	48	42	276, 347, 419, 449	0
2	AP	263/263 (100%)	0.12	16 (6%)	27	30	267, 341, 556, 576	0
2	AQ	263/263 (100%)	0.02	18 (6%)	23	27	295, 397, 566, 605	0
2	AR	263/263 (100%)	0.12	10 (3%)	44	40	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%)	-0.10	6 (2%) 61 51	259, 312, 430, 466	0
2	BB	263/263 (100%)	-0.25	4 (1%) 72 59	282, 346, 455, 506	0
2	BC	263/263 (100%)	-0.02	17 (6%) 25 28	273, 344, 419, 481	0
2	BD	263/263 (100%)	-0.09	7 (2%) 56 47	252, 316, 445, 484	0
2	BE	263/263 (100%)	-0.15	10 (3%) 44 40	274, 342, 448, 477	0
2	BF	263/263 (100%)	0.09	11 (4%) 40 38	258, 361, 457, 487	0
2	BG	263/263 (100%)	0.04	15 (5%) 29 31	252, 346, 496, 557	0
2	BH	263/263 (100%)	-0.15	10 (3%) 44 40	314, 408, 514, 559	0
2	BI	263/263 (100%)	-0.17	4 (1%) 72 59	276, 420, 541, 584	0
2	BJ	263/263 (100%)	-0.19	8 (3%) 52 44	268, 345, 419, 521	0
2	BK	263/263 (100%)	-0.16	3 (1%) 78 65	256, 305, 435, 496	0
2	BL	263/263 (100%)	-0.29	2 (0%) 82 71	283, 341, 452, 534	0
2	BM	263/263 (100%)	-0.10	8 (3%) 52 44	264, 357, 438, 484	0
2	BN	263/263 (100%)	-0.06	9 (3%) 48 42	255, 316, 388, 433	0
2	BO	263/263 (100%)	-0.05	9 (3%) 48 42	276, 348, 418, 453	0
2	BP	263/263 (100%)	0.05	11 (4%) 40 38	261, 365, 541, 549	0
2	BQ	263/263 (100%)	-0.25	3 (1%) 78 65	312, 413, 547, 559	0
2	BR	263/263 (100%)	-0.02	10 (3%) 44 40	308, 418, 537, 556	0
3	AS	298/298 (100%)	-0.06	6 (2%) 65 54	219, 262, 346, 379	0
3	AT	298/298 (100%)	-0.10	4 (1%) 75 62	230, 260, 318, 344	0
3	AU	298/298 (100%)	-0.21	6 (2%) 65 54	228, 269, 334, 364	0
3	AV	298/298 (100%)	-0.06	10 (3%) 48 42	229, 264, 317, 332	0
3	AW	298/298 (100%)	-0.16	2 (0%) 84 72	213, 254, 317, 347	0
3	AX	298/298 (100%)	-0.18	5 (1%) 69 57	216, 255, 347, 401	0
3	BS	298/298 (100%)	-0.17	1 (0%) 90 81	222, 256, 339, 388	0
3	BT	298/298 (100%)	-0.17	3 (1%) 79 66	218, 265, 316, 343	0
3	BU	298/298 (100%)	-0.25	2 (0%) 84 72	228, 262, 338, 382	0
3	BV	298/298 (100%)	-0.14	3 (1%) 79 66	218, 260, 305, 324	0
3	BW	298/298 (100%)	-0.19	2 (0%) 84 72	215, 256, 341, 403	0
3	BX	298/298 (100%)	-0.16	8 (2%) 56 47	228, 272, 370, 407	0
All	All	15276/15276 (100%)	-0.07	465 (3%) 52 44	213, 344, 468, 605	0

All (465) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AM	259	GLY	8.8
2	BO	260	SER	7.0
2	AO	259	GLY	6.9
2	BH	260	SER	6.6
2	BC	257	GLY	6.5
2	AP	222	GLY	6.2
2	AC	184	ASP	6.2
2	AG	167	THR	6.1
2	AR	258	ASN	6.1
2	BN	260	SER	6.0
2	BP	117	GLY	5.9
1	AY	18	SER	5.9
2	AQ	95	ASN	5.9
1	BY	270	ASP	5.8
2	AR	255	THR	5.8
2	AC	45	SER	5.8
2	BM	260	SER	5.7
2	AR	221	VAL	5.4
2	AQ	259	GLY	5.4
2	AI	109	GLY	5.3
2	BF	222	GLY	5.3
2	BM	258	ASN	5.2
2	AI	62	ALA	5.2
2	AG	190	PHE	5.2
2	BP	254	ALA	5.1
2	AG	23	ASP	5.1
2	BP	255	THR	5.0
2	BC	259	GLY	5.0
2	AP	223	HIS	4.9
2	AL	63	GLY	4.9
2	AI	173	GLY	4.9
1	A0	196	SER	4.8
2	BF	252	PRO	4.8
2	BL	197	ILE	4.8
2	AD	64	GLY	4.8
2	AQ	218	GLN	4.8
2	AM	260	SER	4.7
2	AF	259	GLY	4.7
2	BC	190	PHE	4.7
2	BD	179	THR	4.7
2	AI	31	THR	4.7
2	BC	258	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
2	AP	100	SER	4.6
2	AG	256	ARG	4.6
2	AG	191	PHE	4.6
1	AY	132	ALA	4.5
2	AQ	94	ALA	4.5
2	BM	167	THR	4.4
2	AQ	260	SER	4.4
2	BN	261	TYR	4.4
1	A0	32	LEU	4.3
2	AI	36	ARG	4.2
2	AI	107	SER	4.2
2	BI	186	VAL	4.2
2	AC	183	ASN	4.2
1	BZ	244	ALA	4.2
2	BG	62	ALA	4.2
2	BH	259	GLY	4.2
2	BG	257	GLY	4.1
3	BX	298	VAL	4.1
3	AS	204	TYR	4.1
2	BF	258	ASN	4.1
2	BE	260	SER	4.1
2	BR	71	ASN	4.0
1	AY	162	THR	4.0
2	AD	63	GLY	4.0
3	AT	288	GLU	4.0
2	AQ	98	SER	3.9
1	AY	129	THR	3.9
2	AB	87	ASN	3.9
2	BR	3	ILE	3.9
2	AO	130	GLY	3.9
2	BF	49	THR	3.9
2	AO	184	ASP	3.9
2	AI	63	GLY	3.9
2	BE	221	VAL	3.8
2	AM	220	LEU	3.8
2	AI	121	VAL	3.8
2	AQ	246	ALA	3.8
2	AB	255	THR	3.8
2	BO	259	GLY	3.8
2	AO	182	ASN	3.7
1	BZ	140	PRO	3.7
2	BF	50	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	BG	190	PHE	3.7
3	BV	139	TYR	3.7
2	AG	208	VAL	3.7
2	AR	232	HIS	3.7
2	BA	258	ASN	3.7
2	BH	258	ASN	3.7
2	AP	221	VAL	3.6
2	AM	219	SER	3.6
2	BM	257	GLY	3.6
2	AO	185	LEU	3.6
2	BA	257	GLY	3.6
2	BD	187	ILE	3.6
2	AO	260	SER	3.6
2	AO	8	PHE	3.6
2	AN	258	ASN	3.6
1	B0	280	ASP	3.5
3	AV	287	ALA	3.5
2	BM	259	GLY	3.5
2	AN	185	LEU	3.5
2	AF	219	SER	3.5
2	AG	24	GLY	3.5
2	BN	186	VAL	3.5
2	AC	249	ASP	3.5
2	AF	260	SER	3.5
1	A0	276	THR	3.5
2	BB	259	GLY	3.5
2	AQ	258	ASN	3.5
3	BX	258	LEU	3.4
2	AP	254	ALA	3.4
2	BA	259	GLY	3.4
2	BP	88	ILE	3.4
2	AB	86	ALA	3.4
1	A0	330	LEU	3.4
2	BN	184	ASP	3.4
2	AI	65	ARG	3.4
2	BE	259	GLY	3.4
2	BN	185	LEU	3.4
1	AY	19	ASP	3.3
2	AN	260	SER	3.3
2	AG	114	ASN	3.3
1	BY	286	ASP	3.3
2	AE	249	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A0	202	ASN	3.3
2	AF	222	GLY	3.3
3	AV	190	TRP	3.3
2	AI	35	TYR	3.3
2	BC	50	ALA	3.3
2	BO	219	SER	3.3
1	A0	203	LEU	3.2
1	AZ	158	ALA	3.2
2	AG	225	ALA	3.2
2	BE	61	ILE	3.2
2	BR	77	LYS	3.2
2	AL	65	ARG	3.2
2	AL	118	VAL	3.2
2	BJ	247	ASN	3.2
2	AP	231	PHE	3.2
1	AZ	128	THR	3.2
2	AQ	219	SER	3.2
1	AZ	15	TYR	3.2
1	BZ	263	TYR	3.2
1	A0	148	TYR	3.1
1	BZ	116	ILE	3.1
2	AI	99	LEU	3.1
2	AH	259	GLY	3.1
3	AV	201	GLY	3.1
2	AQ	214	PRO	3.1
2	AE	222	GLY	3.1
2	AH	258	ASN	3.1
1	AZ	6	VAL	3.1
2	AC	124	ASP	3.1
2	AJ	251	THR	3.1
2	BG	260	SER	3.1
2	BN	165	THR	3.1
2	AF	23	ASP	3.0
3	BV	296	ASP	3.0
1	B0	75	GLU	3.0
1	B0	209	ALA	3.0
2	BP	215	ALA	3.0
2	AM	188	VAL	3.0
2	BG	88	ILE	3.0
2	AB	62	ALA	3.0
2	AL	254	ALA	3.0
2	BC	251	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	BQ	146	ASP	3.0
2	AL	64	GLY	3.0
1	AZ	233	GLU	3.0
2	AN	181	LYS	3.0
3	BW	1	MET	3.0
2	AP	27	TYR	3.0
1	B0	124	ALA	3.0
2	AH	62	ALA	3.0
2	BI	185	LEU	2.9
2	AA	218	GLN	2.9
1	AZ	278	HIS	2.9
2	AQ	62	ALA	2.9
1	AZ	9	ASN	2.9
2	AI	105	ASN	2.9
2	AF	218	GLN	2.9
1	AZ	331	PRO	2.9
3	AS	286	LYS	2.9
2	AA	259	GLY	2.9
1	A0	199	ASP	2.9
2	BD	182	ASN	2.9
2	BE	257	GLY	2.9
1	AY	128	THR	2.9
2	AF	221	VAL	2.9
2	AL	255	THR	2.9
2	AK	228	ASP	2.9
3	AU	46	ASN	2.9
2	AL	88	ILE	2.8
2	AP	62	ALA	2.8
3	AV	247	GLU	2.8
1	BZ	143	ASN	2.8
3	BX	259	ASN	2.8
3	AV	262	PRO	2.8
2	BF	257	GLY	2.8
2	BC	247	ASN	2.8
1	BY	269	GLY	2.8
2	AG	185	LEU	2.8
2	AM	262	PHE	2.8
2	BF	260	SER	2.8
2	AR	233	ILE	2.8
3	AX	163	THR	2.8
2	AJ	48	ASN	2.8
2	BG	41	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	AU	288	GLU	2.8
2	BJ	59	SER	2.8
3	BV	249	TYR	2.7
2	BR	74	VAL	2.7
2	AN	64	GLY	2.7
2	BL	254	ALA	2.7
2	BR	109	GLY	2.7
2	BG	175	GLN	2.7
2	AC	156	SER	2.7
2	AC	220	LEU	2.7
2	AP	101	ALA	2.7
1	A0	75	GLU	2.7
2	BM	189	ARG	2.7
2	AL	98	SER	2.7
3	BT	157	SER	2.7
1	A0	327	ASN	2.7
2	AI	114	ASN	2.7
1	A0	200	PRO	2.7
2	BP	214	PRO	2.7
2	AL	217	VAL	2.7
2	AP	110	VAL	2.7
1	BZ	232	THR	2.7
2	BA	131	THR	2.7
3	BS	249	TYR	2.7
2	AB	97	VAL	2.7
2	BH	109	GLY	2.7
2	BI	260	SER	2.7
3	AT	35	GLY	2.7
2	AR	228	ASP	2.6
2	BE	220	LEU	2.6
2	AE	259	GLY	2.6
2	AK	63	GLY	2.6
1	AY	1	MET	2.6
2	AP	169	GLU	2.6
2	AH	204	SER	2.6
2	AI	86	ALA	2.6
2	AL	253	ILE	2.6
2	BC	199	LYS	2.6
1	BZ	148	TYR	2.6
2	AD	62	ALA	2.6
3	AW	61	ILE	2.6
2	AI	176	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	BC	219	SER	2.6
2	AF	262	PHE	2.6
2	AG	175	GLN	2.6
2	BG	218	GLN	2.6
2	AN	257	GLY	2.6
2	AP	171	GLY	2.6
2	BC	63	GLY	2.6
2	AQ	233	ILE	2.6
2	BO	159	ILE	2.6
2	BO	65	ARG	2.6
2	BN	7	THR	2.6
2	BC	260	SER	2.6
2	BK	23	ASP	2.6
3	AU	286	LYS	2.6
2	AN	27	TYR	2.6
1	AZ	232	THR	2.6
1	AZ	328	GLU	2.6
2	AG	257	GLY	2.6
2	BJ	61	ILE	2.6
2	BP	144	THR	2.6
2	AF	190	PHE	2.5
2	AC	122	CYS	2.5
2	BE	258	ASN	2.5
2	BJ	199	LYS	2.5
2	AI	98	SER	2.5
3	AV	240	ILE	2.5
1	AZ	8	ASP	2.5
2	AJ	228	ASP	2.5
2	BG	220	LEU	2.5
2	AI	64	GLY	2.5
2	AJ	28	MET	2.5
2	BE	190	PHE	2.5
2	BF	63	GLY	2.5
1	BZ	147	SER	2.5
2	AJ	260	SER	2.5
2	AL	62	ALA	2.5
2	AD	12	ASN	2.5
2	BH	188	VAL	2.5
2	BQ	229	THR	2.5
1	AY	90	ASN	2.5
2	AJ	247	ASN	2.5
2	AL	28	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	AR	257	GLY	2.5
2	AN	204	SER	2.4
2	BH	218	GLN	2.4
2	BP	38	ILE	2.4
3	AX	280	GLU	2.4
1	BZ	265	ALA	2.4
2	AE	196	ASN	2.4
3	BX	46	ASN	2.4
2	BK	63	GLY	2.4
2	AG	220	LEU	2.4
3	AU	219	ASP	2.4
2	AB	258	ASN	2.4
2	BF	251	THR	2.4
2	BG	65	ARG	2.4
2	AK	64	GLY	2.4
2	AL	259	GLY	2.4
1	AY	265	ALA	2.4
2	AL	232	HIS	2.4
2	BB	258	ASN	2.4
2	AH	7	THR	2.4
2	AA	215	ALA	2.4
2	BF	263	ILE	2.4
2	AO	258	ASN	2.4
3	BX	99	GLU	2.4
1	B0	4	ALA	2.4
2	BG	219	SER	2.4
2	BO	62	ALA	2.4
2	BH	137	LYS	2.4
3	BX	260	LEU	2.4
2	AD	116	SER	2.3
2	BB	219	SER	2.3
3	AX	279	MET	2.3
2	BR	228	ASP	2.3
3	AS	203	LEU	2.3
2	BG	87	ASN	2.3
2	BG	259	GLY	2.3
2	AL	174	LEU	2.3
2	BR	70	LEU	2.3
2	AM	187	ILE	2.3
2	AM	258	ASN	2.3
2	BN	164	GLN	2.3
2	AA	260	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	BZ	264	ILE	2.3
2	AC	247	ASN	2.3
2	AN	259	GLY	2.3
2	BO	23	ASP	2.3
2	BM	188	VAL	2.3
2	AJ	229	THR	2.3
2	AL	251	THR	2.3
2	BF	259	GLY	2.3
1	BY	76	VAL	2.3
2	AQ	228	ASP	2.3
2	BA	218	GLN	2.3
2	AR	183	ASN	2.3
2	AC	44	SER	2.3
2	AQ	187	ILE	2.3
1	AZ	209	ALA	2.3
2	AG	255	THR	2.2
2	BQ	233	ILE	2.2
2	AD	161	VAL	2.2
2	AF	220	LEU	2.2
2	AP	259	GLY	2.2
3	BX	2	VAL	2.2
2	BR	33	MET	2.2
2	AH	60	ILE	2.2
2	BC	183	ASN	2.2
3	AU	238	ILE	2.2
2	BC	62	ALA	2.2
2	BO	187	ILE	2.2
3	AV	249	TYR	2.2
2	AD	221	VAL	2.2
2	AJ	225	ALA	2.2
2	BC	189	ARG	2.2
1	BZ	4	ALA	2.2
3	BX	1	MET	2.2
1	AZ	87	LYS	2.2
3	AS	235	GLN	2.2
2	AD	39	ARG	2.2
2	AR	211	PRO	2.2
2	BR	246	ALA	2.2
2	AI	258	ASN	2.2
3	AW	31	PRO	2.2
2	AO	103	THR	2.2
2	BC	262	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	BG	63	GLY	2.2
2	BM	29	MET	2.2
2	BJ	62	ALA	2.2
2	AG	12	ASN	2.2
2	BD	165	THR	2.2
2	BJ	165	THR	2.2
2	AA	186	VAL	2.2
2	BR	126	VAL	2.2
3	AS	234	VAL	2.2
2	BP	39	ARG	2.2
2	AL	222	GLY	2.1
2	AR	259	GLY	2.1
3	BW	69	GLY	2.1
2	BC	191	PHE	2.1
2	AC	185	LEU	2.1
2	AE	5	ASN	2.1
2	AB	2	THR	2.1
3	AV	263	VAL	2.1
2	AB	4	LYS	2.1
1	AZ	90	ASN	2.1
2	AJ	183	ASN	2.1
3	BT	177	THR	2.1
1	AY	77	VAL	2.1
1	AZ	118	SER	2.1
1	B0	352	ALA	2.1
2	AL	225	ALA	2.1
2	BH	117	GLY	2.1
1	BY	331	PRO	2.1
2	AQ	38	ILE	2.1
2	BC	234	ASP	2.1
2	AE	221	VAL	2.1
2	AG	221	VAL	2.1
1	AY	317	THR	2.1
1	BY	128	THR	2.1
3	AX	249	TYR	2.1
2	AP	204	SER	2.1
2	BD	260	SER	2.1
2	BG	86	ALA	2.1
2	AP	220	LEU	2.1
2	BA	23	ASP	2.1
2	BH	23	ASP	2.1
2	BJ	249	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	BH	81	VAL	2.1
1	BZ	302	ASN	2.1
2	AQ	31	THR	2.1
3	BU	5	TYR	2.1
2	AQ	63	GLY	2.1
2	BB	62	ALA	2.1
2	BP	253	ILE	2.1
2	AF	34	ASP	2.1
3	AX	200	MET	2.1
2	BD	258	ASN	2.1
2	AF	216	ALA	2.1
1	AY	233	GLU	2.1
2	AP	116	SER	2.1
3	BU	296	ASP	2.1
2	BD	185	LEU	2.1
1	AZ	16	ASN	2.1
1	AZ	164	ASN	2.1
2	BJ	60	ILE	2.1
3	AV	144	PHE	2.1
3	AV	199	PHE	2.1
2	BO	198	GLN	2.1
2	AL	219	SER	2.1
1	AZ	69	VAL	2.1
2	AG	29	MET	2.0
2	BI	261	TYR	2.0
2	BN	23	ASP	2.0
2	AB	253	ILE	2.0
2	BK	64	GLY	2.0
2	BE	175	GLN	2.0
3	AU	195	GLU	2.0
2	BE	36	ARG	2.0
1	AZ	88	LYS	2.0
2	AK	199	LYS	2.0
1	AY	131	PHE	2.0
2	BP	66	TYR	2.0
2	AB	259	GLY	2.0
3	AT	279	MET	2.0
1	AZ	18	SER	2.0
2	AB	88	ILE	2.0
2	AE	146	ASP	2.0
2	AE	228	ASP	2.0
2	AQ	93	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	AT	163	THR	2.0
3	BT	46	ASN	2.0
3	AS	285	SER	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 oligosaccharides 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, 95th 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	BU	301	1/1	0.96	0.07	269,269,269,269	0
4	CA	BV	301	1/1	0.96	0.12	272,272,272,272	0
4	CA	AW	301	1/1	0.98	0.07	266,266,266,266	0
4	CA	AX	301	1/1	0.98	0.14	275,275,275,275	0
4	CA	BT	301	1/1	0.98	0.07	279,279,279,279	0
4	CA	AS	301	1/1	0.98	0.07	281,281,281,281	0
4	CA	AV	301	1/1	0.98	0.11	276,276,276,276	0
4	CA	BX	301	1/1	0.98	0.10	287,287,287,287	0
4	CA	AT	301	1/1	0.99	0.06	275,275,275,275	0
4	CA	BS	301	1/1	0.99	0.06	267,267,267,267	0
4	CA	BW	301	1/1	0.99	0.05	268,268,268,268	0
4	CA	AU	301	1/1	0.99	0.04	275,275,275,275	0

6.5 Other polymers [i](#)

There are no such residues in this entry.