



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:30 AM UTC

PDB ID : 4L29 / pdb_00004L29
Title : Structure of wtMHC class I with NY-ESO1 double mutant
Authors : Halabelian, L.; Giorgetti, S.; Bellotti, V.; Bolognesi, M.; Ricagno, S.
Deposited on : 2013-06-04
Resolution : 3.09 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
Mogul : 2022.3.0, CSD as543be (2022)
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

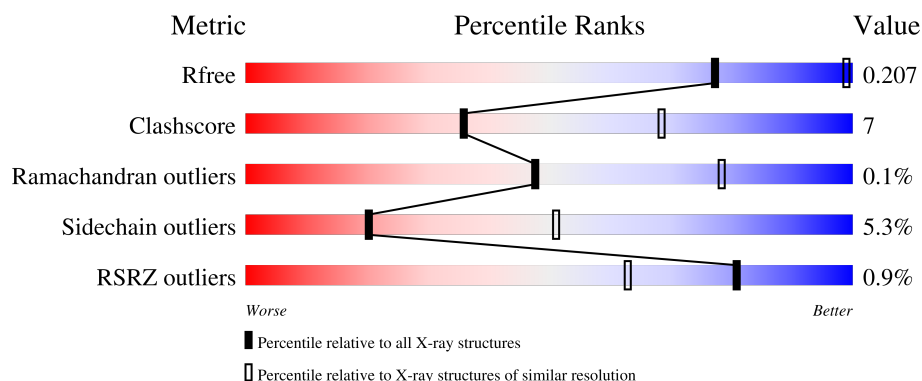
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	276	
1	C	276	
1	E	276	
1	G	276	
1	I	276	

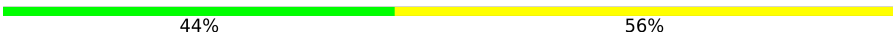
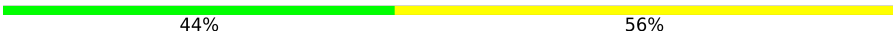
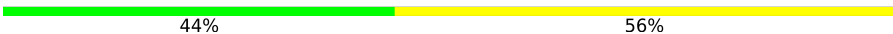
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Mol	Chain	Length	Quality of chain	
1	K	276		
1	M	276		
1	O	276		
1	Q	276		
1	S	276		
1	U	276		
1	W	276		
1	Y	276		
1	a	276		
2	B	100		
2	D	100		
2	F	100		
2	H	100		
2	J	100		
2	L	100		
2	N	100		
2	P	100		
2	R	100		
2	T	100		
2	V	100		
2	X	100		
2	Z	100		
2	b	100		
3	c	9		
3	e	9		

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Mol	Chain	Length	Quality of chain
3	f	9	
3	g	9	
3	h	9	
3	i	9	
3	j	9	
3	k	9	
3	l	9	
3	m	9	
3	n	9	
3	o	9	
3	p	9	
3	q	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44627 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	C	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	E	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	G	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	I	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	K	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	M	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	O	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	Q	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	S	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	U	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	W	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	Y	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	a	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	J	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	N	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	P	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	R	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	T	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	V	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	X	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Z	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	b	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
J	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
P	0	MET	-	initiating methionine	UNP P61769
R	0	MET	-	initiating methionine	UNP P61769
T	0	MET	-	initiating methionine	UNP P61769
V	0	MET	-	initiating methionine	UNP P61769
X	0	MET	-	initiating methionine	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	MET	-	initiating methionine	UNP P61769
b	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called NY-ESO1 DOUBLE MUTANT (1Y, 9V).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	m	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	i	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	k	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	f	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	l	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	h	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	e	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	n	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	p	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	o	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	c	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	g	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	q	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	j	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

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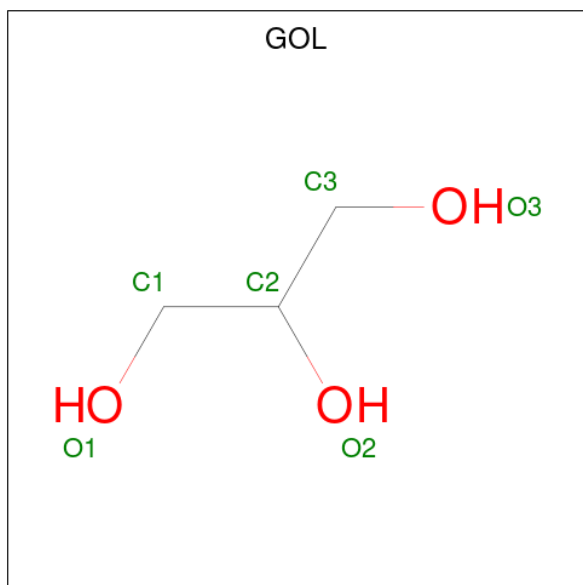
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	G	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	I	3	Total 3	Cl 3	0	0
4	J	1	Total 1	Cl 1	0	0
4	K	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0
4	N	2	Total 2	Cl 2	0	0
4	O	1	Total 1	Cl 1	0	0
4	P	1	Total 1	Cl 1	0	0
4	Q	2	Total 2	Cl 2	0	0
4	R	1	Total 1	Cl 1	0	0
4	S	1	Total 1	Cl 1	0	0
4	T	1	Total 1	Cl 1	0	0
4	U	1	Total 1	Cl 1	0	0
4	V	1	Total 1	Cl 1	0	0
4	W	1	Total 1	Cl 1	0	0
4	Y	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	1	Total	Cl	0	0
			1	1		
4	a	1	Total	Cl	0	0
			1	1		
4	b	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	i	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	f	1	Total	C	O	0	0
			6	3	3		
5	l	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	h	1	Total C O 6 3 3	0	0
5	e	1	Total C O 6 3 3	0	0
5	O	1	Total C O 6 3 3	0	0
5	O	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0
5	o	1	Total C O 6 3 3	0	0
5	c	1	Total C O 6 3 3	0	0
5	g	1	Total C O 6 3 3	0	0
5	Y	1	Total C O 6 3 3	0	0
5	q	1	Total C O 6 3 3	0	0
5	a	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	C	4	Total O 4 4	0	0
6	D	2	Total O 2 2	0	0
6	E	3	Total O 3 3	0	0
6	F	2	Total O 2 2	0	0
6	G	7	Total O 7 7	0	0
6	H	1	Total O 1 1	0	0

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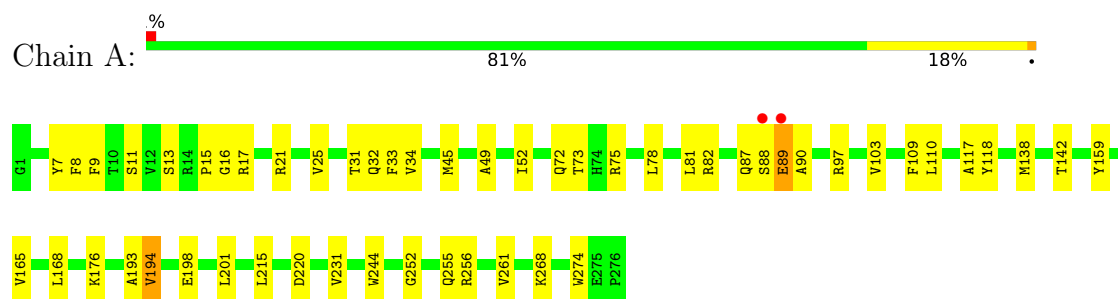
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	3	Total 3	O 3	0	0
6	J	2	Total 2	O 2	0	0
6	K	3	Total 3	O 3	0	0
6	L	3	Total 3	O 3	0	0
6	M	1	Total 1	O 1	0	0
6	P	3	Total 3	O 3	0	0
6	Q	2	Total 2	O 2	0	0
6	R	3	Total 3	O 3	0	0
6	S	1	Total 1	O 1	0	0
6	T	1	Total 1	O 1	0	0
6	U	3	Total 3	O 3	0	0
6	V	2	Total 2	O 2	0	0
6	X	3	Total 3	O 3	0	0
6	Y	2	Total 2	O 2	0	0
6	Z	2	Total 2	O 2	0	0

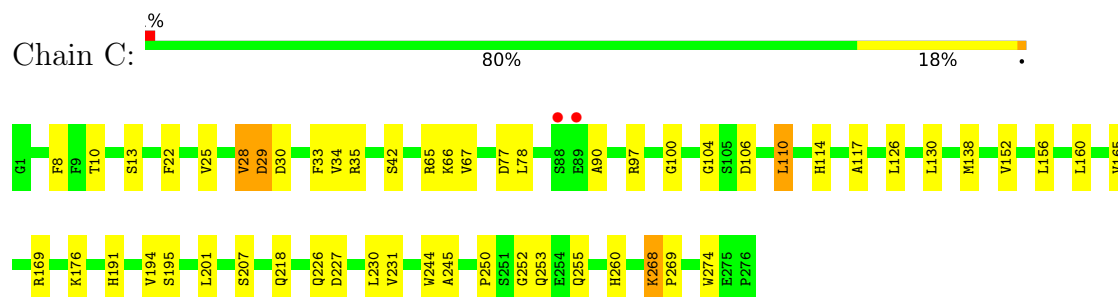
3 Residue-property plots [i](#)

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.

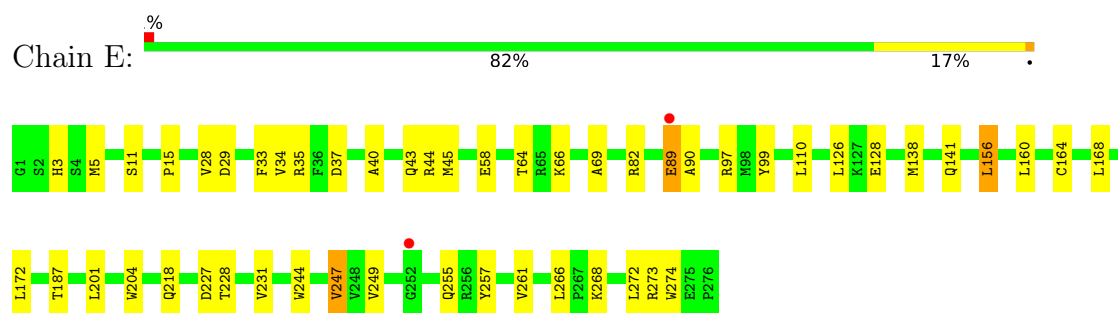
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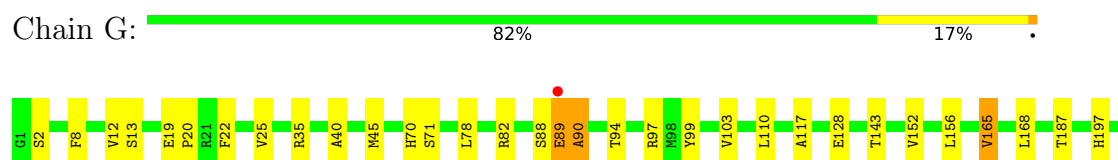
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

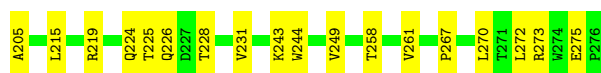


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

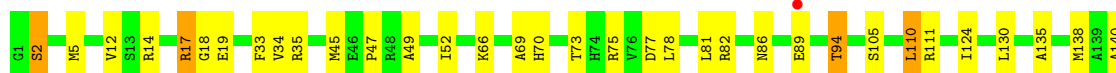
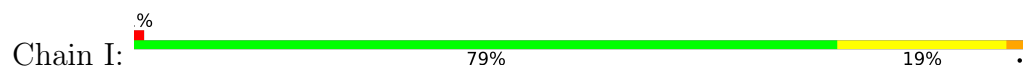


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

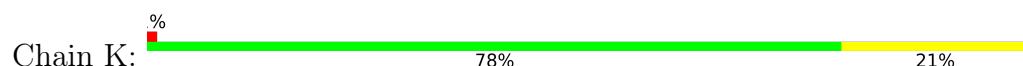




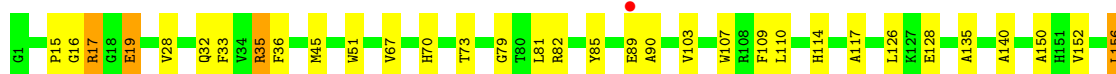
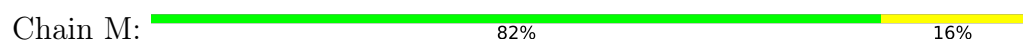
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



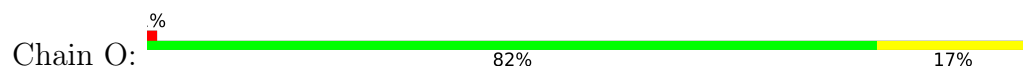
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



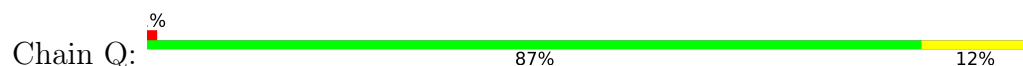
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

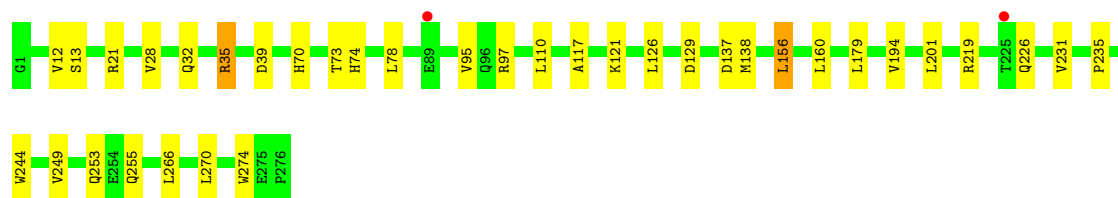


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

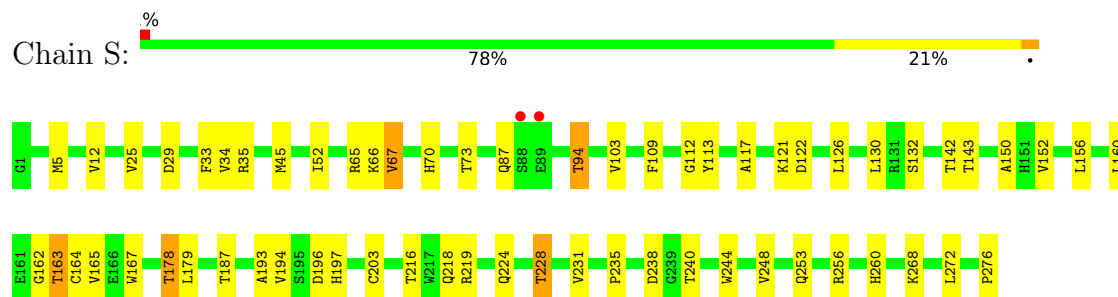


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

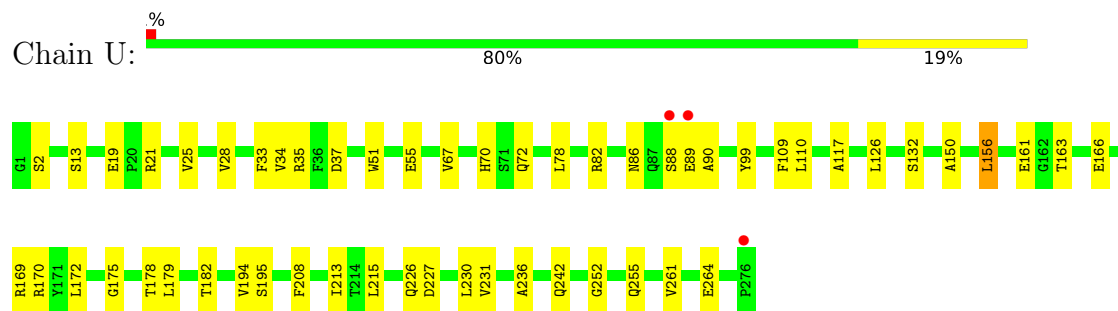




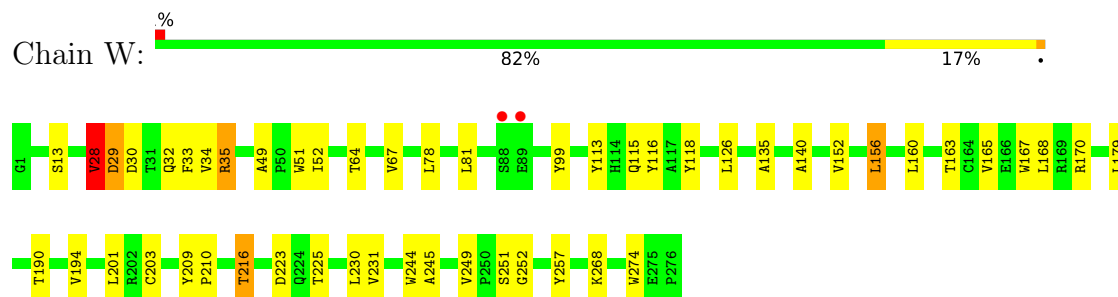
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



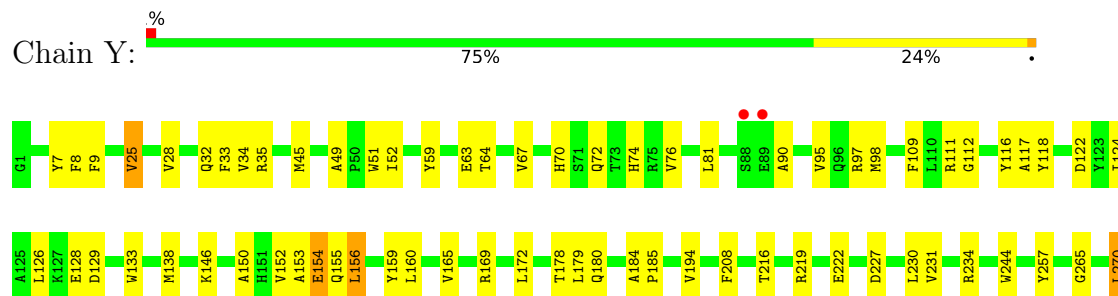
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

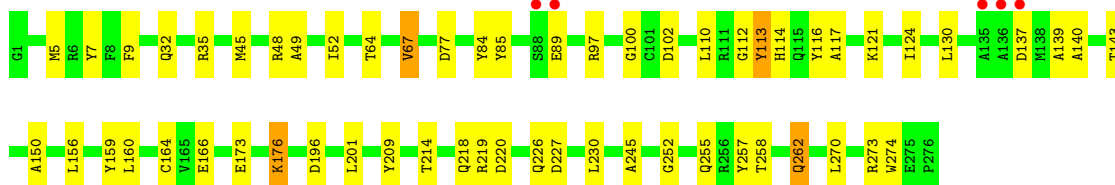
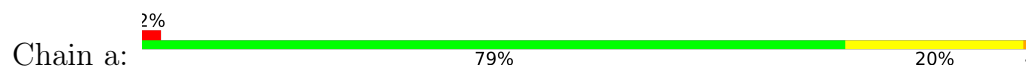


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

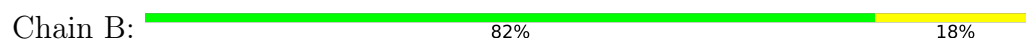




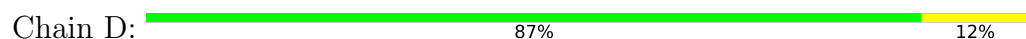
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



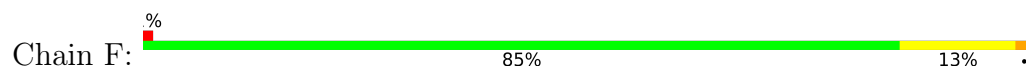
- Molecule 2: Beta-2-microglobulin



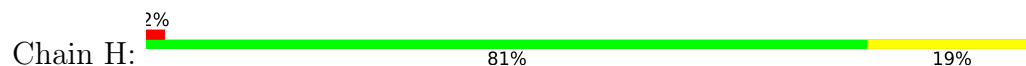
- Molecule 2: Beta-2-microglobulin



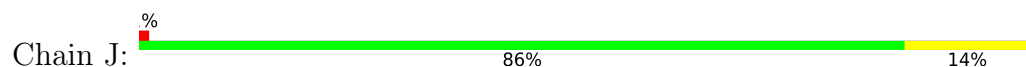
- Molecule 2: Beta-2-microglobulin



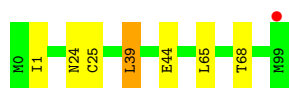
- Molecule 2: Beta-2-microglobulin



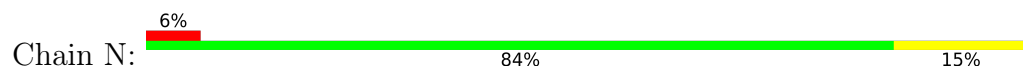
- Molecule 2: Beta-2-microglobulin



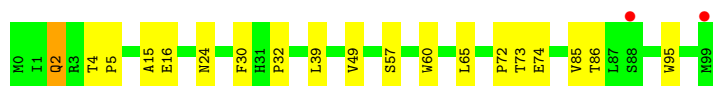
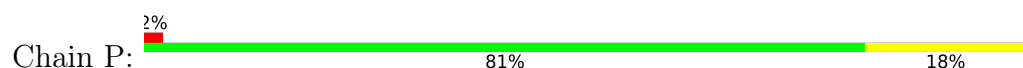
• Molecule 2: Beta-2-microglobulin



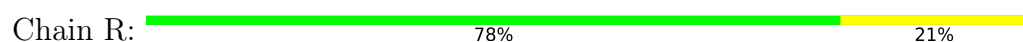
• Molecule 2: Beta-2-microglobulin



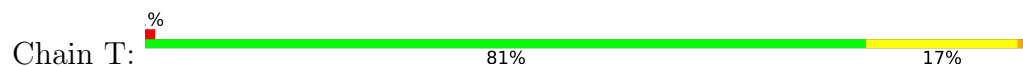
• Molecule 2: Beta-2-microglobulin



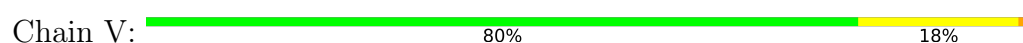
• Molecule 2: Beta-2-microglobulin



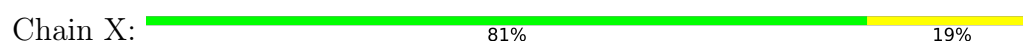
• Molecule 2: Beta-2-microglobulin



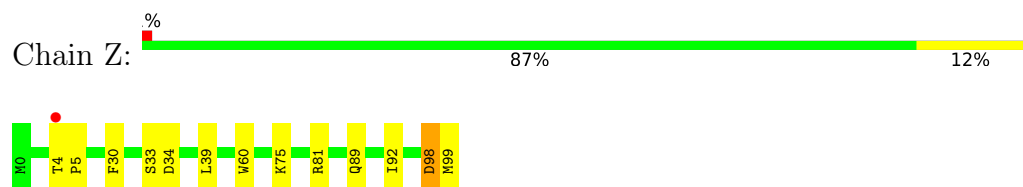
• Molecule 2: Beta-2-microglobulin



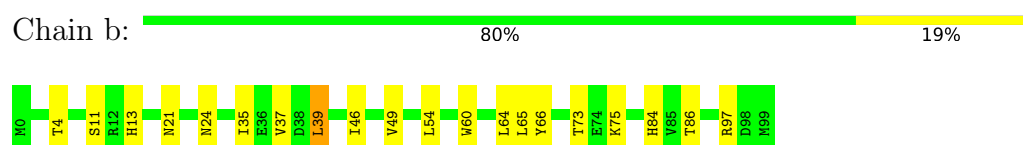
• Molecule 2: Beta-2-microglobulin



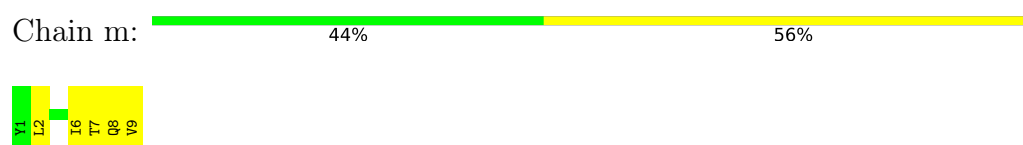
- Molecule 2: Beta-2-microglobulin



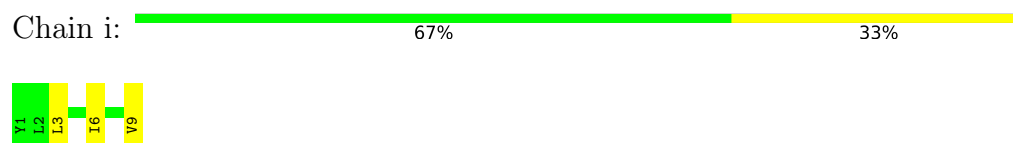
- Molecule 2: Beta-2-microglobulin



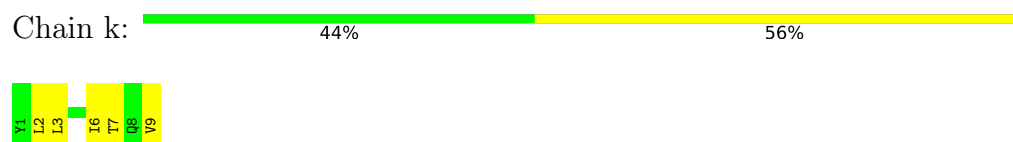
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)



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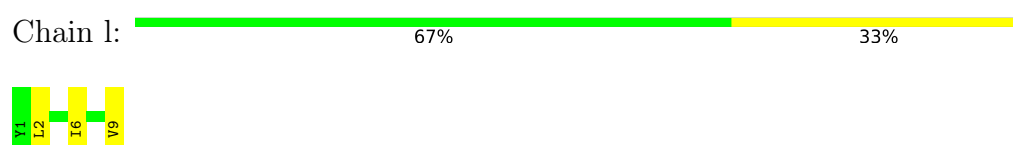
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

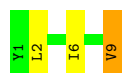


- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)



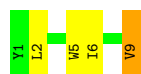
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain h:  67% 22% 11%



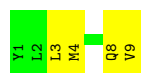
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain e:  56% 33% 11%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain n:  56% 44%



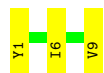
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain p:  78% 22%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain o:  67% 33%



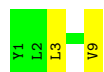
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain c:  89% 11%



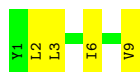
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain g:  78% 22%



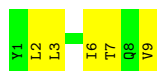
- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain q:  56% 44%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain j:  44% 56%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.57Å 313.36Å 314.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.80 – 3.09 53.80 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (53.80-3.09) 99.1 (53.80-3.09)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.201 0.184 , 0.207	Depositor DCC
R_{free} test set	10973 reflections (5.94%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
Reported twinning fraction	0.671 for H, K, L 0.329 for -H, L, K	Depositor
Outliers	1 of 182843 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	44627	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: CL, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2320	0.77	1/3149 (0.0%)
1	C	0.76	5/2320 (0.2%)	0.80	0/3149
1	E	0.61	0/2320	0.81	0/3149
1	G	0.68	2/2320 (0.1%)	0.79	0/3149
1	I	0.65	1/2320 (0.0%)	0.80	1/3149 (0.0%)
1	K	0.61	0/2320	0.78	1/3149 (0.0%)
1	M	0.60	0/2320	0.78	1/3149 (0.0%)
1	O	0.60	0/2320	0.77	0/3149
1	Q	0.65	0/2320	0.78	0/3149
1	S	0.58	0/2320	0.76	2/3149 (0.1%)
1	U	0.57	0/2320	0.76	1/3149 (0.0%)
1	W	0.66	3/2320 (0.1%)	0.77	2/3149 (0.1%)
1	Y	0.58	0/2320	0.75	0/3149
1	a	0.56	0/2320	0.76	0/3149
2	B	0.57	0/860	0.73	0/1162
2	D	0.59	0/860	0.77	0/1162
2	F	0.62	0/860	0.74	0/1162
2	H	0.57	0/860	0.80	0/1162
2	J	0.57	0/860	0.73	0/1162
2	L	0.58	0/860	0.75	0/1162
2	N	0.60	0/860	0.77	0/1162
2	P	0.56	0/860	0.74	0/1162
2	R	0.56	0/860	0.69	0/1162
2	T	0.66	0/860	0.84	2/1162 (0.2%)
2	V	0.57	0/860	0.73	0/1162
2	X	0.54	0/860	0.74	0/1162
2	Z	0.55	0/860	0.75	0/1162
2	b	0.55	0/860	0.70	0/1162
3	c	0.56	0/84	0.67	0/113
3	e	0.53	0/84	0.69	0/113
3	f	0.58	0/84	0.55	0/113
3	g	0.49	0/84	0.74	0/113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	h	0.51	0/84	0.84	0/113
3	i	0.56	0/84	0.84	0/113
3	j	0.47	0/84	0.67	0/113
3	k	0.62	0/84	0.81	0/113
3	l	0.49	0/84	0.78	0/113
3	m	0.53	0/84	0.80	0/113
3	n	0.53	0/84	0.75	0/113
3	o	0.52	0/84	0.67	0/113
3	p	0.57	0/84	0.68	0/113
3	q	0.54	0/84	0.74	0/113
All	All	0.61	11/45696 (0.0%)	0.77	11/61936 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	29	ASP	CA-C	-9.90	1.44	1.53
1	W	28	VAL	CA-CB	-7.90	1.44	1.54
1	C	29	ASP	C-O	-7.79	1.16	1.24
1	G	90	ALA	CA-CB	-7.73	1.41	1.53
1	C	28	VAL	C-O	-7.15	1.16	1.24
1	W	29	ASP	C-O	-6.84	1.17	1.24
1	C	30	ASP	C-O	-6.12	1.15	1.24
1	G	90	ALA	C-O	-6.00	1.17	1.24
1	C	28	VAL	CA-CB	-5.73	1.47	1.54
1	I	18	GLY	C-O	-5.37	1.17	1.23
1	W	28	VAL	C-O	-5.32	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	47	GLU	N-CA-C	6.77	121.71	113.38
1	I	18	GLY	N-CA-C	6.60	118.77	112.04
1	W	28	VAL	N-CA-C	-5.55	99.65	107.75
1	A	45	MET	N-CA-C	-5.50	101.71	109.96
1	W	28	VAL	CB-CA-C	-5.41	103.09	110.77
1	S	162	GLY	N-CA-C	5.38	115.11	110.21
1	U	231	VAL	CB-CA-C	-5.35	105.70	111.59
1	K	162	GLY	N-CA-C	5.35	115.08	110.21
2	T	48	LYS	N-CA-C	-5.35	106.94	112.93
1	M	275	GLU	N-CA-C	-5.07	103.64	109.93
1	S	29	ASP	CB-CA-C	-5.02	110.77	116.54

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	A	2254	0	2103	47	0
1	C	2254	0	2103	48	0
1	E	2254	0	2103	46	0
1	G	2254	0	2103	31	0
1	I	2254	0	2103	35	0
1	K	2254	0	2103	29	0
1	M	2254	0	2103	42	0
1	O	2254	0	2103	28	0
1	Q	2254	0	2103	26	0
1	S	2254	0	2103	41	0
1	U	2254	0	2103	39	0
1	W	2254	0	2103	33	0
1	Y	2254	0	2103	53	0
1	a	2254	0	2103	44	0
2	B	837	0	803	10	0
2	D	837	0	803	10	0
2	F	837	0	803	6	0
2	H	837	0	803	7	0
2	J	837	0	803	11	0
2	L	837	0	803	4	0
2	N	837	0	803	10	0
2	P	837	0	803	14	0
2	R	837	0	803	13	0
2	T	837	0	803	15	0
2	V	837	0	803	20	0
2	X	837	0	803	11	0
2	Z	837	0	803	5	0
2	b	837	0	803	15	0
3	c	82	0	87	0	0
3	e	82	0	87	5	0
3	f	82	0	87	6	0
3	g	82	0	87	2	0
3	h	82	0	87	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	i	82	0	87	3	0
3	j	82	0	87	10	0
3	k	82	0	87	7	0
3	l	82	0	87	5	0
3	m	82	0	87	7	0
3	n	82	0	87	3	0
3	o	82	0	87	4	0
3	p	82	0	87	4	0
3	q	82	0	87	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	3	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	N	2	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	Y	1	0	0	0	0
4	Z	1	0	0	0	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0
5	A	6	0	8	2	0
5	C	12	0	16	1	0
5	E	6	0	8	3	0
5	K	6	0	8	0	0
5	O	12	0	16	1	0
5	Q	6	0	8	1	0
5	S	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	6	0	8	0	0
5	a	6	0	8	1	0
5	c	6	0	8	1	0
5	e	6	0	8	1	0
5	f	6	0	8	1	0
5	g	6	0	8	1	0
5	h	6	0	8	0	0
5	i	6	0	8	1	0
5	l	6	0	8	0	0
5	o	6	0	8	2	0
5	q	6	0	8	0	0
6	A	2	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
6	E	3	0	0	1	0
6	F	2	0	0	0	0
6	G	7	0	0	0	0
6	H	1	0	0	0	0
6	I	3	0	0	0	0
6	J	2	0	0	1	0
6	K	3	0	0	0	0
6	L	3	0	0	0	0
6	M	1	0	0	0	0
6	P	3	0	0	0	0
6	Q	2	0	0	0	0
6	R	3	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	3	0	0	0	0
6	V	2	0	0	0	0
6	X	3	0	0	0	0
6	Y	2	0	0	0	0
6	Z	2	0	0	0	0
All	All	44627	0	42062	628	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 (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:LEU:HD22	1:K:156:LEU:HD13	1.47	0.97
1:A:90:ALA:HB1	2:N:85:VAL:HG22	1.45	0.97
1:A:231:VAL:HG11	1:A:244:TRP:CE2	2.05	0.91
1:U:126:LEU:HD22	1:U:156:LEU:HD13	1.50	0.90
1:C:90:ALA:HB3	2:V:2:GLN:HE22	1.35	0.88
2:L:39:LEU:HD23	2:L:68:THR:HG22	1.55	0.88
1:K:98:MET:HE2	1:K:115:GLN:OE1	1.76	0.85
1:M:16:GLY:O	1:M:17:ARG:HG2	1.78	0.83
1:C:90:ALA:HB1	2:V:85:VAL:HG13	1.61	0.83
1:E:90:ALA:HB1	2:J:85:VAL:HG22	1.61	0.83
2:X:7:ILE:CD1	2:X:82:VAL:HG21	2.10	0.81
1:U:215:LEU:HD22	1:U:261:VAL:HG22	1.62	0.80
1:Y:126:LEU:HD22	1:Y:156:LEU:HD13	1.63	0.80
1:E:97:ARG:NH2	3:k:6:ILE:HD12	1.97	0.79
1:S:156:LEU:HD21	5:o:101:GOL:O2	1.81	0.79
1:C:90:ALA:CB	2:V:2:GLN:HE22	1.96	0.79
1:W:28:VAL:HG11	1:W:179:LEU:HD13	1.63	0.79
1:a:156:LEU:CD2	1:a:160:LEU:HD11	2.14	0.78
1:E:90:ALA:HB3	2:J:2:GLN:OE1	1.83	0.78
1:C:90:ALA:HB3	2:V:2:GLN:NE2	1.99	0.77
1:I:82:ARG:HD3	1:I:89:GLU:HA	1.66	0.77
1:U:126:LEU:CD2	1:U:156:LEU:HD13	2.14	0.77
1:S:65:ARG:HD3	1:W:190:THR:HG22	1.67	0.76
1:U:215:LEU:CD2	1:U:261:VAL:HG22	2.15	0.76
1:W:51:TRP:CZ2	1:W:179:LEU:HD11	2.21	0.76
2:T:47:GLU:O	2:T:47:GLU:HG3	1.84	0.76
1:C:230:LEU:HD23	1:C:245:ALA:HB2	1.67	0.75
2:b:11:SER:OG	2:b:13:HIS:O	2.04	0.75
1:G:215:LEU:CD2	1:G:261:VAL:HG22	2.16	0.75
1:G:224:GLN:O	1:G:228:THR:HG23	1.86	0.74
1:G:99:TYR:CZ	3:f:3:LEU:HD12	2.22	0.73
1:W:135:ALA:HB1	1:W:140:ALA:HB3	1.69	0.73
1:W:201:LEU:HD22	1:W:274:TRP:CZ2	2.22	0.73
2:X:7:ILE:HD13	2:X:82:VAL:HG21	1.71	0.72
1:M:255:GLN:OE1	1:M:255:GLN:N	2.21	0.72
1:C:90:ALA:HB1	2:V:85:VAL:CG1	2.20	0.71
1:M:252:GLY:HA3	1:a:150:ALA:HB1	1.73	0.70
1:A:82:ARG:HD2	1:A:89:GLU:HA	1.71	0.70
2:B:2:GLN:OE1	1:M:90:ALA:HB3	1.91	0.70
1:K:98:MET:CE	1:K:115:GLN:OE1	2.39	0.69
2:T:39:LEU:HD22	2:T:49:VAL:CG1	2.21	0.69
1:S:218:GLN:OE1	1:S:260:HIS:NE2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:231:VAL:CG1	1:M:244:TRP:CZ2	2.76	0.69
2:b:54:LEU:HA	2:b:64:LEU:HD21	1.74	0.69
1:Q:28:VAL:HG11	1:Q:179:LEU:HD13	1.76	0.68
1:C:90:ALA:CB	2:V:2:GLN:NE2	2.55	0.68
1:E:126:LEU:HD22	1:E:156:LEU:HD13	1.74	0.68
1:S:70:HIS:CD2	3:o:6:ILE:HD13	2.28	0.68
1:I:135:ALA:HB1	1:I:140:ALA:HB3	1.76	0.68
1:Y:231:VAL:HG13	1:Y:244:TRP:CZ2	2.30	0.67
1:A:231:VAL:HG11	1:A:244:TRP:CZ2	2.30	0.66
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.77	0.66
1:Q:137:ASP:HA	1:Q:138:MET:HE2	1.77	0.66
1:C:201:LEU:HD22	1:C:274:TRP:CZ2	2.31	0.66
1:E:228:THR:HG22	1:E:247:VAL:HG23	1.78	0.66
1:K:64:THR:O	1:K:67:VAL:HG12	1.96	0.65
1:M:156:LEU:HD22	1:M:160:LEU:CD1	2.25	0.65
1:C:65:ARG:HD3	1:K:190:THR:HG22	1.79	0.65
1:Y:156:LEU:HD22	1:Y:160:LEU:HD11	1.79	0.65
1:E:90:ALA:CB	2:J:85:VAL:HG22	2.27	0.65
1:Y:231:VAL:CG1	1:Y:244:TRP:CZ2	2.80	0.65
1:a:32:GLN:HE21	1:a:48:ARG:HG3	1.62	0.64
5:A:302:GOL:H12	3:m:7:THR:H	1.61	0.64
1:I:12:VAL:HG22	1:I:94:THR:HG23	1.80	0.64
1:O:40:ALA:O	1:O:43:GLN:NE2	2.30	0.64
2:X:2:GLN:OE1	1:Y:90:ALA:HB3	1.97	0.64
1:Q:117:ALA:HB2	2:R:60:TRP:CE2	2.33	0.64
1:M:231:VAL:HG13	1:M:244:TRP:CZ2	2.33	0.64
2:T:47:GLU:O	2:T:47:GLU:CG	2.45	0.64
1:E:44:ARG:HA	1:E:64:THR:HG23	1.80	0.64
1:Q:266:LEU:HD13	1:Q:270:LEU:HG	1.80	0.63
1:S:163:THR:HG22	1:S:167:TRP:CD1	2.33	0.63
1:M:156:LEU:HD22	1:M:160:LEU:HD11	1.81	0.63
2:V:24:ASN:HB3	2:V:65:LEU:HD11	1.80	0.63
1:Y:126:LEU:HD13	1:Y:133:TRP:CH2	2.34	0.63
1:E:45:MET:CE	3:k:2:LEU:HD11	2.29	0.62
2:P:2:GLN:HB3	2:P:86:THR:HG22	1.80	0.62
2:X:45:ARG:NH1	2:X:47:GLU:OE1	2.30	0.62
1:G:88:SER:C	1:G:90:ALA:H	2.07	0.62
1:C:230:LEU:CD2	1:C:245:ALA:HB2	2.30	0.62
1:O:224:GLN:O	1:O:228:THR:HG23	1.98	0.62
1:A:231:VAL:CG1	1:A:244:TRP:CE2	2.82	0.62
1:I:2:SER:OG	1:I:110:LEU:HD12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:270:LEU:HD22	1:Y:272:LEU:CD2	2.30	0.62
2:T:39:LEU:HD22	2:T:49:VAL:HG11	1.81	0.62
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.35	0.61
1:Y:219:ARG:HG3	1:Y:257:TYR:CZ	2.35	0.61
1:W:49:ALA:O	1:W:52:ILE:HG22	2.00	0.61
1:A:33:PHE:CD1	1:A:34:VAL:HG13	2.35	0.61
1:Y:45:MET:HE1	3:q:2:LEU:HD11	1.81	0.61
1:M:126:LEU:HD22	1:M:156:LEU:HD13	1.82	0.61
2:X:7:ILE:HD11	2:X:82:VAL:HG21	1.80	0.61
2:V:84:HIS:N	2:V:87:LEU:HD12	2.16	0.60
2:V:54:LEU:HA	2:V:64:LEU:HD21	1.83	0.60
1:C:126:LEU:HD23	1:C:130:LEU:HD22	1.83	0.60
2:D:2:GLN:HE22	1:U:88:SER:CB	2.13	0.60
1:Y:49:ALA:O	1:Y:52:ILE:HG22	2.01	0.60
2:b:46:ILE:O	2:b:49:VAL:HG23	2.01	0.60
1:A:90:ALA:CB	2:N:85:VAL:HG22	2.27	0.60
1:M:152:VAL:HG13	5:e:101:GOL:H11	1.84	0.60
1:S:103:VAL:CG1	1:S:165:VAL:HG13	2.32	0.60
1:W:135:ALA:HB1	1:W:140:ALA:CB	2.31	0.60
1:I:70:HIS:CD2	3:l:6:ILE:HD13	2.37	0.59
2:N:25:CYS:HB2	2:N:39:LEU:HD11	1.83	0.59
1:W:231:VAL:HG11	1:W:244:TRP:CZ2	2.37	0.59
1:K:143:THR:HG21	3:h:9:VAL:HG22	1.84	0.59
1:K:116:TYR:HB3	1:K:124:ILE:HG22	1.83	0.59
1:O:99:TYR:CZ	3:n:3:LEU:HD12	2.38	0.59
1:E:231:VAL:CG1	1:E:244:TRP:CZ2	2.86	0.59
1:M:231:VAL:HG11	1:M:244:TRP:CZ2	2.38	0.59
1:U:126:LEU:HD22	1:U:156:LEU:CD1	2.28	0.59
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.38	0.58
1:E:15:PRO:HB2	2:J:85:VAL:HG23	1.85	0.58
1:a:32:GLN:NE2	1:a:48:ARG:HG3	2.18	0.58
1:M:45:MET:HE2	1:M:67:VAL:HB	1.85	0.58
1:O:81:LEU:HD21	3:n:9:VAL:HG11	1.84	0.58
1:I:5:MET:HE2	1:I:164:CYS:SG	2.43	0.58
5:E:302:GOL:H32	3:k:7:THR:H	1.69	0.58
2:T:39:LEU:HD22	2:T:49:VAL:HG13	1.85	0.58
1:U:82:ARG:HD2	1:U:89:GLU:HA	1.86	0.58
1:G:88:SER:C	1:G:90:ALA:N	2.60	0.58
1:A:231:VAL:CG1	1:A:244:TRP:CZ2	2.87	0.57
5:A:302:GOL:C1	3:m:7:THR:H	2.17	0.57
1:a:143:THR:HG21	3:j:9:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:45:MET:HE1	3:j:2:LEU:HD11	1.87	0.57
1:Y:150:ALA:HB1	1:a:252:GLY:HA3	1.85	0.57
1:Y:270:LEU:HD22	1:Y:272:LEU:HD23	1.86	0.57
1:E:37:ASP:HB3	1:E:40:ALA:HB2	1.86	0.57
1:a:49:ALA:O	1:a:52:ILE:HG22	2.04	0.57
1:M:16:GLY:C	1:M:17:ARG:CG	2.77	0.57
1:a:117:ALA:HB2	2:b:60:TRP:CE2	2.40	0.57
1:G:226:GLN:H	1:G:226:GLN:CD	2.12	0.57
1:A:252:GLY:O	1:A:255:GLN:NE2	2.38	0.56
1:C:165:VAL:HG12	1:C:169:ARG:NH1	2.19	0.56
1:C:230:LEU:HD23	1:C:245:ALA:CB	2.35	0.56
1:C:231:VAL:CG1	1:C:244:TRP:CZ2	2.87	0.56
1:E:138:MET:N	1:M:128:GLU:OE2	2.35	0.56
1:M:252:GLY:HA3	1:a:150:ALA:CB	2.35	0.56
1:Y:156:LEU:HD22	1:Y:160:LEU:CD1	2.35	0.56
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.86	0.56
1:W:201:LEU:HD13	1:W:274:TRP:NE1	2.20	0.56
2:X:1:ILE:C	2:X:1:ILE:HD12	2.31	0.56
1:Q:13:SER:HB3	1:Q:78:LEU:HD13	1.86	0.56
1:K:231:VAL:CG1	1:K:244:TRP:CZ2	2.88	0.56
1:Y:8:PHE:HB2	1:Y:25:VAL:HG23	1.88	0.56
3:m:8:GLN:HE21	1:S:193:ALA:HB2	1.71	0.56
1:M:172:LEU:O	1:M:180:GLN:NE2	2.35	0.56
1:A:255:GLN:CD	1:A:255:GLN:H	2.14	0.56
1:U:28:VAL:HG11	1:U:179:LEU:HD13	1.87	0.56
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.88	0.56
1:C:152:VAL:HG13	5:C:302:GOL:H11	1.88	0.56
1:S:12:VAL:HG22	1:S:94:THR:CG2	2.36	0.56
2:T:37:VAL:HG13	2:T:82:VAL:HG22	1.87	0.56
1:G:82:ARG:HD2	1:G:89:GLU:HA	1.87	0.55
2:P:24:ASN:HB3	2:P:65:LEU:HD11	1.86	0.55
1:S:12:VAL:HG22	1:S:94:THR:HG23	1.87	0.55
1:Q:231:VAL:HG13	1:Q:244:TRP:CZ2	2.41	0.55
1:G:88:SER:O	1:G:90:ALA:N	2.40	0.55
1:M:16:GLY:C	1:M:17:ARG:HG2	2.30	0.55
1:A:252:GLY:O	1:U:150:ALA:HB1	2.06	0.55
1:S:224:GLN:O	1:S:228:THR:HG23	2.07	0.55
1:C:231:VAL:HG13	1:C:244:TRP:CZ2	2.42	0.55
1:A:90:ALA:HB1	2:N:85:VAL:CG2	2.31	0.54
1:G:215:LEU:HD23	1:G:261:VAL:HG22	1.87	0.54
1:M:28:VAL:HG23	1:M:33:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:117:ALA:HB2	2:R:60:TRP:CZ2	2.42	0.54
1:Y:72:GLN:O	1:Y:76:VAL:HG23	2.07	0.54
1:C:126:LEU:CD2	1:C:130:LEU:HD22	2.38	0.54
1:a:116:TYR:HB3	1:a:124:ILE:HG22	1.90	0.54
2:P:39:LEU:HD23	2:P:49:VAL:CG2	2.36	0.54
1:I:14:ARG:HB3	1:I:17:ARG:HB3	1.90	0.54
1:O:99:TYR:CE2	3:n:3:LEU:HD12	2.43	0.54
1:O:231:VAL:HG13	1:O:244:TRP:CZ2	2.43	0.54
1:U:110:LEU:C	1:U:110:LEU:HD23	2.32	0.54
1:W:231:VAL:CG1	1:W:244:TRP:CZ2	2.91	0.54
1:A:90:ALA:HB3	2:N:2:GLN:OE1	2.08	0.54
1:A:109:PHE:HB2	1:A:165:VAL:HG21	1.89	0.54
1:I:168:LEU:O	1:I:168:LEU:HD12	2.08	0.54
1:I:110:LEU:HD13	1:I:111:ARG:NH2	2.23	0.53
1:K:11:SER:HA	1:K:21:ARG:O	2.07	0.53
2:D:84:HIS:CE1	2:D:86:THR:HG23	2.42	0.53
2:D:85:VAL:HG22	1:U:90:ALA:HA	1.90	0.53
1:I:258:THR:OG1	1:I:260:HIS:NE2	2.42	0.53
2:R:7:ILE:CD1	2:R:82:VAL:HG21	2.38	0.53
1:U:110:LEU:HD23	1:U:110:LEU:O	2.09	0.53
1:E:231:VAL:HG13	1:E:244:TRP:CZ2	2.43	0.53
5:E:302:GOL:C3	3:k:7:THR:H	2.22	0.53
1:G:35:ARG:NH2	1:G:40:ALA:HB2	2.24	0.53
1:I:165:VAL:HG12	1:I:169:ARG:CZ	2.39	0.53
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.44	0.53
1:Y:70:HIS:CD2	3:q:6:ILE:HD13	2.43	0.53
1:C:90:ALA:CB	2:V:85:VAL:HG13	2.36	0.53
1:C:104:GLY:CA	1:C:110:LEU:HD12	2.39	0.53
1:Q:156:LEU:HD22	1:Q:160:LEU:HG	1.91	0.53
1:C:90:ALA:HB3	2:V:2:GLN:CD	2.34	0.52
1:I:49:ALA:O	1:I:52:ILE:HG22	2.09	0.52
1:Q:70:HIS:CD2	3:p:6:ILE:HD13	2.43	0.52
1:C:250:PRO:HB2	1:C:253:GLN:HE21	1.75	0.52
1:K:130:LEU:HB3	1:K:157:ARG:HG3	1.92	0.52
1:E:33:PHE:CD1	1:E:34:VAL:HG13	2.43	0.52
1:M:81:LEU:HD21	3:e:9:VAL:HG11	1.92	0.52
5:E:302:GOL:H11	3:k:6:ILE:HA	1.91	0.52
1:I:187:THR:HB	1:I:272:LEU:HD11	1.90	0.52
1:a:84:TYR:HB3	1:a:139:ALA:HB1	1.90	0.52
1:A:88:SER:C	1:A:90:ALA:H	2.18	0.52
1:G:143:THR:OG1	3:f:9:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:ARG:HB3	1:G:224:GLN:HE21	1.75	0.52
1:U:70:HIS:NE2	1:U:99:TYR:OH	2.43	0.52
1:S:45:MET:HE1	1:S:67:VAL:HG21	1.91	0.52
1:S:231:VAL:HG13	1:S:244:TRP:CE2	2.45	0.52
1:Y:117:ALA:HB2	2:Z:60:TRP:CE2	2.45	0.52
1:S:231:VAL:CG1	1:S:244:TRP:CE2	2.93	0.52
1:Y:33:PHE:CD1	1:Y:34:VAL:HG13	2.45	0.52
2:B:85:VAL:HG23	1:M:15:PRO:HB2	1.92	0.52
1:U:169:ARG:HA	1:U:172:LEU:HD12	1.92	0.52
1:a:159:TYR:CG	3:j:3:LEU:HD23	2.45	0.52
1:A:72:GLN:HE22	1:A:75:ARG:HH21	1.58	0.51
1:A:159:TYR:HB2	1:S:276:PRO:HB2	1.92	0.51
1:G:45:MET:CE	3:f:2:LEU:HD11	2.40	0.51
1:G:215:LEU:HD22	1:G:261:VAL:HG22	1.88	0.51
1:K:45:MET:CE	3:h:2:LEU:HD11	2.40	0.51
1:K:81:LEU:HD13	1:K:118:TYR:CD1	2.45	0.51
1:O:152:VAL:HG13	5:O:302:GOL:H11	1.93	0.51
1:O:219:ARG:O	1:O:222:GLU:HG3	2.10	0.51
1:Q:253:GLN:HA	1:Q:255:GLN:NE2	2.26	0.51
1:A:11:SER:HA	1:A:21:ARG:O	2.10	0.51
1:A:193:ALA:O	1:U:72:GLN:NE2	2.40	0.51
2:T:23:LEU:HB2	2:T:70:PHE:CE1	2.46	0.51
1:C:33:PHE:CD1	1:C:34:VAL:HG13	2.45	0.51
1:K:231:VAL:HG11	1:K:244:TRP:CZ2	2.46	0.51
1:U:25:VAL:HG21	2:V:55:SER:OG	2.11	0.51
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.92	0.51
1:a:159:TYR:CG	3:j:3:LEU:CD2	2.94	0.51
1:E:261:VAL:HG12	1:E:266:LEU:HD12	1.93	0.50
2:P:2:GLN:HB3	2:P:86:THR:CG2	2.40	0.50
2:P:39:LEU:HD23	2:P:49:VAL:HG21	1.93	0.50
1:C:191:HIS:ND1	3:e:5:TRP:HB2	2.26	0.50
1:G:258:THR:HG22	1:G:273:ARG:HA	1.94	0.50
1:U:117:ALA:HB2	2:V:60:TRP:CE2	2.46	0.50
1:C:201:LEU:HD13	1:C:274:TRP:NE1	2.26	0.50
1:S:117:ALA:HB2	2:T:60:TRP:CE2	2.46	0.50
1:a:230:LEU:HD23	1:a:245:ALA:HB2	1.94	0.50
1:O:12:VAL:HG22	1:O:94:THR:HG23	1.94	0.50
1:O:122:ASP:OD1	2:P:60:TRP:NE1	2.39	0.50
1:K:126:LEU:HD22	1:K:156:LEU:CD1	2.30	0.50
1:A:142:THR:OG1	1:I:111:ARG:NH1	2.45	0.50
1:M:135:ALA:HB1	1:M:140:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:172:LEU:HD23	1:O:179:LEU:HD13	1.94	0.50
1:S:231:VAL:HG13	1:S:244:TRP:CZ2	2.47	0.50
1:Y:45:MET:CE	3:q:2:LEU:HD11	2.41	0.50
1:E:156:LEU:HD22	1:E:160:LEU:HD11	1.93	0.49
1:S:103:VAL:HG11	1:S:165:VAL:HG13	1.93	0.49
1:S:150:ALA:HB1	1:W:252:GLY:HA3	1.94	0.49
1:E:261:VAL:HG11	1:E:266:LEU:HD11	1.94	0.49
1:O:126:LEU:HD22	1:O:156:LEU:HD13	1.93	0.49
1:W:32:GLN:NE2	1:W:35:ARG:HB3	2.27	0.49
1:a:156:LEU:HD22	1:a:160:LEU:HD11	1.93	0.49
1:Q:137:ASP:CA	1:Q:138:MET:HE2	2.41	0.49
1:S:156:LEU:HD21	5:o:101:GOL:C2	2.43	0.49
2:V:25:CYS:HB2	2:V:39:LEU:HD11	1.94	0.49
1:a:100:GLY:O	1:a:160:LEU:HD22	2.13	0.49
1:Y:98:MET:SD	1:Y:98:MET:C	2.96	0.49
1:a:5:MET:HE2	1:a:164:CYS:SG	2.52	0.49
1:a:77:ASP:CG	3:j:9:VAL:HG12	2.36	0.49
1:a:214:THR:HG21	1:a:262:GLN:HE21	1.77	0.49
2:b:37:VAL:HB	2:b:66:TYR:CZ	2.48	0.49
1:U:117:ALA:HB2	2:V:60:TRP:CZ2	2.47	0.49
1:W:249:VAL:HG12	1:W:257:TYR:CZ	2.48	0.49
1:I:244:TRP:CZ3	1:I:246:ALA:HB2	2.48	0.49
2:T:24:ASN:HB3	2:T:65:LEU:HD11	1.94	0.49
1:G:70:HIS:CD2	3:f:6:ILE:HD13	2.47	0.49
1:M:231:VAL:HG11	1:M:244:TRP:CE2	2.48	0.49
1:U:208:PHE:CZ	1:U:213:ILE:HG21	2.48	0.49
1:W:116:TYR:CZ	3:g:9:VAL:HG21	2.47	0.49
1:a:156:LEU:CD2	1:a:160:LEU:CD1	2.88	0.49
1:I:73:THR:HG21	3:l:6:ILE:HG13	1.95	0.49
1:C:90:ALA:HB3	2:V:2:GLN:OE1	2.13	0.48
1:E:201:LEU:HD22	1:E:274:TRP:CZ2	2.48	0.48
1:I:150:ALA:HB3	1:I:152:VAL:HG23	1.95	0.48
1:S:203:CYS:O	1:S:244:TRP:HA	2.13	0.48
1:C:66:LYS:HD2	3:i:3:LEU:O	2.13	0.48
2:J:4:THR:HG22	6:J:202:HOH:O	2.13	0.48
2:J:39:LEU:HD23	2:J:68:THR:HG22	1.95	0.48
1:O:117:ALA:HB2	2:P:60:TRP:CE2	2.48	0.48
1:Q:97:ARG:NH2	3:p:6:ILE:HD12	2.28	0.48
1:a:258:THR:HG22	1:a:273:ARG:HA	1.95	0.48
1:A:8:PHE:HB2	1:A:25:VAL:CG2	2.43	0.48
1:O:45:MET:HE1	1:O:67:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:28:VAL:HG12	1:W:28:VAL:O	1.97	0.48
1:M:79:GLY:O	1:M:82:ARG:HB3	2.13	0.48
1:a:84:TYR:HB3	1:a:139:ALA:CB	2.44	0.48
1:A:138:MET:HE3	1:I:130:LEU:HG	1.95	0.48
1:Y:126:LEU:HD13	1:Y:133:TRP:CZ3	2.48	0.48
1:a:159:TYR:CD1	3:j:3:LEU:HD23	2.49	0.48
1:A:16:GLY:O	2:N:83:ASN:ND2	2.47	0.48
1:C:231:VAL:HG11	1:C:244:TRP:CZ2	2.48	0.48
2:D:85:VAL:HG22	1:U:90:ALA:CA	2.44	0.48
1:a:117:ALA:HB2	2:b:60:TRP:CZ2	2.49	0.48
1:W:209:TYR:CD1	1:W:210:PRO:HA	2.49	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.14	0.47
1:O:78:LEU:CD2	1:O:95:VAL:HG23	2.44	0.47
1:U:21:ARG:NH2	1:U:37:ASP:OD2	2.43	0.47
1:C:138:MET:HG2	1:G:128:GLU:O	2.15	0.47
1:a:219:ARG:O	1:a:220:ASP:C	2.55	0.47
1:E:261:VAL:HG12	1:E:266:LEU:CD1	2.44	0.47
1:K:51:TRP:O	1:K:54:GLN:HG2	2.14	0.47
1:a:64:THR:O	1:a:67:VAL:HG12	2.14	0.47
1:C:165:VAL:HG12	1:C:169:ARG:CZ	2.45	0.47
1:E:66:LYS:O	1:E:69:ALA:HB3	2.14	0.47
1:G:231:VAL:HG11	1:G:244:TRP:CZ2	2.50	0.47
1:S:231:VAL:CG1	1:S:244:TRP:CZ2	2.97	0.47
1:Y:159:TYR:CG	3:q:3:LEU:HD23	2.49	0.47
1:Y:185:PRO:HA	1:Y:208:PHE:HB3	1.97	0.47
1:K:133:TRP:NE1	1:K:153:ALA:HB2	2.29	0.47
1:Q:137:ASP:C	1:Q:138:MET:HE2	2.39	0.47
1:Y:231:VAL:HG13	1:Y:244:TRP:CE2	2.49	0.47
1:C:90:ALA:CB	2:V:2:GLN:OE1	2.62	0.47
1:I:165:VAL:HG12	1:I:169:ARG:NH1	2.30	0.47
1:M:224:GLN:O	1:M:228:THR:HG23	2.13	0.47
1:U:51:TRP:CZ2	1:U:179:LEU:HD11	2.49	0.47
2:X:5:PRO:HB3	2:X:30:PHE:HB3	1.96	0.47
1:Y:153:ALA:HB3	1:Y:154:GLU:OE1	2.15	0.47
2:Z:98:ASP:N	2:Z:98:ASP:OD1	2.48	0.47
1:a:102:ASP:OD1	1:a:113:TYR:OH	2.26	0.47
1:a:218:GLN:O	1:a:257:TYR:HA	2.14	0.47
1:C:97:ARG:NH2	3:i:6:ILE:HD12	2.29	0.47
1:C:252:GLY:HA3	1:M:150:ALA:HB1	1.97	0.47
1:I:47:PRO:HB3	1:I:52:ILE:HG23	1.97	0.47
1:M:45:MET:CE	1:M:67:VAL:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:253:GLN:OE1	1:S:256:ARG:NH1	2.48	0.47
2:X:2:GLN:OE1	1:Y:90:ALA:CB	2.62	0.47
1:K:82:ARG:HG3	1:K:87:GLN:HB2	1.97	0.47
1:Y:109:PHE:HD2	1:Y:165:VAL:HG21	1.80	0.47
1:Y:184:ALA:HB2	1:Y:265:GLY:O	2.15	0.47
1:Y:234:ARG:NH2	2:Z:99:MET:OXT	2.48	0.47
1:M:36:PHE:CD1	1:M:67:VAL:HG11	2.50	0.46
1:S:163:THR:HG22	1:S:167:TRP:HD1	1.78	0.46
1:a:112:GLY:O	1:a:130:LEU:HD21	2.15	0.46
1:Q:137:ASP:C	1:Q:137:ASP:OD1	2.58	0.46
1:S:126:LEU:HD12	1:S:132:SER:O	2.16	0.46
1:S:187:THR:HB	1:S:272:LEU:HD11	1.96	0.46
2:X:35:ILE:O	2:X:35:ILE:HG23	2.15	0.46
1:A:201:LEU:HD22	1:A:274:TRP:CZ2	2.51	0.46
1:C:100:GLY:O	1:C:160:LEU:HD22	2.15	0.46
1:C:218:GLN:OE1	1:C:260:HIS:NE2	2.48	0.46
1:E:187:THR:HB	1:E:272:LEU:HD11	1.98	0.46
1:I:33:PHE:CD1	1:I:34:VAL:HG13	2.51	0.46
1:S:66:LYS:NZ	3:o:1:TYR:CE2	2.84	0.46
1:Y:81:LEU:HD13	1:Y:118:TYR:CD1	2.51	0.46
1:Y:231:VAL:CG1	1:Y:244:TRP:CE2	2.98	0.46
1:G:103:VAL:HG13	1:G:168:LEU:HD23	1.97	0.46
1:G:97:ARG:CZ	3:f:6:ILE:HD12	2.45	0.46
1:a:97:ARG:NH2	3:j:6:ILE:HD12	2.30	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.51	0.46
1:C:28:VAL:O	1:C:29:ASP:HB2	2.16	0.46
1:M:51:TRP:CZ2	1:M:179:LEU:HD11	2.50	0.46
1:A:31:THR:HG22	1:A:32:GLN:O	2.16	0.46
2:D:85:VAL:HG13	1:U:90:ALA:HB1	1.98	0.46
1:O:215:LEU:HD22	1:O:261:VAL:HG22	1.98	0.46
1:K:97:ARG:NH2	3:h:6:ILE:HD12	2.31	0.46
1:O:45:MET:CE	1:O:67:VAL:HB	2.46	0.46
1:S:12:VAL:HG13	1:S:94:THR:HG23	1.98	0.46
2:T:27:VAL:HG23	2:T:30:PHE:CE1	2.50	0.46
1:W:99:TYR:CZ	3:g:3:LEU:HD12	2.51	0.46
1:W:230:LEU:HD23	1:W:245:ALA:HB2	1.97	0.46
1:W:13:SER:HB3	1:W:78:LEU:HD22	1.98	0.45
1:Y:7:TYR:HB3	1:Y:9:PHE:CE2	2.51	0.45
1:U:182:THR:HG21	1:U:264:GLU:HG2	1.97	0.45
1:K:165:VAL:HG12	1:K:169:ARG:CZ	2.46	0.45
1:M:81:LEU:CD2	3:e:9:VAL:HG11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:VAL:HG11	1:E:244:TRP:CE2	2.51	0.45
1:I:172:LEU:HD23	1:I:179:LEU:HD13	1.97	0.45
2:N:49:VAL:HG22	2:N:68:THR:HB	1.99	0.45
2:X:54:LEU:HD11	2:X:62:PHE:HB3	1.98	0.45
1:Y:111:ARG:HG2	1:Y:112:GLY:N	2.31	0.45
1:E:44:ARG:HD2	2:P:16:GLU:HG3	1.98	0.45
2:R:32:PRO:HD2	2:R:85:VAL:HG11	1.99	0.45
1:S:33:PHE:O	1:S:52:ILE:HG21	2.17	0.45
1:Y:146:LYS:NZ	1:a:196:ASP:O	2.40	0.45
1:a:143:THR:HG21	3:j:9:VAL:CG2	2.46	0.45
1:G:8:PHE:HB2	1:G:25:VAL:HG23	1.99	0.45
2:T:39:LEU:HD23	2:T:68:THR:HG22	1.99	0.45
1:E:231:VAL:CG1	1:E:244:TRP:CE2	3.00	0.45
1:O:231:VAL:CG1	1:O:244:TRP:CZ2	3.00	0.45
5:Q:303:GOL:H31	3:p:6:ILE:HA	1.98	0.45
2:R:59:ASP:O	2:R:60:TRP:HB2	2.17	0.45
1:U:33:PHE:CD1	1:U:34:VAL:HG13	2.52	0.45
1:C:90:ALA:CB	2:V:2:GLN:CD	2.88	0.45
1:I:66:LYS:O	1:I:69:ALA:HB3	2.17	0.45
1:I:124:ILE:O	1:I:124:ILE:HG23	2.15	0.45
1:a:137:ASP:H	1:a:140:ALA:HB3	1.81	0.45
2:L:25:CYS:HB2	2:L:39:LEU:HD11	1.99	0.45
2:R:5:PRO:HB3	2:R:30:PHE:HB3	1.99	0.45
1:Y:165:VAL:HG12	1:Y:169:ARG:NH1	2.32	0.45
2:b:54:LEU:CA	2:b:64:LEU:HD21	2.45	0.45
2:H:5:PRO:HB3	2:H:30:PHE:HB3	1.98	0.45
2:H:11:SER:OG	2:H:13:HIS:O	2.32	0.45
1:Y:45:MET:HE1	1:Y:67:VAL:HB	1.99	0.45
1:a:201:LEU:HD22	1:a:274:TRP:CZ2	2.52	0.45
1:A:88:SER:C	1:A:90:ALA:N	2.75	0.44
1:E:40:ALA:HB3	6:E:401:HOH:O	2.16	0.44
2:L:1:ILE:C	2:L:1:ILE:HD12	2.42	0.44
1:M:82:ARG:HD3	1:M:89:GLU:HA	1.99	0.44
1:O:49:ALA:O	1:O:52:ILE:HG22	2.17	0.44
1:A:194:VAL:HG22	1:A:198:GLU:O	2.17	0.44
2:H:40:LEU:HD23	2:H:45:ARG:HA	1.99	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.17	0.44
1:E:231:VAL:HG11	1:E:244:TRP:CZ2	2.52	0.44
2:F:54:LEU:HD12	2:F:64:LEU:HG	1.99	0.44
1:M:103:VAL:HB	1:M:107:TRP:HA	1.99	0.44
1:S:143:THR:OG1	3:o:9:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:156:LEU:HG	5:c:101:GOL:C1	2.47	0.44
1:Y:116:TYR:CE1	3:q:9:VAL:HG21	2.52	0.44
1:Y:152:VAL:O	1:Y:155:GLN:N	2.50	0.44
1:a:219:ARG:O	1:a:219:ARG:HG3	2.16	0.44
1:E:90:ALA:CA	2:J:85:VAL:HG22	2.48	0.44
2:H:34:ASP:O	2:H:84:HIS:HD2	2.00	0.44
1:Q:32:GLN:NE2	1:Q:35:ARG:HB3	2.33	0.44
1:Y:74:HIS:CE1	1:Y:97:ARG:HE	2.35	0.44
1:C:138:MET:HE2	1:C:138:MET:N	2.32	0.44
1:U:13:SER:HB3	1:U:78:LEU:HD13	2.00	0.44
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.53	0.44
1:E:28:VAL:HG23	1:E:33:PHE:CD2	2.52	0.44
1:G:12:VAL:HG22	1:G:94:THR:HG23	1.99	0.44
1:Q:21:ARG:HD3	1:Q:39:ASP:OD2	2.18	0.44
1:E:261:VAL:CG1	1:E:266:LEU:CD1	2.96	0.44
1:G:103:VAL:HG12	1:G:165:VAL:CG1	2.48	0.44
1:K:138:MET:N	1:K:138:MET:HE2	2.33	0.44
1:S:196:ASP:OD2	1:S:197:HIS:N	2.50	0.44
1:a:45:MET:CE	3:j:2:LEU:HD11	2.47	0.44
1:a:201:LEU:HD13	1:a:274:TRP:NE1	2.33	0.44
1:K:214:THR:HG22	1:K:216:THR:HG23	2.00	0.43
1:S:109:PHE:HZ	1:S:130:LEU:HD11	1.83	0.43
1:Y:95:VAL:HG13	1:Y:116:TYR:CE2	2.52	0.43
1:E:3:HIS:HA	1:E:29:ASP:OD1	2.18	0.43
1:G:187:THR:HB	1:G:272:LEU:HD11	2.00	0.43
1:Q:28:VAL:CG1	1:Q:179:LEU:HD13	2.46	0.43
1:Q:231:VAL:CG1	1:Q:244:TRP:CZ2	3.01	0.43
2:R:39:LEU:HD23	2:R:68:THR:HG22	2.00	0.43
1:Y:51:TRP:CE2	1:Y:179:LEU:HD11	2.53	0.43
1:a:255:GLN:HA	1:a:274:TRP:HB2	2.00	0.43
2:b:39:LEU:O	2:b:46:ILE:HD12	2.18	0.43
1:A:252:GLY:HA3	1:U:150:ALA:CB	2.48	0.43
1:E:82:ARG:HD3	1:E:89:GLU:HA	1.99	0.43
1:U:226:GLN:HE21	1:U:226:GLN:HA	1.83	0.43
1:K:8:PHE:HB2	1:K:25:VAL:CG2	2.48	0.43
1:M:231:VAL:CG1	1:M:244:TRP:CE2	3.02	0.43
2:T:2:GLN:HB3	2:T:86:THR:HG22	1.99	0.43
1:W:81:LEU:HD13	1:W:118:TYR:CD1	2.54	0.43
1:Y:219:ARG:HG3	1:Y:257:TYR:CE2	2.54	0.43
5:a:302:GOL:H32	3:j:6:ILE:HA	1.99	0.43
2:R:40:LEU:HD23	2:R:45:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:25:VAL:HG12	1:Y:32:GLN:NE2	2.33	0.43
1:a:114:HIS:ND1	1:a:114:HIS:C	2.76	0.43
1:A:103:VAL:HG13	1:A:168:LEU:HD23	2.00	0.43
1:C:8:PHE:HB2	1:C:25:VAL:HG22	2.00	0.43
1:E:99:TYR:CZ	3:k:3:LEU:HD12	2.53	0.43
1:E:138:MET:SD	1:M:110:LEU:HD22	2.59	0.43
1:E:247:VAL:HG13	1:E:249:VAL:HG13	2.00	0.43
1:G:152:VAL:HG13	5:f:101:GOL:H12	1.99	0.43
2:P:5:PRO:HB3	2:P:30:PHE:HB3	2.00	0.43
1:S:103:VAL:HG12	1:S:165:VAL:HG13	2.01	0.43
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.00	0.43
2:R:7:ILE:HD13	2:R:82:VAL:HG21	1.99	0.43
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.48	0.43
2:F:51:HIS:HB3	2:F:66:TYR:CD2	2.54	0.43
1:U:82:ARG:CD	1:U:89:GLU:HA	2.49	0.43
2:V:68:THR:HG23	2:V:69:GLU:O	2.19	0.43
1:I:191:HIS:HB2	1:I:274:TRP:CH2	2.54	0.43
1:I:244:TRP:HZ3	1:I:246:ALA:HB2	1.83	0.43
1:Q:12:VAL:O	1:Q:21:ARG:N	2.52	0.43
1:U:252:GLY:O	1:U:255:GLN:NE2	2.51	0.43
1:C:28:VAL:O	1:C:29:ASP:C	2.53	0.43
1:E:43:GLN:HE21	2:P:74:GLU:HG2	1.84	0.43
1:W:203:CYS:O	1:W:244:TRP:HB2	2.19	0.43
1:A:7:TYR:HB3	1:A:9:PHE:CE2	2.55	0.42
1:A:88:SER:O	1:A:90:ALA:N	2.52	0.42
1:C:77:ASP:CG	3:i:9:VAL:HG12	2.43	0.42
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.54	0.42
2:P:2:GLN:HG3	2:P:32:PRO:HD3	2.01	0.42
1:Y:270:LEU:HD22	1:Y:272:LEU:HD21	1.99	0.42
1:a:7:TYR:HB3	1:a:9:PHE:CE2	2.54	0.42
2:b:73:THR:O	2:b:97:ARG:NH2	2.52	0.42
1:C:97:ARG:HH11	1:C:114:HIS:CE1	2.36	0.42
2:H:23:LEU:O	2:H:67:TYR:HA	2.19	0.42
1:I:45:MET:CE	3:l:2:LEU:HD11	2.49	0.42
1:M:32:GLN:NE2	1:M:35:ARG:HB3	2.34	0.42
1:M:109:PHE:CD2	1:M:161:GLU:HA	2.54	0.42
2:T:37:VAL:HG21	2:T:66:TYR:CE1	2.54	0.42
1:U:110:LEU:C	1:U:110:LEU:CD2	2.91	0.42
1:W:216:THR:HG21	1:W:223:ASP:OD2	2.19	0.42
1:a:173:GLU:O	1:a:176:LYS:HB2	2.18	0.42
1:C:268:LYS:HG2	1:C:269:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:LEU:HD21	3:l:9:VAL:HG11	2.00	0.42
2:J:24:ASN:HB3	2:J:65:LEU:HD11	2.01	0.42
1:K:133:TRP:HE1	1:K:153:ALA:HB2	1.84	0.42
1:K:175:GLY:O	1:K:179:LEU:N	2.50	0.42
1:Q:129:ASP:C	1:Q:129:ASP:OD1	2.62	0.42
1:A:97:ARG:NH2	3:m:6:ILE:HD12	2.35	0.42
2:B:10:TYR:CD1	2:B:10:TYR:N	2.87	0.42
2:F:7:ILE:HB	2:F:93:VAL:HG21	2.01	0.42
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.53	0.42
2:H:21:ASN:OD1	2:H:22:PHE:N	2.48	0.42
1:M:45:MET:CE	3:e:2:LEU:HD11	2.50	0.42
1:O:78:LEU:HD23	1:O:95:VAL:HG23	2.02	0.42
1:U:109:PHE:CD2	1:U:161:GLU:HA	2.54	0.42
1:W:30:ASP:HB2	1:W:209:TYR:HE1	1.84	0.42
1:S:5:MET:HE2	1:S:164:CYS:SG	2.59	0.42
1:U:194:VAL:HG23	1:U:195:SER:N	2.34	0.42
2:b:24:ASN:HB3	2:b:65:LEU:HD11	2.01	0.42
2:F:98:ASP:OD1	2:F:98:ASP:N	2.53	0.42
1:Q:73:THR:HG21	3:p:6:ILE:HG13	2.01	0.42
1:U:236:ALA:HB2	1:U:242:GLN:HE21	1.84	0.42
1:Y:67:VAL:HB	3:q:2:LEU:HD11	2.01	0.42
2:Z:5:PRO:HB3	2:Z:30:PHE:HB3	2.02	0.42
1:A:15:PRO:HG2	2:N:85:VAL:HG23	2.01	0.42
1:I:165:VAL:CG1	1:I:169:ARG:CZ	2.97	0.42
1:O:104:GLY:HA2	1:O:110:LEU:HD12	2.01	0.42
1:S:235:PRO:HG2	2:T:65:LEU:HD22	2.01	0.42
2:T:23:LEU:O	2:T:67:TYR:HA	2.19	0.42
1:W:64:THR:O	1:W:67:VAL:HG12	2.19	0.42
1:C:10:THR:HG21	2:D:54:LEU:HD23	2.00	0.42
1:M:255:GLN:HA	1:M:274:TRP:HB2	2.02	0.42
1:O:12:VAL:CG2	1:O:94:THR:HG23	2.50	0.42
1:S:73:THR:HG21	3:o:6:ILE:HG13	2.02	0.42
1:W:28:VAL:O	1:W:29:ASP:HB2	2.20	0.42
1:Y:59:TYR:O	1:Y:63:GLU:HG2	2.20	0.42
1:Y:172:LEU:O	1:Y:180:GLN:NE2	2.52	0.42
2:D:33:SER:HB2	2:D:54:LEU:HD21	2.02	0.42
1:E:28:VAL:HG23	1:E:33:PHE:CE2	2.55	0.42
1:K:135:ALA:HB1	1:K:140:ALA:CB	2.50	0.42
1:G:231:VAL:O	1:G:243:LYS:NZ	2.41	0.41
1:I:156:LEU:HD22	1:I:160:LEU:CD1	2.50	0.41
1:O:109:PHE:HD2	1:O:165:VAL:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:219:ARG:HG3	1:O:257:TYR:CZ	2.55	0.41
1:A:7:TYR:CZ	3:m:2:LEU:HD23	2.55	0.41
1:A:109:PHE:CD1	1:A:109:PHE:C	2.98	0.41
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.47	0.41
1:C:13:SER:HB3	1:C:78:LEU:HD13	2.02	0.41
1:E:168:LEU:HD12	1:E:172:LEU:HG	2.03	0.41
1:E:218:GLN:O	1:E:257:TYR:HA	2.21	0.41
3:f:3:LEU:O	3:f:4:MET:C	2.63	0.41
2:P:15:ALA:HB2	2:P:95:TRP:HZ2	1.84	0.41
2:R:2:GLN:HB3	2:R:86:THR:HG22	2.01	0.41
1:S:238:ASP:OD1	1:S:240:THR:OG1	2.36	0.41
1:W:152:VAL:HG13	5:g:101:GOL:H11	2.02	0.41
1:W:230:LEU:CD2	1:W:245:ALA:HB2	2.50	0.41
1:Y:116:TYR:HB3	1:Y:124:ILE:HG22	2.01	0.41
1:K:266:LEU:O	1:K:267:PRO:C	2.61	0.41
1:M:70:HIS:HA	3:e:6:ILE:HD11	2.02	0.41
1:M:114:HIS:ND1	1:M:114:HIS:C	2.78	0.41
1:O:13:SER:HG	1:O:93:HIS:H	1.67	0.41
1:W:33:PHE:CD1	1:W:34:VAL:HG13	2.55	0.41
1:W:160:LEU:O	1:W:165:VAL:HG23	2.19	0.41
1:G:19:GLU:HB3	1:G:20:PRO:HD2	2.01	0.41
2:N:24:ASN:HB3	2:N:65:LEU:HD11	2.02	0.41
1:A:87:GLN:O	1:A:88:SER:C	2.63	0.41
2:B:37:VAL:HB	2:B:66:TYR:CZ	2.55	0.41
1:E:90:ALA:HB1	2:J:85:VAL:CG2	2.41	0.41
2:J:23:LEU:O	2:J:67:TYR:HA	2.20	0.41
2:J:31:HIS:ND1	2:J:32:PRO:HA	2.35	0.41
1:M:19:GLU:OE1	1:M:19:GLU:CA	2.69	0.41
2:P:72:PRO:C	2:P:73:THR:HG23	2.46	0.41
1:Y:51:TRP:CZ2	1:Y:179:LEU:HD11	2.54	0.41
2:b:54:LEU:HD12	2:b:64:LEU:HG	2.03	0.41
1:A:7:TYR:CE2	3:m:2:LEU:HD23	2.54	0.41
2:B:23:LEU:HB3	2:B:68:THR:HG22	2.02	0.41
1:C:22:PHE:HE2	1:C:67:VAL:HG22	1.85	0.41
1:W:231:VAL:HG11	1:W:244:TRP:CE2	2.55	0.41
1:E:187:THR:HA	1:E:204:TRP:O	2.20	0.41
1:E:201:LEU:HD13	1:E:274:TRP:NE1	2.35	0.41
1:E:249:VAL:HG12	1:E:257:TYR:CZ	2.56	0.41
1:Q:235:PRO:HG2	2:R:65:LEU:HD22	2.02	0.41
1:S:231:VAL:HG11	1:S:244:TRP:CE2	2.56	0.41
1:W:126:LEU:HD22	1:W:156:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:52:ILE:HD12	1:Y:52:ILE:HA	1.95	0.41
2:Z:81:ARG:HB2	2:Z:92:ILE:HD13	2.03	0.41
1:a:85:TYR:CE2	1:a:139:ALA:HB3	2.55	0.41
1:A:252:GLY:C	1:U:150:ALA:HB1	2.45	0.41
1:I:138:MET:HG2	1:M:85:TYR:CE1	2.56	0.41
1:S:112:GLY:HA3	1:S:160:LEU:HD13	2.03	0.41
1:Y:95:VAL:HG11	1:Y:116:TYR:OH	2.21	0.41
1:C:65:ARG:HD2	5:i:101:GOL:O2	2.21	0.41
1:E:5:MET:HE2	1:E:164:CYS:SG	2.61	0.41
1:E:37:ASP:HB3	1:E:40:ALA:CB	2.50	0.41
1:E:45:MET:HE1	3:k:2:LEU:HD11	2.03	0.41
1:G:22:PHE:CD2	1:G:71:SER:HB3	2.55	0.41
2:P:85:VAL:HG13	2:P:86:THR:N	2.36	0.41
1:Q:201:LEU:HD13	1:Q:274:TRP:NE1	2.36	0.41
2:R:3:ARG:HB3	2:R:29:GLY:O	2.21	0.41
1:S:45:MET:HE1	1:S:67:VAL:CG2	2.51	0.41
1:S:150:ALA:HB3	1:S:152:VAL:HG23	2.03	0.41
1:W:126:LEU:HD22	1:W:156:LEU:CD1	2.51	0.41
1:Y:28:VAL:HG11	1:Y:179:LEU:HD13	2.03	0.41
2:b:37:VAL:HG11	2:b:66:TYR:CD1	2.56	0.41
2:b:54:LEU:HD13	2:b:64:LEU:HD11	2.03	0.41
1:E:44:ARG:HA	1:E:64:THR:CG2	2.49	0.41
1:K:82:ARG:CD	1:K:89:GLU:HA	2.51	0.41
2:L:24:ASN:HB3	2:L:65:LEU:HD11	2.03	0.41
1:A:73:THR:HG21	3:m:6:ILE:HG13	2.02	0.40
1:C:117:ALA:HB2	2:D:60:TRP:CZ2	2.56	0.40
1:O:176:LYS:O	1:O:177:GLU:C	2.64	0.40
1:Q:126:LEU:HD22	1:Q:156:LEU:HD13	2.03	0.40
1:U:175:GLY:O	1:U:179:LEU:N	2.51	0.40
2:V:0:MET:HE2	2:V:0:MET:HB3	1.93	0.40
2:b:84:HIS:CE1	2:b:86:THR:HG23	2.56	0.40
2:B:7:ILE:HG12	2:B:27:VAL:HG12	2.03	0.40
1:I:77:ASP:O	1:I:78:LEU:C	2.63	0.40
1:Q:74:HIS:HD2	1:Q:95:VAL:HG11	1.86	0.40
1:W:167:TRP:CE3	1:W:170:ARG:HD3	2.56	0.40
1:a:209:TYR:CD2	1:a:209:TYR:C	2.99	0.40
1:G:205:ALA:HB2	1:G:215:LEU:HD21	2.03	0.40
1:I:266:LEU:O	1:I:267:PRO:C	2.63	0.40
1:K:182:THR:HG21	1:K:264:GLU:HG2	2.03	0.40
2:R:24:ASN:HB3	2:R:65:LEU:HD11	2.04	0.40
2:b:13:HIS:HB2	2:b:21:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:LEU:HA	2:F:44:GLU:O	2.21	0.40
1:I:70:HIS:HA	3:I:6:ILE:HD11	2.03	0.40
1:K:28:VAL:HG11	1:K:179:LEU:HD13	2.03	0.40
1:S:178:THR:OG1	1:S:179:LEU:N	2.53	0.40
1:U:70:HIS:HE2	1:U:99:TYR:HH	1.63	0.40
1:I:19:GLU:HG2	1:I:75:ARG:HH22	1.87	0.40
1:O:95:VAL:HG13	1:O:116:TYR:CE2	2.57	0.40
1:O:216:THR:O	1:O:260:HIS:N	2.55	0.40
1:Q:78:LEU:CD2	1:Q:95:VAL:HG23	2.52	0.40
1:U:55:GLU:OE2	1:U:170:ARG:NE	2.53	0.40
2:X:96:ASP:OD2	2:X:99:MET:HE3	2.22	0.40
1:Y:64:THR:O	1:Y:67:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	263 (96%)	10 (4%)	1 (0%)	30	61
1	C	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	E	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	G	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	30	61
1	I	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	K	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	M	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	O	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	Q	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	S	274/276 (99%)	264 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	W	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	Y	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
1	a	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	H	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	J	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	N	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	P	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	R	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
2	T	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	V	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	X	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	Z	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	b	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	12	41
3	c	7/9 (78%)	7 (100%)	0	0	100	100
3	e	7/9 (78%)	7 (100%)	0	0	100	100
3	f	7/9 (78%)	7 (100%)	0	0	100	100
3	g	7/9 (78%)	7 (100%)	0	0	100	100
3	h	7/9 (78%)	7 (100%)	0	0	100	100
3	i	7/9 (78%)	7 (100%)	0	0	100	100
3	j	7/9 (78%)	7 (100%)	0	0	100	100
3	k	7/9 (78%)	7 (100%)	0	0	100	100
3	l	7/9 (78%)	7 (100%)	0	0	100	100
3	m	7/9 (78%)	7 (100%)	0	0	100	100
3	n	7/9 (78%)	7 (100%)	0	0	100	100
3	o	7/9 (78%)	7 (100%)	0	0	100	100
3	p	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	5306/5390 (98%)	5121 (96%)	182 (3%)	3 (0%)	48	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	G	267	PRO
2	b	35	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	227 (98%)	5 (2%)	45	71
1	C	232/232 (100%)	219 (94%)	13 (6%)	19	49
1	E	232/232 (100%)	219 (94%)	13 (6%)	19	49
1	G	232/232 (100%)	222 (96%)	10 (4%)	26	57
1	I	232/232 (100%)	217 (94%)	15 (6%)	15	44
1	K	232/232 (100%)	215 (93%)	17 (7%)	13	40
1	M	232/232 (100%)	222 (96%)	10 (4%)	26	57
1	O	232/232 (100%)	220 (95%)	12 (5%)	21	51
1	Q	232/232 (100%)	224 (97%)	8 (3%)	32	63
1	S	232/232 (100%)	214 (92%)	18 (8%)	11	38
1	U	232/232 (100%)	220 (95%)	12 (5%)	21	51
1	W	232/232 (100%)	220 (95%)	12 (5%)	21	51
1	Y	232/232 (100%)	217 (94%)	15 (6%)	15	44
1	a	232/232 (100%)	220 (95%)	12 (5%)	21	51
2	B	95/95 (100%)	90 (95%)	5 (5%)	20	51
2	D	95/95 (100%)	90 (95%)	5 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	95/95 (100%)	89 (94%)	6 (6%)	16	45
2	H	95/95 (100%)	89 (94%)	6 (6%)	16	45
2	J	95/95 (100%)	92 (97%)	3 (3%)	34	64
2	L	95/95 (100%)	93 (98%)	2 (2%)	47	71
2	N	95/95 (100%)	88 (93%)	7 (7%)	13	40
2	P	95/95 (100%)	92 (97%)	3 (3%)	34	64
2	R	95/95 (100%)	90 (95%)	5 (5%)	20	51
2	T	95/95 (100%)	93 (98%)	2 (2%)	47	71
2	V	95/95 (100%)	88 (93%)	7 (7%)	13	40
2	X	95/95 (100%)	89 (94%)	6 (6%)	16	45
2	Z	95/95 (100%)	88 (93%)	7 (7%)	13	40
2	b	95/95 (100%)	92 (97%)	3 (3%)	34	64
3	c	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	e	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	f	9/9 (100%)	7 (78%)	2 (22%)	1	4
3	g	9/9 (100%)	9 (100%)	0	100	100
3	h	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	i	9/9 (100%)	9 (100%)	0	100	100
3	j	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	k	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	l	9/9 (100%)	9 (100%)	0	100	100
3	m	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	n	9/9 (100%)	7 (78%)	2 (22%)	1	4
3	o	9/9 (100%)	9 (100%)	0	100	100
3	p	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	q	9/9 (100%)	9 (100%)	0	100	100
All	All	4704/4704 (100%)	4454 (95%)	250 (5%)	20	51

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	194	VAL
1	A	268	LYS
2	B	4	THR
2	B	57	SER
2	B	77	GLU
2	B	89	GLN
2	B	97	ARG
3	m	9	VAL
1	C	35	ARG
1	C	42	SER
1	C	106	ASP
1	C	110	LEU
1	C	156	LEU
1	C	176	LYS
1	C	194	VAL
1	C	195	SER
1	C	207	SER
1	C	226	GLN
1	C	227	ASP
1	C	255	GLN
1	C	268	LYS
2	D	2	GLN
2	D	39	LEU
2	D	45	ARG
2	D	97	ARG
2	D	98	ASP
1	E	11	SER
1	E	35	ARG
1	E	58	GLU
1	E	89	GLU
1	E	110	LEU
1	E	128	GLU
1	E	141	GLN
1	E	156	LEU
1	E	227	ASP
1	E	247	VAL
1	E	255	GLN
1	E	268	LYS
1	E	273	ARG
2	F	36	GLU
2	F	39	LEU

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Mol	Chain	Res	Type
2	F	70	PHE
2	F	85	VAL
2	F	89	GLN
2	F	98	ASP
3	k	9	VAL
1	G	2	SER
1	G	89	GLU
1	G	110	LEU
1	G	156	LEU
1	G	165	VAL
1	G	197	HIS
1	G	225	THR
1	G	249	VAL
1	G	270	LEU
1	G	275	GLU
2	H	4	THR
2	H	39	LEU
2	H	47	GLU
2	H	75	LYS
2	H	85	VAL
2	H	89	GLN
3	f	7	THR
3	f	9	VAL
1	I	2	SER
1	I	17	ARG
1	I	35	ARG
1	I	86	ASN
1	I	94	THR
1	I	105	SER
1	I	110	LEU
1	I	156	LEU
1	I	168	LEU
1	I	194	VAL
1	I	228	THR
1	I	230	LEU
1	I	249	VAL
1	I	258	THR
1	I	268	LYS
2	J	47	GLU
2	J	49	VAL
2	J	92	ILE
1	K	2	SER

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Mol	Chain	Res	Type
1	K	6	ARG
1	K	34	VAL
1	K	35	ARG
1	K	58	GLU
1	K	72	GLN
1	K	110	LEU
1	K	111	ARG
1	K	132	SER
1	K	156	LEU
1	K	178	THR
1	K	194	VAL
1	K	207	SER
1	K	225	THR
1	K	226	GLN
1	K	228	THR
1	K	275	GLU
2	L	39	LEU
2	L	44	GLU
3	h	9	VAL
1	M	17	ARG
1	M	19	GLU
1	M	35	ARG
1	M	73	THR
1	M	156	LEU
1	M	194	VAL
1	M	230	LEU
1	M	249	VAL
1	M	268	LYS
1	M	275	GLU
2	N	4	THR
2	N	34	ASP
2	N	38	ASP
2	N	39	LEU
2	N	58	LYS
2	N	75	LYS
2	N	77	GLU
3	e	9	VAL
1	O	4	SER
1	O	35	ARG
1	O	89	GLU
1	O	128	GLU
1	O	163	THR

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Mol	Chain	Res	Type
1	O	194	VAL
1	O	207	SER
1	O	222	GLU
1	O	224	GLN
1	O	227	ASP
1	O	249	VAL
1	O	268	LYS
2	P	2	GLN
2	P	4	THR
2	P	57	SER
3	n	4	MET
3	n	8	GLN
1	Q	35	ARG
1	Q	110	LEU
1	Q	121	LYS
1	Q	156	LEU
1	Q	194	VAL
1	Q	219	ARG
1	Q	226	GLN
1	Q	249	VAL
2	R	0	MET
2	R	3	ARG
2	R	50	GLU
2	R	75	LYS
2	R	77	GLU
3	p	9	VAL
1	S	25	VAL
1	S	34	VAL
1	S	35	ARG
1	S	67	VAL
1	S	87	GLN
1	S	94	THR
1	S	113	TYR
1	S	121	LYS
1	S	122	ASP
1	S	142	THR
1	S	163	THR
1	S	178	THR
1	S	194	VAL
1	S	216	THR
1	S	219	ARG
1	S	228	THR

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Mol	Chain	Res	Type
1	S	248	VAL
1	S	268	LYS
2	T	39	LEU
2	T	75	LYS
1	U	2	SER
1	U	19	GLU
1	U	35	ARG
1	U	67	VAL
1	U	86	ASN
1	U	132	SER
1	U	156	LEU
1	U	163	THR
1	U	166	GLU
1	U	178	THR
1	U	227	ASP
1	U	230	LEU
2	V	4	THR
2	V	48	LYS
2	V	63	TYR
2	V	68	THR
2	V	85	VAL
2	V	97	ARG
2	V	98	ASP
3	c	9	VAL
1	W	28	VAL
1	W	35	ARG
1	W	113	TYR
1	W	115	GLN
1	W	156	LEU
1	W	163	THR
1	W	168	LEU
1	W	194	VAL
1	W	216	THR
1	W	225	THR
1	W	251	SER
1	W	268	LYS
2	X	9	VAL
2	X	39	LEU
2	X	48	LYS
2	X	58	LYS
2	X	76	ASP
2	X	92	ILE

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Mol	Chain	Res	Type
1	Y	25	VAL
1	Y	35	ARG
1	Y	122	ASP
1	Y	128	GLU
1	Y	129	ASP
1	Y	138	MET
1	Y	154	GLU
1	Y	156	LEU
1	Y	178	THR
1	Y	194	VAL
1	Y	216	THR
1	Y	222	GLU
1	Y	227	ASP
1	Y	230	LEU
1	Y	270	LEU
2	Z	4	THR
2	Z	33	SER
2	Z	34	ASP
2	Z	39	LEU
2	Z	75	LYS
2	Z	89	GLN
2	Z	98	ASP
1	a	35	ARG
1	a	67	VAL
1	a	89	GLU
1	a	110	LEU
1	a	113	TYR
1	a	121	LYS
1	a	166	GLU
1	a	176	LYS
1	a	226	GLN
1	a	227	ASP
1	a	262	GLN
1	a	270	LEU
2	b	4	THR
2	b	39	LEU
2	b	75	LYS
3	j	7	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	262	GLN
2	B	13	HIS
1	C	72	GLN
1	C	145	HIS
1	C	188	HIS
1	C	262	GLN
2	D	2	GLN
1	E	43	GLN
1	E	96	GLN
1	E	218	GLN
1	E	255	GLN
2	F	24	ASN
2	F	31	HIS
1	G	54	GLN
1	G	141	GLN
1	G	218	GLN
1	G	224	GLN
1	G	226	GLN
2	H	13	HIS
1	I	155	GLN
2	J	8	GLN
2	J	13	HIS
1	M	86	ASN
1	M	145	HIS
1	M	155	GLN
1	M	242	GLN
1	O	180	GLN
1	O	191	HIS
1	Q	70	HIS
1	Q	96	GLN
1	Q	141	GLN
1	Q	188	HIS
1	S	32	GLN
1	S	87	GLN
1	S	155	GLN
1	S	224	GLN
2	T	24	ASN
1	U	155	GLN
1	U	226	GLN
1	U	242	GLN
1	U	255	GLN
2	V	13	HIS

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Mol	Chain	Res	Type
1	W	54	GLN
1	W	115	GLN
1	W	141	GLN
1	W	151	HIS
1	W	188	HIS
1	Y	32	GLN
1	Y	54	GLN
1	Y	151	HIS
1	a	32	GLN
1	a	87	GLN
1	a	96	GLN
1	a	155	GLN
1	a	226	GLN
1	a	262	GLN
2	b	13	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	f	101	-	5,5,5	0.58	0	5,5,5	0.91	0
5	GOL	c	101	-	5,5,5	0.41	0	5,5,5	0.47	0
5	GOL	Y	302	-	5,5,5	0.52	0	5,5,5	0.28	0
5	GOL	C	302	-	5,5,5	0.55	0	5,5,5	0.38	0
5	GOL	C	303	-	5,5,5	0.38	0	5,5,5	0.24	0
5	GOL	E	302	-	5,5,5	0.56	0	5,5,5	0.83	0
5	GOL	S	302	-	5,5,5	0.43	0	5,5,5	0.59	0
5	GOL	l	101	-	5,5,5	0.26	0	5,5,5	0.40	0
5	GOL	K	302	-	5,5,5	0.39	0	5,5,5	0.66	0
5	GOL	a	302	-	5,5,5	0.51	0	5,5,5	0.51	0
5	GOL	O	303	-	5,5,5	0.41	0	5,5,5	0.30	0
5	GOL	i	101	-	5,5,5	0.53	0	5,5,5	0.48	0
5	GOL	o	101	-	5,5,5	0.49	0	5,5,5	0.29	0
5	GOL	e	101	-	5,5,5	0.53	0	5,5,5	0.38	0
5	GOL	O	302	-	5,5,5	0.42	0	5,5,5	0.31	0
5	GOL	Q	303	-	5,5,5	0.62	0	5,5,5	0.47	0
5	GOL	g	101	-	5,5,5	0.53	0	5,5,5	0.26	0
5	GOL	q	101	-	5,5,5	0.44	0	5,5,5	0.31	0
5	GOL	h	101	-	5,5,5	0.53	0	5,5,5	0.55	0
5	GOL	A	302	-	5,5,5	0.64	0	5,5,5	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	f	101	-	-	2/4/4/4	-
5	GOL	c	101	-	-	2/4/4/4	-
5	GOL	Y	302	-	-	2/4/4/4	-
5	GOL	C	302	-	-	2/4/4/4	-
5	GOL	C	303	-	-	2/4/4/4	-
5	GOL	E	302	-	-	2/4/4/4	-
5	GOL	S	302	-	-	0/4/4/4	-
5	GOL	l	101	-	-	4/4/4/4	-
5	GOL	K	302	-	-	0/4/4/4	-
5	GOL	a	302	-	-	2/4/4/4	-
5	GOL	O	303	-	-	2/4/4/4	-
5	GOL	i	101	-	-	2/4/4/4	-
5	GOL	o	101	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	e	101	-	-	2/4/4/4	-
5	GOL	O	302	-	-	2/4/4/4	-
5	GOL	Q	303	-	-	2/4/4/4	-
5	GOL	g	101	-	-	2/4/4/4	-
5	GOL	q	101	-	-	0/4/4/4	-
5	GOL	h	101	-	-	3/4/4/4	-
5	GOL	A	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	GOL	C1-C2-C3-O3
5	C	303	GOL	O1-C1-C2-C3
5	f	101	GOL	O1-C1-C2-C3
5	l	101	GOL	O1-C1-C2-C3
5	l	101	GOL	C1-C2-C3-O3
5	e	101	GOL	C1-C2-C3-O3
5	Q	303	GOL	O1-C1-C2-C3
5	c	101	GOL	O1-C1-C2-C3
5	g	101	GOL	C1-C2-C3-O3
5	Y	302	GOL	O1-C1-C2-C3
5	C	303	GOL	O1-C1-C2-O2
5	f	101	GOL	O1-C1-C2-O2
5	Y	302	GOL	O1-C1-C2-O2
5	i	101	GOL	O1-C1-C2-C3
5	E	302	GOL	O1-C1-C2-C3
5	h	101	GOL	C1-C2-C3-O3
5	O	302	GOL	C1-C2-C3-O3
5	O	303	GOL	O1-C1-C2-C3
5	a	302	GOL	O1-C1-C2-C3
5	i	101	GOL	O1-C1-C2-O2
5	l	101	GOL	O1-C1-C2-O2
5	Q	303	GOL	O1-C1-C2-O2
5	a	302	GOL	O1-C1-C2-O2
5	A	302	GOL	O2-C2-C3-O3
5	l	101	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	e	101	GOL	O2-C2-C3-O3
5	O	303	GOL	O1-C1-C2-O2
5	c	101	GOL	O1-C1-C2-O2
5	g	101	GOL	O2-C2-C3-O3
5	h	101	GOL	O2-C2-C3-O3
5	O	302	GOL	O2-C2-C3-O3
5	C	302	GOL	O2-C2-C3-O3
5	E	302	GOL	O2-C2-C3-O3
5	h	101	GOL	O1-C1-C2-O2
5	C	302	GOL	C1-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	f	101	GOL	1	0
5	c	101	GOL	1	0
5	C	302	GOL	1	0
5	E	302	GOL	3	0
5	a	302	GOL	1	0
5	i	101	GOL	1	0
5	o	101	GOL	2	0
5	e	101	GOL	1	0
5	O	302	GOL	1	0
5	Q	303	GOL	1	0
5	g	101	GOL	1	0
5	A	302	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	276/276 (100%)	-0.06	2 (0%) 84 68	29, 51, 71, 87	2 (0%)
1	C	276/276 (100%)	-0.18	2 (0%) 84 68	26, 47, 68, 82	2 (0%)
1	E	276/276 (100%)	-0.24	2 (0%) 84 68	28, 49, 66, 81	1 (0%)
1	G	276/276 (100%)	-0.23	1 (0%) 88 76	31, 50, 69, 80	1 (0%)
1	I	276/276 (100%)	-0.13	2 (0%) 84 68	30, 49, 71, 83	1 (0%)
1	K	276/276 (100%)	-0.10	4 (1%) 73 53	29, 51, 65, 72	2 (0%)
1	M	276/276 (100%)	-0.07	1 (0%) 88 76	29, 53, 70, 83	1 (0%)
1	O	276/276 (100%)	-0.11	2 (0%) 84 68	29, 54, 69, 78	2 (0%)
1	Q	276/276 (100%)	-0.19	2 (0%) 84 68	31, 48, 63, 80	1 (0%)
1	S	276/276 (100%)	0.07	2 (0%) 84 68	31, 58, 74, 82	2 (0%)
1	U	276/276 (100%)	0.01	3 (1%) 78 59	29, 56, 72, 102	2 (0%)
1	W	276/276 (100%)	-0.03	2 (0%) 84 68	31, 59, 74, 87	2 (0%)
1	Y	276/276 (100%)	0.02	2 (0%) 84 68	34, 58, 73, 78	2 (0%)
1	a	276/276 (100%)	0.12	5 (1%) 67 47	35, 62, 78, 98	2 (0%)
2	B	100/100 (100%)	-0.02	0 100 100	38, 53, 71, 93	0
2	D	100/100 (100%)	0.01	0 100 100	34, 50, 72, 89	0
2	F	100/100 (100%)	-0.13	1 (1%) 79 61	34, 52, 69, 83	0
2	H	100/100 (100%)	-0.03	2 (2%) 65 44	39, 57, 73, 113	0
2	J	100/100 (100%)	-0.14	1 (1%) 79 61	38, 53, 70, 85	0
2	L	100/100 (100%)	-0.01	1 (1%) 79 61	38, 53, 70, 86	0
2	N	100/100 (100%)	0.07	6 (6%) 27 15	42, 55, 73, 155	0
2	P	100/100 (100%)	-0.03	2 (2%) 65 44	41, 56, 79, 116	0
2	R	100/100 (100%)	-0.16	0 100 100	37, 52, 69, 80	0
2	T	100/100 (100%)	0.07	1 (1%) 79 61	43, 60, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	V	100/100 (100%)	-0.03	0 100 100	42, 57, 71, 84	0
2	X	100/100 (100%)	-0.11	0 100 100	45, 57, 73, 84	0
2	Z	100/100 (100%)	0.11	1 (1%) 79 61	44, 58, 75, 83	0
2	b	100/100 (100%)	-0.06	0 100 100	48, 61, 75, 85	0
3	c	9/9 (100%)	0.02	0 100 100	58, 58, 60, 62	0
3	e	9/9 (100%)	-0.24	0 100 100	52, 55, 56, 57	0
3	f	9/9 (100%)	-0.06	0 100 100	42, 44, 50, 50	0
3	g	9/9 (100%)	-0.03	0 100 100	50, 52, 56, 56	0
3	h	9/9 (100%)	-0.18	0 100 100	47, 49, 53, 54	0
3	i	9/9 (100%)	-0.20	0 100 100	40, 41, 43, 45	0
3	j	9/9 (100%)	0.23	0 100 100	56, 61, 66, 66	0
3	k	9/9 (100%)	-0.31	0 100 100	39, 43, 48, 49	0
3	l	9/9 (100%)	-0.17	0 100 100	39, 42, 48, 48	0
3	m	9/9 (100%)	-0.02	0 100 100	42, 47, 49, 51	0
3	n	9/9 (100%)	-0.11	0 100 100	53, 55, 58, 58	0
3	o	9/9 (100%)	0.22	0 100 100	55, 61, 64, 64	0
3	p	9/9 (100%)	0.02	0 100 100	38, 42, 45, 46	0
3	q	9/9 (100%)	0.33	0 100 100	67, 71, 73, 73	0
All	All	5390/5390 (100%)	-0.07	47 (0%) 81 63	26, 54, 73, 155	23 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	88	SER	13.6
1	K	88	SER	12.9
1	U	88	SER	12.3
1	O	88	SER	12.3
1	S	89	GLU	12.0
1	C	88	SER	11.2
1	a	88	SER	11.1
1	S	88	SER	11.1
1	A	88	SER	11.0
1	U	89	GLU	10.2
1	a	89	GLU	10.0
1	O	89	GLU	9.9
1	I	89	GLU	9.8

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Mol	Chain	Res	Type	RSRZ
1	M	89	GLU	9.6
1	G	89	GLU	9.6
1	K	89	GLU	9.2
1	Q	89	GLU	8.9
1	C	89	GLU	8.9
1	Y	89	GLU	8.4
1	A	89	GLU	8.3
1	W	89	GLU	7.5
1	E	89	GLU	6.7
2	N	95	TRP	4.1
2	P	99	MET	3.5
1	a	135	ALA	3.0
2	N	99	MET	2.9
2	N	97	ARG	2.9
2	J	99	MET	2.9
1	K	86	ASN	2.8
2	N	77	GLU	2.6
1	E	252	GLY	2.5
1	W	88	SER	2.4
2	H	99	MET	2.4
1	Q	225	THR	2.4
2	H	98	ASP	2.4
2	F	69	GLU	2.3
1	a	137	ASP	2.3
1	U	276	PRO	2.2
1	I	276	PRO	2.2
2	N	0	MET	2.2
2	T	74	GLU	2.2
2	N	98	ASP	2.2
2	P	88	SER	2.1
2	Z	4	THR	2.1
1	a	136	ALA	2.1
2	L	99	MET	2.0
1	K	132	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	GOL	O	303	6/6	0.81	0.16	79,80,81,82	0
5	GOL	c	101	6/6	0.81	0.20	60,61,62,63	0
5	GOL	a	302	6/6	0.81	0.23	57,58,59,59	0
5	GOL	Y	302	6/6	0.82	0.20	58,59,59,60	0
5	GOL	C	303	6/6	0.82	0.16	55,57,58,58	0
5	GOL	K	302	6/6	0.85	0.16	50,52,54,54	0
5	GOL	o	101	6/6	0.87	0.21	58,58,58,58	0
5	GOL	e	101	6/6	0.87	0.26	51,53,54,55	0
4	CL	N	101	1/1	0.88	0.12	65,65,65,65	0
5	GOL	S	302	6/6	0.88	0.16	53,55,55,55	0
5	GOL	A	302	6/6	0.90	0.13	25,28,28,29	0
4	CL	L	101	1/1	0.90	0.13	74,74,74,74	0
4	CL	S	301	1/1	0.90	0.08	52,52,52,52	0
4	CL	V	101	1/1	0.90	0.14	69,69,69,69	0
4	CL	Z	101	1/1	0.90	0.10	59,59,59,59	0
5	GOL	f	101	6/6	0.91	0.17	35,37,37,38	0
5	GOL	O	302	6/6	0.91	0.16	53,54,55,56	0
5	GOL	g	101	6/6	0.91	0.15	56,56,57,57	0
4	CL	J	101	1/1	0.91	0.10	67,67,67,67	0
5	GOL	q	101	6/6	0.91	0.18	61,61,62,62	0
5	GOL	h	101	6/6	0.91	0.17	50,51,52,52	0
4	CL	N	102	1/1	0.92	0.12	50,50,50,50	0
4	CL	Y	301	1/1	0.92	0.16	60,60,60,60	0
4	CL	D	101	1/1	0.93	0.17	76,76,76,76	0
4	CL	F	101	1/1	0.93	0.14	68,68,68,68	0
4	CL	H	101	1/1	0.93	0.13	83,83,83,83	0
4	CL	A	301	1/1	0.93	0.15	66,66,66,66	0
5	GOL	i	101	6/6	0.93	0.15	68,68,69,69	0
4	CL	K	301	1/1	0.93	0.22	69,69,69,69	0
4	CL	P	101	1/1	0.94	0.15	70,70,70,70	0
4	CL	R	101	1/1	0.94	0.20	72,72,72,72	0
4	CL	O	301	1/1	0.94	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	E	302	6/6	0.94	0.14	38,39,43,45	0
4	CL	a	301	1/1	0.94	0.10	67,67,67,67	0
5	GOL	l	101	6/6	0.94	0.10	35,38,39,41	0
5	GOL	C	302	6/6	0.95	0.14	37,39,40,41	0
4	CL	T	101	1/1	0.95	0.10	63,63,63,63	0
4	CL	B	101	1/1	0.95	0.09	64,64,64,64	0
5	GOL	Q	303	6/6	0.96	0.11	36,37,38,39	0
4	CL	I	301	1/1	0.96	0.23	57,57,57,57	0
4	CL	U	301	1/1	0.96	0.21	64,64,64,64	0
4	CL	Q	301	1/1	0.96	0.18	46,46,46,46	0
4	CL	C	301	1/1	0.97	0.20	60,60,60,60	0
4	CL	G	301	1/1	0.97	0.12	54,54,54,54	0
4	CL	Q	302	1/1	0.97	0.12	57,57,57,57	0
4	CL	b	101	1/1	0.97	0.10	73,73,73,73	0
4	CL	I	302	1/1	0.97	0.14	52,52,52,52	0
4	CL	W	301	1/1	0.97	0.18	59,59,59,59	0
4	CL	E	301	1/1	0.98	0.06	44,44,44,44	0
4	CL	I	303	1/1	0.99	0.14	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.