



# Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 03:12 PM GMT

PDB ID : 4L29  
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 validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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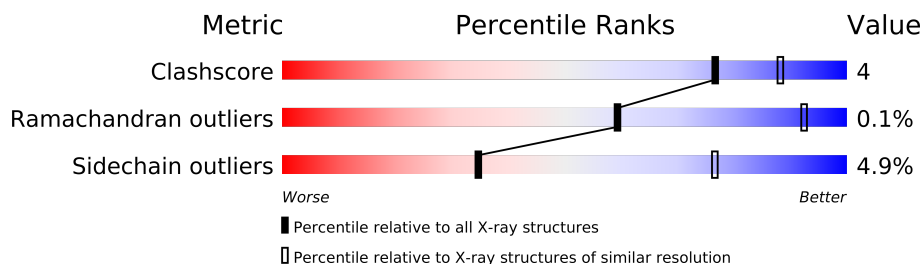
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	276	
1	C	276	
1	E	276	
1	G	276	
1	I	276	
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	

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Mol	Chain	Length	Quality of chain
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	
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 hydrogen and 0 are deuterium.

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 837	C 533	N 141	O 159	S 4	0	0	0
2	D	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	F	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	H	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	J	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	L	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	N	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	P	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	R	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	T	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	V	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	X	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	Z	100	Total 837	C 533	N 141	O 159	S 4	0	0	0
2	b	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

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 (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		

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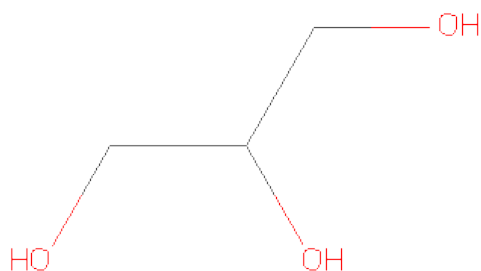
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	W	1	Total 1	Cl 1	0	0
4	N	2	Total 2	Cl 2	0	0
4	S	1	Total 1	Cl 1	0	0
4	J	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	b	1	Total 1	Cl 1	0	0
4	V	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	R	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	I	3	Total 3	Cl 3	0	0
4	Z	1	Total 1	Cl 1	0	0
4	a	1	Total 1	Cl 1	0	0
4	U	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0
4	G	1	Total 1	Cl 1	0	0
4	Q	2	Total 2	Cl 2	0	0
4	H	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	T	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Cl	0	0
			1	1		
4	Y	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: 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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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

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

Note EDS failed to run properly.

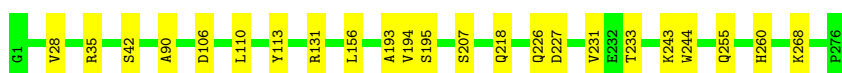
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A: 



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

Chain C: 



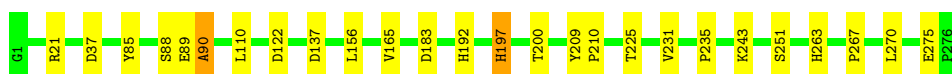
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain E: 



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

Chain G: 



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

Chain I: 



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

Chain K: 



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

Chain M:



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

Chain O:



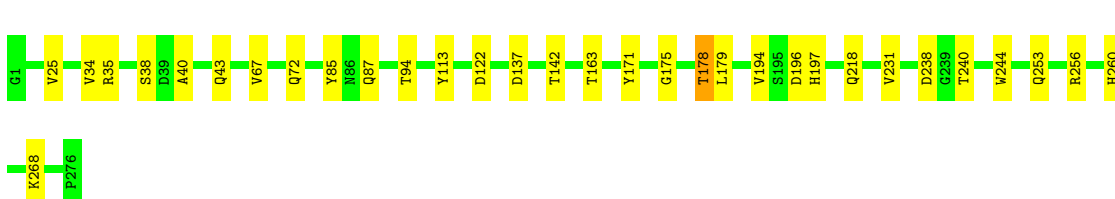
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain Q:



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

Chain S:



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

Chain U:



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

Chain W:



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

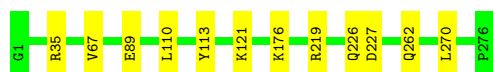
Chain Y:



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

Chain a:





- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain D:



- Molecule 2: Beta-2-microglobulin

Chain F:



- Molecule 2: Beta-2-microglobulin

Chain H:



- Molecule 2: Beta-2-microglobulin

Chain J:



- Molecule 2: Beta-2-microglobulin

Chain L:



- Molecule 2: Beta-2-microglobulin

Chain N:



- Molecule 2: Beta-2-microglobulin

Chain P:



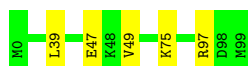
- Molecule 2: Beta-2-microglobulin

Chain R:



- Molecule 2: Beta-2-microglobulin

Chain T:



- Molecule 2: Beta-2-microglobulin

Chain V:



- Molecule 2: Beta-2-microglobulin

Chain X:



- Molecule 2: Beta-2-microglobulin

Chain Z:



- Molecule 2: Beta-2-microglobulin

Chain b:



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

Chain m:



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

Chain i:

There are no outlier residues recorded for this chain.

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

Chain k: 

There are no outlier residues recorded for this chain.

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

Chain f: 



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

Chain l: 

There are no outlier residues recorded for this chain.

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

Chain h: 



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

Chain e: 

There are no outlier residues recorded for this chain.

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

Chain n: 



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

Chain p: 

There are no outlier residues recorded for this chain.

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

Chain o: 

There are no outlier residues recorded for this chain.

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

Chain c: 



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

Chain g: 

There are no outlier residues recorded for this chain.

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

Chain q: 

There are no outlier residues recorded for this chain.

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

Chain j: 





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.57Å 313.36Å 314.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.80 – 3.09	Depositor
% Data completeness (in resolution range)	98.8 (53.80-3.09)	Depositor
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.201	Depositor
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.061	Xtriage
Estimated twinning fraction	0.671 for H, K, L 0.329 for -H, L, K 0.017 for -h,l,k	Xtriage
Reported twinning fraction	0.671 for H, K, L 0.329 for -H, L, K	Depositor
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 182843 reflections (0.001%)	Xtriage
Total number of atoms	44627	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.49	0/2320	0.64	0/3149
1	C	0.58	1/2320 (0.0%)	0.65	0/3149
1	E	0.49	0/2320	0.64	0/3149
1	G	0.52	1/2320 (0.0%)	0.61	0/3149
1	I	0.51	0/2320	0.61	0/3149
1	K	0.49	0/2320	0.63	0/3149
1	M	0.48	0/2320	0.62	0/3149
1	O	0.46	0/2320	0.60	0/3149
1	Q	0.52	0/2320	0.64	0/3149
1	S	0.47	0/2320	0.61	0/3149
1	U	0.47	0/2320	0.58	0/3149
1	W	0.52	1/2320 (0.0%)	0.61	0/3149
1	Y	0.47	0/2320	0.60	0/3149
1	a	0.44	0/2320	0.59	0/3149
2	B	0.47	0/860	0.59	0/1162
2	D	0.53	0/860	0.63	0/1162
2	F	0.50	0/860	0.59	0/1162
2	H	0.48	0/860	0.60	0/1162
2	J	0.50	0/860	0.57	0/1162
2	L	0.50	0/860	0.60	0/1162
2	N	0.50	0/860	0.61	0/1162
2	P	0.46	0/860	0.58	0/1162
2	R	0.47	0/860	0.56	0/1162
2	T	0.56	1/860 (0.1%)	0.63	0/1162
2	V	0.49	0/860	0.58	0/1162
2	X	0.48	0/860	0.59	0/1162
2	Z	0.45	0/860	0.58	0/1162
2	b	0.46	0/860	0.56	0/1162
3	c	0.51	0/84	0.55	0/113
3	e	0.43	0/84	0.58	0/113
3	f	0.45	0/84	0.50	0/113
3	g	0.46	0/84	0.51	0/113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	h	0.48	0/84	0.58	0/113
3	i	0.46	0/84	0.62	0/113
3	j	0.46	0/84	0.53	0/113
3	k	0.51	0/84	0.59	0/113
3	l	0.42	0/84	0.59	0/113
3	m	0.46	0/84	0.69	0/113
3	n	0.45	0/84	0.68	0/113
3	o	0.45	0/84	0.48	0/113
3	p	0.48	0/84	0.57	0/113
3	q	0.43	0/84	0.54	0/113
All	All	0.49	4/45696 (0.0%)	0.61	0/61936

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	49	VAL	CB-CG1	-5.63	1.41	1.52
1	C	28	VAL	CB-CG1	-5.37	1.41	1.52
1	G	90	ALA	CA-CB	-5.34	1.41	1.52
1	W	28	VAL	CA-CB	-5.01	1.44	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	0	16	0
1	C	2254	0	0	7	0
1	E	2254	0	0	7	0
1	G	2254	0	0	11	0
1	I	2254	0	0	7	0
1	K	2254	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2254	0	0	15	0
1	O	2254	0	0	7	0
1	Q	2254	0	0	9	0
1	S	2254	0	0	12	0
1	U	2254	0	0	7	0
1	W	2254	0	0	3	0
1	Y	2254	0	0	11	0
1	a	2254	0	0	0	0
2	B	837	0	0	4	0
2	D	837	0	0	1	0
2	F	837	0	0	1	0
2	H	837	0	0	7	0
2	J	837	0	0	2	0
2	L	837	0	0	0	0
2	N	837	0	0	2	0
2	P	837	0	0	2	0
2	R	837	0	0	2	0
2	T	837	0	0	1	0
2	V	837	0	0	5	0
2	X	837	0	0	3	0
2	Z	837	0	0	2	0
2	b	837	0	0	0	0
3	c	82	0	87	0	0
3	e	82	0	87	0	0
3	f	82	0	87	0	0
3	g	82	0	87	0	0
3	h	82	0	87	0	0
3	i	82	0	87	0	0
3	j	82	0	87	0	0
3	k	82	0	87	0	0
3	l	82	0	87	0	0
3	m	82	0	87	0	0
3	n	82	0	87	0	0
3	o	82	0	87	0	0
3	p	82	0	87	0	0
3	q	82	0	87	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	0	0
5	C	12	0	16	0	0
5	E	6	0	8	0	0
5	K	6	0	8	0	0
5	O	12	0	16	0	0
5	Q	6	0	8	0	0
5	S	6	0	8	0	0
5	Y	6	0	8	0	0
5	a	6	0	8	0	0
5	c	6	0	8	0	0
5	e	6	0	8	0	0
5	f	6	0	8	0	0
5	g	6	0	8	0	0
5	h	6	0	8	0	0
5	i	6	0	8	0	0
5	l	6	0	8	0	0
5	o	6	0	8	0	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	1378	125	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:11:SER:OG	2:B:13:HIS:O	2.56	0.75
1:M:255:GLN:N	1:M:255:GLN:OE1	2.21	0.73
1:K:98:MET:CE	1:K:115:GLN:OE1	2.39	0.71
1:C:90:ALA:CB	2:V:2:GLN:NE2	2.55	0.69
1:S:218:GLN:OE1	1:S:260:HIS:NE2	2.24	0.69
1:M:231:VAL:CG1	1:M:244:TRP:CZ2	2.76	0.69
1:Y:231:VAL:CG1	1:Y:244:TRP:CZ2	2.80	0.65
2:X:45:ARG:NH1	2:X:47:GLU:OE1	2.30	0.64
1:O:40:ALA:O	1:O:43:GLN:NE2	2.30	0.64
2:T:47:GLU:O	2:T:47:GLU:CG	2.45	0.64
1:Q:122:ASP:OD1	2:R:60:TRP:NE1	2.31	0.63
1:A:231:VAL:CG1	1:A:244:TRP:CE2	2.82	0.63
1:M:172:LEU:O	1:M:180:GLN:NE2	2.35	0.59
1:E:231:VAL:CG1	1:E:244:TRP:CZ2	2.86	0.59
1:E:138:MET:N	1:M:128:GLU:OE2	2.35	0.59
1:A:93:HIS:ND1	1:A:119:ASP:OD2	2.70	0.58
1:A:231:VAL:CG1	1:A:244:TRP:CZ2	2.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:GLY:O	1:A:255:GLN:NE2	2.38	0.56
1:C:231:VAL:CG1	1:C:244:TRP:CZ2	2.87	0.56
2:V:41:LYS:NZ	4:V:101:CL:CL	2.75	0.56
1:K:231:VAL:CG1	1:K:244:TRP:CZ2	2.88	0.56
1:G:88:SER:O	1:G:90:ALA:N	2.40	0.55
1:O:122:ASP:OD1	2:P:60:TRP:NE1	2.39	0.55
1:G:231:VAL:O	1:G:243:LYS:NZ	2.41	0.54
1:A:193:ALA:O	1:U:72:GLN:NE2	2.40	0.54
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.54	0.54
1:W:231:VAL:CG1	1:W:244:TRP:CZ2	2.91	0.54
1:M:85:TYR:OH	1:M:137:ASP:OD2	2.25	0.54
1:A:196:ASP:O	1:Y:146:LYS:NZ	148.26	0.53
1:G:88:SER:C	1:G:90:ALA:N	2.60	0.53
1:I:258:THR:OG1	1:I:260:HIS:NE2	2.42	0.53
1:A:6:ARG:NE	1:A:113:TYR:OH	2.97	0.53
1:M:16:GLY:C	1:M:17:ARG:CG	2.77	0.53
1:U:21:ARG:NH2	1:U:37:ASP:OD2	2.43	0.52
1:C:193:ALA:O	1:M:72:GLN:NE2	2.42	0.52
1:I:102:ASP:OD1	1:I:113:TYR:OH	2.26	0.52
1:U:70:HIS:NE2	1:U:99:TYR:OH	2.43	0.52
1:S:231:VAL:CG1	1:S:244:TRP:CE2	2.93	0.52
1:A:156:LEU:CD2	1:A:160:LEU:CD1	4.68	0.51
1:M:16:GLY:O	1:M:17:ARG:CG	2.59	0.50
1:A:142:THR:OG1	1:I:111:ARG:NH1	2.45	0.50
1:G:192:HIS:O	1:G:200:THR:N	2.46	0.49
1:M:122:ASP:OD1	2:N:60:TRP:NE1	2.47	0.48
1:G:122:ASP:OD1	2:H:60:TRP:NE1	2.47	0.48
1:S:38:SER:O	1:S:43:GLN:NE2	2.47	0.48
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.47	0.48
1:O:96:GLN:NE2	2:P:60:TRP:O	2.47	0.48
2:H:51:HIS:ND1	2:H:52:SER:O	2.47	0.48
1:G:210:PRO:O	1:G:263:HIS:NE2	2.47	0.48
1:A:16:GLY:O	2:N:83:ASN:ND2	2.47	0.48
2:X:2:GLN:OE1	1:Y:90:ALA:CB	2.62	0.47
1:I:122:ASP:OD1	2:J:60:TRP:NE1	2.47	0.47
2:H:11:SER:OG	2:H:13:HIS:O	2.32	0.47
1:S:231:VAL:CG1	1:S:244:TRP:CZ2	2.97	0.47
1:G:21:ARG:NH2	1:G:37:ASP:OD2	2.47	0.47
1:C:90:ALA:CB	2:V:2:GLN:OE1	2.62	0.47
2:H:39:LEU:O	2:H:46:ILE:N	2.48	0.47
2:Z:98:ASP:OD1	2:Z:98:ASP:N	2.48	0.47
1:W:55:GLU:OE2	1:W:170:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:253:GLN:OE1	1:S:256:ARG:NH1	2.48	0.47
1:Y:234:ARG:NH2	2:Z:99:MET:OXT	2.48	0.47
1:A:151:HIS:ND1	1:A:154:GLU:OE2	2.49	0.46
2:H:21:ASN:OD1	2:H:22:PHE:N	2.48	0.46
1:Y:231:VAL:CG1	1:Y:244:TRP:CE2	2.98	0.46
1:E:146:LYS:NZ	1:O:196:ASP:O	2.49	0.46
1:C:218:GLN:OE1	1:C:260:HIS:NE2	2.48	0.46
2:H:25:CYS:N	2:H:66:TYR:O	2.49	0.46
2:B:2:GLN:OE1	1:M:90:ALA:CB	2.65	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
1:G:197:HIS:O	1:G:251:SER:N	2.50	0.45
1:K:175:GLY:O	1:K:179:LEU:N	2.50	0.44
1:Y:98:MET:SD	1:Y:98:MET:C	2.96	0.44
1:Y:152:VAL:O	1:Y:155:GLN:N	2.50	0.44
1:Q:231:VAL:CG1	1:Q:244:TRP:CZ2	3.01	0.44
1:G:85:TYR:OH	1:G:137:ASP:OD2	2.36	0.44
1:S:72:GLN:NE2	1:W:193:ALA:O	2.50	0.44
1:S:238:ASP:OD1	1:S:240:THR:OG1	2.36	0.44
1:U:175:GLY:O	1:U:179:LEU:N	2.51	0.44
1:Q:171:TYR:O	1:Q:175:GLY:N	2.50	0.44
1:Q:13:SER:O	1:Q:92:SER:OG	2.35	0.44
1:E:261:VAL:CG1	1:E:266:LEU:CD1	2.96	0.44
1:S:196:ASP:OD2	1:S:197:HIS:N	2.50	0.44
1:U:252:GLY:O	1:U:255:GLN:NE2	2.51	0.43
1:O:156:LEU:O	1:O:160:LEU:N	2.51	0.43
1:A:146:LYS:NZ	1:M:196:ASP:O	49.90	0.43
1:M:231:VAL:CG1	1:M:244:TRP:CE2	3.02	0.43
1:S:85:TYR:OH	1:S:137:ASP:OD2	2.35	0.43
1:G:235:PRO:O	2:H:10:TYR:OH	2.36	0.43
1:Y:252:GLY:O	1:Y:255:GLN:NE2	2.52	0.43
1:I:165:VAL:CG1	1:I:169:ARG:CZ	2.97	0.43
1:A:219:ARG:O	1:A:220:ASP:C	2.93	0.43
1:Q:141:GLN:O	1:Q:145:HIS:ND1	2.52	0.43
1:Q:12:VAL:O	1:Q:21:ARG:N	2.52	0.43
1:I:42:SER:OG	1:I:46:GLU:OE2	2.37	0.43
1:A:88:SER:O	1:A:90:ALA:N	2.52	0.42
2:B:73:THR:O	2:B:97:ARG:NH2	2.97	0.42
1:S:171:TYR:O	1:S:175:GLY:N	2.52	0.42
1:E:89:GLU:O	1:E:89:GLU:CG	2.65	0.42
2:B:10:TYR:N	2:B:10:TYR:CD1	2.87	0.42
2:J:59:ASP:OD1	2:J:61:SER:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:98:ASP:OD1	2:F:98:ASP:N	2.53	0.42
1:C:90:ALA:CB	2:V:2:GLN:CD	2.88	0.42
1:Y:172:LEU:O	1:Y:180:GLN:NE2	2.52	0.42
1:Q:85:TYR:OH	1:Q:137:ASP:OD2	2.38	0.41
1:M:238:ASP:OD1	1:M:240:THR:OG1	2.38	0.41
1:G:183:ASP:N	1:G:209:TYR:O	2.53	0.41
1:U:55:GLU:OE2	1:U:170:ARG:NE	2.53	0.41
1:Y:14:ARG:NH2	1:Y:19:GLU:O	2.54	0.41
1:Q:137:ASP:OD1	1:Q:137:ASP:C	2.58	0.41
1:K:102:ASP:OD1	1:K:113:TYR:OH	2.39	0.41
1:C:233:THR:OG1	1:C:243:LYS:NZ	2.54	0.41
1:M:19:GLU:CA	1:M:19:GLU:OE1	2.69	0.41
2:V:84:HIS:ND1	2:V:86:THR:OG1	2.54	0.41
2:X:7:ILE:CD1	2:X:82:VAL:CG2	2.99	0.41
1:E:59:TYR:OH	1:E:171:TYR:OH	2.39	0.41
1:Y:38:SER:O	1:Y:43:GLN:NE2	2.53	0.41
1:M:38:SER:O	1:M:43:GLN:NE2	2.54	0.40
1:S:40:ALA:O	1:S:43:GLN:NE2	2.54	0.40
2:D:21:ASN:OD1	2:D:22:PHE:N	2.54	0.40
1:U:171:TYR:O	1:U:175:GLY:N	2.54	0.40
1:I:220:ASP:OD2	1:I:256:ARG:NH2	2.54	0.40
1:S:178:THR:OG1	1:S:179:LEU:N	2.53	0.40
1:Q:234:ARG:NH1	2:R:99:MET:OXT	2.55	0.40
1:O:216:THR:O	1:O:260:HIS:N	2.55	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%)	43	84
1	C	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	E	274/276 (99%)	262 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	43	84
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
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%)	22	68
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
3	q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	5306/5390 (98%)	5121 (96%)	182 (3%)	3 (0%)	59	92

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%)	229 (99%)	3 (1%)	80	95
1	C	232/232 (100%)	218 (94%)	14 (6%)	27	67
1	E	232/232 (100%)	217 (94%)	15 (6%)	24	65
1	G	232/232 (100%)	224 (97%)	8 (3%)	49	86
1	I	232/232 (100%)	220 (95%)	12 (5%)	32	73
1	K	232/232 (100%)	215 (93%)	17 (7%)	20	59
1	M	232/232 (100%)	223 (96%)	9 (4%)	43	83
1	O	232/232 (100%)	221 (95%)	11 (5%)	36	78
1	Q	232/232 (100%)	228 (98%)	4 (2%)	73	94
1	S	232/232 (100%)	219 (94%)	13 (6%)	30	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	232/232 (100%)	219 (94%)	13 (6%)	30	70
1	W	232/232 (100%)	221 (95%)	11 (5%)	36	78
1	Y	232/232 (100%)	218 (94%)	14 (6%)	27	67
1	a	232/232 (100%)	220 (95%)	12 (5%)	32	73
2	B	95/95 (100%)	89 (94%)	6 (6%)	25	66
2	D	95/95 (100%)	90 (95%)	5 (5%)	32	72
2	F	95/95 (100%)	90 (95%)	5 (5%)	32	72
2	H	95/95 (100%)	89 (94%)	6 (6%)	25	66
2	J	95/95 (100%)	92 (97%)	3 (3%)	51	87
2	L	95/95 (100%)	91 (96%)	4 (4%)	40	81
2	N	95/95 (100%)	89 (94%)	6 (6%)	25	66
2	P	95/95 (100%)	92 (97%)	3 (3%)	51	87
2	R	95/95 (100%)	89 (94%)	6 (6%)	25	66
2	T	95/95 (100%)	92 (97%)	3 (3%)	51	87
2	V	95/95 (100%)	90 (95%)	5 (5%)	32	72
2	X	95/95 (100%)	89 (94%)	6 (6%)	25	66
2	Z	95/95 (100%)	88 (93%)	7 (7%)	20	59
2	b	95/95 (100%)	90 (95%)	5 (5%)	32	72
3	c	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	e	9/9 (100%)	9 (100%)	0	100	100
3	f	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	g	9/9 (100%)	9 (100%)	0	100	100
3	h	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	i	9/9 (100%)	9 (100%)	0	100	100
3	j	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	k	9/9 (100%)	9 (100%)	0	100	100
3	l	9/9 (100%)	9 (100%)	0	100	100
3	m	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	n	9/9 (100%)	8 (89%)	1 (11%)	9	33
3	o	9/9 (100%)	9 (100%)	0	100	100
3	p	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q	9/9 (100%)	9 (100%)	0	100	100
All	All	4704/4704 (100%)	4472 (95%)	232 (5%)	35	76

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	110	LEU
1	A	113	TYR
2	B	4	THR
2	B	57	SER
2	B	70	PHE
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	113	TYR
1	C	131	ARG
1	C	156	LEU
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	39	LEU
2	D	45	ARG
2	D	70	PHE
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	113	TYR
1	E	128	GLU

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Mol	Chain	Res	Type
1	E	131	ARG
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
2	F	70	PHE
2	F	85	VAL
2	F	89	GLN
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	270	LEU
1	G	275	GLU
2	H	4	THR
2	H	47	GLU
2	H	70	PHE
2	H	75	LYS
2	H	85	VAL
2	H	89	GLN
3	f	7	THR
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	230	LEU
1	I	268	LYS
2	J	47	GLU
2	J	49	VAL

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Mol	Chain	Res	Type
2	J	70	PHE
1	K	2	SER
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	113	TYR
1	K	132	SER
1	K	156	LEU
1	K	178	THR
1	K	194	VAL
1	K	207	SER
1	K	226	GLN
1	K	228	THR
1	K	275	GLU
2	L	39	LEU
2	L	44	GLU
2	L	51	HIS
2	L	70	PHE
3	h	9	VAL
1	M	17	ARG
1	M	19	GLU
1	M	35	ARG
1	M	113	TYR
1	M	156	LEU
1	M	194	VAL
1	M	230	LEU
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
1	O	4	SER
1	O	35	ARG
1	O	89	GLU
1	O	113	TYR

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Mol	Chain	Res	Type
1	O	163	THR
1	O	194	VAL
1	O	207	SER
1	O	222	GLU
1	O	224	GLN
1	O	227	ASP
1	O	268	LYS
2	P	4	THR
2	P	57	SER
2	P	70	PHE
3	n	4	MET
1	Q	35	ARG
1	Q	110	LEU
1	Q	156	LEU
1	Q	181	ARG
2	R	0	MET
2	R	2	GLN
2	R	3	ARG
2	R	48	LYS
2	R	50	GLU
2	R	77	GLU
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	122	ASP
1	S	142	THR
1	S	163	THR
1	S	178	THR
1	S	194	VAL
1	S	268	LYS
2	T	39	LEU
2	T	75	LYS
2	T	97	ARG
1	U	2	SER
1	U	19	GLU
1	U	35	ARG
1	U	67	VAL
1	U	86	ASN

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Mol	Chain	Res	Type
1	U	113	TYR
1	U	127	LYS
1	U	132	SER
1	U	156	LEU
1	U	163	THR
1	U	178	THR
1	U	207	SER
1	U	230	LEU
2	V	4	THR
2	V	48	LYS
2	V	63	TYR
2	V	68	THR
2	V	97	ARG
3	c	9	VAL
1	W	35	ARG
1	W	113	TYR
1	W	115	GLN
1	W	122	ASP
1	W	156	LEU
1	W	163	THR
1	W	168	LEU
1	W	216	THR
1	W	225	THR
1	W	251	SER
1	W	268	LYS
2	X	39	LEU
2	X	48	LYS
2	X	58	LYS
2	X	70	PHE
2	X	76	ASP
2	X	98	ASP
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

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Mol	Chain	Res	Type
1	Y	227	ASP
1	Y	230	LEU
1	Y	270	LEU
2	Z	4	THR
2	Z	34	ASP
2	Z	39	LEU
2	Z	70	PHE
2	Z	75	LYS
2	Z	98	ASP
2	Z	99	MET
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	176	LYS
1	a	219	ARG
1	a	226	GLN
1	a	227	ASP
1	a	262	GLN
1	a	270	LEU
2	b	4	THR
2	b	11	SER
2	b	39	LEU
2	b	70	PHE
2	b	75	LYS
3	j	7	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 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	A	302	-	5,5,5	0.57	0	5,5,5	0.80	0
5	GOL	C	302	-	5,5,5	0.49	0	5,5,5	0.36	0
5	GOL	C	303	-	5,5,5	0.33	0	5,5,5	0.24	0
5	GOL	E	302	-	5,5,5	0.50	0	5,5,5	0.85	0
5	GOL	K	302	-	5,5,5	0.31	0	5,5,5	0.63	0
5	GOL	O	302	-	5,5,5	0.39	0	5,5,5	0.29	0
5	GOL	O	303	-	5,5,5	0.36	0	5,5,5	0.31	0
5	GOL	Q	303	-	5,5,5	0.56	0	5,5,5	0.49	0
5	GOL	S	302	-	5,5,5	0.33	0	5,5,5	0.56	0
5	GOL	Y	302	-	5,5,5	0.44	0	5,5,5	0.31	0
5	GOL	a	302	-	5,5,5	0.43	0	5,5,5	0.52	0
5	GOL	c	101	-	5,5,5	0.38	0	5,5,5	0.47	0
5	GOL	e	101	-	5,5,5	0.46	0	5,5,5	0.40	0
5	GOL	f	101	-	5,5,5	0.51	0	5,5,5	0.88	0
5	GOL	g	101	-	5,5,5	0.47	0	5,5,5	0.29	0
5	GOL	h	101	-	5,5,5	0.47	0	5,5,5	0.53	0
5	GOL	i	101	-	5,5,5	0.46	0	5,5,5	0.54	0
5	GOL	l	101	-	5,5,5	0.21	0	5,5,5	0.38	0
5	GOL	o	101	-	5,5,5	0.42	0	5,5,5	0.31	0
5	GOL	q	101	-	5,5,5	0.39	0	5,5,5	0.29	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	A	302	-	-	0/4/4/4	0/0/0/0
5	GOL	C	302	-	-	0/4/4/4	0/0/0/0
5	GOL	C	303	-	-	0/4/4/4	0/0/0/0
5	GOL	E	302	-	-	0/4/4/4	0/0/0/0
5	GOL	K	302	-	-	0/4/4/4	0/0/0/0
5	GOL	O	302	-	-	0/4/4/4	0/0/0/0
5	GOL	O	303	-	-	0/4/4/4	0/0/0/0
5	GOL	Q	303	-	-	0/4/4/4	0/0/0/0
5	GOL	S	302	-	-	0/4/4/4	0/0/0/0
5	GOL	Y	302	-	-	0/4/4/4	0/0/0/0
5	GOL	a	302	-	-	0/4/4/4	0/0/0/0
5	GOL	c	101	-	-	0/4/4/4	0/0/0/0
5	GOL	e	101	-	-	0/4/4/4	0/0/0/0
5	GOL	f	101	-	-	0/4/4/4	0/0/0/0
5	GOL	g	101	-	-	0/4/4/4	0/0/0/0
5	GOL	h	101	-	-	0/4/4/4	0/0/0/0
5	GOL	i	101	-	-	0/4/4/4	0/0/0/0
5	GOL	l	101	-	-	0/4/4/4	0/0/0/0
5	GOL	o	101	-	-	0/4/4/4	0/0/0/0
5	GOL	q	101	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.