



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:18 PM GMT

PDB ID : 3TBV  
Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTO-COMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (A2G,V3P,Y4A)  
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Deposited on : 2011-08-08  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

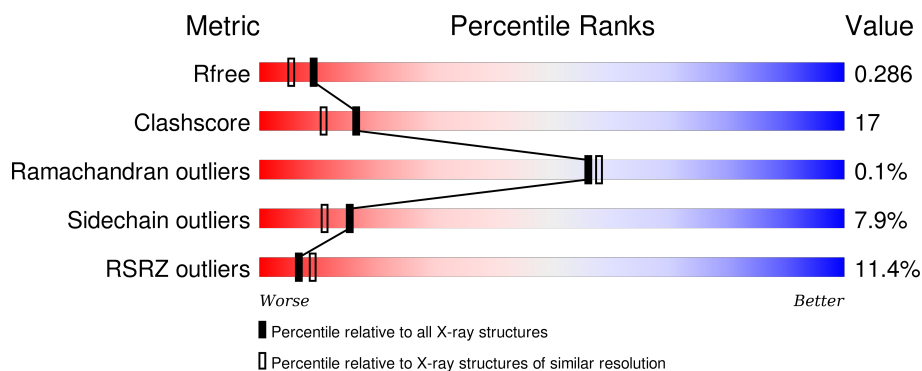
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	338	<div> <div>12%</div> <div>57%</div> <div>20%</div> <div>•</div> <div>18%</div> </div>
1	C	338	<div> <div>10%</div> <div>58%</div> <div>19%</div> <div>•</div> <div>18%</div> </div>
1	E	338	<div> <div>11%</div> <div>60%</div> <div>17%</div> <div>• •</div> <div>18%</div> </div>
1	G	338	<div> <div>15%</div> <div>59%</div> <div>19%</div> <div>• •</div> <div>18%</div> </div>
2	B	99	<div> <div>3%</div> <div>75%</div> <div>20%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	99	
2	F	99	
2	H	99	
3	I	9	
3	J	9	
3	K	9	
3	L	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	339	-	-	-	X
4	SO4	F	100	-	-	X	-
5	GOL	A	340	-	-	-	X
5	GOL	B	100	-	-	-	X
5	GOL	E	341	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13548 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	C	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	E	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	G	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	D	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	F	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	H	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

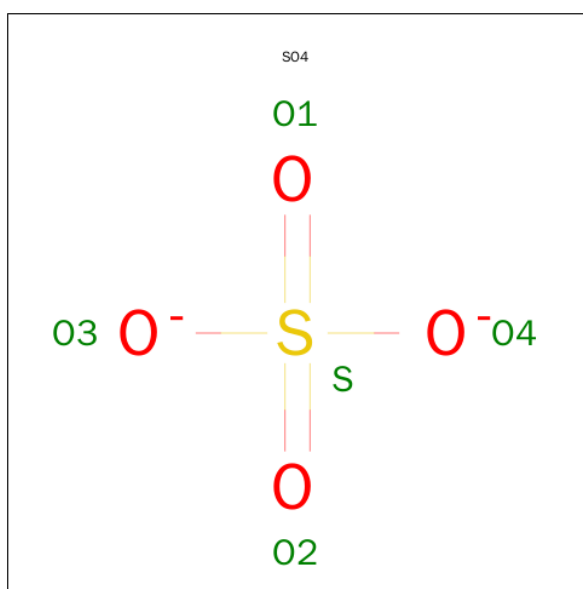
- Molecule 3 is a protein called Glycoprotein G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	J	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	K	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	L	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLY	ALA	ENGINEERED MUTATION	UNP P07399
I	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
I	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
I	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
J	2	GLY	ALA	ENGINEERED MUTATION	UNP P07399
J	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
J	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
J	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
K	2	GLY	ALA	ENGINEERED MUTATION	UNP P07399
K	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
K	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
K	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
L	2	GLY	ALA	ENGINEERED MUTATION	UNP P07399
L	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
L	4	ALA	TYR	ENGINEERED MUTATION	UNP P07399
L	9	MET	CYS	ENGINEERED MUTATION	UNP P07399

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	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	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	132	Total	O	0	0
			132	132		

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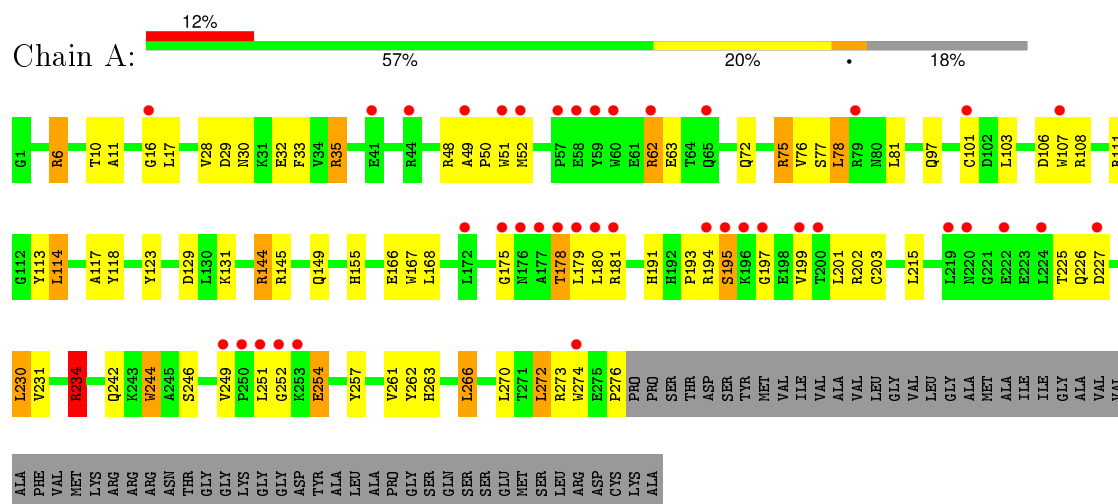
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	67	Total 67	O 67	0	0
6	C	164	Total 164	O 164	0	0
6	D	77	Total 77	O 77	0	0
6	E	154	Total 154	O 154	0	0
6	F	69	Total 69	O 69	0	0
6	G	128	Total 128	O 128	0	0
6	H	74	Total 74	O 74	0	0
6	I	4	Total 4	O 4	0	0
6	J	9	Total 9	O 9	0	0
6	K	10	Total 10	O 10	0	0
6	L	2	Total 2	O 2	0	0

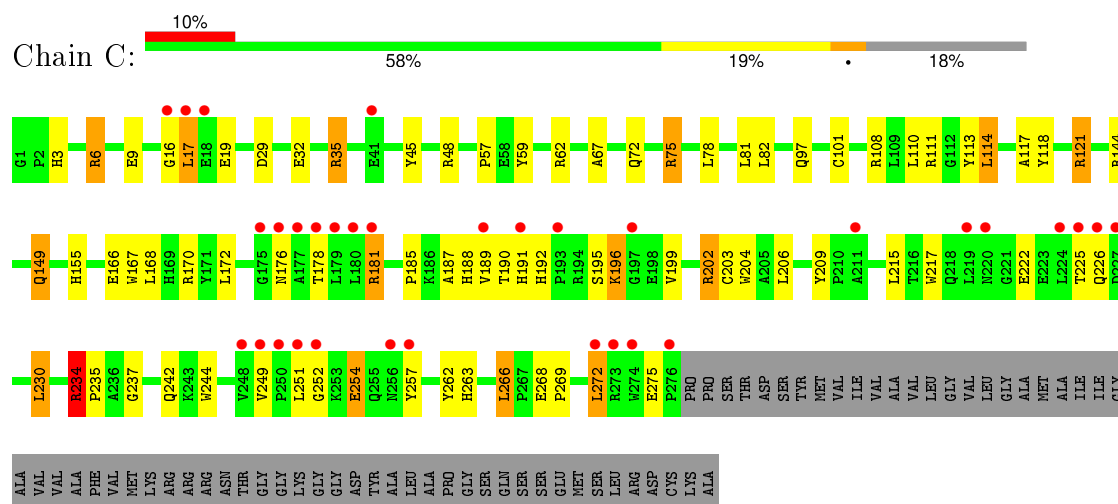
### 3 Residue-property plots

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.

- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



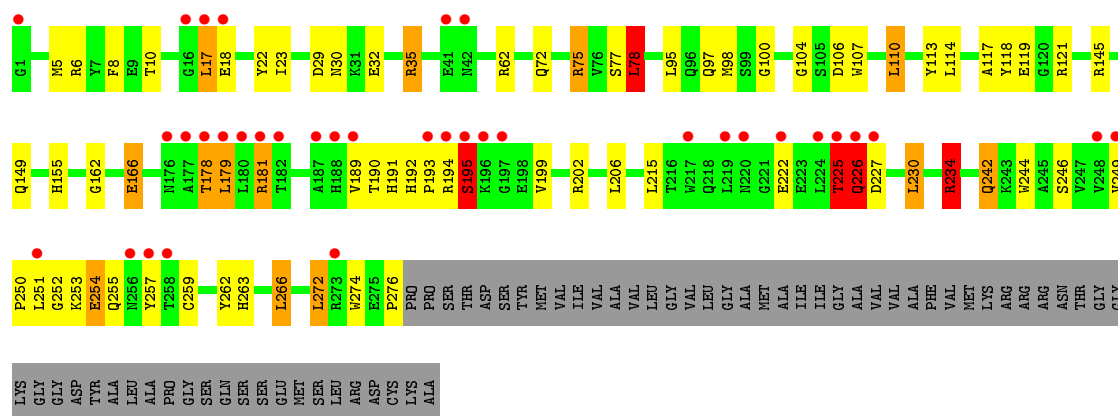
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



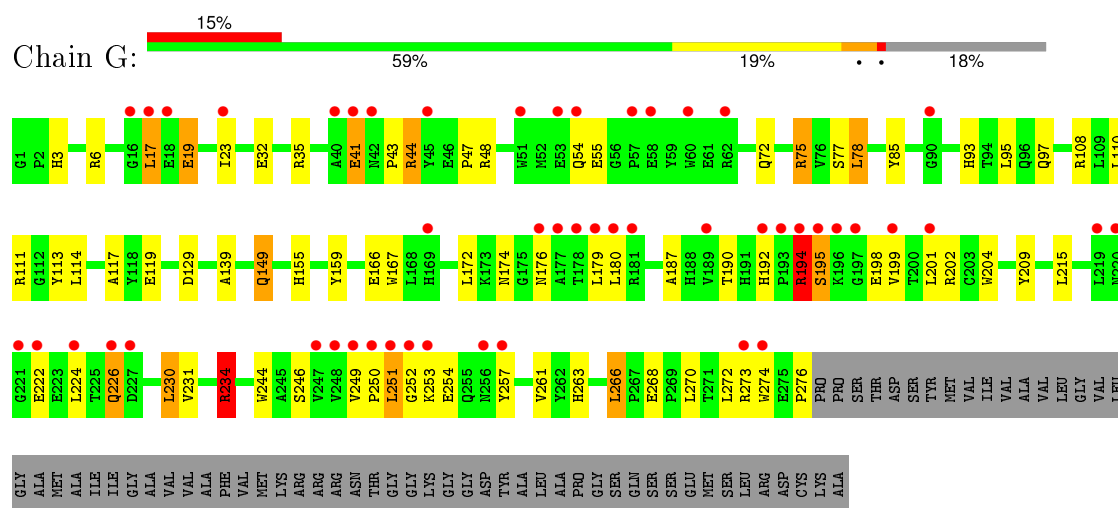
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



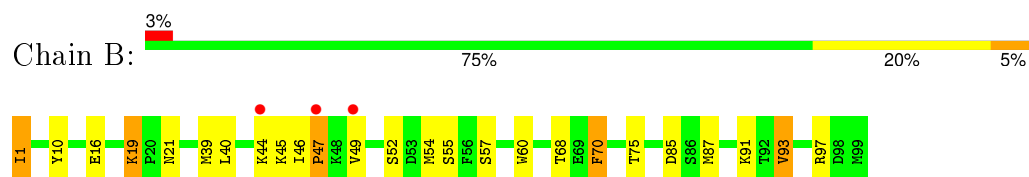




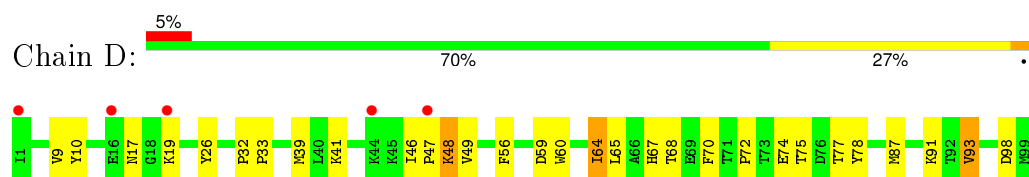
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



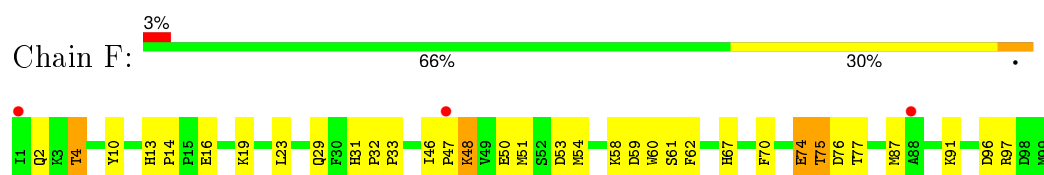
- Molecule 2: Beta-2-microglobulin



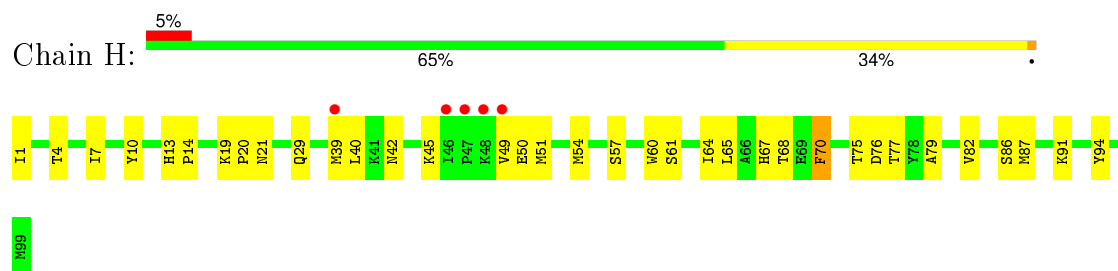
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



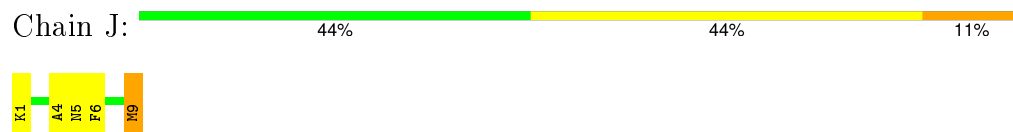
## ● Molecule 2: Beta-2-microglobulin



## ● Molecule 3: Glycoprotein G1



## ● Molecule 3: Glycoprotein G1



## ● Molecule 3: Glycoprotein G1



## ● Molecule 3: Glycoprotein G1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.58Å 126.47Å 102.11Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	49.51 – 2.10 63.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.51-2.10) 99.1 (63.24-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.225 , 0.278 0.236 , 0.286	Depositor DCC
$R_{free}$ test set	6804 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 135592 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.1085e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.91	3/2331 (0.1%)	1.02	7/3166 (0.2%)
1	C	0.91	2/2331 (0.1%)	0.96	10/3166 (0.3%)
1	E	0.96	0/2331	1.06	11/3166 (0.3%)
1	G	0.88	0/2331	0.96	4/3166 (0.1%)
2	B	0.99	1/846 (0.1%)	0.97	0/1148
2	D	0.90	1/846 (0.1%)	0.96	1/1148 (0.1%)
2	F	0.98	1/846 (0.1%)	0.95	2/1148 (0.2%)
2	H	0.92	0/846	0.94	2/1148 (0.2%)
3	I	3.52	1/66 (1.5%)	1.19	0/86
3	J	3.30	2/66 (3.0%)	1.27	0/86
3	K	3.26	1/66 (1.5%)	1.05	0/86
3	L	1.94	1/66 (1.5%)	1.13	0/86
All	All	1.01	13/12972 (0.1%)	0.99	37/17600 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
All	All	0	2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	9	MET	C-OXT	27.14	1.75	1.23
3	K	9	MET	C-OXT	24.50	1.69	1.23
3	J	9	MET	C-OXT	23.53	1.68	1.23
3	L	9	MET	C-OXT	12.89	1.47	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	ALA	CA-CB	7.34	1.67	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-19.77	110.42	120.30
1	A	234	ARG	NE-CZ-NH1	18.44	129.52	120.30
1	E	234	ARG	NE-CZ-NH1	17.34	128.97	120.30
1	E	234	ARG	NE-CZ-NH2	-15.07	112.76	120.30
1	G	234	ARG	NE-CZ-NH1	14.79	127.69	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	GLY	Peptide
1	G	194	ARG	Peptide

## 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	2264	0	2136	68	0
1	C	2264	0	2136	72	0
1	E	2264	0	2136	83	0
1	G	2264	0	2136	68	0
2	B	820	0	796	31	0
2	D	820	0	796	43	0
2	F	820	0	796	31	0
2	H	820	0	796	36	0
3	I	65	0	66	7	0
3	J	65	0	66	9	0
3	K	65	0	66	11	0
3	L	65	0	66	6	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	3	0
5	A	12	0	16	3	0
5	B	6	0	8	3	0
5	E	12	0	16	9	0
5	H	12	0	16	3	0
6	A	132	0	0	5	0
6	B	67	0	0	6	0
6	C	164	0	0	8	0
6	D	77	0	0	2	0
6	E	154	0	0	1	0
6	F	69	0	0	4	0
6	G	128	0	0	4	0
6	H	74	0	0	1	0
6	I	4	0	0	0	0
6	J	9	0	0	0	0
6	K	10	0	0	0	0
6	L	2	0	0	0	0
All	All	13548	0	12048	411	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 17.

The worst 5 of 411 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:9:MET:C	3:J:9:MET:OXT	1.68	1.30
3:K:9:MET:C	3:K:9:MET:OXT	1.69	1.29
3:I:9:MET:OXT	3:I:9:MET:C	1.74	1.23
1:E:226:GLN:CD	1:E:226:GLN:O	1.75	1.22
1:E:226:GLN:O	1:E:226:GLN:NE2	1.94	0.98

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	274/338 (81%)	257 (94%)	17 (6%)	0	100	100
1	C	274/338 (81%)	260 (95%)	14 (5%)	0	100	100
1	E	274/338 (81%)	259 (94%)	15 (6%)	0	100	100
1	G	274/338 (81%)	261 (95%)	13 (5%)	0	100	100
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19	13
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	F	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	H	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	19	13
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	K	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1512/1784 (85%)	1433 (95%)	77 (5%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	ASN
2	B	47	PRO

### 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	234/280 (84%)	217 (93%)	17 (7%)	17	13
1	C	234/280 (84%)	212 (91%)	22 (9%)	11	7
1	E	234/280 (84%)	212 (91%)	22 (9%)	11	7
1	G	234/280 (84%)	212 (91%)	22 (9%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/94 (100%)	88 (94%)	6 (6%)	22	18
2	D	94/94 (100%)	88 (94%)	6 (6%)	22	18
2	F	94/94 (100%)	87 (93%)	7 (7%)	17	13
2	H	94/94 (100%)	91 (97%)	3 (3%)	46	48
3	I	6/6 (100%)	6 (100%)	0	100	100
3	J	6/6 (100%)	6 (100%)	0	100	100
3	K	6/6 (100%)	6 (100%)	0	100	100
3	L	6/6 (100%)	6 (100%)	0	100	100
All	All	1336/1520 (88%)	1231 (92%)	105 (8%)	15	11

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	74	GLU
1	E	166	GLU
1	G	251	LEU
2	D	75	THR
1	E	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	34	HIS
1	E	97	GLN
1	G	174	ASN
1	C	176	ASN
1	C	192	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	339	-	4,4,4	0.27	0	6,6,6	0.25	0
5	GOL	A	340	-	5,5,5	0.70	0	5,5,5	0.83	0
5	GOL	A	341	-	5,5,5	0.62	0	5,5,5	0.36	0
5	GOL	B	100	-	5,5,5	0.53	0	5,5,5	0.96	0
4	SO4	C	339	-	4,4,4	0.32	0	6,6,6	1.30	1 (16%)
4	SO4	E	339	-	4,4,4	0.20	0	6,6,6	0.39	0
5	GOL	E	340	-	5,5,5	0.62	0	5,5,5	1.53	2 (40%)
5	GOL	E	341	-	5,5,5	0.33	0	5,5,5	0.34	0
4	SO4	F	100	-	4,4,4	0.40	0	6,6,6	0.40	0
5	GOL	H	100	-	5,5,5	0.51	0	5,5,5	1.00	0
5	GOL	H	101	-	5,5,5	0.52	0	5,5,5	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	339	-	-	0/0/0/0	0/0/0/0
5	GOL	A	340	-	-	0/4/4/4	0/0/0/0
5	GOL	A	341	-	-	0/4/4/4	0/0/0/0
5	GOL	B	100	-	-	0/4/4/4	0/0/0/0
4	SO4	C	339	-	-	0/0/0/0	0/0/0/0
4	SO4	E	339	-	-	0/0/0/0	0/0/0/0
5	GOL	E	340	-	-	0/4/4/4	0/0/0/0
5	GOL	E	341	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	F	100	-	-	0/0/0/0	0/0/0/0
5	GOL	H	100	-	-	0/4/4/4	0/0/0/0
5	GOL	H	101	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	340	GOL	C3-C2-C1	-2.37	101.83	111.12
5	E	340	GOL	O2-C2-C3	2.13	118.40	108.65
4	C	339	SO4	O2-S-O1	2.56	117.61	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	340	GOL	2	0
5	A	341	GOL	1	0
5	B	100	GOL	3	0
5	E	340	GOL	3	0
5	E	341	GOL	6	0
4	F	100	SO4	3	0
5	H	101	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/338 (81%)	1.13	40 (14%) 3 5	20, 52, 113, 192	0
1	C	276/338 (81%)	0.93	33 (11%) 6 8	20, 47, 112, 203	0
1	E	276/338 (81%)	1.08	36 (13%) 5 6	20, 46, 129, 193	0
1	G	276/338 (81%)	1.12	50 (18%) 2 2	19, 51, 116, 190	0
2	B	99/99 (100%)	0.54	3 (3%) 54 62	25, 41, 72, 101	0
2	D	99/99 (100%)	0.72	5 (5%) 32 40	24, 47, 82, 95	0
2	F	99/99 (100%)	0.60	3 (3%) 54 62	25, 46, 73, 100	0
2	H	99/99 (100%)	0.65	5 (5%) 32 40	26, 44, 74, 95	0
3	I	9/9 (100%)	0.30	0 100 100	30, 35, 51, 54	0
3	J	9/9 (100%)	0.02	0 100 100	22, 29, 33, 38	0
3	K	9/9 (100%)	0.16	0 100 100	20, 30, 36, 36	0
3	L	9/9 (100%)	0.28	0 100 100	25, 29, 45, 53	0
All	All	1536/1784 (86%)	0.93	175 (11%) 7 9	19, 47, 112, 203	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	THR	22.9
1	A	178	THR	19.3
1	E	177	ALA	18.5
1	G	178	THR	15.8
1	E	179	LEU	15.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	340	6/6	0.90	0.45	12.96	41,54,66,71	0
4	SO4	C	339	5/5	0.89	0.26	7.63	56,61,74,80	0
5	GOL	B	100	6/6	0.83	0.26	4.81	58,65,75,78	0
5	GOL	E	340	6/6	0.90	0.16	1.56	35,50,56,59	0
5	GOL	H	100	6/6	0.92	0.17	1.36	50,53,60,65	0
4	SO4	A	339	5/5	0.96	0.23	0.93	50,70,79,88	0
4	SO4	E	339	5/5	0.94	0.16	-0.44	66,70,76,84	0
5	GOL	A	341	6/6	0.61	0.19	-	51,60,64,65	0
5	GOL	E	341	6/6	0.91	0.10	-	46,49,54,73	0
4	SO4	F	100	5/5	0.90	0.33	-	68,70,84,91	0
5	GOL	H	101	6/6	0.85	0.26	-	48,58,59,66	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.