



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:47 am GMT

PDB ID : 5LBS  
Title : structural basis of Zika and Dengue virus potent antibody cross-neutralization  
Authors : VANEY, M.C.; ROUVINSKI, A.; BARBA-SPAETH, G.; REY, F.A.  
Deposited on : 2016-06-17  
Resolution : 2.41 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

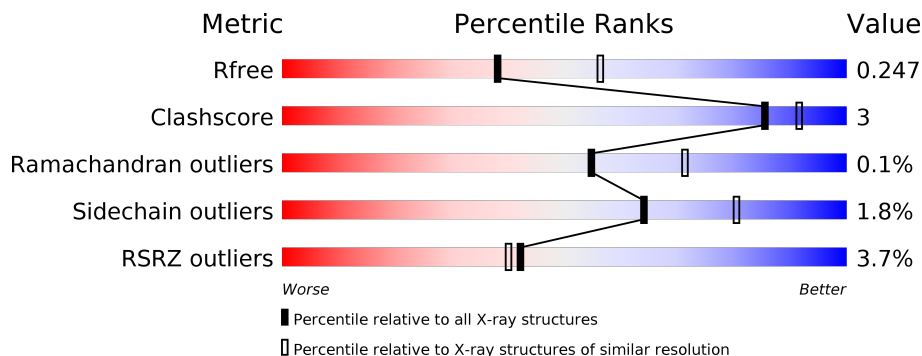
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	447	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>12%</div> </div> </div>
1	B	447	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>
2	H	141	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>
2	I	141	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
3	L	147	<div> <div></div> <div> <div></div> <div>71%</div> <div>•</div> <div>24%</div> </div> </div>
3	M	147	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>•</div> <div>24%</div> </div> </div>

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	EDO	H	201	-	-	-	X
4	EDO	I	201	-	-	-	X
4	EDO	L	202	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9815 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 envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	1	0
			3013	1886	524	578	25			
1	B	386	Total	C	N	O	S	0	0	0
			2968	1861	519	564	24			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP A0A120IIH9
A	410	PRO	-	expression tag	UNP A0A120IIH9
A	411	PHE	-	expression tag	UNP A0A120IIH9
A	412	GLU	-	expression tag	UNP A0A120IIH9
A	413	ASP	-	expression tag	UNP A0A120IIH9
A	414	ASP	-	expression tag	UNP A0A120IIH9
A	415	ASP	-	expression tag	UNP A0A120IIH9
A	416	ASP	-	expression tag	UNP A0A120IIH9
A	417	LYS	-	expression tag	UNP A0A120IIH9
A	418	ALA	-	expression tag	UNP A0A120IIH9
A	419	GLY	-	expression tag	UNP A0A120IIH9
A	420	TRP	-	expression tag	UNP A0A120IIH9
A	421	SER	-	expression tag	UNP A0A120IIH9
A	422	HIS	-	expression tag	UNP A0A120IIH9
A	423	PRO	-	expression tag	UNP A0A120IIH9
A	424	GLN	-	expression tag	UNP A0A120IIH9
A	425	PHE	-	expression tag	UNP A0A120IIH9
A	426	GLU	-	expression tag	UNP A0A120IIH9
A	427	LYS	-	expression tag	UNP A0A120IIH9
A	428	GLY	-	expression tag	UNP A0A120IIH9
A	429	GLY	-	expression tag	UNP A0A120IIH9
A	430	GLY	-	expression tag	UNP A0A120IIH9
A	431	SER	-	expression tag	UNP A0A120IIH9
A	432	GLY	-	expression tag	UNP A0A120IIH9
A	433	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLY	-	expression tag	UNP A0A120IIH9
A	435	SER	-	expression tag	UNP A0A120IIH9
A	436	GLY	-	expression tag	UNP A0A120IIH9
A	437	GLY	-	expression tag	UNP A0A120IIH9
A	438	GLY	-	expression tag	UNP A0A120IIH9
A	439	SER	-	expression tag	UNP A0A120IIH9
A	440	TRP	-	expression tag	UNP A0A120IIH9
A	441	SER	-	expression tag	UNP A0A120IIH9
A	442	HIS	-	expression tag	UNP A0A120IIH9
A	443	PRO	-	expression tag	UNP A0A120IIH9
A	444	GLN	-	expression tag	UNP A0A120IIH9
A	445	PHE	-	expression tag	UNP A0A120IIH9
A	446	GLU	-	expression tag	UNP A0A120IIH9
A	447	LYS	-	expression tag	UNP A0A120IIH9
B	409	GLY	-	expression tag	UNP A0A120IIH9
B	410	PRO	-	expression tag	UNP A0A120IIH9
B	411	PHE	-	expression tag	UNP A0A120IIH9
B	412	GLU	-	expression tag	UNP A0A120IIH9
B	413	ASP	-	expression tag	UNP A0A120IIH9
B	414	ASP	-	expression tag	UNP A0A120IIH9
B	415	ASP	-	expression tag	UNP A0A120IIH9
B	416	ASP	-	expression tag	UNP A0A120IIH9
B	417	LYS	-	expression tag	UNP A0A120IIH9
B	418	ALA	-	expression tag	UNP A0A120IIH9
B	419	GLY	-	expression tag	UNP A0A120IIH9
B	420	TRP	-	expression tag	UNP A0A120IIH9
B	421	SER	-	expression tag	UNP A0A120IIH9
B	422	HIS	-	expression tag	UNP A0A120IIH9
B	423	PRO	-	expression tag	UNP A0A120IIH9
B	424	GLN	-	expression tag	UNP A0A120IIH9
B	425	PHE	-	expression tag	UNP A0A120IIH9
B	426	GLU	-	expression tag	UNP A0A120IIH9
B	427	LYS	-	expression tag	UNP A0A120IIH9
B	428	GLY	-	expression tag	UNP A0A120IIH9
B	429	GLY	-	expression tag	UNP A0A120IIH9
B	430	GLY	-	expression tag	UNP A0A120IIH9
B	431	SER	-	expression tag	UNP A0A120IIH9
B	432	GLY	-	expression tag	UNP A0A120IIH9
B	433	GLY	-	expression tag	UNP A0A120IIH9
B	434	GLY	-	expression tag	UNP A0A120IIH9
B	435	SER	-	expression tag	UNP A0A120IIH9
B	436	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	GLY	-	expression tag	UNP A0A120IIH9
B	438	GLY	-	expression tag	UNP A0A120IIH9
B	439	SER	-	expression tag	UNP A0A120IIH9
B	440	TRP	-	expression tag	UNP A0A120IIH9
B	441	SER	-	expression tag	UNP A0A120IIH9
B	442	HIS	-	expression tag	UNP A0A120IIH9
B	443	PRO	-	expression tag	UNP A0A120IIH9
B	444	GLN	-	expression tag	UNP A0A120IIH9
B	445	PHE	-	expression tag	UNP A0A120IIH9
B	446	GLU	-	expression tag	UNP A0A120IIH9
B	447	LYS	-	expression tag	UNP A0A120IIH9

- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	121	Total	C	N	O	S	0	0	0
			932	591	151	185	5			
2	I	122	Total	C	N	O	S	0	0	0
			938	594	152	187	5			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8.

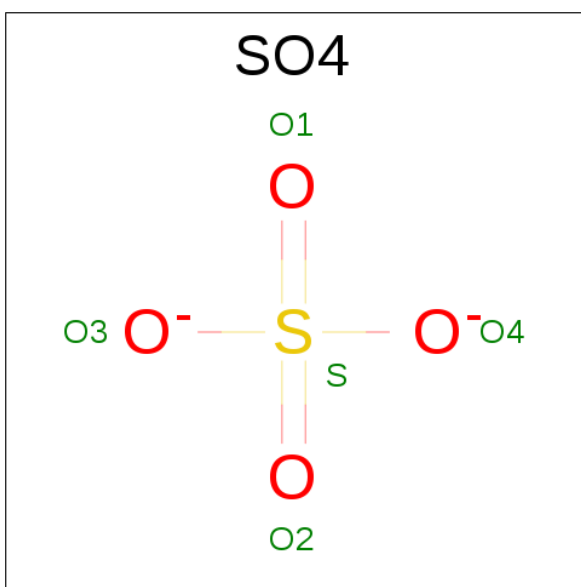
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	111	Total	C	N	O	S	0	0	0
			861	547	147	165	2			
3	M	112	Total	C	N	O	S	0	0	1
			864	548	148	166	2			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

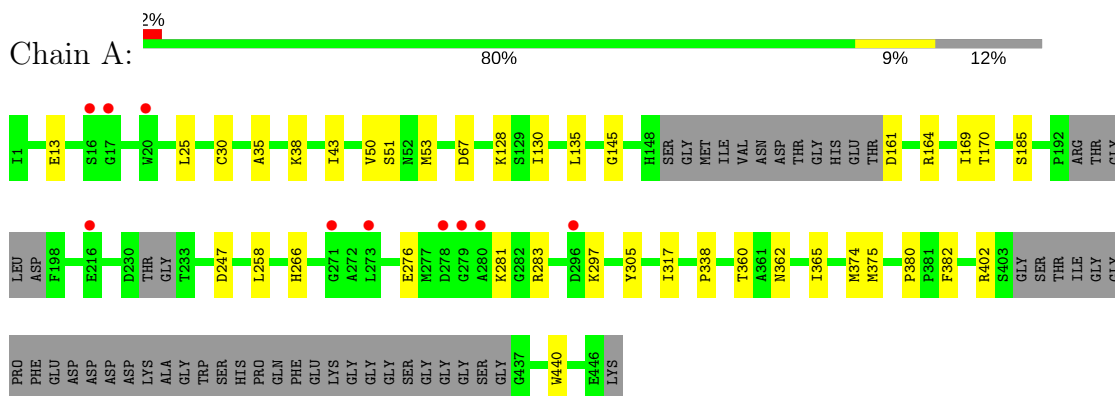
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	15	Total	O	0	0
			15	15		
6	H	25	Total	O	0	0
			25	25		
6	I	10	Total	O	0	0
			10	10		
6	L	52	Total	O	0	0
			52	52		
6	M	25	Total	O	0	0
			25	25		



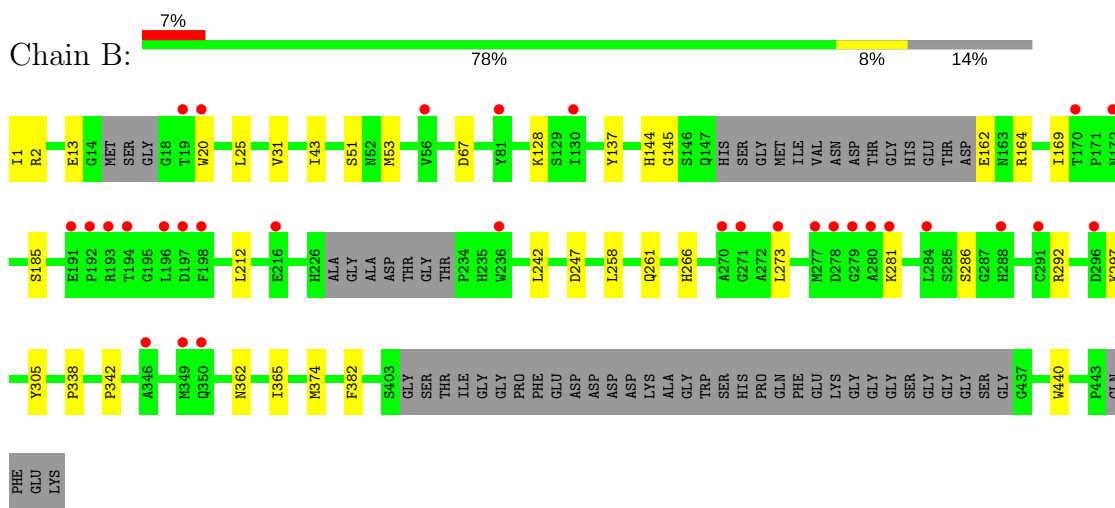
### 3 Residue-property plots [i](#)

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

- Molecule 1: envelope protein E



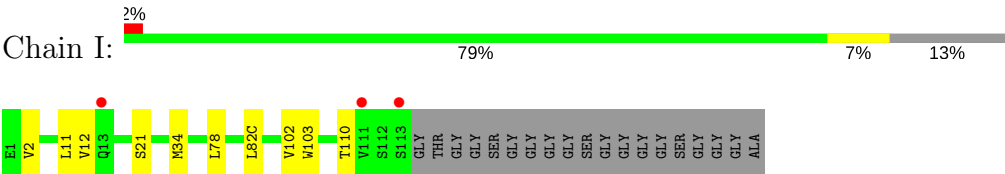
- Molecule 1: envelope protein E



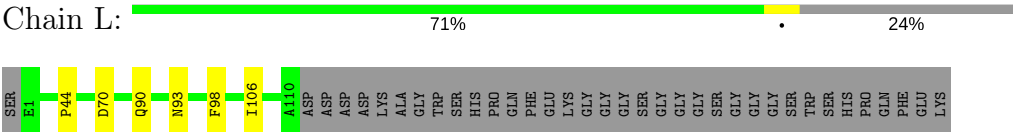
- Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8



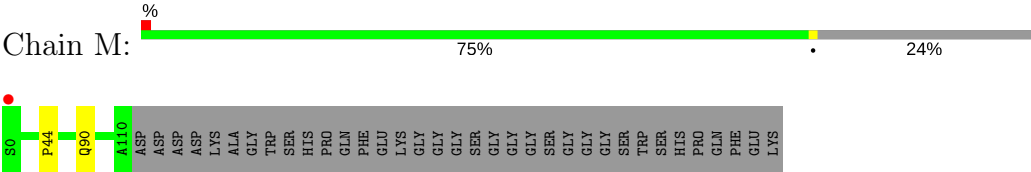
- Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8



● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8



● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE1 C8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.80Å 121.35Å 257.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 2.41 39.96 – 2.41	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.96-2.41) 87.3 (39.96-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.194 , 0.217 0.215 , 0.247	Depositor DCC
$R_{free}$ test set	3204 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9815	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 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

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	0.43	0/3079	0.57	0/4167
1	B	0.40	0/3031	0.55	0/4101
2	H	0.37	0/956	0.53	0/1297
2	I	0.36	0/962	0.53	0/1305
3	L	0.42	0/884	0.61	0/1206
3	M	0.40	0/887	0.60	0/1210
All	All	0.40	0/9799	0.56	0/13286

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3013	0	2931	16	0
1	B	2968	0	2906	21	0
2	H	932	0	868	6	0
2	I	938	0	873	5	0
3	L	861	0	841	3	0
3	M	864	0	842	1	0
4	A	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	8	0	12	0	0
4	I	4	0	6	0	0
4	L	12	0	18	4	0
4	M	8	0	12	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	I	5	0	0	0	0
6	A	53	0	0	0	0
6	B	15	0	0	1	0
6	H	25	0	0	0	0
6	I	10	0	0	0	0
6	L	52	0	0	1	0
6	M	25	0	0	0	0
All	All	9815	0	9327	49	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 3.

All (49) 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:B:1:ILE:HG22	1:B:2:ARG:O	1.93	0.69
1:B:362:ASN:HB3	1:B:440:TRP:CZ2	2.32	0.63
1:B:242:LEU:HA	1:B:258:LEU:HD12	1.84	0.59
2:H:46:GLU:HG3	4:L:203:EDO:H21	1.86	0.57
1:A:135:LEU:O	1:A:170:THR:HG22	2.04	0.57
1:A:317:ILE:HG23	4:L:201:EDO:H21	1.86	0.56
1:B:1:ILE:HG21	1:B:144:HIS:CE1	2.41	0.55
1:A:382:PHE:HB3	1:B:382:PHE:HB3	1.88	0.55
1:B:1:ILE:HG22	1:B:2:ARG:N	2.24	0.52
1:A:362:ASN:HB3	1:A:440:TRP:CZ2	2.46	0.51
1:B:1:ILE:CG2	1:B:2:ARG:N	2.74	0.50
1:B:162:GLU:HG3	1:B:164:ARG:H	1.76	0.50
1:A:25:LEU:HD21	1:A:43:ILE:HG12	1.93	0.49
1:B:25:LEU:HD21	1:B:43:ILE:HG12	1.93	0.49
3:L:70:ASP:HB3	6:L:350:HOH:O	2.12	0.49
1:B:1:ILE:HG12	1:B:145:GLY:HA2	1.94	0.48
1:B:51:SER:HB3	1:B:281:LYS:HG2	1.95	0.48
1:A:161:ASP:HB3	1:A:164:ARG:HG2	1.96	0.47
1:B:261:GLN:HA	6:B:603:HOH:O	2.13	0.47
2:H:11:LEU:HD12	2:H:110:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG21	1:A:130:ILE:HG23	1.97	0.47
1:B:273:LEU:HD23	1:B:286:SER:HB3	1.97	0.46
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.98	0.46
2:I:11:LEU:HD12	2:I:110:THR:HB	1.97	0.46
1:A:51:SER:HB3	1:A:281:LYS:HG2	1.98	0.46
2:H:46:GLU:HA	4:L:203:EDO:H11	1.98	0.46
1:B:137:TYR:HB2	1:B:169:ILE:HG13	1.97	0.46
2:I:12:VAL:HG11	2:I:82(C):LEU:HD13	1.98	0.45
2:I:103:TRP:CE3	3:M:44:PRO:HD2	2.52	0.45
1:B:53:MET:HB3	1:B:128:LYS:HB3	1.99	0.44
1:B:185:SER:HB3	1:B:297:LYS:HD3	1.99	0.44
1:A:380:PRO:HG2	1:A:402:ARG:HD2	1.99	0.44
1:A:145:GLY:HA3	1:A:360[A]:THR:HG23	2.00	0.44
1:B:20:TRP:CE3	1:B:292:ARG:HB3	2.53	0.44
1:B:305:TYR:CE2	1:B:338:PRO:HB2	2.53	0.44
1:A:185:SER:HB3	1:A:297:LYS:HD3	1.99	0.44
1:A:338:PRO:HA	1:A:365:ILE:O	2.19	0.43
2:H:103:TRP:CE3	3:L:44:PRO:HD2	2.55	0.42
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.01	0.42
2:I:34:MET:HB3	2:I:78:LEU:HD22	2.02	0.42
3:L:98:PHE:H	4:L:203:EDO:H12	1.85	0.42
1:A:53:MET:HB3	1:A:128:LYS:HB3	2.02	0.42
1:A:276:GLU:HB2	1:A:283:ARG:HB2	2.02	0.41
2:I:2:VAL:HG12	2:I:102:VAL:HG21	2.02	0.41
1:B:338:PRO:HA	1:B:365:ILE:O	2.19	0.41
1:A:305:TYR:CE2	1:A:338:PRO:HB2	2.56	0.41
1:B:212:LEU:HB2	1:B:273:LEU:HB2	2.03	0.41
1:A:35:ALA:HB3	1:A:38:LYS:HB2	2.02	0.40
1:B:31:VAL:HB	1:B:43:ILE:HG23	2.03	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	385/447 (86%)	376 (98%)	9 (2%)	0	100	100
1	B	376/447 (84%)	366 (97%)	10 (3%)	0	100	100
2	H	119/141 (84%)	116 (98%)	3 (2%)	0	100	100
2	I	120/141 (85%)	117 (98%)	3 (2%)	0	100	100
3	L	109/147 (74%)	106 (97%)	2 (2%)	1 (1%)	20	28
3	M	110/147 (75%)	107 (97%)	3 (3%)	0	100	100
All	All	1219/1470 (83%)	1188 (98%)	30 (2%)	1 (0%)	55	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	93	ASN

### 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	328/367 (89%)	319 (97%)	9 (3%)	50	69
1	B	325/367 (89%)	319 (98%)	6 (2%)	64	80
2	H	99/105 (94%)	99 (100%)	0	100	100
2	I	100/105 (95%)	99 (99%)	1 (1%)	80	90
3	L	92/117 (79%)	90 (98%)	2 (2%)	57	75
3	M	93/117 (80%)	92 (99%)	1 (1%)	78	89
All	All	1037/1178 (88%)	1018 (98%)	19 (2%)	64	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	30	CYS
1	A	67	ASP
1	A	169	ILE

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Mol	Chain	Res	Type
1	A	247	ASP
1	A	258	LEU
1	A	266	HIS
1	A	374	MET
1	A	375	MET
1	B	13	GLU
1	B	67	ASP
1	B	247	ASP
1	B	266	HIS
1	B	342	PRO
1	B	374	MET
2	I	21	SER
3	L	90	GLN
3	L	106	ILE
3	M	90	GLN

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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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	EDO	A	801	-	3,3,3	0.57	0	2,2,2	0.34	0
4	EDO	A	802	-	3,3,3	0.56	0	2,2,2	0.32	0
4	EDO	A	803	-	3,3,3	0.47	0	2,2,2	0.53	0
5	SO4	A	804	-	4,4,4	0.18	0	6,6,6	0.11	0
5	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.15	0
4	EDO	H	201	-	3,3,3	0.68	0	2,2,2	0.20	0
4	EDO	H	202	-	3,3,3	0.58	0	2,2,2	0.20	0
4	EDO	I	201	-	3,3,3	0.59	0	2,2,2	0.34	0
5	SO4	I	202	-	4,4,4	0.22	0	6,6,6	0.08	0
4	EDO	L	201	-	3,3,3	0.54	0	2,2,2	0.41	0
4	EDO	L	202	-	3,3,3	0.51	0	2,2,2	0.42	0
4	EDO	L	203	-	3,3,3	0.46	0	2,2,2	0.46	0
4	EDO	M	801	-	3,3,3	0.58	0	2,2,2	0.34	0
4	EDO	M	802	-	3,3,3	0.67	0	2,2,2	0.28	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	EDO	A	801	-	-	0/1/1/1	0/0/0/0
4	EDO	A	802	-	-	0/1/1/1	0/0/0/0
4	EDO	A	803	-	-	0/1/1/1	0/0/0/0
5	SO4	A	804	-	-	0/0/0/0	0/0/0/0
5	SO4	B	501	-	-	0/0/0/0	0/0/0/0
4	EDO	H	201	-	-	0/1/1/1	0/0/0/0
4	EDO	H	202	-	-	0/1/1/1	0/0/0/0
4	EDO	I	201	-	-	0/1/1/1	0/0/0/0
5	SO4	I	202	-	-	0/0/0/0	0/0/0/0
4	EDO	L	201	-	-	0/1/1/1	0/0/0/0
4	EDO	L	202	-	-	0/1/1/1	0/0/0/0
4	EDO	L	203	-	-	0/1/1/1	0/0/0/0
4	EDO	M	801	-	-	0/1/1/1	0/0/0/0
4	EDO	M	802	-	-	0/1/1/1	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	201	EDO	1	0
4	L	203	EDO	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	394/447 (88%)	0.07	10 (2%) 58 54	16, 53, 102, 125	0
1	B	386/447 (86%)	0.50	31 (8%) 13 11	38, 71, 106, 145	0
2	H	121/141 (85%)	-0.09	1 (0%) 86 84	15, 37, 73, 106	0
2	I	122/141 (86%)	-0.02	3 (2%) 58 54	28, 53, 90, 133	0
3	L	111/147 (75%)	-0.43	0 100 100	11, 24, 48, 75	0
3	M	112/147 (76%)	-0.41	1 (0%) 84 82	20, 35, 55, 81	0
All	All	1246/1470 (84%)	0.09	46 (3%) 42 40	11, 54, 101, 145	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	12.6
1	A	271	GLY	7.3
1	B	349	MET	6.8
1	B	350	GLN	5.7
1	A	278	ASP	5.6
1	B	193	ARG	5.2
1	A	280	ALA	4.9
1	B	278	ASP	4.9
1	B	20	TRP	4.9
1	B	280	ALA	4.9
1	B	279	GLY	4.5
1	B	191	GLU	4.5
1	B	196	LEU	4.3
1	B	281	LYS	4.2
1	B	192	PRO	4.0
1	A	16	SER	4.0
1	B	271	GLY	3.9
1	A	273	LEU	3.6
1	B	273	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLU	3.2
1	B	170	THR	3.2
2	I	113	SER	3.2
1	A	20	TRP	3.1
1	B	172	ASN	3.1
1	B	198	PHE	2.9
1	B	216	GLU	2.8
1	B	56	VAL	2.8
1	B	277	MET	2.8
2	I	13	GLN	2.8
1	B	197	ASP	2.8
1	B	346	ALA	2.8
1	B	291	CYS	2.8
2	H	13	GLN	2.7
1	B	288	HIS	2.6
1	A	17	GLY	2.5
1	B	130	ILE	2.5
1	B	236	TRP	2.5
1	B	270	ALA	2.5
1	B	296	ASP	2.4
1	B	194	THR	2.4
3	M	0	SER	2.3
1	A	296	ASP	2.3
2	I	111	VAL	2.2
1	B	19	THR	2.2
1	B	81	TYR	2.1
1	B	284	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	EDO	L	202	4/4	0.84	0.37	5.15	65,66,67,68	0
4	EDO	I	201	4/4	0.94	0.20	4.11	44,46,46,46	0
4	EDO	H	201	4/4	0.73	0.22	3.94	59,60,61,61	0
5	SO4	B	501	5/5	0.92	0.19	1.44	91,91,92,92	0
5	SO4	A	804	5/5	0.95	0.21	1.27	75,76,76,77	0
4	EDO	L	203	4/4	0.93	0.21	1.16	12,21,29,34	0
5	SO4	I	202	5/5	0.95	0.17	1.06	89,90,90,90	0
4	EDO	H	202	4/4	0.96	0.13	-0.30	36,36,37,38	0
4	EDO	A	801	4/4	0.93	0.12	-0.81	48,49,49,50	0
4	EDO	A	802	4/4	0.94	0.10	-	50,50,51,52	0
4	EDO	M	802	4/4	0.88	0.17	-	44,46,46,46	0
4	EDO	A	803	4/4	0.88	0.20	-	46,46,47,48	0
4	EDO	L	201	4/4	0.95	0.13	-	24,25,25,27	0
4	EDO	M	801	4/4	0.85	0.18	-	72,73,73,73	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.