



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:48 PM GMT

PDB ID : 4RWY  
Title : Crystal structure of VH1-46 germline-derived CD4-binding site-directed anti-body 8ANC131 in complex with HIV-1 clade B YU2 gp120  
Authors : Acharya, P.; Luongo, T.S.; Kwong, P.D.  
Deposited on : 2014-12-08  
Resolution : 2.13 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

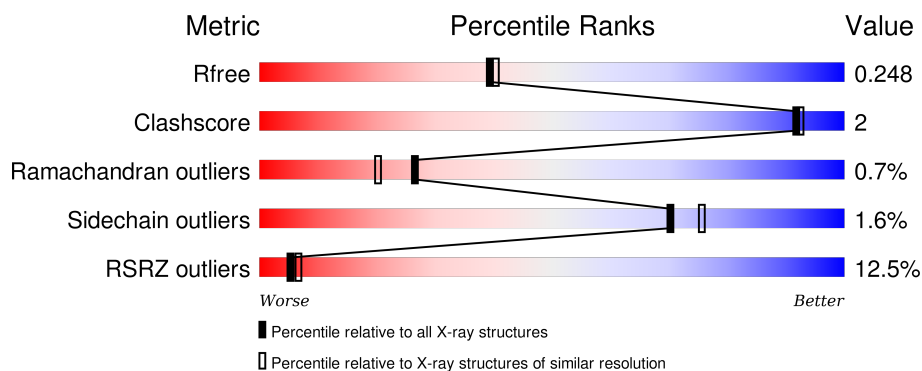
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	376	<div> <div>14%</div> <div>86%</div> <div>10%</div> </div>
2	H	227	<div> <div>11%</div> <div>94%</div> <div>6%</div> </div>
3	L	213	<div> <div>9%</div> <div>91%</div> <div>7%</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	NAG	A	506	-	-	-	X
6	EDO	A	508	-	-	-	X
6	EDO	H	301	-	-	-	X
6	EDO	H	304	-	-	-	X
7	NA	H	305	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12412 atoms, of which 6038 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 HIV-1 YU2 gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	337	5256	1667	2600	461	507	21	0	5	0

- Molecule 2 is a protein called Antibody 8ANC131 Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	227	3408	1077	1699	296	329	7	0	0	0

- Molecule 3 is a protein called Antibody 8ANC131 Light chain.

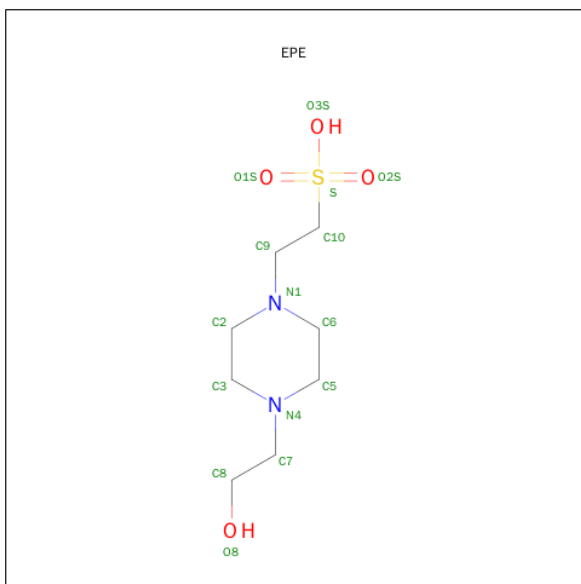
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	213	3270	1036	1612	291	326	5	0	1	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 6 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
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Na	0	0
			1	1		

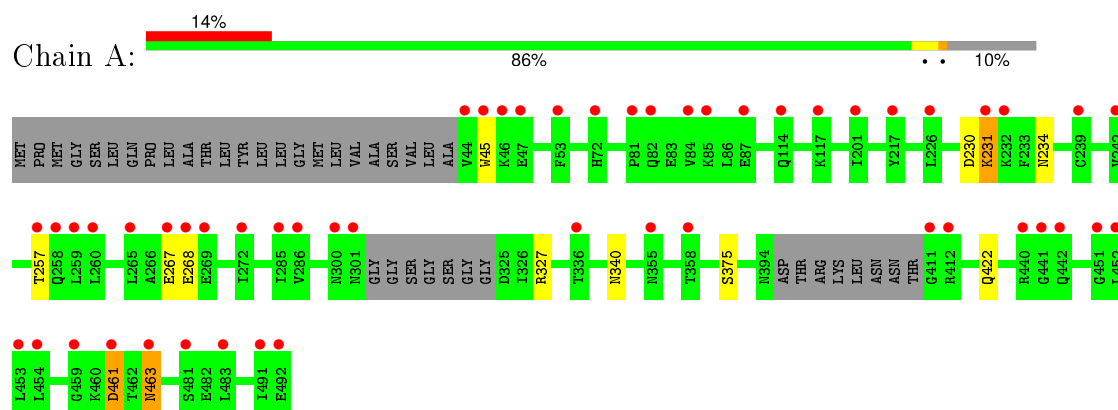
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total	O	0	0
			80	80		
8	H	82	Total	O	0	0
			82	82		
8	L	69	Total	O	0	0
			69	69		

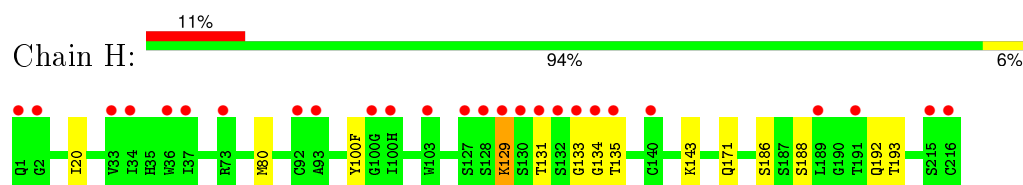
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

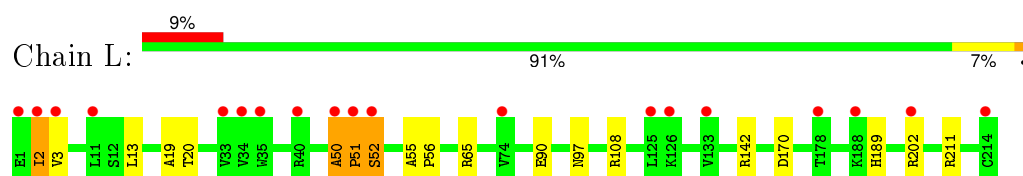
- Molecule 1: HIV-1 YU2 gp120



- Molecule 2: Antibody 8ANC131 Heavy chain



- Molecule 3: Antibody 8ANC131 Light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.25Å 67.14Å 214.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.84 – 2.13 28.84 – 2.13	Depositor EDS
% Data completeness (in resolution range)	79.3 (28.84-2.13) 73.6 (28.84-2.13)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, $R_{free}$	0.219 , 0.254 0.217 , 0.248	Depositor DCC
$R_{free}$ test set	1967 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.4	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 43325 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, EPE, NAG, 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	0.22	0/2738	0.40	0/3716
2	H	0.22	0/1749	0.42	0/2378
3	L	0.22	0/1700	0.42	0/2308
All	All	0.22	0/6187	0.41	0/8402

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
3	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	50	ALA	Peptide

### 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	2656	2600	2583	6	0
2	H	1709	1699	1696	9	0
3	L	1658	1612	1611	11	0
4	A	84	80	78	1	0
5	A	15	17	17	0	0
6	A	4	6	6	0	0
6	H	16	24	24	0	0
7	H	1	0	0	0	0
8	A	80	0	0	1	0
8	H	82	0	0	3	0
8	L	69	0	0	1	0
All	All	6374	6038	6015	25	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 2.

All (25) 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:L:189:HIS:O	3:L:211:ARG:NH1	2.29	0.66
2:H:134:GLY:O	2:H:186:SER:N	2.33	0.61
3:L:142:ARG:NH1	8:L:323:HOH:O	2.33	0.61
2:H:131:THR:OG1	2:H:135:THR:O	2.15	0.60
1:A:234:ASN:HD22	4:A:502:NAG:H83	1.69	0.57
3:L:50:ALA:HB1	3:L:51:PRO:CD	2.38	0.54
1:A:463:ASN:ND2	1:A:463:ASN:O	2.40	0.53
3:L:2:ILE:O	3:L:97:ASN:ND2	2.42	0.53
1:A:231:LYS:NZ	8:A:663:HOH:O	2.43	0.51
2:H:143:LYS:NZ	2:H:171:GLN:OE1	2.43	0.51
2:H:129:LYS:NZ	2:H:133:GLY:O	2.44	0.50
2:H:188:SER:O	2:H:192:GLN:N	2.45	0.49
3:L:51:PRO:HA	3:L:52:SER:CB	2.43	0.49
2:H:80:MET:O	8:H:458:HOH:O	2.20	0.48
1:A:327:ARG:NH2	1:A:422:GLN:OE1	2.48	0.45
1:A:461:ASP:N	1:A:461:ASP:OD1	2.49	0.45
2:H:80:MET:N	8:H:458:HOH:O	2.43	0.44
2:H:100(F):TYR:HB2	3:L:50:ALA:HB2	2.00	0.43
3:L:108:ARG:NE	3:L:170:ASP:O	2.50	0.43
3:L:2:ILE:HG22	3:L:3:VAL:N	2.35	0.42
1:A:257:THR:O	1:A:375:SER:N	2.52	0.42
3:L:202:ARG:H	3:L:202:ARG:HD2	1.85	0.42
3:L:13:LEU:CD1	3:L:19:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:55:ALA:HB1	3:L:56:PRO:HD2	2.03	0.41
2:H:20:ILE:N	8:H:458:HOH:O	2.53	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/376 (89%)	325 (97%)	9 (3%)	2 (1%)	30	24
2	H	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	39	36
3	L	212/213 (100%)	204 (96%)	6 (3%)	2 (1%)	21	14
All	All	773/816 (95%)	747 (97%)	21 (3%)	5 (1%)	26	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	TRP
2	H	129	LYS
3	L	2	ILE
1	A	268	GLU
3	L	51	PRO

### 5.3.2 Protein sidechains [i](#)

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	303/328 (92%)	297 (98%)	6 (2%)	63	67
2	H	190/190 (100%)	189 (100%)	1 (0%)	92	95
3	L	186/185 (100%)	182 (98%)	4 (2%)	60	63
All	All	679/703 (97%)	668 (98%)	11 (2%)	70	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ASP
1	A	231	LYS
1	A	267	GLU
1	A	340	ASN
1	A	461	ASP
1	A	463	ASN
2	H	193	THR
3	L	20	THR
3	L	52	SER
3	L	65	ARG
3	L	90	GLU

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 ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z  > 2$
4	NAG	A	501	1	14,14,15	0.20	0	15,19,21	0.39	0
4	NAG	A	502	1	14,14,15	0.18	0	15,19,21	0.39	0
4	NAG	A	503	1	14,14,15	0.25	0	15,19,21	0.40	0
4	NAG	A	504	1	14,14,15	0.20	0	15,19,21	0.39	0
4	NAG	A	505	1	14,14,15	0.23	0	15,19,21	0.33	0
4	NAG	A	506	1	14,14,15	0.31	0	15,19,21	0.35	0
5	EPE	A	507	-	15,15,15	0.78	1 (6%)	19,20,20	1.94	5 (26%)
6	EDO	A	508	-	3,3,3	0.45	0	2,2,2	0.29	0
6	EDO	H	301	-	3,3,3	0.45	0	2,2,2	0.34	0
6	EDO	H	302	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	H	303	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	H	304	-	3,3,3	0.44	0	2,2,2	0.37	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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	0/6/23/26	0/1/1/1
5	EPE	A	507	-	-	0/9/19/19	0/1/1/1
6	EDO	A	508	-	-	0/1/1/1	0/0/0/0
6	EDO	H	301	-	-	0/1/1/1	0/0/0/0
6	EDO	H	302	-	-	0/1/1/1	0/0/0/0
6	EDO	H	303	-	-	0/1/1/1	0/0/0/0
6	EDO	H	304	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	507	EPE	C10-S	2.69	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	507	EPE	O3S-S-C10	2.36	109.89	104.99
5	A	507	EPE	O1S-S-C10	3.45	109.31	106.87
5	A	507	EPE	C5-N4-C3	3.66	117.07	108.87
5	A	507	EPE	C7-N4-C5	3.69	119.27	111.25
5	A	507	EPE	O2S-S-C10	3.69	109.48	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	NAG	1	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	337/376 (89%)	0.99	52 (15%) 3 4	35, 54, 94, 135	0
2	H	227/227 (100%)	0.79	26 (11%) 6 9	31, 45, 92, 196	1 (0%)
3	L	213/213 (100%)	0.72	19 (8%) 12 16	36, 53, 83, 142	0
All	All	777/816 (95%)	0.86	97 (12%) 5 7	31, 51, 92, 196	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	GLY	15.1
1	A	411	GLY	14.0
2	H	1	GLN	9.0
2	H	132	SER	8.0
2	H	134	GLY	6.5
2	H	73	ARG	6.1
1	A	452	LEU	6.0
3	L	202	ARG	5.7
3	L	52	SER	5.3
1	A	44	VAL	5.1
2	H	2	GLY	5.0
1	A	231	LYS	4.7
3	L	1	GLU	4.5
3	L	51	PRO	4.4
1	A	259	LEU	4.4
2	H	127	SER	4.4
1	A	441	GLY	4.3
1	A	84	VAL	4.3
1	A	453	LEU	4.2
3	L	214	CYS	4.0
2	H	129	LYS	4.0
1	A	301	ASN	4.0
3	L	2	ILE	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	131	THR	3.9
3	L	50	ALA	3.9
2	H	216	CYS	3.7
1	A	286	VAL	3.7
1	A	451	GLY	3.7
1	A	440	ARG	3.5
2	H	130	SER	3.5
1	A	257	THR	3.5
1	A	300	ASN	3.5
1	A	285	ILE	3.5
2	H	215	SER	3.3
1	A	242	VAL	3.3
1	A	201	ILE	3.3
3	L	126	LYS	3.3
1	A	492	GLU	3.2
2	H	191	THR	3.2
3	L	3	VAL	3.1
2	H	100(H)	ILE	3.1
1	A	45	TRP	3.0
1	A	232	LYS	3.0
1	A	46	LYS	3.0
1	A	81	PRO	2.9
1	A	87	GLU	2.9
3	L	188	LYS	2.9
1	A	268	GLU	2.8
1	A	442	GLN	2.8
1	A	82	GLN	2.8
2	H	128	SER	2.8
1	A	454	LEU	2.7
3	L	34	VAL	2.7
1	A	258	GLN	2.7
1	A	461	ASP	2.6
1	A	85	LYS	2.6
2	H	92	CYS	2.6
1	A	412	ARG	2.5
1	A	217	TYR	2.5
1	A	265	LEU	2.5
1	A	260	LEU	2.5
3	L	35	TRP	2.4
1	A	483	LEU	2.4
1	A	114	GLN	2.4
3	L	33	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	491[A]	ILE	2.3
3	L	11	LEU	2.3
3	L	40	ARG	2.3
1	A	481	SER	2.3
3	L	133	VAL	2.3
1	A	239	CYS	2.3
1	A	358	THR	2.3
2	H	135	THR	2.3
2	H	37	ILE	2.3
1	A	267	GLU	2.2
2	H	36	TRP	2.2
1	A	272	ILE	2.2
1	A	269	GLU	2.2
3	L	74	VAL	2.2
1	A	459	GLY	2.2
2	H	93	ALA	2.2
1	A	463	ASN	2.2
1	A	53	PHE	2.2
2	H	34	ILE	2.1
1	A	47	GLU	2.1
1	A	355	ASN	2.1
1	A	117	LYS	2.1
1	A	336	THR	2.1
2	H	103	TRP	2.1
2	H	100(G)	GLY	2.1
2	H	189	LEU	2.1
1	A	226	LEU	2.0
3	L	125	LEU	2.0
2	H	33	VAL	2.0
1	A	72	HIS	2.0
2	H	140	CYS	2.0
3	L	178	THR	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 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
7	NA	H	305	1/1	0.89	0.57	20.48	60,60,60,60	0
6	EDO	H	304	4/4	0.52	0.31	7.01	80,96,96,97	0
4	NAG	A	506	14/15	0.74	0.25	3.97	75,100,129,129	0
6	EDO	H	301	4/4	0.67	0.25	2.88	70,85,85,85	0
6	EDO	A	508	4/4	0.81	0.30	2.33	91,110,113,113	0
4	NAG	A	505	14/15	0.82	0.20	1.45	102,118,140,144	0
4	NAG	A	501	14/15	0.79	0.24	1.15	85,93,111,113	0
4	NAG	A	504	14/15	0.86	0.29	0.74	51,57,68,68	0
6	EDO	H	303	4/4	0.93	0.25	0.57	51,61,63,63	0
4	NAG	A	502	14/15	0.88	0.15	0.51	54,62,73,74	0
5	EPE	A	507	15/15	0.96	0.17	-0.41	42,50,54,55	0
4	NAG	A	503	14/15	0.90	0.14	-0.77	40,46,55,55	0
6	EDO	H	302	4/4	0.64	0.41	-	70,84,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.