



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 10, 2016 – 05:53 AM EDT

PDB ID : 5F9O  
Title : Crystal structure of broadly neutralizing VH1-46 germline-derived CD4-binding site-directed antibody CH235.09 in complex with HIV-1 clade A/E 93TH057 gp120  
Authors : Joyce, M.G.; Mascola, J.R.; Kwong, P.D.  
Deposited on : 2015-12-10  
Resolution : 1.86 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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-20027107

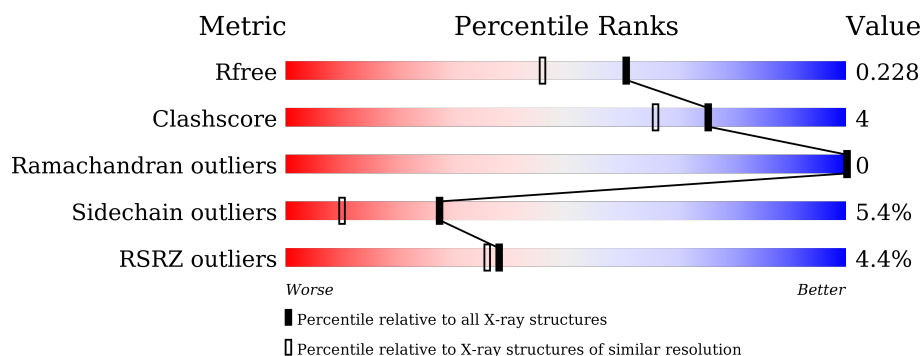
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	G	352	<div> <div>7%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
2	H	234	<div> <div>3%</div> <div>85%</div> <div>7%</div> <div>6%</div> </div>
3	L	213	<div> <div>%</div> <div>89%</div> <div>9%</div> <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	NAG	G	502	-	-	-	X
4	NAG	G	505	-	-	-	X
4	NAG	G	507	-	-	-	X
4	NAG	G	508	-	-	-	X
4	NAG	G	512	-	-	-	X
5	EPE	G	513	-	-	X	X
5	EPE	G	514	-	-	X	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6648 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	341	Total	C	N	O	S	0	0	0
			2671	1678	464	506	23			

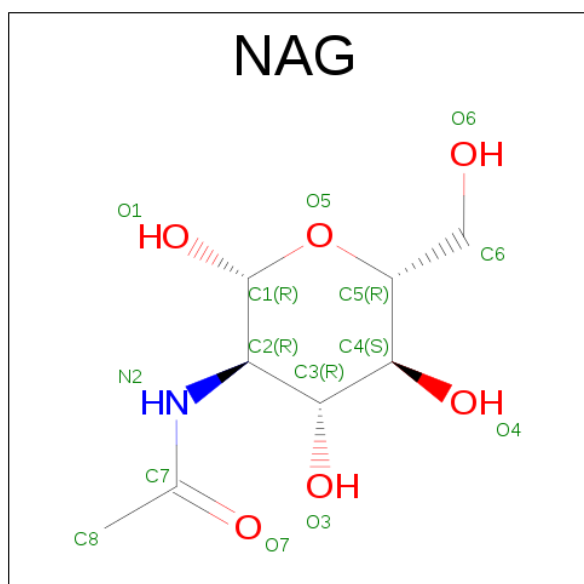
- Molecule 2 is a protein called CH235.9 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1661	1047	287	316	11			

- Molecule 3 is a protein called CH235.09 Light chain.

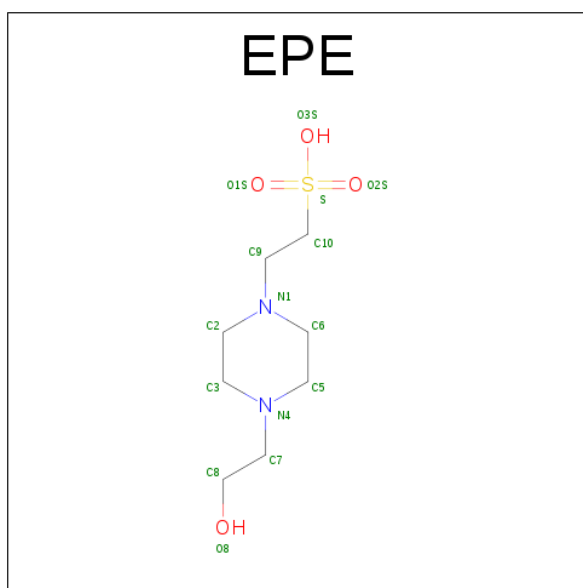
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1635	1022	285	323	5			

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



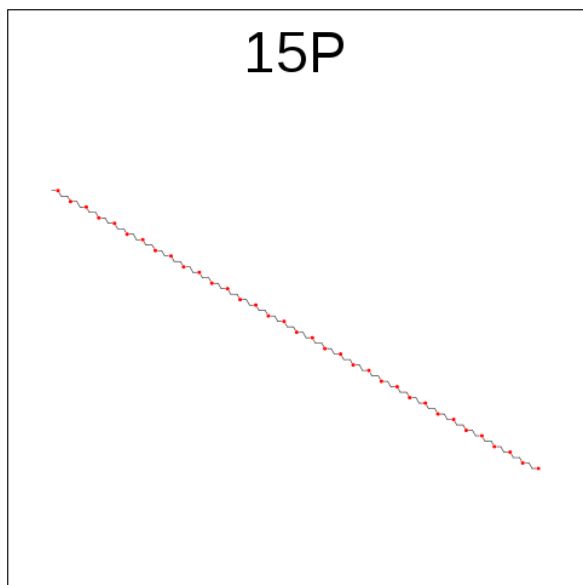
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula:  $C_{69}H_{140}O_{35}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			23	15	8		

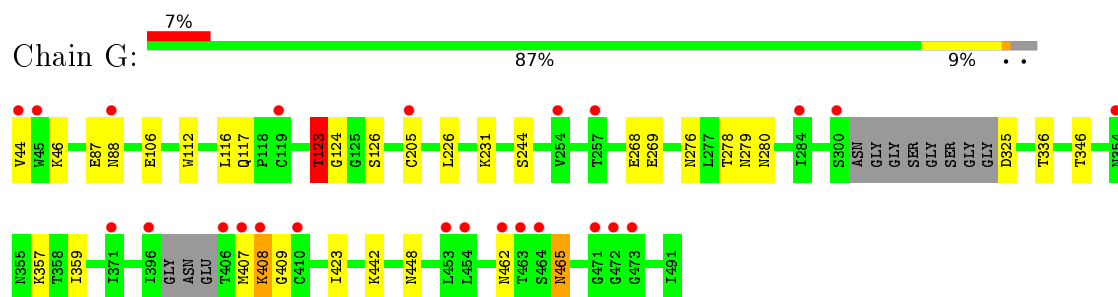
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	191	Total	O	0	0
			191	191		
7	H	141	Total	O	0	0
			141	141		
7	L	128	Total	O	0	0
			128	128		

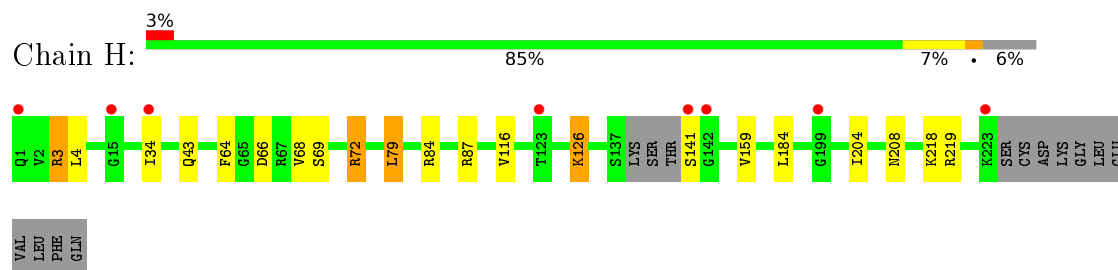
### 3 Residue-property plots [i](#)

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.

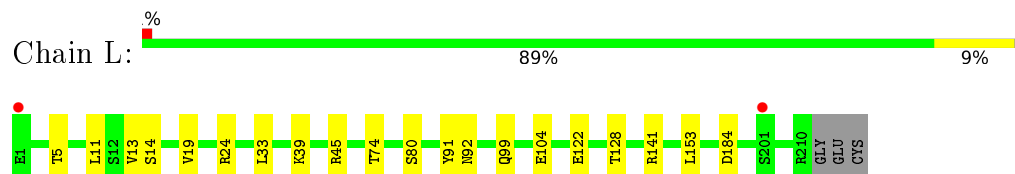
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 2: CH235.9 Heavy chain



- Molecule 3: CH235.09 Light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.53Å 67.80Å 225.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.81 – 1.86 35.81 – 1.86	Depositor EDS
% Data completeness (in resolution range)	89.2 (35.81-1.86) 85.6 (35.81-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.204 , 0.221 0.213 , 0.228	Depositor DCC
$R_{free}$ test set	3410 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 73940 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: 15P, EPE, NAG

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	G	0.41	0/2727	0.48	0/3701
2	H	0.31	0/1702	0.54	0/2313
3	L	0.36	0/1670	0.51	0/2267
All	All	0.37	0/6099	0.51	0/8281

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	G	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
1	G	123	THR	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	G	2671	0	2610	26	1
2	H	1661	0	1624	11	0
3	L	1635	0	1596	9	0
4	G	168	0	156	9	1
5	G	30	0	35	0	18
6	G	23	0	29	0	0
7	G	191	0	0	8	0
7	H	141	0	0	1	0
7	L	128	0	0	4	0
All	All	6648	0	6050	47	19

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 4.

The worst 5 of 47 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:G:325:ASP:OD1	7:G:601:HOH:O	1.88	0.91
3:L:141:ARG:NH1	7:L:301:HOH:O	2.10	0.84
1:G:106:GLU:OE2	7:G:602:HOH:O	1.98	0.81
1:G:442:LYS:NZ	7:G:603:HOH:O	2.18	0.77
2:H:69:SER:OG	2:H:84:ARG:NH1	2.18	0.75

The worst 5 of 19 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:513:EPE:O1S	5:G:514:EPE:O3S[3_554]	0.03	2.17
5:G:513:EPE:S	5:G:514:EPE:S[3_554]	0.07	2.13
5:G:513:EPE:C10	5:G:514:EPE:C10[3_554]	0.11	2.09
5:G:513:EPE:O8	5:G:514:EPE:O8[3_554]	0.15	2.05
5:G:513:EPE:O2S	5:G:514:EPE:O2S[3_554]	0.23	1.97

## 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	G	335/352 (95%)	327 (98%)	8 (2%)	0	100	100
2	H	216/234 (92%)	211 (98%)	5 (2%)	0	100	100
3	L	208/213 (98%)	203 (98%)	5 (2%)	0	100	100
All	All	759/799 (95%)	741 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	G	305/310 (98%)	291 (95%)	14 (5%)	33	14
2	H	183/196 (93%)	173 (94%)	10 (6%)	27	9
3	L	183/185 (99%)	171 (93%)	12 (7%)	21	6
All	All	671/691 (97%)	635 (95%)	36 (5%)	27	10

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	72	ARG
2	H	126	LYS
3	L	104	GLU
2	H	87	ARG
2	H	141	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	444	ASN
3	L	159	GLN

### 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 ⓘ

15 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	NAG	G	501	1	14,14,15	0.28	0	15,19,21	0.53	0
4	NAG	G	502	1	14,14,15	0.28	0	15,19,21	0.54	0
4	NAG	G	503	1	14,14,15	0.27	0	15,19,21	0.53	0
4	NAG	G	504	1	14,14,15	0.31	0	15,19,21	0.38	0
4	NAG	G	505	1	14,14,15	0.97	1 (7%)	15,19,21	1.06	1 (6%)
4	NAG	G	506	1	14,14,15	0.22	0	15,19,21	0.47	0
4	NAG	G	507	1	14,14,15	0.28	0	15,19,21	0.54	0
4	NAG	G	508	1	14,14,15	0.15	0	15,19,21	1.14	1 (6%)
4	NAG	G	509	1	14,14,15	0.43	0	15,19,21	0.48	0
4	NAG	G	510	1	14,14,15	0.28	0	15,19,21	0.48	0
4	NAG	G	511	1	14,14,15	0.19	0	15,19,21	0.32	0
4	NAG	G	512	1	14,14,15	0.43	0	15,19,21	1.24	1 (6%)
5	EPE	G	513	5	15,15,15	2.64	4 (26%)	19,20,20	2.01	2 (10%)
5	EPE	G	514	5	15,15,15	2.63	4 (26%)	19,20,20	2.78	6 (31%)
6	15P	G	515	-	22,22,103	0.86	0	21,21,102	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	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	1	-	1/6/23/26	0/1/1/1
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
4	NAG	G	509	1	-	0/6/23/26	0/1/1/1
4	NAG	G	510	1	-	0/6/23/26	0/1/1/1
4	NAG	G	511	1	-	0/6/23/26	0/1/1/1
4	NAG	G	512	1	-	0/6/23/26	0/1/1/1
5	EPE	G	513	5	-	0/9/19/19	0/1/1/1
5	EPE	G	514	5	-	0/9/19/19	0/1/1/1
6	15P	G	515	-	-	0/20/20/101	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	513	EPE	C10-S	-8.72	1.64	1.77
5	G	514	EPE	C10-S	-8.23	1.65	1.77
5	G	514	EPE	O1S-S	-3.21	1.35	1.45
5	G	514	EPE	O3S-S	-3.14	1.36	1.47
5	G	513	EPE	O2S-S	-3.07	1.36	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	514	EPE	C9-N1-C2	-2.59	105.61	111.25
5	G	514	EPE	O2S-S-O1S	-2.36	107.28	113.96
5	G	514	EPE	C7-N4-C5	-2.18	106.50	111.25
5	G	514	EPE	C9-N1-C6	2.20	116.03	111.25
5	G	513	EPE	O3S-S-C10	2.38	109.94	104.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	502	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	501	NAG	1	0
4	G	502	NAG	2	0
4	G	505	NAG	1	0
4	G	507	NAG	2	0
4	G	508	NAG	1	0
4	G	512	NAG	2	1
5	G	513	EPE	0	18
5	G	514	EPE	0	18

## 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	G	341/352 (96%)	0.41	24 (7%) 19 18	26, 40, 74, 146	0
2	H	220/234 (94%)	0.26	8 (3%) 46 44	25, 36, 60, 122	0
3	L	210/213 (98%)	0.06	2 (0%) 84 84	25, 40, 61, 85	0
All	All	771/799 (96%)	0.27	34 (4%) 38 36	25, 39, 65, 146	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	142	GLY	5.9
1	G	396	ILE	5.0
2	H	223	LYS	4.6
1	G	406	THR	4.0
1	G	407	MET	3.8

### 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	507	14/15	0.64	0.32	8.15	61,67,68,70	0
4	NAG	G	505	14/15	0.61	0.47	7.76	113,127,130,131	0
4	NAG	G	502	14/15	0.81	0.24	3.68	97,102,105,105	0
5	EPE	G	513	15/15	0.91	0.19	2.93	109,114,124,135	0
4	NAG	G	508	14/15	0.83	0.29	2.86	85,94,99,99	0
5	EPE	G	514	15/15	0.90	0.18	2.52	100,114,150,151	15
4	NAG	G	512	14/15	0.69	0.29	2.35	95,101,105,107	0
6	15P	G	515	23/104	0.89	0.15	1.13	43,45,50,55	0
4	NAG	G	511	14/15	0.87	0.25	1.06	86,90,96,98	0
4	NAG	G	506	14/15	0.88	0.19	0.82	46,51,62,62	0
4	NAG	G	510	14/15	0.92	0.16	0.47	50,54,59,59	0
4	NAG	G	504	14/15	0.90	0.12	-0.23	39,46,51,53	0
4	NAG	G	503	14/15	0.82	0.21	-	78,81,95,96	0
4	NAG	G	501	14/15	0.62	0.80	-	115,116,117,118	0
4	NAG	G	509	14/15	0.63	0.54	-	111,119,121,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.