



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:31 AM UTC

PDB ID : 4RX4 / pdb\_00004rx4  
Title : Crystal structure of VH1-46 germline-derived CD4-binding site-directed antibody 8ANC134 in complex with HIV-1 clade A Q842.d12 gp120  
Authors : Zhou, T.; Acharya, P.; Moquin, S.; Kwong, P.D.  
Deposited on : 2014-12-08  
Resolution : 3.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

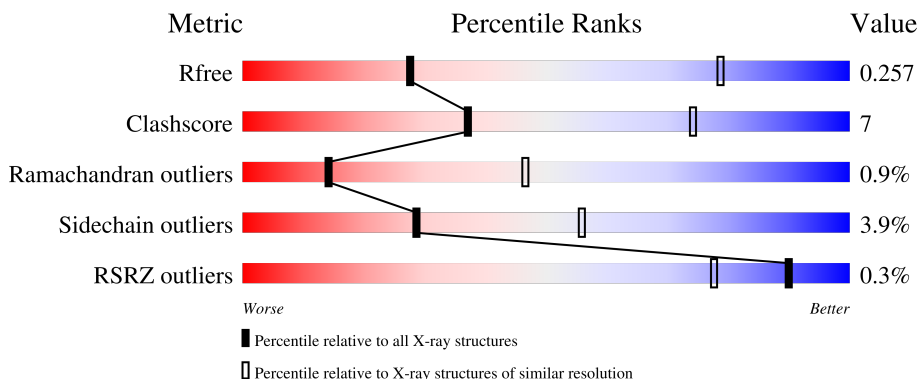
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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))
$R_{free}$	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	E	354	 70% 19% 10%
1	G	354	 70% 19% 8%
2	A	229	 78% 18%
2	H	229	 80% 14% 5%
3	D	213	 84% 14%

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Mol	Chain	Length	Quality of chain
3	L	213	 84% 13% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23562 atoms, of which 11587 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 Clade A Q842.d12 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	G	325	5094	1627	2504	459	483	21	0	0	0
1	E	320	5026	1606	2472	452	475	21	0	0	0

- Molecule 2 is a protein called 8ANC134 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	H	217	3258	1038	1623	280	311	6	0	0	0
2	A	222	3300	1060	1627	287	319	7	0	0	0

- Molecule 3 is a protein called 8ANC134 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	L	212	3226	1025	1586	285	325	5	0	0	0
3	D	213	3240	1030	1591	286	328	5	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

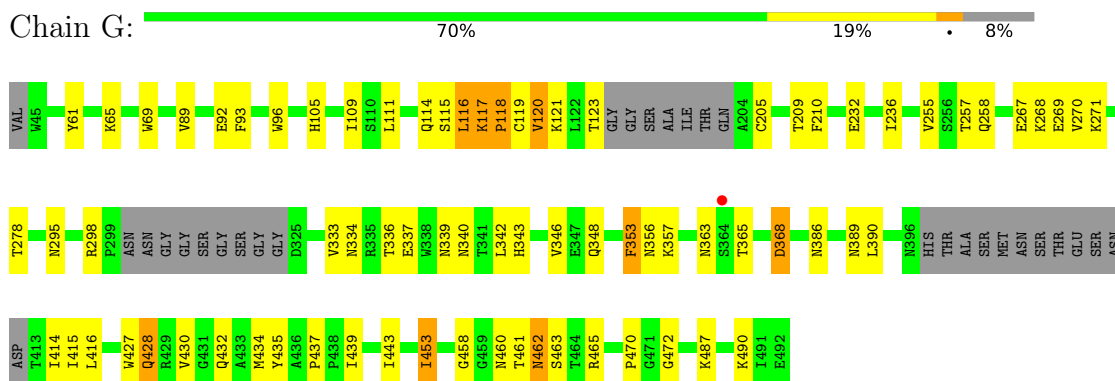


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	G	1	10	2	6	2	0	0
6	G	1	10	2	6	2	0	0
6	G	1	10	2	6	2	0	0
6	G	1	10	2	6	2	0	0
6	E	1	10	2	6	2	0	0

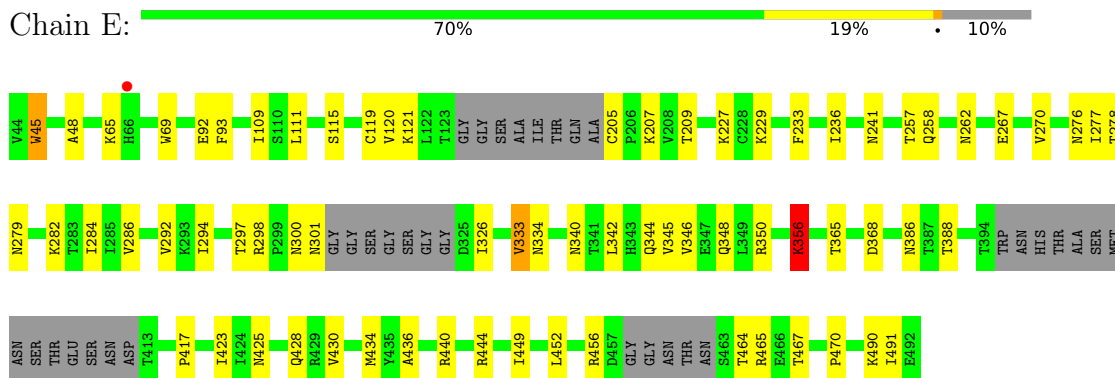
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

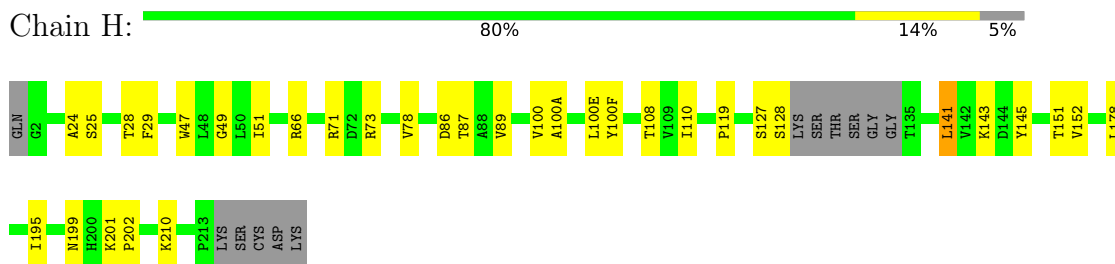
- Molecule 1: HIV-1 Clade A Q842.d12 gp120



- Molecule 1: HIV-1 Clade A Q842.d12 gp120



- Molecule 2: 8ANC134 Heavy chain



- Molecule 2: 8ANC134 Heavy chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.35Å 220.35Å 118.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.90 – 3.45 26.90 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.90-3.45) 93.0 (26.90-3.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.46Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, $R_{free}$	0.208 , 0.253 0.214 , 0.257	Depositor DCC
$R_{free}$ test set	1406 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.6	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 105.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 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	E	0.52	0/2607	1.03	9/3535 (0.3%)
1	G	0.55	0/2646	1.02	13/3590 (0.4%)
2	A	0.53	0/1711	0.91	2/2326 (0.1%)
2	H	0.54	0/1673	0.90	2/2277 (0.1%)
3	D	0.51	0/1687	0.92	4/2291 (0.2%)
3	L	0.48	0/1678	0.88	2/2279 (0.1%)
All	All	0.52	0/12002	0.96	32/16298 (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	E	0	1
3	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	100	VAL	N-CA-C	8.87	120.94	107.99
1	G	267	GLU	N-CA-C	7.28	119.30	111.36
1	E	257	THR	N-CA-C	7.07	121.18	109.95
3	L	54	ARG	N-CA-C	6.93	120.69	109.40
1	G	257	THR	N-CA-C	6.69	120.58	109.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	50	GLY	Peptide
1	E	356	LYS	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	E	2554	2472	2505	40	0
1	G	2590	2504	2530	41	0
2	A	1673	1627	1667	25	0
2	H	1635	1623	1628	23	0
3	D	1649	1591	1597	18	0
3	L	1640	1586	1589	23	0
4	E	70	70	65	6	0
4	G	84	84	78	4	0
5	A	5	0	0	0	0
5	D	20	0	0	1	0
5	E	5	0	0	0	0
5	G	15	0	0	1	0
5	L	15	0	0	0	0
6	E	4	6	6	0	0
6	G	16	24	24	1	0
All	All	11975	11587	11689	167	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 7.

The worst 5 of 167 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:E:241:ASN:ND2	4:E:504:NAG:O5	2.14	0.80
1:G:298:ARG:NH2	1:G:439:ILE:O	2.23	0.72
1:G:365:THR:HG21	6:G:513:EDO:H21	1.73	0.69
1:E:276:ASN:ND2	4:E:501:NAG:O7	2.25	0.69
1:G:353:PHE:HA	1:G:356:ASN:HB2	1.74	0.69

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	E	310/354 (88%)	295 (95%)	11 (4%)	4 (1%)	9	39
1	G	317/354 (90%)	299 (94%)	13 (4%)	5 (2%)	7	36
2	A	218/229 (95%)	209 (96%)	8 (4%)	1 (0%)	24	57
2	H	213/229 (93%)	206 (97%)	7 (3%)	0	100	100
3	D	211/213 (99%)	204 (97%)	4 (2%)	3 (1%)	9	38
3	L	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
All	All	1479/1592 (93%)	1418 (96%)	48 (3%)	13 (1%)	14	46

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	465	ARG
3	D	2	ILE
3	D	53	ASP
1	G	118	PRO
1	G	120	VAL

### 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	E	289/312 (93%)	281 (97%)	8 (3%)	38	62
1	G	292/312 (94%)	273 (94%)	19 (6%)	15	43
2	A	186/191 (97%)	182 (98%)	4 (2%)	45	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	181/191 (95%)	179 (99%)	2 (1%)	65	75
3	D	185/185 (100%)	175 (95%)	10 (5%)	20	47
3	L	184/185 (100%)	175 (95%)	9 (5%)	22	50
All	All	1317/1376 (96%)	1265 (96%)	52 (4%)	28	56

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	154	LEU
1	E	365	THR
3	D	90	GLU
3	L	169	LYS
1	E	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	137	ASN
3	D	49	HIS
3	L	199	GLN
3	D	124	GLN
2	A	30	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

28 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	502	-	14,14,15	0.44	0	17,19,21	0.64	0
4	NAG	G	506	1	14,14,15	0.43	0	17,19,21	0.56	0
4	NAG	G	503	1	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
4	NAG	E	504	-	14,14,15	0.23	0	17,19,21	0.61	1 (5%)
4	NAG	E	502	1	14,14,15	0.34	0	17,19,21	0.51	0
6	EDO	G	508	-	3,3,3	0.60	0	2,2,2	0.08	0
5	SO4	G	507	-	4,4,4	0.27	0	6,6,6	0.09	0
4	NAG	G	501	1	14,14,15	0.84	1 (7%)	17,19,21	0.99	1 (5%)
5	SO4	D	304	-	4,4,4	0.23	0	6,6,6	0.22	0
5	SO4	D	302	-	4,4,4	0.21	0	6,6,6	0.08	0
4	NAG	E	501	1	14,14,15	0.55	0	17,19,21	1.00	1 (5%)
5	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.20	0
5	SO4	L	402	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	L	403	-	4,4,4	0.26	0	6,6,6	0.27	0
4	NAG	G	505	1	14,14,15	0.40	0	17,19,21	0.43	0
6	EDO	G	509	-	3,3,3	0.54	0	2,2,2	0.20	0
6	EDO	G	513	-	3,3,3	0.27	0	2,2,2	0.60	0
6	EDO	E	507	-	3,3,3	0.46	0	2,2,2	0.32	0
4	NAG	E	505	-	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
4	NAG	G	504	1	14,14,15	0.63	1 (7%)	17,19,21	0.85	1 (5%)
4	NAG	E	503	1	14,14,15	0.43	0	17,19,21	0.45	0
5	SO4	G	512	-	4,4,4	0.25	0	6,6,6	0.24	0
5	SO4	D	303	-	4,4,4	0.25	0	6,6,6	0.11	0
6	EDO	G	510	-	3,3,3	0.51	0	2,2,2	0.19	0
5	SO4	L	401	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	D	301	-	4,4,4	0.22	0	6,6,6	0.15	0
5	SO4	G	511	-	4,4,4	0.26	0	6,6,6	0.18	0
5	SO4	E	506	-	4,4,4	0.23	0	6,6,6	0.12	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	502	-	-	1/6/23/26	0/1/1/1
4	NAG	G	506	1	-	2/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	505	1	-	3/6/23/26	0/1/1/1
4	NAG	E	504	-	-	4/6/23/26	0/1/1/1
4	NAG	E	502	1	-	2/6/23/26	0/1/1/1
6	EDO	G	509	-	-	1/1/1/1	-
6	EDO	G	513	-	-	1/1/1/1	-
6	EDO	E	507	-	-	1/1/1/1	-
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	505	-	-	0/6/23/26	0/1/1/1
6	EDO	G	508	-	-	1/1/1/1	-
6	EDO	G	510	-	-	1/1/1/1	-
4	NAG	G	504	1	-	4/6/23/26	0/1/1/1
4	NAG	E	503	1	-	0/6/23/26	0/1/1/1
4	NAG	E	501	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	501	NAG	C1-C2	2.43	1.55	1.52
4	G	504	NAG	O5-C1	-2.12	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	501	NAG	C1-O5-C5	3.68	117.11	112.19
4	E	501	NAG	C2-N2-C7	3.11	127.07	122.90
4	G	503	NAG	C1-O5-C5	2.57	115.64	112.19
4	E	505	NAG	C1-O5-C5	2.34	115.32	112.19
4	G	504	NAG	C1-O5-C5	2.18	115.11	112.19

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	502	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	E	501	NAG	C1-C2-N2-C7
4	E	501	NAG	C4-C5-C6-O6
4	E	501	NAG	O5-C5-C6-O6
4	E	504	NAG	O5-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	502	NAG	1	0
4	G	506	NAG	1	0
4	E	504	NAG	2	0
4	E	502	NAG	1	0
5	G	507	SO4	1	0
4	E	501	NAG	2	0
4	G	505	NAG	1	0
6	G	513	EDO	1	0
4	G	504	NAG	1	0
4	E	503	NAG	1	0
5	D	301	SO4	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 [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	E	320/354 (90%)	-0.14	1 (0%) 90 77	90, 154, 239, 351	0
1	G	325/354 (91%)	-0.24	1 (0%) 90 77	77, 132, 211, 346	0
2	A	222/229 (96%)	-0.48	1 (0%) 87 70	76, 109, 176, 312	0
2	H	217/229 (94%)	-0.44	0 100 100	64, 113, 197, 293	0
3	D	213/213 (100%)	-0.38	1 (0%) 87 70	88, 134, 175, 203	0
3	L	212/213 (99%)	-0.43	0 100 100	70, 127, 182, 217	0
All	All	1509/1592 (94%)	-0.33	4 (0%) 90 77	64, 129, 205, 351	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	364	SER	3.6
2	A	128	SER	2.8
1	E	66	HIS	2.7
3	D	51	PRO	2.3

### 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 oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	L	403	5/5	0.37	0.16	254,255,256,257	0
4	NAG	G	502	14/15	0.40	0.13	121,161,198,200	0
5	SO4	D	303	5/5	0.43	0.18	187,188,189,189	0
4	NAG	G	506	14/15	0.48	0.12	141,190,230,233	0
5	SO4	G	512	5/5	0.48	0.21	267,268,269,271	0
5	SO4	G	507	5/5	0.51	0.10	193,193,195,195	0
5	SO4	D	304	5/5	0.54	0.13	263,264,264,265	0
5	SO4	A	301	5/5	0.57	0.17	199,200,200,201	0
6	EDO	G	510	4/4	0.58	0.11	95,114,123,123	0
4	NAG	E	502	14/15	0.64	0.11	119,150,200,200	0
4	NAG	E	505	14/15	0.71	0.13	139,192,248,248	0
4	NAG	E	504	14/15	0.71	0.09	147,185,222,228	0
5	SO4	D	302	5/5	0.72	0.15	184,185,186,186	0
6	EDO	G	513	4/4	0.73	0.32	151,182,183,183	0
5	SO4	D	301	5/5	0.75	0.08	171,172,173,174	0
4	NAG	G	505	14/15	0.75	0.11	171,190,227,227	0
5	SO4	L	402	5/5	0.78	0.08	189,190,190,192	0
6	EDO	G	509	4/4	0.79	0.19	94,113,121,122	0
5	SO4	G	511	5/5	0.80	0.10	154,155,157,159	0
4	NAG	G	503	14/15	0.83	0.07	130,137,163,164	0
6	EDO	G	508	4/4	0.84	0.07	90,108,114,114	0
5	SO4	L	401	5/5	0.85	0.10	183,183,185,186	0
4	NAG	E	503	14/15	0.85	0.11	133,166,199,199	0
6	EDO	E	507	4/4	0.85	0.08	94,113,118,118	0
4	NAG	E	501	14/15	0.86	0.11	150,180,194,194	0
4	NAG	G	504	14/15	0.89	0.09	107,156,203,203	0
5	SO4	E	506	5/5	0.90	0.12	176,176,177,179	0
4	NAG	G	501	14/15	0.92	0.11	73,155,186,189	0

## 6.5 Other polymers

There are no such residues in this entry.