



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 05:37 AM EST

PDB ID : 5D02  
Title : Neisseria meningitidis 3 deoxy-D-arabino-heptulosonate 7-phosphate synthase  
Glu176Gln variant  
Authors : Heyes, L.C.  
Deposited on : 2015-08-02  
Resolution : 1.87 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

<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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

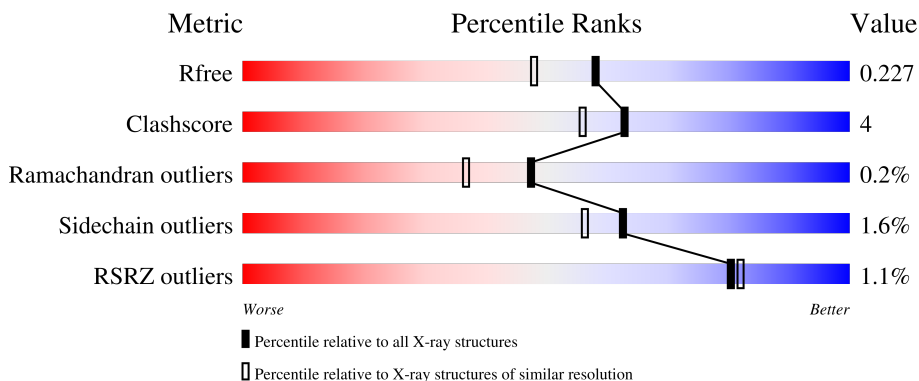
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	A	351	 % 90% 5% 5%
1	B	351	 89% 6% 5%
1	C	351	 3% 86% 8% 5%
1	D	351	 % 89% 5% 5%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	PEP	C	402	-	-	X	-
5	EDO	D	403	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10904 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 Phospho-2-dehydro-3-deoxyheptonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2572	1608	465	485	14	0	3	0
1	B	335	2555	1602	461	478	14	0	2	0
1	C	333	2532	1583	457	478	14	0	1	0
1	D	334	2531	1584	456	477	14	0	2	0

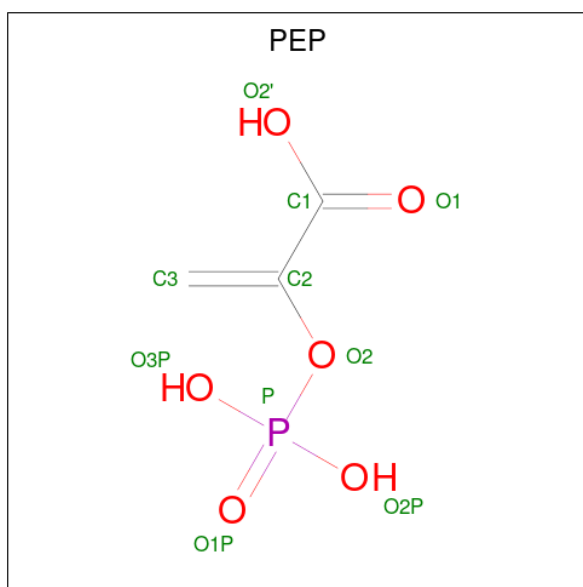
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLN	GLU	engineered mutation	UNP Q9K169
B	176	GLN	GLU	engineered mutation	UNP Q9K169
C	176	GLN	GLU	engineered mutation	UNP Q9K169
D	176	GLN	GLU	engineered mutation	UNP Q9K169

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

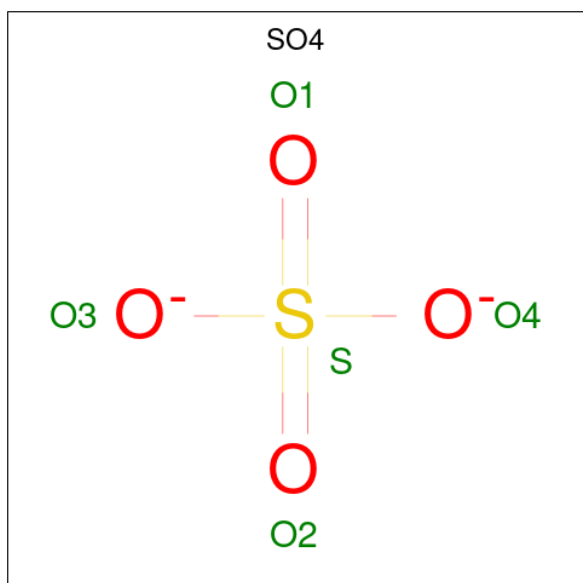
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C<sub>3</sub>H<sub>5</sub>O<sub>6</sub>P).



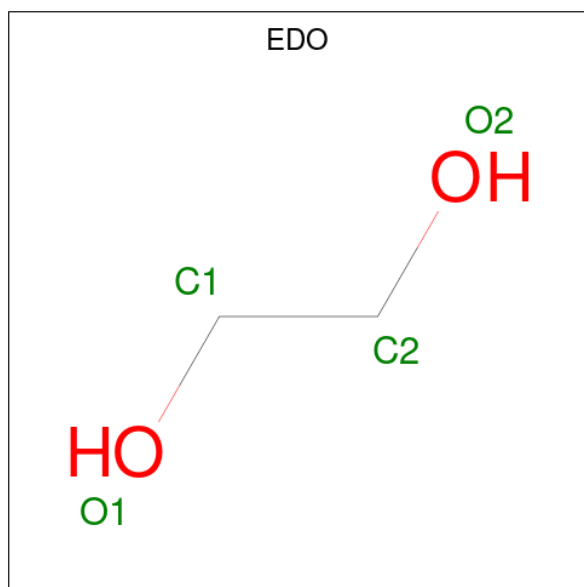
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
3	B	1	10	3	6	1	0	0
3	C	1	10	3	6	1	0	0
3	D	1	10	3	6	1	0	0

- 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	D	1	Total O S 5 4 1	0	0

- Molecule 5 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
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	187	Total O 187 187	0	0
6	B	170	Total O 170 170	0	0
6	C	141	Total O 141 141	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	D	142	Total 142	O 142	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.

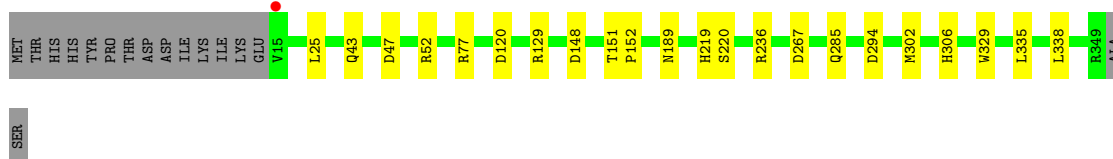
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

Chain A: 




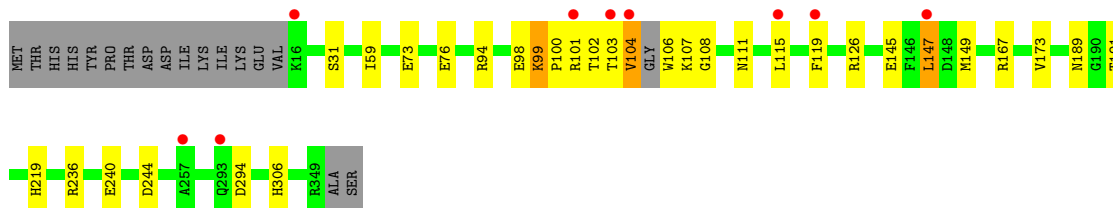
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

Chain B: 

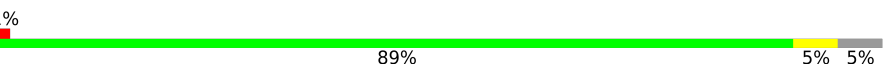


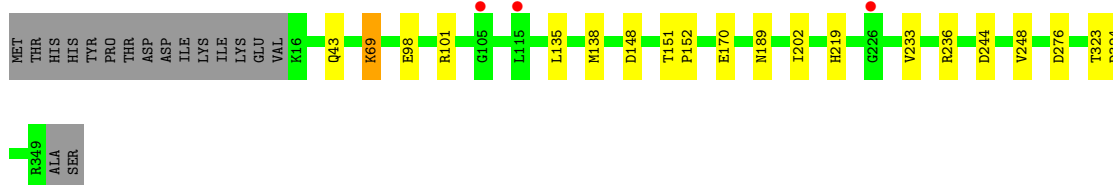
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

Chain C: 



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.54Å 135.55Å 76.01Å 90.00° 96.27° 90.00°	Depositor
Resolution (Å)	75.55 – 1.87 43.01 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.55-1.87) 99.9 (43.01-1.87)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.87Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.176 , 0.221 0.185 , 0.227	Depositor DCC
$R_{free}$ test set	7573 reflections (6.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: EDO, MN, PEP, 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	0.59	0/2621	0.73	2/3550 (0.1%)
1	B	0.60	0/2604	0.71	0/3529
1	C	0.59	0/2580	0.75	5/3499 (0.1%)
1	D	0.56	0/2580	0.69	1/3501 (0.0%)
All	All	0.59	0/10385	0.72	8/14079 (0.1%)

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	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	167	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	244	ASP	CB-CG-OD1	6.08	123.77	118.30
1	C	167	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	102	THR	N-CA-C	-5.58	95.93	111.00
1	A	279	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	104	VAL	N-CA-C	5.06	124.67	111.00
1	D	101	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	99	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	A	2572	0	2522	20	0
1	B	2555	0	2503	19	0
1	C	2532	0	2467	39	0
1	D	2531	0	2462	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	4	0
3	D	10	0	2	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	B	8	0	12	1	0
5	C	8	0	12	2	0
5	D	4	0	6	5	0
6	A	187	0	0	2	0
6	B	170	0	0	0	0
6	C	141	0	0	5	0
6	D	142	0	0	3	0
All	All	10904	0	9992	87	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 4.

All (87) 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:C:219[B]:HIS:NE2	1:D:219[B]:HIS:CE1	1.76	1.51
1:C:219[B]:HIS:CD2	1:D:219[B]:HIS:CE1	2.10	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219[B]:HIS:HE2	1:D:219[B]:HIS:CE1	1.36	1.36
1:C:101:ARG:HG3	1:C:104:VAL:O	1.49	1.11
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:CD2	2.40	1.09
1:B:47:ASP:OD1	1:B:52:ARG:NH2	1.89	1.06
1:A:219[A]:HIS:NE2	1:D:219[A]:HIS:CD2	2.30	1.00
5:C:404:EDO:H11	6:C:512:HOH:O	1.66	0.93
1:C:219[B]:HIS:CD2	1:D:219[B]:HIS:HE1	1.87	0.92
1:B:219[A]:HIS:CE1	1:C:219[A]:HIS:NE2	2.39	0.90
1:B:219[A]:HIS:CE1	1:C:219[A]:HIS:HE2	1.93	0.87
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:HD2	1.94	0.85
1:A:219[A]:HIS:CG	1:D:219[A]:HIS:HE2	1.98	0.82
1:C:219[B]:HIS:CD2	1:D:219[B]:HIS:ND1	2.48	0.82
1:A:219[A]:HIS:ND1	1:B:219[A]:HIS:CE1	2.49	0.81
1:A:219[A]:HIS:CD2	1:D:219[A]:HIS:NE2	2.51	0.79
1:A:219[A]:HIS:CG	1:D:219[A]:HIS:NE2	2.52	0.78
1:D:323:THR:HA	5:D:403:EDO:H11	1.67	0.77
1:C:219[B]:HIS:NE2	1:D:219[B]:HIS:NE2	2.04	0.76
1:B:219[A]:HIS:CE1	1:C:219[A]:HIS:CD2	2.76	0.73
1:B:148[B]:ASP:OD1	1:B:151:THR:OG1	2.05	0.72
1:C:219[B]:HIS:NE2	1:D:219[B]:HIS:ND1	2.35	0.72
1:B:219[A]:HIS:ND1	1:C:219[A]:HIS:NE2	2.38	0.71
1:D:323:THR:CA	5:D:403:EDO:H11	2.22	0.70
1:C:103:THR:C	1:C:104:VAL:HG23	2.12	0.70
1:A:219[A]:HIS:CD2	6:A:527:HOH:O	2.47	0.67
1:A:219[A]:HIS:CE1	1:D:219[A]:HIS:NE2	2.63	0.67
1:D:323:THR:C	5:D:403:EDO:H11	2.16	0.66
1:C:145:GLU:OE1	6:C:501:HOH:O	2.12	0.65
1:C:219[B]:HIS:HD2	1:D:219[B]:HIS:CE1	2.06	0.64
1:C:147:LEU:HD12	1:C:147:LEU:O	1.98	0.63
1:C:101:ARG:CG	1:C:104:VAL:O	2.37	0.62
3:C:402:PEP:C3	6:C:501:HOH:O	2.47	0.61
1:C:219[B]:HIS:NE2	1:D:219[B]:HIS:CD2	2.70	0.60
1:C:107:LYS:O	1:C:111:ASN:HB3	2.01	0.60
1:A:219[A]:HIS:CE1	1:B:219[A]:HIS:HE1	2.19	0.60
1:C:103:THR:O	1:C:104:VAL:HG23	2.03	0.59
1:A:219[A]:HIS:CD2	1:D:219[A]:HIS:CD2	2.90	0.59
1:A:219[A]:HIS:CE1	1:B:219[A]:HIS:CE1	2.90	0.59
1:C:59:ILE:HG22	1:C:94:ARG:HG3	1.84	0.58
1:C:106:TRP:NE1	1:C:115:LEU:HD23	2.20	0.56
1:B:120:ASP:HA	5:B:403:EDO:H11	1.87	0.56
1:C:98:GLU:HG2	1:C:99:LYS:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219[A]:HIS:ND1	1:D:219[A]:HIS:NE2	2.52	0.55
1:A:148[B]:ASP:OD1	1:A:151:THR:OG1	2.23	0.55
1:C:106:TRP:HE1	1:C:115:LEU:HD23	1.74	0.52
1:C:219[B]:HIS:HD2	1:D:219[B]:HIS:HE1	1.51	0.52
1:C:106:TRP:NE1	1:C:115:LEU:CD2	2.72	0.52
1:D:323:THR:HA	5:D:403:EDO:C1	2.38	0.52
1:B:285:GLN:HA	1:B:338:LEU:HD21	1.92	0.51
1:D:98:GLU:OE2	1:D:148[B]:ASP:OD1	2.28	0.51
1:C:149:MET:SD	1:C:173:VAL:CG1	2.99	0.51
1:D:202:ILE:HD11	1:D:233:VAL:HG13	1.93	0.50
1:A:219[A]:HIS:HD2	6:A:527:HOH:O	1.91	0.49
1:C:145:GLU:OE1	3:C:402:PEP:H31	2.13	0.49
1:A:25:LEU:HD23	1:A:129:ARG:CZ	2.45	0.47
1:B:219[B]:HIS:HD2	1:B:220:SER:O	1.98	0.46
3:C:402:PEP:H31	6:C:501:HOH:O	2.14	0.46
1:C:98:GLU:HG3	1:C:108:GLY:HA3	1.97	0.45
1:C:191:THR:HG21	1:D:170:GLU:OE2	2.17	0.45
1:B:267:ASP:HA	1:B:302:MET:HB3	1.98	0.44
1:C:219[B]:HIS:NE2	1:D:219[B]:HIS:CG	2.85	0.44
3:C:402:PEP:O2P	3:C:402:PEP:H32	2.18	0.44
1:D:151:THR:N	1:D:152:PRO:CD	2.81	0.44
1:A:151:THR:N	1:A:152:PRO:CD	2.81	0.43
1:C:31:SER:HB3	5:C:404:EDO:O1	2.18	0.43
1:B:335:LEU:C	1:B:335:LEU:HD23	2.38	0.43
1:C:103:THR:C	1:C:104:VAL:CG2	2.85	0.43
1:C:100:PRO:HB3	1:C:147:LEU:HD21	1.99	0.43
1:B:77:ARG:HB3	1:B:329:TRP:CZ2	2.54	0.42
1:D:148[B]:ASP:HB3	6:D:536:HOH:O	2.19	0.42
1:B:25:LEU:HD23	1:B:129:ARG:CZ	2.50	0.42
1:B:151:THR:N	1:B:152:PRO:CD	2.83	0.41
1:D:135:LEU:O	1:D:138:MET:HG2	2.20	0.41
1:B:219[A]:HIS:NE2	1:D:219[A]:HIS:NE2	2.68	0.41
1:C:126:ARG:HD2	6:C:580:HOH:O	2.20	0.41
1:D:276:ASP:HA	6:D:514:HOH:O	2.20	0.41
1:C:73:GLU:O	1:C:76:GLU:HG2	2.20	0.41
1:C:98:GLU:HG2	1:C:99:LYS:H	1.85	0.41
1:A:103:THR:OG1	1:A:104:VAL:N	2.53	0.41
1:A:135:LEU:O	1:A:138:MET:HG2	2.21	0.41
1:C:111:ASN:O	1:C:119:PHE:HA	2.21	0.41
1:D:324:ASP:OD1	5:D:403:EDO:H22	2.20	0.41
1:A:268:CYS:HA	1:A:283:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219[A]:HIS:NE2	1:C:219[A]:HIS:CD2	2.89	0.40
1:D:69:LYS:HD2	6:D:639:HOH:O	2.22	0.40
1:D:244:ASP:O	1:D:248:VAL:HG23	2.22	0.40

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	335/351 (95%)	327 (98%)	7 (2%)	1 (0%)	41	30
1	B	335/351 (95%)	326 (97%)	8 (2%)	1 (0%)	41	30
1	C	330/351 (94%)	320 (97%)	9 (3%)	1 (0%)	41	30
1	D	334/351 (95%)	324 (97%)	10 (3%)	0	100	100
All	All	1334/1404 (95%)	1297 (97%)	34 (2%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	ASP
1	A	294	ASP
1	B	294	ASP

### 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	267/289 (92%)	263 (98%)	4 (2%)	65	59
1	B	263/289 (91%)	259 (98%)	4 (2%)	65	59
1	C	262/289 (91%)	257 (98%)	5 (2%)	57	49
1	D	260/289 (90%)	256 (98%)	4 (2%)	65	59
All	All	1052/1156 (91%)	1035 (98%)	17 (2%)	62	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	189	ASN
1	A	236	ARG
1	A	306	HIS
1	B	43	GLN
1	B	189	ASN
1	B	236	ARG
1	B	306	HIS
1	C	147	LEU
1	C	189	ASN
1	C	236	ARG
1	C	240	GLU
1	C	306	HIS
1	D	43	GLN
1	D	69	LYS
1	D	189	ASN
1	D	236	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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
3	PEP	A	402	-	9,9,9	3.15	2 (22%)	11,13,13	1.60	3 (27%)
5	EDO	D	403	-	3,3,3	0.41	0	2,2,2	0.28	0
5	EDO	C	403	-	3,3,3	0.37	0	2,2,2	0.47	0
5	EDO	C	404	-	3,3,3	0.24	0	2,2,2	0.44	0
3	PEP	D	402	-	9,9,9	2.41	2 (22%)	11,13,13	2.02	5 (45%)
4	SO4	A	403	-	4,4,4	0.53	0	6,6,6	0.41	0
3	PEP	C	402	-	9,9,9	5.96	2 (22%)	11,13,13	3.14	6 (54%)
5	EDO	B	403	-	3,3,3	0.28	0	2,2,2	0.76	0
5	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.38	0
4	SO4	D	404	-	4,4,4	0.45	0	6,6,6	0.20	0
3	PEP	B	402	-	9,9,9	2.49	2 (22%)	11,13,13	3.00	4 (36%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEP	A	402	-	-	4/9/9/9	-
5	EDO	D	403	-	-	1/1/1/1	-
5	EDO	C	403	-	-	1/1/1/1	-
5	EDO	C	404	-	-	1/1/1/1	-
3	PEP	D	402	-	-	4/9/9/9	-
3	PEP	C	402	-	-	4/9/9/9	-
5	EDO	B	403	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	404	-	-	1/1/1/1	-
3	PEP	B	402	-	-	4/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PEP	C2-C1	-17.20	1.32	1.49
3	A	402	PEP	C2-C1	-7.58	1.42	1.49
3	D	402	PEP	C2-C1	-6.20	1.43	1.49
3	B	402	PEP	C2-C1	-6.13	1.43	1.49
3	A	402	PEP	P-O2	4.72	1.66	1.59
3	C	402	PEP	P-O2	4.09	1.65	1.59
3	B	402	PEP	P-O2	3.36	1.64	1.59
3	D	402	PEP	O2'-C1	-2.13	1.24	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PEP	O1-C1-C2	-7.03	111.19	121.79
3	B	402	PEP	O1-C1-C2	-6.81	111.53	121.79
3	B	402	PEP	O2'-C1-C2	5.36	123.06	113.91
3	C	402	PEP	C3-C2-C1	-4.36	114.66	122.73
3	D	402	PEP	O1-C1-C2	-4.32	115.27	121.79
3	C	402	PEP	O2'-C1-O1	3.41	131.41	123.61
3	B	402	PEP	O2P-P-O2	-3.17	95.60	105.25
3	A	402	PEP	O1-C1-C2	-2.99	117.27	121.79
3	A	402	PEP	O2P-P-O2	-2.94	96.29	105.25
3	D	402	PEP	O2-P-O1P	-2.83	99.27	109.32
3	B	402	PEP	O3P-P-O2P	2.77	118.24	107.64
3	C	402	PEP	O2-C2-C3	2.58	129.75	124.79
3	A	402	PEP	O2P-P-O1P	2.49	120.43	110.68
3	C	402	PEP	O2P-P-O1P	2.40	120.07	110.68
3	D	402	PEP	O3P-P-O2P	2.25	116.24	107.64
3	D	402	PEP	O2'-C1-C2	2.13	117.54	113.91
3	D	402	PEP	O2P-P-O1P	2.12	118.99	110.68
3	C	402	PEP	O2'-C1-C2	2.02	117.35	113.91

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PEP	O1-C1-C2-C3
3	A	402	PEP	O1-C1-C2-O2
3	A	402	PEP	O2'-C1-C2-C3
3	A	402	PEP	O2'-C1-C2-O2
3	B	402	PEP	O1-C1-C2-C3
3	B	402	PEP	O1-C1-C2-O2
3	B	402	PEP	O2'-C1-C2-C3
3	B	402	PEP	O2'-C1-C2-O2
3	C	402	PEP	O1-C1-C2-C3
3	C	402	PEP	O2'-C1-C2-C3
3	D	402	PEP	O1-C1-C2-C3
3	D	402	PEP	O1-C1-C2-O2
3	D	402	PEP	O2'-C1-C2-C3
3	D	402	PEP	O2'-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
5	C	403	EDO	O1-C1-C2-O2
5	C	404	EDO	O1-C1-C2-O2
3	C	402	PEP	O1-C1-C2-O2
3	C	402	PEP	O2'-C1-C2-O2
5	B	403	EDO	O1-C1-C2-O2
5	D	403	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	403	EDO	5	0
5	C	404	EDO	2	0
3	C	402	PEP	4	0
5	B	403	EDO	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	A	334/351 (95%)	-0.28	2 (0%) 89 90	22, 34, 50, 74	0
1	B	335/351 (95%)	-0.24	1 (0%) 94 94	22, 37, 54, 67	0
1	C	333/351 (94%)	-0.11	9 (2%) 54 56	23, 36, 59, 86	0
1	D	334/351 (95%)	-0.19	3 (0%) 84 85	27, 40, 56, 78	0
All	All	1336/1404 (95%)	-0.21	15 (1%) 80 82	22, 37, 56, 86	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	VAL	4.9
1	C	115	LEU	3.6
1	C	147	LEU	3.1
1	D	105	GLY	2.7
1	C	293	GLN	2.7
1	C	257	ALA	2.7
1	B	15	VAL	2.7
1	C	119	PHE	2.5
1	C	103	THR	2.5
1	D	115	LEU	2.5
1	C	16	LYS	2.2
1	D	226	GLY	2.2
1	A	292	GLU	2.1
1	A	291	LEU	2.1
1	C	101	ARG	2.1

### 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 monosaccharides 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	EDO	B	404	4/4	0.82	0.14	56,57,59,60	0
5	EDO	D	403	4/4	0.85	0.44	50,54,54,56	0
3	PEP	C	402	10/10	0.87	0.15	27,35,52,57	0
5	EDO	B	403	4/4	0.90	0.27	41,44,48,49	0
5	EDO	C	403	4/4	0.91	0.14	58,61,63,67	0
4	SO4	D	404	5/5	0.91	0.28	73,76,85,86	0
4	SO4	A	403	5/5	0.93	0.17	63,73,73,80	0
3	PEP	B	402	10/10	0.93	0.09	32,37,41,42	0
5	EDO	C	404	4/4	0.94	0.46	40,42,42,44	0
3	PEP	A	402	10/10	0.94	0.11	24,34,36,37	0
3	PEP	D	402	10/10	0.96	0.09	38,42,45,48	0
2	MN	D	401	1/1	0.97	0.04	39,39,39,39	0
2	MN	B	401	1/1	0.99	0.04	37,37,37,37	0
2	MN	C	401	1/1	0.99	0.08	36,36,36,36	0
2	MN	A	401	1/1	1.00	0.08	26,26,26,26	0

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

There are no such residues in this entry.