



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2025 – 01:32 pm BST

PDB ID : 9FL1 / pdb\_00009fl1  
Title : Apo Glyceraldehyde 3-phosphate Dehydrogenase (GapA) from *Helicobacter pylori*  
Authors : Elliott, P.R.; Moody, P.C.E.  
Deposited on : 2024-06-04  
Resolution : 1.74 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

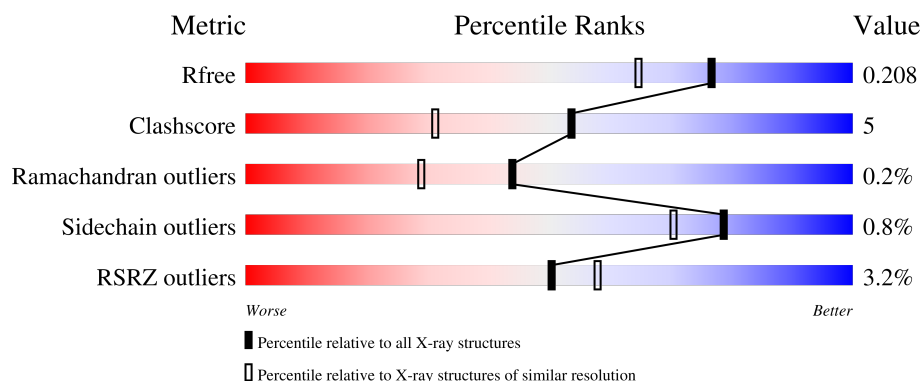
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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))
$R_{free}$	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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	330	<div> <div>5%</div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	B	330	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>..</div> </div>
1	C	330	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	D	330	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

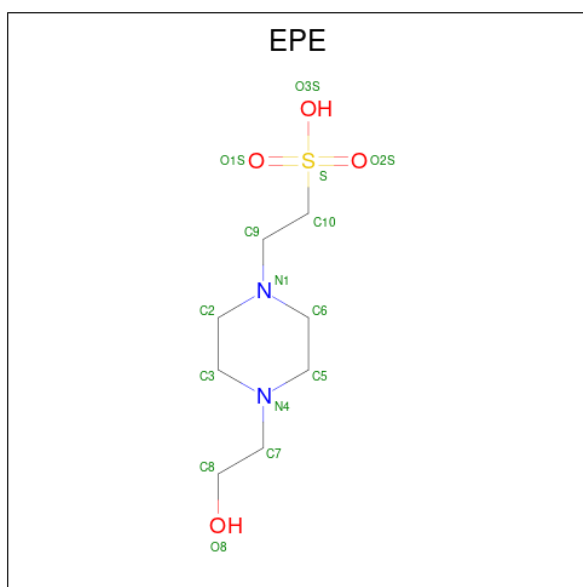
There are 5 unique types of molecules in this entry. The entry contains 11093 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase (Gap).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	7	0
			2469	1552	438	471	8			
1	B	318	Total	C	N	O	S	0	15	0
			2552	1599	458	485	10			
1	C	317	Total	C	N	O	S	0	6	0
			2476	1559	438	471	8			
1	D	318	Total	C	N	O	S	0	10	0
			2515	1577	450	479	9			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: 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
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	4	Total	Na	0	0
			4	4		
4	C	4	Total	Na	0	0
			4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		

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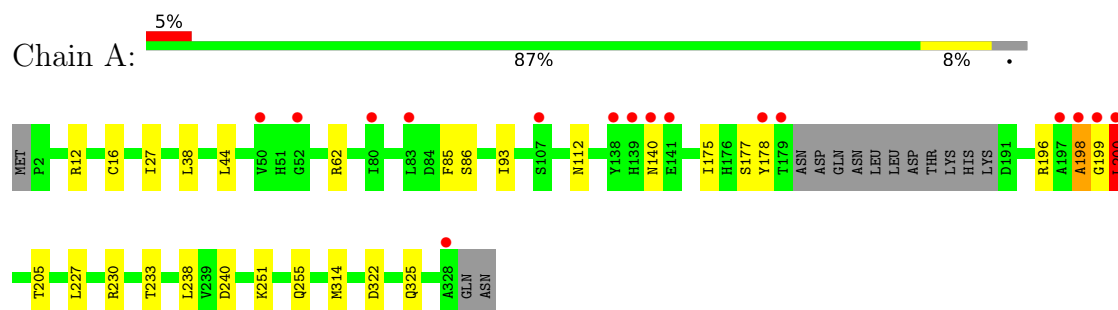
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	301	Total 301	O 301	0	0
5	C	223	Total 223	O 223	0	0
5	D	289	Total 289	O 289	0	0

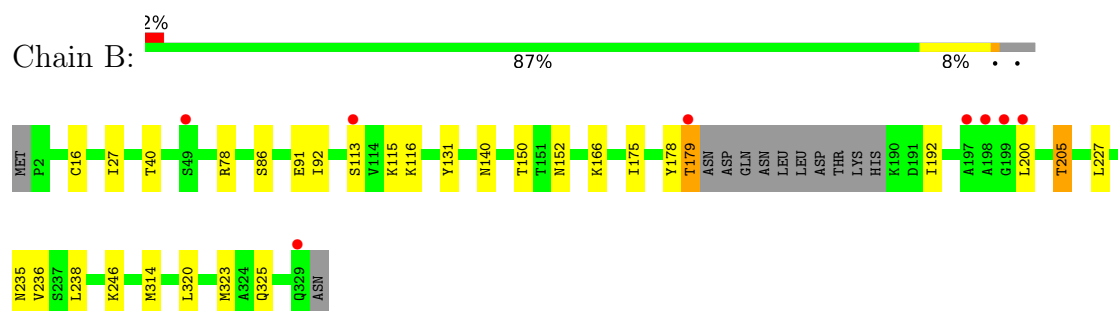
### 3 Residue-property plots [i](#)

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.

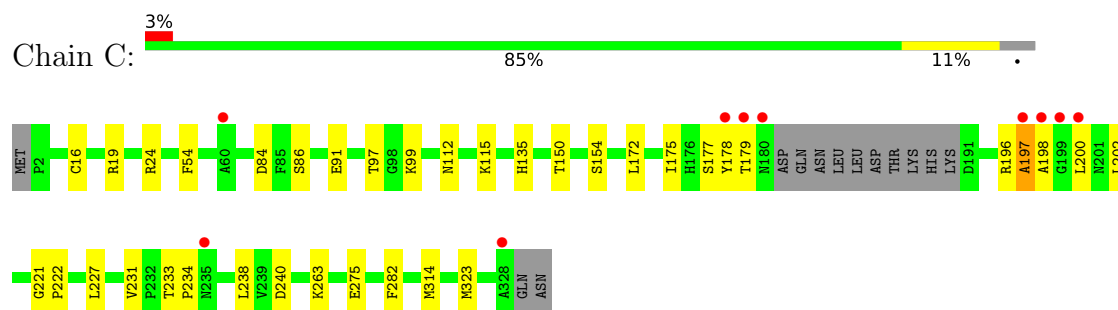
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase (Gap)



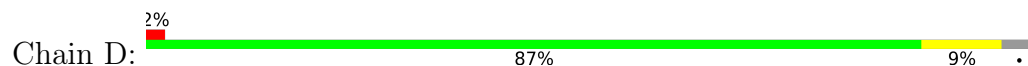
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase (Gap)

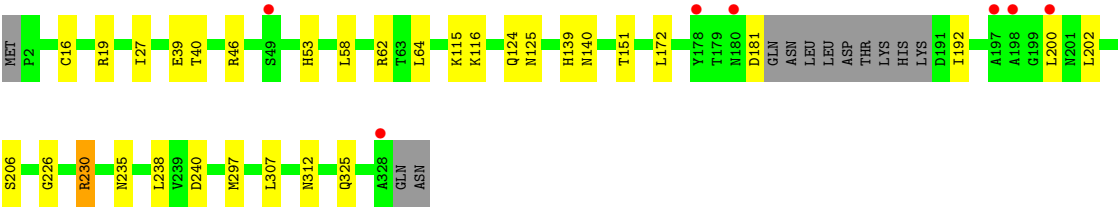


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase (Gap)



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase (Gap)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.16Å 100.62Å 97.79Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	95.35 – 1.74 95.35 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (95.35-1.74) 99.1 (95.35-1.74)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.150 , 0.200 0.164 , 0.208	Depositor DCC
$R_{free}$ test set	7445 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, EPE

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	0.62	0/2511	1.03	3/3402 (0.1%)
1	B	0.63	0/2590	1.01	4/3505 (0.1%)
1	C	0.61	0/2514	0.99	2/3406 (0.1%)
1	D	0.62	0/2553	1.01	4/3457 (0.1%)
All	All	0.62	0/10168	1.01	13/13770 (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	D	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASN	CA-CB-CG	-6.50	106.10	112.60
1	C	240	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	200	LEU	N-CA-CB	5.85	120.38	110.49
1	B	320	LEU	N-CA-CB	-5.83	101.55	110.12
1	B	236	VAL	N-CA-CB	5.47	117.61	111.21
1	D	39	GLU	CB-CG-CD	5.32	121.65	112.60
1	D	151	THR	CA-CB-OG1	-5.22	101.77	109.60
1	D	312	ASN	CB-CA-C	5.20	120.35	110.27
1	B	205	THR	OG1-CB-CG2	-5.16	98.99	109.30
1	D	240	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	282	PHE	CA-CB-CG	-5.12	108.69	113.80
1	A	322	ASP	CA-CB-CG	5.09	117.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	230	ARG	Sidechain

## 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	2469	0	2513	35	0
1	B	2552	0	2594	25	0
1	C	2476	0	2522	33	0
1	D	2515	0	2556	18	0
2	A	15	0	18	0	0
2	B	15	0	18	0	0
2	C	15	0	18	1	0
2	D	15	0	18	1	0
3	A	6	0	8	3	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	193	0	0	2	0
5	B	301	0	0	9	0
5	C	223	0	0	4	0
5	D	289	0	0	7	0
All	All	11093	0	10265	98	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 5.

All (98) 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:16[B]:CYS:SG	1:B:314[B]:MET:SD	2.57	1.03
1:D:16[B]:CYS:SG	5:D:602:HOH:O	2.40	0.79
1:C:231:VAL:HG23	1:C:233:THR:HG22	1.68	0.76
1:B:152:ASN:HB3	5:B:716:HOH:O	1.89	0.72
1:A:199:GLY:O	1:A:200:LEU:CD2	2.37	0.72
1:A:199:GLY:O	1:A:200:LEU:HD22	1.92	0.69
1:A:12:ARG:NH1	3:A:402:GOL:H11	2.07	0.69
1:C:16[B]:CYS:SG	1:C:314:MET:SD	2.92	0.67
1:B:150:THR:HG23	5:B:621:HOH:O	1.95	0.66
1:B:323[A]:MET:HA	1:B:323[A]:MET:HE2	1.78	0.64
1:B:205:THR:HG22	5:B:518:HOH:O	1.98	0.63
1:A:199:GLY:C	1:A:200:LEU:HD22	2.23	0.63
1:A:200:LEU:CD2	1:C:179:THR:CG2	2.79	0.61
1:A:200:LEU:HD21	1:C:179:THR:CG2	2.32	0.59
1:C:115:LYS:HE2	5:C:642:HOH:O	2.03	0.58
1:A:16[B]:CYS:SG	1:A:314:MET:SD	3.03	0.57
1:C:175:ILE:HD13	1:C:238:LEU:HD22	1.86	0.57
1:B:140[B]:ASN:O	1:B:140[B]:ASN:ND2	2.38	0.57
1:A:200:LEU:CD2	1:C:179:THR:HG21	2.35	0.57
1:B:86[B]:SER:OG	1:B:113[B]:SER:HB3	2.05	0.57
1:D:27:ILE:HD11	1:D:325:GLN:HG2	1.88	0.55
1:D:230:ARG:NH1	5:D:503:HOH:O	2.41	0.54
2:D:401:EPE:H71	5:D:540:HOH:O	2.08	0.54
1:A:12:ARG:HH11	3:A:402:GOL:H11	1.71	0.54
1:A:27:ILE:HD11	1:A:325:GLN:HG2	1.90	0.54
1:B:27:ILE:HD11	1:B:325:GLN:HG2	1.90	0.54
1:A:178:TYR:CE1	1:A:198:ALA:HB1	2.42	0.54
1:A:178:TYR:OH	1:A:198:ALA:C	2.51	0.54
1:B:131:TYR:HD1	1:B:323[A]:MET:CE	2.21	0.53
1:A:251:LYS:NZ	1:A:255:GLN:HE22	2.06	0.53
1:C:233:THR:HG21	1:D:202:LEU:HD21	1.91	0.53
1:B:178:TYR:O	1:B:179:THR:CB	2.57	0.53
1:A:175:ILE:HD11	1:B:175[B]:ILE:HD11	1.91	0.52
1:A:200:LEU:CD2	1:C:179:THR:HG22	2.38	0.52
1:A:85:PHE:CD2	1:A:93:ILE:HD12	2.46	0.51
1:A:200:LEU:HD21	1:C:179:THR:HG21	1.92	0.51
1:C:177:SER:OG	1:C:233:THR:HG23	2.11	0.50
1:B:78:ARG:NH1	5:B:506:HOH:O	2.43	0.50
1:A:177[A]:SER:HB3	1:A:233:THR:O	2.13	0.49
1:B:166:LYS:HE2	5:B:556:HOH:O	2.13	0.49
1:D:58:LEU:HD23	1:D:64:LEU:HD23	1.94	0.49
1:D:140:ASN:HB2	5:D:714:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:THR:HG21	5:C:698:HOH:O	2.13	0.48
1:B:178:TYR:O	1:B:179:THR:HB	2.13	0.48
1:C:19:ARG:HD3	1:C:54[B]:PHE:CD2	2.48	0.48
1:D:62[B]:ARG:NE	5:D:501:HOH:O	2.29	0.48
1:A:199:GLY:O	1:A:200:LEU:HD23	2.12	0.47
1:D:62[A]:ARG:NH2	5:D:507:HOH:O	2.47	0.47
1:D:124:GLN:HG2	1:D:125:ASN:ND2	2.29	0.47
1:A:200:LEU:HD22	1:C:179:THR:CG2	2.44	0.47
1:A:205:THR:HG21	1:A:230:ARG:HD2	1.97	0.47
1:C:19:ARG:HD3	1:C:54[B]:PHE:CG	2.50	0.47
1:B:40:THR:HG23	1:D:192:ILE:CD1	2.45	0.46
1:B:131:TYR:HD1	1:B:323[A]:MET:HE1	1.81	0.45
1:C:86:SER:OG	1:C:112:ASN:HB2	2.15	0.45
1:B:227:LEU:C	1:B:227:LEU:HD12	2.41	0.45
1:B:246:LYS:HD2	5:B:639:HOH:O	2.17	0.45
1:C:233:THR:OG1	1:C:234:PRO:HD2	2.16	0.45
1:C:275:GLU:HG2	5:C:695:HOH:O	2.15	0.45
1:C:97:THR:HB	1:C:99:LYS:HE2	1.99	0.45
1:C:227[B]:LEU:HD21	1:D:307:LEU:HD11	1.99	0.44
1:B:91:GLU:OE2	1:B:115:LYS:NZ	2.44	0.44
1:B:192:ILE:CD1	1:D:40:THR:HG23	2.48	0.44
1:A:178:TYR:OH	1:A:198:ALA:O	2.36	0.43
1:D:172:LEU:O	1:D:226:GLY:HA3	2.19	0.43
1:C:24:ARG:HA	2:C:401:EPE:H71	2.00	0.43
1:C:227[A]:LEU:HD23	1:D:297:MET:HE3	2.00	0.43
1:A:198:ALA:O	1:A:199:GLY:C	2.61	0.43
1:A:200:LEU:HD22	1:C:179:THR:HG21	2.01	0.43
1:B:115:LYS:HE3	5:B:514:HOH:O	2.18	0.43
1:A:238:LEU:C	1:A:238:LEU:HD23	2.43	0.42
1:C:221:GLY:N	1:C:222:PRO:CD	2.82	0.42
1:C:196:ARG:O	1:C:198:ALA:N	2.53	0.42
1:A:86:SER:HB3	1:A:112:ASN:HB2	2.01	0.42
1:A:38:LEU:HD23	1:A:62:ARG:NH2	2.34	0.42
1:A:175:ILE:CD1	1:B:175[B]:ILE:HD11	2.48	0.42
1:C:202:LEU:HD22	1:C:231:VAL:HG12	2.01	0.42
1:C:135:HIS:CB	1:C:323:MET:HE1	2.50	0.42
1:A:44:LEU:HD22	3:A:402:GOL:H12	2.02	0.41
1:A:196:ARG:HG3	5:B:631:HOH:O	2.19	0.41
1:B:92:ILE:HD12	1:B:116:LYS:HB2	2.01	0.41
1:A:255:GLN:CD	5:A:565:HOH:O	2.64	0.41
1:C:135:HIS:HB3	1:C:323:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:N	5:A:517:HOH:O	2.52	0.41
1:B:238:LEU:C	1:B:238:LEU:HD23	2.45	0.41
1:D:46:ARG:O	1:D:53[B]:HIS:HA	2.21	0.41
1:A:227:LEU:C	1:A:227:LEU:HD12	2.46	0.41
1:D:238:LEU:HD23	1:D:238:LEU:C	2.46	0.41
1:C:196:ARG:O	1:C:197:ALA:C	2.64	0.41
1:A:251:LYS:HZ3	1:A:255:GLN:NE2	2.19	0.41
1:C:263:LYS:NZ	5:C:508:HOH:O	2.54	0.41
1:D:19[B]:ARG:HD3	5:D:705:HOH:O	2.21	0.40
1:C:84:ASP:OD1	1:C:86:SER:HB2	2.20	0.40
1:D:115:LYS:O	1:D:116[A]:LYS:HD3	2.21	0.40
1:A:251:LYS:NZ	1:A:255:GLN:NE2	2.70	0.40
1:B:115:LYS:HE2	5:B:753:HOH:O	2.22	0.40
1:C:154:SER:HB2	1:C:172:LEU:CD2	2.51	0.40
1:C:178:TYR:CZ	1:C:198:ALA:HB1	2.56	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	319/330 (97%)	306 (96%)	11 (3%)	2 (1%)	22	8
1	B	329/330 (100%)	316 (96%)	13 (4%)	0	100	100
1	C	319/330 (97%)	308 (97%)	10 (3%)	1 (0%)	37	23
1	D	324/330 (98%)	312 (96%)	12 (4%)	0	100	100
All	All	1291/1320 (98%)	1242 (96%)	46 (4%)	3 (0%)	44	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA
1	A	200	LEU
1	C	197	ALA

### 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	276/283 (98%)	276 (100%)	0	100	100
1	B	286/283 (101%)	284 (99%)	2 (1%)	81	74
1	C	276/283 (98%)	273 (99%)	3 (1%)	70	55
1	D	281/283 (99%)	276 (98%)	5 (2%)	54	32
All	All	1119/1132 (99%)	1109 (99%)	10 (1%)	79	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	THR
1	B	200	LEU
1	C	91[A]	GLU
1	C	91[B]	GLU
1	C	200	LEU
1	D	139	HIS
1	D	181	ASP
1	D	200	LEU
1	D	206	SER
1	D	235	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	295	GLN
1	B	43	HIS
1	B	244	ASN

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Mol	Chain	Res	Type
1	B	256	HIS
1	C	244	ASN
1	C	295	GLN
1	D	57	GLN
1	D	81	ASN
1	D	125	ASN
1	D	235	ASN
1	D	256	HIS

### 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 [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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$
2	EPE	D	401	-	15,15,15	0.56	0	18,20,20	1.74	1 (5%)
2	EPE	B	401	-	15,15,15	0.75	1 (6%)	18,20,20	1.13	1 (5%)
2	EPE	A	401	-	15,15,15	0.60	1 (6%)	18,20,20	0.65	0
2	EPE	C	401	-	15,15,15	0.62	1 (6%)	18,20,20	0.71	0
3	GOL	A	402	-	5,5,5	0.24	0	5,5,5	0.49	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
2	EPE	D	401	-	-	3/9/19/19	0/1/1/1
2	EPE	B	401	-	-	3/9/19/19	0/1/1/1
2	EPE	A	401	-	-	3/9/19/19	0/1/1/1
2	EPE	C	401	-	-	3/9/19/19	0/1/1/1
3	GOL	A	402	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	EPE	O3S-S	2.54	1.56	1.47
2	C	401	EPE	O3S-S	2.17	1.55	1.47
2	A	401	EPE	O3S-S	2.14	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	EPE	O3S-S-C10	-6.48	95.29	105.77
2	B	401	EPE	O2S-S-C10	-3.24	103.01	106.92

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EPE	C9-C10-S-O1S
2	A	401	EPE	C9-C10-S-O2S
2	A	401	EPE	C9-C10-S-O3S
2	C	401	EPE	N4-C7-C8-O8
2	D	401	EPE	C10-C9-N1-C2
2	D	401	EPE	N4-C7-C8-O8
2	B	401	EPE	C8-C7-N4-C5
2	B	401	EPE	C8-C7-N4-C3
2	C	401	EPE	C8-C7-N4-C3
2	B	401	EPE	C9-C10-S-O1S
2	D	401	EPE	C9-C10-S-O1S
2	C	401	EPE	C8-C7-N4-C5

There are no ring outliers.



3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	EPE	1	0
2	C	401	EPE	1	0
3	A	402	GOL	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	316/330 (95%)	0.17	16 (5%) 34 41	13, 32, 58, 75	7 (2%)
1	B	318/330 (96%)	-0.32	8 (2%) 58 65	9, 22, 40, 64	15 (4%)
1	C	317/330 (96%)	-0.09	10 (3%) 50 58	11, 28, 49, 69	6 (1%)
1	D	318/330 (96%)	-0.30	7 (2%) 62 68	10, 24, 39, 72	10 (3%)
All	All	1269/1320 (96%)	-0.14	41 (3%) 50 58	9, 26, 51, 75	38 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	4.2
1	B	197	ALA	4.0
1	C	198	ALA	3.8
1	C	197	ALA	3.7
1	A	179	THR	3.6
1	B	49	SER	3.5
1	D	198	ALA	3.4
1	C	200	LEU	3.3
1	A	328	ALA	3.2
1	D	197	ALA	3.2
1	B	200	LEU	3.1
1	A	50	VAL	3.1
1	C	180	ASN	3.0
1	D	180	ASN	3.0
1	A	139	HIS	3.0
1	A	197	ALA	3.0
1	D	178	TYR	3.0
1	D	200	LEU	2.9
1	B	329	GLN	2.9
1	B	179	THR	2.9
1	C	179	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	49	SER	2.8
1	A	178	TYR	2.7
1	A	138	TYR	2.5
1	B	113[A]	SER	2.4
1	B	198	ALA	2.4
1	C	178	TYR	2.3
1	A	199	GLY	2.3
1	C	328	ALA	2.3
1	A	141	GLU	2.2
1	C	235	ASN	2.2
1	A	80	ILE	2.2
1	A	107	SER	2.2
1	A	52	GLY	2.2
1	C	199	GLY	2.2
1	A	198	ALA	2.2
1	A	140	ASN	2.2
1	C	60	ALA	2.1
1	D	328	ALA	2.1
1	B	199	GLY	2.1
1	A	83	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 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
2	EPE	C	401	15/15	0.75	0.20	60,76,96,98	0
3	GOL	A	402	6/6	0.86	0.14	34,43,48,56	0
2	EPE	A	401	15/15	0.87	0.13	55,64,70,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EPE	B	401	15/15	0.90	0.15	39,51,62,65	0
2	EPE	D	401	15/15	0.94	0.10	40,44,52,55	0
4	NA	C	405	1/1	0.96	0.12	50,50,50,50	0
4	NA	B	405	1/1	0.97	0.10	46,46,46,46	0
4	NA	C	403	1/1	0.97	0.14	51,51,51,51	0
4	NA	C	404	1/1	0.97	0.08	36,36,36,36	0
4	NA	B	404	1/1	0.97	0.17	47,47,47,47	0
4	NA	B	403	1/1	0.98	0.06	41,41,41,41	0
4	NA	A	403	1/1	0.98	0.11	52,52,52,52	0
4	NA	C	402	1/1	0.99	0.14	30,30,30,30	0
4	NA	B	402	1/1	1.00	0.11	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.