



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 11:24 PM EDT

PDB ID : 1Z7A  
Title : Crystal structure of probable Polysaccharide deacetylase from *Pseudomonas aeruginosa* PAO1  
Authors : Chang, C.; Skarina, T.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2005-03-24  
Resolution : 1.71 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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)	:	2.39

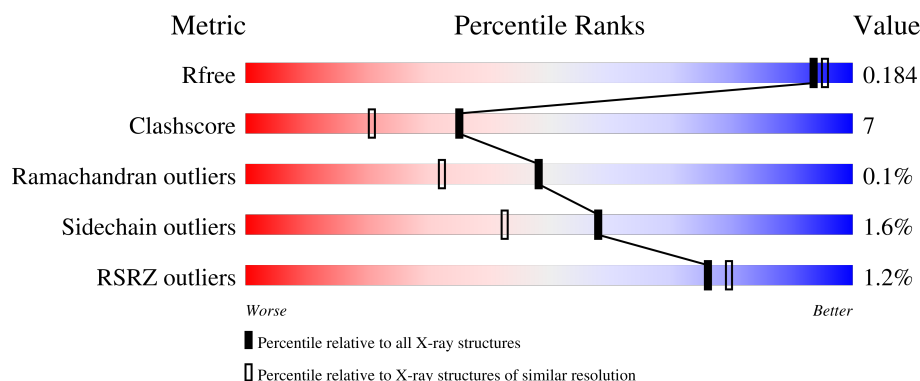
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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.





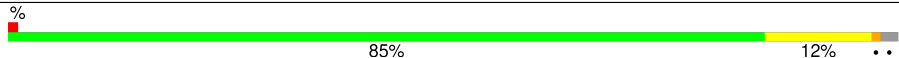
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 85%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>12%</span> <span>..</span> </div> </div>
1	B	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 8%, green 89%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>89%</span> <span>8%</span> <span>.</span> </div> </div>
1	C	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 90%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>7%</span> <span>.</span> </div> </div>
1	D	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 87%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>10%</span> <span>.</span> </div> </div>
1	E	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 6%, green 90%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>6%</span> <span>..</span> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	308	
1	G	308	
1	H	308	

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
3	GOL	A	311	-	-	X	-
4	IPA	B	313	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22756 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 conserved hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	Se	8	15	0
			2560	1623	458	465	3	11			
1	B	301	Total	C	N	O	S	Se	8	15	0
			2559	1624	461	460	3	11			
1	C	300	Total	C	N	O	S	Se	8	18	0
			2571	1631	463	463	3	11			
1	D	300	Total	C	N	O	S	Se	0	16	0
			2555	1625	456	460	3	11			
1	E	301	Total	C	N	O	S	Se	0	10	0
			2514	1595	447	458	3	11			
1	F	301	Total	C	N	O	S	Se	0	16	0
			2554	1625	456	459	3	11			
1	G	301	Total	C	N	O	S	Se	0	18	0
			2562	1632	456	460	3	11			
1	H	301	Total	C	N	O	S	Se	0	19	0
			2590	1644	467	465	3	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	GB 9947474
A	57	MSE	MET	modified residue	GB 9947474
A	69	MSE	MET	modified residue	GB 9947474
A	71	MSE	MET	modified residue	GB 9947474
A	104	MSE	MET	modified residue	GB 9947474
A	116	MSE	MET	modified residue	GB 9947474
A	136	MSE	MET	modified residue	GB 9947474
A	145	MSE	MET	modified residue	GB 9947474
A	177	MSE	MET	modified residue	GB 9947474
A	218	MSE	MET	modified residue	GB 9947474
A	253	MSE	MET	modified residue	GB 9947474
A	269	MSE	MET	modified residue	GB 9947474
B	1	MSE	MET	modified residue	GB 9947474

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	MSE	MET	modified residue	GB 9947474
B	69	MSE	MET	modified residue	GB 9947474
B	71	MSE	MET	modified residue	GB 9947474
B	104	MSE	MET	modified residue	GB 9947474
B	116	MSE	MET	modified residue	GB 9947474
B	136	MSE	MET	modified residue	GB 9947474
B	145	MSE	MET	modified residue	GB 9947474
B	177	MSE	MET	modified residue	GB 9947474
B	218	MSE	MET	modified residue	GB 9947474
B	253	MSE	MET	modified residue	GB 9947474
B	269	MSE	MET	modified residue	GB 9947474
C	1	MSE	MET	modified residue	GB 9947474
C	57	MSE	MET	modified residue	GB 9947474
C	69	MSE	MET	modified residue	GB 9947474
C	71	MSE	MET	modified residue	GB 9947474
C	104	MSE	MET	modified residue	GB 9947474
C	116	MSE	MET	modified residue	GB 9947474
C	136	MSE	MET	modified residue	GB 9947474
C	145	MSE	MET	modified residue	GB 9947474
C	177	MSE	MET	modified residue	GB 9947474
C	218	MSE	MET	modified residue	GB 9947474
C	253	MSE	MET	modified residue	GB 9947474
C	269	MSE	MET	modified residue	GB 9947474
D	1	MSE	MET	modified residue	GB 9947474
D	57	MSE	MET	modified residue	GB 9947474
D	69	MSE	MET	modified residue	GB 9947474
D	71	MSE	MET	modified residue	GB 9947474
D	104	MSE	MET	modified residue	GB 9947474
D	116	MSE	MET	modified residue	GB 9947474
D	136	MSE	MET	modified residue	GB 9947474
D	145	MSE	MET	modified residue	GB 9947474
D	177	MSE	MET	modified residue	GB 9947474
D	218	MSE	MET	modified residue	GB 9947474
D	253	MSE	MET	modified residue	GB 9947474
D	269	MSE	MET	modified residue	GB 9947474
E	1	MSE	MET	modified residue	GB 9947474
E	57	MSE	MET	modified residue	GB 9947474
E	69	MSE	MET	modified residue	GB 9947474
E	71	MSE	MET	modified residue	GB 9947474
E	104	MSE	MET	modified residue	GB 9947474
E	116	MSE	MET	modified residue	GB 9947474
E	136	MSE	MET	modified residue	GB 9947474

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	145	MSE	MET	modified residue	GB 9947474
E	177	MSE	MET	modified residue	GB 9947474
E	218	MSE	MET	modified residue	GB 9947474
E	253	MSE	MET	modified residue	GB 9947474
E	269	MSE	MET	modified residue	GB 9947474
F	1	MSE	MET	modified residue	GB 9947474
F	57	MSE	MET	modified residue	GB 9947474
F	69	MSE	MET	modified residue	GB 9947474
F	71	MSE	MET	modified residue	GB 9947474
F	104	MSE	MET	modified residue	GB 9947474
F	116	MSE	MET	modified residue	GB 9947474
F	136	MSE	MET	modified residue	GB 9947474
F	145	MSE	MET	modified residue	GB 9947474
F	177	MSE	MET	modified residue	GB 9947474
F	218	MSE	MET	modified residue	GB 9947474
F	253	MSE	MET	modified residue	GB 9947474
F	269	MSE	MET	modified residue	GB 9947474
G	1	MSE	MET	modified residue	GB 9947474
G	57	MSE	MET	modified residue	GB 9947474
G	69	MSE	MET	modified residue	GB 9947474
G	71	MSE	MET	modified residue	GB 9947474
G	104	MSE	MET	modified residue	GB 9947474
G	116	MSE	MET	modified residue	GB 9947474
G	136	MSE	MET	modified residue	GB 9947474
G	145	MSE	MET	modified residue	GB 9947474
G	177	MSE	MET	modified residue	GB 9947474
G	218	MSE	MET	modified residue	GB 9947474
G	253	MSE	MET	modified residue	GB 9947474
G	269	MSE	MET	modified residue	GB 9947474
H	1	MSE	MET	modified residue	GB 9947474
H	57	MSE	MET	modified residue	GB 9947474
H	69	MSE	MET	modified residue	GB 9947474
H	71	MSE	MET	modified residue	GB 9947474
H	104	MSE	MET	modified residue	GB 9947474
H	116	MSE	MET	modified residue	GB 9947474
H	136	MSE	MET	modified residue	GB 9947474
H	145	MSE	MET	modified residue	GB 9947474
H	177	MSE	MET	modified residue	GB 9947474
H	218	MSE	MET	modified residue	GB 9947474
H	253	MSE	MET	modified residue	GB 9947474
H	269	MSE	MET	modified residue	GB 9947474

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



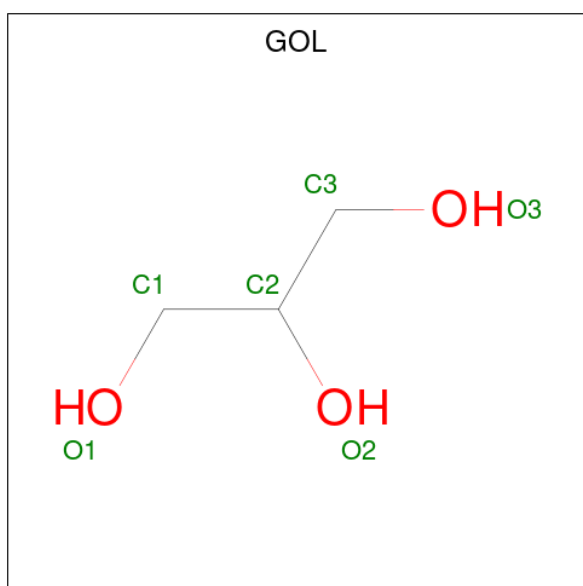
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



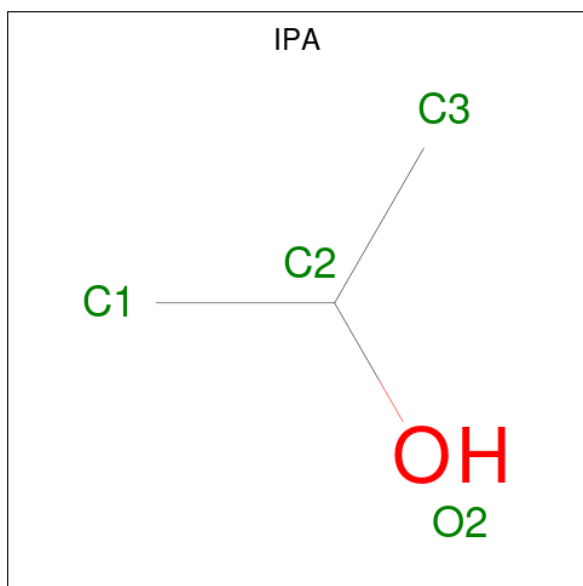
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

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

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	C	1	Total	C	O	0	0
			4	3	1		
4	D	1	Total	C	O	0	0
			4	3	1		
4	E	1	Total	C	O	0	0
			4	3	1		
4	F	1	Total	C	O	0	0
			4	3	1		
4	H	1	Total	C	O	0	0
			4	3	1		

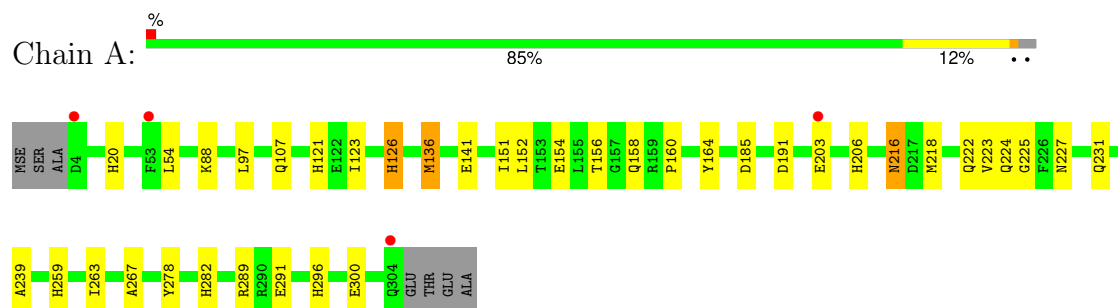
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	268	Total 268	O 268	0	0
5	B	269	Total 269	O 269	0	0
5	C	279	Total 279	O 279	0	0
5	D	265	Total 265	O 265	0	0
5	E	268	Total 268	O 268	0	0
5	F	270	Total 270	O 270	0	0
5	G	256	Total 256	O 256	0	0
5	H	266	Total 266	O 266	0	0

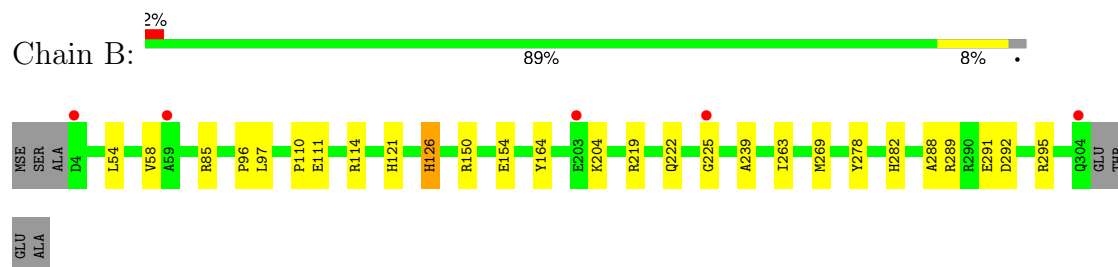
### 3 Residue-property plots [i](#)

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.

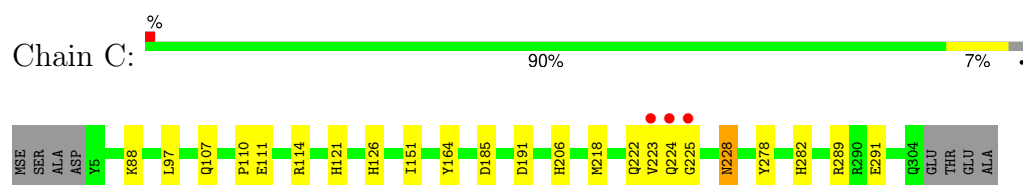
- Molecule 1: conserved hypothetical protein



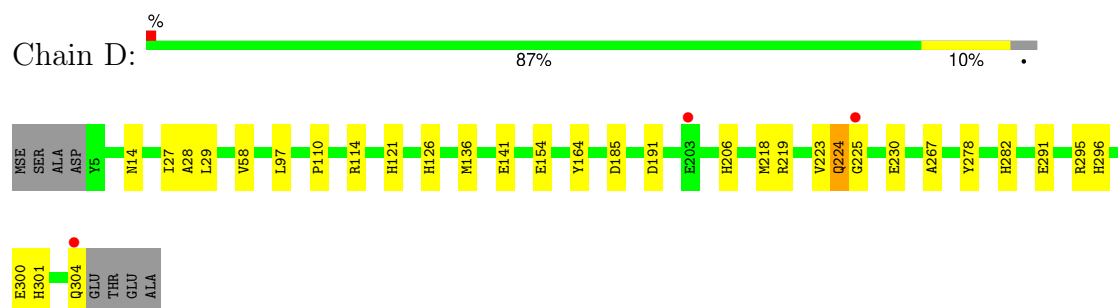
- Molecule 1: conserved hypothetical protein



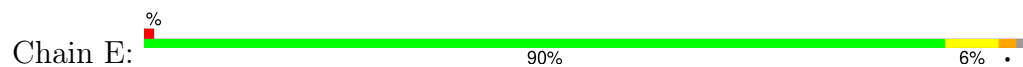
- Molecule 1: conserved hypothetical protein



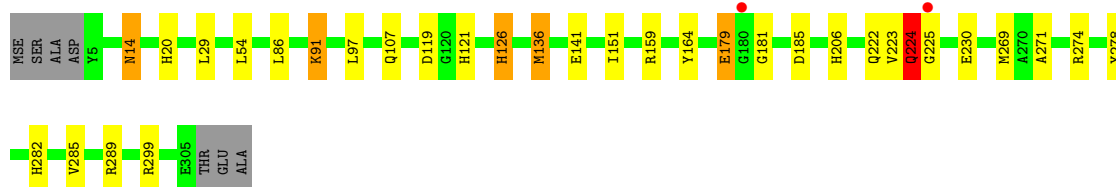
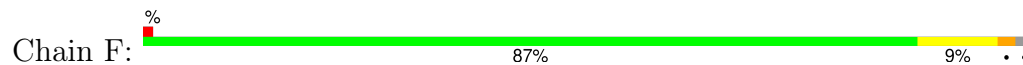
- Molecule 1: conserved hypothetical protein



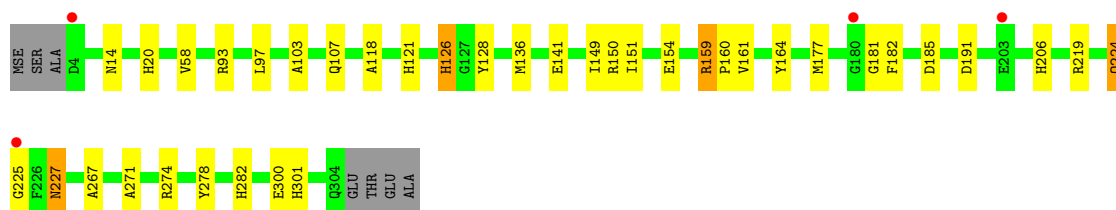
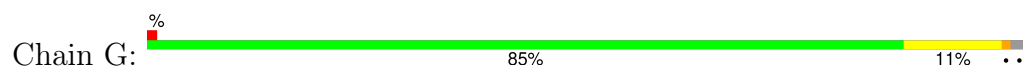
- Molecule 1: conserved hypothetical protein



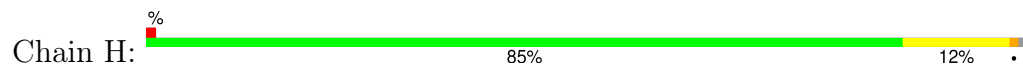
- Molecule 1: conserved hypothetical protein



- Molecule 1: conserved hypothetical protein



- Molecule 1: conserved hypothetical protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.65Å 101.77Å 100.99Å 60.71° 61.24° 89.90°	Depositor
Resolution (Å)	50.00 – 1.71 50.00 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.71) 95.9 (50.00-1.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.151 , 0.175 0.162 , 0.184	Depositor DCC
$R_{free}$ test set	15394 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage

*Continued on next page...*

<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.

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.005 for $h+k-l, l, h$ 0.005 for $l, h+k-l, k$ 0.003 for $h-l, k-l, h+k-l$ 0.003 for $-k+l, -h+l, -h-k+l$ 0.139 for $-k, h, -k+l$ 0.139 for $k, -h, -h+l$ 0.004 for $k-l, -h+l, k$ 0.004 for $-h-k+l, l, -h+l$ 0.005 for $-k+l, h-l, h$ 0.005 for $l, -h-k+l, -k+l$ 0.005 for $-l, h+k-l, h-l$ 0.005 for $-h+l, k-l, -h$ 0.004 for $h-l, -k+l, -k$ 0.004 for $h+k-l, -l, k-l$ 0.012 for $-h+l, -k+l, l$ 0.017 for $h, -k, h-l$ 0.021 for $-h, k, k-l$ 0.013 for $-l, -h-k+l, -h$ 0.012 for $-h-k+l, -l, -k$ 0.014 for $k, h, h+k-l$ 0.027 for $-k, -h, -l$ 0.012 for $k-l, h-l, -l$ 0.087 for $-h, -k, -h-k+l$	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22756	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/2656	0.59	0/3578
1	B	0.53	0/2664	0.60	0/3585
1	C	0.53	0/2679	0.61	0/3608
1	D	0.53	0/2663	0.59	0/3585
1	E	0.52	0/2595	0.59	0/3498
1	F	0.53	0/2662	0.64	2/3587 (0.1%)
1	G	0.53	0/2677	0.61	0/3608
1	H	0.52	0/2690	0.62	0/3623
All	All	0.53	0/21286	0.61	2/28672 (0.0%)

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	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	GLY	N-CA-C	-10.45	86.98	113.10
1	F	224	GLN	N-CA-C	5.70	126.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	224	GLN	Peptide

## 5.2 Too-close contacts

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	2560	0	2459	44	0
1	B	2559	0	2475	26	0
1	C	2571	0	2485	34	0
1	D	2555	0	2478	39	0
1	E	2514	0	2395	61	0
1	F	2554	0	2473	50	0
1	G	2562	0	2474	36	0
1	H	2590	0	2493	59	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
2	E	12	0	18	0	0
2	F	8	0	12	0	0
2	G	12	0	18	0	0
2	H	12	0	18	0	0
3	A	6	0	8	6	0
3	B	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	4	0	8	0	0
4	B	8	0	16	5	0
4	C	4	0	8	0	0
4	D	4	0	8	0	0
4	E	4	0	8	1	0
4	F	4	0	8	0	0
4	H	4	0	8	2	0
5	A	268	0	0	7	0
5	B	269	0	0	3	0
5	C	279	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	265	0	0	4	0
5	E	268	0	0	8	0
5	F	270	0	0	12	0
5	G	256	0	0	6	0
5	H	266	0	0	6	0
All	All	22756	0	19966	294	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.

All (294) 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:111[B]:GLU:OE2	1:B:114[B]:ARG:NH2	1.59	1.36
1:C:223[A]:VAL:HG23	1:D:223[A]:VAL:CG1	1.61	1.31
1:F:269[MSE]:HG3	5:F:493:HOH:O	1.11	1.27
1:E:223[B]:VAL:HG13	1:F:223[B]:VAL:CG2	1.66	1.23
1:A:223[A]:VAL:HG21	1:D:223[A]:VAL:HG13	1.28	1.15
1:C:223[A]:VAL:HG23	1:D:223[A]:VAL:HG12	1.27	1.14
1:E:223[B]:VAL:HG13	1:F:223[B]:VAL:HG21	1.15	1.14
1:E:223[B]:VAL:CG1	1:H:223[B]:VAL:HG23	1.80	1.11
1:A:223[A]:VAL:CG2	1:D:223[A]:VAL:HG13	1.78	1.11
1:A:223[B]:VAL:HG11	1:D:223[B]:VAL:HG12	1.28	1.10
1:B:111[B]:GLU:OE2	1:B:114[B]:ARG:CZ	2.00	1.10
1:E:223[B]:VAL:HG12	1:H:223[B]:VAL:HG23	1.08	1.05
1:H:219[A]:ARG:HH21	1:H:224[A]:GLN:NE2	1.57	1.03
1:E:224[B]:GLN:NE2	1:H:225[B]:GLY:C	2.12	1.03
1:E:225[A]:GLY:O	1:H:227[A]:ASN:CB	2.07	1.02
1:B:111[B]:GLU:OE2	1:B:114[B]:ARG:NE	1.94	0.98
1:E:224[B]:GLN:NE2	1:H:225[B]:GLY:O	1.95	0.97
1:E:225[A]:GLY:O	1:H:227[A]:ASN:HB3	1.63	0.97
1:H:219[A]:ARG:HH21	1:H:224[A]:GLN:HE22	1.17	0.93
1:E:223[B]:VAL:HG12	1:H:223[B]:VAL:CG2	1.99	0.90
1:B:288:ALA:HA	4:B:313:IPA:H12	1.53	0.90
1:E:224[B]:GLN:HG3	1:H:225[B]:GLY:H	1.37	0.89
1:E:223[B]:VAL:O	1:E:224[B]:GLN:HB2	1.71	0.89
1:E:219[A]:ARG:HH21	1:E:224[A]:GLN:NE2	1.70	0.89
1:H:227[B]:ASN:HD22	1:H:231:GLN:HE22	1.19	0.88
1:C:218:MSE:HG3	1:C:222:GLN:NE2	1.89	0.88
1:C:218:MSE:HG3	1:C:222:GLN:HE21	1.37	0.87
1:E:88:LYS:NZ	1:F:14:ASN:HD21	1.73	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:311:GOL:H12	5:A:513:HOH:O	1.74	0.87
1:A:223[B]:VAL:CG1	1:D:223[B]:VAL:HG12	2.05	0.87
1:B:292:ASP:OD2	4:B:313:IPA:H13	1.75	0.85
1:E:223[B]:VAL:CG1	1:F:223[B]:VAL:HG21	2.03	0.84
1:F:86:LEU:CD2	5:F:493:HOH:O	2.26	0.84
1:E:224[B]:GLN:CG	1:H:225[B]:GLY:H	1.90	0.84
1:G:159[B]:ARG:CZ	1:G:181:GLY:O	2.27	0.83
1:A:152:LEU:O	1:A:156[B]:THR:HG22	1.78	0.83
4:B:313:IPA:H31	1:G:118:ALA:O	1.79	0.82
1:F:86:LEU:HD21	5:F:493:HOH:O	1.81	0.80
1:B:58:VAL:HG21	1:C:224[A]:GLN:HG3	1.64	0.80
1:G:219[A]:ARG:HH21	1:G:224:GLN:NE2	1.80	0.80
1:A:160:PRO:HA	3:A:311:GOL:H32	1.64	0.80
1:E:225[A]:GLY:O	1:H:227[A]:ASN:HB2	1.80	0.80
1:A:224[B]:GLN:HG3	1:D:58:VAL:HG11	1.63	0.79
1:E:224[B]:GLN:NE2	1:H:225[B]:GLY:CA	2.45	0.78
1:G:93[B]:ARG:NH2	5:G:551:HOH:O	2.16	0.78
1:G:159[B]:ARG:NH1	1:G:181:GLY:O	2.17	0.78
1:B:111[B]:GLU:CD	1:B:114[B]:ARG:HE	1.86	0.78
1:D:219[A]:ARG:HH21	1:D:224:GLN:NE2	1.83	0.77
1:G:14:ASN:ND2	5:G:552:HOH:O	2.17	0.77
1:E:181:GLY:O	5:E:512:HOH:O	2.04	0.77
1:F:230[A]:GLU:OE1	1:F:274[A]:ARG:NH1	2.17	0.76
1:C:185:ASP:OD1	1:C:206:HIS:HE1	1.67	0.76
1:F:185:ASP:OD1	1:F:206:HIS:HE1	1.69	0.76
1:C:111[A]:GLU:CD	1:C:114[A]:ARG:HH21	1.89	0.76
1:A:185:ASP:OD1	1:A:206:HIS:HE1	1.70	0.74
1:C:223[A]:VAL:CG2	1:D:223[A]:VAL:CG1	2.54	0.74
1:F:29[B]:LEU:CD1	1:F:285:VAL:HG13	2.17	0.74
1:H:300[A]:GLU:HG3	1:H:301:HIS:CD2	2.23	0.74
1:C:228:ASN:C	1:C:228:ASN:HD22	1.90	0.74
1:C:222:GLN:HG2	5:C:587:HOH:O	1.89	0.72
1:E:223[B]:VAL:CG1	1:H:223[B]:VAL:CG2	2.62	0.72
1:D:185:ASP:OD1	1:D:206:HIS:HE1	1.71	0.72
1:H:97:LEU:H	1:H:121:HIS:HD2	1.37	0.71
1:A:223[A]:VAL:HG21	1:D:223[A]:VAL:CG1	2.16	0.71
1:E:88:LYS:HZ2	1:F:14:ASN:HD21	1.37	0.71
1:F:29[B]:LEU:HD13	1:F:285:VAL:CG1	2.21	0.71
1:H:97:LEU:H	1:H:121:HIS:CD2	2.08	0.70
1:F:136:MSE:HG2	1:F:141:GLU:HB2	1.74	0.70
1:H:219[A]:ARG:NH2	1:H:224[A]:GLN:HE22	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224[B]:GLN:HA	1:F:224:GLN:HG3	1.74	0.69
1:H:185:ASP:OD1	1:H:206:HIS:HE1	1.77	0.68
1:C:223[A]:VAL:HG23	1:D:223[A]:VAL:HG11	1.66	0.68
1:F:271:ALA:HA	1:F:274[B]:ARG:HG2	1.75	0.68
1:G:206:HIS:HD2	5:G:430:HOH:O	1.75	0.68
1:E:97:LEU:H	1:E:121:HIS:HD2	1.41	0.68
1:E:185:ASP:OD1	1:E:206:HIS:HE1	1.77	0.68
1:A:123:ILE:O	3:A:311:GOL:H31	1.94	0.68
1:G:97:LEU:H	1:G:121:HIS:HD2	1.42	0.68
1:E:118:ALA:HB1	4:E:313:IPA:H33	1.74	0.68
1:H:181:GLY:O	5:H:488:HOH:O	2.12	0.67
1:B:97:LEU:H	1:B:121:HIS:HD2	1.43	0.67
1:F:29[B]:LEU:HD13	1:F:285:VAL:HG13	1.73	0.67
1:D:296:HIS:CE1	1:D:300[A]:GLU:HG3	2.30	0.67
1:B:97:LEU:H	1:B:121:HIS:CD2	2.12	0.67
1:E:219[A]:ARG:HH21	1:E:224[A]:GLN:HE22	1.40	0.66
1:F:97:LEU:H	1:F:121:HIS:HD2	1.43	0.66
1:D:206:HIS:HD2	5:D:434:HOH:O	1.77	0.66
1:A:156[B]:THR:HG23	1:A:158:GLN:H	1.59	0.66
1:C:111[A]:GLU:OE2	1:C:114[A]:ARG:NH2	2.29	0.66
1:F:97:LEU:H	1:F:121:HIS:CD2	2.14	0.66
1:F:299[B]:ARG:HG2	5:F:488:HOH:O	1.96	0.66
1:E:97:LEU:H	1:E:121:HIS:CD2	2.13	0.66
1:G:300[A]:GLU:HG3	1:G:301:HIS:CD2	2.31	0.66
1:E:48:LYS:HG3	5:E:507:HOH:O	1.95	0.65
1:A:216:ASN:HD22	1:A:218:MSE:H	1.44	0.65
1:G:97:LEU:H	1:G:121:HIS:CD2	2.13	0.65
1:F:159[B]:ARG:NH2	1:F:179:GLU:OE2	2.29	0.65
1:B:121:HIS:HE1	5:B:346:HOH:O	1.79	0.65
1:E:224[B]:GLN:CG	1:H:225[B]:GLY:N	2.60	0.64
1:F:181:GLY:O	5:F:460:HOH:O	2.15	0.64
1:D:121:HIS:HE1	5:D:342:HOH:O	1.81	0.64
1:G:121:HIS:HE1	5:G:333:HOH:O	1.80	0.64
1:F:121:HIS:HE1	5:F:339:HOH:O	1.80	0.63
1:F:206:HIS:HD2	5:F:435:HOH:O	1.80	0.63
1:C:121:HIS:HE1	5:C:359:HOH:O	1.82	0.63
1:D:154[A]:GLU:HG3	5:D:470:HOH:O	1.97	0.63
1:A:136:MSE:HG2	1:A:141:GLU:HB2	1.81	0.63
1:A:97:LEU:H	1:A:121:HIS:CD2	2.15	0.62
1:C:206:HIS:HD2	5:C:443:HOH:O	1.80	0.62
1:A:121:HIS:HE1	5:A:337:HOH:O	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159[A]:ARG:NH2	1:H:179:GLU:OE2	2.33	0.62
1:G:185:ASP:OD1	1:G:206:HIS:HE1	1.82	0.62
1:F:86:LEU:HD23	5:F:493:HOH:O	1.94	0.62
1:E:93:ARG:NH1	1:E:273:GLU:OE2	2.33	0.61
1:C:97:LEU:H	1:C:121:HIS:HD2	1.48	0.61
1:A:160:PRO:CA	3:A:311:GOL:H32	2.29	0.61
1:F:179:GLU:OE1	1:F:181:GLY:N	2.31	0.61
1:A:97:LEU:H	1:A:121:HIS:HD2	1.49	0.61
1:C:97:LEU:H	1:C:121:HIS:CD2	2.18	0.61
1:A:156[B]:THR:HG21	3:A:311:GOL:O3	2.01	0.61
1:E:88:LYS:NZ	1:F:14:ASN:ND2	2.46	0.61
1:A:224[B]:GLN:CG	1:D:58:VAL:HG11	2.30	0.61
1:E:6:PRO:O	5:E:541:HOH:O	2.16	0.61
1:A:223[A]:VAL:HG22	1:D:223[A]:VAL:HG13	1.80	0.60
1:G:219[A]:ARG:HH21	1:G:224:GLN:HE22	1.47	0.60
1:H:121:HIS:HE1	5:H:326:HOH:O	1.85	0.60
1:E:154:GLU:HG3	5:E:491:HOH:O	2.01	0.59
1:H:93:ARG:NH1	1:H:273:GLU:OE2	2.35	0.59
1:E:121:HIS:HE1	5:E:338:HOH:O	1.86	0.59
1:H:154[A]:GLU:HG3	5:H:462:HOH:O	2.03	0.59
1:D:97:LEU:H	1:D:121:HIS:HD2	1.51	0.59
1:H:233:PHE:CD1	1:H:274[B]:ARG:HG3	2.38	0.58
1:G:149[B]:ILE:HD12	1:G:160:PRO:HG2	1.84	0.58
1:G:58:VAL:HG11	1:H:224[A]:GLN:HB3	1.84	0.58
1:D:97:LEU:H	1:D:121:HIS:CD2	2.21	0.58
1:C:88:LYS:HE3	1:D:14:ASN:HD21	1.69	0.57
1:E:224[B]:GLN:CA	1:F:224:GLN:HG3	2.34	0.57
1:F:107:GLN:OE1	5:F:566:HOH:O	2.17	0.57
1:C:289[A]:ARG:CZ	1:C:291[A]:GLU:OE2	2.54	0.56
1:E:223[B]:VAL:HG13	1:F:223[B]:VAL:HG22	1.78	0.56
1:E:224[B]:GLN:HE22	1:H:225[B]:GLY:C	2.06	0.56
1:G:58:VAL:HG22	1:H:222[B]:GLN:CD	2.25	0.56
1:H:114[B]:ARG:NH1	5:H:557:HOH:O	2.38	0.56
1:C:223[A]:VAL:CG2	1:D:223[A]:VAL:HG12	2.17	0.56
1:D:27[B]:ILE:HD13	1:D:28:ALA:N	2.20	0.55
1:D:219[A]:ARG:HH21	1:D:224:GLN:HE22	1.54	0.55
1:E:179:GLU:OE1	1:E:181:GLY:N	2.38	0.55
1:C:111[A]:GLU:CD	1:C:114[A]:ARG:NH2	2.59	0.55
1:H:219[A]:ARG:NH2	1:H:224[A]:GLN:NE2	2.42	0.55
1:H:227[B]:ASN:HD22	1:H:231:GLN:NE2	1.97	0.54
1:G:149[B]:ILE:HD11	1:G:182:PHE:HZ	1.73	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154[A]:GLU:HG3	5:A:482:HOH:O	2.06	0.54
1:B:58:VAL:HG21	1:C:224[A]:GLN:CG	2.36	0.54
1:F:159[B]:ARG:HH22	1:F:179:GLU:CD	2.10	0.54
1:B:126:HIS:HA	1:B:164:TYR:O	2.08	0.54
1:D:219[B]:ARG:HE	1:D:225:GLY:HA2	1.73	0.53
1:D:136:MSE:HG2	1:D:141:GLU:HB2	1.89	0.53
1:G:126:HIS:HA	1:G:164:TYR:O	2.08	0.53
1:C:218:MSE:CG	1:C:222:GLN:NE2	2.69	0.53
1:A:54:LEU:CD2	1:A:222[A]:GLN:NE2	2.72	0.53
1:E:278:TYR:O	1:E:282:HIS:HD2	1.92	0.53
1:F:20:HIS:HD2	5:F:523:HOH:O	1.92	0.53
1:F:278:TYR:O	1:F:282:HIS:HD2	1.91	0.53
1:G:159[B]:ARG:NH1	1:G:161:VAL:HG12	2.22	0.53
1:B:96:PRO:HG3	4:B:313:IPA:H11	1.90	0.52
1:C:126:HIS:HA	1:C:164:TYR:O	2.08	0.52
1:F:126:HIS:HA	1:F:164:TYR:O	2.09	0.52
1:E:219[B]:ARG:HE	1:E:225[B]:GLY:HA2	1.74	0.52
1:F:289[B]:ARG:NH1	5:F:514:HOH:O	2.42	0.52
1:G:227[A]:ASN:ND2	1:H:225[A]:GLY:HA2	2.25	0.52
1:H:136:MSE:HG2	1:H:141:GLU:HB2	1.90	0.52
1:F:91:LYS:HE3	1:F:119:ASP:OD1	2.09	0.52
1:H:278:TYR:O	1:H:282:HIS:HD2	1.92	0.52
1:A:278:TYR:O	1:A:282:HIS:HD2	1.92	0.52
1:E:206:HIS:HD2	5:E:460:HOH:O	1.93	0.52
1:F:29[B]:LEU:HD11	1:F:285:VAL:HG13	1.90	0.51
1:A:206:HIS:HD2	5:A:451:HOH:O	1.92	0.51
1:C:107[A]:GLN:HG3	1:C:151:ILE:HG21	1.93	0.51
1:D:278:TYR:O	1:D:282:HIS:HD2	1.93	0.51
1:E:88:LYS:HZ1	1:F:14:ASN:ND2	2.08	0.51
1:G:271:ALA:HA	1:G:274[A]:ARG:HG2	1.92	0.51
1:H:126:HIS:HA	1:H:164:TYR:O	2.10	0.51
1:C:228:ASN:C	1:C:228:ASN:ND2	2.63	0.51
1:A:216:ASN:HD21	1:A:259:HIS:HE1	1.59	0.51
1:D:27[B]:ILE:HD12	1:D:29:LEU:CD2	2.41	0.51
1:E:126:HIS:HA	1:E:164:TYR:O	2.10	0.51
1:F:54:LEU:HD23	1:F:222[B]:GLN:NE2	2.25	0.51
1:C:185:ASP:OD1	1:C:206:HIS:CE1	2.56	0.50
1:E:88:LYS:HZ1	1:F:14:ASN:HD21	1.54	0.50
1:G:278:TYR:O	1:G:282:HIS:HD2	1.94	0.50
1:H:264:GLY:HA2	5:H:570:HOH:O	2.11	0.50
1:C:278:TYR:O	1:C:282:HIS:HD2	1.95	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:GLN:C	1:E:224[B]:GLN:H	2.13	0.50
1:E:159:ARG:NE	5:E:450:HOH:O	2.44	0.50
1:H:159[A]:ARG:HH22	1:H:179:GLU:CD	2.14	0.50
1:A:296:HIS:CE1	1:A:300[B]:GLU:HG3	2.47	0.50
1:H:179:GLU:OE1	1:H:181:GLY:N	2.41	0.49
1:E:219[A]:ARG:NH2	1:E:224[A]:GLN:HE22	2.07	0.49
1:A:126:HIS:HA	1:A:164:TYR:O	2.12	0.49
1:E:224[B]:GLN:HG3	1:H:224[B]:GLN:N	2.27	0.49
1:A:216:ASN:ND2	1:A:218:MSE:H	2.09	0.49
1:B:111[A]:GLU:OE1	1:B:114[A]:ARG:NH2	2.37	0.49
1:D:185:ASP:OD1	1:D:206:HIS:CE1	2.61	0.49
1:F:54:LEU:CD2	1:F:222[B]:GLN:NE2	2.76	0.49
1:H:138:GLU:OE2	1:H:142:ARG:NH2	2.45	0.49
1:B:204:LYS:HG2	5:B:582:HOH:O	2.12	0.48
1:B:278:TYR:O	1:B:282:HIS:HD2	1.96	0.48
1:C:218:MSE:CG	1:C:222:GLN:HE21	2.18	0.48
1:A:20:HIS:HE1	5:A:535:HOH:O	1.97	0.48
1:E:224[B]:GLN:HG2	5:E:480:HOH:O	2.13	0.48
1:D:300[B]:GLU:HG3	1:D:301:HIS:CD2	2.48	0.48
1:G:300[A]:GLU:HG3	1:G:301:HIS:NE2	2.29	0.48
1:F:54:LEU:HD23	1:F:222[B]:GLN:HE22	1.78	0.48
1:H:118:ALA:HB1	4:H:313:IPA:C1	2.44	0.47
1:H:300[A]:GLU:HG3	1:H:301:HIS:NE2	2.28	0.47
1:C:110:PRO:O	1:C:114[B]:ARG:HG3	2.14	0.47
1:E:223[B]:VAL:O	1:E:224[B]:GLN:CB	2.51	0.47
1:B:289[B]:ARG:CZ	1:B:291[B]:GLU:OE2	2.61	0.47
1:H:271:ALA:HA	1:H:274[B]:ARG:HG2	1.95	0.47
1:D:126:HIS:HA	1:D:164:TYR:O	2.14	0.47
1:H:118:ALA:HB1	4:H:313:IPA:H11	1.96	0.47
1:F:224:GLN:CD	1:F:224:GLN:O	2.53	0.46
1:A:218:MSE:HE1	5:A:400:HOH:O	2.14	0.46
1:F:185:ASP:OD1	1:F:206:HIS:CE1	2.58	0.46
1:E:223[B]:VAL:HG12	1:E:223[B]:VAL:O	2.16	0.46
1:F:91:LYS:HE3	1:F:119:ASP:CG	2.35	0.46
1:A:227:ASN:N	1:A:231:GLN:OE1	2.45	0.46
1:H:159[B]:ARG:NE	5:H:490:HOH:O	2.49	0.46
1:E:223[B]:VAL:O	1:H:223[B]:VAL:HA	2.16	0.45
1:A:185:ASP:OD1	1:A:206:HIS:CE1	2.60	0.45
1:A:136:MSE:HE3	1:A:136:MSE:HB2	1.81	0.45
1:G:107[B]:GLN:HG3	1:G:151:ILE:HG21	1.98	0.45
1:A:54:LEU:HD23	1:A:222[A]:GLN:HE22	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ALA:HB2	1:B:239:ALA:HB2	1.99	0.45
1:E:224[B]:GLN:HE21	1:H:225[B]:GLY:C	1.86	0.45
1:B:54:LEU:CD2	1:B:222[A]:GLN:NE2	2.79	0.44
1:A:203:GLU:CD	1:A:203:GLU:H	2.20	0.44
1:B:150:ARG:O	1:B:154[A]:GLU:HG2	2.16	0.44
1:G:20:HIS:HD2	5:G:560:HOH:O	2.00	0.44
1:C:218:MSE:HE2	1:C:222:GLN:NE2	2.32	0.44
1:E:185:ASP:OD1	1:E:206:HIS:CE1	2.65	0.44
1:A:54:LEU:HD23	1:A:222[A]:GLN:NE2	2.33	0.44
1:C:223[A]:VAL:HG23	1:D:223[A]:VAL:HG13	1.81	0.44
1:D:218:MSE:HE1	5:D:418:HOH:O	2.16	0.44
1:F:282:HIS:HE1	5:F:570:HOH:O	2.00	0.44
1:A:107:GLN:HG3	1:A:151:ILE:HG21	2.00	0.43
1:F:29[B]:LEU:CD1	1:F:285:VAL:CG1	2.86	0.43
1:G:219[B]:ARG:HE	1:G:225:GLY:HA2	1.83	0.43
1:B:219[B]:ARG:HE	1:B:225:GLY:HA2	1.83	0.43
1:C:223[A]:VAL:CG2	1:D:223[A]:VAL:HG11	2.37	0.43
1:G:136:MSE:HG2	1:G:141:GLU:HB2	1.99	0.43
1:A:223[B]:VAL:HG11	1:D:223[B]:VAL:CG1	2.20	0.43
1:E:224[A]:GLN:HB3	1:H:58:VAL:HG11	1.99	0.43
1:G:149[B]:ILE:HD11	1:G:182:PHE:CZ	2.51	0.43
4:B:313:IPA:C3	5:G:518:HOH:O	2.66	0.43
1:G:150:ARG:NH1	1:G:154[A]:GLU:OE2	2.52	0.43
1:G:219[A]:ARG:NH2	1:G:224:GLN:HE22	2.13	0.43
1:B:114[B]:ARG:NH1	5:B:578:HOH:O	2.51	0.43
1:F:179:GLU:OE1	1:F:181:GLY:CA	2.67	0.42
1:H:159[A]:ARG:HH12	1:H:181:GLY:HA3	1.84	0.42
1:E:177:MSE:HG2	1:E:206:HIS:CG	2.54	0.42
1:E:224[B]:GLN:NE2	1:H:225[B]:GLY:N	2.67	0.42
1:A:156[B]:THR:HG21	3:A:311:GOL:O2	2.20	0.42
1:C:218:MSE:O	1:C:222:GLN:HG3	2.20	0.42
1:H:48:LYS:HA	1:H:48:LYS:HD3	1.93	0.42
1:A:289[A]:ARG:CZ	1:A:291:GLU:OE2	2.68	0.41
1:A:88:LYS:NZ	5:A:457:HOH:O	2.51	0.41
1:A:239:ALA:HB2	1:D:267:ALA:HB2	2.02	0.41
1:D:110:PRO:O	1:D:114[B]:ARG:HG3	2.19	0.41
1:B:110:PRO:O	1:B:114[B]:ARG:HG3	2.21	0.41
1:F:107:GLN:HG3	1:F:151:ILE:HG21	2.02	0.41
1:E:88:LYS:HZ2	1:F:14:ASN:ND2	2.11	0.41
1:B:85:ARG:HG2	1:B:269:MSE:SE	2.71	0.41
1:E:219[A]:ARG:NH2	1:E:224[A]:GLN:NE2	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:MSE:HE3	1:G:136:MSE:HB2	2.00	0.41
1:D:291[A]:GLU:HG2	1:D:295[A]:ARG:HH11	1.48	0.41
1:F:271:ALA:HA	1:F:274[B]:ARG:CG	2.49	0.41
1:G:103:ALA:HB3	1:G:128:TYR:HA	2.03	0.41
1:H:117:VAL:HG22	1:H:123[B]:ILE:CD1	2.51	0.41
1:D:136:MSE:HE3	1:D:136:MSE:HB2	1.90	0.40
1:G:267:ALA:HB2	1:H:239:ALA:HB2	2.03	0.40
1:B:291[B]:GLU:OE1	1:B:295[B]:ARG:NH1	2.54	0.40
1:G:58:VAL:CG2	1:H:222[B]:GLN:HG2	2.51	0.40
1:G:177:MSE:HG2	1:G:206:HIS:CG	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	314/308 (102%)	307 (98%)	7 (2%)	0	100	100
1	B	314/308 (102%)	305 (97%)	9 (3%)	0	100	100
1	C	316/308 (103%)	308 (98%)	8 (2%)	0	100	100
1	D	314/308 (102%)	305 (97%)	9 (3%)	0	100	100
1	E	309/308 (100%)	296 (96%)	9 (3%)	4 (1%)	10	2
1	F	315/308 (102%)	307 (98%)	8 (2%)	0	100	100
1	G	317/308 (103%)	310 (98%)	7 (2%)	0	100	100
1	H	318/308 (103%)	312 (98%)	6 (2%)	0	100	100
All	All	2517/2464 (102%)	2450 (97%)	63 (2%)	4 (0%)	48	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	224[A]	GLN
1	E	224[B]	GLN
1	E	223[A]	VAL
1	E	223[B]	VAL

### 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	268/247 (108%)	263 (98%)	5 (2%)	52	35
1	B	268/247 (108%)	266 (99%)	2 (1%)	81	74
1	C	270/247 (109%)	268 (99%)	2 (1%)	81	74
1	D	269/247 (109%)	264 (98%)	5 (2%)	52	35
1	E	260/247 (105%)	255 (98%)	5 (2%)	52	35
1	F	268/247 (108%)	262 (98%)	6 (2%)	47	29
1	G	269/247 (109%)	262 (97%)	7 (3%)	41	22
1	H	270/247 (109%)	263 (97%)	7 (3%)	41	22
All	All	2142/1976 (108%)	2103 (98%)	39 (2%)	58	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	136	MSE
1	A	191	ASP
1	A	216	ASN
1	A	263	ILE
1	B	126	HIS
1	B	263	ILE
1	C	191	ASP
1	C	228	ASN
1	D	191	ASP
1	D	224	GLN
1	D	230[A]	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	230[B]	GLU
1	D	304	GLN
1	E	48	LYS
1	E	126	HIS
1	E	179	GLU
1	E	300[A]	GLU
1	E	300[B]	GLU
1	F	14	ASN
1	F	91	LYS
1	F	126	HIS
1	F	136	MSE
1	F	179	GLU
1	F	224	GLN
1	G	126	HIS
1	G	159[A]	ARG
1	G	159[B]	ARG
1	G	191	ASP
1	G	224	GLN
1	G	227[A]	ASN
1	G	227[B]	ASN
1	H	126	HIS
1	H	178[A]	GLU
1	H	178[B]	GLU
1	H	179	GLU
1	H	191	ASP
1	H	274[A]	ARG
1	H	274[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	20	HIS
1	A	121	HIS
1	A	158	GLN
1	A	206	HIS
1	A	216	ASN
1	A	282	HIS
1	B	14	ASN
1	B	20	HIS
1	B	121	HIS
1	B	158	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	282	HIS
1	C	14	ASN
1	C	121	HIS
1	C	140	GLN
1	C	158	GLN
1	C	206	HIS
1	C	222	GLN
1	C	228	ASN
1	C	282	HIS
1	C	298	HIS
1	D	14	ASN
1	D	20	HIS
1	D	121	HIS
1	D	206	HIS
1	D	224	GLN
1	D	282	HIS
1	D	298	HIS
1	E	14	ASN
1	E	20	HIS
1	E	121	HIS
1	E	206	HIS
1	E	282	HIS
1	F	14	ASN
1	F	20	HIS
1	F	121	HIS
1	F	140	GLN
1	F	206	HIS
1	F	282	HIS
1	G	14	ASN
1	G	20	HIS
1	G	121	HIS
1	G	206	HIS
1	G	224	GLN
1	G	282	HIS
1	G	298	HIS
1	H	14	ASN
1	H	20	HIS
1	H	121	HIS
1	H	206	HIS
1	H	282	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](#)

34 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	IPA	A	312	-	3,3,3	0.51	0	3,3,3	0.46	0
2	EDO	C	310	-	3,3,3	0.40	0	2,2,2	0.57	0
4	IPA	E	313	-	3,3,3	0.47	0	3,3,3	0.64	0
2	EDO	E	310	-	3,3,3	0.51	0	2,2,2	0.28	0
2	EDO	B	309	-	3,3,3	0.41	0	2,2,2	0.63	0
2	EDO	E	309	-	3,3,3	0.46	0	2,2,2	0.32	0
3	GOL	B	311	-	5,5,5	0.32	0	5,5,5	0.84	0
2	EDO	D	309	-	3,3,3	0.42	0	2,2,2	0.50	0
2	EDO	G	310	-	3,3,3	0.44	0	2,2,2	0.49	0
2	EDO	A	309	-	3,3,3	0.46	0	2,2,2	0.45	0
2	EDO	A	310	-	3,3,3	0.41	0	2,2,2	0.59	0
4	IPA	C	311	-	3,3,3	0.52	0	3,3,3	0.44	0
3	GOL	D	311	-	5,5,5	0.37	0	5,5,5	1.08	0
2	EDO	D	310	-	3,3,3	0.41	0	2,2,2	0.48	0
4	IPA	B	313	-	3,3,3	0.37	0	3,3,3	0.87	0
3	GOL	E	312	-	5,5,5	0.28	0	5,5,5	0.74	0
3	GOL	A	311	-	5,5,5	0.45	0	5,5,5	0.70	0
2	EDO	F	310	-	3,3,3	0.40	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	IPA	F	312	-	3,3,3	0.44	0	3,3,3	0.36	0
4	IPA	H	313	-	3,3,3	0.44	0	3,3,3	0.60	0
2	EDO	G	309	-	3,3,3	0.50	0	2,2,2	0.50	0
3	GOL	H	312	-	5,5,5	0.32	0	5,5,5	0.77	0
3	GOL	G	312	-	5,5,5	0.32	0	5,5,5	0.99	0
3	GOL	F	311	-	5,5,5	0.33	0	5,5,5	0.90	0
2	EDO	H	309	-	3,3,3	0.41	0	2,2,2	0.47	0
2	EDO	H	310	-	3,3,3	0.50	0	2,2,2	0.52	0
4	IPA	D	312	-	3,3,3	0.53	0	3,3,3	0.30	0
4	IPA	B	312	-	3,3,3	0.52	0	3,3,3	0.38	0
2	EDO	E	311	-	3,3,3	0.45	0	2,2,2	0.42	0
2	EDO	F	309	-	3,3,3	0.38	0	2,2,2	0.56	0
2	EDO	H	311	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	G	311	-	3,3,3	0.42	0	2,2,2	0.53	0
2	EDO	C	309	-	3,3,3	0.49	0	2,2,2	0.41	0
2	EDO	B	310	-	3,3,3	0.32	0	2,2,2	0.72	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	EDO	C	310	-	-	1/1/1/1	-
2	EDO	E	310	-	-	1/1/1/1	-
2	EDO	B	309	-	-	1/1/1/1	-
2	EDO	E	309	-	-	1/1/1/1	-
3	GOL	B	311	-	-	2/4/4/4	-
2	EDO	D	309	-	-	0/1/1/1	-
2	EDO	G	310	-	-	0/1/1/1	-
2	EDO	A	309	-	-	0/1/1/1	-
2	EDO	A	310	-	-	1/1/1/1	-
3	GOL	D	311	-	-	3/4/4/4	-
2	EDO	D	310	-	-	0/1/1/1	-
3	GOL	E	312	-	-	2/4/4/4	-
3	GOL	A	311	-	-	2/4/4/4	-
2	EDO	F	310	-	-	1/1/1/1	-
2	EDO	G	309	-	-	0/1/1/1	-
3	GOL	H	312	-	-	0/4/4/4	-
3	GOL	G	312	-	-	2/4/4/4	-
3	GOL	F	311	-	-	1/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	H	309	-	-	0/1/1/1	-
2	EDO	H	310	-	-	0/1/1/1	-
2	EDO	E	311	-	-	1/1/1/1	-
2	EDO	F	309	-	-	1/1/1/1	-
2	EDO	H	311	-	-	1/1/1/1	-
2	EDO	G	311	-	-	0/1/1/1	-
2	EDO	C	309	-	-	0/1/1/1	-
2	EDO	B	310	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	311	GOL	O1-C1-C2-C3
3	G	312	GOL	C1-C2-C3-O3
3	B	311	GOL	C1-C2-C3-O3
3	D	311	GOL	C1-C2-C3-O3
3	F	311	GOL	C1-C2-C3-O3
3	A	311	GOL	O1-C1-C2-O2
3	B	311	GOL	O2-C2-C3-O3
3	G	312	GOL	O2-C2-C3-O3
2	A	310	EDO	O1-C1-C2-O2
3	D	311	GOL	O2-C2-C3-O3
2	C	310	EDO	O1-C1-C2-O2
2	E	311	EDO	O1-C1-C2-O2
3	E	312	GOL	O2-C2-C3-O3
2	B	309	EDO	O1-C1-C2-O2
2	E	310	EDO	O1-C1-C2-O2
3	E	312	GOL	C1-C2-C3-O3
3	D	311	GOL	O1-C1-C2-O2
2	B	310	EDO	O1-C1-C2-O2
2	H	311	EDO	O1-C1-C2-O2
2	E	309	EDO	O1-C1-C2-O2
2	F	309	EDO	O1-C1-C2-O2
2	F	310	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	313	IPA	1	0
4	B	313	IPA	5	0
3	A	311	GOL	6	0
4	H	313	IPA	2	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	290/308 (94%)	-0.51	4 (1%) 73 77	3, 7, 15, 24	15 (5%)
1	B	290/308 (94%)	-0.51	5 (1%) 69 72	3, 7, 16, 25	16 (5%)
1	C	289/308 (93%)	-0.57	3 (1%) 79 82	3, 6, 15, 25	20 (6%)
1	D	289/308 (93%)	-0.54	3 (1%) 79 82	3, 6, 15, 25	16 (5%)
1	E	290/308 (94%)	-0.50	4 (1%) 73 77	4, 7, 17, 26	10 (3%)
1	F	290/308 (94%)	-0.58	2 (0%) 84 87	3, 7, 17, 26	16 (5%)
1	G	290/308 (94%)	-0.55	4 (1%) 73 77	3, 7, 16, 25	18 (6%)
1	H	290/308 (94%)	-0.53	3 (1%) 79 82	2, 7, 16, 26	19 (6%)
All	All	2318/2464 (94%)	-0.54	28 (1%) 76 79	2, 7, 16, 26	130 (5%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	180	GLY	5.1
1	E	180	GLY	4.7
1	F	180	GLY	4.6
1	G	180	GLY	3.5
1	C	225	GLY	3.4
1	B	225	GLY	3.2
1	F	225	GLY	3.0
1	A	203	GLU	2.9
1	C	224[A]	GLN	2.9
1	E	225[A]	GLY	2.8
1	B	4	ASP	2.8
1	H	225[A]	GLY	2.8
1	D	225	GLY	2.8
1	B	59	ALA	2.6
1	A	53	PHE	2.5
1	H	203	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	59	ALA	2.5
1	A	304	GLN	2.4
1	G	225	GLY	2.4
1	D	203	GLU	2.3
1	A	4	ASP	2.3
1	B	203	GLU	2.3
1	G	203	GLU	2.2
1	C	223[A]	VAL	2.2
1	D	304	GLN	2.2
1	E	4	ASP	2.1
1	B	304	GLN	2.1
1	G	4	ASP	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
4	IPA	D	312	4/4	0.68	0.22	44,45,46,46	0
4	IPA	E	313	4/4	0.70	0.25	23,25,25,27	0
4	IPA	B	313	4/4	0.71	0.17	27,27,28,28	0
4	IPA	H	313	4/4	0.73	0.21	34,34,35,36	0
2	EDO	G	309	4/4	0.76	0.13	21,23,23,26	0
4	IPA	B	312	4/4	0.78	0.17	36,37,38,38	0
2	EDO	E	310	4/4	0.79	0.11	28,29,29,32	0
4	IPA	A	312	4/4	0.85	0.16	34,34,34,35	0
2	EDO	G	310	4/4	0.85	0.12	26,29,30,32	0
2	EDO	H	309	4/4	0.86	0.14	34,34,35,35	0
3	GOL	A	311	6/6	0.87	0.20	16,22,26,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IPA	C	311	4/4	0.87	0.14	33,33,33,33	0
3	GOL	B	311	6/6	0.87	0.12	19,23,23,24	0
2	EDO	F	309	4/4	0.87	0.10	28,29,30,30	0
2	EDO	H	310	4/4	0.87	0.09	17,20,20,24	0
3	GOL	H	312	6/6	0.89	0.08	15,19,20,22	0
4	IPA	F	312	4/4	0.89	0.10	18,20,21,22	0
2	EDO	A	310	4/4	0.89	0.10	20,23,25,28	0
2	EDO	H	311	4/4	0.90	0.10	21,24,25,28	0
3	GOL	D	311	6/6	0.90	0.10	15,20,21,21	0
3	GOL	G	312	6/6	0.90	0.08	14,19,21,21	0
2	EDO	F	310	4/4	0.90	0.09	21,23,24,27	0
2	EDO	G	311	4/4	0.91	0.09	21,23,25,28	0
3	GOL	F	311	6/6	0.91	0.09	17,21,22,23	0
2	EDO	C	310	4/4	0.91	0.09	23,25,26,30	0
2	EDO	A	309	4/4	0.92	0.07	17,18,18,19	0
2	EDO	D	309	4/4	0.92	0.10	19,19,20,20	0
2	EDO	E	309	4/4	0.92	0.07	22,25,25,28	0
3	GOL	E	312	6/6	0.92	0.09	15,16,18,18	0
2	EDO	B	309	4/4	0.92	0.06	21,21,21,23	0
2	EDO	B	310	4/4	0.93	0.07	16,19,20,24	0
2	EDO	E	311	4/4	0.94	0.07	19,23,24,28	0
2	EDO	C	309	4/4	0.94	0.07	18,19,19,20	0
2	EDO	D	310	4/4	0.94	0.07	21,22,24,27	0

## 6.5 Other polymers

There are no such residues in this entry.