



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:20 PM GMT

PDB ID : 4URR  
Title : Tailspike protein of Sf6 bacteriophage bound to Shigella flexneri O- antigen octasaccharide fragment  
Authors : Gohlke, U.; Heinemann, U.; Seckler, R.; Barbirz, S.  
Deposited on : 2014-07-01  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

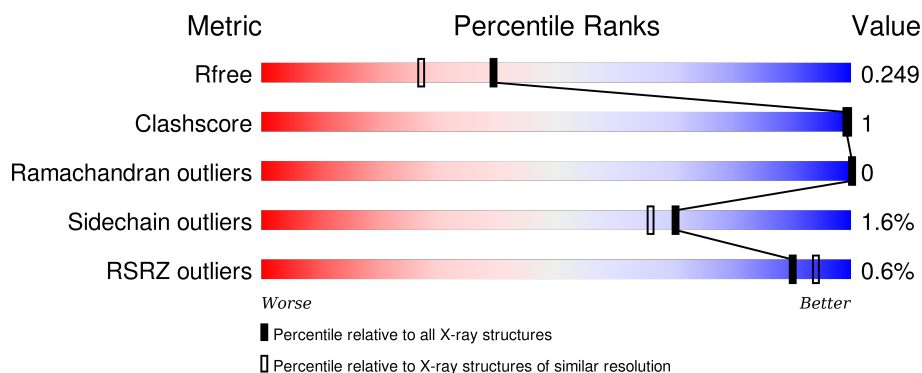
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



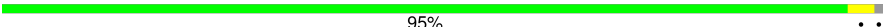
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	 97% ..
1	B	514	 96% ..
1	C	514	 96% ..
1	D	514	 96% ..
1	E	514	 96% ..

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Mol	Chain	Length	Quality of chain
1	F	514	

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
2	RAM	B	1	-	-	-	X
2	RAM	E	1	-	-	-	X
2	RAM	E	8	-	-	-	X
2	RAM	F	4	-	-	-	X
2	RAM	F	8	-	-	-	X
3	MN	A	1624	-	-	-	X
5	EDO	E	1624	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25129 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 BIFUNCTIONAL TAIL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	3	0
			3848	2407	665	757	19			
1	B	508	Total	C	N	O	S	0	4	0
			3838	2399	662	758	19			
1	C	509	Total	C	N	O	S	0	2	0
			3828	2392	662	755	19			
1	D	508	Total	C	N	O	S	0	2	0
			3820	2389	659	753	19			
1	E	508	Total	C	N	O	S	0	4	0
			3839	2399	663	758	19			
1	F	508	Total	C	N	O	S	0	3	0
			3833	2397	661	756	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
A	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3
B	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
B	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3
C	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
C	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3
D	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
D	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3
E	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
E	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3
F	366	ALA	GLU	ENGINEERED MUTATION	UNP Q9XJP3
F	399	ALA	ASP	ENGINEERED MUTATION	UNP Q9XJP3

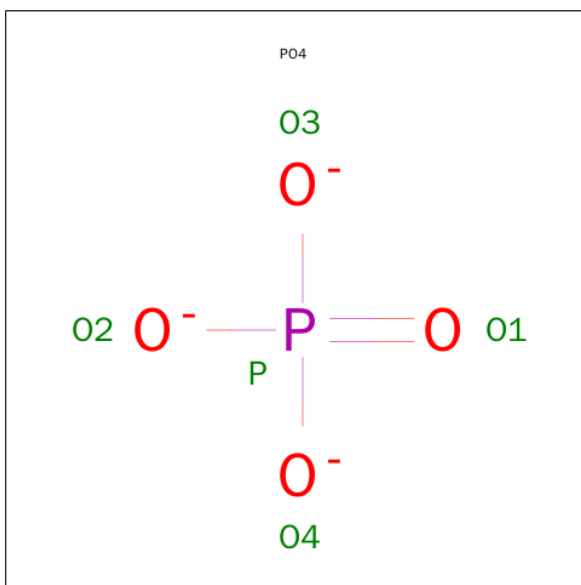
- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	8	Total	C	N	O	0	0
			89	52	2	35		
2	B	8	Total	C	N	O	0	0
			89	52	2	35		
2	C	8	Total	C	N	O	0	0
			89	52	2	35		
2	D	8	Total	C	N	O	0	0
			89	52	2	35		
2	E	8	Total	C	N	O	0	0
			89	52	2	35		
2	F	8	Total	C	N	O	0	0
			89	52	2	35		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

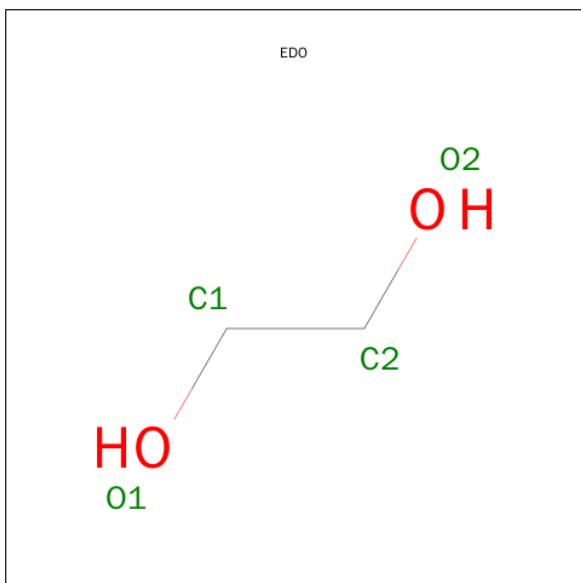
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Mn	0	0
			3	3		
3	E	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	3	Total	Mn	0	0
			3	3		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

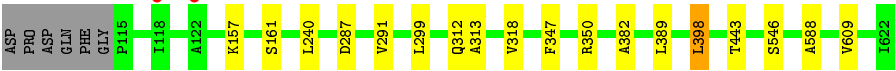


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	317	Total O 317 317	0	0
6	B	234	Total O 234 234	0	0
6	C	254	Total O 254 254	0	0
6	D	246	Total O 246 246	0	0
6	E	257	Total O 257 257	0	0
6	F	231	Total O 231 231	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.99Å 138.90Å 136.07Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	45.33 – 1.95 45.33 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.33-1.95) 99.9 (45.33-1.95)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.196 , 0.236 0.209 , 0.249	Depositor DCC
$R_{free}$ test set	11034 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.8	EDS
Estimated twinning fraction	0.080 for -h,-l,-k 0.067 for -h,l,k 0.085 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	4 of 223380 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	25129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.76 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6050e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RAM, PO4, MN, NAG, 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	0.54	0/3918	0.71	0/5327
1	B	0.50	0/3909	0.70	0/5317
1	C	0.53	0/3898	0.70	0/5302
1	D	0.49	0/3894	0.69	0/5296
1	E	0.52	0/3909	0.69	0/5318
1	F	0.53	0/3903	0.70	0/5309
All	All	0.52	0/23431	0.70	0/31869

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	176	TYR	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	3848	0	3779	5	0
1	B	3838	0	3759	5	0
1	C	3828	0	3750	5	0
1	D	3820	0	3750	5	0
1	E	3839	0	3760	5	0
1	F	3833	0	3758	5	0
2	A	89	0	81	0	0
2	B	89	0	81	1	0
2	C	89	0	81	1	0
2	D	89	0	81	0	0
2	E	89	0	81	1	0
2	F	89	0	81	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	F	10	0	0	0	0
5	B	8	0	12	0	0
5	E	8	0	12	0	0
5	F	4	0	6	0	0
6	A	317	0	0	0	0
6	B	234	0	0	1	0
6	C	254	0	0	0	0
6	D	246	0	0	0	0
6	E	257	0	0	0	0
6	F	231	0	0	0	0
All	All	25129	0	23072	29	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 1.

All (29) 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:F:588:ALA:HB1	1:F:609[B]:VAL:HG21	1.95	0.48
1:A:389:LEU:HD22	2:C:8:RAM:H61	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASN:O	1:D:179[A]:ILE:HG12	2.14	0.48
1:E:588:ALA:HB1	1:E:609[B]:VAL:HG11	1.96	0.47
1:E:318:VAL:HA	1:E:347:PHE:O	2.16	0.46
2:E:8:RAM:H61	1:F:389:LEU:HD22	1.97	0.46
1:B:318:VAL:HA	1:B:347:PHE:O	2.16	0.45
1:C:382:ALA:HB1	1:C:398:LEU:HG	1.98	0.45
1:A:382:ALA:HB1	1:A:398:LEU:HG	1.99	0.45
1:C:175:ASN:O	1:C:179:ILE:HG12	2.17	0.45
1:F:382:ALA:HB1	1:F:398:LEU:HG	2.00	0.44
1:E:382:ALA:HB1	1:E:398:LEU:HG	1.99	0.44
1:B:382:ALA:HB1	1:B:398:LEU:HG	1.99	0.44
1:F:291:VAL:O	1:F:313:ALA:HA	2.18	0.44
1:D:382:ALA:HB1	1:D:398:LEU:HG	1.99	0.44
1:B:231:ALA:HB2	1:B:239:VAL:HG22	2.00	0.44
1:F:318:VAL:HA	1:F:347:PHE:O	2.18	0.44
1:C:480:SER:HA	1:C:503:ASP:O	2.19	0.43
1:E:175:ASN:O	1:E:179:ILE:HG12	2.18	0.43
1:A:318:VAL:HA	1:A:347:PHE:O	2.19	0.42
2:B:8:RAM:H61	1:C:389:LEU:HD22	2.01	0.41
1:B:277:VAL:HG22	6:B:2109:HOH:O	2.20	0.41
1:D:182:ALA:HB1	1:D:195:LEU:HD11	2.01	0.41
1:E:480:SER:HA	1:E:503:ASP:O	2.20	0.41
1:D:318:VAL:HA	1:D:347:PHE:O	2.20	0.41
1:D:480:SER:HA	1:D:503:ASP:O	2.21	0.40
1:A:450:SER:HA	1:A:480:SER:O	2.21	0.40
1:C:318:VAL:HA	1:C:347:PHE:O	2.21	0.40
1:A:590:SER:OG	1:B:595:SER:HB3	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	511/514 (99%)	488 (96%)	23 (4%)	0	100	100
1	B	510/514 (99%)	489 (96%)	21 (4%)	0	100	100
1	C	509/514 (99%)	486 (96%)	23 (4%)	0	100	100
1	D	508/514 (99%)	488 (96%)	20 (4%)	0	100	100
1	E	510/514 (99%)	489 (96%)	21 (4%)	0	100	100
1	F	509/514 (99%)	488 (96%)	21 (4%)	0	100	100
All	All	3057/3084 (99%)	2928 (96%)	129 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/424 (100%)	418 (99%)	5 (1%)	78	75
1	B	423/424 (100%)	417 (99%)	6 (1%)	74	70
1	C	421/424 (99%)	414 (98%)	7 (2%)	68	63
1	D	421/424 (99%)	416 (99%)	5 (1%)	78	75
1	E	423/424 (100%)	417 (99%)	6 (1%)	74	70
1	F	422/424 (100%)	411 (97%)	11 (3%)	54	43
All	All	2533/2544 (100%)	2493 (98%)	40 (2%)	70	66

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	299	LEU
1	A	312	GLN
1	A	398	LEU
1	A	546	SER
1	B	119	GLU
1	B	161	SER

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Mol	Chain	Res	Type
1	B	287	ASP
1	B	299	LEU
1	B	312	GLN
1	B	398	LEU
1	C	119	GLU
1	C	161	SER
1	C	299	LEU
1	C	312	GLN
1	C	350	ARG
1	C	398	LEU
1	C	546	SER
1	D	119	GLU
1	D	299	LEU
1	D	312	GLN
1	D	398	LEU
1	D	403	SER
1	E	299	LEU
1	E	312	GLN
1	E	350	ARG
1	E	398	LEU
1	E	546	SER
1	E	607	SER
1	F	157	LYS
1	F	161	SER
1	F	240	LEU
1	F	287	ASP
1	F	299	LEU
1	F	312	GLN
1	F	350	ARG
1	F	398	LEU
1	F	443[A]	THR
1	F	443[B]	THR
1	F	546	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

48 carbohydrates 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	$\# Z  > 2$
2	RAM	A	1	2	10,10,11	0.38	0	13,14,16	0.40	0
2	NAG	A	2	2	14,14,15	0.21	0	15,19,21	0.59	0
2	RAM	A	3	2	10,10,11	0.28	0	13,14,16	0.57	0
2	RAM	A	4	2	10,10,11	0.29	0	13,14,16	0.48	0
2	RAM	A	5	2	10,10,11	0.36	0	13,14,16	0.54	0
2	NAG	A	6	2	14,14,15	0.32	0	15,19,21	0.56	0
2	RAM	A	7	2	10,10,11	0.25	0	13,14,16	0.40	0
2	RAM	A	8	2	11,11,11	0.29	0	16,16,16	0.60	0
2	RAM	B	1	2	10,10,11	0.34	0	13,14,16	0.54	0
2	NAG	B	2	2	14,14,15	0.28	0	15,19,21	0.56	0
2	RAM	B	3	2	10,10,11	0.24	0	13,14,16	0.42	0
2	RAM	B	4	2	10,10,11	0.28	0	13,14,16	0.43	0
2	RAM	B	5	2	10,10,11	0.33	0	13,14,16	0.55	0
2	NAG	B	6	2	14,14,15	0.32	0	15,19,21	0.55	0
2	RAM	B	7	2	10,10,11	0.34	0	13,14,16	0.52	0
2	RAM	B	8	2	11,11,11	0.14	0	16,16,16	0.45	0
2	RAM	C	1	2	10,10,11	0.38	0	13,14,16	0.47	0
2	NAG	C	2	2	14,14,15	0.30	0	15,19,21	0.61	0
2	RAM	C	3	2	10,10,11	0.37	0	13,14,16	0.59	0
2	RAM	C	4	2	10,10,11	0.30	0	13,14,16	0.67	0
2	RAM	C	5	2	10,10,11	0.33	0	13,14,16	0.54	0
2	NAG	C	6	2	14,14,15	0.31	0	15,19,21	0.65	0
2	RAM	C	7	2	10,10,11	0.34	0	13,14,16	0.51	0
2	RAM	C	8	2	11,11,11	0.24	0	16,16,16	0.51	0
2	RAM	D	1	2	10,10,11	0.25	0	13,14,16	0.37	0
2	NAG	D	2	2	14,14,15	0.27	0	15,19,21	0.56	0
2	RAM	D	3	2	10,10,11	0.22	0	13,14,16	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RAM	D	4	2	10,10,11	0.26	0	13,14,16	0.52	0
2	RAM	D	5	2	10,10,11	0.30	0	13,14,16	0.47	0
2	NAG	D	6	2	14,14,15	0.28	0	15,19,21	0.61	0
2	RAM	D	7	2	10,10,11	0.28	0	13,14,16	0.43	0
2	RAM	D	8	2	11,11,11	0.13	0	16,16,16	0.45	0
2	RAM	E	1	2	10,10,11	0.29	0	13,14,16	0.35	0
2	NAG	E	2	2	14,14,15	0.27	0	15,19,21	0.54	0
2	RAM	E	3	2	10,10,11	0.31	0	13,14,16	0.61	0
2	RAM	E	4	2	10,10,11	0.24	0	13,14,16	0.52	0
2	RAM	E	5	2	10,10,11	0.30	0	13,14,16	0.47	0
2	NAG	E	6	2	14,14,15	0.33	0	15,19,21	0.61	0
2	RAM	E	7	2	10,10,11	0.38	0	13,14,16	0.55	0
2	RAM	E	8	2	11,11,11	0.13	0	16,16,16	0.46	0
2	RAM	F	1	2	10,10,11	0.35	0	13,14,16	0.43	0
2	NAG	F	2	2	14,14,15	0.27	0	15,19,21	0.61	0
2	RAM	F	3	2	10,10,11	0.28	0	13,14,16	0.47	0
2	RAM	F	4	2	10,10,11	0.31	0	13,14,16	0.56	0
2	RAM	F	5	2	10,10,11	0.39	0	13,14,16	0.64	0
2	NAG	F	6	2	14,14,15	0.28	0	15,19,21	0.63	0
2	RAM	F	7	2	10,10,11	0.33	0	13,14,16	0.54	0
2	RAM	F	8	2	11,11,11	0.39	0	16,16,16	0.80	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	RAM	A	1	2	-	0/0/17/20	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	RAM	A	3	2	-	0/0/17/20	0/1/1/1
2	RAM	A	4	2	-	0/0/17/20	0/1/1/1
2	RAM	A	5	2	-	0/0/17/20	0/1/1/1
2	NAG	A	6	2	-	0/6/23/26	0/1/1/1
2	RAM	A	7	2	-	0/0/17/20	0/1/1/1
2	RAM	A	8	2	-	0/0/20/20	0/1/1/1
2	RAM	B	1	2	-	0/0/17/20	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	RAM	B	3	2	-	0/0/17/20	0/1/1/1
2	RAM	B	4	2	-	0/0/17/20	0/1/1/1
2	RAM	B	5	2	-	0/0/17/20	0/1/1/1
2	NAG	B	6	2	-	0/6/23/26	0/1/1/1
2	RAM	B	7	2	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RAM	B	8	2	-	0/0/20/20	0/1/1/1
2	RAM	C	1	2	-	0/0/17/20	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	RAM	C	3	2	-	0/0/17/20	0/1/1/1
2	RAM	C	4	2	-	0/0/17/20	0/1/1/1
2	RAM	C	5	2	-	0/0/17/20	0/1/1/1
2	NAG	C	6	2	-	0/6/23/26	0/1/1/1
2	RAM	C	7	2	-	0/0/17/20	0/1/1/1
2	RAM	C	8	2	-	0/0/20/20	0/1/1/1
2	RAM	D	1	2	-	0/0/17/20	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	RAM	D	3	2	-	0/0/17/20	0/1/1/1
2	RAM	D	4	2	-	0/0/17/20	0/1/1/1
2	RAM	D	5	2	-	0/0/17/20	0/1/1/1
2	NAG	D	6	2	-	0/6/23/26	0/1/1/1
2	RAM	D	7	2	-	0/0/17/20	0/1/1/1
2	RAM	D	8	2	-	0/0/20/20	0/1/1/1
2	RAM	E	1	2	-	0/0/17/20	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	RAM	E	3	2	-	0/0/17/20	0/1/1/1
2	RAM	E	4	2	-	0/0/17/20	0/1/1/1
2	RAM	E	5	2	-	0/0/17/20	0/1/1/1
2	NAG	E	6	2	-	0/6/23/26	0/1/1/1
2	RAM	E	7	2	-	0/0/17/20	0/1/1/1
2	RAM	E	8	2	-	0/0/20/20	0/1/1/1
2	RAM	F	1	2	-	0/0/17/20	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	RAM	F	3	2	-	0/0/17/20	0/1/1/1
2	RAM	F	4	2	-	0/0/17/20	0/1/1/1
2	RAM	F	5	2	-	0/0/17/20	0/1/1/1
2	NAG	F	6	2	-	0/6/23/26	0/1/1/1
2	RAM	F	7	2	-	0/0/17/20	0/1/1/1
2	RAM	F	8	2	-	0/0/20/20	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	RAM	1	0
2	C	8	RAM	1	0
2	E	8	RAM	1	0

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 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	$\# Z  > 2$
4	PO4	A	1626	-	4,4,4	1.11	0	6,6,6	0.26	0
4	PO4	B	1623	-	4,4,4	1.28	1 (25%)	6,6,6	0.25	0
5	EDO	B	1625	-	3,3,3	0.89	0	2,2,2	0.02	0
5	EDO	B	1626	-	3,3,3	0.66	0	2,2,2	0.16	0
5	EDO	E	1624	-	3,3,3	0.65	0	2,2,2	0.51	0
5	EDO	E	1625	-	3,3,3	0.65	0	2,2,2	0.24	0
4	PO4	F	1623	-	4,4,4	1.31	0	6,6,6	0.25	0
4	PO4	F	1625	-	4,4,4	1.28	0	6,6,6	0.27	0
5	EDO	F	1626	-	3,3,3	0.90	0	2,2,2	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	1626	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1623	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1625	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1626	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1624	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1625	-	-	0/1/1/1	0/0/0/0
4	PO4	F	1623	-	-	0/0/0/0	0/0/0/0
4	PO4	F	1625	-	-	0/0/0/0	0/0/0/0
5	EDO	F	1626	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1623	PO4	P-O2	2.16	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	509/514 (99%)	-0.30	2 (0%) 93 95	6, 13, 31, 45	0
1	B	508/514 (98%)	-0.19	2 (0%) 93 95	10, 18, 33, 51	0
1	C	509/514 (99%)	-0.29	1 (0%) 95 97	6, 15, 30, 51	0
1	D	508/514 (98%)	-0.07	5 (0%) 84 89	7, 20, 38, 63	0
1	E	508/514 (98%)	-0.03	5 (0%) 84 89	6, 19, 40, 65	0
1	F	508/514 (98%)	-0.24	2 (0%) 93 95	6, 14, 35, 67	0
All	All	3050/3084 (98%)	-0.19	17 (0%) 90 94	6, 17, 35, 67	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	LEU	5.6
1	E	117	LEU	4.8
1	D	127	TYR	3.4
1	B	340	ASN	3.3
1	F	118	ILE	2.9
1	C	114	GLY	2.7
1	A	609	VAL	2.7
1	F	122	ALA	2.4
1	D	168	ILE	2.4
1	E	132	THR	2.4
1	E	134	GLY	2.3
1	E	340[A]	ASN	2.3
1	D	360	SER	2.2
1	E	127	TYR	2.2
1	A	610	GLY	2.2
1	B	610	GLY	2.2
1	D	124	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	RAM	E	8	11/11	0.84	0.18	6.21	40,47,51,53	0
2	RAM	F	8	11/11	0.89	0.15	3.63	35,47,51,54	0
2	RAM	E	1	10/11	0.93	0.12	2.96	18,24,29,30	0
2	RAM	B	1	10/11	0.89	0.14	2.79	20,28,34,34	0
2	RAM	F	4	10/11	0.91	0.12	2.07	18,24,28,29	0
2	NAG	B	2	14/15	0.94	0.12	1.98	19,23,38,42	0
2	RAM	C	3	10/11	0.92	0.10	1.53	16,23,30,33	0
2	NAG	C	6	14/15	0.96	0.10	0.86	13,18,22,28	0
2	RAM	C	4	10/11	0.95	0.09	0.75	9,14,21,22	0
2	RAM	D	1	10/11	0.91	0.13	0.72	20,27,30,37	0
2	RAM	C	1	10/11	0.96	0.10	0.66	6,10,18,19	0
2	NAG	D	6	14/15	0.89	0.12	0.28	29,34,39,40	0
2	NAG	B	6	14/15	0.94	0.11	-0.01	23,27,30,30	0
2	RAM	A	1	10/11	0.96	0.08	-0.13	10,16,19,19	0
2	NAG	E	6	14/15	0.96	0.10	-0.41	9,20,31,32	0
2	RAM	B	3	10/11	0.92	0.11	-0.46	26,32,33,34	0
2	RAM	A	4	10/11	0.97	0.09	-0.72	9,11,17,26	0
2	RAM	D	4	10/11	0.96	0.10	-0.75	14,24,26,31	0
2	RAM	E	4	10/11	0.96	0.08	-0.83	14,17,20,22	0
2	NAG	F	6	14/15	0.95	0.09	-1.09	15,23,25,25	0
2	RAM	F	1	10/11	0.94	0.09	-1.10	13,23,30,33	0
2	RAM	B	4	10/11	0.96	0.09	-1.31	12,16,18,23	0
2	RAM	D	5	10/11	0.89	0.13	-	20,31,34,35	0
2	RAM	C	7	10/11	0.94	0.11	-	19,26,28,30	0
2	RAM	F	3	10/11	0.89	0.13	-	29,31,33,38	0
2	NAG	D	2	14/15	0.88	0.16	-	25,35,45,49	0
2	NAG	C	2	14/15	0.93	0.12	-	7,20,25,35	0
2	RAM	E	5	10/11	0.95	0.10	-	14,20,25,27	0
2	RAM	B	5	10/11	0.93	0.16	-	18,29,35,38	0
2	RAM	B	8	11/11	0.84	0.21	-	34,47,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RAM	A	7	10/11	0.94	0.09	-	27,34,38,39	0
2	RAM	D	3	10/11	0.89	0.12	-	31,36,39,44	0
2	NAG	A	2	14/15	0.95	0.09	-	10,17,22,24	0
2	RAM	D	7	10/11	0.84	0.14	-	34,36,38,45	0
2	RAM	C	5	10/11	0.95	0.10	-	15,19,23,24	0
2	RAM	A	8	11/11	0.83	0.20	-	46,52,56,57	0
2	RAM	F	7	10/11	0.92	0.14	-	21,26,29,29	0
2	RAM	A	3	10/11	0.92	0.11	-	21,29,34,35	0
2	RAM	D	8	11/11	0.88	0.16	-	40,44,48,51	0
2	RAM	B	7	10/11	0.91	0.11	-	20,26,29,32	0
2	RAM	A	5	10/11	0.94	0.11	-	14,22,26,30	0
2	RAM	C	8	11/11	0.88	0.14	-	26,36,41,41	0
2	NAG	A	6	14/15	0.92	0.12	-	18,22,25,25	0
2	NAG	E	2	14/15	0.92	0.13	-	14,26,38,43	0
2	RAM	E	7	10/11	0.92	0.14	-	23,26,28,30	0
2	NAG	F	2	14/15	0.86	0.13	-	23,35,40,42	0
2	RAM	E	3	10/11	0.92	0.11	-	13,21,24,26	0
2	RAM	F	5	10/11	0.89	0.15	-	23,26,27,29	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	A	1624	1/1	1.00	0.14	4.22	4,4,4,4	1
5	EDO	E	1624	4/4	0.97	0.11	2.18	19,20,22,22	0
5	EDO	F	1626	4/4	0.92	0.13	1.67	21,32,37,38	0
5	EDO	E	1625	4/4	0.90	0.17	1.56	26,32,35,36	0
3	MN	D	1624	1/1	0.99	0.08	-0.34	6,6,6,6	1
4	PO4	F	1625	5/5	0.95	0.09	-0.75	35,40,41,42	0
3	MN	C	1623	1/1	0.99	0.04	-1.88	19,19,19,19	0
3	MN	A	1623	1/1	1.00	0.05	-2.43	13,13,13,13	0
3	MN	E	1623	1/1	1.00	0.04	-2.44	26,26,26,26	0
3	MN	D	1623	1/1	1.00	0.05	-2.86	32,32,32,32	0
3	MN	B	1624	1/1	1.00	0.04	-3.63	13,13,13,13	0
3	MN	F	1624	1/1	0.99	0.03	-3.98	28,28,28,28	0
5	EDO	B	1625	4/4	0.68	0.20	-	36,37,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	F	1623	5/5	0.95	0.13	-	37,40,41,42	0
4	PO4	B	1623	5/5	0.98	0.07	-	23,23,24,30	0
4	PO4	A	1626	5/5	0.98	0.09	-	23,24,25,29	0
5	EDO	B	1626	4/4	0.84	0.25	-	40,43,46,47	0
3	MN	D	1625	1/1	0.97	0.07	-	23,23,23,23	1
3	MN	A	1625	1/1	0.98	0.05	-	14,14,14,14	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.