



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 03:22 PM EDT

PDB ID : 3NEV  
Title : Crystal structure of YagE, a prophage protein from E. coli K12 in complex with KDGal  
Authors : Bhaskar, V.; Kumar, P.M.; Manicka, S.; Krishnaswamy, S.  
Deposited on : 2010-06-09  
Resolution : 2.19 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

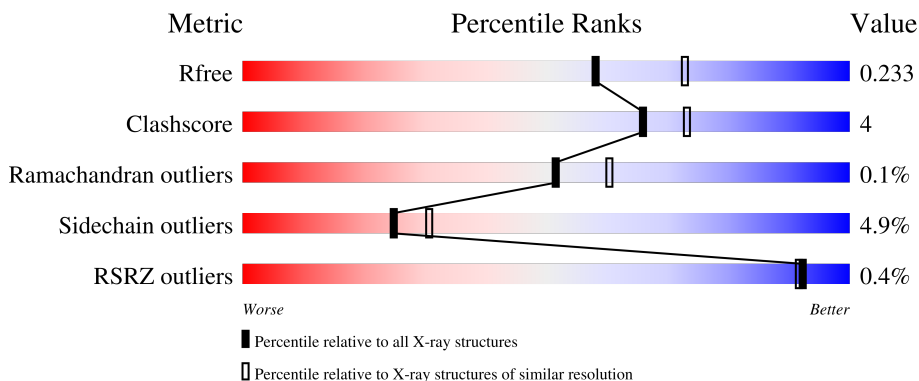
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	298	
1	B	298	
1	C	298	
1	D	298	

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	EDO	B	4	-	-	X	-
2	EDO	D	8	-	-	X	-
3	RSH	A	1	X	-	-	-
3	RSH	B	2	X	-	-	-
3	RSH	C	3	X	X	X	-
3	RSH	D	4	X	-	-	-

## 2 Entry composition [i](#)

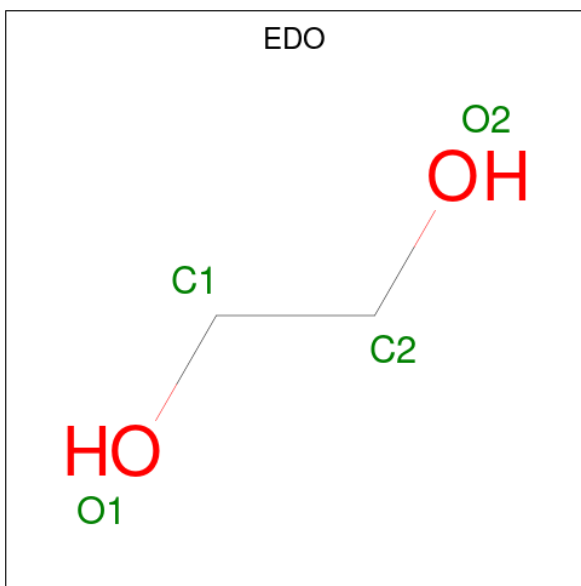
There are 4 unique types of molecules in this entry. The entry contains 9667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein yagE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	Total 2275	C 1456	N 391	O 422	S 6	0	2	0
1	B	298	Total 2263	C 1449	N 388	O 420	S 6	0	1	0
1	C	298	Total 2297	C 1468	N 397	O 426	S 6	0	4	0
1	D	298	Total 2266	C 1452	N 388	O 420	S 6	0	1	0

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



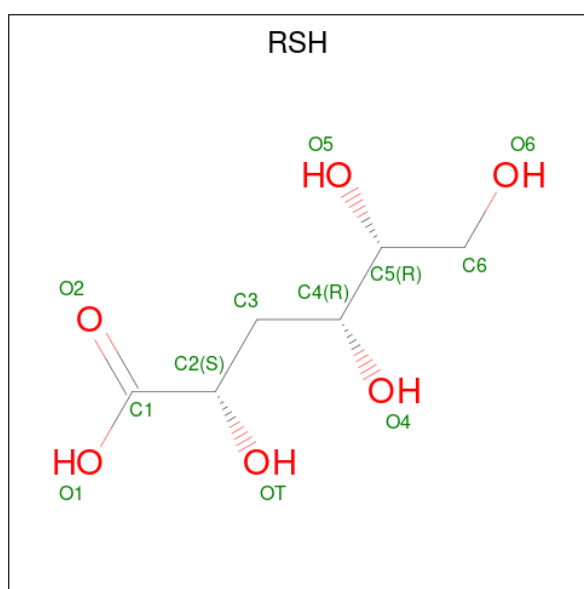
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is 3-DEOXY-D-LYXO-HEXONIC ACID (three-letter code: RSH) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	121	Total 121	O 121	0	0
4	B	124	Total 124	O 124	0	0
4	C	130	Total 130	O 130	0	0
4	D	115	Total 115	O 115	0	0

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

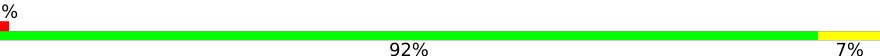
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein yagE

Chain A:  91% 7%




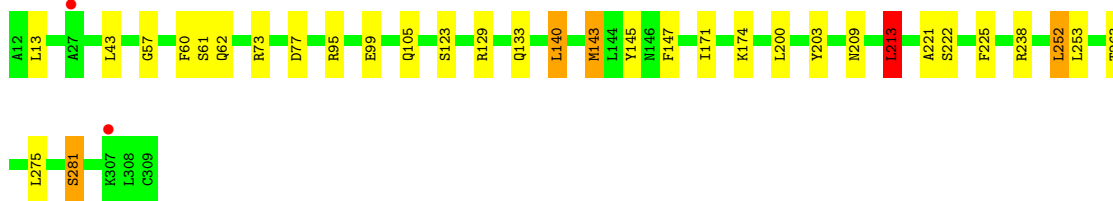
- Molecule 1: Uncharacterized protein yagE

Chain B:  92% 7%




- Molecule 1: Uncharacterized protein yagE

Chain C:  89% 9%



- Molecule 1: Uncharacterized protein yagE

Chain D:  90% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.86Å 155.13Å 55.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.19 49.18 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.18-2.19) 99.1 (49.18-2.19)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.197 , 0.237 0.195 , 0.233	Depositor DCC
$R_{free}$ test set	3178 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtrriage
Anisotropy	0.890	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.85 % 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 3.9754e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: RSH, 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	1.11	4/2325 (0.2%)	0.90	3/3169 (0.1%)
1	B	1.09	2/2312 (0.1%)	0.91	7/3151 (0.2%)
1	C	1.05	4/2348 (0.2%)	0.89	3/3200 (0.1%)
1	D	1.07	1/2315 (0.0%)	0.89	7/3155 (0.2%)
All	All	1.08	11/9300 (0.1%)	0.90	20/12675 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	ALA	CA-CB	-12.41	1.26	1.52
1	B	12	ALA	N-CA	-6.41	1.33	1.46
1	C	281	SER	CB-OG	-6.29	1.34	1.42
1	A	113	VAL	CB-CG1	5.83	1.65	1.52
1	A	119	TYR	CD1-CE1	5.77	1.48	1.39
1	A	99	GLU	CG-CD	5.62	1.60	1.51
1	A	203	TYR	CD2-CE2	5.36	1.47	1.39
1	C	60	PHE	CE1-CZ	5.34	1.47	1.37
1	C	203	TYR	CD1-CE1	5.32	1.47	1.39
1	D	12	ALA	CA-CB	-5.19	1.41	1.52
1	C	99	GLU	CG-CD	5.11	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	D	184	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	B	12	ALA	N-CA-CB	-6.15	101.49	110.10
1	A	292	ASP	CB-CG-OD1	5.77	123.50	118.30
1	C	213	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	213	LEU	CA-CB-CG	5.68	128.36	115.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	213	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	73	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	D	43	LEU	CB-CG-CD1	5.43	120.23	111.00
1	B	186	MET	CG-SD-CE	5.42	108.88	100.20
1	D	200	LEU	CB-CG-CD1	5.41	120.20	111.00
1	B	95	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	252	LEU	CB-CG-CD1	5.27	119.96	111.00
1	D	213	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	121	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	D	184	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	252	LEU	CB-CG-CD1	5.18	119.80	111.00
1	A	129	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	D	252	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2275	0	2285	17	0
1	B	2263	0	2278	14	0
1	C	2297	0	2311	17	0
1	D	2266	0	2287	14	0
2	A	8	0	12	2	0
2	B	8	0	12	5	0
2	C	8	0	12	0	0
2	D	8	0	12	10	0
3	A	11	0	9	4	0
3	B	11	0	9	4	0
3	C	11	0	9	6	0
3	D	11	0	9	4	0
4	A	121	0	0	1	0
4	B	124	0	0	2	0
4	C	130	0	0	7	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	115	0	0	7	0
All	All	9667	0	9245	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (69) 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:D:174:LYS:HZ1	3:D:4:RSH:C2	1.33	1.32
1:B:174:LYS:HZ3	3:B:2:RSH:C2	1.36	1.31
1:A:174:LYS:HZ1	3:A:1:RSH:C2	1.37	1.26
1:C:174:LYS:HZ3	3:C:3:RSH:C2	1.41	1.18
1:B:174:LYS:HZ1	3:B:2:RSH:C2	1.53	1.05
2:D:8:EDO:H11	4:D:332:HOH:O	1.59	1.02
1:C:174:LYS:HZ1	3:C:3:RSH:C2	1.54	0.99
1:D:174:LYS:HZ3	3:D:4:RSH:C2	1.56	0.97
2:D:8:EDO:H12	4:D:366:HOH:O	1.65	0.95
1:A:174:LYS:HZ2	3:A:1:RSH:C2	1.56	0.92
4:C:454:HOH:O	2:D:8:EDO:H11	1.81	0.81
4:C:454:HOH:O	2:D:8:EDO:C1	2.31	0.79
4:B:459:HOH:O	1:D:260:GLN:HG3	1.83	0.78
1:C:129[B]:ARG:NH2	4:C:454:HOH:O	2.22	0.71
1:C:129[A]:ARG:HD3	1:C:133:GLN:NE2	2.06	0.70
2:D:8:EDO:C1	4:D:332:HOH:O	2.29	0.66
1:B:105:GLN:HB2	1:B:140:LEU:HD22	1.79	0.63
1:B:130:TYR:HA	2:B:4:EDO:H11	1.80	0.63
1:B:221:ALA:HB2	3:B:2:RSH:H6C2	1.83	0.61
2:D:8:EDO:H21	4:D:313:HOH:O	2.01	0.59
1:A:105:GLN:HB2	1:A:140:LEU:HD22	1.85	0.59
2:D:8:EDO:H22	4:D:332:HOH:O	2.03	0.58
1:D:105:GLN:HB2	1:D:140:LEU:HD22	1.84	0.58
1:C:105:GLN:HB2	1:C:140:LEU:HD22	1.85	0.57
1:A:233:LEU:C	1:A:233:LEU:HD23	2.26	0.56
1:C:221:ALA:HB2	3:C:3:RSH:H6C2	1.88	0.56
3:C:3:RSH:H3C1	4:C:392:HOH:O	2.05	0.56
1:A:174:LYS:NZ	3:A:1:RSH:C1	2.61	0.53
1:C:57:GLY:HA3	4:C:460:HOH:O	2.10	0.52
1:C:238:ARG:NH2	4:C:391:HOH:O	2.42	0.51
2:D:8:EDO:C2	4:D:332:HOH:O	2.55	0.50
1:B:129:ARG:NH1	2:B:4:EDO:O2	2.44	0.50

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HH11	2:A:5:EDO:H12	1.77	0.49
1:A:129:ARG:HD3	2:A:5:EDO:H12	1.95	0.48
1:A:253:LEU:HB3	1:C:213:LEU:HD13	1.96	0.48
1:B:130:TYR:CA	2:B:4:EDO:H11	2.43	0.47
1:C:171:ILE:HD12	1:C:171:ILE:C	2.35	0.46
1:C:222:SER:HA	1:C:225:PHE:CE1	2.51	0.45
1:D:258:MET:HB3	1:D:302:LEU:HD23	1.98	0.45
1:A:263:THR:HA	1:A:264:PRO:C	2.36	0.45
1:B:174:LYS:NZ	3:B:2:RSH:C1	2.64	0.45
1:D:61:SER:OG	1:D:62:GLN:NE2	2.47	0.44
1:D:221:ALA:HB2	3:D:4:RSH:H6C2	1.99	0.44
1:B:24:ILE:HG22	1:B:32:ASP:HB3	1.99	0.44
1:C:174:LYS:NZ	3:C:3:RSH:C1	2.65	0.44
1:A:297:ALA:O	1:A:301:THR:HG23	2.18	0.44
1:A:213:LEU:HD13	1:C:253:LEU:HB3	2.00	0.44
1:A:209:ASN:HD21	1:C:209:ASN:HD21	1.64	0.43
1:D:60:PHE:CG	2:D:6:EDO:H12	2.53	0.43
1:B:126:ASN:O	2:B:4:EDO:H22	2.18	0.43
1:A:174:LYS:CE	3:A:1:RSH:C2	2.85	0.43
1:C:95:ARG:HG3	1:D:286:PRO:HG2	2.01	0.43
1:A:233:LEU:HD23	1:A:233:LEU:O	2.19	0.43
1:B:129:ARG:HD3	4:B:441:HOH:O	2.18	0.42
1:D:252:LEU:O	1:D:256:PRO:HD3	2.19	0.42
1:B:60:PHE:CG	1:B:61:SER:N	2.87	0.42
1:B:233:LEU:C	1:B:233:LEU:HD23	2.40	0.42
1:D:263:THR:HA	1:D:264:PRO:C	2.40	0.42
1:C:61:SER:OG	1:C:62:GLN:NE2	2.53	0.42
2:D:8:EDO:C1	4:D:456:HOH:O	2.68	0.42
1:D:233:LEU:HD23	1:D:233:LEU:C	2.41	0.41
1:B:129:ARG:NH2	2:B:4:EDO:O2	2.54	0.41
1:A:281:SER:OG	1:A:283[B]:HIS:HD2	2.04	0.41
1:A:143:MET:HE3	1:A:143:MET:HB2	1.98	0.41
1:A:77:ASP:CG	4:A:494:HOH:O	2.58	0.41
3:C:3:RSH:O1	4:C:392:HOH:O	2.21	0.41
1:D:174:LYS:NZ	3:D:4:RSH:C3	2.69	0.41
1:D:300:LYS:O	1:D:304:GLN:HG3	2.21	0.41
1:C:143:MET:HE3	1:C:143:MET:HB2	1.94	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	298/298 (100%)	291 (98%)	7 (2%)	0	100	100
1	B	297/298 (100%)	291 (98%)	6 (2%)	0	100	100
1	C	300/298 (101%)	292 (97%)	7 (2%)	1 (0%)	41	46
1	D	297/298 (100%)	291 (98%)	6 (2%)	0	100	100
All	All	1192/1192 (100%)	1165 (98%)	26 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/243 (100%)	231 (95%)	12 (5%)	25	31
1	B	241/243 (99%)	230 (95%)	11 (5%)	27	34
1	C	246/243 (101%)	233 (95%)	13 (5%)	22	27
1	D	242/243 (100%)	231 (96%)	11 (4%)	27	34
All	All	972/972 (100%)	925 (95%)	47 (5%)	25	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	77	ASP
1	A	140	LEU
1	A	143	MET
1	A	145	TYR
1	A	147	PHE
1	A	200	LEU
1	A	213	LEU
1	A	252	LEU
1	A	263	THR
1	A	275	LEU
1	A	301	THR
1	B	43	LEU
1	B	129	ARG
1	B	140	LEU
1	B	143	MET
1	B	145	TYR
1	B	147	PHE
1	B	200	LEU
1	B	213	LEU
1	B	252	LEU
1	B	263	THR
1	B	275	LEU
1	C	13	LEU
1	C	43	LEU
1	C	77	ASP
1	C	140	LEU
1	C	143	MET
1	C	145	TYR
1	C	147	PHE
1	C	200	LEU
1	C	213	LEU
1	C	252	LEU
1	C	263	THR
1	C	275	LEU
1	C	281	SER
1	D	43	LEU
1	D	129	ARG
1	D	140	LEU
1	D	143	MET
1	D	145	TYR
1	D	147	PHE
1	D	200	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	213	LEU
1	D	252	LEU
1	D	263	THR
1	D	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	305	GLN
1	B	62	GLN
1	B	102	GLN
1	B	305	GLN
1	C	62	GLN
1	C	102	GLN
1	C	305	GLN
1	D	62	GLN
1	D	305	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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
3	RSH	C	3	1	10,10,11	2.35	1 (10%)	11,12,14	2.45	6 (54%)
2	EDO	A	2	-	3,3,3	0.39	0	2,2,2	0.07	0
2	EDO	B	3	-	3,3,3	0.44	0	2,2,2	1.94	1 (50%)
2	EDO	A	5	-	3,3,3	0.41	0	2,2,2	0.67	0
3	RSH	D	4	1	10,10,11	2.31	1 (10%)	11,12,14	2.49	3 (27%)
2	EDO	C	7	-	3,3,3	0.52	0	2,2,2	0.73	0
3	RSH	A	1	1	10,10,11	2.52	2 (20%)	11,12,14	2.59	3 (27%)
2	EDO	B	4	-	3,3,3	0.26	0	2,2,2	1.13	0
2	EDO	C	1	-	3,3,3	0.71	0	2,2,2	0.93	0
2	EDO	D	6	-	3,3,3	0.32	0	2,2,2	1.82	1 (50%)
2	EDO	D	8	-	3,3,3	0.73	0	2,2,2	0.39	0
3	RSH	B	2	1	10,10,11	2.18	1 (10%)	11,12,14	2.56	3 (27%)

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
3	RSH	C	3	1	2/2/3/4	7/11/11/14	-
2	EDO	A	2	-	-	1/1/1/1	-
2	EDO	B	3	-	-	0/1/1/1	-
2	EDO	A	5	-	-	0/1/1/1	-
3	RSH	D	4	1	2/2/3/4	5/11/11/14	-
2	EDO	C	7	-	-	1/1/1/1	-
3	RSH	A	1	1	2/2/3/4	4/11/11/14	-
2	EDO	B	4	-	-	1/1/1/1	-
2	EDO	C	1	-	-	0/1/1/1	-
2	EDO	D	6	-	-	0/1/1/1	-
2	EDO	D	8	-	-	1/1/1/1	-
3	RSH	B	2	1	2/2/3/4	5/11/11/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	RSH	C2-C1	-7.14	1.34	1.50

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	RSH	C2-C1	-6.62	1.35	1.50
3	D	4	RSH	C2-C1	-6.57	1.35	1.50
3	B	2	RSH	C2-C1	-6.10	1.36	1.50
3	A	1	RSH	C6-C5	2.21	1.58	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	RSH	C3-C2-C1	6.00	128.42	112.51
3	A	1	RSH	O6-C6-C5	5.72	123.53	111.07
3	C	3	RSH	O6-C6-C5	5.17	122.35	111.07
3	D	4	RSH	C3-C2-C1	5.07	125.95	112.51
3	D	4	RSH	O6-C6-C5	4.97	121.91	111.07
3	A	1	RSH	C3-C2-C1	4.64	124.83	112.51
3	B	2	RSH	O6-C6-C5	3.82	119.41	111.07
3	C	3	RSH	C3-C2-C1	3.60	122.06	112.51
3	A	1	RSH	C6-C5-C4	3.21	120.08	113.11
3	B	2	RSH	C6-C5-C4	3.15	119.94	113.11
2	B	3	EDO	O2-C2-C1	-2.74	92.23	111.91
3	C	3	RSH	C3-C4-C5	-2.68	106.99	113.35
2	D	6	EDO	O1-C1-C2	-2.55	93.59	111.91
3	C	3	RSH	O4-C4-C5	2.28	114.42	109.72
3	D	4	RSH	C6-C5-C4	2.13	117.74	113.11
3	C	3	RSH	O1-C1-C2	2.10	120.78	114.03
3	C	3	RSH	C6-C5-C4	2.06	117.57	113.11

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	RSH	C4
3	A	1	RSH	C5
3	B	2	RSH	C4
3	B	2	RSH	C5
3	C	3	RSH	C4
3	C	3	RSH	C5
3	D	4	RSH	C4
3	D	4	RSH	C5

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	RSH	C2-C3-C4-O4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	1	RSH	C4-C5-C6-O6
3	A	1	RSH	O5-C5-C6-O6
3	B	2	RSH	C2-C3-C4-O4
3	B	2	RSH	C4-C5-C6-O6
3	B	2	RSH	O5-C5-C6-O6
3	C	3	RSH	C2-C3-C4-O4
3	C	3	RSH	C2-C3-C4-C5
3	C	3	RSH	O5-C5-C6-O6
3	D	4	RSH	C2-C3-C4-O4
3	C	3	RSH	C4-C5-C6-O6
3	D	4	RSH	O5-C5-C6-O6
3	D	4	RSH	C4-C5-C6-O6
2	D	8	EDO	O1-C1-C2-O2
3	A	1	RSH	C2-C3-C4-C5
3	B	2	RSH	C2-C3-C4-C5
3	D	4	RSH	C2-C3-C4-C5
2	B	4	EDO	O1-C1-C2-O2
2	C	7	EDO	O1-C1-C2-O2
3	C	3	RSH	O1-C1-C2-C3
3	C	3	RSH	O2-C1-C2-C3
2	A	2	EDO	O1-C1-C2-O2
3	B	2	RSH	C1-C2-C3-C4
3	C	3	RSH	C1-C2-C3-C4
3	D	4	RSH	C1-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	RSH	6	0
2	A	5	EDO	2	0
3	D	4	RSH	4	0
3	A	1	RSH	4	0
2	B	4	EDO	5	0
2	D	6	EDO	1	0
2	D	8	EDO	9	0
3	B	2	RSH	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	298/298 (100%)	-0.38	0 <a href="#">100</a>   <a href="#">100</a>	11, 19, 32, 43	0
1	B	298/298 (100%)	-0.34	2 (0%) <a href="#">87</a>   <a href="#">86</a>	11, 18, 32, 43	0
1	C	298/298 (100%)	-0.39	2 (0%) <a href="#">87</a>   <a href="#">86</a>	11, 18, 32, 43	0
1	D	298/298 (100%)	-0.42	1 (0%) <a href="#">94</a>   <a href="#">93</a>	11, 18, 32, 43	0
All	All	1192/1192 (100%)	-0.38	5 (0%) <a href="#">92</a>   <a href="#">91</a>	11, 18, 32, 43	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	LYS	2.9
1	B	309	CYS	2.6
1	D	307	LYS	2.2
1	C	307	LYS	2.2
1	C	27	ALA	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	EDO	C	7	4/4	0.80	0.25	52,55,57,58	0
2	EDO	D	8	4/4	0.82	0.17	28,29,31,33	0
2	EDO	A	5	4/4	0.89	0.13	47,47,47,48	0
3	RSH	A	1	11/12	0.90	0.14	29,34,40,41	0
2	EDO	B	4	4/4	0.92	0.20	32,33,36,37	0
3	RSH	D	4	11/12	0.93	0.12	28,32,36,36	0
2	EDO	B	3	4/4	0.94	0.17	21,23,26,30	0
3	RSH	B	2	11/12	0.94	0.11	22,28,31,33	0
3	RSH	C	3	11/12	0.94	0.11	21,27,34,37	0
2	EDO	C	1	4/4	0.94	0.11	14,15,17,20	0
2	EDO	A	2	4/4	0.95	0.13	19,19,22,25	0
2	EDO	D	6	4/4	0.97	0.12	20,24,24,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.