



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:19 PM GMT

PDB ID : 3QRC  
Title : The crystal structure of Ail, the attachment invasion locus protein of *Yersinia pestis*, in complex with the heparin analogue sucrose octasulfate  
Authors : Yamashita, S.; Lukacik, P.; Noinaj, N.; Buchanan, S.K.  
Deposited on : 2011-02-17  
Resolution : 1.85 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	184	-	-	-	X
3	C8E	B	183	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2701 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.

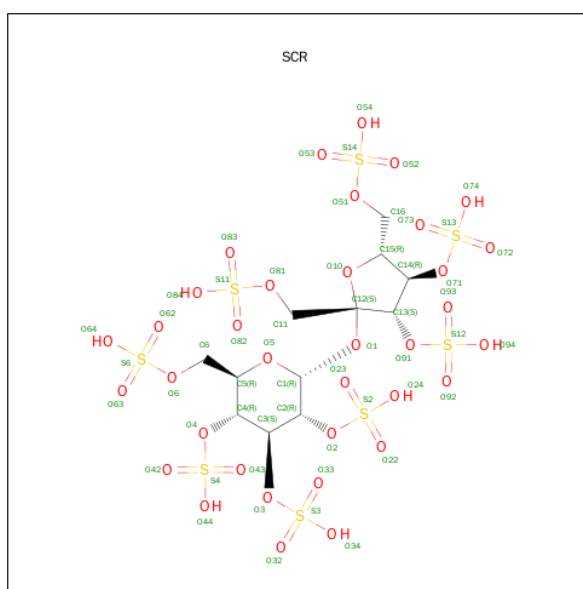
- Molecule 1 is a protein called Attachment invasion locus protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	1	0
			1188	767	198	222	1			
1	B	154	Total	C	N	O	S	0	0	0
			1190	768	202	218	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	INITIATING METHIONINE	UNP Q0WCZ9
B	26	MET	-	INITIATING METHIONINE	UNP Q0WCZ9

- Molecule 2 is SUGAR (SUCROSE OCTASULFATE) (three-letter code: SCR) (formula:  $C_{12}H_{22}O_{35}S_8$ ).



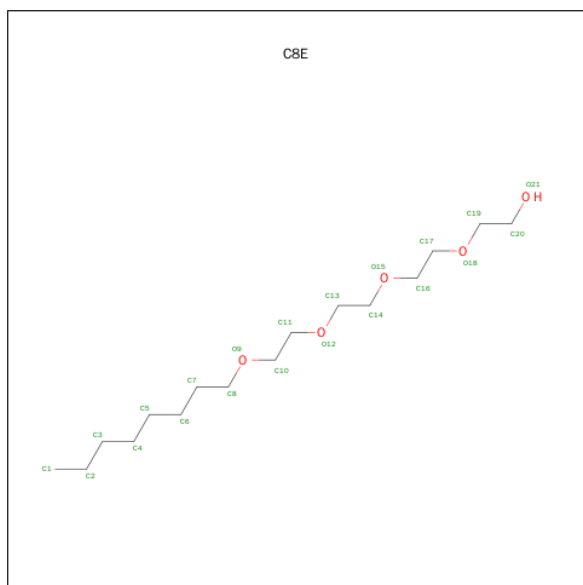
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			55	12	35	8		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			55	12	35	8		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			15	12	3		
3	B	1	Total	C	O	0	0
			9	8	1		
3	B	1	Total	C	O	0	0
			9	8	1		
3	B	1	Total	C		0	0
			8	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		

Continued on next page...

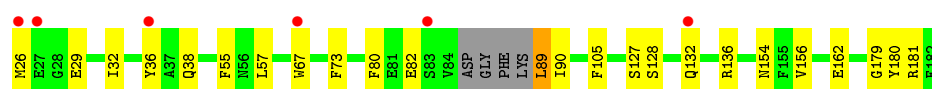
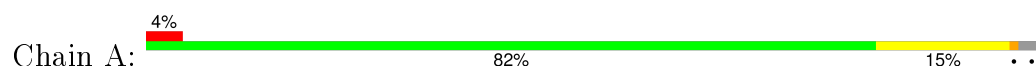
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	60	Total	O	0	0
			60	60		

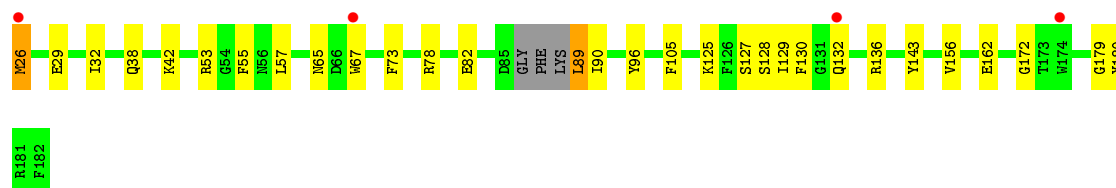
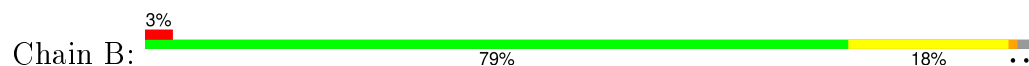
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Attachment invasion locus protein



- Molecule 1: Attachment invasion locus protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.38 Å 91.38 Å 47.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.93 – 1.85 32.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.93-1.85) 100.0 (32.93-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.85 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.204 , 0.221 0.202 , 0.219	Depositor DCC
$R_{free}$ test set	1887 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.3	EDS
Estimated twinning fraction	0.467 for -h,-k,l 0.034 for h,-h-k,-l 0.030 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 37771 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: C8E, SCR

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	0.61	2/1222 (0.2%)	0.67	1/1646 (0.1%)
1	B	0.60	2/1220 (0.2%)	0.67	1/1640 (0.1%)
All	All	0.60	4/2442 (0.2%)	0.67	2/3286 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	CD-OE2	-11.22	1.13	1.25
1	B	162	GLU	CD-OE1	-10.93	1.13	1.25
1	A	162	GLU	CD-OE1	-10.71	1.13	1.25
1	B	162	GLU	CD-OE2	-10.65	1.14	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	GLU	OE1-CD-OE2	-12.86	107.87	123.30
1	A	162	GLU	OE1-CD-OE2	-12.84	107.89	123.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1188	0	1103	28	0
1	B	1190	0	1120	34	0
2	A	55	0	20	1	0
2	B	55	0	20	1	0
3	A	30	0	51	6	0
3	B	62	0	108	8	0
4	A	61	0	0	2	0
4	B	60	0	0	1	0
All	All	2701	0	2422	58	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 12.

All (58) 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:A:36[B]:TYR:HE1	1:B:67:TRP:CH2	1.73	1.06
1:A:36[B]:TYR:CE1	1:B:67:TRP:CH2	2.55	0.95
1:A:36[B]:TYR:HE1	1:B:67:TRP:HH2	1.12	0.94
1:A:80:PHE:HZ	1:A:82:GLU:OE2	1.60	0.82
1:B:26:MET:HB3	1:B:65:ASN:OD1	1.87	0.74
1:B:53:ARG:NH1	1:B:78:ARG:NH1	2.37	0.72
1:A:136:ARG:HG2	3:A:184:C8E:H102	1.72	0.70
1:B:136:ARG:HG2	3:B:183:C8E:H101	1.76	0.67
1:A:80:PHE:CZ	1:A:82:GLU:OE2	2.47	0.65
1:B:96:TYR:CB	3:B:183:C8E:H13	2.29	0.63
1:B:82:GLU:O	1:B:89:LEU:HA	1.99	0.61
1:A:82:GLU:O	1:A:89:LEU:HA	1.98	0.61
1:A:90:ILE:HD13	1:A:128:SER:HB2	1.82	0.61
1:B:90:ILE:HD13	1:B:128:SER:HB2	1.83	0.61
1:B:96:TYR:HB2	3:B:183:C8E:H13	1.82	0.61
1:B:125:LYS:NZ	2:B:187:SCR:O74	2.34	0.60
1:B:129:ILE:HD12	1:B:130:PHE:CD2	2.36	0.60
1:A:136:ARG:HD3	3:A:184:C8E:H132	1.86	0.58
1:A:90:ILE:HD13	1:A:128:SER:CB	2.33	0.58
1:A:36[B]:TYR:CE1	1:B:67:TRP:HH2	2.03	0.56
1:B:90:ILE:HD13	1:B:128:SER:CB	2.34	0.56
1:B:67:TRP:CD1	1:B:105:PHE:CD1	2.94	0.56
1:A:36[B]:TYR:CE1	1:B:67:TRP:CZ2	2.93	0.56
1:B:26:MET:N	1:B:29:GLU:HG3	2.21	0.56
1:A:67:TRP:CD1	1:A:105:PHE:CD1	2.93	0.55
1:B:53:ARG:HH12	1:B:78:ARG:NH1	2.04	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:MET:N	1:A:29:GLU:HG3	2.20	0.55
1:B:53:ARG:HH11	1:B:78:ARG:CZ	2.20	0.55
1:A:156:VAL:HG12	1:A:179:GLY:C	2.28	0.54
1:B:156:VAL:HG12	1:B:179:GLY:C	2.29	0.54
1:A:55:PHE:HB3	1:B:105:PHE:CD1	2.43	0.53
1:B:53:ARG:NH1	1:B:78:ARG:CZ	2.72	0.52
1:A:36[B]:TYR:OH	1:A:38:GLN:NE2	2.33	0.51
1:A:154:ASN:HB3	3:A:183:C8E:H82	1.93	0.50
1:B:38:GLN:OE1	3:B:186:C8E:H22	2.12	0.49
1:B:96:TYR:HB3	3:B:183:C8E:H13	1.95	0.48
1:A:67:TRP:CD1	1:A:105:PHE:HD1	2.29	0.48
1:A:180:TYR:CE1	1:B:143:TYR:HD1	2.31	0.48
1:B:180:TYR:HB3	3:B:184:C8E:H52	1.96	0.47
1:B:67:TRP:CD1	1:B:105:PHE:HD1	2.31	0.47
1:B:172:GLY:O	3:B:186:C8E:H51	2.15	0.47
1:B:32:ILE:HD11	1:B:57:LEU:HD11	1.98	0.46
1:B:127:SER:HA	1:B:132:GLN:O	2.15	0.46
1:A:32:ILE:HD11	1:A:57:LEU:HD11	1.97	0.45
1:A:136:ARG:HE	3:A:184:C8E:C11	2.29	0.45
1:A:127:SER:HA	1:A:132:GLN:O	2.16	0.45
1:A:36[B]:TYR:CD1	1:B:67:TRP:CZ2	3.04	0.45
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.72	0.45
1:A:29:GLU:HG3	4:A:196:HOH:O	2.18	0.44
2:A:1:SCR:H1	2:A:1:SCR:H111	1.86	0.44
3:B:183:C8E:H132	3:B:183:C8E:H101	1.82	0.43
3:A:184:C8E:H101	3:A:184:C8E:H71	1.31	0.43
1:B:55:PHE:CZ	1:B:73:PHE:HE2	2.37	0.42
1:A:80:PHE:CZ	1:A:82:GLU:HG3	2.55	0.42
1:A:55:PHE:CZ	1:A:73:PHE:HE2	2.38	0.41
1:A:181:ARG:NH2	4:A:196:HOH:O	2.47	0.41
1:B:65:ASN:HB2	4:B:228:HOH:O	2.21	0.41
3:A:184:C8E:H101	3:A:184:C8E:H131	1.45	0.41

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	150/157 (96%)	148 (99%)	2 (1%)	0	100	100
1	B	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
All	All	300/314 (96%)	295 (98%)	5 (2%)	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	114/128 (89%)	113 (99%)	1 (1%)	84	79
1	B	114/128 (89%)	112 (98%)	2 (2%)	66	52
All	All	228/256 (89%)	225 (99%)	3 (1%)	76	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	B	26	MET
1	B	89	LEU

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
2	SCR	A	1	-	56,56,56	4.48	33 (58%)	79,92,92	1.80	16 (20%)
3	C8E	A	183	-	8,8,20	0.25	0	7,7,19	0.59	0
3	C8E	A	184	-	20,20,20	0.40	0	19,19,19	0.51	0
3	C8E	B	1	-	20,20,20	0.38	0	19,19,19	0.37	0
3	C8E	B	183	-	14,14,20	0.39	0	13,13,19	0.43	0
3	C8E	B	184	-	8,8,20	0.23	0	7,7,19	0.63	0
3	C8E	B	185	-	8,8,20	0.24	0	7,7,19	0.53	0
3	C8E	B	186	-	7,7,20	0.28	0	6,6,19	0.33	0
2	SCR	B	187	-	56,56,56	4.86	43 (76%)	79,92,92	1.61	14 (17%)

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	SCR	A	1	-	-	0/48/88/88	0/2/2/2
3	C8E	A	183	-	-	0/6/6/18	0/0/0/0
3	C8E	A	184	-	-	0/18/18/18	0/0/0/0
3	C8E	B	1	-	-	0/18/18/18	0/0/0/0
3	C8E	B	183	-	-	0/12/12/18	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	B	184	-	-	0/6/6/18	0/0/0/0
3	C8E	B	185	-	-	0/6/6/18	0/0/0/0
3	C8E	B	186	-	-	0/5/5/18	0/0/0/0
2	SCR	B	187	-	-	0/48/88/88	0/2/2/2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	SCR	C4-C3	-21.13	1.06	1.52
2	A	1	SCR	C4-C3	-20.07	1.09	1.52
2	A	1	SCR	O5-C1	-12.54	1.09	1.41
2	B	187	SCR	O5-C1	-12.30	1.10	1.41
2	A	1	SCR	C11-C12	-8.02	1.42	1.52
2	B	187	SCR	C11-C12	-7.52	1.42	1.52
2	A	1	SCR	O3-C3	-5.01	1.35	1.46
2	A	1	SCR	C12-C13	-4.12	1.47	1.54
2	A	1	SCR	O2-C2	-3.81	1.38	1.46
2	A	1	SCR	O81-C11	-3.77	1.39	1.45
2	B	187	SCR	C12-C13	-3.66	1.48	1.54
2	B	187	SCR	O3-C3	-3.65	1.38	1.46
2	A	1	SCR	O4-C4	-3.44	1.39	1.46
2	A	1	SCR	O91-C13	-3.42	1.38	1.47
2	B	187	SCR	O2-C2	-3.23	1.39	1.46
2	A	1	SCR	O71-C14	-3.22	1.39	1.46
2	B	187	SCR	O4-C4	-3.16	1.39	1.46
2	B	187	SCR	O81-C11	-2.84	1.40	1.45
2	A	1	SCR	O10-C12	-2.63	1.36	1.42
2	B	187	SCR	O71-C14	-2.53	1.41	1.46
2	B	187	SCR	O91-C13	-2.45	1.41	1.47
2	A	1	SCR	C14-C15	-2.42	1.45	1.52
2	B	187	SCR	O10-C12	-2.16	1.37	1.42
2	B	187	SCR	C14-C15	-2.01	1.47	1.52
2	B	187	SCR	O44-S4	2.05	1.61	1.50
2	B	187	SCR	O94-S12	2.09	1.61	1.50
2	B	187	SCR	O4-S4	2.10	1.63	1.57
2	B	187	SCR	O3-S3	2.11	1.63	1.57
2	B	187	SCR	O54-S14	2.28	1.62	1.50
2	A	1	SCR	O22-S2	2.33	1.53	1.45
2	B	187	SCR	O91-S12	2.34	1.64	1.57
2	A	1	SCR	O32-S3	2.39	1.53	1.45
2	B	187	SCR	O2-S2	2.40	1.64	1.57
2	A	1	SCR	O33-S3	2.48	1.54	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SCR	O23-S2	2.51	1.54	1.45
2	B	187	SCR	O64-S6	2.57	1.63	1.50
2	B	187	SCR	O71-S13	2.64	1.65	1.57
2	A	1	SCR	O81-S11	2.79	1.66	1.57
2	A	1	SCR	O43-S4	2.83	1.55	1.45
2	A	1	SCR	O93-S12	2.91	1.55	1.45
2	A	1	SCR	O6-S6	3.01	1.66	1.57
2	A	1	SCR	O42-S4	3.14	1.56	1.45
2	A	1	SCR	C4-C5	3.14	1.61	1.52
2	B	187	SCR	O6-S6	3.25	1.67	1.57
2	B	187	SCR	C4-C5	3.28	1.62	1.52
2	B	187	SCR	O81-S11	3.31	1.67	1.57
2	A	1	SCR	O82-S11	3.46	1.57	1.45
2	A	1	SCR	O83-S11	3.53	1.58	1.45
2	B	187	SCR	O92-S12	3.60	1.58	1.45
2	B	187	SCR	O51-S14	3.62	1.68	1.57
2	A	1	SCR	O73-S13	3.84	1.59	1.45
2	A	1	SCR	O51-S14	3.91	1.69	1.57
2	A	1	SCR	O63-S6	4.10	1.60	1.45
2	B	187	SCR	O33-S3	4.22	1.60	1.45
2	A	1	SCR	O72-S13	4.34	1.61	1.45
2	B	187	SCR	O22-S2	4.40	1.61	1.45
2	B	187	SCR	O23-S2	4.45	1.61	1.45
2	B	187	SCR	O32-S3	4.46	1.61	1.45
2	B	187	SCR	O43-S4	4.49	1.61	1.45
2	A	1	SCR	O53-S14	4.50	1.61	1.45
2	A	1	SCR	C1-C2	4.54	1.64	1.52
2	B	187	SCR	O42-S4	4.57	1.61	1.45
2	B	187	SCR	O93-S12	4.64	1.62	1.45
2	B	187	SCR	C1-C2	4.72	1.65	1.52
2	B	187	SCR	O82-S11	4.78	1.62	1.45
2	B	187	SCR	O73-S13	4.78	1.62	1.45
2	A	1	SCR	O52-S14	4.87	1.63	1.45
2	B	187	SCR	O83-S11	4.91	1.63	1.45
2	B	187	SCR	O63-S6	4.94	1.63	1.45
2	B	187	SCR	O72-S13	5.12	1.63	1.45
2	B	187	SCR	O53-S14	5.23	1.64	1.45
2	B	187	SCR	O52-S14	5.24	1.64	1.45
2	A	1	SCR	O5-C5	6.36	1.60	1.44
2	B	187	SCR	O5-C5	7.32	1.62	1.44
2	A	1	SCR	C3-C2	8.51	1.70	1.52
2	B	187	SCR	C3-C2	8.74	1.71	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SCR	C12-O1-C1	-3.50	108.30	117.53
2	B	187	SCR	C12-O1-C1	-3.41	108.55	117.53
2	A	1	SCR	O10-C15-C14	-3.18	98.15	103.52
2	B	187	SCR	O5-C1-C2	-2.82	103.79	109.47
2	B	187	SCR	O63-S6-O62	-2.75	100.49	112.46
2	B	187	SCR	O10-C15-C14	-2.53	99.25	103.52
2	B	187	SCR	O64-S6-O62	-2.27	100.03	108.56
2	A	1	SCR	O5-C1-C2	-2.23	104.98	109.47
2	A	1	SCR	O6-S6-O63	2.01	113.02	106.77
2	A	1	SCR	O3-S3-O33	2.11	113.72	106.86
2	A	1	SCR	O71-C14-C15	2.18	114.82	109.09
2	A	1	SCR	O6-C6-C5	2.23	112.19	107.90
2	B	187	SCR	O5-C5-C6	2.35	111.41	106.61
2	A	1	SCR	O5-C5-C6	2.57	111.86	106.61
2	A	1	SCR	O81-S11-O83	2.63	114.95	106.77
2	A	1	SCR	C4-O4-S4	2.68	123.88	118.77
2	B	187	SCR	O71-C14-C15	2.69	116.14	109.09
2	A	1	SCR	O5-C5-C4	2.71	115.47	109.75
2	A	1	SCR	O4-C4-C3	2.74	114.54	108.48
2	B	187	SCR	O10-C15-C16	2.89	116.06	109.49
2	B	187	SCR	O64-S6-O63	2.97	119.73	108.56
2	B	187	SCR	O6-S6-O63	3.07	116.31	106.77
2	A	1	SCR	O64-S6-O63	3.08	120.13	108.56
2	B	187	SCR	O6-C6-C5	3.18	114.01	107.90
2	A	1	SCR	O10-C15-C16	3.32	117.05	109.49
2	B	187	SCR	O5-C5-C4	3.44	117.00	109.75
2	B	187	SCR	O3-C3-C4	3.52	116.27	108.48
2	A	1	SCR	O3-C3-C4	4.17	117.71	108.48
2	B	187	SCR	O51-C16-C15	6.19	119.82	107.90
2	A	1	SCR	O51-C16-C15	8.27	123.81	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SCR	1	0
3	A	183	C8E	1	0
3	A	184	C8E	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	183	C8E	5	0
3	B	184	C8E	1	0
3	B	186	C8E	2	0
2	B	187	SCR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	153/157 (97%)	-0.11	6 (3%) 43 40	18, 32, 67, 109	0
1	B	154/157 (98%)	-0.16	4 (2%) 59 57	18, 32, 70, 119	0
All	All	307/314 (97%)	-0.13	10 (3%) 50 47	18, 32, 69, 119	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	MET	5.9
1	A	27	GLU	5.6
1	A	26	MET	4.9
1	A	67	TRP	4.0
1	B	67	TRP	3.0
1	A	83	SER	2.6
1	B	174	TRP	2.3
1	A	132	GLN	2.2
1	B	132	GLN	2.1
1	A	36[A]	TYR	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
3	C8E	B	183	15/21	0.90	0.17	4.10	26,45,69,69	0
3	C8E	A	184	21/21	0.88	0.17	3.44	23,51,66,72	0
3	C8E	B	1	21/21	0.95	0.11	1.93	34,56,87,92	0
3	C8E	B	185	9/21	0.95	0.11	1.59	31,44,56,61	0
3	C8E	B	186	8/21	0.84	0.15	1.37	45,50,70,74	0
3	C8E	A	183	9/21	0.81	0.14	1.13	37,40,60,70	0
3	C8E	B	184	9/21	0.87	0.13	1.10	33,40,60,74	0
2	SCR	B	187	55/55	0.96	0.10	0.79	33,46,86,96	0
2	SCR	A	1	55/55	0.96	0.09	-0.05	33,46,86,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.