



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2R8E
Title : Crystal structure of YrbI from Escherichia coli in complex with Mg
Authors : Tsodikov, O.V.; Aggarwal, P.; Rubin, J.R.; Stuckey, J.A.; Woodard, R.; Biswas, T.
Deposited on : 2007-09-10
Resolution : 1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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

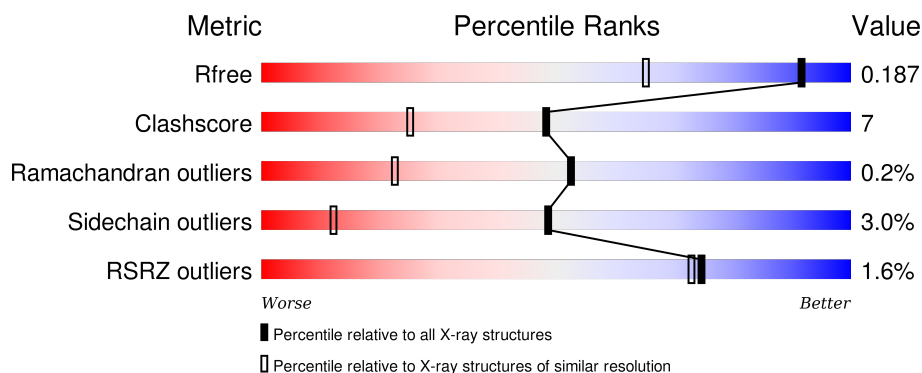
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.



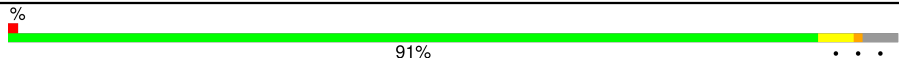


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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 ≥ 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	188	<div> <div>2%</div> <div>79%</div> <div>11%</div> <div>8%</div> </div>
1	B	188	<div> <div>3%</div> <div>79%</div> <div>11%</div> <div>8%</div> </div>
1	C	188	<div> <div>2%</div> <div>80%</div> <div>10%</div> <div>8%</div> </div>
1	D	188	<div> <div>3%</div> <div>77%</div> <div>12%</div> <div>8%</div> </div>
1	E	188	<div> <div>0%</div> <div>93%</div> <div>5%</div> <div>2%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	
1	G	188	
1	H	188	

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	MG	H	208	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12808 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 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1289	817	221	244	7			
1	B	173	Total	C	N	O	S	0	0	0
			1289	817	221	244	7			
1	C	173	Total	C	N	O	S	0	0	0
			1286	816	221	242	7			
1	D	173	Total	C	N	O	S	0	0	0
			1289	817	221	244	7			
1	E	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	F	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	G	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	H	181	Total	C	N	O	S	0	0	0
			1351	855	232	257	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Cl 1	0	0
3	G	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0

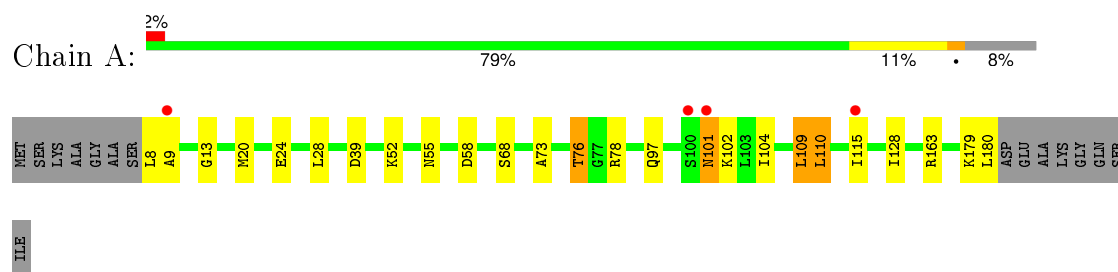
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total 274	O 274	0	0
4	B	270	Total 270	O 270	0	0
4	C	276	Total 276	O 276	0	0
4	D	277	Total 277	O 277	0	0
4	E	283	Total 283	O 283	0	0
4	F	274	Total 274	O 274	0	0
4	G	282	Total 282	O 282	0	0
4	H	296	Total 296	O 296	0	0

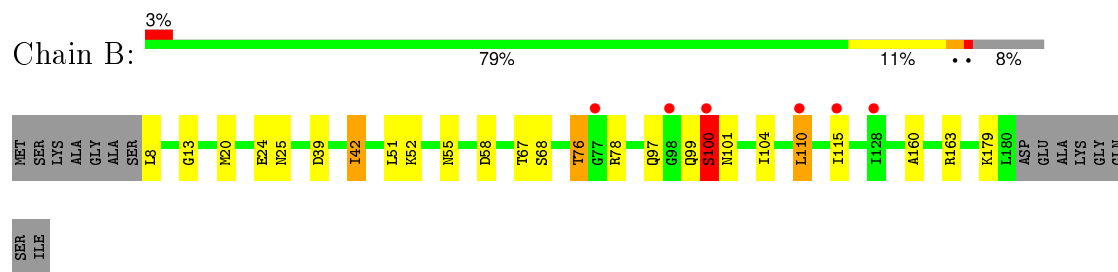
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

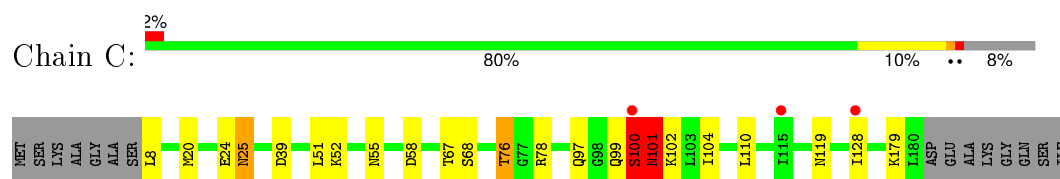
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



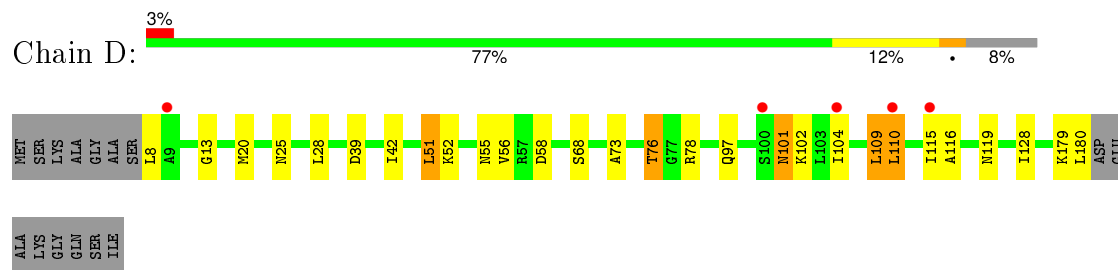
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



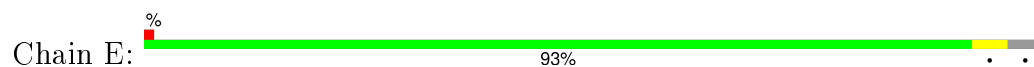
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



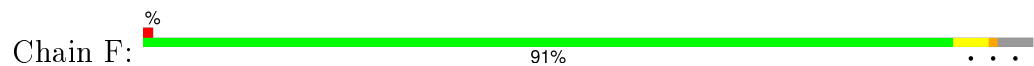
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



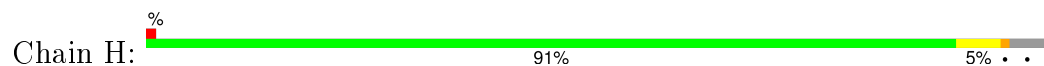
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



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- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.88 Å 83.00 Å 85.86 Å 118.84° 118.77° 90.06°	Depositor
Resolution (Å)	29.34 – 1.40 29.34 – 1.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.34-1.40) 68.3 (29.34-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.30 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.159 , 0.188 0.157 , 0.187	Depositor DCC
R_{free} test set	15730 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
Estimated twinning fraction	0.467 for k,-h,h+l 0.467 for -k,h,k+l 0.015 for h,-k,-h-l 0.015 for -h,k,-k-l 0.015 for k,h,-h-k-l 0.014 for -k,-h,-l 0.477 for -h,-k,h+k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 331074 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12808	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

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	0.51	0/1305	0.70	1/1772 (0.1%)
1	B	0.53	0/1305	0.74	1/1772 (0.1%)
1	C	0.50	0/1302	0.72	2/1768 (0.1%)
1	D	0.51	0/1305	0.68	1/1772 (0.1%)
1	E	0.49	0/1368	0.64	0/1853
1	F	0.50	0/1368	0.64	0/1853
1	G	0.50	0/1372	0.70	1/1858 (0.1%)
1	H	0.48	0/1367	0.65	0/1852
All	All	0.50	0/10692	0.68	6/14500 (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	B	1	2
1	C	2	2
All	All	3	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	76	THR	CB-CA-C	-7.76	90.66	111.60
1	B	100	SER	N-CA-C	6.61	128.83	111.00
1	C	100	SER	N-CA-C	6.10	127.47	111.00
1	A	101	ASN	CB-CA-C	-5.31	99.77	110.40
1	D	51	LEU	CA-CB-CG	5.28	127.43	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	100	SER	CA
1	C	100	SER	CA
1	C	101	ASN	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	SER	Peptide
1	B	99	GLN	Peptide
1	C	100	SER	Peptide
1	C	99	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	1289	0	1315	26	0
1	B	1289	0	1315	32	0
1	C	1286	0	1313	23	0
1	D	1289	0	1315	33	0
1	E	1352	0	1381	10	0
1	F	1352	0	1381	8	0
1	G	1356	0	1385	11	0
1	H	1351	0	1386	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	274	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	270	0	0	19	0
4	C	276	0	0	16	0
4	D	277	0	0	18	0
4	E	283	0	0	9	0
4	F	274	0	0	9	0
4	G	282	0	0	8	0
4	H	296	0	0	8	0
All	All	12808	0	10791	156	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.

The worst 5 of 156 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:E:163:ARG:HD2	4:E:569:HOH:O	1.05	1.23
1:B:39:ASP:HB2	4:B:380:HOH:O	1.39	1.21
1:C:39:ASP:HB2	4:C:373:HOH:O	1.41	1.19
1:C:52:LYS:HG3	4:C:267:HOH:O	1.47	1.15
1:A:52:LYS:HG3	4:A:284:HOH:O	1.47	1.14

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	171/188 (91%)	168 (98%)	3 (2%)	0	100	100
1	B	171/188 (91%)	167 (98%)	3 (2%)	1 (1%)	30	8
1	C	171/188 (91%)	166 (97%)	3 (2%)	2 (1%)	16	2
1	D	171/188 (91%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	F	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	G	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	H	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
All	All	1400/1504 (93%)	1376 (98%)	21 (2%)	3 (0%)	52	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	SER
1	C	100	SER
1	C	101	ASN

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	134/147 (91%)	130 (97%)	4 (3%)	48	12
1	B	134/147 (91%)	129 (96%)	5 (4%)	41	9
1	C	133/147 (90%)	128 (96%)	5 (4%)	40	8
1	D	134/147 (91%)	127 (95%)	7 (5%)	29	4
1	E	141/147 (96%)	139 (99%)	2 (1%)	74	45
1	F	141/147 (96%)	138 (98%)	3 (2%)	61	24
1	G	142/147 (97%)	137 (96%)	5 (4%)	43	9
1	H	141/147 (96%)	139 (99%)	2 (1%)	74	45
All	All	1100/1176 (94%)	1067 (97%)	33 (3%)	48	12

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	ASN

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Mol	Chain	Res	Type
1	D	109	LEU
1	G	181	ASP
1	D	51	LEU
1	D	76	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	94	HIS
1	F	94	HIS
1	H	94	HIS
1	E	119	ASN
1	F	55	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

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, 95th 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 ²)	Q<0.9
1	A	173/188 (92%)	0.06	4 (2%) 64 62	12, 18, 27, 34	0
1	B	173/188 (92%)	0.15	6 (3%) 48 44	12, 18, 27, 32	0
1	C	173/188 (92%)	0.05	3 (1%) 73 71	12, 18, 27, 33	0
1	D	173/188 (92%)	0.12	5 (2%) 55 52	12, 18, 27, 34	0
1	E	181/188 (96%)	-0.11	1 (0%) 90 89	12, 18, 25, 31	0
1	F	181/188 (96%)	-0.05	1 (0%) 90 89	12, 18, 25, 31	0
1	G	181/188 (96%)	-0.02	0 100 100	12, 18, 25, 31	0
1	H	181/188 (96%)	0.10	2 (1%) 82 81	12, 18, 25, 33	0
All	All	1416/1504 (94%)	0.04	22 (1%) 74 73	12, 18, 27, 34	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	SER	5.7
1	A	100	SER	4.8
1	H	8	LEU	4.6
1	D	100	SER	4.6
1	B	100	SER	4.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 95th 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 ²)	Q<0.9
2	MG	H	208	1/1	0.99	0.13	4.29	13,13,13,13	0
2	MG	A	201	1/1	1.00	0.06	-1.19	12,12,12,12	0
3	CL	E	306	1/1	0.97	0.06	-1.80	17,17,17,17	0
2	MG	C	203	1/1	0.99	0.06	-1.85	12,12,12,12	0
2	MG	E	205	1/1	0.98	0.06	-1.86	13,13,13,13	0
2	MG	D	204	1/1	0.99	0.05	-2.04	13,13,13,13	0
3	CL	H	308	1/1	0.97	0.05	-2.22	17,17,17,17	0
2	MG	B	202	1/1	0.99	0.06	-2.24	13,13,13,13	0
3	CL	F	305	1/1	0.98	0.04	-2.53	17,17,17,17	0
2	MG	F	206	1/1	0.98	0.05	-2.66	13,13,13,13	0
2	MG	G	207	1/1	0.98	0.05	-3.36	13,13,13,13	0
3	CL	G	307	1/1	0.99	0.04	-3.59	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.