



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:50 pm GMT

PDB ID : 1PB0  
Title : YCDX PROTEIN IN AUTOINHIBITED STATE  
Authors : Teplyakov, A.; Obmolova, G.; Khil, P.P.; Camerini-Otero, R.D.; Gilliland, G.L.  
Deposited on : 2003-05-14  
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtrriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

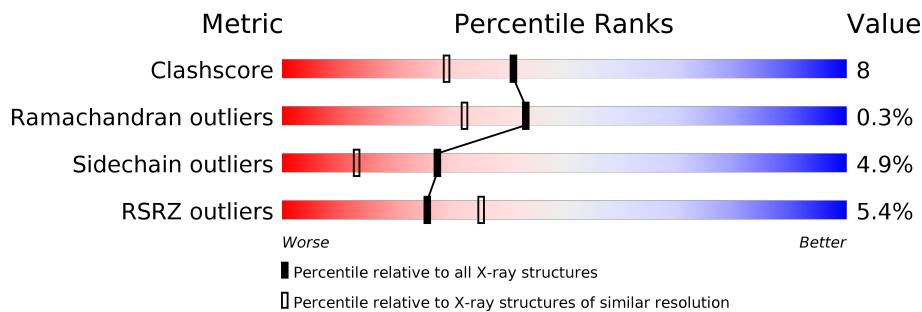
# 1 Overall quality at a glance

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))
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (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	245	 3% 86% 9% . .
1	B	245	 9% 73% 18% 5% .
1	C	245	 3% 84% 10% . .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6181 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 Hypothetical protein ycdX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	236	1813	1149	317	336	11	0	0	1
1	B	235	1811	1148	316	336	11	0	0	0
1	C	235	1811	1148	316	336	11	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

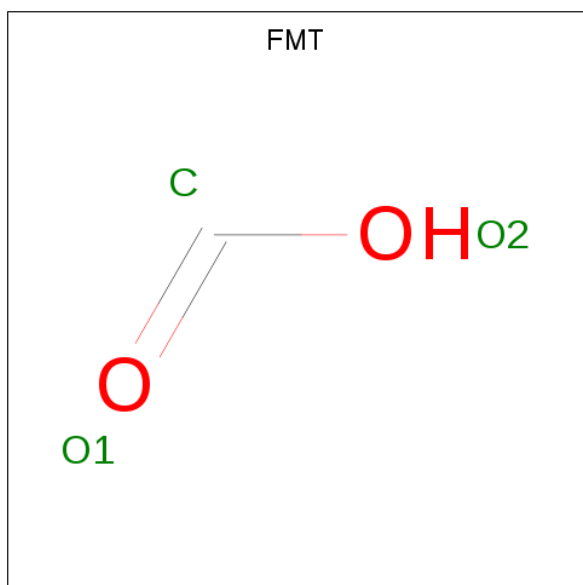
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Zn 3	0	0
2	A	3	Total 3	Zn 3	0	0
2	C	3	Total 3	Zn 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

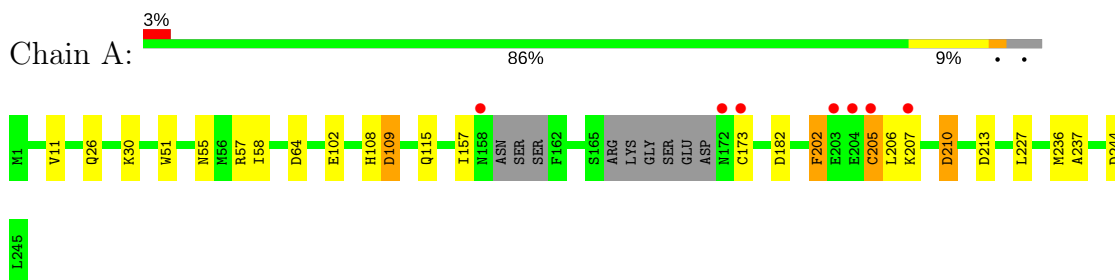
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total	O	0	0
			267	267		
5	B	176	Total	O	0	0
			176	176		
5	C	256	Total	O	0	0
			256	256		

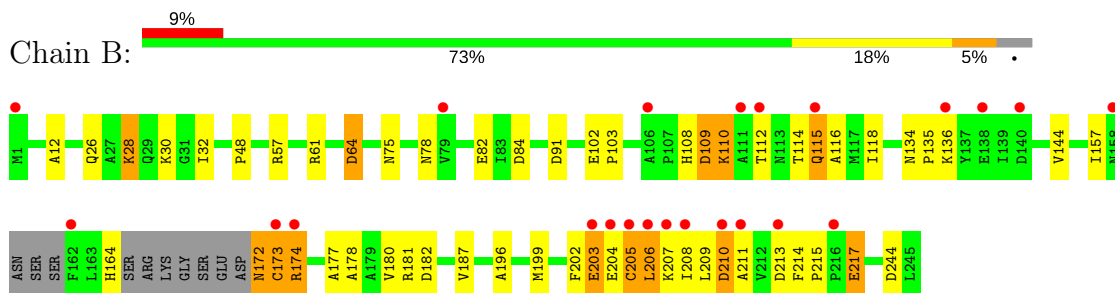
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

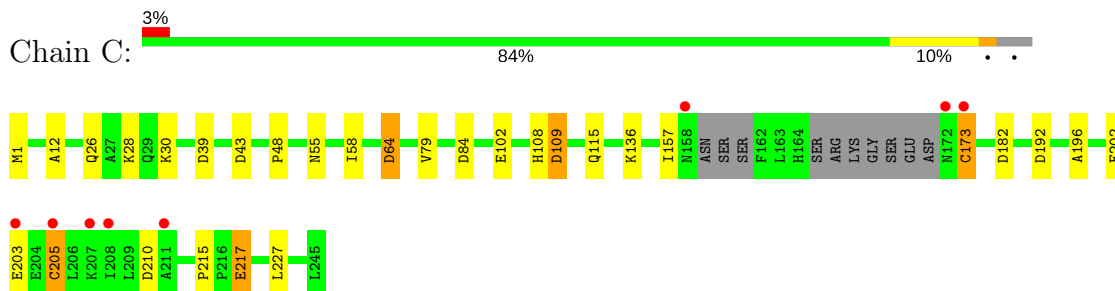
- Molecule 1: Hypothetical protein ycdX



- Molecule 1: Hypothetical protein ycdX



- Molecule 1: Hypothetical protein ycdX



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.13Å 77.33Å 82.28Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 20.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-1.95) 97.9 (20.97-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.164 , (Not available) 0.169 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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, 0.333 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: ZN, FMT, SO4

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	0.66	0/1856	0.82	6/2518 (0.2%)
1	B	0.56	0/1854	0.80	8/2515 (0.3%)
1	C	0.63	0/1854	0.83	8/2515 (0.3%)
All	All	0.62	0/5564	0.82	22/7548 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	ASP	CB-CG-OD2	8.06	125.56	118.30
1	B	84	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	84	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	64	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	39	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	43	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	210	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	244	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	213	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	182	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	213	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	244	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	91	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	182	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	64	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	109	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	182	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	210	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	64	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	109	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	210	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ASP	CB-CG-OD2	5.05	122.84	118.30

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	1813	0	1766	16	0
1	B	1811	0	1765	49	0
1	C	1811	0	1765	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	3	0	1	0	0
4	B	9	0	3	1	0
4	C	6	0	2	0	0
5	A	267	0	0	1	0
5	B	176	0	0	3	0
5	C	256	0	0	0	0
All	All	6181	0	5302	83	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 8.

All (83) 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:C:26:GLN:NE2	1:C:30:LYS:HE3	1.35	1.34
1:A:26:GLN:NE2	1:A:30:LYS:HE3	1.64	1.10
1:C:26:GLN:HE21	1:C:30:LYS:CE	1.71	1.03
1:C:26:GLN:NE2	1:C:30:LYS:CE	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HE21	1:A:30:LYS:HE3	1.33	0.89
1:B:28:LYS:HD2	1:B:64:ASP:HB3	1.51	0.88
1:C:26:GLN:HE21	1:C:30:LYS:HE3	1.08	0.88
1:B:78:ASN:OD1	1:B:82:GLU:HG3	1.76	0.84
1:B:28:LYS:HD2	1:B:64:ASP:CB	2.06	0.83
1:B:115:GLN:HE21	1:B:115:GLN:N	1.80	0.79
1:A:26:GLN:HE21	1:A:30:LYS:CE	1.96	0.78
1:C:102:GLU:OE1	1:C:136:LYS:HE2	1.87	0.74
1:A:202:PHE:O	1:A:206:LEU:HG	1.90	0.72
1:B:173:CYS:SG	1:B:205:CYS:HB3	2.30	0.71
1:B:174:ARG:HG3	1:B:208:ILE:CG2	2.21	0.71
1:B:217:GLU:CD	1:B:217:GLU:H	1.93	0.70
1:B:114:THR:O	1:B:115:GLN:C	2.30	0.68
1:B:26:GLN:HG2	1:B:196:ALA:O	1.94	0.68
1:B:174:ARG:HG3	1:B:208:ILE:HG21	1.75	0.67
1:C:79:VAL:HB	1:C:115:GLN:HE21	1.62	0.65
1:B:206:LEU:O	1:B:209:LEU:HB2	1.97	0.65
1:B:136:LYS:HE3	1:B:164:HIS:C	2.17	0.64
1:B:26:GLN:HG3	1:B:30:LYS:HE3	1.79	0.64
1:A:157:ILE:HG22	1:A:205:CYS:SG	2.38	0.64
1:B:115:GLN:H	1:B:115:GLN:HE21	1.43	0.63
1:B:26:GLN:CG	1:B:30:LYS:HE3	2.28	0.63
1:C:173:CYS:SG	1:C:205:CYS:HB3	2.39	0.62
1:C:26:GLN:HE21	1:C:30:LYS:NZ	1.95	0.62
1:B:157:ILE:CG2	1:B:205:CYS:HB2	2.28	0.62
1:B:115:GLN:CA	1:B:115:GLN:HE21	2.12	0.61
1:B:134:ASN:OD1	1:B:136:LYS:HG3	2.00	0.61
1:A:30:LYS:HD2	5:A:1378:HOH:O	2.02	0.59
1:A:227:LEU:C	1:A:227:LEU:HD13	2.24	0.58
1:A:157:ILE:CG2	1:A:205:CYS:HB2	2.34	0.57
1:B:28:LYS:CD	1:B:64:ASP:HB3	2.30	0.57
1:B:75:ASN:HB3	5:B:1421:HOH:O	2.06	0.56
1:C:217:GLU:H	1:C:217:GLU:CD	2.09	0.56
1:A:26:GLN:HE21	1:A:30:LYS:NZ	2.04	0.55
1:A:157:ILE:CG2	1:A:205:CYS:CB	2.85	0.55
1:C:157:ILE:HG22	1:C:205:CYS:SG	2.48	0.54
1:B:214:PHE:CG	1:B:215:PRO:HD2	2.43	0.54
1:B:157:ILE:HG22	1:B:205:CYS:SG	2.48	0.54
1:B:118:ILE:HG13	1:B:144:VAL:HG22	1.91	0.53
1:A:157:ILE:HG21	1:A:205:CYS:HB2	1.91	0.52
1:B:177:ALA:HB1	1:B:209:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:NE2	1:A:30:LYS:CE	2.50	0.52
1:C:26:GLN:HG2	1:C:196:ALA:O	2.10	0.52
1:B:103:PRO:HB2	5:B:1460:HOH:O	2.10	0.51
1:B:108:HIS:HB3	1:B:112:THR:HB	1.93	0.51
1:B:180:VAL:HG11	1:B:187:VAL:HG13	1.93	0.51
1:B:26:GLN:HG3	1:B:30:LYS:HD2	1.93	0.49
1:C:227:LEU:C	1:C:227:LEU:HD13	2.33	0.49
1:B:174:ARG:HG3	1:B:208:ILE:HG23	1.95	0.48
1:B:109:ASP:O	1:B:112:THR:N	2.47	0.48
1:B:217:GLU:N	1:B:217:GLU:CD	2.66	0.48
1:C:215:PRO:HB2	1:C:217:GLU:OE2	2.13	0.48
1:B:12:ALA:HB1	1:B:48:PRO:HB3	1.96	0.48
1:B:32:ILE:CD1	1:B:199:MET:HG2	2.44	0.47
1:C:157:ILE:HG21	1:C:205:CYS:HB2	1.97	0.46
1:A:108:HIS:CG	1:A:109:ASP:H	2.34	0.46
1:B:32:ILE:HD12	1:B:199:MET:HG2	1.97	0.46
1:C:108:HIS:CG	1:C:109:ASP:H	2.35	0.45
1:A:236:MET:HG2	1:A:237:ALA:O	2.17	0.45
1:B:178:ALA:O	1:B:181:ARG:HB3	2.16	0.45
1:B:157:ILE:CG2	1:B:205:CYS:CB	2.96	0.44
1:B:172:ASN:N	1:B:172:ASN:OD1	2.51	0.44
1:B:208:ILE:O	1:B:211:ALA:HB3	2.17	0.43
1:B:103:PRO:CB	5:B:1460:HOH:O	2.65	0.43
1:B:114:THR:C	1:B:116:ALA:N	2.72	0.43
1:C:28:LYS:HD2	1:C:64:ASP:HB3	2.01	0.43
1:C:157:ILE:CG2	1:C:205:CYS:CB	2.97	0.43
1:B:109:ASP:O	1:B:110:LYS:C	2.57	0.42
1:B:134:ASN:HA	1:B:135:PRO:HD3	1.90	0.42
1:C:12:ALA:HB1	1:C:48:PRO:HB3	2.02	0.41
1:B:109:ASP:OD1	1:B:110:LYS:N	2.53	0.41
1:B:174:ARG:CG	1:B:208:ILE:HG23	2.50	0.41
1:B:61:ARG:H	4:B:1326:FMT:C	2.34	0.41
1:A:55:ASN:O	1:A:58:ILE:HG12	2.21	0.41
1:A:51:TRP:HH2	1:B:103:PRO:HG3	1.86	0.41
1:C:55:ASN:O	1:C:58:ILE:HG12	2.21	0.41
1:B:203:GLU:HG3	1:B:203:GLU:H	1.42	0.40
1:B:157:ILE:HG21	1:B:205:CYS:HB2	2.01	0.40
1:B:102:GLU:N	1:B:103:PRO:CD	2.84	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	230/245 (94%)	224 (97%)	5 (2%)	1 (0%)	36	24
1	B	229/245 (94%)	216 (94%)	12 (5%)	1 (0%)	36	24
1	C	229/245 (94%)	221 (96%)	8 (4%)	0	100	100
All	All	688/735 (94%)	661 (96%)	25 (4%)	2 (0%)	43	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	B	110	LYS

### 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	190/200 (95%)	182 (96%)	8 (4%)	32	18
1	B	190/200 (95%)	176 (93%)	14 (7%)	15	5
1	C	190/200 (95%)	184 (97%)	6 (3%)	42	30
All	All	570/600 (95%)	542 (95%)	28 (5%)	27	13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG

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Mol	Chain	Res	Type
1	A	102	GLU
1	A	115	GLN
1	A	173	CYS
1	A	202	PHE
1	A	205	CYS
1	A	207	LYS
1	A	210	ASP
1	B	28	LYS
1	B	57	ARG
1	B	115	GLN
1	B	172	ASN
1	B	173	CYS
1	B	174	ARG
1	B	202	PHE
1	B	203	GLU
1	B	204	GLU
1	B	205	CYS
1	B	206	LEU
1	B	207	LYS
1	B	210	ASP
1	B	217	GLU
1	C	1	MET
1	C	173	CYS
1	C	202	PHE
1	C	203	GLU
1	C	205	CYS
1	C	217	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	B	115	GLN
1	B	172	ASN
1	C	26	GLN
1	C	29	GLN
1	C	115	GLN

### 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](#)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\# Z  > 2$
3	SO4	A	1305	-	4,4,4	0.31	0	6,6,6	0.31	0
4	FMT	A	1306	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	1324	-	4,4,4	0.14	0	6,6,6	0.39	0
4	FMT	B	1307	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1318	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1326	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	B	1334	-	4,4,4	0.15	0	6,6,6	0.39	0
4	FMT	C	1317	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	1336	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	C	1344	-	4,4,4	0.21	0	6,6,6	0.25	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
3	SO4	A	1305	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1306	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1324	-	-	0/0/0/0	0/0/0/0
4	FMT	B	1307	-	-	0/0/0/0	0/0/0/0
4	FMT	B	1318	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMT	B	1326	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1334	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1317	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1336	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1344	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1326	FMT	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

### 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	236/245 (96%)	-0.26	7 (2%) 50 59	10, 17, 45, 68	0
1	B	235/245 (95%)	0.33	23 (9%) 7 13	10, 25, 61, 99	0
1	C	235/245 (95%)	-0.24	8 (3%) 45 55	10, 17, 44, 72	0
All	All	706/735 (96%)	-0.06	38 (5%) 26 35	10, 19, 53, 99	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	CYS	5.3
1	B	174	ARG	5.1
1	B	204	GLU	4.9
1	B	106	ALA	4.8
1	B	173	CYS	4.6
1	A	204	GLU	4.2
1	B	203	GLU	4.1
1	B	111	ALA	3.8
1	B	162	PHE	3.8
1	C	173	CYS	3.7
1	C	158	ASN	3.7
1	C	208	ILE	3.4
1	B	208	ILE	3.3
1	B	211	ALA	3.3
1	A	205	CYS	3.3
1	A	158	ASN	3.2
1	B	206	LEU	3.1
1	B	115	GLN	3.1
1	B	158	ASN	3.0
1	A	173	CYS	2.8
1	C	207	LYS	2.7
1	B	216	PRO	2.7
1	B	140	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	203	GLU	2.5
1	A	172	ASN	2.5
1	B	210	ASP	2.5
1	C	203	GLU	2.5
1	B	112	THR	2.4
1	B	213	ASP	2.4
1	B	138	GLU	2.4
1	B	207	LYS	2.3
1	A	207	LYS	2.3
1	B	136	LYS	2.3
1	C	172	ASN	2.3
1	B	1	MET	2.2
1	C	205	CYS	2.1
1	C	211	ALA	2.1
1	B	79	VAL	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 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. 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( $\text{\AA}^2$ )	Q<0.9
4	FMT	B	1307	3/3	0.78	0.12	55,55,58,62	0
4	FMT	C	1317	3/3	0.85	0.10	39,39,40,42	0
3	SO4	A	1305	5/5	0.89	0.28	30,39,51,60	0
4	FMT	B	1318	3/3	0.92	0.07	39,39,41,46	0
4	FMT	B	1326	3/3	0.93	0.10	27,27,30,31	0
3	SO4	B	1334	5/5	0.96	0.18	23,31,39,42	0
4	FMT	A	1306	3/3	0.96	0.09	20,20,20,29	0
4	FMT	C	1336	3/3	0.97	0.07	19,19,26,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1324	5/5	0.97	0.14	17,29,34,40	0
3	SO4	C	1344	5/5	0.98	0.15	22,28,32,33	0
2	ZN	B	1313	1/1	0.98	0.04	24,24,24,24	0
2	ZN	B	1312	1/1	0.99	0.04	19,19,19,19	0
2	ZN	B	1311	1/1	1.00	0.04	18,18,18,18	0
2	ZN	A	1303	1/1	1.00	0.03	17,17,17,17	0
2	ZN	C	1321	1/1	1.00	0.03	14,14,14,14	0
2	ZN	A	1301	1/1	1.00	0.04	15,15,15,15	0
2	ZN	A	1302	1/1	1.00	0.03	15,15,15,15	0
2	ZN	C	1323	1/1	1.00	0.03	17,17,17,17	0
2	ZN	C	1322	1/1	1.00	0.04	16,16,16,16	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.