wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 02:35 PM JST

PDB ID	:	5ZI9
Title	:	Crystal structure of type-II LOG from Streptomyces coelicolor A3
Authors	:	Seo, H.; Kim, K.-J.
Deposited on	:	2018-03-14
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

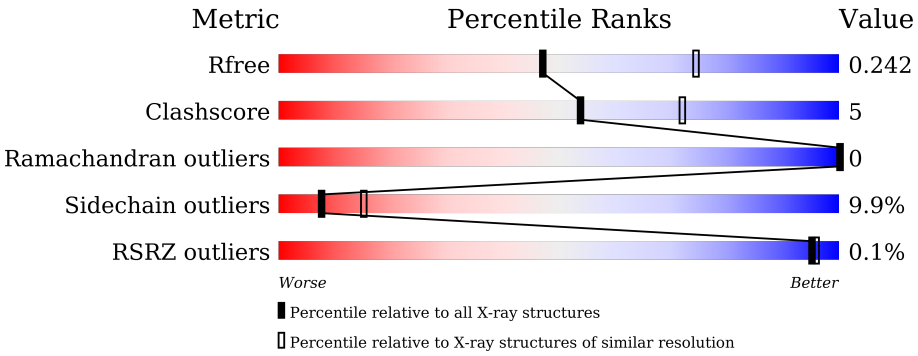
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 >=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 <=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	260	68% 10% • 20%
1	B	260	73% 17% • 8%
1	C	260	66% 13% • 20%
1	D	260	75% 15% • 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	B	502	-	X	X	-
3	FLC	C	502	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7147 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 Cytokinin riboside 5'-monophosphate phosphoribohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	1	0
			1608	1045	265	294	4			
1	B	240	Total	C	N	O	S	0	1	0
			1864	1194	321	345	4			
1	C	209	Total	C	N	O	S	0	1	0
			1608	1045	265	294	4			
1	D	240	Total	C	N	O	S	0	1	0
			1864	1194	321	345	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	LEU	-	expression tag	UNP Q9FBL8
A	254	GLU	-	expression tag	UNP Q9FBL8
A	255	HIS	-	expression tag	UNP Q9FBL8
A	256	HIS	-	expression tag	UNP Q9FBL8
A	257	HIS	-	expression tag	UNP Q9FBL8
A	258	HIS	-	expression tag	UNP Q9FBL8
A	259	HIS	-	expression tag	UNP Q9FBL8
A	260	HIS	-	expression tag	UNP Q9FBL8
B	253	LEU	-	expression tag	UNP Q9FBL8
B	254	GLU	-	expression tag	UNP Q9FBL8
B	255	HIS	-	expression tag	UNP Q9FBL8
B	256	HIS	-	expression tag	UNP Q9FBL8
B	257	HIS	-	expression tag	UNP Q9FBL8
B	258	HIS	-	expression tag	UNP Q9FBL8
B	259	HIS	-	expression tag	UNP Q9FBL8
B	260	HIS	-	expression tag	UNP Q9FBL8
C	253	LEU	-	expression tag	UNP Q9FBL8
C	254	GLU	-	expression tag	UNP Q9FBL8
C	255	HIS	-	expression tag	UNP Q9FBL8
C	256	HIS	-	expression tag	UNP Q9FBL8
C	257	HIS	-	expression tag	UNP Q9FBL8

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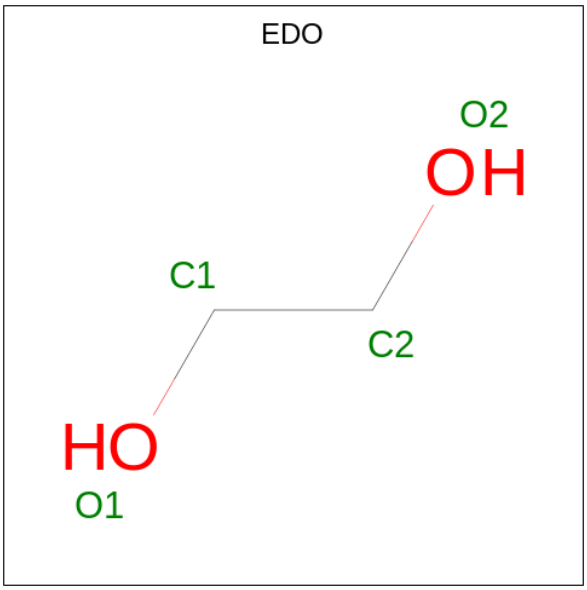
Chain	Residue	Modelled	Actual	Comment	Reference
C	258	HIS	-	expression tag	UNP Q9FBL8
C	259	HIS	-	expression tag	UNP Q9FBL8
C	260	HIS	-	expression tag	UNP Q9FBL8
D	253	LEU	-	expression tag	UNP Q9FBL8
D	254	GLU	-	expression tag	UNP Q9FBL8
D	255	HIS	-	expression tag	UNP Q9FBL8
D	256	HIS	-	expression tag	UNP Q9FBL8
D	257	HIS	-	expression tag	UNP Q9FBL8
D	258	HIS	-	expression tag	UNP Q9FBL8
D	259	HIS	-	expression tag	UNP Q9FBL8
D	260	HIS	-	expression tag	UNP Q9FBL8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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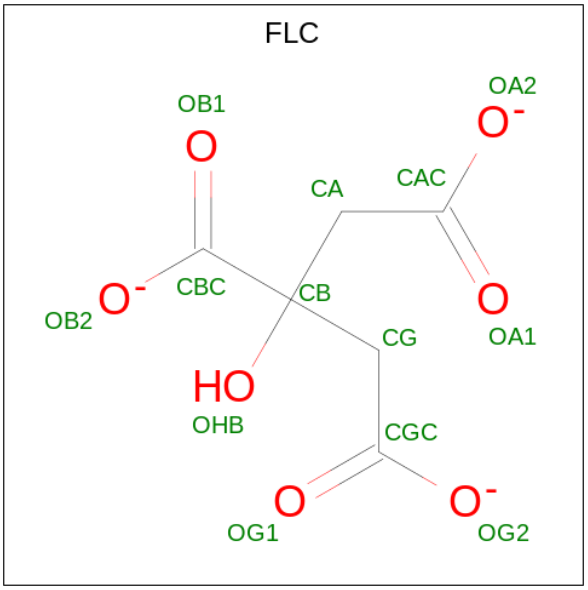
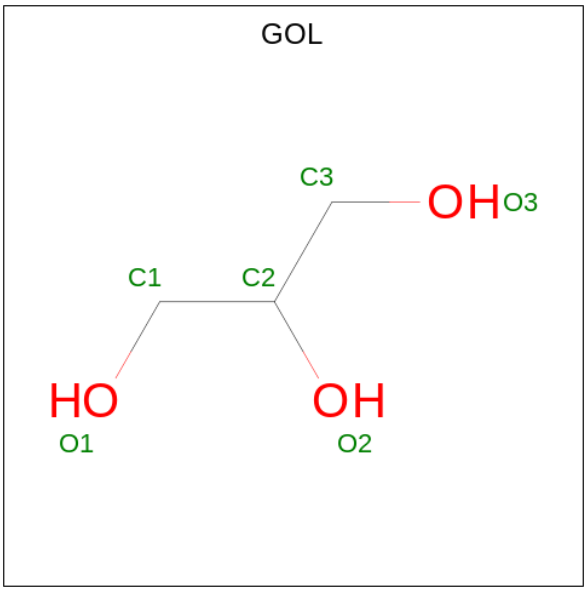
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

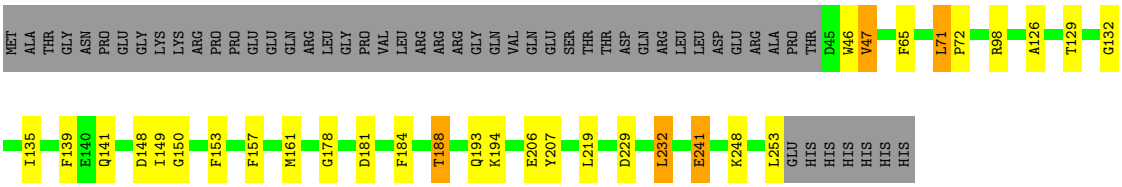
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	17	Total O 17 17	0	0
5	C	16	Total O 16 16	0	0
5	D	21	Total O 21 21	0	0

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.

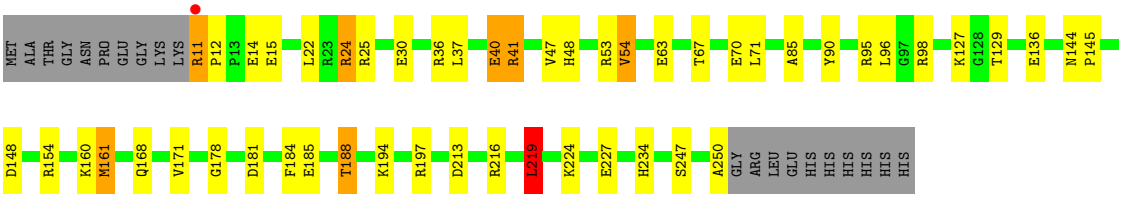
• Molecule 1: Cytokinin riboside 5'-monophosphate phosphoribohydrolase

Chain A:



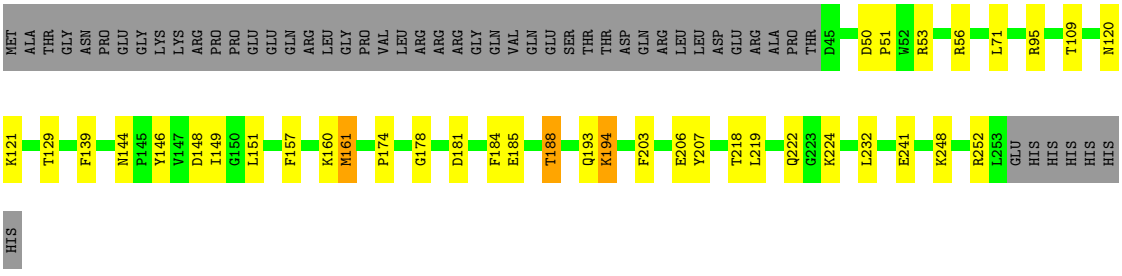
• Molecule 1: Cytokinin riboside 5'-monophosphate phosphoribohydrolase

Chain B:



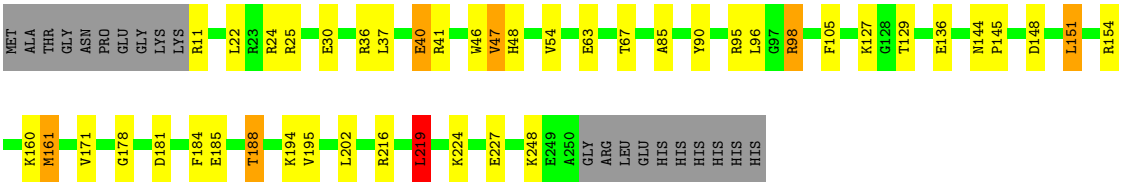
• Molecule 1: Cytokinin riboside 5'-monophosphate phosphoribohydrolase

Chain C:



• Molecule 1: Cytokinin riboside 5'-monophosphate phosphoribohydrolase

Chain D:


MET
ALA
THR
GLY
ASN
PRO
GLU
GLY
LYS
LYS
R11
L22
R23
R24
R25
E30
R36
L37
E40
R41
W46
V47
H48
V54
E63
T67
A85
Y90
R95
L96
G97
R98
F105
K127
G128
T129
E136
N144
P145
D148
L151
R154
K160
M161
V171
G178
D181
F184
E185
T188
K194
V195
L202
R216
L219
K224
E227
K248
E249
A250
GLY
ARG
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	206.77Å 206.77Å 206.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.21 – 2.50 31.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (146.21-2.50) 98.0 (31.90-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.185 , 0.237 0.193 , 0.242	Depositor DCC
R_{free} test set	2395 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 19.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.487 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, FLC, 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	0.76	0/1647	0.85	1/2235 (0.0%)
1	B	0.74	0/1906	0.91	5/2586 (0.2%)
1	C	0.74	0/1647	0.86	3/2235 (0.1%)
1	D	0.75	0/1906	0.90	4/2586 (0.2%)
All	All	0.75	0/7106	0.88	13/9642 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	24	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	98	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	24	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	252	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	98	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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	1608	0	1595	20	1
1	B	1864	0	1854	24	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1608	0	1595	21	1
1	D	1864	0	1854	20	1
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	1	0
3	A	13	0	5	0	0
3	B	26	0	10	4	0
3	C	13	0	5	1	0
3	D	26	0	10	1	0
4	A	12	0	16	4	0
4	C	12	0	16	4	0
5	A	15	0	0	2	0
5	B	17	0	0	0	0
5	C	16	0	0	2	0
5	D	21	0	0	0	0
All	All	7147	0	7008	75	2

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 5.

The worst 5 of 75 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:248:LYS:NZ	4:C:504:GOL:H12	1.86	0.90
1:C:53:ARG:NH1	4:C:503:GOL:O1	2.10	0.84
1:A:181:ASP:OD1	5:A:601:HOH:O	1.99	0.79
1:A:194:LYS:NZ	1:B:136:GLU:O	2.16	0.79
1:B:11:ARG:N	1:B:12:PRO:HD2	1.98	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASP:OD1	1:D:25:ARG:NH2[7_555]	2.00	0.20
1:A:148:ASP:OD1	1:B:25:ARG:NH2[10_555]	2.15	0.05

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	208/260 (80%)	208 (100%)	0	0	100	100
1	B	239/260 (92%)	231 (97%)	8 (3%)	0	100	100
1	C	208/260 (80%)	205 (99%)	3 (1%)	0	100	100
1	D	239/260 (92%)	233 (98%)	6 (2%)	0	100	100
All	All	894/1040 (86%)	877 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	163/207 (79%)	151 (93%)	12 (7%)	13	27
1	B	192/207 (93%)	169 (88%)	23 (12%)	5	9
1	C	163/207 (79%)	149 (91%)	14 (9%)	10	20
1	D	192/207 (93%)	169 (88%)	23 (12%)	5	9
All	All	710/828 (86%)	638 (90%)	72 (10%)	8	14

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	95[A]	ARG
1	D	248	LYS
1	D	98	ARG

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Mol	Chain	Res	Type
1	D	161	MET
1	B	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	191	GLN
1	C	120	ASN
1	D	27	GLN
1	D	58	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)

18 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	EDO	B	500	-	3,3,3	0.80	0	2,2,2	0.18	0
3	FLC	B	502	-	12,12,12	1.60	2 (16%)	17,17,17	2.01	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	A	500	-	3,3,3	0.42	0	2,2,2	0.64	0
4	GOL	A	503	-	5,5,5	0.34	0	5,5,5	1.12	0
4	GOL	C	503	-	5,5,5	0.80	0	5,5,5	0.76	0
3	FLC	D	502	-	12,12,12	1.71	3 (25%)	17,17,17	2.62	5 (29%)
2	EDO	D	503	-	3,3,3	0.73	0	2,2,2	0.62	0
4	GOL	C	504	-	5,5,5	0.25	0	5,5,5	0.71	0
2	EDO	D	500	-	3,3,3	0.71	0	2,2,2	0.40	0
2	EDO	B	503	-	3,3,3	0.71	0	2,2,2	0.59	0
3	FLC	B	501	-	12,12,12	1.44	3 (25%)	17,17,17	1.77	4 (23%)
3	FLC	A	502	-	12,12,12	1.97	5 (41%)	17,17,17	2.34	7 (41%)
2	EDO	C	500	-	3,3,3	0.59	0	2,2,2	0.73	0
4	GOL	A	504	-	5,5,5	0.32	0	5,5,5	0.50	0
2	EDO	C	501	-	3,3,3	0.46	0	2,2,2	0.57	0
3	FLC	D	501	-	12,12,12	1.27	0	17,17,17	1.36	2 (11%)
3	FLC	C	502	-	12,12,12	1.59	3 (25%)	17,17,17	2.41	8 (47%)
2	EDO	A	501	-	3,3,3	0.45	0	2,2,2	0.55	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	EDO	B	500	-	-	0/1/1/1	-
3	FLC	B	502	-	-	12/16/16/16	-
2	EDO	A	500	-	-	0/1/1/1	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	C	503	-	-	3/4/4/4	-
3	FLC	D	502	-	-	8/16/16/16	-
2	EDO	D	503	-	-	0/1/1/1	-
4	GOL	C	504	-	-	2/4/4/4	-
2	EDO	D	500	-	-	1/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
3	FLC	B	501	-	-	2/16/16/16	-
3	FLC	A	502	-	-	1/16/16/16	-
2	EDO	C	500	-	-	0/1/1/1	-
4	GOL	A	504	-	-	2/4/4/4	-
2	EDO	C	501	-	-	0/1/1/1	-
3	FLC	D	501	-	-	3/16/16/16	-
3	FLC	C	502	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	501	-	-	0/1/1/1	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	FLC	CB-CBC	-3.61	1.49	1.53
3	B	502	FLC	OG2-CGC	-3.45	1.19	1.30
3	D	502	FLC	CB-CBC	3.21	1.56	1.53
3	C	502	FLC	OG2-CGC	-3.12	1.20	1.30
3	A	502	FLC	OG2-CGC	-3.11	1.20	1.30

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	FLC	OB2-CBC-CB	6.93	125.08	113.05
3	D	502	FLC	OHB-CB-CBC	5.87	117.11	108.86
3	D	502	FLC	CG-CB-CBC	-5.69	97.88	110.11
3	B	502	FLC	OB2-CBC-CB	5.32	122.29	113.05
3	B	501	FLC	OB2-CBC-CB	4.53	120.92	113.05

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	FLC	CG-CB-CBC-OB1
3	B	502	FLC	CG-CB-CBC-OB2
3	B	502	FLC	OHB-CB-CBC-OB1
3	B	502	FLC	OHB-CB-CBC-OB2
3	C	502	FLC	CA-CB-CBC-OB1

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FLC	4	0
4	A	503	GOL	1	0
4	C	503	GOL	1	0
3	D	502	FLC	1	0
2	D	503	EDO	1	0
4	C	504	GOL	3	0
4	A	504	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	FLC	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^{th} 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	209/260 (80%)	-0.17	0 100 100	18, 27, 48, 77	0
1	B	240/260 (92%)	-0.09	1 (0%) 92 93	18, 32, 52, 66	0
1	C	209/260 (80%)	-0.17	0 100 100	18, 27, 47, 79	0
1	D	240/260 (92%)	-0.10	0 100 100	18, 31, 51, 65	0
All	All	898/1040 (86%)	-0.13	1 (0%) 95 96	18, 30, 51, 79	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	ARG	3.1

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 monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
4	GOL	A	503	6/6	0.87	0.19	36,37,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FLC	C	502	13/13	0.88	0.20	34,44,54,68	0
3	FLC	B	502	13/13	0.90	0.15	33,39,47,48	0
2	EDO	D	503	4/4	0.91	0.13	27,32,33,36	0
4	GOL	C	504	6/6	0.91	0.23	20,20,20,20	0
2	EDO	B	503	4/4	0.92	0.17	30,32,33,39	0
3	FLC	D	502	13/13	0.92	0.15	33,39,50,51	0
3	FLC	A	502	13/13	0.92	0.19	39,42,54,63	0
2	EDO	D	500	4/4	0.92	0.13	34,37,39,39	0
3	FLC	B	501	13/13	0.93	0.15	48,57,64,67	0
4	GOL	C	503	6/6	0.93	0.14	39,40,42,42	0
2	EDO	B	500	4/4	0.93	0.11	33,38,38,38	0
2	EDO	C	501	4/4	0.94	0.13	31,32,33,33	0
3	FLC	D	501	13/13	0.95	0.14	42,51,54,54	0
4	GOL	A	504	6/6	0.95	0.19	20,20,20,20	0
2	EDO	C	500	4/4	0.97	0.14	27,27,27,28	0
2	EDO	A	500	4/4	0.97	0.13	26,26,27,28	0
2	EDO	A	501	4/4	0.98	0.16	33,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.