wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 02:24 PM EDT

PDB ID	:	3E05
Title	:	CRYSTAL STRUCTURE OF Precorrin-6y C5,15-methyltransferase FROM Geobacter metallireducens GS-15
Authors	:	Patskovsky, Y.; Ramagopal, U.A.; Toro, R.; Dickey, M.; Hu, S.; Maletic, M.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-07-30
Resolution	:	1.80 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 (i)) were used in the production of this report:

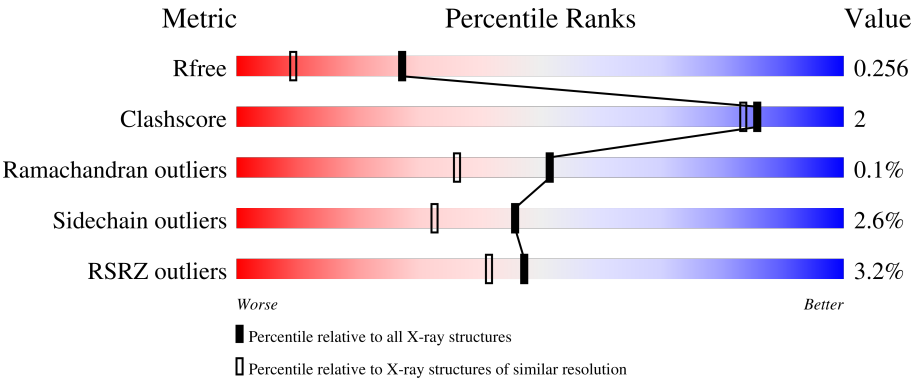
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	204	84% 8% 8%
1	B	204	89% 5% 6%
1	C	204	89% • 7%
1	D	204	4% 85% 7% • 6%

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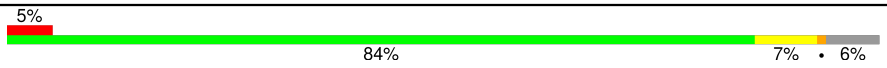
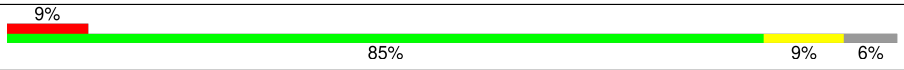
Mol	Chain	Length	Quality of chain
1	E	204	
1	F	204	
1	G	204	
1	H	204	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12584 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 Precorrin-6Y C5,15-methyltransferase (Decarboxylating).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	3	0
			1488	949	248	285	6			
1	B	192	Total	C	N	O	S	0	5	0
			1520	972	251	291	6			
1	C	190	Total	C	N	O	S	0	6	0
			1519	976	253	283	7			
1	D	192	Total	C	N	O	S	0	7	0
			1537	984	254	293	6			
1	E	191	Total	C	N	O	S	0	4	0
			1509	966	250	286	7			
1	F	187	Total	C	N	O	S	0	2	0
			1464	933	247	278	6			
1	G	189	Total	C	N	O	S	0	4	0
			1495	959	246	283	7			
1	H	191	Total	C	N	O	S	0	3	0
			1495	952	251	286	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	MET	-	expression tag	UNP Q39YF0
A	210	SER	-	expression tag	UNP Q39YF0
A	406	GLY	-	expression tag	UNP Q39YF0
A	407	HIS	-	expression tag	UNP Q39YF0
A	408	HIS	-	expression tag	UNP Q39YF0
A	409	HIS	-	expression tag	UNP Q39YF0
A	410	HIS	-	expression tag	UNP Q39YF0
A	411	HIS	-	expression tag	UNP Q39YF0
A	412	HIS	-	expression tag	UNP Q39YF0
B	209	MET	-	expression tag	UNP Q39YF0
B	210	SER	-	expression tag	UNP Q39YF0
B	406	GLY	-	expression tag	UNP Q39YF0
B	407	HIS	-	expression tag	UNP Q39YF0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	expression tag	UNP Q39YF0
B	409	HIS	-	expression tag	UNP Q39YF0
B	410	HIS	-	expression tag	UNP Q39YF0
B	411	HIS	-	expression tag	UNP Q39YF0
B	412	HIS	-	expression tag	UNP Q39YF0
C	209	MET	-	expression tag	UNP Q39YF0
C	210	SER	-	expression tag	UNP Q39YF0
C	406	GLY	-	expression tag	UNP Q39YF0
C	407	HIS	-	expression tag	UNP Q39YF0
C	408	HIS	-	expression tag	UNP Q39YF0
C	409	HIS	-	expression tag	UNP Q39YF0
C	410	HIS	-	expression tag	UNP Q39YF0
C	411	HIS	-	expression tag	UNP Q39YF0
C	412	HIS	-	expression tag	UNP Q39YF0
D	209	MET	-	expression tag	UNP Q39YF0
D	210	SER	-	expression tag	UNP Q39YF0
D	406	GLY	-	expression tag	UNP Q39YF0
D	407	HIS	-	expression tag	UNP Q39YF0
D	408	HIS	-	expression tag	UNP Q39YF0
D	409	HIS	-	expression tag	UNP Q39YF0
D	410	HIS	-	expression tag	UNP Q39YF0
D	411	HIS	-	expression tag	UNP Q39YF0
D	412	HIS	-	expression tag	UNP Q39YF0
E	209	MET	-	expression tag	UNP Q39YF0
E	210	SER	-	expression tag	UNP Q39YF0
E	406	GLY	-	expression tag	UNP Q39YF0
E	407	HIS	-	expression tag	UNP Q39YF0
E	408	HIS	-	expression tag	UNP Q39YF0
E	409	HIS	-	expression tag	UNP Q39YF0
E	410	HIS	-	expression tag	UNP Q39YF0
E	411	HIS	-	expression tag	UNP Q39YF0
E	412	HIS	-	expression tag	UNP Q39YF0
F	209	MET	-	expression tag	UNP Q39YF0
F	210	SER	-	expression tag	UNP Q39YF0
F	406	GLY	-	expression tag	UNP Q39YF0
F	407	HIS	-	expression tag	UNP Q39YF0
F	408	HIS	-	expression tag	UNP Q39YF0
F	409	HIS	-	expression tag	UNP Q39YF0
F	410	HIS	-	expression tag	UNP Q39YF0
F	411	HIS	-	expression tag	UNP Q39YF0
F	412	HIS	-	expression tag	UNP Q39YF0
G	209	MET	-	expression tag	UNP Q39YF0

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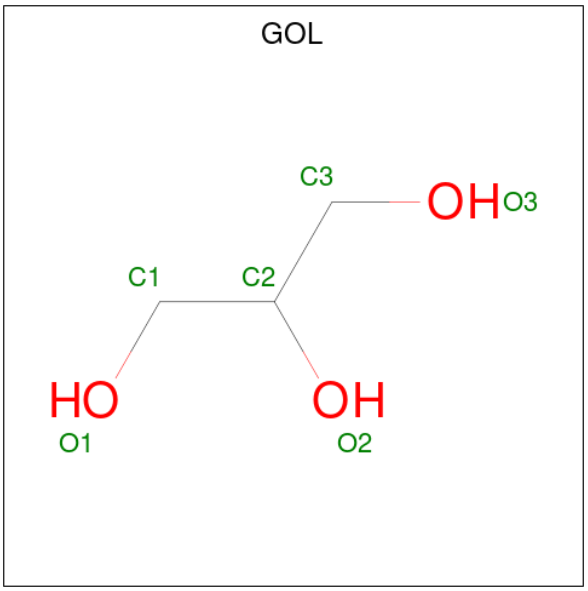
Chain	Residue	Modelled	Actual	Comment	Reference
G	210	SER	-	expression tag	UNP Q39YF0
G	406	GLY	-	expression tag	UNP Q39YF0
G	407	HIS	-	expression tag	UNP Q39YF0
G	408	HIS	-	expression tag	UNP Q39YF0
G	409	HIS	-	expression tag	UNP Q39YF0
G	410	HIS	-	expression tag	UNP Q39YF0
G	411	HIS	-	expression tag	UNP Q39YF0
G	412	HIS	-	expression tag	UNP Q39YF0
H	209	MET	-	expression tag	UNP Q39YF0
H	210	SER	-	expression tag	UNP Q39YF0
H	406	GLY	-	expression tag	UNP Q39YF0
H	407	HIS	-	expression tag	UNP Q39YF0
H	408	HIS	-	expression tag	UNP Q39YF0
H	409	HIS	-	expression tag	UNP Q39YF0
H	410	HIS	-	expression tag	UNP Q39YF0
H	411	HIS	-	expression tag	UNP Q39YF0
H	412	HIS	-	expression tag	UNP Q39YF0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

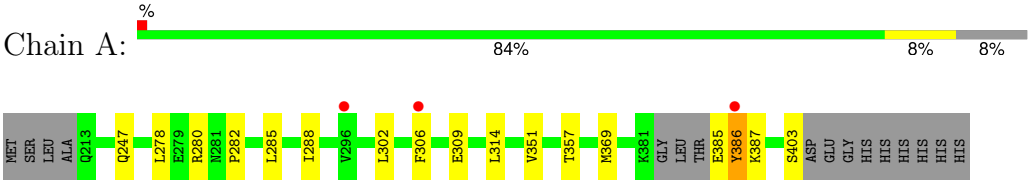
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 70 70	0	0
4	B	90	Total O 90 90	0	0
4	C	87	Total O 87 87	0	0
4	D	66	Total O 66 66	0	0
4	E	57	Total O 57 57	0	0
4	F	63	Total O 63 63	0	0
4	G	60	Total O 60 60	0	0
4	H	44	Total O 44 44	0	0

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.

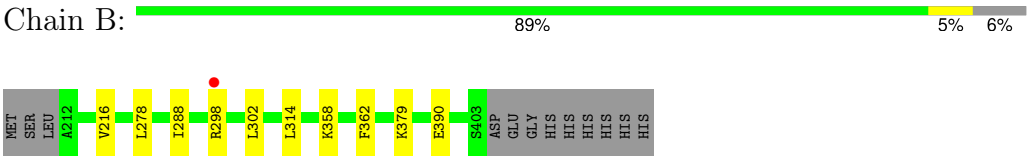
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain A:



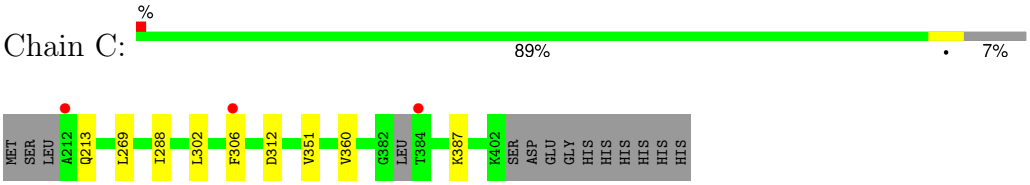
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain B:



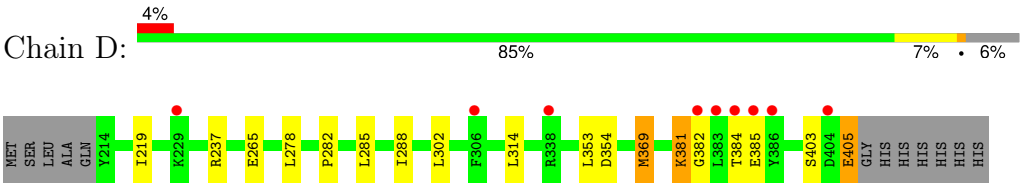
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain C:



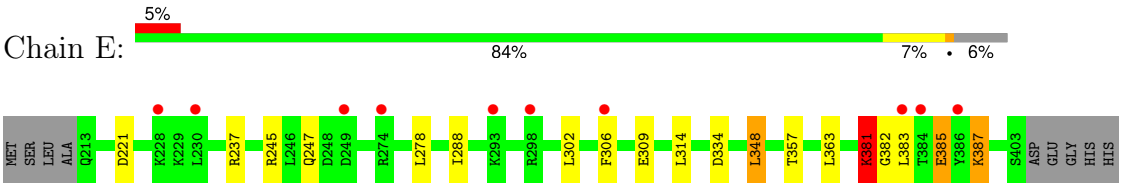
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain D:



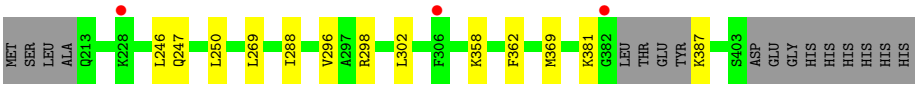
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain E:



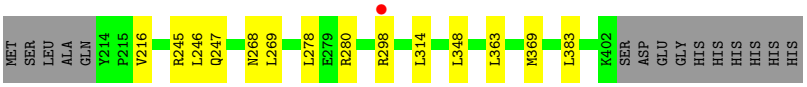
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain F:



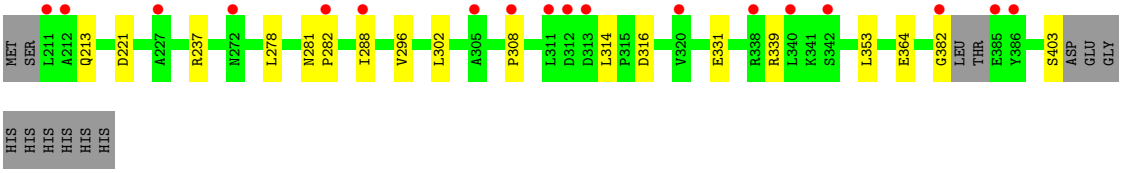
• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain G:



• Molecule 1: Precorrin-6Y C5,15-methyltransferase (Decarboxylating)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.71Å 83.45Å 149.06Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 49.26 – 1.76	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-1.80) 92.4 (49.26-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.262 0.213 , 0.256	Depositor DCC
R_{free} test set	4198 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12584	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: CL, GOL

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	0.53	0/1521	0.65	0/2058
1	B	0.48	0/1561	0.62	0/2115
1	C	0.52	0/1562	0.65	0/2110
1	D	0.48	0/1584	0.61	0/2145
1	E	0.54	0/1547	0.67	0/2095
1	F	0.51	0/1493	0.62	0/2019
1	G	0.47	0/1532	0.65	0/2074
1	H	0.47	0/1527	0.63	0/2066
All	All	0.50	0/12327	0.64	0/16682

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	A	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	GLU	Peptide
1	D	381	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	381	LYS	Peptide

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	1488	0	1502	10	0
1	B	1520	0	1541	6	0
1	C	1519	0	1553	4	0
1	D	1537	0	1566	12	0
1	E	1509	0	1535	10	0
1	F	1464	0	1487	6	0
1	G	1495	0	1527	4	0
1	H	1495	0	1511	9	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	A	6	0	8	0	0
3	B	6	0	8	2	0
4	A	70	0	0	1	0
4	B	90	0	0	0	0
4	C	87	0	0	1	0
4	D	66	0	0	0	0
4	E	57	0	0	0	0
4	F	63	0	0	0	0
4	G	60	0	0	1	0
4	H	44	0	0	0	0
All	All	12584	0	12238	54	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 2.

The worst 5 of 54 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:386:TYR:CD2	1:A:386:TYR:O	2.30	0.85
1:B:390:GLU:HB2	3:B:413:GOL:H31	1.76	0.67
1:B:379:LYS:HG3	3:B:413:GOL:H32	1.78	0.65
1:A:386:TYR:O	1:A:386:TYR:HD2	1.80	0.64
1:H:221:ASP:OD1	1:H:237:ARG:NH2	2.32	0.63

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	187/204 (92%)	184 (98%)	3 (2%)	0	100	100
1	B	195/204 (96%)	192 (98%)	3 (2%)	0	100	100
1	C	191/204 (94%)	188 (98%)	3 (2%)	0	100	100
1	D	197/204 (97%)	190 (96%)	7 (4%)	0	100	100
1	E	193/204 (95%)	187 (97%)	4 (2%)	2 (1%)	15	5
1	F	185/204 (91%)	181 (98%)	4 (2%)	0	100	100
1	G	191/204 (94%)	185 (97%)	6 (3%)	0	100	100
1	H	190/204 (93%)	188 (99%)	2 (1%)	0	100	100
All	All	1529/1632 (94%)	1495 (98%)	32 (2%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	381	LYS
1	E	382	GLY

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	163/173 (94%)	158 (97%)	5 (3%)	40 25
1	B	167/173 (96%)	166 (99%)	1 (1%)	86 84
1	C	166/173 (96%)	161 (97%)	5 (3%)	41 27
1	D	170/173 (98%)	168 (99%)	2 (1%)	71 65
1	E	166/173 (96%)	155 (93%)	11 (7%)	16 5
1	F	160/173 (92%)	157 (98%)	3 (2%)	57 46
1	G	164/173 (95%)	157 (96%)	7 (4%)	29 14
1	H	162/173 (94%)	159 (98%)	3 (2%)	57 46
All	All	1318/1384 (95%)	1281 (97%)	37 (3%)	46 30

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	247	GLN
1	H	296	VAL
1	G	280	ARG
1	G	369[B]	MET
1	D	405	GLU

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

Mol	Chain	Res	Type
1	A	349	ASN
1	D	349	ASN
1	E	349	ASN
1	G	234	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)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	GOL	B	413	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	A	413	-	5,5,5	0.41	0	5,5,5	0.34	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	GOL	B	413	-	-	2/4/4/4	-
3	GOL	A	413	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	413	GOL	O1-C1-C2-C3
3	B	413	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	413	GOL	2	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	188/204 (92%)	-0.12	3 (1%) 72 68	21, 37, 61, 98	0
1	B	192/204 (94%)	-0.01	1 (0%) 91 89	24, 36, 58, 76	0
1	C	190/204 (93%)	0.04	3 (1%) 72 68	23, 36, 61, 86	0
1	D	192/204 (94%)	-0.06	9 (4%) 31 25	23, 37, 64, 105	0
1	E	191/204 (93%)	0.16	10 (5%) 27 22	23, 38, 65, 85	0
1	F	187/204 (91%)	-0.06	3 (1%) 72 68	25, 38, 61, 82	0
1	G	189/204 (92%)	-0.01	1 (0%) 91 89	22, 38, 61, 74	0
1	H	191/204 (93%)	0.55	18 (9%) 8 6	26, 39, 63, 99	0
All	All	1520/1632 (93%)	0.06	48 (3%) 47 41	21, 38, 62, 105	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	211	LEU	8.3
1	A	386	TYR	6.3
1	D	382	GLY	5.7
1	H	386	TYR	5.3
1	D	383	LEU	5.3

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 (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^{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
3	GOL	B	413	6/6	0.81	0.25	48,56,59,59	0
3	GOL	A	413	6/6	0.83	0.13	35,45,51,52	0
2	CL	H	1	1/1	0.98	0.07	48,48,48,48	0
2	CL	D	1	1/1	0.98	0.09	37,37,37,37	0
2	CL	E	1	1/1	0.98	0.05	38,38,38,38	0
2	CL	F	1	1/1	0.99	0.07	34,34,34,34	0
2	CL	C	1	1/1	0.99	0.10	29,29,29,29	0
2	CL	A	1	1/1	0.99	0.07	34,34,34,34	0
2	CL	B	1	1/1	0.99	0.13	29,29,29,29	0
2	CL	G	1	1/1	1.00	0.06	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.