wwPDB X-ray Structure Validation Summary Report (i)

Jun 7, 2020 – 02:38 am BST

PDB ID	:	6I34
Title	:	Crystal structure of Neanderthal glycine decarboxylase (P-protein)
Authors	:	Van Laer, B.; Kapp, U.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on	:	2018-11-05
Resolution	:	2.10 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 following versions of software and data (see references (1)) were used in the production of this report:

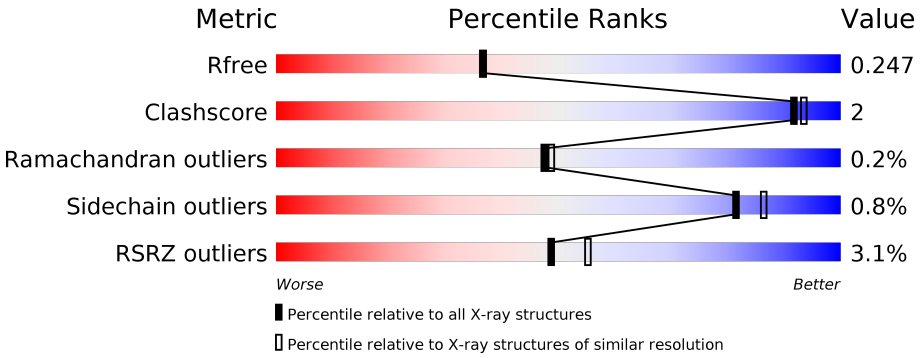
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	984	2% 93%
1	B	984	4% 93%
1	C	984	2% 92% 5%
1	D	984	4% 91% 5%

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	EDO	C	1102	-	-	X	-
4	PEG	A	1105	-	-	X	-
4	PEG	C	1106	-	-	X	-

2 Entry composition

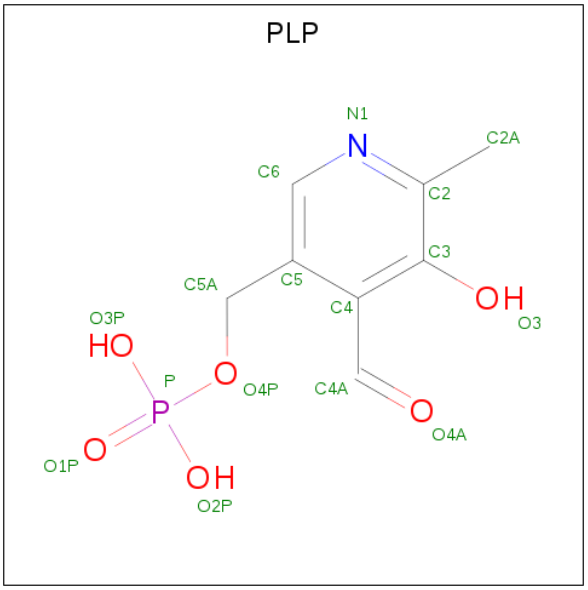
There are 6 unique types of molecules in this entry. The entry contains 31302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neanderthal Glycine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	2	0
			7450	4694	1319	1382	55			
1	B	954	Total	C	N	O	S	0	1	0
			7454	4696	1320	1384	54			
1	C	953	Total	C	N	O	S	0	0	0
			7436	4687	1317	1378	54			
1	D	953	Total	C	N	O	S	0	0	0
			7434	4685	1314	1381	54			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



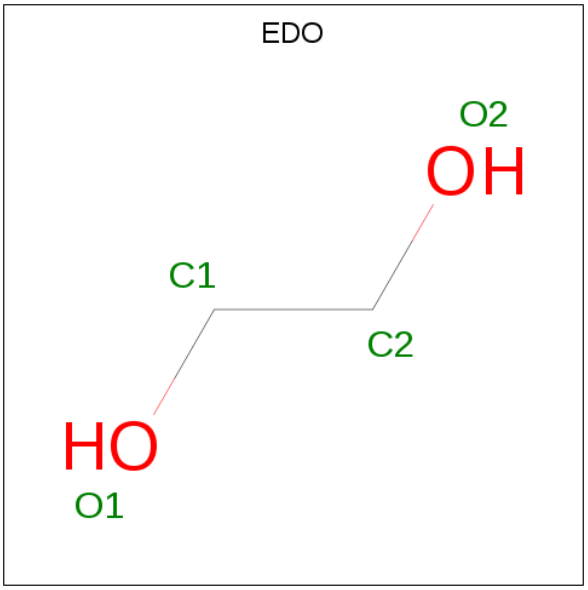
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 15 8 1 5 1	0	0
2	D	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



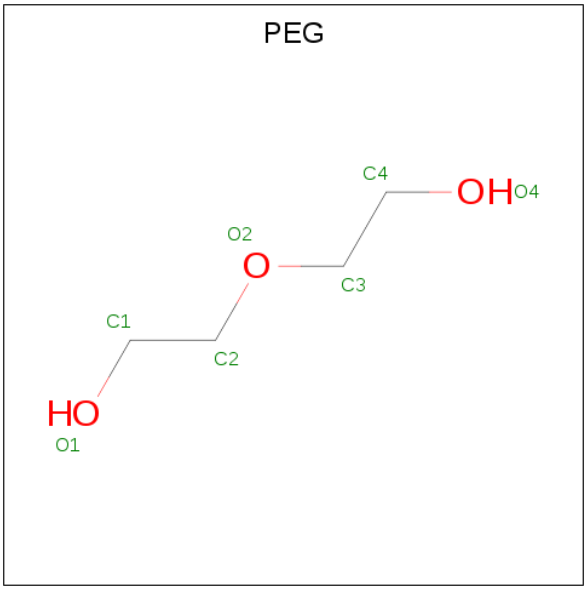
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

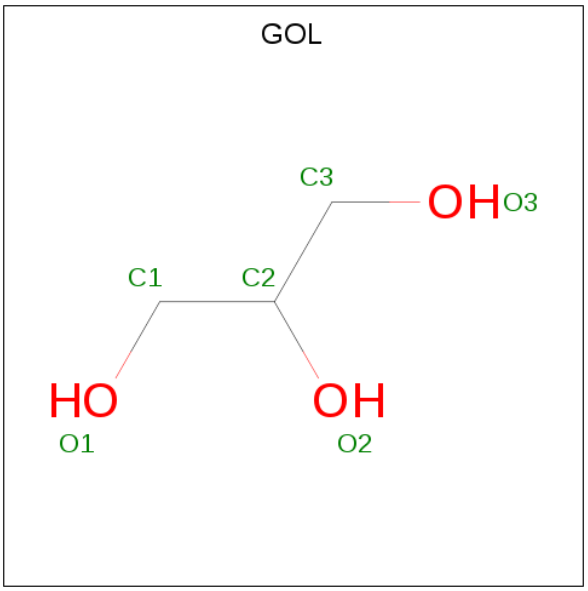
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

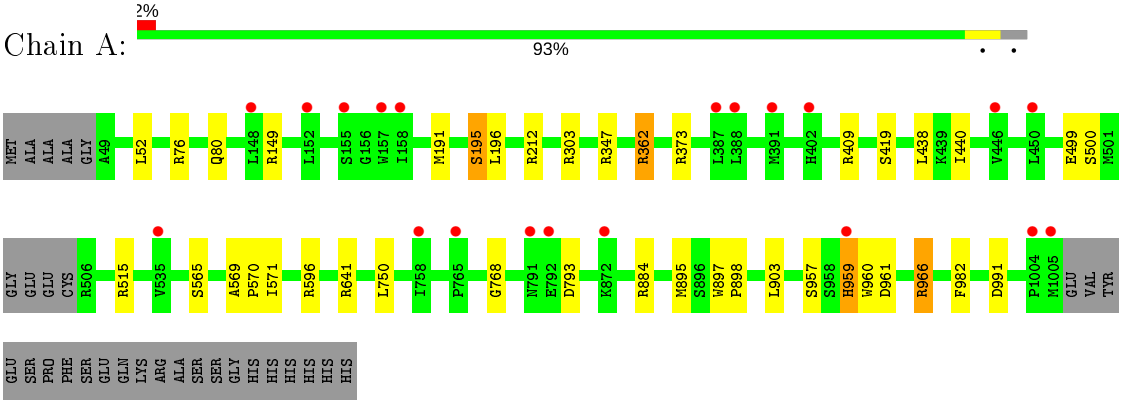
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	403	Total O 403 403	0	0
6	B	282	Total O 282 282	0	0
6	C	404	Total O 404 404	0	0
6	D	270	Total O 270 270	0	0

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 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.

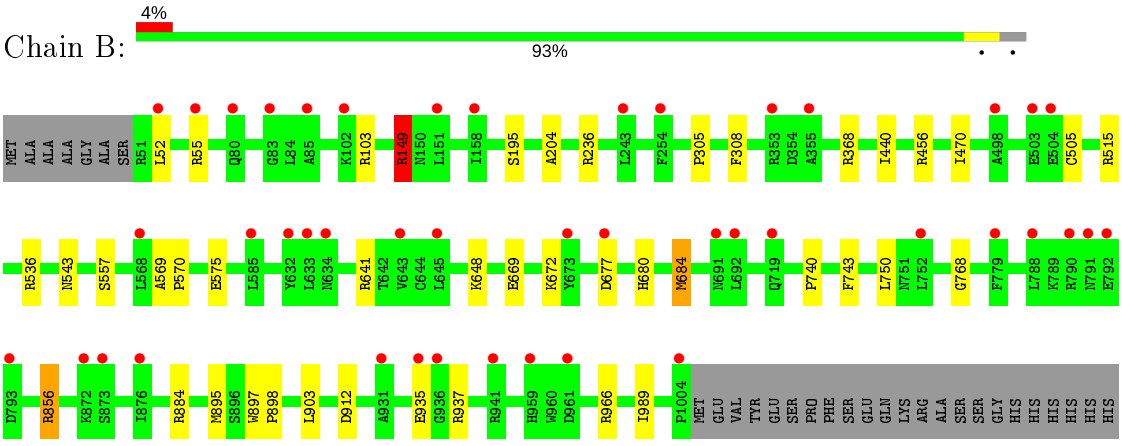
- Molecule 1: Neanderthal Glycine decarboxylase

Chain A:



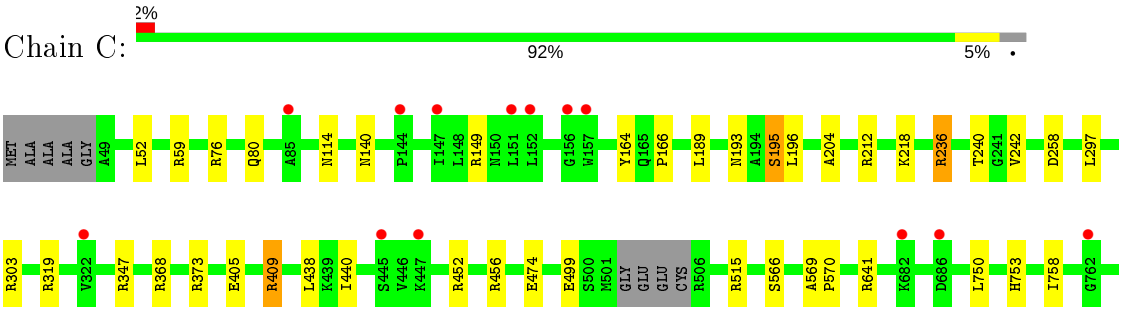
- Molecule 1: Neanderthal Glycine decarboxylase

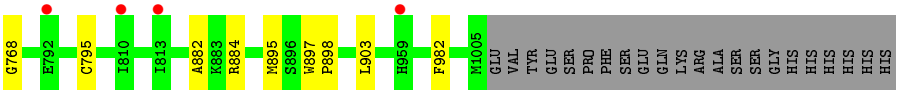
Chain B:



- Molecule 1: Neanderthal Glycine decarboxylase

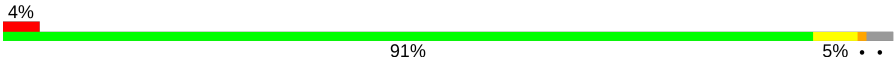
Chain C:

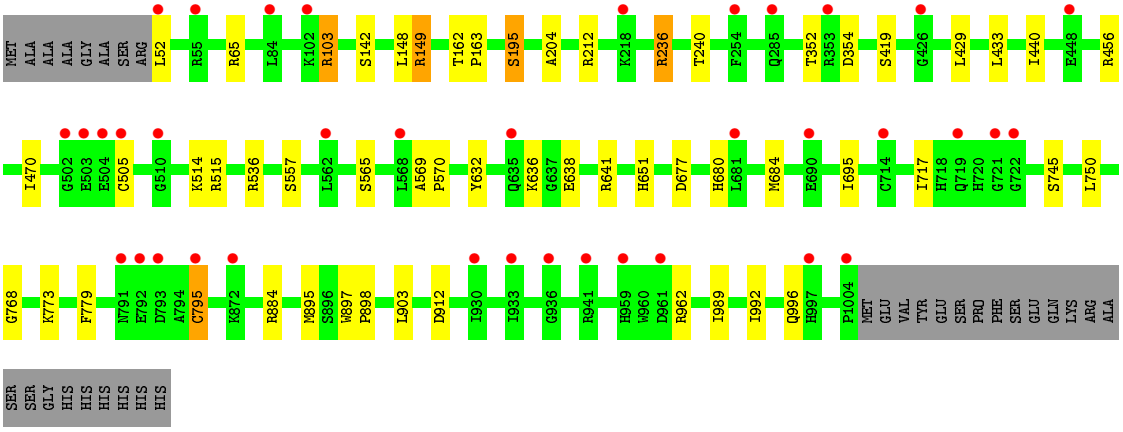




- Molecule 1: Neanderthal Glycine decarboxylase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.87Å 124.38Å 201.30Å 90.00° 98.57° 90.00°	Depositor
Resolution (Å)	47.90 – 2.10 47.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.90-2.10) 99.8 (47.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.216 , 0.243 0.223 , 0.247	Depositor DCC
R_{free} test set	12259 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	31302	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9183e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, PEG, EDO, PLP

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	0.86	0/7617	0.88	13/10316 (0.1%)
1	B	0.79	1/7622 (0.0%)	0.86	14/10323 (0.1%)
1	C	0.85	2/7603 (0.0%)	0.87	14/10296 (0.1%)
1	D	0.82	1/7602 (0.0%)	0.86	15/10297 (0.1%)
All	All	0.83	4/30444 (0.0%)	0.87	56/41232 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	795	CYS	CB-SG	-7.37	1.69	1.82
1	B	575	GLU	CD-OE1	6.26	1.32	1.25
1	C	795	CYS	CB-SG	-5.22	1.73	1.81
1	C	566	SER	CB-OG	5.21	1.49	1.42

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	966	ARG	NE-CZ-NH2	10.94	125.77	120.30
1	A	966	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	D	677	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	966	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	B	149	ARG	NE-CZ-NH2	-8.30	116.15	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	7450	0	7375	15	0
1	B	7454	0	7376	22	0
1	C	7436	0	7367	26	0
1	D	7434	0	7356	30	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	7	0	0
3	A	12	0	18	0	0
3	B	12	0	18	0	0
3	C	12	0	18	5	0
3	D	8	0	12	0	0
4	A	7	0	10	5	0
4	B	7	0	10	1	0
4	C	14	0	20	6	0
4	D	7	0	10	0	0
5	A	12	0	16	0	0
5	C	12	0	16	0	0
5	D	6	0	8	1	0
6	A	403	0	0	3	0
6	B	282	0	0	2	0
6	C	404	0	0	1	0
6	D	270	0	0	1	0
All	All	31302	0	29655	93	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 93 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:B:856:ARG:HH11	1:B:856:ARG:HG3	1.11	1.15
1:C:474:GLU:HB2	3:C:1102:EDO:H11	1.36	1.01
1:C:895:MET:SD	1:C:903:LEU:HD22	2.15	0.86
1:C:319:ARG:HB2	3:C:1102:EDO:H21	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASN:HB3	4:C:1106:PEG:H12	1.67	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	951/984 (97%)	923 (97%)	25 (3%)	3 (0%)	41	41
1	B	953/984 (97%)	926 (97%)	26 (3%)	1 (0%)	51	54
1	C	949/984 (96%)	925 (98%)	23 (2%)	1 (0%)	51	54
1	D	951/984 (97%)	925 (97%)	25 (3%)	1 (0%)	51	54
All	All	3804/3936 (97%)	3699 (97%)	99 (3%)	6 (0%)	47	49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	B	195	SER
1	C	195	SER
1	D	195	SER
1	A	959	HIS

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	807/829 (97%)	800 (99%)	7 (1%)	78	84
1	B	807/829 (97%)	800 (99%)	7 (1%)	78	84
1	C	805/829 (97%)	800 (99%)	5 (1%)	86	90
1	D	805/829 (97%)	799 (99%)	6 (1%)	84	88
All	All	3224/3316 (97%)	3199 (99%)	25 (1%)	81	86

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	672	LYS
1	B	989	ILE
1	D	557	SER
1	B	856	ARG
1	C	52	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

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

25 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	$\#\|Z\| > 2$
5	GOL	D	1105	-	5,5,5	0.53	0	5,5,5	0.44	0
3	EDO	A	1103	-	3,3,3	0.55	0	2,2,2	0.37	0
3	EDO	A	1102	-	3,3,3	0.78	0	2,2,2	0.34	0
4	PEG	B	1105	-	6,6,6	0.68	0	5,5,5	0.72	0
3	EDO	D	1104	-	3,3,3	0.65	0	2,2,2	0.18	0
3	EDO	C	1102	-	3,3,3	0.51	0	2,2,2	0.73	0
2	PLP	D	1102	1	15,15,16	3.49	3 (20%)	20,22,23	2.03	6 (30%)
4	PEG	A	1105	-	6,6,6	0.54	0	5,5,5	0.57	0
2	PLP	C	1101	1	15,15,16	2.93	3 (20%)	20,22,23	2.28	5 (25%)
5	GOL	C	1108	-	5,5,5	0.85	0	5,5,5	1.18	0
2	PLP	A	1101	1	15,15,16	2.43	3 (20%)	20,22,23	2.13	4 (20%)
3	EDO	C	1103	-	3,3,3	0.62	0	2,2,2	0.43	0
2	PLP	B	1101	1	15,15,16	3.42	3 (20%)	20,22,23	1.93	5 (25%)
3	EDO	C	1104	-	3,3,3	0.87	0	2,2,2	0.60	0
3	EDO	A	1104	-	3,3,3	0.39	0	2,2,2	0.52	0
5	GOL	C	1107	-	5,5,5	0.30	0	5,5,5	0.31	0
5	GOL	A	1107	-	5,5,5	0.24	0	5,5,5	0.70	0
3	EDO	B	1104	-	3,3,3	0.36	0	2,2,2	0.54	0
4	PEG	C	1106	-	6,6,6	0.53	0	5,5,5	0.70	0
4	PEG	C	1105	-	6,6,6	0.57	0	5,5,5	1.38	0
4	PEG	D	1101	-	6,6,6	0.74	0	5,5,5	0.89	0
3	EDO	B	1102	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	D	1103	-	3,3,3	0.92	0	2,2,2	1.07	0
3	EDO	B	1103	-	3,3,3	0.36	0	2,2,2	0.79	0
5	GOL	A	1106	-	5,5,5	0.61	0	5,5,5	0.94	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
5	GOL	D	1105	-	-	4/4/4/4	-
3	EDO	A	1103	-	-	1/1/1/1	-
3	EDO	A	1102	-	-	1/1/1/1	-
4	PEG	B	1105	-	-	2/4/4/4	-
3	EDO	D	1104	-	-	0/1/1/1	-
3	EDO	C	1102	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	1102	1	-	0/6/6/8	0/1/1/1
4	PEG	A	1105	-	-	1/4/4/4	-
2	PLP	C	1101	1	-	4/6/6/8	0/1/1/1
5	GOL	C	1108	-	-	4/4/4/4	-
2	PLP	A	1101	1	-	2/6/6/8	0/1/1/1
3	EDO	C	1103	-	-	0/1/1/1	-
2	PLP	B	1101	1	-	0/6/6/8	0/1/1/1
3	EDO	C	1104	-	-	1/1/1/1	-
3	EDO	A	1104	-	-	1/1/1/1	-
5	GOL	C	1107	-	-	0/4/4/4	-
5	GOL	A	1107	-	-	2/4/4/4	-
3	EDO	B	1104	-	-	1/1/1/1	-
4	PEG	C	1106	-	-	3/4/4/4	-
4	PEG	C	1105	-	-	3/4/4/4	-
4	PEG	D	1101	-	-	3/4/4/4	-
3	EDO	B	1102	-	-	1/1/1/1	-
3	EDO	D	1103	-	-	0/1/1/1	-
3	EDO	B	1103	-	-	1/1/1/1	-
5	GOL	A	1106	-	-	2/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	PLP	C3-C2	8.92	1.49	1.40
2	C	1101	PLP	C3-C2	8.81	1.49	1.40
2	D	1102	PLP	C3-C2	8.66	1.49	1.40
2	B	1101	PLP	C5-C4	8.41	1.49	1.40
2	D	1102	PLP	C5-C4	8.39	1.49	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	PLP	O4P-C5A-C5	5.90	120.60	109.35
2	C	1101	PLP	O2P-P-O4P	5.49	121.35	106.73
2	C	1101	PLP	O4P-C5A-C5	5.32	119.49	109.35
2	A	1101	PLP	O4P-P-O1P	4.59	119.36	106.47
2	D	1102	PLP	O3P-P-O4P	-4.35	95.16	106.73

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1105	GOL	O1-C1-C2-C3
2	C	1101	PLP	C4-C5-C5A-O4P
2	C	1101	PLP	C6-C5-C5A-O4P
2	C	1101	PLP	C5A-O4P-P-O1P
5	C	1108	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1105	GOL	1	0
4	B	1105	PEG	1	0
3	C	1102	EDO	5	0
4	A	1105	PEG	5	0
4	C	1106	PEG	4	0
4	C	1105	PEG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	953/984 (96%)	0.02	20 (2%)	63	68	16, 29, 49, 81	0
1	B	954/984 (96%)	0.24	44 (4%)	32	38	21, 41, 67, 99	0
1	C	953/984 (96%)	0.04	17 (1%)	68	72	18, 29, 51, 97	0
1	D	953/984 (96%)	0.21	37 (3%)	39	45	21, 40, 64, 90	0
All	All	3813/3936 (96%)	0.13	118 (3%)	49	55	16, 34, 61, 99	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	6.9
1	C	792	GLU	5.9
1	A	959	HIS	4.1
1	B	102	LYS	4.0
1	B	55	ARG	4.0

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

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	PEG	A	1105	7/7	0.67	0.26	37,51,54,64	0
4	PEG	D	1101	7/7	0.71	0.26	38,41,63,65	0
3	EDO	D	1103	4/4	0.72	0.26	38,41,42,56	0
4	PEG	C	1105	7/7	0.73	0.24	37,43,48,53	0
5	GOL	C	1108	6/6	0.77	0.33	43,47,56,56	0
3	EDO	B	1103	4/4	0.77	0.27	44,50,50,53	0
4	PEG	B	1105	7/7	0.78	0.23	36,39,45,49	0
3	EDO	D	1104	4/4	0.81	0.39	33,37,46,50	0
3	EDO	C	1104	4/4	0.82	0.24	37,38,49,54	0
3	EDO	A	1102	4/4	0.83	0.25	35,35,41,44	0
3	EDO	C	1103	4/4	0.84	0.14	36,41,48,51	0
3	EDO	C	1102	4/4	0.84	0.26	38,42,45,47	0
3	EDO	B	1104	4/4	0.85	0.14	51,53,54,56	0
5	GOL	C	1107	6/6	0.86	0.15	40,51,59,64	0
5	GOL	D	1105	6/6	0.87	0.21	47,60,62,70	0
5	GOL	A	1106	6/6	0.87	0.27	34,46,48,52	0
3	EDO	B	1102	4/4	0.88	0.35	35,44,45,48	0
3	EDO	A	1104	4/4	0.89	0.18	52,55,62,66	0
5	GOL	A	1107	6/6	0.90	0.18	40,51,52,56	0
4	PEG	C	1106	7/7	0.91	0.15	31,38,48,52	0
3	EDO	A	1103	4/4	0.92	0.12	38,39,39,51	0
2	PLP	D	1102	15/16	0.96	0.17	30,38,49,51	0
2	PLP	C	1101	15/16	0.97	0.17	16,20,28,29	0
2	PLP	B	1101	15/16	0.97	0.13	29,39,45,50	0
2	PLP	A	1101	15/16	0.98	0.18	18,23,30,32	0

6.5 Other polymers (i)

There are no such residues in this entry.