wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2023 – 10:04 PM EDT

PDB ID	:	3V5C
Title	:	Crystal structure of the mutant E234A of Galacturonate Dehydratase from GEOBACILLUS SP. complexed with Mg
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Groninger-Poe, F.; Gerlt, J.A.; Almo, S.C.
Deposited on	:	2011-12-16
Resolution	:	1.53 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:

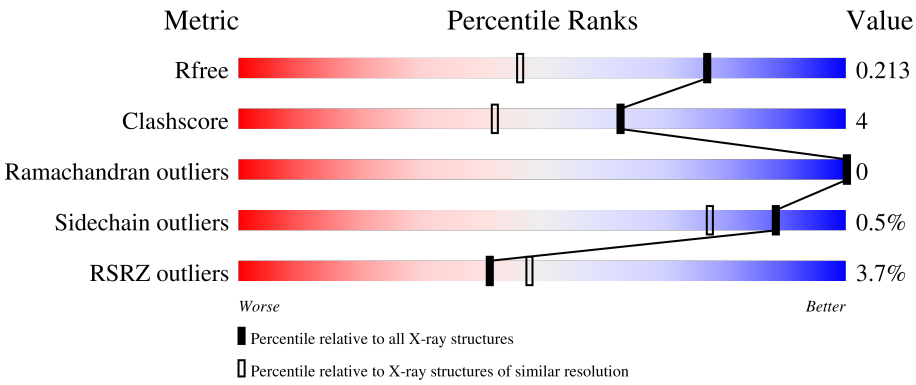
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	392	2% 90% 8% •
1	B	392	% 88% 8% •
1	C	392	4% 89% 9% •
1	D	392	7% 83% 12% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13728 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3100	1956	549	583	12	0	7	0
1	B	376	3005	1900	526	568	11	0	5	0
1	C	385	3072	1941	539	580	12	0	5	0
1	D	376	3004	1900	528	565	11	0	4	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP D3EID5
A	3	LEU	-	expression tag	UNP D3EID5
A	234	ALA	GLU	engineered mutation	UNP D3EID5
A	385	GLU	-	expression tag	UNP D3EID5
A	386	GLY	-	expression tag	UNP D3EID5
A	387	HIS	-	expression tag	UNP D3EID5
A	388	HIS	-	expression tag	UNP D3EID5
A	389	HIS	-	expression tag	UNP D3EID5
A	390	HIS	-	expression tag	UNP D3EID5
A	391	HIS	-	expression tag	UNP D3EID5
A	392	HIS	-	expression tag	UNP D3EID5
B	2	SER	-	expression tag	UNP D3EID5
B	3	LEU	-	expression tag	UNP D3EID5
B	234	ALA	GLU	engineered mutation	UNP D3EID5
B	385	GLU	-	expression tag	UNP D3EID5
B	386	GLY	-	expression tag	UNP D3EID5
B	387	HIS	-	expression tag	UNP D3EID5
B	388	HIS	-	expression tag	UNP D3EID5
B	389	HIS	-	expression tag	UNP D3EID5
B	390	HIS	-	expression tag	UNP D3EID5
B	391	HIS	-	expression tag	UNP D3EID5

Continued on next page...

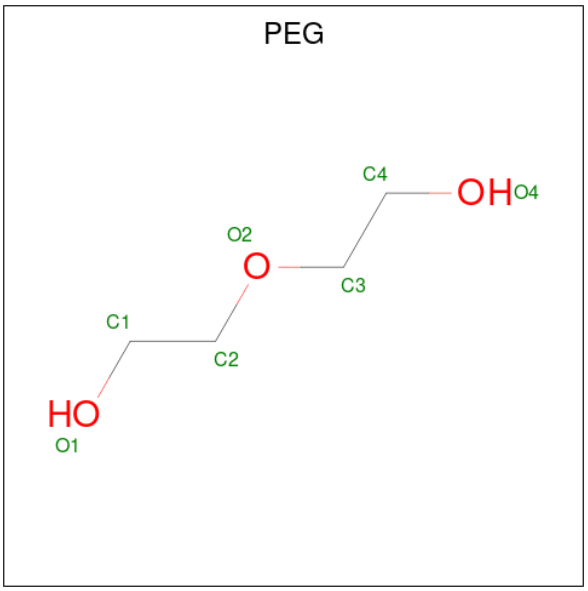
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP D3EID5
C	2	SER	-	expression tag	UNP D3EID5
C	3	LEU	-	expression tag	UNP D3EID5
C	234	ALA	GLU	engineered mutation	UNP D3EID5
C	385	GLU	-	expression tag	UNP D3EID5
C	386	GLY	-	expression tag	UNP D3EID5
C	387	HIS	-	expression tag	UNP D3EID5
C	388	HIS	-	expression tag	UNP D3EID5
C	389	HIS	-	expression tag	UNP D3EID5
C	390	HIS	-	expression tag	UNP D3EID5
C	391	HIS	-	expression tag	UNP D3EID5
C	392	HIS	-	expression tag	UNP D3EID5
D	2	SER	-	expression tag	UNP D3EID5
D	3	LEU	-	expression tag	UNP D3EID5
D	234	ALA	GLU	engineered mutation	UNP D3EID5
D	385	GLU	-	expression tag	UNP D3EID5
D	386	GLY	-	expression tag	UNP D3EID5
D	387	HIS	-	expression tag	UNP D3EID5
D	388	HIS	-	expression tag	UNP D3EID5
D	389	HIS	-	expression tag	UNP D3EID5
D	390	HIS	-	expression tag	UNP D3EID5
D	391	HIS	-	expression tag	UNP D3EID5
D	392	HIS	-	expression tag	UNP D3EID5

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	3	3	3	0	0
2	C	1	1	1	0	0
2	D	2	2	2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is water.

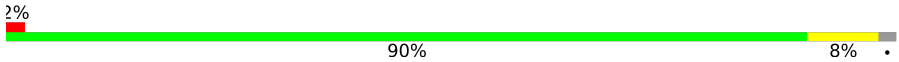
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	487	487	487	0	0
			Total	O		
4	B	387	387	387	0	0
			Total	O		
4	C	385	385	385	0	0
			Total	O		
4	D	239	239	239	0	0

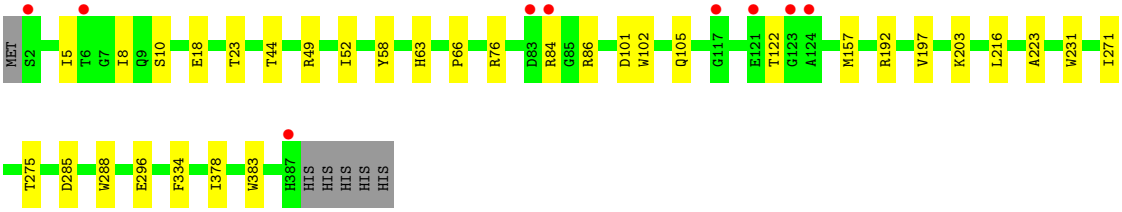
3 Residue-property plots (i)

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: Mandelate racemase/muconate lactonizing protein

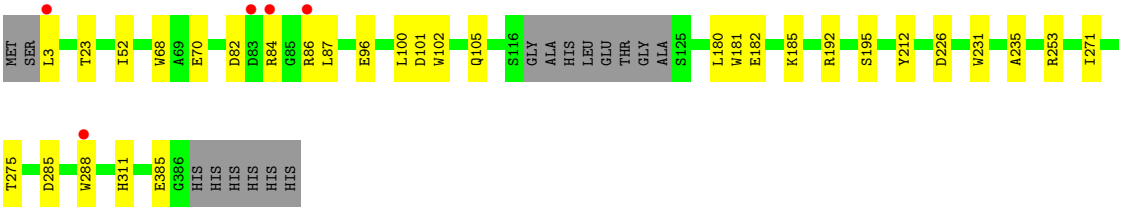
Chain A:





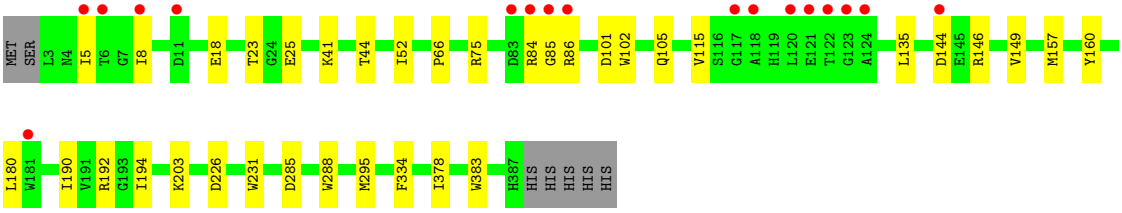
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain B:



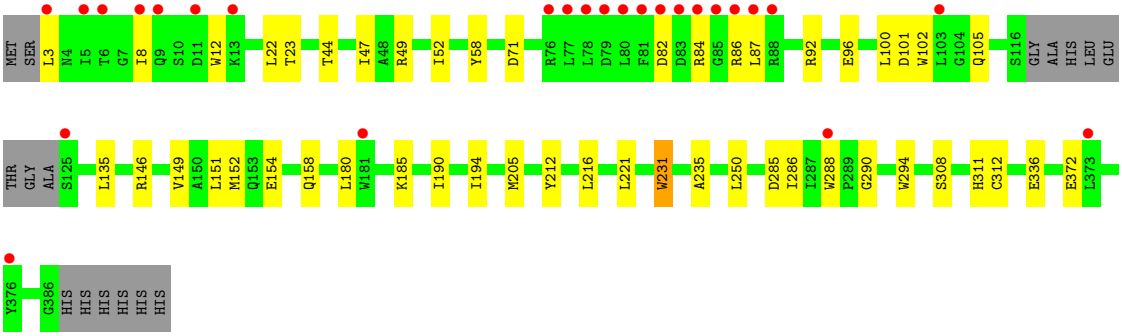
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain C:



• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:


MET SER L3 N4 I5 T6 G7 I8 Q9 S10 D11 W12 K13 L22 T23 T44 I47 A48 R49 I52 Y58 D71 R76 L77 L78 D79 L80 F81 D82 D83 R84 G85 R86 L87 R88 R92 E96 L100 D101 W102 L103 G104 Q105 S116 GLY ALA HIS LEU GLU
THR GLY ALA S125 L135 R146 V149 A150 L151 M152 Q153 E154 Q158 L180 W181 K185 I190 I194 M205 Y212 L216 L221 W231 A235 L250 D285 I286 I287 W288 P289 G290 W294 S308 H311 C312 E336 E372 L373
Y376 G386 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.27Å 65.86Å 151.22Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	40.47 – 1.53 40.47 – 1.53	Depositor EDS
% Data completeness (in resolution range)	87.6 (40.47-1.53) 87.6 (40.47-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.53Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.185 , 0.216 0.182 , 0.213	Depositor DCC
R_{free} test set	10061 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13728	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 63.92 % 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 8.9722e-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 (i)

5.1 Standard geometry (i)

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

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	0.39	0/3171	0.59	0/4295
1	B	0.36	0/3073	0.56	0/4163
1	C	0.32	0/3143	0.53	0/4259
1	D	0.30	0/3072	0.49	0/4161
All	All	0.34	0/12459	0.55	0/16878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3100	0	2989	21	0
1	B	3005	0	2898	21	0
1	C	3072	0	2958	26	0
1	D	3004	0	2902	39	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	20	1	0
3	C	21	0	30	3	0
4	A	487	0	0	4	0
4	B	387	0	0	4	0
4	C	385	0	0	3	0
4	D	239	0	0	3	0
All	All	13728	0	11807	104	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 4.

The worst 5 of 104 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:84:ARG:HD3	1:A:86:ARG:HH21	1.17	1.08
1:C:84:ARG:HD3	1:C:86:ARG:HH21	1.35	0.91
1:A:157:MET:SD	1:A:197:VAL:HG13	2.15	0.86
1:D:84:ARG:HD3	1:D:86:ARG:HH21	1.45	0.80
1:B:84:ARG:HD3	1:B:86:ARG:HH21	1.46	0.79

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	391/392 (100%)	388 (99%)	3 (1%)	0	100	100
1	B	377/392 (96%)	373 (99%)	4 (1%)	0	100	100
1	C	388/392 (99%)	384 (99%)	4 (1%)	0	100	100
1	D	376/392 (96%)	372 (99%)	4 (1%)	0	100	100
All	All	1532/1568 (98%)	1517 (99%)	15 (1%)	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	316/315 (100%)	314 (99%)	2 (1%)	86	72
1	B	308/315 (98%)	307 (100%)	1 (0%)	92	84
1	C	313/315 (99%)	312 (100%)	1 (0%)	92	84
1	D	307/315 (98%)	305 (99%)	2 (1%)	84	68
All	All	1244/1260 (99%)	1238 (100%)	6 (0%)	88	77

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	231	TRP
1	D	71	ASP
1	D	231	TRP
1	A	231	TRP
1	A	63	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	PEG	B	397	-	6,6,6	0.41	0	5,5,5	0.33	0
3	PEG	C	396	-	6,6,6	0.44	0	5,5,5	0.20	0
3	PEG	B	396	-	6,6,6	0.52	0	5,5,5	0.08	0
3	PEG	C	395	-	6,6,6	0.44	0	5,5,5	0.25	0
3	PEG	A	394	-	6,6,6	0.41	0	5,5,5	0.31	0
3	PEG	C	394	-	6,6,6	0.47	0	5,5,5	0.27	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	PEG	B	397	-	-	1/4/4/4	-
3	PEG	C	396	-	-	2/4/4/4	-
3	PEG	B	396	-	-	1/4/4/4	-
3	PEG	C	395	-	-	1/4/4/4	-
3	PEG	A	394	-	-	2/4/4/4	-
3	PEG	C	394	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	394	PEG	O1-C1-C2-O2
3	A	394	PEG	O1-C1-C2-O2
3	B	396	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	396	PEG	O2-C3-C4-O4
3	A	394	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	397	PEG	1	0
3	C	396	PEG	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	386/392 (98%)	-0.19	9 (2%)	60	66	9, 15, 30, 54	0
1	B	376/392 (95%)	-0.20	5 (1%)	77	81	11, 18, 33, 67	0
1	C	385/392 (98%)	-0.09	17 (4%)	34	39	12, 19, 38, 59	0
1	D	376/392 (95%)	0.27	26 (6%)	16	19	16, 26, 51, 81	0
All	All	1523/1568 (97%)	-0.06	57 (3%)	41	48	9, 19, 39, 81	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	ILE	9.5
1	D	83	ASP	6.0
1	A	6	THR	6.0
1	B	83	ASP	5.9
1	D	86	ARG	5.2

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 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, 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	B-factors(Å^2)	Q<0.9
3	PEG	C	394	7/7	0.72	0.21	30,32,41,52	0
3	PEG	B	396	7/7	0.77	0.18	33,37,41,42	0
3	PEG	C	396	7/7	0.83	0.13	33,36,43,43	0
3	PEG	C	395	7/7	0.85	0.19	33,36,39,44	0
3	PEG	B	397	7/7	0.89	0.17	36,37,39,41	0
3	PEG	A	394	7/7	0.92	0.14	29,35,42,43	0
2	MG	B	394	1/1	0.96	0.15	29,29,29,29	0
2	MG	D	394	1/1	0.97	0.14	31,31,31,31	0
2	MG	D	393	1/1	0.98	0.10	18,18,18,18	0
2	MG	B	395	1/1	0.98	0.12	29,29,29,29	0
2	MG	A	393	1/1	0.99	0.12	11,11,11,11	0
2	MG	B	393	1/1	1.00	0.08	13,13,13,13	0
2	MG	C	393	1/1	1.00	0.11	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.