



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2022 – 01:13 am BST

PDB ID : 7ZM9
Title : Ketosynthase domain 3 of Brevibacillus Brevis orphan BGC11
Authors : Tittes, Y.U.; Herbst, D.A.; Jakob, R.P.; Maier, T.
Deposited on : 2022-04-19
Resolution : 1.62 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.30
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

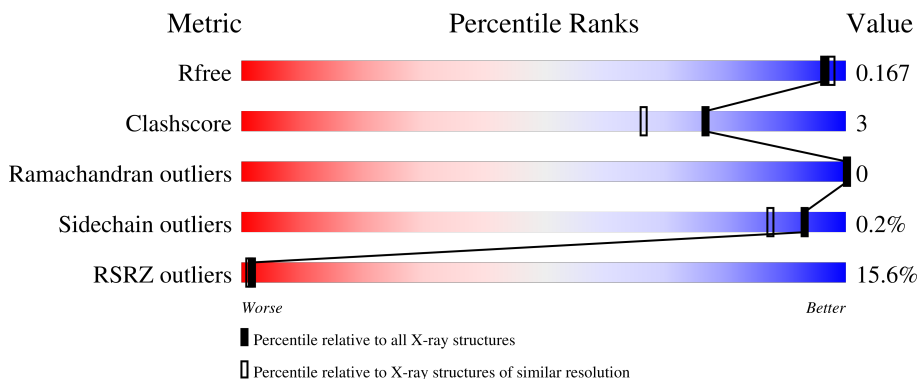
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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 $\leq 5\%$. 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	609	

2 Entry composition [i](#)

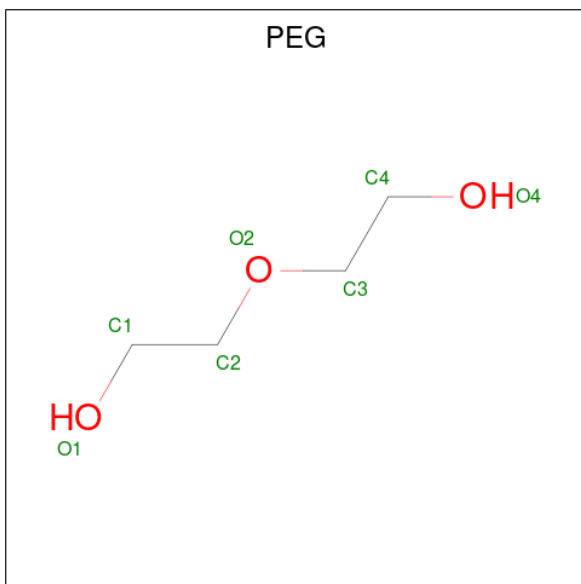
There are 4 unique types of molecules in this entry. The entry contains 9888 atoms, of which 4653 are hydrogens and 0 are deuteriums.

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 Putative polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	596	9260	2957	4589	788	903	23	0	4	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

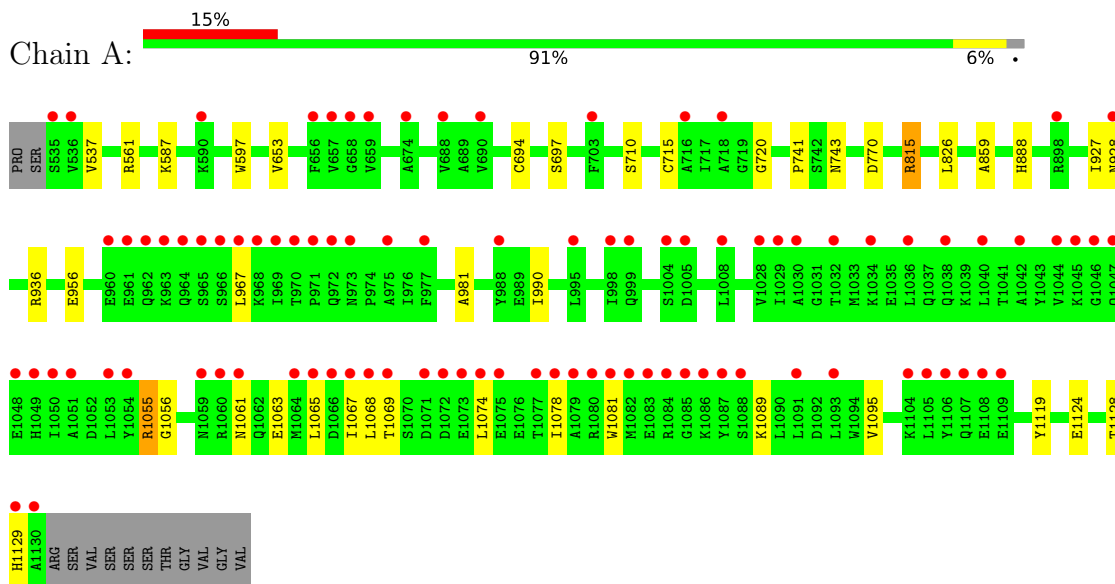
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	518	Total	O	0	0
			518	518		

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: Putative polyketide synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.78Å 92.69Å 99.27Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	60.48 – 1.62 60.48 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.7 (60.48-1.62) 99.7 (60.48-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.62Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.152 , 0.168 0.152 , 0.167	Depositor DCC
R_{free} test set	2000 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.658	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PEG, CSD, 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	0.61	2/4778 (0.0%)	0.69	6/6477 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	956	GLU	CB-CG	-5.56	1.41	1.52
1	A	710	SER	CB-OG	-5.25	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	826	LEU	CB-CG-CD2	6.57	122.17	111.00
1	A	770	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	815	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	936	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	561	ARG	CG-CD-NE	-5.51	100.24	111.80
1	A	826	LEU	CB-CG-CD1	5.16	119.78	111.00

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	4671	4589	4588	27	0
2	A	28	40	40	2	0
3	A	18	24	23	2	0
4	A	518	0	0	2	0
All	All	5235	4653	4651	28	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 3.

All (28) 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:1068:LEU:HD13	1:A:1074:LEU:HD13	1.80	0.64
1:A:1068:LEU:HD13	1:A:1074:LEU:CD1	2.28	0.63
1:A:1074:LEU:O	1:A:1074:LEU:HD23	1.99	0.62
1:A:1061:ASN:O	1:A:1065:LEU:HG	2.00	0.61
1:A:1124:GLU:HA	3:A:1207:GOL:H2	1.86	0.57
1:A:1055:ARG:C	1:A:1095:VAL:HG11	2.27	0.55
1:A:1056:GLY:HA3	1:A:1095:VAL:HG12	1.90	0.54
1:A:967:LEU:HD22	1:A:967:LEU:N	2.25	0.52
1:A:587:LYS:HE3	1:A:741:PRO:HG3	1.92	0.51
1:A:1056:GLY:N	1:A:1095:VAL:CG1	2.74	0.50
2:A:1201:PEG:O1	4:A:1301:HOH:O	2.19	0.50
1:A:1119:TYR:HA	2:A:1201:PEG:H41	1.94	0.50
1:A:1128:THR:HG23	1:A:1129:HIS:N	2.26	0.49
1:A:1068:LEU:HD12	1:A:1069:THR:N	2.28	0.49
1:A:697:SER:HB3	1:A:720:GLY:HA3	1.95	0.48
1:A:1081:TRP:CZ2	1:A:1089:LYS:HE2	2.49	0.47
1:A:1056:GLY:CA	1:A:1095:VAL:HG12	2.46	0.46
1:A:928:ASN:CG	1:A:928:ASN:O	2.54	0.45
1:A:981:ALA:HB2	1:A:990:ILE:HD12	1.97	0.45
1:A:859:ALA:HB2	3:A:1206:GOL:H2	1.99	0.45
1:A:653:VAL:HG22	1:A:715[B]:CYS:SG	2.58	0.44
1:A:537:VAL:HG21	1:A:815:ARG:HG3	2.00	0.44
1:A:927:ILE:O	1:A:928:ASN:HB3	2.16	0.44
1:A:597:TRP:CD2	1:A:743:ASN:HB3	2.53	0.44
1:A:1074:LEU:CD2	1:A:1078:ILE:CD1	2.97	0.43
1:A:888:HIS:HE1	4:A:1709:HOH:O	2.01	0.43
1:A:1067:ILE:O	1:A:1067:ILE:HG22	2.20	0.42
1:A:1063:GLU:OE1	1:A:1063:GLU:HA	2.22	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	598/609 (98%)	582 (97%)	16 (3%)	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	500/506 (99%)	499 (100%)	1 (0%)	93 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1055	ARG

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](#)

1 non-standard protein/DNA/RNA residue is 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
1	CSD	A	694	1	3,7,8	1.02	0	1,8,10	2.32	1 (100%)

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
1	CSD	A	694	1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	CSD	OD1-SG-CB	-2.32	101.12	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	694	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 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
3	GOL	A	1207	-	5,5,5	0.93	0	5,5,5	0.69	0
2	PEG	A	1201	-	6,6,6	0.73	0	5,5,5	0.67	0
2	PEG	A	1203	-	6,6,6	0.47	0	5,5,5	0.27	0
3	GOL	A	1206	-	5,5,5	2.14	2 (40%)	5,5,5	1.28	0
2	PEG	A	1202	-	6,6,6	0.43	0	5,5,5	0.62	0
3	GOL	A	1205	-	5,5,5	1.05	0	5,5,5	0.99	0
2	PEG	A	1204	-	6,6,6	0.51	0	5,5,5	0.53	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	A	1207	-	-	0/4/4/4	-
2	PEG	A	1201	-	-	1/4/4/4	-
2	PEG	A	1203	-	-	1/4/4/4	-
3	GOL	A	1206	-	-	3/4/4/4	-
2	PEG	A	1202	-	-	2/4/4/4	-
3	GOL	A	1205	-	-	2/4/4/4	-
2	PEG	A	1204	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1206	GOL	C3-C2	3.48	1.66	1.51
3	A	1206	GOL	O2-C2	-3.02	1.34	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1205	GOL	O1-C1-C2-C3
3	A	1206	GOL	O1-C1-C2-O2
3	A	1206	GOL	O1-C1-C2-C3
2	A	1203	PEG	O1-C1-C2-O2
2	A	1202	PEG	O1-C1-C2-O2
3	A	1205	GOL	O1-C1-C2-O2
2	A	1202	PEG	O2-C3-C4-O4
3	A	1206	GOL	O2-C2-C3-O3
2	A	1201	PEG	C1-C2-O2-C3
2	A	1204	PEG	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1207	GOL	1	0
2	A	1201	PEG	2	0
3	A	1206	GOL	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, 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	595/609 (97%)	0.74	93 (15%) 2 1	23, 45, 109, 166	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	963	LYS	12.2
1	A	965	SER	10.2
1	A	967	LEU	9.6
1	A	1130	ALA	8.9
1	A	1072	ASP	7.8
1	A	962	GLN	7.6
1	A	964	GLN	6.9
1	A	1084	ARG	6.7
1	A	1068	LEU	6.2
1	A	966	SER	6.2
1	A	1067	ILE	6.0
1	A	1108	GLU	5.4
1	A	1081	TRP	5.4
1	A	1048	GLU	5.4
1	A	1065	LEU	5.3
1	A	1078	ILE	4.6
1	A	1107	GLN	4.6
1	A	961	GLU	4.4
1	A	1079	ALA	4.4
1	A	1051	ALA	4.4
1	A	1109	GLU	4.3
1	A	968	LYS	4.1
1	A	1050	ILE	4.1
1	A	1008	LEU	4.0
1	A	1074	LEU	3.9
1	A	1083	GLU	3.9
1	A	969	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	535	SER	3.9
1	A	1045	LYS	3.8
1	A	1049	HIS	3.7
1	A	1077	THR	3.7
1	A	1044	VAL	3.6
1	A	1129	HIS	3.6
1	A	1036	LEU	3.6
1	A	1080	ARG	3.5
1	A	1059	ASN	3.5
1	A	1082	MET	3.5
1	A	1087	TYR	3.5
1	A	972	GLN	3.5
1	A	703	PHE	3.4
1	A	1029	ILE	3.4
1	A	1053	LEU	3.3
1	A	1032	THR	3.3
1	A	1064	MET	3.3
1	A	1085	GLY	3.3
1	A	1028	VAL	3.2
1	A	977	PHE	3.1
1	A	1073	GLU	3.1
1	A	1038	GLN	3.0
1	A	674	ALA	3.0
1	A	1104	LYS	3.0
1	A	536	VAL	3.0
1	A	1054	TYR	2.9
1	A	690[A]	VAL	2.8
1	A	1042	ALA	2.8
1	A	1066	ASP	2.8
1	A	928	ASN	2.8
1	A	1040	LEU	2.8
1	A	973	ASN	2.7
1	A	1030	ALA	2.7
1	A	1106	TYR	2.7
1	A	1004	SER	2.7
1	A	1093	LEU	2.7
1	A	1086	LYS	2.7
1	A	658	GLY	2.6
1	A	1047	GLN	2.6
1	A	1034	LYS	2.6
1	A	1061	ASN	2.6
1	A	659	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	656	PHE	2.6
1	A	975	ALA	2.6
1	A	971	PRO	2.5
1	A	1105	LEU	2.5
1	A	1069	THR	2.4
1	A	1091	LEU	2.4
1	A	718	ALA	2.4
1	A	1088	SER	2.4
1	A	995	LEU	2.3
1	A	1075	GLU	2.3
1	A	898	ARG	2.3
1	A	1060	ARG	2.3
1	A	998	ILE	2.3
1	A	1046	GLY	2.2
1	A	716	ALA	2.2
1	A	999	GLN	2.2
1	A	688	VAL	2.2
1	A	590	LYS	2.1
1	A	960	GLU	2.1
1	A	970	THR	2.1
1	A	988	TYR	2.1
1	A	1071	ASP	2.0
1	A	657	VAL	2.0
1	A	1005	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	694	8/9	0.95	0.12	27,33,45,56	0

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
2	PEG	A	1201	7/7	0.57	0.28	64,79,96,96	0
2	PEG	A	1203	7/7	0.68	0.20	75,92,108,108	0
3	GOL	A	1205	6/6	0.74	0.30	89,107,111,112	0
3	GOL	A	1207	6/6	0.74	0.36	74,92,107,111	0
2	PEG	A	1202	7/7	0.81	0.19	75,90,95,95	0
2	PEG	A	1204	7/7	0.82	0.14	58,81,100,100	0
3	GOL	A	1206	6/6	0.83	0.24	36,68,82,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.