Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2021 – 03:08 PM GMT

PDB ID	:	6ZT8
Title	:	X-ray structure of mutated arabinofuranosidase
Authors	:	Tandrup, T.; Lo Leggio, L.; Zhao, J.; Bissaro, B.; Barbe, S.; Andre, I.; Dumon, C.; O'Donohue, M.J.; Faure, R.
Deposited on	:	2020-07-17
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

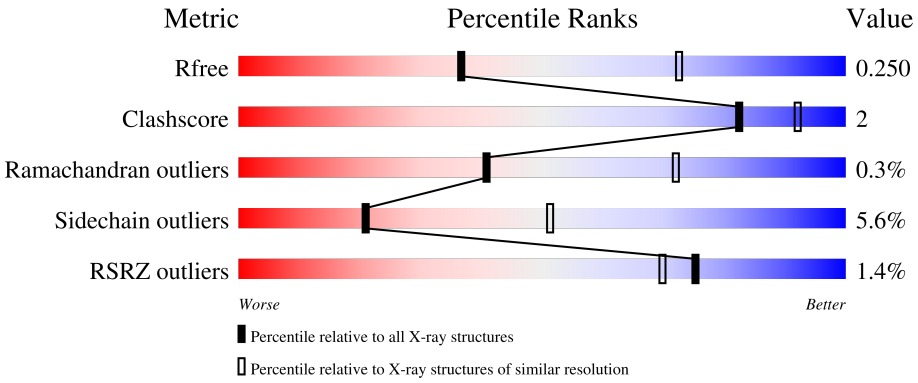
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	496	2% 87% 11%
1	B	496	2% 86% 12%
1	C	496	2% 88% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11916 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.

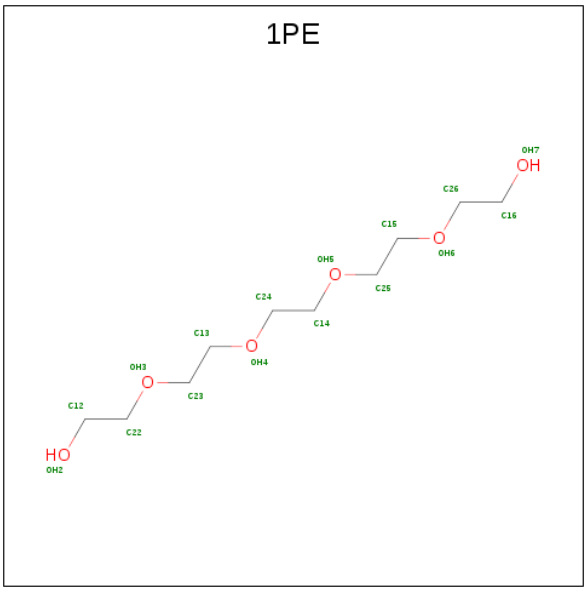
- Molecule 1 is a protein called Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	1	0
			3916	2480	686	726	24			
1	B	490	Total	C	N	O	S	0	2	0
			3921	2483	686	728	24			
1	C	490	Total	C	N	O	S	0	0	0
			3911	2477	685	725	24			

There are 12 discrepancies between the modelled and reference sequences:

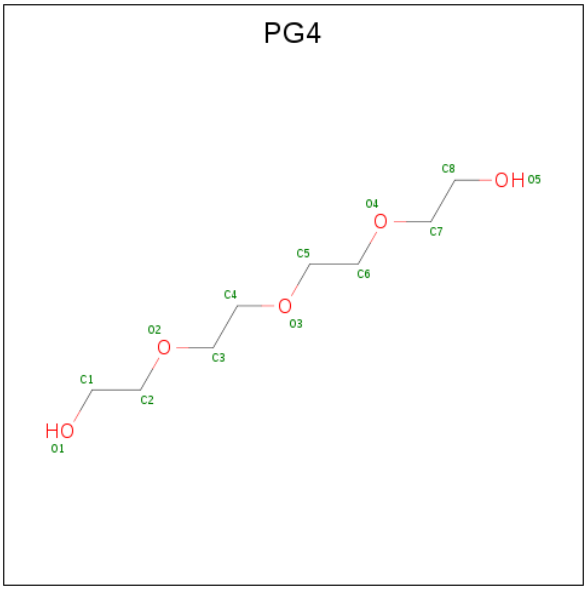
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	HIS	ARG	conflict	UNP O69262
A	216	TRP	ASN	conflict	UNP O69262
A	274	GLU	ARG	conflict	UNP O69262
A	352	MET	LEU	conflict	UNP O69262
B	69	HIS	ARG	conflict	UNP O69262
B	216	TRP	ASN	conflict	UNP O69262
B	274	GLU	ARG	conflict	UNP O69262
B	352	MET	LEU	conflict	UNP O69262
C	69	HIS	ARG	conflict	UNP O69262
C	216	TRP	ASN	conflict	UNP O69262
C	274	GLU	ARG	conflict	UNP O69262
C	352	MET	LEU	conflict	UNP O69262

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 10 6	0	0
2	B	1	Total C O 16 10 6	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0

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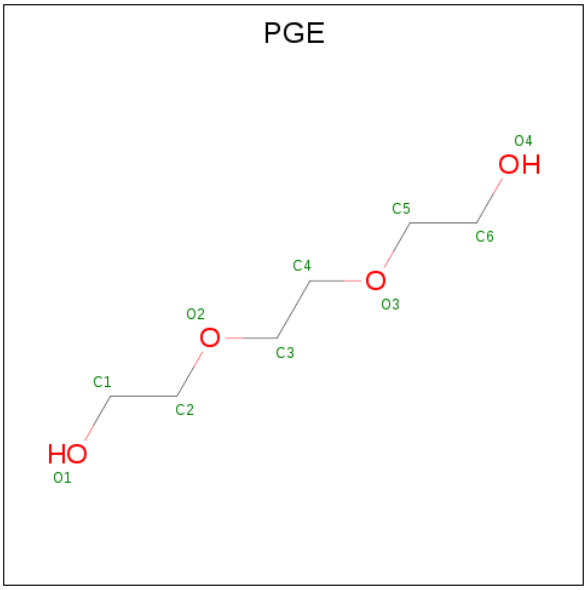
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 6 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0

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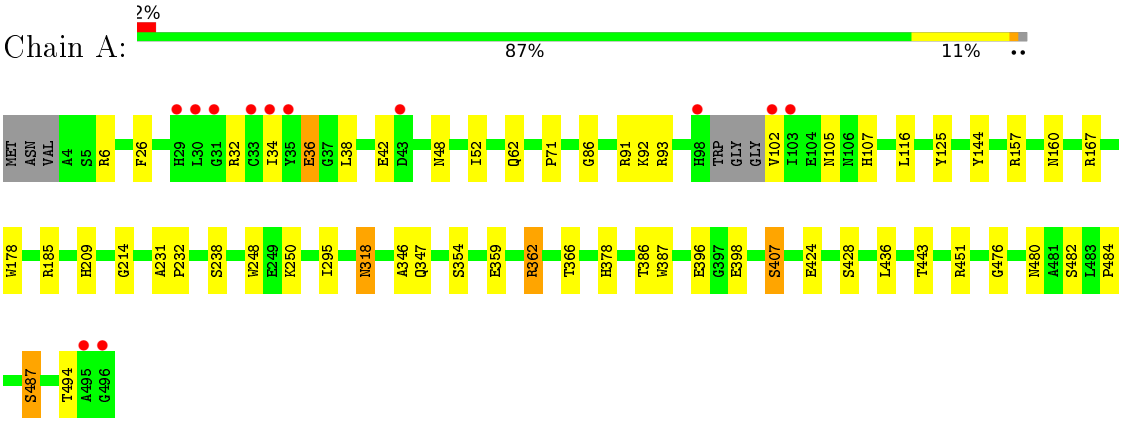
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	23	Total O 23 23	0	0
6	C	21	Total O 21 21	0	0

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.

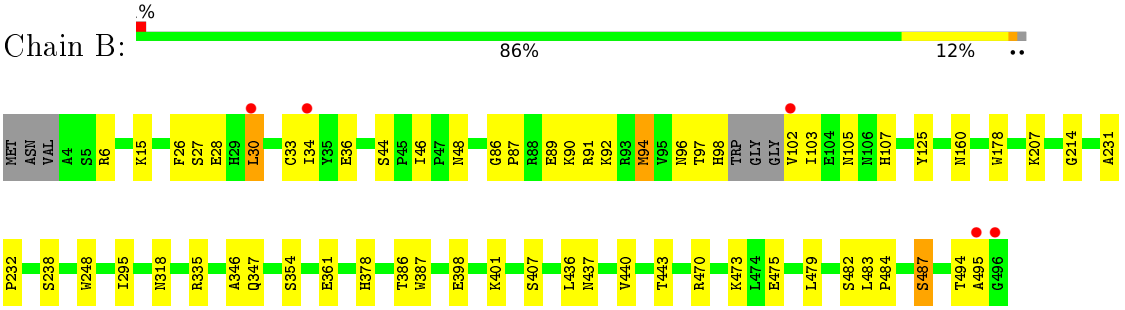
- Molecule 1: Alpha-L-arabinofuranosidase

Chain A:



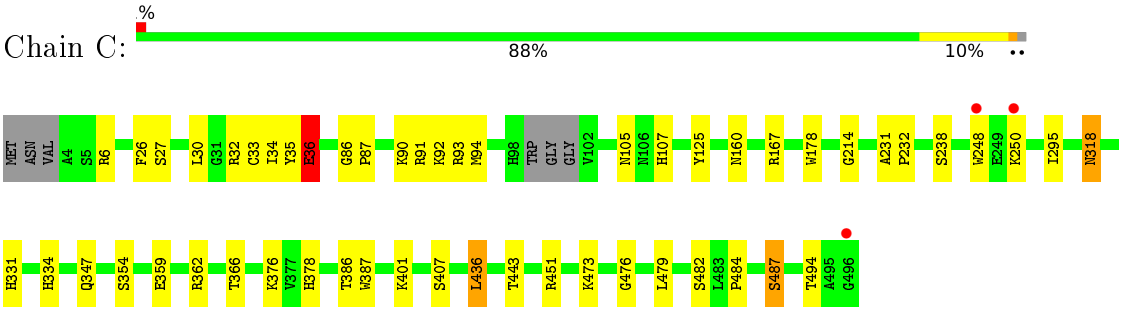
- Molecule 1: Alpha-L-arabinofuranosidase

Chain B:



- Molecule 1: Alpha-L-arabinofuranosidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	156.63Å 156.63Å 376.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.00 – 2.80 48.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.80) 100.0 (48.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.209 , 0.247 0.214 , 0.250	Depositor DCC
R_{free} test set	672 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11916	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: PG4, PGE, CL, 1PE

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	0.50	0/4027	0.69	0/5467
1	B	0.49	0/4035	0.71	0/5478
1	C	0.50	0/4019	0.70	0/5456
All	All	0.50	0/12081	0.70	0/16401

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	8
1	B	0	3
1	C	0	4
All	All	0	15

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	VAL	Peptide
1	A	167	ARG	Sidechain
1	A	185	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	451	ARG	Sidechain
1	A	6	ARG	Sidechain
1	A	91	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	93	ARG	Sidechain
1	B	335	ARG	Sidechain
1	B	6	ARG	Sidechain
1	B	91	ARG	Sidechain
1	C	167	ARG	Sidechain
1	C	451	ARG	Sidechain
1	C	91	ARG	Sidechain
1	C	93	ARG	Sidechain

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	3916	0	3754	19	0
1	B	3921	0	3758	19	0
1	C	3911	0	3748	19	0
2	A	16	0	22	0	0
2	B	16	0	22	0	0
3	A	13	0	18	0	0
3	B	26	0	36	0	0
3	C	13	0	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	10	0	14	1	0
6	A	27	0	0	1	0
6	B	23	0	0	0	0
6	C	21	0	0	0	0
All	All	11916	0	11390	57	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.

All (57) 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:32:ARG:NH1	1:A:36:GLU:OE2	2.19	0.75
1:A:34:ILE:O	1:A:34:ILE:HG22	1.87	0.72
1:C:35:TYR:O	1:C:36:GLU:HB3	1.92	0.68
1:C:32:ARG:HD2	1:C:36:GLU:HG2	1.80	0.63
1:A:359:GLU:OE1	1:A:362:ARG:NH1	2.33	0.62
1:C:359:GLU:OE1	1:C:362:ARG:NH1	2.33	0.60
1:B:27:SER:HB2	1:B:33:CYS:SG	2.44	0.57
1:B:44:SER:OG	1:B:46:ILE:HD12	2.05	0.56
1:A:34:ILE:O	1:A:34:ILE:CG2	2.54	0.55
1:C:27:SER:HB2	1:C:33:CYS:SG	2.47	0.54
1:B:94:MET:HB3	1:B:102:VAL:HG12	1.91	0.53
1:A:396:GLU:HB2	1:A:398:GLU:HG3	1.92	0.51
1:C:378:HIS:ND1	1:C:407:SER:HB3	2.27	0.50
1:A:52:ILE:HD13	1:A:116:LEU:HD13	1.94	0.50
1:A:86:GLY:HA2	1:A:160:ASN:OD1	2.12	0.49
1:B:86:GLY:HA2	1:B:160:ASN:OD1	2.13	0.48
1:B:238:SER:HA	1:B:295:ILE:O	2.13	0.48
1:C:86:GLY:HA2	1:C:160:ASN:OD1	2.14	0.48
1:A:484:PRO:O	1:A:487:SER:HB3	2.15	0.47
1:A:378:HIS:ND1	1:A:407:SER:HB3	2.30	0.47
1:B:484:PRO:O	1:B:487:SER:HB3	2.15	0.47
1:C:376:LYS:O	5:C:502:PGE:H6	2.15	0.46
1:A:238:SER:HA	1:A:295:ILE:O	2.15	0.46
1:B:378:HIS:ND1	1:B:407:SER:HB3	2.30	0.46
1:C:484:PRO:O	1:C:487:SER:HB3	2.15	0.46
1:B:214:GLY:HA3	1:B:238:SER:O	2.15	0.46
1:B:103:ILE:HG22	1:B:103:ILE:O	2.16	0.46
1:B:87:PRO:HB2	1:B:90:LYS:HG2	1.97	0.45
1:C:214:GLY:HA3	1:C:238:SER:O	2.16	0.45
1:A:209:HIS:ND1	6:A:603:HOH:O	2.36	0.45
1:B:105:ASN:ND2	1:B:107:HIS:CG	2.85	0.45
1:A:105:ASN:ND2	1:A:107:HIS:CG	2.85	0.45
1:C:105:ASN:ND2	1:C:107:HIS:CG	2.85	0.44
1:A:214:GLY:HA3	1:A:238:SER:O	2.17	0.44
1:C:436:LEU:HD12	1:C:436:LEU:HA	1.90	0.44
1:C:231:ALA:HB3	1:C:232:PRO:HD3	2.00	0.44
1:C:238:SER:HA	1:C:295:ILE:O	2.17	0.43
1:A:346:ALA:HA	1:A:347:GLN:HA	1.78	0.42
1:B:28:GLU:OE2	1:B:30:LEU:HD13	2.19	0.42
1:B:346:ALA:HA	1:B:347:GLN:HA	1.79	0.42
1:A:231:ALA:HB3	1:A:232:PRO:HD3	2.00	0.42
1:B:27:SER:OG	1:B:34:ILE:HD11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:SER:OG	1:C:34:ILE:HD11	2.20	0.42
1:C:87:PRO:HB2	1:C:90:LYS:HG3	2.01	0.42
1:A:480[B]:ASN:HD22	1:A:480[B]:ASN:H	1.67	0.41
1:B:479:LEU:C	1:B:479:LEU:HD23	2.41	0.41
1:C:331:HIS:O	1:C:334:HIS:HB2	2.21	0.41
1:B:347:GLN:O	1:B:354:SER:HA	2.21	0.41
1:A:318:ASN:HB3	1:A:366:THR:HB	2.02	0.41
1:B:231:ALA:HB3	1:B:232:PRO:HD3	2.03	0.41
1:A:347:GLN:O	1:A:354:SER:HA	2.22	0.40
1:B:96:ASN:HD21	1:B:98:HIS:HB2	1.85	0.40
1:B:440:VAL:HG12	1:B:495:ALA:HA	2.02	0.40
1:A:144:TYR:O	1:A:157:ARG:HD3	2.21	0.40
1:C:347:GLN:O	1:C:354:SER:HA	2.22	0.40
1:C:318:ASN:HB3	1:C:366:THR:HB	2.03	0.40
1:C:479:LEU:C	1:C:479:LEU:HD23	2.41	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	487/496 (98%)	460 (94%)	25 (5%)	2 (0%)	34	66
1	B	488/496 (98%)	460 (94%)	27 (6%)	1 (0%)	47	78
1	C	486/496 (98%)	461 (95%)	23 (5%)	2 (0%)	34	66
All	All	1461/1488 (98%)	1381 (94%)	75 (5%)	5 (0%)	41	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	476	GLY

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Mol	Chain	Res	Type
1	B	36	GLU
1	C	36	GLU
1	C	476	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	416/419 (99%)	394 (95%)	22 (5%)	22	54
1	B	417/419 (100%)	389 (93%)	28 (7%)	16	43
1	C	415/419 (99%)	395 (95%)	20 (5%)	25	58
All	All	1248/1257 (99%)	1178 (94%)	70 (6%)	21	51

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	38	LEU
1	A	42	GLU
1	A	48	ASN
1	A	62	GLN
1	A	71	PRO
1	A	92	LYS
1	A	125	TYR
1	A	178	TRP
1	A	248	TRP
1	A	250	LYS
1	A	318	ASN
1	A	386	THR
1	A	387	TRP
1	A	407	SER
1	A	424	GLU
1	A	428	SER
1	A	436	LEU
1	A	443	THR

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Mol	Chain	Res	Type
1	A	482	SER
1	A	487	SER
1	A	494	THR
1	B	15	LYS
1	B	26	PHE
1	B	30	LEU
1	B	48	ASN
1	B	89	GLU
1	B	92	LYS
1	B	94	MET
1	B	97	THR
1	B	125	TYR
1	B	178	TRP
1	B	207	LYS
1	B	248	TRP
1	B	318	ASN
1	B	361	GLU
1	B	386	THR
1	B	387	TRP
1	B	398	GLU
1	B	401	LYS
1	B	436	LEU
1	B	437	ASN
1	B	443	THR
1	B	470	ARG
1	B	473	LYS
1	B	475	GLU
1	B	482	SER
1	B	483	LEU
1	B	487	SER
1	B	494	THR
1	C	6	ARG
1	C	26	PHE
1	C	30	LEU
1	C	36	GLU
1	C	92	LYS
1	C	94	MET
1	C	125	TYR
1	C	178	TRP
1	C	248	TRP
1	C	250	LYS
1	C	318	ASN

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Mol	Chain	Res	Type
1	C	386	THR
1	C	387	TRP
1	C	401	LYS
1	C	436	LEU
1	C	443	THR
1	C	473	LYS
1	C	482	SER
1	C	487	SER
1	C	494	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	98	HIS
1	A	175	ASN
1	A	183	ASN
1	A	235	HIS
1	A	240	HIS
1	B	48	ASN
1	B	175	ASN
1	B	183	ASN
1	B	235	HIS
1	B	240	HIS
1	B	437	ASN
1	C	48	ASN
1	C	175	ASN
1	C	183	ASN
1	C	229	GLN
1	C	235	HIS
1	C	240	HIS
1	C	480	ASN

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, 3 are monoatomic - leaving 7 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	PG4	C	501	-	12,12,12	1.00	0	11,11,11	0.80	0
3	PG4	B	503	-	12,12,12	0.66	0	11,11,11	0.77	0
5	PGE	C	502	-	9,9,9	0.60	0	8,8,8	0.62	0
3	PG4	A	502	-	12,12,12	0.65	0	11,11,11	0.70	0
3	PG4	B	502	-	12,12,12	0.90	0	11,11,11	0.90	0
2	1PE	B	501	-	15,15,15	0.50	0	14,14,14	0.47	0
2	1PE	A	501	-	15,15,15	0.83	0	14,14,14	0.75	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	PG4	C	501	-	-	6/10/10/10	-
3	PG4	B	503	-	-	5/10/10/10	-
5	PGE	C	502	-	-	3/7/7/7	-
3	PG4	A	502	-	-	4/10/10/10	-
3	PG4	B	502	-	-	5/10/10/10	-
2	1PE	B	501	-	-	8/13/13/13	-
2	1PE	A	501	-	-	5/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	1PE	C12-C22-OH3-C23
2	B	501	1PE	OH7-C16-C26-OH6
3	B	503	PG4	C5-C6-O4-C7
3	C	501	PG4	O3-C5-C6-O4
3	C	501	PG4	O2-C3-C4-O3
3	B	502	PG4	O1-C1-C2-O2
3	B	502	PG4	O2-C3-C4-O3
2	A	501	1PE	OH6-C15-C25-OH5
3	B	503	PG4	O4-C7-C8-O5
3	A	502	PG4	C3-C4-O3-C5
2	B	501	1PE	OH4-C13-C23-OH3
2	A	501	1PE	OH5-C14-C24-OH4
5	C	502	PGE	O3-C5-C6-O4
2	A	501	1PE	OH7-C16-C26-OH6
3	C	501	PG4	O4-C7-C8-O5
3	B	503	PG4	O1-C1-C2-O2
3	A	502	PG4	O4-C7-C8-O5
3	A	502	PG4	O2-C3-C4-O3
2	B	501	1PE	C15-C25-OH5-C14
2	B	501	1PE	OH5-C14-C24-OH4
2	A	501	1PE	OH4-C13-C23-OH3
2	B	501	1PE	C25-C15-OH6-C26
3	B	502	PG4	C3-C4-O3-C5
3	C	501	PG4	C6-C5-O3-C4
5	C	502	PGE	C4-C3-O2-C2
3	B	503	PG4	C1-C2-O2-C3
3	B	502	PG4	C1-C2-O2-C3
3	B	502	PG4	O3-C5-C6-O4
3	B	503	PG4	O2-C3-C4-O3
2	B	501	1PE	C16-C26-OH6-C15
3	C	501	PG4	C8-C7-O4-C6
2	A	501	1PE	C24-C14-OH5-C25
3	A	502	PG4	O3-C5-C6-O4
5	C	502	PGE	C3-C4-O3-C5
3	C	501	PG4	C4-C3-O2-C2
2	B	501	1PE	OH6-C15-C25-OH5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	PGE	1	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	490/496 (98%)	-0.28	12 (2%) 59 49	35, 52, 102, 163	0
1	B	490/496 (98%)	-0.27	5 (1%) 82 77	33, 58, 98, 137	0
1	C	490/496 (98%)	-0.24	3 (0%) 89 86	33, 57, 94, 122	0
All	All	1470/1488 (98%)	-0.26	20 (1%) 75 70	33, 56, 97, 163	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	CYS	12.0
1	A	30	LEU	4.0
1	B	30	LEU	4.0
1	A	102	VAL	3.8
1	B	102	VAL	3.7
1	A	98	HIS	3.2
1	C	496	GLY	3.2
1	A	496	GLY	3.1
1	B	496	GLY	3.1
1	A	29	HIS	3.0
1	C	248	TRP	2.7
1	A	35	TYR	2.6
1	A	495	ALA	2.5
1	A	34	ILE	2.5
1	C	250	LYS	2.2
1	B	495	ALA	2.2
1	A	31	GLY	2.2
1	A	43	ASP	2.1
1	B	34	ILE	2.0
1	A	103	ILE	2.0

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, 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	PG4	B	502	13/13	0.78	0.23	51,74,86,88	0
3	PG4	C	501	13/13	0.79	0.32	61,77,109,112	0
3	PG4	A	502	13/13	0.83	0.30	60,69,77,81	0
3	PG4	B	503	13/13	0.84	0.27	83,93,111,111	0
2	1PE	B	501	16/16	0.89	0.22	63,73,110,112	0
2	1PE	A	501	16/16	0.89	0.17	46,70,94,98	0
4	CL	C	503	1/1	0.91	0.17	54,54,54,54	0
5	PGE	C	502	10/10	0.93	0.13	47,54,56,57	0
4	CL	A	503	1/1	0.96	0.13	55,55,55,55	0
4	CL	B	504	1/1	0.97	0.17	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.