



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PUZ
Title : Crystal Structure of a pre-translocation state MBP-Maltose transporter complex bound to AMP-PNP
Authors : Oldham, M.L.; Chen, J.
Deposited on : 2010-12-06
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

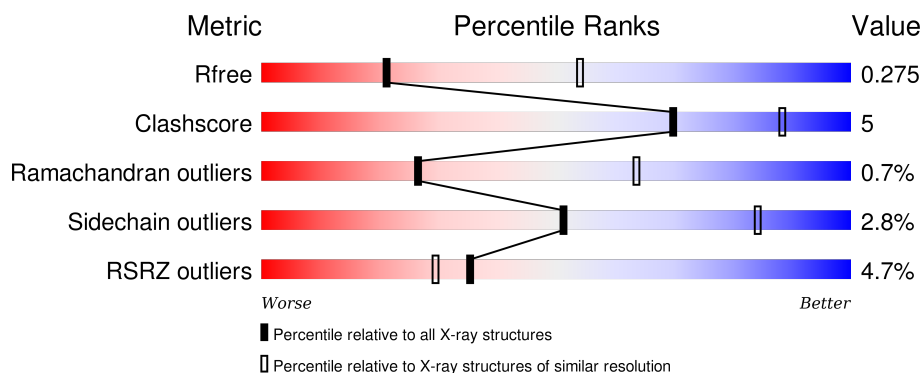
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	E	370	<div> <div>0%</div> <div>87% 13%</div> </div>
2	F	514	<div> <div>5%</div> <div>83% 10% 6%</div> </div>
3	G	296	<div> <div>3%</div> <div>81% 11% 5%</div> </div>
4	A	381	<div> <div>3%</div> <div>82% 15%</div> </div>
4	B	381	<div> <div>9%</div> <div>84% 12%</div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PGV	F	4001	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14697 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 Maltose transporter subunit; periplasmic-binding component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	370	Total	C	N	O	S	0	0	0
			2880	1854	469	549	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	69	CYS	GLY	ENGINEERED MUTATION	UNP B1XC33
E	337	CYS	SER	ENGINEERED MUTATION	UNP B1XC33

- Molecule 2 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	481	Total	C	N	O	S	0	0	0
			3732	2452	594	669	17			

- Molecule 3 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	282	Total	C	N	O	S	0	0	0
			2182	1461	348	364	9			

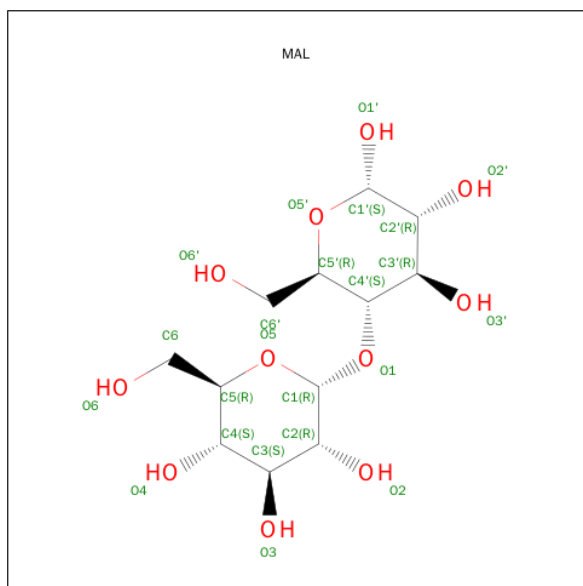
- Molecule 4 is a protein called Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			
4	B	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP B1XC34
A	373	SER	-	EXPRESSION TAG	UNP B1XC34
A	374	ALA	-	EXPRESSION TAG	UNP B1XC34
A	375	SER	-	EXPRESSION TAG	UNP B1XC34
A	376	HIS	-	EXPRESSION TAG	UNP B1XC34
A	377	HIS	-	EXPRESSION TAG	UNP B1XC34
A	378	HIS	-	EXPRESSION TAG	UNP B1XC34
A	379	HIS	-	EXPRESSION TAG	UNP B1XC34
A	380	HIS	-	EXPRESSION TAG	UNP B1XC34
A	381	HIS	-	EXPRESSION TAG	UNP B1XC34
B	372	ALA	-	EXPRESSION TAG	UNP B1XC34
B	373	SER	-	EXPRESSION TAG	UNP B1XC34
B	374	ALA	-	EXPRESSION TAG	UNP B1XC34
B	375	SER	-	EXPRESSION TAG	UNP B1XC34
B	376	HIS	-	EXPRESSION TAG	UNP B1XC34
B	377	HIS	-	EXPRESSION TAG	UNP B1XC34
B	378	HIS	-	EXPRESSION TAG	UNP B1XC34
B	379	HIS	-	EXPRESSION TAG	UNP B1XC34
B	380	HIS	-	EXPRESSION TAG	UNP B1XC34
B	381	HIS	-	EXPRESSION TAG	UNP B1XC34

- Molecule 5 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



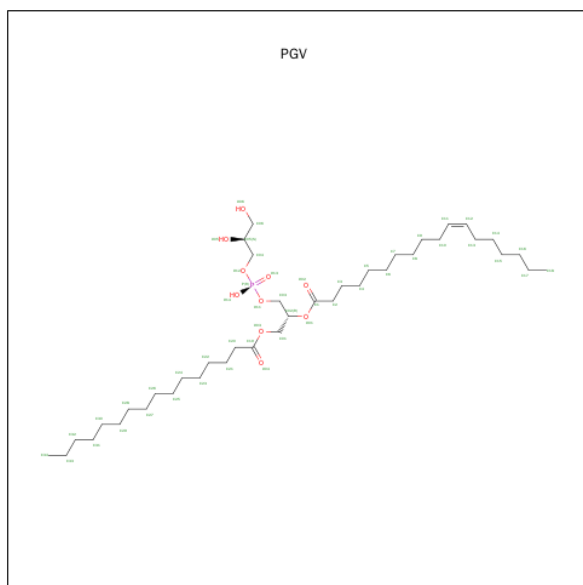
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			23	12	11		

- Molecule 6 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).

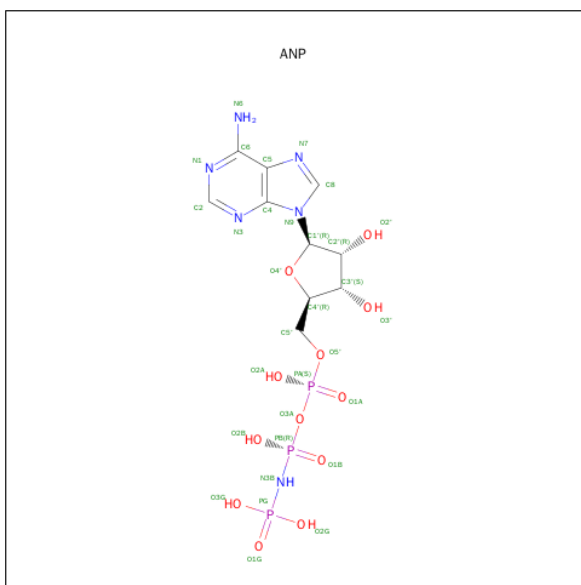


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

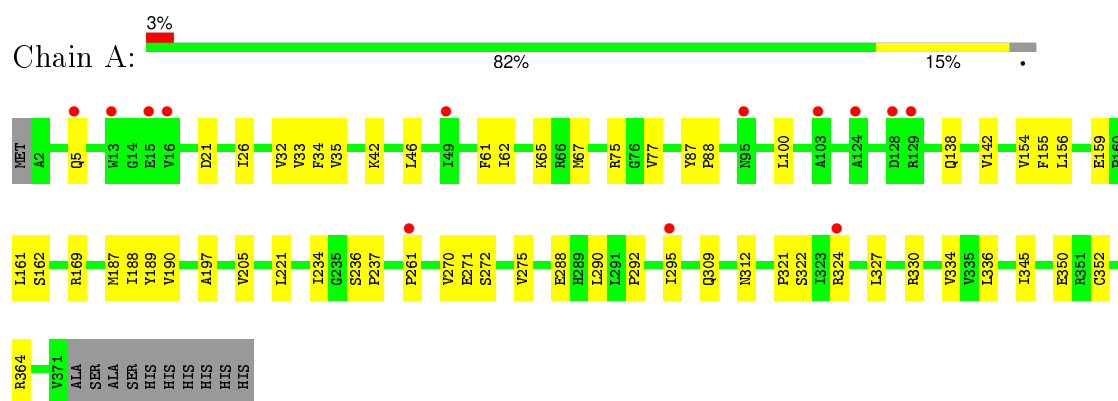
- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



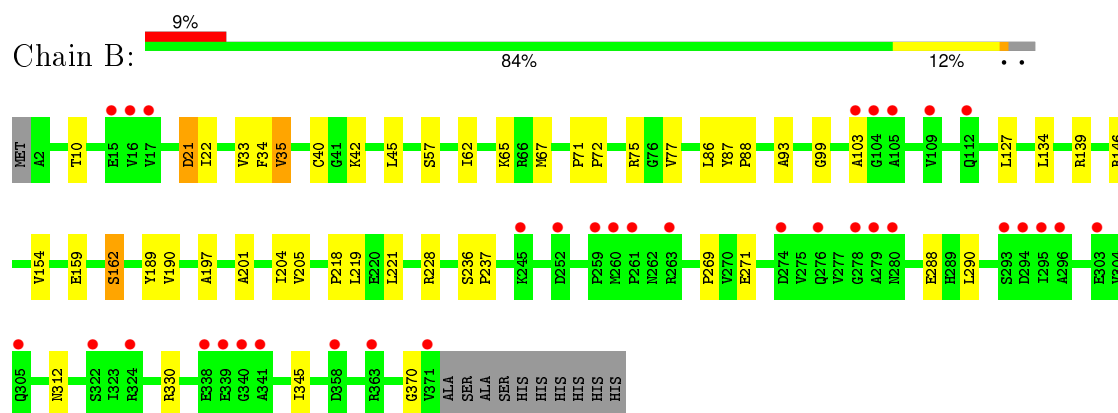
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 27	C 10	N 6	O 9	P 2	0	0
8	B	1	Total 27	C 10	N 6	O 9	P 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total O 3 3	0	0
9	B	5	Total O 5 5	0	0



- Molecule 4: Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.02Å 93.36Å 119.76Å 90.05° 102.57° 105.01°	Depositor
Resolution (Å)	19.95 – 2.90 19.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.0 (19.95-2.90) 76.6 (19.90-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.237 , 0.279 0.234 , 0.275	Depositor DCC
R_{free} test set	2864 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55543 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14697	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PGV, MG, ANP, MAL

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	E	0.31	0/2949	0.45	0/4001
2	F	0.33	0/3823	0.47	0/5203
3	G	0.34	0/2242	0.48	0/3065
4	A	0.30	0/2921	0.48	0/3961
4	B	0.30	0/2921	0.47	0/3961
All	All	0.32	0/14856	0.47	0/20191

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	E	2880	0	2859	29	0
2	F	3732	0	3759	28	0
3	G	2182	0	2271	20	0
4	A	2871	0	2936	36	0
4	B	2871	0	2937	30	0
5	E	23	0	22	0	0
5	F	23	0	22	2	0
6	F	51	0	76	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	27	0	12	0	0
8	B	27	0	12	0	0
9	A	3	0	0	0	0
9	B	5	0	0	0	0
All	All	14697	0	14906	134	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 5.

The worst 5 of 134 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)
4:B:236:SER:HB3	4:B:237:PRO:HD3	1.54	0.89
4:A:236:SER:HB3	4:A:237:PRO:HD3	1.58	0.84
3:G:91:VAL:O	3:G:95:SER:HB2	1.82	0.78
4:A:159:GLU:HB3	4:A:162:SER:HB2	1.67	0.75
1:E:277:LYS:HD3	2:F:200:SER:HB3	1.71	0.71

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	E	368/370 (100%)	354 (96%)	12 (3%)	2 (0%)	34	71
2	F	477/514 (93%)	457 (96%)	18 (4%)	2 (0%)	39	74
3	G	280/296 (95%)	258 (92%)	17 (6%)	5 (2%)	11	37
4	A	368/381 (97%)	349 (95%)	18 (5%)	1 (0%)	46	79
4	B	368/381 (97%)	354 (96%)	11 (3%)	3 (1%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1861/1942 (96%)	1772 (95%)	76 (4%)	13 (1%)	26 63

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ASN
2	F	355	PHE
3	G	8	SER
4	B	103	ALA
2	F	58	ALA

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	E	298/298 (100%)	294 (99%)	4 (1%)	76 94
2	F	391/424 (92%)	379 (97%)	12 (3%)	47 82
3	G	228/237 (96%)	214 (94%)	14 (6%)	23 56
4	A	314/323 (97%)	307 (98%)	7 (2%)	60 88
4	B	314/323 (97%)	307 (98%)	7 (2%)	60 88
All	All	1545/1605 (96%)	1501 (97%)	44 (3%)	51 84

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	19	LEU
3	G	74	ILE
4	B	162	SER
3	G	21	LEU
3	G	54	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	116	GLN
4	B	366	HIS
4	B	264	GLN
2	F	440	ASN
4	B	255	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
8	ANP	A	2501	7	22,29,33	1.51	3 (13%)	24,45,52	2.09	5 (20%)
8	ANP	B	2502	7	22,29,33	1.52	3 (13%)	24,45,52	2.09	5 (20%)
5	MAL	E	2002	-	24,24,24	0.45	0	35,35,35	0.62	0
5	MAL	F	2001	-	24,24,24	0.48	0	35,35,35	0.99	1 (2%)
6	PGV	F	4001	-	50,50,50	1.05	3 (6%)	51,56,56	1.03	3 (5%)

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
8	ANP	A	2501	7	-	0/9/32/38	0/3/3/3
8	ANP	B	2502	7	-	0/9/32/38	0/3/3/3
5	MAL	E	2002	-	-	0/8/48/48	0/2/2/2
5	MAL	F	2001	-	-	0/8/48/48	0/2/2/2
6	PGV	F	4001	-	-	0/55/55/55	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2501	ANP	PB-O3A	2.00	1.61	1.59
8	B	2502	ANP	PB-O3A	2.12	1.61	1.59
8	B	2502	ANP	C5-C4	3.24	1.47	1.40
8	A	2501	ANP	C5-C4	3.30	1.47	1.40
6	F	4001	PGV	C12-C11	3.68	1.53	1.31

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2502	ANP	N3-C2-N1	-7.33	123.28	128.89
8	A	2501	ANP	N3-C2-N1	-7.32	123.29	128.89
8	A	2501	ANP	PA-O3A-PB	-3.82	122.00	132.73
8	B	2502	ANP	PA-O3A-PB	-3.09	124.06	132.73
8	B	2502	ANP	C4-C5-N7	-2.96	106.75	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2001	MAL	2	0
6	F	4001	PGV	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 [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	E	370/370 (100%)	-0.35	5 (1%) 78 76	44, 75, 114, 139	0
2	F	481/514 (93%)	0.04	26 (5%) 29 23	45, 89, 181, 261	0
3	G	282/296 (95%)	-0.19	10 (3%) 48 40	44, 72, 115, 143	0
4	A	370/381 (97%)	-0.03	13 (3%) 48 40	58, 88, 123, 148	0
4	B	370/381 (97%)	0.30	34 (9%) 11 7	57, 100, 215, 277	0
All	All	1873/1942 (96%)	-0.03	88 (4%) 35 29	44, 85, 166, 277	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	322	SER	7.3
2	F	18	SER	7.0
2	F	40	TYR	6.8
3	G	8	SER	6.6
4	B	276	GLN	6.1

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	PGV	F	4001	51/51	0.81	0.29	2.17	89,97,103,104	0
8	ANP	A	2501	27/31	0.90	0.21	0.50	72,85,94,97	0
8	ANP	B	2502	27/31	0.92	0.18	0.02	74,87,95,98	0
5	MAL	F	2001	23/23	0.94	0.14	-0.18	45,47,50,51	0
5	MAL	E	2002	23/23	0.98	0.12	-0.58	47,53,58,58	0
7	MG	A	1501	1/1	0.98	0.15	-	51,51,51,51	0
7	MG	B	1502	1/1	0.98	0.14	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.