

## wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 20, 2023 – 12:21 AM JST

PDB ID	:	7C6X
Title	:	Crystal structure of beta-glycosides-binding protein (W41A) of ABC trans-
		porter in an open state (Form I)
Authors	:	Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.
Deposited on	:	2020-05-22
Resolution	:	2.65  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 (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
$\mathrm{EDS}$	:	2.36
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)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.65 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374(2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	А	423	87%	10%	••
1	В	423	88%	9%	·
1	С	423	2% <b>8</b> 9%	8%	••
1	D	423	87%	9%	
1	Е	423	88%	8%	•••
1	F	423	% 89%	8%	••



Mol	Chain	Length	Quality of chain		
1	G	423	90%	8%	
1	Н	423	87%	9%	•••
1	Ι	423	% 	10%	•••
1	J	423	87%	9%	••
1	K	423	89%	8%	·
1	L	423	88%	8%	••



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 38371 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	419	Total	С	Ν	0	S	0	1	0
	A	410	3153	2026	544	573	10	0	1	0
1	р	412	Total	С	Ν	0	S	0	0	0
	D	410	3145	2021	541	573	10	0	0	0
1	С	413	Total	С	Ν	0	S	0	0	Ο
1		415	3145	2021	541	573	10	0	0	0
1	Л	413	Total	С	Ν	0	S	0	1	Ο
1	D	415	3153	2026	544	573	10	0	I	0
1	F	413	Total	С	Ν	0	S	0	0	0
		410	3145	2021	541	573	10		0	0
1	Б	419	Total	С	Ν	0	S	0	0	0
	Г	410	3145	2021	541	573	10	0	0	U
1	C	416	Total	С	Ν	0	S	0	1	0
	G	410	3181	2042	551	578	10	0	1	0
1	ц	412	Total	С	Ν	0	S	0	1	0
	п	410	3153	2026	544	573	10	0	1	0
1	т	412	Total	С	Ν	0	S	0	1	0
	1	410	3153	2026	544	573	10	0	L	0
1	т	412	Total	С	Ν	0	S	0	0	0
	J	410	3145	2021	541	573	10		0	0
1	K	413	Total	С	Ν	0	S	0	0	0
	IX	410	3145	2021	541	573	10	U	U	U
1	т	413	Total	С	Ν	0	S	0	0	0
		410	3145	2021	541	573	10	0	U	U

• Molecule 1 is a protein called Sugar ABC transporter, periplasmic sugar-binding protein.

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	MET	-	initiating methionine	UNP Q53W80
А	41	ALA	TRP	engineered mutation	UNP Q53W80
А	417	HIS	-	expression tag	UNP Q53W80
А	418	HIS	-	expression tag	UNP Q53W80
А	419	HIS	-	expression tag	UNP Q53W80



7	C	6	Х

Chain	Residue	Modelled	Actual	Comment	Reference
А	420	HIS	-	expression tag	UNP Q53W80
А	421	HIS	-	expression tag	UNP Q53W80
А	422	HIS	_	expression tag	UNP Q53W80
В	0	MET	-	initiating methionine	UNP Q53W80
В	41	ALA	TRP	engineered mutation	UNP Q53W80
В	417	HIS	-	expression tag	UNP Q53W80
В	418	HIS	_	expression tag	UNP Q53W80
В	419	HIS	-	expression tag	UNP Q53W80
В	420	HIS	-	expression tag	UNP Q53W80
В	421	HIS	-	expression tag	UNP Q53W80
В	422	HIS	-	expression tag	UNP Q53W80
С	0	MET	_	initiating methionine	UNP Q53W80
С	41	ALA	TRP	engineered mutation	UNP Q53W80
С	417	HIS	-	expression tag	UNP Q53W80
С	418	HIS	-	expression tag	UNP Q53W80
С	419	HIS	-	expression tag	UNP Q53W80
С	420	HIS	-	expression tag	UNP Q53W80
С	421	HIS	-	expression tag	UNP Q53W80
С	422	HIS	-	expression tag	UNP Q53W80
D	0	MET	-	initiating methionine	UNP Q53W80
D	41	ALA	TRP	engineered mutation	UNP Q53W80
D	417	HIS	-	expression tag	UNP Q53W80
D	418	HIS	-	expression tag	UNP Q53W80
D	419	HIS	-	expression tag	UNP Q53W80
D	420	HIS	-	expression tag	UNP Q53W80
D	421	HIS	-	expression tag	UNP Q53W80
D	422	HIS	-	expression tag	UNP Q53W80
Е	0	MET	-	initiating methionine	UNP Q53W80
Е	41	ALA	TRP	engineered mutation	UNP Q53W80
Е	417	HIS	-	expression tag	UNP Q53W80
Е	418	HIS	-	expression tag	UNP Q53W80
Е	419	HIS	-	expression tag	UNP Q53W80
Е	420	HIS	-	expression tag	UNP Q53W80
Е	421	HIS	-	expression tag	UNP Q53W80
Е	422	HIS	-	expression tag	UNP Q53W80
F	0	MET	-	initiating methionine	UNP Q53W80
F	41	ALA	TRP	engineered mutation	UNP Q53W80
F	417	HIS	-	expression tag	UNP Q53W80
F	418	HIS	-	expression tag	UNP Q53W80
F	419	HIS	-	expression tag	UNP Q53W80
F	420	HIS	-	expression tag	UNP Q53W80
F	421	HIS	-	expression tag	UNP Q53W80



7(	26	Х

Chain	Residue	Modelled	Actual	Comment	Reference
F	422	HIS	-	expression tag	UNP Q53W80
G	0	MET	-	initiating methionine	UNP Q53W80
G	41	ALA	TRP	engineered mutation	UNP Q53W80
G	417	HIS	-	expression tag	UNP Q53W80
G	418	HIS	-	expression tag	UNP Q53W80
G	419	HIS	-	expression tag	UNP Q53W80
G	420	HIS	-	expression tag	UNP Q53W80
G	421	HIS	-	expression tag	UNP Q53W80
G	422	HIS	-	expression tag	UNP Q53W80
Н	0	MET	-	initiating methionine	UNP Q53W80
Н	41	ALA	TRP	engineered mutation	UNP Q53W80
Н	417	HIS	-	expression tag	UNP Q53W80
Н	418	HIS	-	expression tag	UNP Q53W80
Н	419	HIS	-	expression tag	UNP Q53W80
Н	420	HIS	-	expression tag	UNP Q53W80
Н	421	HIS	-	expression tag	UNP Q53W80
Н	422	HIS	-	expression tag	UNP Q53W80
Ι	0	MET	-	initiating methionine	UNP Q53W80
Ι	41	ALA	TRP	engineered mutation	UNP Q53W80
Ι	417	HIS	-	expression tag	UNP Q53W80
Ι	418	HIS	-	expression tag	UNP Q53W80
Ι	419	HIS	-	expression tag	UNP Q53W80
Ι	420	HIS	-	expression tag	UNP Q53W80
Ι	421	HIS	-	expression tag	UNP Q53W80
Ι	422	HIS	-	expression tag	UNP Q53W80
J	0	MET	-	initiating methionine	UNP Q53W80
J	41	ALA	TRP	engineered mutation	UNP Q53W80
J	417	HIS	-	expression tag	UNP Q53W80
J	418	HIS	-	expression tag	UNP Q53W80
J	419	HIS	-	expression tag	UNP Q53W80
J	420	HIS	-	expression tag	UNP Q53W80
J	421	HIS	-	expression tag	UNP Q53W80
J	422	HIS	-	expression tag	UNP Q53W80
K	0	MET	-	initiating methionine	UNP Q53W80
K	41	ALA	TRP	engineered mutation	UNP Q53W80
K	417	HIS	-	expression tag	UNP Q53W80
K	418	HIS	-	expression tag	UNP Q53W80
K	419	HIS	-	expression tag	UNP Q53W80
K	420	HIS	-	expression tag	UNP $Q53W80$
K	421	HIS	-	expression tag	UNP Q53W80
K	422	HIS	-	expression tag	UNP $Q53W80$
L	0	MET	-	initiating methionine	UNP Q53W80



Chain	Residue	Modelled	Actual	Comment	Reference
L	41	ALA	TRP	engineered mutation	UNP Q53W80
L	417	HIS	-	expression tag	UNP Q53W80
L	418	HIS	-	expression tag	UNP Q53W80
L	419	HIS	-	expression tag	UNP Q53W80
L	420	HIS	-	expression tag	UNP Q53W80
L	421	HIS	-	expression tag	UNP Q53W80
L	422	HIS	-	expression tag	UNP Q53W80

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Cl 1 1	0	0
2	В	1	Total Cl 1 1	0	0
2	С	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0
2	Ε	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	Н	2	Total Cl 2 2	0	0
2	Ι	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	К	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
4	Е	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 2	0	0



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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	$\mathbf{F}$	1	Total         C         O           10         6         4	0	0
5	G	1	Total         C         O           10         6         4	0	0
5	K	1	Total         C         O           10         6         4	0	0
5	L	1	Total C O 10 6 4	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
6	В	53	Total O 53 53	0	0
6	С	33	Total         O           33         33	0	0
6	D	43	Total         O           43         43	0	0
6	Е	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
6	F	33	Total         O           33         33	0	0
6	G	31	Total O 31 31	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	40	Total         O           40         40	0	0
6	Ι	44	Total         O           44         44	0	0
6	J	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
6	K	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
6	L	51	$\begin{array}{cc} \text{Total} & \text{O} \\ 51 & 51 \end{array}$	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: Sugar ABC transporter, periplasmic sugar-binding protein



## 

• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



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## 

• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Cha	in	J											8	7%											9%	·	•		
MET GLN I.YS	13	A24	P25	A29 H30	A41	G42	V43	A51	V56	L94 P95	R107	R119	Y122	K129	<mark>0143</mark>	R158	L166	N175	R196	E230	<mark>Q244</mark>	F251	M257	R260	F270	K277	K309 P310	E323	R327
<b>0</b> 330	L335	R339	F347	R354	1357	<b>Q358</b>	<mark>0361</mark>	Y366	1 360	W372	E376	L383	0392	G393 R394	E398	L415	HIS	SIH	SIH	CTII									

• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

С	hə	ii	1	K	•													8	9%									8%	, .	i.			
MET	GLN	T3		K20		P25	-	A29	H30	A51	ATE C		W67	E85	R110	Y122	N134	E137	L166	E193	R196 Q197	E230	q244	F251	M257	1258 Q259	E265	F270	K309		E323	R339	
R354	Y366		W372	COCII	1 383	G384	M385	-	E398	L415	ARG	SIH	SIH	SIH	SIH																		

• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Cha	in	L:											8	38%	_										8%	6•	•		
MET GLN MET	T3	E17	K20	A24	P25	D40	A51	V56	R107	R119	Y122	N134	E137	E146	K153	R158	W177	R196	419/ A198	R201	P209	E230	E233	<mark>Q244</mark>	F251	M257	R260	E265	F270
K309 P310	L335 P336	01011	N 04 Z	K354	R364 T365	1300	W372	H382	M385	L415	HIS	STH	STH	STH															



### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	80.99Å 116.40Å 132.14Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$83.39^{\circ}$ $88.73^{\circ}$ $89.95^{\circ}$	Depositor
$\mathbf{P}_{\text{osolution}}(\hat{\mathbf{A}})$	82.19 - 2.65	Depositor
Resolution (A)	82.19 - 2.65	EDS
% Data completeness	88.1 (82.19-2.65)	Depositor
(in resolution range)	88.1 (82.19-2.65)	EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.65 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.243 , $0.268$	Depositor
$\mathbf{n},  \mathbf{n}_{free}$	0.248 , $0.273$	DCC
$R_{free}$ test set	6334 reflections $(4.84%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , -14.1	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.129 for h,-k,-l	Xtriage
Poported twinning fraction	0.865 for H, K, L	Depositor
Reported twinning fraction	0.135 for h,-k,-l	Depositor
Outliers	0 of 130990 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	38371	wwPDB-VP
Average B, all atoms $(Å^2)$	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: PGE, CL, PEG, EDO

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).

Mal	Chain	Bo	ond lengths	В	ond angles
MOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.88	7/3242~(0.2%)	0.89	2/4414~(0.0%)
1	В	0.79	1/3231~(0.0%)	0.87	2/4400~(0.0%)
1	С	0.83	5/3231~(0.2%)	0.86	2/4400~(0.0%)
1	D	0.84	5/3242~(0.2%)	0.90	8/4414~(0.2%)
1	Ε	0.85	3/3231~(0.1%)	0.88	3/4400~(0.1%)
1	F	0.86	5/3231~(0.2%)	0.89	5/4400~(0.1%)
1	G	0.83	5/3272~(0.2%)	0.89	1/4455~(0.0%)
1	Н	0.83	3/3242~(0.1%)	0.87	3/4414~(0.1%)
1	Ι	0.84	4/3242~(0.1%)	0.91	6/4414~(0.1%)
1	J	0.85	3/3231~(0.1%)	0.91	3/4400~(0.1%)
1	Κ	0.85	3/3231~(0.1%)	0.92	5/4400~(0.1%)
1	L	0.85	4/3231~(0.1%)	0.92	5/4400~(0.1%)
All	All	0.84	48/38857~(0.1%)	0.89	45/52911 (0.1%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	5	GLU	CD-OE2	9.23	1.35	1.25
1	Ι	398	GLU	CD-OE2	9.11	1.35	1.25
1	С	137	GLU	CD-OE2	7.86	1.34	1.25
1	J	398	GLU	CD-OE1	7.77	1.34	1.25
1	F	5	GLU	CD-OE2	7.71	1.34	1.25

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Ι	151[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	Ι	151[B]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	L	158	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	L	119	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	D	151[A]	ARG	NE-CZ-NH1	7.83	124.22	120.30



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	А	3153	0	3121	23	1
1	В	3145	0	3108	39	0
1	С	3145	0	3108	20	1
1	D	3153	0	3121	24	1
1	Е	3145	0	3108	23	0
1	F	3145	0	3108	15	0
1	G	3181	0	3139	15	0
1	Н	3153	0	3121	47	0
1	Ι	3153	0	3121	30	0
1	J	3145	0	3108	23	1
1	Κ	3145	0	3108	19	0
1	L	3145	0	3108	24	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	2	0	0	0	0
2	Ε	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	2	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0
2	Κ	1	0	0	0	0
2	L	1	0	0	0	0
3	В	7	0	10	1	0
3	D	7	0	10	0	0
3	Ι	7	0	10	0	0
4	Е	4	0	6	0	0
5	F	10	0	14	1	0
5	G	10	0	14	2	0
5	K	10	0	14	3	0
5	L	10	0	14	0	0
6	A	42	0	0	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	53	0	0	5	0
6	С	33	0	0	3	0
6	D	43	0	0	5	0
6	Е	47	0	0	8	0
6	F	33	0	0	2	0
6	G	31	0	0	1	0
6	Н	40	0	0	7	0
6	Ι	44	0	0	4	0
6	J	32	0	0	4	0
6	Κ	35	0	0	1	0
6	L	51	0	0	3	0
All	All	38371	0	37471	257	2

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.

The worst 5 of 257 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:108:GLN:O	1:H:107:ARG:NH1	1.73	1.19
1:A:54:SER:O	1:I:196:ARG:NH2	1.88	1.07
1:B:110:THR:CG2	1:H:107:ARG:NE	2.22	1.02
1:L:335:LEU:HD23	1:L:336:PRO:HD2	1.43	1.01
1:K:354:ARG:HD2	6:K:607:HOH:O	1.58	1.01

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLN:NE2	1:D:137:GLU:O[1_445]	1.70	0.50
1:C:391:ALA:O	1:J:158:ARG:NH2[1_565]	2.14	0.06

#### 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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	412/423~(97%)	405~(98%)	7 (2%)	0	100 100
1	В	411/423~(97%)	406 (99%)	5 (1%)	0	100 100
1	С	411/423~(97%)	405~(98%)	6 (2%)	0	100 100
1	D	412/423~(97%)	407 (99%)	5 (1%)	0	100 100
1	Е	411/423~(97%)	405 (98%)	6 (2%)	0	100 100
1	F	411/423~(97%)	404 (98%)	7 (2%)	0	100 100
1	G	415/423~(98%)	410 (99%)	5 (1%)	0	100 100
1	Н	412/423~(97%)	406 (98%)	6 (2%)	0	100 100
1	Ι	412/423~(97%)	406 (98%)	6 (2%)	0	100 100
1	J	411/423~(97%)	406 (99%)	5 (1%)	0	100 100
1	Κ	411/423~(97%)	405~(98%)	6 (2%)	0	100 100
1	L	411/423 (97%)	406 (99%)	5 (1%)	0	100 100
All	All	4940/5076~(97%)	4871 (99%)	69 (1%)	0	100 100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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	А	312/321~(97%)	298~(96%)	14 (4%)	27 42
1	В	311/321~(97%)	303~(97%)	8 (3%)	46 64
1	С	311/321~(97%)	302~(97%)	9~(3%)	42 60
1	D	312/321~(97%)	304 (97%)	8 (3%)	46 64
1	Е	311/321~(97%)	300 (96%)	11 (4%)	36 52
1	F	311/321 (97%)	301 (97%)	10 (3%)	39 56
1	G	315/321~(98%)	307~(98%)	8 (2%)	47 66



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	Н	312/321~(97%)	305~(98%)	7~(2%)	52	70
1	Ι	312/321~(97%)	301~(96%)	11 (4%)	36	52
1	J	311/321~(97%)	297~(96%)	14 (4%)	27	42
1	Κ	311/321~(97%)	300~(96%)	11 (4%)	36	52
1	L	311/321~(97%)	298~(96%)	13~(4%)	30	45
All	All	3740/3852~(97%)	3616 (97%)	124 (3%)	38	54

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	277	LYS
1	Κ	383	LEU
1	Н	230	GLU
1	Κ	323	GLU
1	L	201	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	F	358	GLN
1	L	361	GLN
1	G	392	GLN
1	Κ	382	HIS
1	G	382	HIS

#### 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 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	Dec	Tink	B	ond leng	$\operatorname{gths}$	B	Bond angles			
	inton Type Chan	Unain	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
5	PGE	K	502	-	$9,\!9,\!9$	0.31	0	8,8,8	0.22	0		
3	PEG	В	502	-	$6,\!6,\!6$	0.23	0	$5,\!5,\!5$	0.10	0		
4	EDO	Е	502	-	3,3,3	0.63	0	2,2,2	0.62	0		
5	PGE	L	502	-	9,9,9	0.41	0	8,8,8	0.21	0		
3	PEG	Ι	502	-	6,6,6	0.32	0	$5,\!5,\!5$	0.20	0		
3	PEG	D	503	-	6,6,6	0.28	0	$5,\!5,\!5$	0.25	0		
5	PGE	F	502	-	9,9,9	0.44	0	8,8,8	0.22	0		
5	PGE	G	502	-	9,9,9	0.30	0	8,8,8	0.26	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	PGE	К	502	-	-	6/7/7/7	-
3	PEG	В	502	-	-	2/4/4/4	-
4	EDO	Е	502	-	-	0/1/1/1	-
5	PGE	L	502	-	-	4/7/7/7	-
3	PEG	Ι	502	-	-	3/4/4/4	-
3	PEG	D	503	-	-	3/4/4/4	-
5	PGE	F	502	-	-	4/7/7/7	-
5	PGE	G	502	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	G	502	PGE	C4-C3-O2-C2
5	L	502	PGE	O2-C3-C4-O3
5	F	502	PGE	O2-C3-C4-O3
3	D	503	PEG	O2-C3-C4-O4
5	G	502	PGE	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Κ	502	PGE	3	0
3	В	502	PEG	1	0
5	F	502	PGE	1	0
5	G	502	PGE	2	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,  $95^{th}$  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	А	413/423~(97%)	-0.06	2 (0%) 91 91	5, 11, 26, 57	0
1	В	413/423~(97%)	-0.08	1 (0%) 95 96	5, 13, 26, 45	0
1	С	413/423~(97%)	0.01	7 (1%) 70 67	5, 15, 27, 57	0
1	D	413/423~(97%)	-0.11	2 (0%) 91 91	5, 11, 29, 56	0
1	Е	413/423~(97%)	-0.16	1 (0%) 95 96	5, 11, 23, 34	0
1	F	413/423 (97%)	-0.07	6 (1%) 73 71	5, 13, 28, 51	0
1	G	416/423 (98%)	-0.07	1 (0%) 95 96	5, 14, 28, 45	0
1	Н	413/423~(97%)	-0.09	1 (0%) 95 96	6, 13, 27, 56	0
1	Ι	413/423~(97%)	-0.11	5 (1%) 79 77	5, 12, 27, 53	0
1	J	413/423~(97%)	-0.14	2 (0%) 91 91	5, 10, 23, 36	0
1	K	413/423 (97%)	-0.18	0 100 100	5, 10, 21, 34	0
1	L	413/423 (97%)	-0.16	0 100 100	5, 11, 22, 38	0
All	All	$495\overline{9/5076}~(97\%)$	-0.10	28 (0%) 89 89	5, 12, 26, 57	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	198	ALA	4.0
1	С	199	GLY	3.8
1	Ι	199	GLY	3.5
1	D	266	ALA	3.2
1	F	198	ALA	3.0

#### 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
5	PGE	K	502	10/10	0.88	0.19	$13,\!17,\!18,\!19$	0
3	PEG	Ι	502	7/7	0.89	0.21	17,18,24,25	0
3	PEG	В	502	7/7	0.90	0.17	18,19,20,21	0
5	PGE	G	502	10/10	0.90	0.17	16,19,20,21	0
3	PEG	D	503	7/7	0.90	0.17	11,12,14,14	0
5	PGE	L	502	10/10	0.92	0.17	18,21,22,22	0
5	PGE	F	502	10/10	0.93	0.14	13,15,17,17	0
4	EDO	Е	502	4/4	0.93	0.12	7,7,7,7	0
2	CL	D	501	1/1	0.95	0.08	3,3,3,3	0
2	CL	Ι	501	1/1	0.96	0.07	10,10,10,10	0
2	CL	L	501	1/1	0.97	0.13	13,13,13,13	0
2	CL	Н	502	1/1	0.97	0.05	0,0,0,0	0
2	CL	А	501	1/1	0.97	0.06	0,0,0,0	0
2	CL	D	502	1/1	0.98	0.04	0,0,0,0	0
2	CL	J	501	1/1	0.98	0.05	10,10,10,10	0
2	CL	K	501	1/1	0.98	0.06	14,14,14,14	0
2	CL	F	501	1/1	0.98	0.06	13,13,13,13	0
2	CL	Н	501	1/1	0.98	0.13	3, 3, 3, 3	0
2	CL	В	501	1/1	0.98	0.04	9,9,9,9	0
2	CL	G	501	1/1	0.99	0.05	9,9,9,9	0
2	CL	Е	501	1/1	0.99	0.06	7,7,7,7	0
2	CL	С	501	1/1	0.99	0.07	13,13,13,13	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

