Full wwPDB X-ray Structure Validation Report

Nov 20, 2023 – 12:21 AM JST

PDB ID	:	7C6X
Title	:	Crystal structure of beta-glycosides-binding protein (W41A) of ABC transporter 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 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:

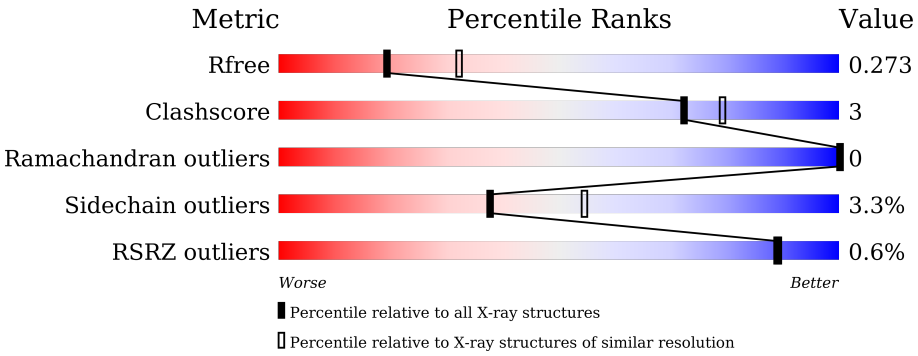
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-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.



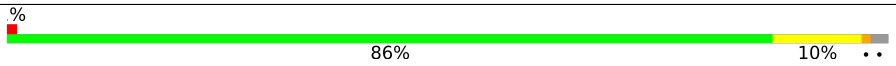
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	A	423	87% 10%
1	B	423	88% 9%
1	C	423	2% 89% 8%
1	D	423	87% 9%
1	E	423	88% 8%
1	F	423	% 89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3153	2026	544	573	10			
1	B	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	C	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	D	413	Total	C	N	O	S	0	1	0
			3153	2026	544	573	10			
1	E	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	F	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	G	416	Total	C	N	O	S	0	1	0
			3181	2042	551	578	10			
1	H	413	Total	C	N	O	S	0	1	0
			3153	2026	544	573	10			
1	I	413	Total	C	N	O	S	0	1	0
			3153	2026	544	573	10			
1	J	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	K	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			
1	L	413	Total	C	N	O	S	0	0	0
			3145	2021	541	573	10			

There are 96 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
A	422	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	41	ALA	TRP	engineered mutation	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80
B	421	HIS	-	expression tag	UNP Q53W80
B	422	HIS	-	expression tag	UNP Q53W80
C	0	MET	-	initiating methionine	UNP Q53W80
C	41	ALA	TRP	engineered mutation	UNP Q53W80
C	417	HIS	-	expression tag	UNP Q53W80
C	418	HIS	-	expression tag	UNP Q53W80
C	419	HIS	-	expression tag	UNP Q53W80
C	420	HIS	-	expression tag	UNP Q53W80
C	421	HIS	-	expression tag	UNP Q53W80
C	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
E	0	MET	-	initiating methionine	UNP Q53W80
E	41	ALA	TRP	engineered mutation	UNP Q53W80
E	417	HIS	-	expression tag	UNP Q53W80
E	418	HIS	-	expression tag	UNP Q53W80
E	419	HIS	-	expression tag	UNP Q53W80
E	420	HIS	-	expression tag	UNP Q53W80
E	421	HIS	-	expression tag	UNP Q53W80
E	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

Continued on next page...

Continued from previous page...

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
H	0	MET	-	initiating methionine	UNP Q53W80
H	41	ALA	TRP	engineered mutation	UNP Q53W80
H	417	HIS	-	expression tag	UNP Q53W80
H	418	HIS	-	expression tag	UNP Q53W80
H	419	HIS	-	expression tag	UNP Q53W80
H	420	HIS	-	expression tag	UNP Q53W80
H	421	HIS	-	expression tag	UNP Q53W80
H	422	HIS	-	expression tag	UNP Q53W80
I	0	MET	-	initiating methionine	UNP Q53W80
I	41	ALA	TRP	engineered mutation	UNP Q53W80
I	417	HIS	-	expression tag	UNP Q53W80
I	418	HIS	-	expression tag	UNP Q53W80
I	419	HIS	-	expression tag	UNP Q53W80
I	420	HIS	-	expression tag	UNP Q53W80
I	421	HIS	-	expression tag	UNP Q53W80
I	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

Continued on next page...

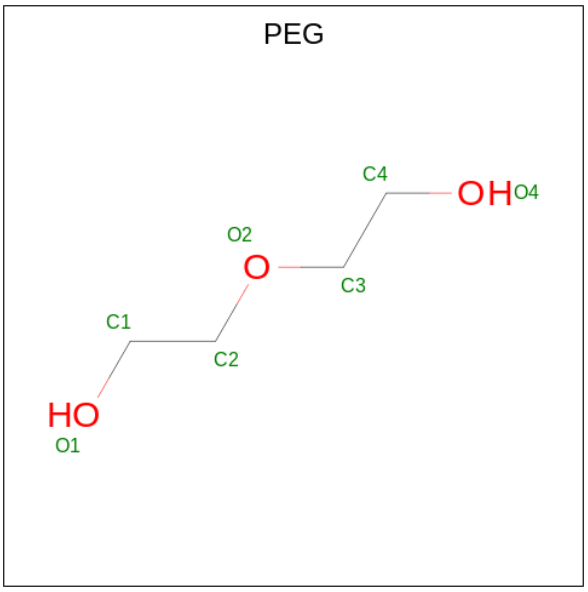
Continued from previous page...

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).

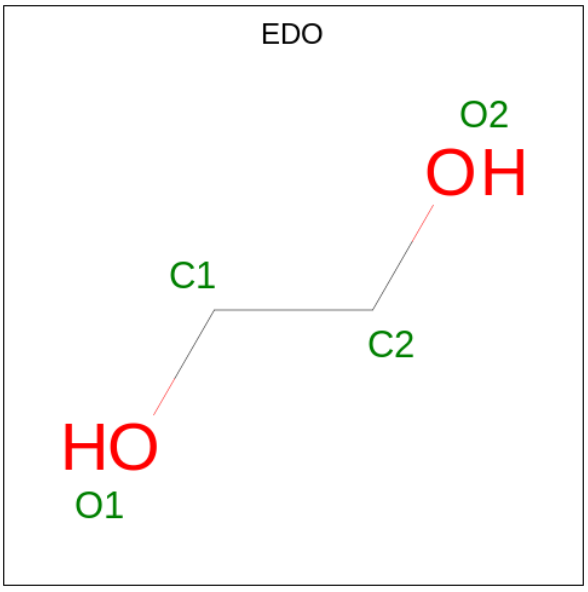
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	2	Total Cl 2 2	0	0
2	I	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

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



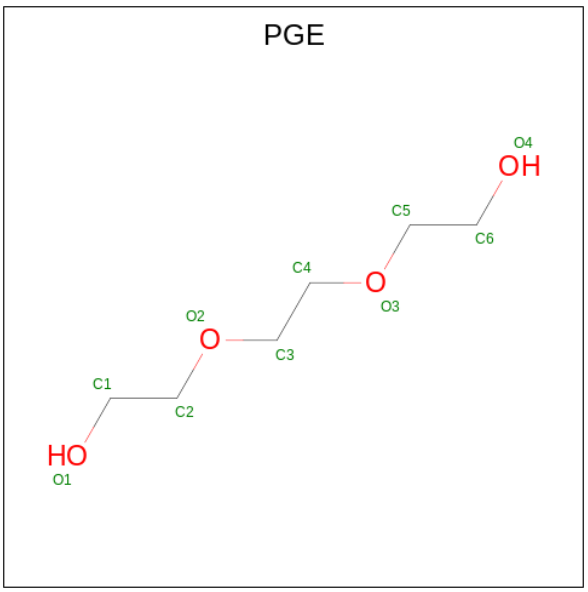
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	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	A	42	Total O 42 42	0	0
6	B	53	Total O 53 53	0	0
6	C	33	Total O 33 33	0	0
6	D	43	Total O 43 43	0	0
6	E	47	Total O 47 47	0	0
6	F	33	Total O 33 33	0	0
6	G	31	Total O 31 31	0	0

Continued on next page...

Continued from previous page...

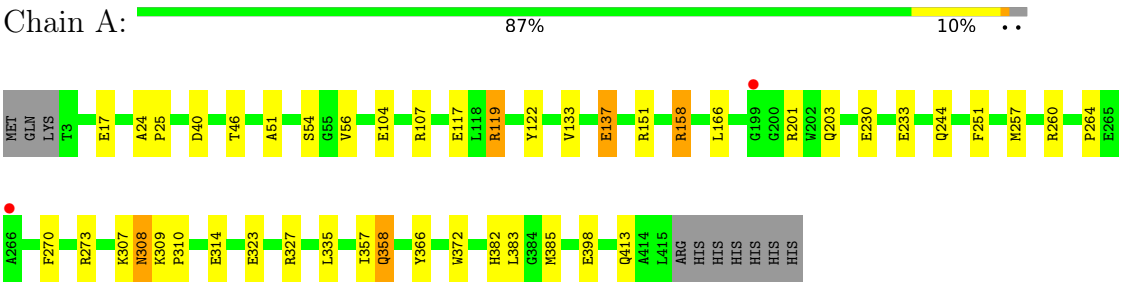
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	40	Total O 40 40	0	0
6	I	44	Total O 44 44	0	0
6	J	32	Total O 32 32	0	0
6	K	35	Total O 35 35	0	0
6	L	51	Total O 51 51	0	0

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.

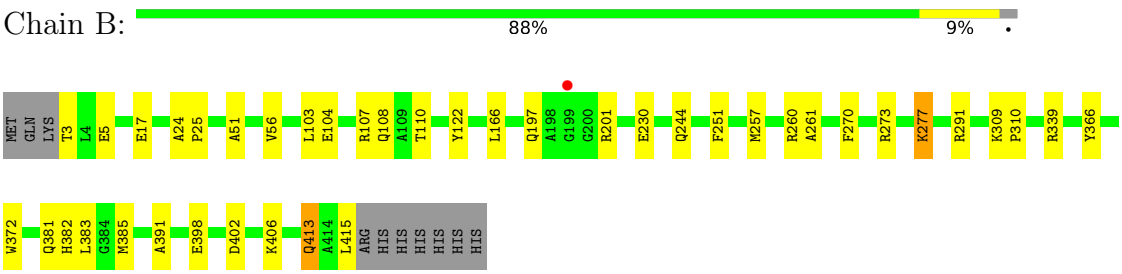
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain A:



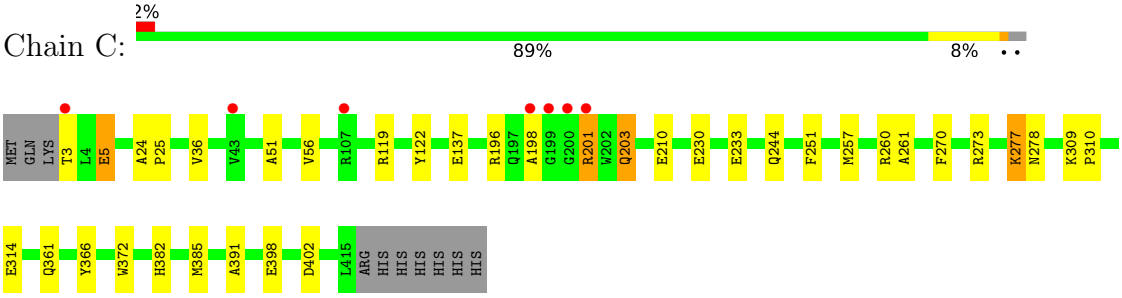
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain B:



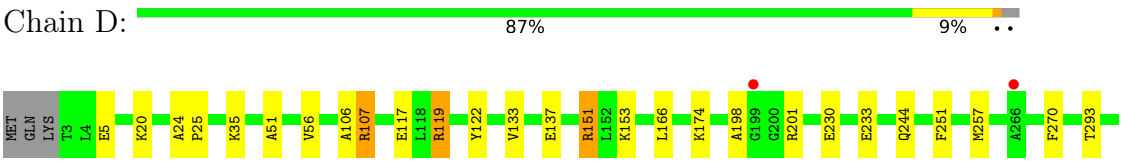
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain C:

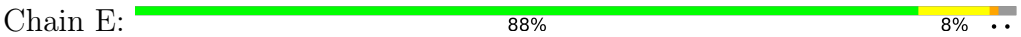


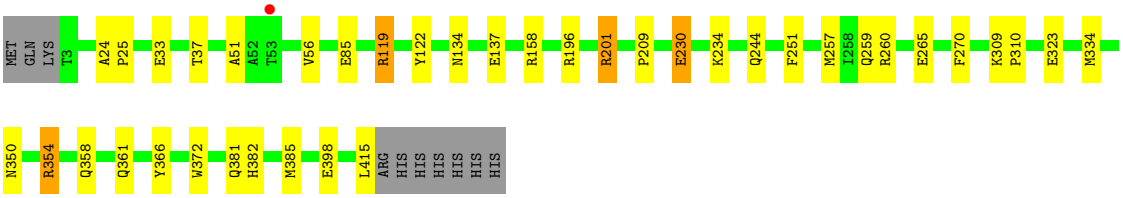
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain D:

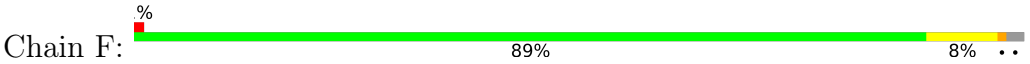


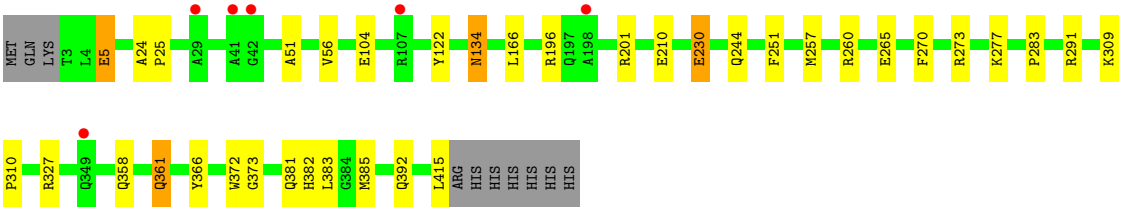
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



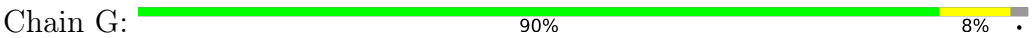


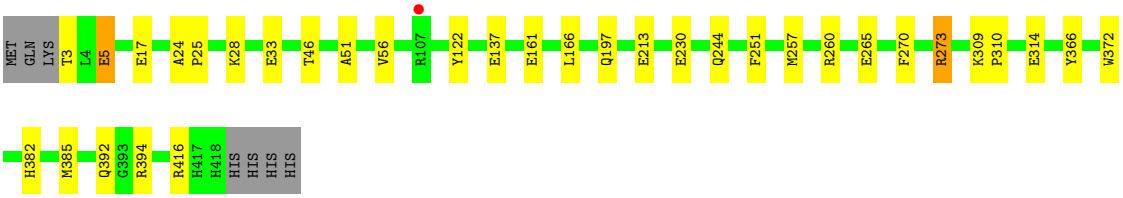
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



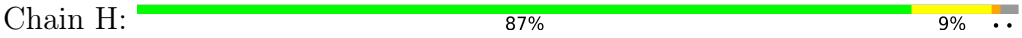


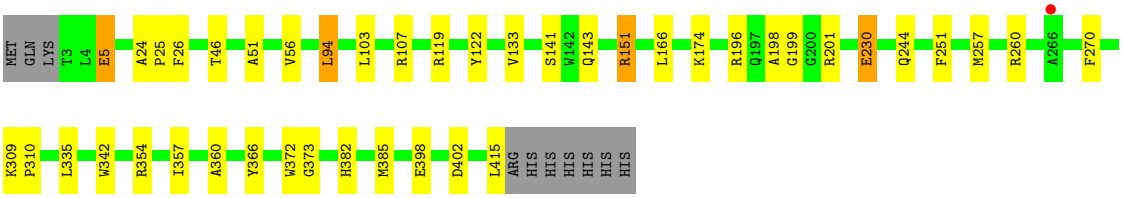
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



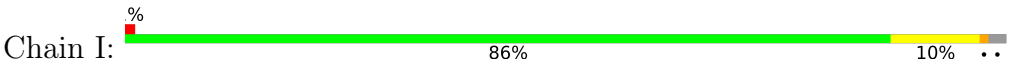


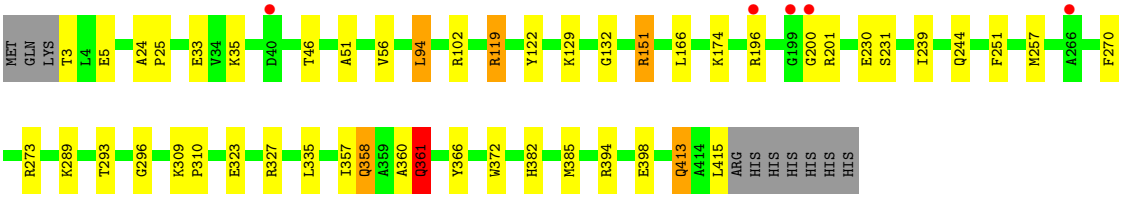
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein





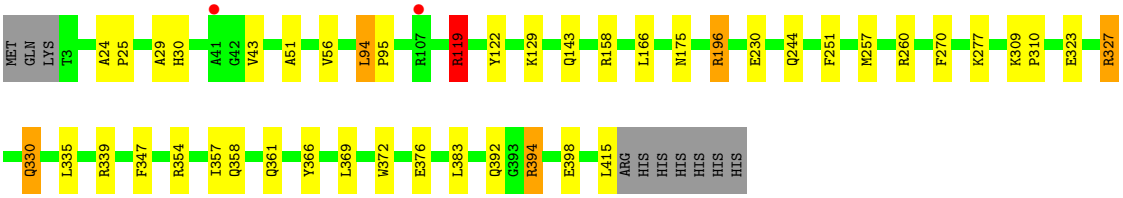
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein





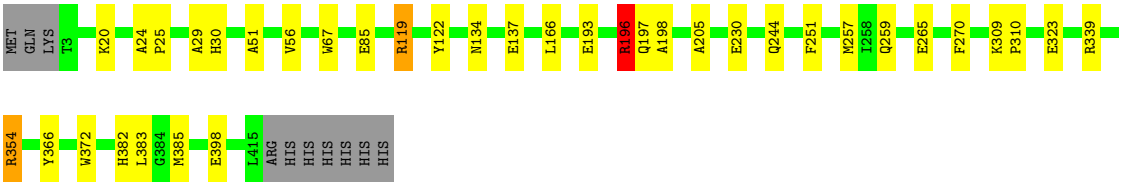
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain J:



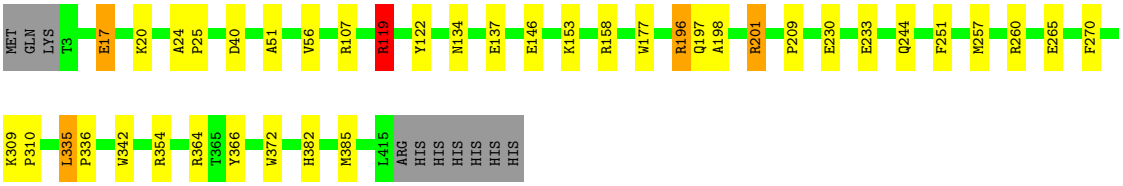
• Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.99Å 116.40Å 132.14Å 83.39° 88.73° 89.95°	Depositor
Resolution (Å)	82.19 – 2.65 82.19 – 2.65	Depositor EDS
% Data completeness (in resolution range)	88.1 (82.19-2.65) 88.1 (82.19-2.65)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.243 , 0.268 0.248 , 0.273	Depositor DCC
R_{free} test set	6334 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^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
Reported twinning fraction	0.865 for H, K, L 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.*

[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: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.88	7/3242 (0.2%)	0.89	2/4414 (0.0%)
1	B	0.79	1/3231 (0.0%)	0.87	2/4400 (0.0%)
1	C	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	E	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	H	0.83	3/3242 (0.1%)	0.87	3/4414 (0.1%)
1	I	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	K	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%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	GLU	CD-OE2	9.23	1.35	1.25
1	I	398	GLU	CD-OE2	9.11	1.35	1.25
1	C	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
1	A	137	GLU	CD-OE2	7.54	1.33	1.25
1	G	5	GLU	CD-OE2	7.09	1.33	1.25
1	F	265	GLU	CD-OE2	7.03	1.33	1.25
1	H	230	GLU	CD-OE2	6.82	1.33	1.25
1	F	230	GLU	CD-OE2	6.54	1.32	1.25
1	A	117	GLU	CD-OE1	6.53	1.32	1.25
1	A	117	GLU	CD-OE2	6.49	1.32	1.25
1	G	33	GLU	CD-OE2	6.24	1.32	1.25
1	G	314	GLU	CD-OE1	6.20	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	85	GLU	CD-OE1	6.16	1.32	1.25
1	A	323	GLU	CD-OE1	6.16	1.32	1.25
1	A	398	GLU	CD-OE1	-6.06	1.19	1.25
1	D	5	GLU	CD-OE2	5.99	1.32	1.25
1	E	398	GLU	CD-OE1	5.99	1.32	1.25
1	I	5	GLU	CD-OE2	5.96	1.32	1.25
1	D	398	GLU	CD-OE1	5.95	1.32	1.25
1	G	137	GLU	CD-OE2	5.90	1.32	1.25
1	L	17	GLU	CD-OE2	5.85	1.32	1.25
1	D	314	GLU	CD-OE2	5.79	1.32	1.25
1	D	233	GLU	CD-OE1	5.73	1.31	1.25
1	C	210	GLU	CD-OE1	5.64	1.31	1.25
1	D	117	GLU	CD-OE1	5.58	1.31	1.25
1	J	376	GLU	CD-OE2	-5.58	1.19	1.25
1	I	296	GLY	C-O	5.57	1.32	1.23
1	H	5	GLU	CD-OE2	5.55	1.31	1.25
1	L	137	GLU	CD-OE1	5.48	1.31	1.25
1	A	104	GLU	CD-OE1	5.46	1.31	1.25
1	K	193	GLU	CD-OE2	5.46	1.31	1.25
1	K	398	GLU	CD-OE1	5.39	1.31	1.25
1	C	233	GLU	CD-OE1	5.36	1.31	1.25
1	F	104	GLU	CD-OE1	5.34	1.31	1.25
1	E	137	GLU	CD-OE1	5.34	1.31	1.25
1	I	323	GLU	CD-OE1	5.32	1.31	1.25
1	G	213	GLU	CD-OE2	5.30	1.31	1.25
1	C	314	GLU	CD-OE1	5.29	1.31	1.25
1	H	230	GLU	CD-OE1	5.27	1.31	1.25
1	B	5	GLU	CD-OE1	5.26	1.31	1.25
1	L	233	GLU	CD-OE2	5.25	1.31	1.25
1	K	193	GLU	CD-OE1	5.23	1.31	1.25
1	J	323	GLU	CD-OE1	5.16	1.31	1.25
1	A	314	GLU	CD-OE1	5.11	1.31	1.25
1	L	146	GLU	CD-OE1	5.04	1.31	1.25
1	F	210	GLU	CD-OE1	5.01	1.31	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	151[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	I	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	151[A]	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	D	151[B]	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	L	134	ASN	N-CA-CB	7.71	124.47	110.60
1	A	308	ASN	N-CA-CB	7.46	124.03	110.60
1	I	394	ARG	CB-CG-CD	7.37	130.77	111.60
1	K	119	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	308	ASN	N-CA-CB	7.22	123.60	110.60
1	K	137	GLU	CB-CA-C	7.00	124.39	110.40
1	F	134	ASN	CB-CA-C	6.88	124.15	110.40
1	K	196	ARG	CB-CG-CD	6.73	129.10	111.60
1	F	291	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	G	273	ARG	CB-CG-CD	6.64	128.87	111.60
1	K	354	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	291	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	J	119	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	D	354	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	H	151[A]	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	H	151[B]	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	K	339	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	F	361	GLN	CB-CA-C	-5.97	98.45	110.40
1	F	361	GLN	CA-CB-CG	5.95	126.49	113.40
1	I	327	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	D	107	ARG	CB-CA-C	5.82	122.05	110.40
1	E	415	LEU	CA-C-O	5.73	132.13	120.10
1	F	327	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	C	402	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	D	354	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	J	196	ARG	CG-CD-NE	-5.51	100.22	111.80
1	I	361	GLN	CB-CA-C	5.48	121.36	110.40
1	E	119	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	402	ASP	CB-CG-OD1	5.36	123.12	118.30
1	L	364	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	107	ARG	CB-CG-CD	5.25	125.24	111.60
1	A	119	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	I	361	GLN	CB-CG-CD	-5.21	98.05	111.60
1	L	354	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	E	201	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	415	LEU	CA-C-O	5.13	130.88	120.10
1	B	339	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	339	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	J	394	ARG	NE-CZ-NH1	5.03	122.81	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	A	3153	0	3121	23	1
1	B	3145	0	3108	39	0
1	C	3145	0	3108	20	1
1	D	3153	0	3121	24	1
1	E	3145	0	3108	23	0
1	F	3145	0	3108	15	0
1	G	3181	0	3139	15	0
1	H	3153	0	3121	47	0
1	I	3153	0	3121	30	0
1	J	3145	0	3108	23	1
1	K	3145	0	3108	19	0
1	L	3145	0	3108	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	B	7	0	10	1	0
3	D	7	0	10	0	0
3	I	7	0	10	0	0
4	E	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
6	B	53	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	33	0	0	3	0
6	D	43	0	0	5	0
6	E	47	0	0	8	0
6	F	33	0	0	2	0
6	G	31	0	0	1	0
6	H	40	0	0	7	0
6	I	44	0	0	4	0
6	J	32	0	0	4	0
6	K	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.

All (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
1:K:67:TRP:HE1	5:K:502:PGE:H62	1.26	0.96
1:B:110:THR:CG2	1:H:107:ARG:CD	2.44	0.95
1:B:110:THR:HG21	1:H:107:ARG:NE	1.81	0.94
1:B:110:THR:CG2	1:H:107:ARG:HD3	1.99	0.92
1:L:177:TRP:HD1	6:L:624:HOH:O	1.52	0.92
1:B:110:THR:HG23	1:H:107:ARG:CD	2.01	0.91
1:H:198:ALA:O	1:H:201:ARG:NH1	2.05	0.90
1:G:3:THR:N	6:G:601:HOH:O	2.05	0.88
1:B:110:THR:HG21	1:H:107:ARG:HE	1.38	0.88
1:B:110:THR:HG23	1:H:107:ARG:NE	1.89	0.88
1:B:103:LEU:H	1:H:107:ARG:NH2	1.76	0.83
1:K:67:TRP:NE1	5:K:502:PGE:H62	1.94	0.82
1:D:35:LYS:HG3	6:D:628:HOH:O	1.82	0.80
1:D:198:ALA:O	1:D:201:ARG:NH1	2.14	0.80
1:L:177:TRP:CD1	6:L:624:HOH:O	2.32	0.79
1:H:94:LEU:CD1	1:H:342:TRP:HH2	1.95	0.78
1:H:94:LEU:HD12	1:H:342:TRP:CH2	2.18	0.78
1:B:103:LEU:H	1:H:107:ARG:HH22	1.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:LEU:HD11	1:H:357:ILE:HD13	1.66	0.78
1:L:335:LEU:HD23	1:L:336:PRO:CD	2.14	0.78
1:H:94:LEU:HD12	1:H:342:TRP:HH2	1.51	0.75
1:H:143:GLN:OE1	1:I:361:GLN:NE2	2.20	0.72
1:C:277:LYS:HG3	1:C:278:ASN:ND2	2.07	0.70
1:B:413:GLN:OE1	1:I:196:ARG:HD2	1.91	0.70
1:C:198:ALA:O	1:C:201:ARG:HG3	1.92	0.69
1:J:335:LEU:HD11	1:J:357:ILE:HD13	1.75	0.68
1:K:67:TRP:HE1	5:K:502:PGE:C6	2.05	0.68
1:H:94:LEU:CD1	1:H:342:TRP:CH2	2.76	0.67
1:I:335:LEU:HD11	1:I:357:ILE:HD13	1.76	0.67
1:B:110:THR:HG21	1:H:107:ARG:CD	2.20	0.65
1:A:335:LEU:HD11	1:A:357:ILE:HD13	1.78	0.64
1:B:197:GLN:OE1	1:H:199:GLY:N	2.30	0.64
1:A:335:LEU:HD11	1:A:357:ILE:CD1	2.29	0.63
1:A:158:ARG:NE	6:A:601:HOH:O	2.31	0.62
1:A:307:LYS:NZ	1:I:415:LEU:O	2.32	0.62
1:L:119:ARG:CG	1:L:119:ARG:HH21	2.13	0.62
1:L:335:LEU:HD22	1:L:342:TRP:NE1	2.15	0.62
1:J:392:GLN:HG3	1:J:394:ARG:HD3	1.81	0.61
1:G:265:GLU:OE1	1:G:273:ARG:HD3	2.01	0.60
1:J:415:LEU:C	6:J:604:HOH:O	2.40	0.60
1:B:107:ARG:HD2	1:H:103:LEU:HD21	1.84	0.60
1:B:110:THR:HG21	1:H:107:ARG:HD3	1.82	0.59
1:B:3:THR:N	6:B:601:HOH:O	2.36	0.58
1:E:209:PRO:HG3	1:K:29:ALA:O	2.03	0.58
1:B:261:ALA:O	1:L:198:ALA:HB1	2.05	0.57
1:E:230:GLU:OE2	1:E:234:LYS:NZ	2.36	0.57
1:C:261:ALA:O	1:K:198:ALA:HB1	2.06	0.56
1:H:141:SER:OG	1:I:358:GLN:OE1	2.23	0.56
1:J:29:ALA:O	1:L:209:PRO:HG3	2.05	0.56
5:G:502:PGE:H2	1:H:373:GLY:HA3	1.88	0.56
1:A:133:VAL:HG22	1:A:151[A]:ARG:NH2	2.21	0.56
1:A:264:PRO:HG3	1:J:327:ARG:HD3	1.87	0.55
1:H:354:ARG:HD2	1:I:151[A]:ARG:NH2	2.20	0.55
1:D:398:GLU:HB3	6:D:641:HOH:O	2.06	0.55
1:B:103:LEU:N	1:H:107:ARG:HH22	2.02	0.54
1:E:33:GLU:HG3	6:E:626:HOH:O	2.07	0.54
1:B:402:ASP:HB2	6:B:630:HOH:O	2.07	0.54
1:J:94:LEU:HD22	1:J:95:PRO:HD2	1.89	0.54
1:B:277:LYS:HZ2	1:L:196:ARG:HD2	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:GLN:HG2	6:J:605:HOH:O	2.08	0.54
1:C:277:LYS:HA	1:K:197:GLN:O	2.09	0.53
1:D:35:LYS:CE	6:D:628:HOH:O	2.56	0.53
1:D:308:ASN:ND2	1:D:311:LEU:CB	2.71	0.53
1:J:119:ARG:HG3	1:J:119:ARG:HH11	1.74	0.53
1:E:209:PRO:HB3	1:K:30:HIS:HA	1.92	0.52
1:D:133:VAL:HG22	1:D:151[A]:ARG:NH2	2.23	0.52
1:C:398:GLU:HG2	6:C:614:HOH:O	2.08	0.52
1:K:196:ARG:HG2	1:K:205:ALA:HB2	1.91	0.52
6:B:631:HOH:O	1:L:201:ARG:HG2	2.10	0.52
1:D:122:TYR:CZ	1:D:257:MET:HB2	2.45	0.52
1:H:133:VAL:HG22	1:H:151[A]:ARG:NH2	2.24	0.52
1:D:308:ASN:ND2	1:D:311:LEU:HB3	2.25	0.51
1:E:334:MET:CE	6:E:631:HOH:O	2.57	0.51
1:H:122:TYR:CZ	1:H:257:MET:HB2	2.46	0.51
1:J:30:HIS:HA	1:L:209:PRO:HB3	1.93	0.51
1:A:133:VAL:HG22	1:A:151[A]:ARG:HH21	1.75	0.51
1:I:122:TYR:CZ	1:I:257:MET:HB2	2.46	0.50
1:F:283:PRO:HG2	1:F:358:GLN:HE21	1.76	0.50
1:L:17:GLU:HG3	6:L:637:HOH:O	2.12	0.50
1:C:122:TYR:CZ	1:C:257:MET:HB2	2.47	0.50
1:H:5:GLU:HG2	6:H:617:HOH:O	2.10	0.50
1:H:26:PHE:HA	6:H:629:HOH:O	2.10	0.50
1:I:231:SER:OG	1:I:239:ILE:CD1	2.59	0.50
1:A:122:TYR:CZ	1:A:257:MET:HB2	2.46	0.50
1:J:43:VAL:HG22	1:J:43:VAL:O	2.11	0.50
1:G:122:TYR:CZ	1:G:257:MET:HB2	2.47	0.50
1:G:161:GLU:OE2	1:G:273:ARG:NH1	2.46	0.49
1:H:133:VAL:HG22	1:H:151[A]:ARG:HH21	1.77	0.49
1:L:122:TYR:CZ	1:L:257:MET:HB2	2.47	0.49
1:B:122:TYR:CZ	1:B:257:MET:HB2	2.47	0.49
1:B:277:LYS:NZ	1:L:196:ARG:HD2	2.27	0.49
1:J:122:TYR:CZ	1:J:257:MET:HB2	2.47	0.49
1:E:122:TYR:CZ	1:E:257:MET:HB2	2.48	0.49
1:H:94:LEU:HD11	1:H:342:TRP:HH2	1.77	0.49
1:D:133:VAL:HG22	1:D:151[A]:ARG:HH21	1.78	0.49
1:A:309:LYS:HD2	1:I:413:GLN:OE1	2.12	0.49
1:F:122:TYR:CZ	1:F:257:MET:HB2	2.48	0.49
1:K:122:TYR:CZ	1:K:257:MET:HB2	2.48	0.49
1:B:398:GLU:HG2	6:B:627:HOH:O	2.12	0.48
1:B:415:LEU:C	6:B:609:HOH:O	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:GLN:HE22	1:J:347:PHE:HZ	1.55	0.48
1:H:174:LYS:HG2	6:H:612:HOH:O	2.12	0.48
1:C:3:THR:N	6:C:602:HOH:O	2.46	0.48
1:L:244:GLN:HG2	1:L:270:PHE:CG	2.49	0.48
1:B:406:LYS:NZ	1:I:200:GLY:HA3	2.29	0.48
1:E:381:GLN:OE1	1:J:56:VAL:HG12	2.13	0.47
1:H:24:ALA:HB3	1:H:25:PRO:HD3	1.96	0.47
1:F:244:GLN:HG2	1:F:270:PHE:CG	2.49	0.47
1:G:161:GLU:CD	1:G:273:ARG:NH1	2.68	0.47
1:G:244:GLN:HG2	1:G:270:PHE:CG	2.50	0.47
1:J:244:GLN:HG2	1:J:270:PHE:CG	2.50	0.47
1:B:244:GLN:HG2	1:B:270:PHE:CG	2.50	0.47
1:C:244:GLN:HG2	1:C:270:PHE:CG	2.49	0.47
1:F:24:ALA:HB3	1:F:25:PRO:HD3	1.97	0.47
1:I:231:SER:OG	1:I:239:ILE:HD11	2.14	0.47
1:L:119:ARG:HH21	1:L:119:ARG:HG2	1.79	0.47
1:E:244:GLN:HG2	1:E:270:PHE:CG	2.50	0.47
1:J:24:ALA:HB3	1:J:25:PRO:HD3	1.98	0.46
1:D:244:GLN:HG2	1:D:270:PHE:CG	2.50	0.46
1:E:24:ALA:HB3	1:E:25:PRO:HD3	1.97	0.46
1:A:327:ARG:HD3	6:A:627:HOH:O	2.15	0.46
1:E:350:ASN:HB2	6:E:608:HOH:O	2.14	0.46
1:F:373:GLY:HA3	5:F:502:PGE:O4	2.14	0.46
1:H:46:THR:HG22	6:H:619:HOH:O	2.14	0.46
1:B:391:ALA:O	1:E:158:ARG:NH1	2.43	0.46
1:B:24:ALA:HB3	1:B:25:PRO:HD3	1.98	0.46
1:E:382:HIS:CD2	1:E:385:MET:HE3	2.51	0.46
1:K:244:GLN:HG2	1:K:270:PHE:CG	2.51	0.46
1:B:273:ARG:HA	1:B:273:ARG:NE	2.31	0.46
1:C:273:ARG:HA	1:C:273:ARG:NE	2.31	0.46
1:I:102:ARG:CD	6:I:607:HOH:O	2.63	0.46
1:C:309:LYS:HB2	1:C:310:PRO:HD3	1.98	0.45
1:I:273:ARG:HA	1:I:273:ARG:NE	2.31	0.45
1:H:244:GLN:HG2	1:H:270:PHE:CG	2.51	0.45
1:K:24:ALA:HB3	1:K:25:PRO:HD3	1.99	0.45
1:I:244:GLN:HG2	1:I:270:PHE:CG	2.51	0.45
1:L:335:LEU:CD2	1:L:336:PRO:HD2	2.30	0.45
1:I:174:LYS:HG2	6:I:616:HOH:O	2.16	0.45
1:C:277:LYS:HB3	1:K:196:ARG:NH1	2.32	0.45
1:J:119:ARG:HH11	1:J:119:ARG:CG	2.28	0.45
1:K:382:HIS:CD2	1:K:385:MET:HE3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:309:LYS:HB2	1:H:310:PRO:HD3	1.98	0.45
1:A:24:ALA:HB3	1:A:25:PRO:HD3	1.97	0.45
1:B:366:TYR:CG	1:B:372:TRP:CZ2	3.05	0.45
1:F:273:ARG:HA	1:F:273:ARG:NE	2.32	0.45
1:F:366:TYR:CG	1:F:372:TRP:CZ2	3.05	0.45
1:I:366:TYR:CG	1:I:372:TRP:CZ2	3.05	0.45
1:J:366:TYR:CG	1:J:372:TRP:CZ2	3.05	0.45
1:L:382:HIS:CD2	1:L:385:MET:HE3	2.52	0.45
1:A:244:GLN:HG2	1:A:270:PHE:CG	2.51	0.45
1:E:334:MET:HE3	6:E:631:HOH:O	2.17	0.45
1:G:46:THR:OG1	5:G:502:PGE:H22	2.17	0.44
1:L:24:ALA:HB3	1:L:25:PRO:HD3	1.99	0.44
1:D:24:ALA:HB3	1:D:25:PRO:HD3	1.99	0.44
1:F:361:GLN:CG	6:F:625:HOH:O	2.65	0.44
1:G:24:ALA:HB3	1:G:25:PRO:HD3	1.99	0.44
1:A:309:LYS:HB2	1:A:310:PRO:HD3	1.98	0.44
1:H:94:LEU:HD21	1:H:360:ALA:O	2.16	0.44
1:B:108:GLN:O	1:H:107:ARG:CZ	2.57	0.44
1:L:309:LYS:HB2	1:L:310:PRO:HD3	2.00	0.44
1:C:398:GLU:OE1	6:C:601:HOH:O	2.21	0.44
1:G:366:TYR:CG	1:G:372:TRP:CZ2	3.05	0.44
1:C:24:ALA:HB3	1:C:25:PRO:HD3	2.00	0.44
1:G:392:GLN:NE2	1:G:394:ARG:HH11	2.16	0.44
1:A:366:TYR:CG	1:A:372:TRP:CZ2	3.06	0.44
1:E:354:ARG:NE	6:E:601:HOH:O	2.40	0.44
1:F:392:GLN:NE2	1:I:35:LYS:NZ	2.66	0.44
1:H:366:TYR:CG	1:H:372:TRP:CZ2	3.05	0.44
1:B:382:HIS:CD2	1:B:385:MET:HE3	2.53	0.44
1:D:309:LYS:HB2	1:D:310:PRO:HD3	2.00	0.44
1:D:366:TYR:CG	1:D:372:TRP:CZ2	3.05	0.44
1:I:24:ALA:HB3	1:I:25:PRO:HD3	1.98	0.44
1:K:366:TYR:CG	1:K:372:TRP:CZ2	3.06	0.44
1:A:273:ARG:HA	1:A:273:ARG:NE	2.33	0.43
1:E:334:MET:HE2	6:E:631:HOH:O	2.18	0.43
1:B:309:LYS:HB2	1:B:310:PRO:HD3	2.00	0.43
1:C:36:VAL:O	1:D:174:LYS:NZ	2.43	0.43
1:C:366:TYR:CG	1:C:372:TRP:CZ2	3.06	0.43
1:H:354:ARG:NH2	1:I:132:GLY:O	2.45	0.43
1:J:369:LEU:HA	6:J:608:HOH:O	2.18	0.43
1:E:366:TYR:CG	1:E:372:TRP:CZ2	3.06	0.43
1:L:366:TYR:CG	1:L:372:TRP:CZ2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD11	1:D:357:ILE:HD13	2.00	0.43
1:H:382:HIS:CD2	1:H:385:MET:HE3	2.53	0.43
1:A:46:THR:HG21	3:B:502:PEG:H11	2.01	0.43
1:G:51:ALA:HA	1:G:56:VAL:O	2.19	0.43
1:J:361:GLN:CD	6:J:601:HOH:O	2.57	0.43
1:I:51:ALA:HA	1:I:56:VAL:O	2.19	0.43
1:I:309:LYS:HB2	1:I:310:PRO:HD3	1.99	0.43
1:J:166:LEU:HD12	1:J:166:LEU:N	2.34	0.43
1:A:166:LEU:N	1:A:166:LEU:HD12	2.34	0.43
1:F:51:ALA:HA	1:F:56:VAL:O	2.19	0.43
1:I:102:ARG:NE	6:I:607:HOH:O	2.52	0.43
1:D:174:LYS:HG2	6:D:616:HOH:O	2.18	0.43
1:E:209:PRO:HB3	1:K:29:ALA:O	2.19	0.43
1:H:398:GLU:HB3	6:H:614:HOH:O	2.19	0.42
1:J:309:LYS:HB2	1:J:310:PRO:HD3	2.01	0.42
1:A:51:ALA:HA	1:A:56:VAL:O	2.20	0.42
1:F:382:HIS:CD2	1:F:385:MET:HE3	2.54	0.42
1:G:309:LYS:HB2	1:G:310:PRO:HD3	2.01	0.42
1:F:415:LEU:C	6:F:609:HOH:O	2.58	0.42
1:E:309:LYS:HB2	1:E:310:PRO:HD3	2.01	0.42
1:A:382:HIS:CD2	1:A:385:MET:CE	3.02	0.42
1:D:308:ASN:ND2	1:D:311:LEU:CD2	2.83	0.42
1:I:382:HIS:CD2	1:I:385:MET:CE	3.03	0.42
1:C:51:ALA:HA	1:C:56:VAL:O	2.20	0.42
1:K:309:LYS:HB2	1:K:310:PRO:HD3	2.01	0.42
1:A:233:GLU:OE1	1:B:17:GLU:HG2	2.19	0.42
1:F:382:HIS:CD2	1:F:385:MET:CE	3.03	0.42
1:I:166:LEU:HD12	1:I:166:LEU:N	2.35	0.42
1:B:104:GLU:HG3	6:H:606:HOH:O	2.19	0.41
1:C:196:ARG:NH2	1:C:203:GLN:HE22	2.18	0.41
1:D:51:ALA:HA	1:D:56:VAL:O	2.20	0.41
1:E:119:ARG:NH2	6:E:606:HOH:O	2.53	0.41
1:B:166:LEU:HD12	1:B:166:LEU:N	2.35	0.41
1:L:51:ALA:HA	1:L:56:VAL:O	2.20	0.41
1:D:35:LYS:HE2	6:D:628:HOH:O	2.18	0.41
1:E:382:HIS:CD2	1:E:385:MET:CE	3.03	0.41
1:H:94:LEU:HD23	6:H:613:HOH:O	2.19	0.41
1:H:166:LEU:N	1:H:166:LEU:HD12	2.35	0.41
1:H:382:HIS:CD2	1:H:385:MET:CE	3.03	0.41
1:B:51:ALA:HA	1:B:56:VAL:O	2.20	0.41
1:B:382:HIS:CD2	1:B:385:MET:CE	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLN:HG2	1:C:270:PHE:CD1	2.55	0.41
1:D:166:LEU:N	1:D:166:LEU:HD12	2.35	0.41
1:K:51:ALA:HA	1:K:56:VAL:O	2.20	0.41
1:F:166:LEU:N	1:F:166:LEU:HD12	2.35	0.41
1:H:51:ALA:HA	1:H:56:VAL:O	2.20	0.41
1:D:20:LYS:HD2	1:D:20:LYS:HA	1.91	0.41
1:G:244:GLN:HG2	1:G:270:PHE:CD1	2.56	0.41
1:E:259:GLN:HG3	6:E:615:HOH:O	2.19	0.41
1:G:166:LEU:HD12	1:G:166:LEU:N	2.35	0.41
1:I:94:LEU:HD11	1:I:360:ALA:O	2.21	0.41
1:K:166:LEU:N	1:K:166:LEU:HD12	2.36	0.41
1:E:51:ALA:HA	1:E:56:VAL:O	2.20	0.41
1:I:102:ARG:HD2	6:I:607:HOH:O	2.21	0.41
1:A:137:GLU:OE2	1:A:151[A]:ARG:NH1	2.54	0.41
1:E:37:THR:HA	1:J:175:ASN:ND2	2.36	0.41
1:J:51:ALA:HA	1:J:56:VAL:O	2.20	0.41
1:D:106:ALA:C	1:D:107:ARG:HD2	2.41	0.40
1:I:119:ARG:O	1:I:293:THR:HG23	2.22	0.40
1:A:158:ARG:CD	6:A:601:HOH:O	2.70	0.40
1:D:119:ARG:O	1:D:293:THR:HG23	2.22	0.40
1:F:309:LYS:HB2	1:F:310:PRO:HD3	2.04	0.40
1:G:382:HIS:CD2	1:G:385:MET:CE	3.04	0.40
1:B:277:LYS:NZ	1:L:196:ARG:CD	2.85	0.40
1:C:382:HIS:CD2	1:C:385:MET:CE	3.04	0.40
1:H:141:SER:HB2	1:I:361:GLN:NE2	2.37	0.40
1:I:3:THR:HA	1:I:33:GLU:O	2.21	0.40
1:L:382:HIS:CD2	1:L:385:MET:CE	3.04	0.40
1:C:382:HIS:CD2	1:C:385:MET:HE3	2.56	0.40
1:D:382:HIS:ND1	1:D:385:MET:HE3	2.37	0.40

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.

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	412/423 (97%)	405 (98%)	7 (2%)	0	100	100
1	B	411/423 (97%)	406 (99%)	5 (1%)	0	100	100
1	C	411/423 (97%)	405 (98%)	6 (2%)	0	100	100
1	D	412/423 (97%)	407 (99%)	5 (1%)	0	100	100
1	E	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	H	412/423 (97%)	406 (98%)	6 (2%)	0	100	100
1	I	412/423 (97%)	406 (98%)	6 (2%)	0	100	100
1	J	411/423 (97%)	406 (99%)	5 (1%)	0	100	100
1	K	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

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	312/321 (97%)	298 (96%)	14 (4%)	27	42
1	B	311/321 (97%)	303 (97%)	8 (3%)	46	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	311/321 (97%)	302 (97%)	9 (3%)	42	60
1	D	312/321 (97%)	304 (97%)	8 (3%)	46	64
1	E	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
1	H	312/321 (97%)	305 (98%)	7 (2%)	52	70
1	I	312/321 (97%)	301 (96%)	11 (4%)	36	52
1	J	311/321 (97%)	297 (96%)	14 (4%)	27	42
1	K	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

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	40	ASP
1	A	107	ARG
1	A	119	ARG
1	A	158	ARG
1	A	201	ARG
1	A	203	GLN
1	A	230	GLU
1	A	251	PHE
1	A	260	ARG
1	A	308	ASN
1	A	358	GLN
1	A	383	LEU
1	A	413	GLN
1	B	201	ARG
1	B	230	GLU
1	B	251	PHE
1	B	260	ARG
1	B	277	LYS
1	B	381	GLN
1	B	383	LEU
1	B	413	GLN
1	C	5	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	ARG
1	C	201	ARG
1	C	203	GLN
1	C	230	GLU
1	C	251	PHE
1	C	260	ARG
1	C	277	LYS
1	C	361	GLN
1	D	119	ARG
1	D	153	LYS
1	D	230	GLU
1	D	251	PHE
1	D	327	ARG
1	D	335	LEU
1	D	358	GLN
1	D	402	ASP
1	E	134	ASN
1	E	196	ARG
1	E	201	ARG
1	E	230	GLU
1	E	251	PHE
1	E	260	ARG
1	E	265	GLU
1	E	323	GLU
1	E	354	ARG
1	E	358	GLN
1	E	361	GLN
1	F	5	GLU
1	F	134	ASN
1	F	196	ARG
1	F	201	ARG
1	F	230	GLU
1	F	251	PHE
1	F	260	ARG
1	F	277	LYS
1	F	381	GLN
1	F	383	LEU
1	G	5	GLU
1	G	17	GLU
1	G	28	LYS
1	G	197	GLN
1	G	230	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	251	PHE
1	G	260	ARG
1	G	416	ARG
1	H	94	LEU
1	H	119	ARG
1	H	196	ARG
1	H	230	GLU
1	H	251	PHE
1	H	260	ARG
1	H	402	ASP
1	I	46	THR
1	I	94	LEU
1	I	119	ARG
1	I	129	LYS
1	I	201	ARG
1	I	230	GLU
1	I	251	PHE
1	I	289	LYS
1	I	358	GLN
1	I	361	GLN
1	I	413	GLN
1	J	94	LEU
1	J	119	ARG
1	J	129	LYS
1	J	196	ARG
1	J	230	GLU
1	J	251	PHE
1	J	260	ARG
1	J	277	LYS
1	J	327	ARG
1	J	330	GLN
1	J	339	ARG
1	J	354	ARG
1	J	358	GLN
1	J	383	LEU
1	K	20	LYS
1	K	85	GLU
1	K	119	ARG
1	K	134	ASN
1	K	196	ARG
1	K	230	GLU
1	K	251	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	259	GLN
1	K	265	GLU
1	K	323	GLU
1	K	383	LEU
1	L	20	LYS
1	L	40	ASP
1	L	107	ARG
1	L	119	ARG
1	L	153	LYS
1	L	196	ARG
1	L	197	GLN
1	L	201	ARG
1	L	230	GLU
1	L	251	PHE
1	L	260	ARG
1	L	265	GLU
1	L	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	HIS
1	A	392	GLN
1	C	203	GLN
1	C	278	ASN
1	C	358	GLN
1	C	392	GLN
1	D	203	GLN
1	D	262	GLN
1	D	308	ASN
1	D	392	GLN
1	E	134	ASN
1	E	197	GLN
1	E	358	GLN
1	E	382	HIS
1	F	358	GLN
1	F	392	GLN
1	G	382	HIS
1	G	392	GLN
1	I	134	ASN
1	I	203	GLN
1	J	11	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	62	GLN
1	J	175	ASN
1	K	134	ASN
1	K	382	HIS
1	L	197	GLN
1	L	259	GLN
1	L	361	GLN
1	L	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	Res	Link	Bond lengths			Bond angles		
					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	B	502	-	6,6,6	0.23	0	5,5,5	0.10	0
4	EDO	E	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	I	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	K	502	-	-	6/7/7/7	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	E	502	-	-	0/1/1/1	-
5	PGE	L	502	-	-	4/7/7/7	-
3	PEG	I	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.

All (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
5	K	502	PGE	O2-C3-C4-O3
5	F	502	PGE	O1-C1-C2-O2
5	L	502	PGE	O3-C5-C6-O4
3	I	502	PEG	O2-C3-C4-O4
5	F	502	PGE	O3-C5-C6-O4
5	K	502	PGE	O3-C5-C6-O4
5	K	502	PGE	C4-C3-O2-C2
3	I	502	PEG	O1-C1-C2-O2
5	G	502	PGE	O2-C3-C4-O3
3	D	503	PEG	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	L	502	PGE	C1-C2-O2-C3
3	B	502	PEG	O1-C1-C2-O2
3	I	502	PEG	C4-C3-O2-C2
5	G	502	PGE	C3-C4-O3-C5
5	K	502	PGE	C3-C4-O3-C5
3	B	502	PEG	C4-C3-O2-C2
5	F	502	PGE	C6-C5-O3-C4
5	L	502	PGE	C3-C4-O3-C5
5	K	502	PGE	C1-C2-O2-C3
5	K	502	PGE	C6-C5-O3-C4
3	D	503	PEG	O1-C1-C2-O2
5	G	502	PGE	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	502	PGE	3	0
3	B	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

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	413/423 (97%)	-0.06	2 (0%) 91 91	5, 11, 26, 57	0
1	B	413/423 (97%)	-0.08	1 (0%) 95 96	5, 13, 26, 45	0
1	C	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	E	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	H	413/423 (97%)	-0.09	1 (0%) 95 96	6, 13, 27, 56	0
1	I	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	4959/5076 (97%)	-0.10	28 (0%) 89 89	5, 12, 26, 57	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	ALA	4.0
1	C	199	GLY	3.8
1	I	199	GLY	3.5
1	D	266	ALA	3.2
1	F	198	ALA	3.0
1	H	266	ALA	3.0
1	B	199	GLY	2.8
1	A	199	GLY	2.7
1	E	53	THR	2.5
1	F	42	GLY	2.4
1	A	266	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	107	ARG	2.4
1	C	200	GLY	2.4
1	C	107	ARG	2.3
1	F	41	ALA	2.2
1	I	200	GLY	2.2
1	I	40	ASP	2.2
1	D	199	GLY	2.2
1	I	266	ALA	2.2
1	J	107	ARG	2.2
1	F	29	ALA	2.1
1	F	349	GLN	2.1
1	J	41	ALA	2.1
1	C	201	ARG	2.1
1	F	107	ARG	2.1
1	I	196	ARG	2.1
1	C	3	THR	2.1
1	C	43	VAL	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
5	PGE	K	502	10/10	0.88	0.19	13,17,18,19	0
3	PEG	I	502	7/7	0.89	0.21	17,18,24,25	0
3	PEG	B	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	F	502	10/10	0.93	0.14	13,15,17,17	0
4	EDO	E	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	I	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	H	502	1/1	0.97	0.05	0,0,0,0	0
2	CL	A	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	H	501	1/1	0.98	0.13	3,3,3,3	0
2	CL	B	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	E	501	1/1	0.99	0.06	7,7,7,7	0
2	CL	C	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.