Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:05 PM GMT

PDB ID	:	4KHZ
Title	:	Crystal structure of the maltose-binding protein/maltose transporter complex in an pre-translocation conformation bound to maltoheptaose
Authors	:	Oldham, M.L.; Chen, S.; Chen, J.
Deposited on	:	2013-05-01
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

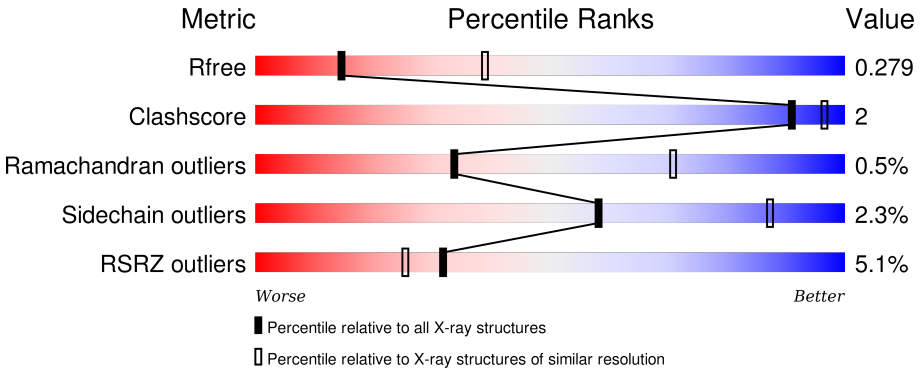
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	380	2% 91% 6%
2	F	514	6% 89% 5% 6%
3	G	296	4% 83% 11% 5%
4	A	381	4% 88% 8%
4	B	381	7% 90% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14715 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-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	370	Total	C	N	O	S	0	0	0
			2877	1853	469	549	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	372	SER	-	EXPRESSION TAG	UNP P0AEX9
E	373	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	374	SER	-	EXPRESSION TAG	UNP P0AEX9
E	375	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	376	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	377	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	378	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	379	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	380	HIS	-	EXPRESSION TAG	UNP P0AEX9

- Molecule 2 is a protein called Maltose transport system permease protein MalF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	483	Total	C	N	O	S	0	0	0
			3750	2464	597	672	17			

- Molecule 3 is a protein called Binding-protein-dependent transport systems inner membrane component.

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 Binding-protein-dependent transport systems inner membrane component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	370	Total	C	N	O	S	0	1	0
			2879	1820	515	531	13			
4	B	368	Total	C	N	O	S	0	0	0
			2855	1806	511	525	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP C9QV42
A	373	SER	-	EXPRESSION TAG	UNP C9QV42
A	374	ALA	-	EXPRESSION TAG	UNP C9QV42
A	375	SER	-	EXPRESSION TAG	UNP C9QV42
A	376	HIS	-	EXPRESSION TAG	UNP C9QV42
A	377	HIS	-	EXPRESSION TAG	UNP C9QV42
A	378	HIS	-	EXPRESSION TAG	UNP C9QV42
A	379	HIS	-	EXPRESSION TAG	UNP C9QV42
A	380	HIS	-	EXPRESSION TAG	UNP C9QV42
A	381	HIS	-	EXPRESSION TAG	UNP C9QV42
B	372	ALA	-	EXPRESSION TAG	UNP C9QV42
B	373	SER	-	EXPRESSION TAG	UNP C9QV42
B	374	ALA	-	EXPRESSION TAG	UNP C9QV42
B	375	SER	-	EXPRESSION TAG	UNP C9QV42
B	376	HIS	-	EXPRESSION TAG	UNP C9QV42
B	377	HIS	-	EXPRESSION TAG	UNP C9QV42
B	378	HIS	-	EXPRESSION TAG	UNP C9QV42
B	379	HIS	-	EXPRESSION TAG	UNP C9QV42
B	380	HIS	-	EXPRESSION TAG	UNP C9QV42
B	381	HIS	-	EXPRESSION TAG	UNP C9QV42

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

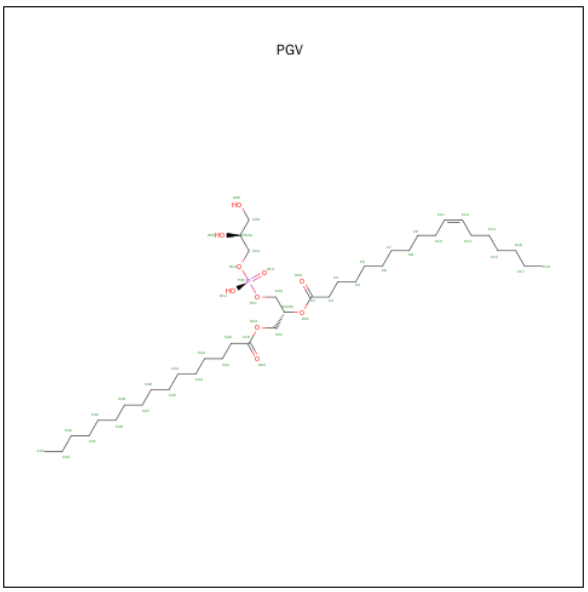
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	4	Total	C	O	0	0
			45	24	21		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	3	Total	C	O	0	0
			23	12	11		

- Molecule 7 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE

(three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

- Molecule 8 is water.

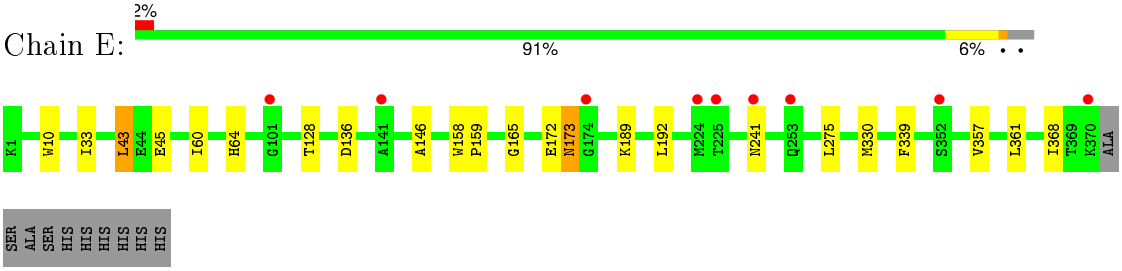
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	21	Total	O	0	0
			21	21		
8	F	11	Total	O	0	0
			11	11		
8	G	5	Total	O	0	0
			5	5		
8	A	9	Total	O	0	0
			9	9		
8	B	7	Total	O	0	0
			7	7		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

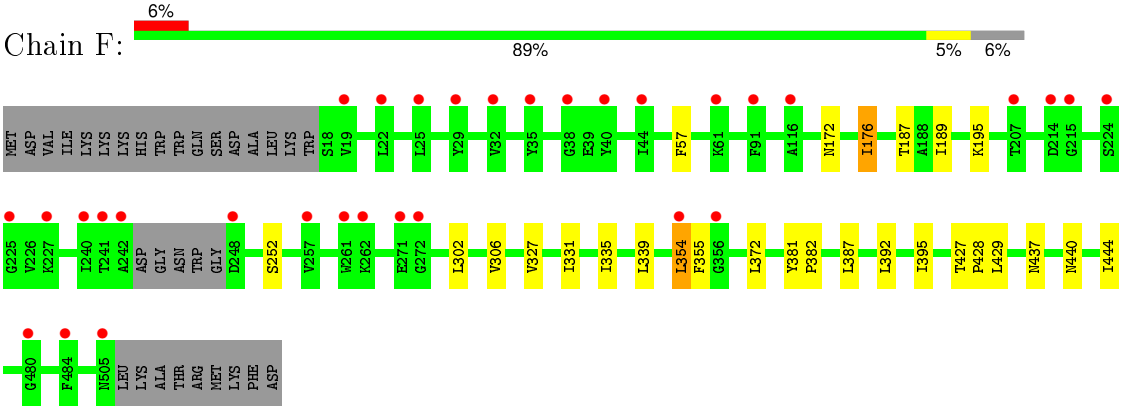
- Molecule 1: Maltose-binding periplasmic protein

Chain E:



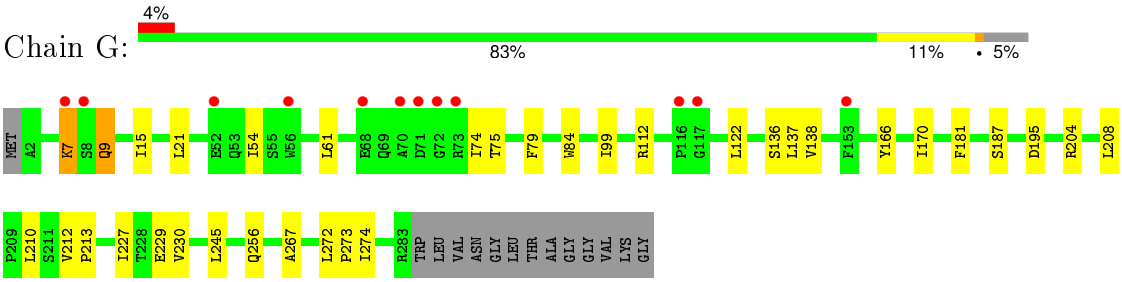
- Molecule 2: Maltose transport system permease protein MalF

Chain F:



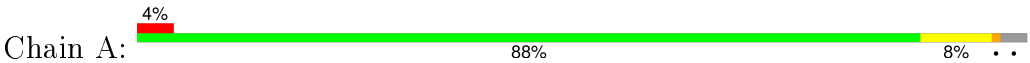
- Molecule 3: Binding-protein-dependent transport systems inner membrane component

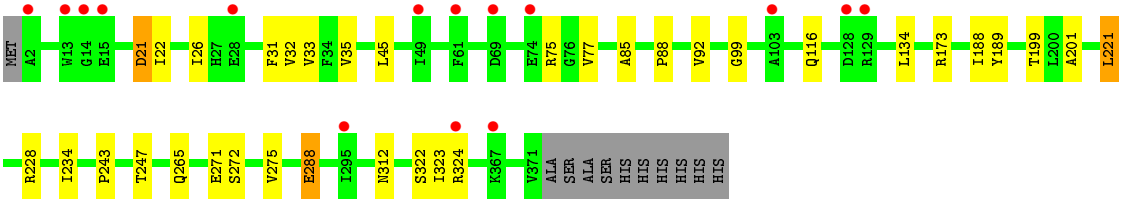
Chain G:



- Molecule 4: Binding-protein-dependent transport systems inner membrane component

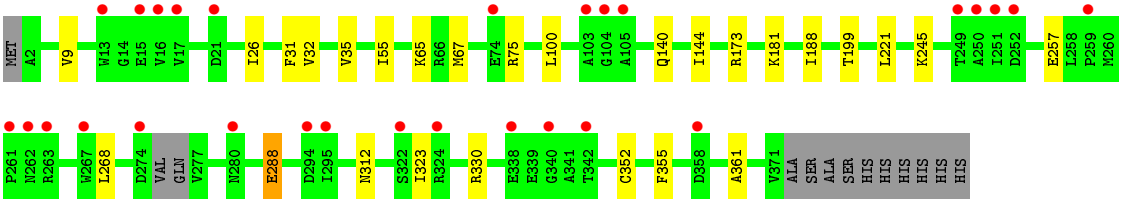
Chain A:





• Molecule 4: Binding-protein-dependent transport systems inner membrane component

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.25Å 92.22Å 117.81Å 90.73° 101.68° 103.60°	Depositor
Resolution (Å)	19.81 – 2.90 19.80 – 2.89	Depositor EDS
% Data completeness (in resolution range)	71.7 (19.81-2.90) 71.5 (19.80-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.283 0.241 , 0.279	Depositor DCC
R_{free} test set	2438 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 48502 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, GLC

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	0.26	0/2946	0.42	0/3998
2	F	0.27	0/3841	0.42	0/5228
3	G	0.27	0/2242	0.44	0/3065
4	A	0.25	0/2929	0.45	0/3972
4	B	0.25	0/2904	0.44	0/3936
All	All	0.26	0/14862	0.43	0/20199

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

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	2877	0	2859	10	0
2	F	3750	0	3783	14	0
3	G	2182	0	2271	14	0
4	A	2879	0	2940	20	0
4	B	2855	0	2919	14	0
5	E	45	0	39	0	0
6	F	23	0	19	1	0
7	F	51	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	9	0	0	0	0
8	B	7	0	0	0	0
8	E	21	0	0	0	0
8	F	11	0	0	0	0
8	G	5	0	0	0	0
All	All	14715	0	14906	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (66) 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:E:136:ASP:HA	1:E:146:ALA:HB2	1.81	0.61
4:A:247:THR:HG21	4:A:265:GLN:HE21	1.68	0.59
1:E:43:LEU:HD11	1:E:60:ILE:CD1	2.34	0.58
4:A:243:PRO:HD3	4:A:323:ILE:HD12	1.85	0.57
3:G:210:LEU:HD21	4:A:88:PRO:HD2	1.85	0.56
4:B:26:ILE:HG23	4:B:32:VAL:HG21	1.88	0.55
1:E:189:LYS:HG2	1:E:361:LEU:HD12	1.87	0.55
3:G:9:GLN:HE21	3:G:9:GLN:HA	1.72	0.54
2:F:327:VAL:HG13	2:F:331:ILE:HD11	1.88	0.54
1:E:10:TRP:HB3	1:E:43:LEU:HD13	1.91	0.53
3:G:136:SER:O	3:G:138:VAL:N	2.42	0.52
4:B:173:ARG:NH1	4:B:199:THR:HG21	2.25	0.52
4:A:247:THR:HG21	4:A:265:GLN:NE2	2.27	0.50
4:A:22:ILE:HD11	4:A:45:LEU:HD21	1.94	0.50
4:A:33:VAL:CG2	4:A:201:ALA:HB2	2.42	0.50
4:A:243:PRO:CD	4:A:323:ILE:HD12	2.42	0.49
1:E:33:ILE:HD13	1:E:275:LEU:HD13	1.94	0.49
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.48	0.49
2:F:392:LEU:HD12	2:F:395:ILE:HD12	1.93	0.48
2:F:381:TYR:N	2:F:382:PRO:HD2	2.29	0.48
4:A:75:ARG:HB2	4:A:77:VAL:HG12	1.96	0.48
1:E:339:PHE:HA	1:E:368:ILE:HD12	1.96	0.48
2:F:331:ILE:HD12	3:G:267:ALA:HB1	1.96	0.47
4:B:67:MET:CE	4:B:75:ARG:HA	2.44	0.47
2:F:387:LEU:CD2	2:F:429:LEU:HD13	2.45	0.47
1:E:64:HIS:NE2	1:E:330:MET:O	2.42	0.47
2:F:387:LEU:HD21	2:F:429:LEU:HD13	1.96	0.46
4:B:355:PHE:CE2	4:B:361:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:LEU:HB3	4:A:234:ILE:HD12	1.97	0.46
4:A:92:VAL:HG22	4:A:134:LEU:HD11	1.98	0.46
4:A:272:SER:O	4:A:275:VAL:HG22	2.16	0.46
3:G:112:ARG:NH2	3:G:181:PHE:O	2.49	0.46
3:G:166:TYR:CE1	3:G:229:GLU:HG2	2.51	0.46
2:F:437:ASN:HD21	6:F:603:GLC:H62	1.80	0.45
3:G:227:ILE:HG21	3:G:274:ILE:HD11	1.97	0.45
1:E:192:LEU:HD23	1:E:357:VAL:HG13	1.97	0.45
1:E:158:TRP:N	1:E:159:PRO:CD	2.80	0.45
4:A:26:ILE:HG23	4:A:32:VAL:HG21	1.99	0.44
2:F:189:ILE:HD12	2:F:195:LYS:HG2	1.99	0.44
4:A:92:VAL:CG2	4:A:134:LEU:HD11	2.48	0.44
4:B:26:ILE:HD13	4:B:188:ILE:HD12	2.00	0.43
3:G:272:LEU:N	3:G:273:PRO:HD2	2.33	0.43
4:B:268:LEU:HD22	4:B:352:CYS:HB2	2.00	0.43
3:G:99:ILE:HG23	3:G:170:ILE:HG22	2.01	0.42
3:G:204:ARG:HA	3:G:208:LEU:HD12	2.01	0.42
4:A:288:GLU:HG2	4:B:312:ASN:HB2	2.02	0.42
1:E:172:GLU:O	1:E:173:ASN:C	2.57	0.42
2:F:302:LEU:O	2:F:306:VAL:HG23	2.19	0.42
2:F:335:ILE:O	2:F:339:LEU:HG	2.20	0.42
2:F:354:LEU:HD12	2:F:355:PHE:H	1.85	0.42
4:B:288:GLU:HG3	4:B:330:ARG:HD3	2.00	0.42
3:G:195:ASP:HB3	4:A:99:GLY:HA2	2.01	0.42
4:B:140:GLN:NE2	4:B:144:ILE:HD11	2.35	0.42
4:B:140:GLN:HE22	4:B:144:ILE:HD11	1.86	0.41
3:G:187:SER:HB3	4:A:85:ALA:HB2	2.01	0.41
4:A:26:ILE:HD13	4:A:188:ILE:HD12	2.01	0.41
2:F:372:LEU:HD11	2:F:444:ILE:HD13	2.03	0.41
4:B:55:ILE:N	4:B:55:ILE:HD12	2.34	0.41
4:B:9:VAL:HG13	4:B:55:ILE:HG23	2.03	0.41
4:A:312:ASN:HB2	4:B:288:GLU:HG2	2.03	0.41
3:G:212:VAL:N	3:G:213:PRO:CD	2.84	0.41
4:A:33:VAL:HG22	4:A:189:TYR:HB3	2.03	0.41
4:A:173:ARG:NH1	4:A:199:THR:HG21	2.36	0.41
2:F:427:THR:N	2:F:428:PRO:HD2	2.37	0.40
2:F:172:ASN:O	2:F:176:ILE:HG23	2.20	0.40
4:B:245:LYS:O	4:B:257:GLU:N	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	368/380 (97%)	353 (96%)	12 (3%)	3 (1%)	24	60
2	F	479/514 (93%)	447 (93%)	31 (6%)	1 (0%)	52	84
3	G	280/296 (95%)	260 (93%)	17 (6%)	3 (1%)	17	51
4	A	369/381 (97%)	348 (94%)	19 (5%)	2 (0%)	34	71
4	B	364/381 (96%)	345 (95%)	18 (5%)	1 (0%)	46	79
All	All	1860/1952 (95%)	1753 (94%)	97 (5%)	10 (0%)	34	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ASN
3	G	137	LEU
3	G	7	LYS
4	A	21	ASP
4	A	322	SER
3	G	230	VAL
1	E	241	ASN
4	B	323	ILE
2	F	252	SER
1	E	165	GLY

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	297/305 (97%)	294 (99%)	3 (1%)	82 95
2	F	394/424 (93%)	389 (99%)	5 (1%)	76 94
3	G	228/237 (96%)	217 (95%)	11 (5%)	31 67
4	A	315/323 (98%)	306 (97%)	9 (3%)	50 83
4	B	312/323 (97%)	305 (98%)	7 (2%)	60 88
All	All	1546/1612 (96%)	1511 (98%)	35 (2%)	58 87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	LEU
1	E	45	GLU
1	E	128	THR
2	F	57	PHE
2	F	176	ILE
2	F	187	THR
2	F	354	LEU
2	F	440	ASN
3	G	7	LYS
3	G	9	GLN
3	G	15	ILE
3	G	21	LEU
3	G	54	ILE
3	G	61	LEU
3	G	74	ILE
3	G	75	THR
3	G	122	LEU
3	G	245	LEU
3	G	256	GLN
4	A	21	ASP
4	A	31	PHE
4	A	35	VAL
4	A	116	GLN
4	A	221	LEU
4	A	228	ARG
4	A	271	GLU
4	A	288	GLU
4	A	324	ARG
4	B	31	PHE
4	B	35	VAL
4	B	65	LYS

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Mol	Chain	Res	Type
4	B	100	LEU
4	B	181	LYS
4	B	221	LEU
4	B	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	158	GLN
2	F	208	GLN
2	F	376	ASN
2	F	437	ASN
2	F	440	ASN
3	G	9	GLN
3	G	69	GLN
3	G	250	GLN
4	A	116	GLN
4	A	255	GLN
4	A	265	GLN
4	A	305	GLN
4	B	305	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

Of 7 carbohydrates modelled in this entry, 1 is modelled with single atom - leaving 6 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	GLC	E	501	5	12,12,12	0.51	0	17,17,17	0.51	0
5	GLC	E	502	5	11,11,12	0.62	0	14,15,17	0.89	0
5	GLC	E	503	5	11,11,12	0.69	0	14,15,17	0.94	1 (7%)
5	GLC	E	504	5	11,11,12	0.50	0	14,15,17	1.32	1 (7%)
6	GLC	F	602	6	11,11,12	0.52	0	14,15,17	1.27	2 (14%)
6	GLC	F	603	6	11,11,12	0.59	0	14,15,17	1.03	2 (14%)

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	GLC	E	501	5	-	0/2/22/22	0/1/1/1
5	GLC	E	502	5	-	0/2/19/22	0/1/1/1
5	GLC	E	503	5	-	0/2/19/22	0/1/1/1
5	GLC	E	504	5	-	0/2/19/22	0/1/1/1
6	GLC	F	602	6	-	0/2/19/22	0/1/1/1
6	GLC	F	603	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	503	GLC	O5-C1-C2	-2.39	106.97	110.86
6	F	603	GLC	C1-C2-C3	2.11	112.04	109.54
6	F	602	GLC	C1-C2-C3	2.16	112.09	109.54
6	F	603	GLC	C1-O5-C5	2.34	115.22	112.25
6	F	602	GLC	C1-O5-C5	3.56	116.77	112.25
5	E	504	GLC	C1-O5-C5	4.14	117.50	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	603	GLC	1	0

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PGV	F	604	-	50,50,50	1.06	3 (6%)	51,56,56	1.00	2 (3%)

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
7	PGV	F	604	-	-	0/55/55/55	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	604	PGV	C12-C11	3.71	1.53	1.31
7	F	604	PGV	O01-C1	3.99	1.46	1.34
7	F	604	PGV	O03-C19	4.10	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	604	PGV	O03-C19-C20	2.71	120.17	111.90
7	F	604	PGV	O01-C1-C2	3.93	120.06	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	E	370/380 (97%)	-0.15	9 (2%)	62	57	57, 82, 117, 133	0
2	F	483/514 (93%)	0.24	32 (6%)	22	16	63, 101, 154, 189	0
3	G	282/296 (95%)	-0.03	12 (4%)	39	32	58, 86, 145, 170	0
4	A	370/381 (97%)	-0.00	15 (4%)	41	34	69, 91, 123, 176	0
4	B	368/381 (96%)	0.25	28 (7%)	17	11	66, 100, 170, 218	0
All	All	1873/1952 (95%)	0.08	96 (5%)	32	25	57, 94, 150, 218	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	280	ASN	6.5
4	A	15	GLU	6.1
4	B	340	GLY	5.9
2	F	40	TYR	5.9
2	F	354	LEU	5.4
4	B	105	ALA	5.4
3	G	71	ASP	5.0
4	A	324	ARG	4.9
4	B	263	ARG	4.8
4	B	251	ILE	4.8
4	A	128	ASP	4.7
4	B	322	SER	4.7
3	G	116	PRO	4.6
4	B	261	PRO	4.3
4	B	250	ALA	4.2
4	A	69	ASP	4.2
3	G	73	ARG	4.1
4	B	249	THR	4.0
3	G	8	SER	4.0
2	F	29	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
4	B	259	PRO	3.9
2	F	35	TYR	3.9
2	F	225	GLY	3.9
3	G	52	GLU	3.8
3	G	70	ALA	3.8
2	F	227	LYS	3.8
4	B	252	ASP	3.8
2	F	480	GLY	3.7
2	F	271	GLU	3.5
2	F	356	GLY	3.3
2	F	61	LYS	3.3
4	B	16	VAL	3.3
2	F	242	ALA	3.3
2	F	240	ILE	3.1
4	B	17	VAL	3.1
2	F	19	VAL	3.1
4	A	28	GLU	3.1
2	F	215	GLY	3.1
2	F	262	LYS	3.0
4	B	338	GLU	3.0
4	B	262	ASN	3.0
1	E	224	MET	2.9
2	F	32	VAL	2.9
4	B	274	ASP	2.9
4	B	358	ASP	2.9
4	A	14	GLY	2.9
4	B	295	ILE	2.9
4	B	324	ARG	2.8
1	E	174	GLY	2.8
2	F	207	THR	2.8
4	B	294	ASP	2.8
3	G	7	LYS	2.7
1	E	241	ASN	2.7
3	G	72	GLY	2.6
2	F	484	PHE	2.5
4	B	74	GLU	2.5
2	F	257	VAL	2.4
4	A	13	TRP	2.4
2	F	25	LEU	2.4
2	F	38	GLY	2.4
2	F	44	ILE	2.4
2	F	261	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	342	THR	2.4
4	B	13	TRP	2.4
2	F	22	LEU	2.3
4	A	74	GLU	2.3
3	G	56	TRP	2.3
2	F	505	ASN	2.3
4	B	103	ALA	2.3
1	E	370	LYS	2.2
4	A	295	ILE	2.2
4	A	103	ALA	2.2
4	B	104	GLY	2.2
1	E	253	GLN	2.2
2	F	241	THR	2.2
4	B	267	TRP	2.2
4	A	129	ARG	2.2
4	A	49	ILE	2.2
4	A	367	LYS	2.1
4	B	15	GLU	2.1
1	E	225	THR	2.1
2	F	224	SER	2.1
1	E	141	ALA	2.1
3	G	153	PHE	2.1
2	F	116	ALA	2.1
1	E	101	GLY	2.1
2	F	91	PHE	2.1
3	G	117	GLY	2.1
1	E	352	SER	2.1
2	F	214	ASP	2.0
2	F	248	ASP	2.0
4	A	2	ALA	2.0
4	A	61	PHE	2.0
3	G	68	GLU	2.0
2	F	272	GLY	2.0
4	B	21	ASP	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	GLC	F	603	11/12	0.97	0.18	0.92	61,62,63,63	0
5	GLC	E	504	11/12	0.93	0.27	0.90	78,81,84,84	0
5	GLC	E	501	12/12	0.98	0.13	-0.43	59,62,63,65	0
6	GLC	F	602	11/12	0.95	0.10	-1.28	62,62,64,64	0
5	GLC	E	503	11/12	0.96	0.11	-1.47	73,74,77,77	0
5	GLC	E	502	11/12	0.97	0.12	-1.74	67,70,72,72	0
6	GLC	F	601	1/12	0.98	0.08	-	66,66,66,66	0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
7	PGV	F	604	51/51	0.79	0.29	1.42	100,108,121,122	0

6.5 Other polymers (i)

There are no such residues in this entry.