



wwPDB X-ray Structure Validation Summary Report

Aug 7, 2014 – 09:19 PM EDT

PDB ID : 4D11
Title : GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 peptide and manganese (Lower resolution dataset)
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2014-05-01
Resolution : 2.85 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

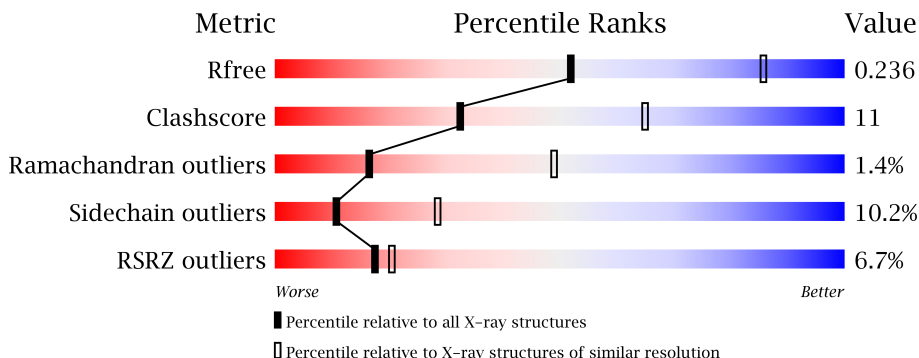
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.85 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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	
1	D	571	
1	E	571	
1	F	571	
2	C	571	
3	L	6	
3	O	6	
3	P	6	
3	X	6	
3	Z	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	BBK	B	1572	-	X
5	BBK	D	1572	-	X
5	BBK	E	1571	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21829 atoms, of which 0 are hydrogen and 0 are deuterium.

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 POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	20	0	0
			3938	2477	715	722	24			
1	B	482	Total	C	N	O	S	20	1	0
			3877	2441	703	710	23			
1	D	487	Total	C	N	O	S	20	0	0
			3916	2465	711	716	24			
1	E	487	Total	C	N	O	S	20	0	0
			3917	2465	711	717	24			
1	F	276	Total	C	N	O	S	8	0	0
			2246	1419	406	407	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
B	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
D	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
E	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
F	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

- Molecule 2 is a protein called POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	436	Total	C	N	O	S	20	0	0
			3560	2249	646	644	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	SER	GLY	CONFLICT	UNP Q10471
C	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

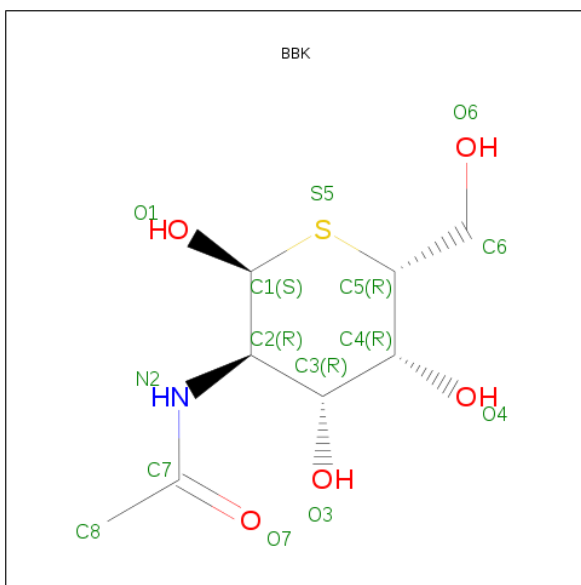
- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	O	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	P	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	Z	5	Total	C	N	O	S	0	0	0
			31	18	5	7	1			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

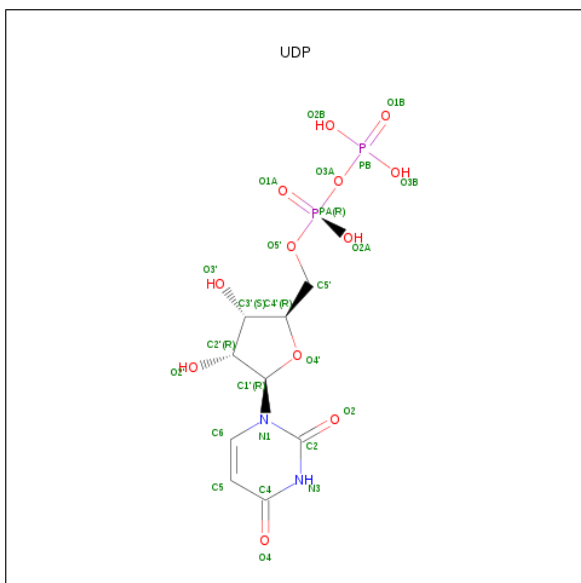
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-5-THIO-ALPHA-D-GALACTOPYRANOSE) (three-letter code: BBK) (formula: C₈H₁₅NO₅S).

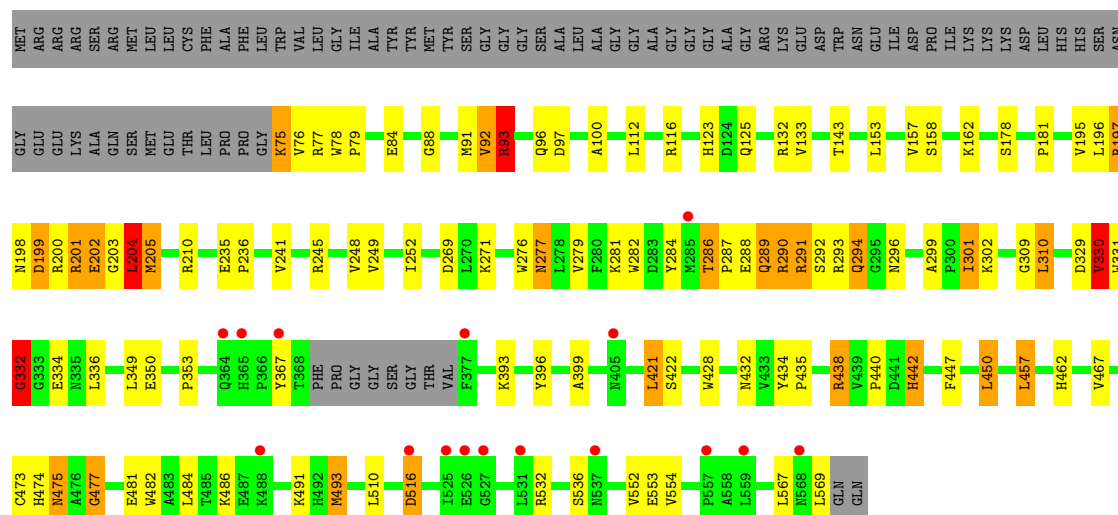


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

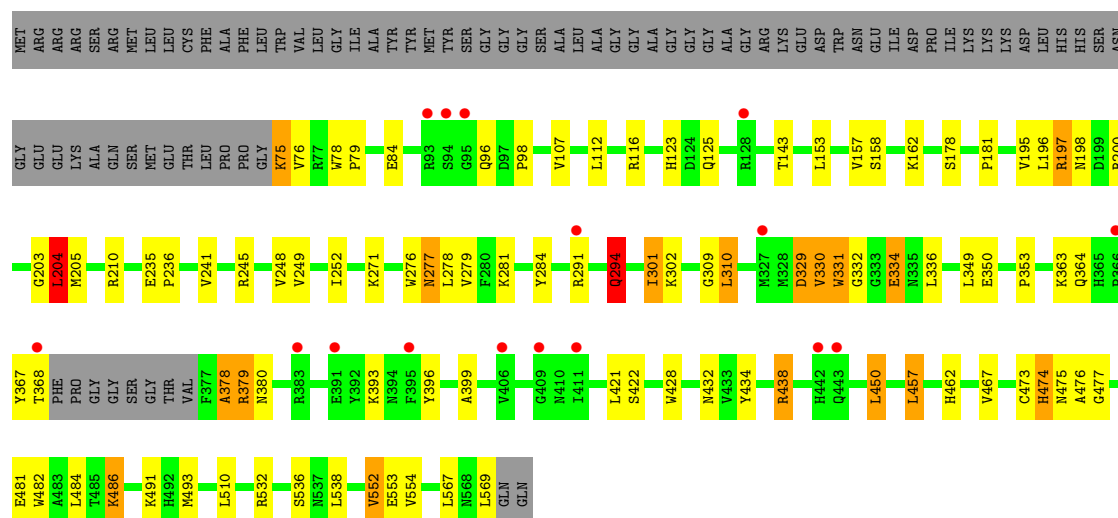


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		



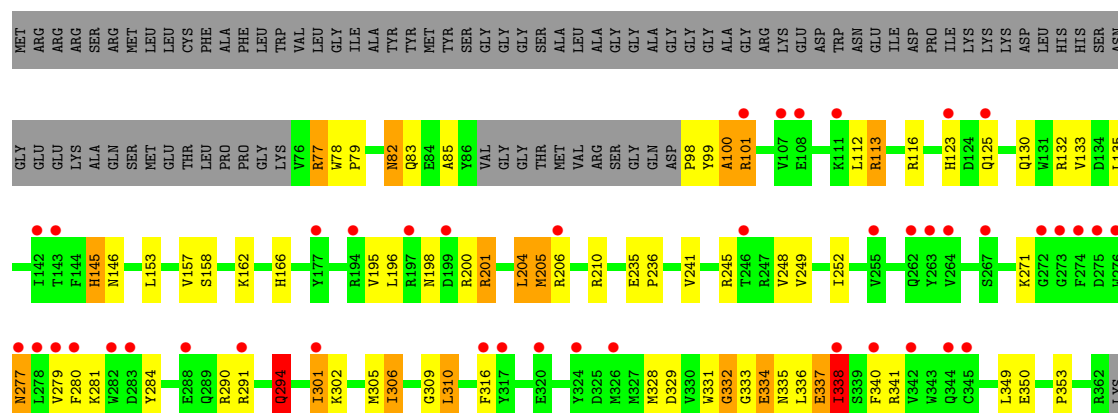
• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain E:



• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain F:



[illegible]

- Molecule 2: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain C:

T566 L567 M568 L569 GLN GLN	GLY	R438	G309	K162	GLY	MET
	SER		L310		GLU	ARG
	LEU	H442			LYS	ARG
	ILE		G322	S178		ARG
	K509	I445			ALA	SER
	L510	A446	D325	P181	GLN	ARG
	Q511	F447			SER	MET
			D329	V195	MET	LEU
	R514	Q451	W330	L196	GLU	LEU
	E515		G332	R197	THR	CYS
D517	T454		M198	PRO	PHE	
S518	N455	N385	D199	LEU	ALA	
R519	C456	L386	R200	PRO	PHE	
Q520	L457			S74	LEU	
K521	D458	L349	L204	K75	TRP	
M522	T459	E350	M205	V76	VAL	
E523	L460		R210	R77	LEU	
Q524	G461	P353		W78	GLY	
L525	H462		E235	P79	ILE	
I526	PHE	K363	E236		ALA	
E526	ALA	Q364	P236	E84	ALA	
G527	ASP	R365	E239	G89	TYR	
N528	GLY	P366	R240	THR	MET	
S529	VAL	TYR	V241	MET	SER	
K530	VAL	THR	R245	VAL	GLY	
L531	GLY	PHE		ARG	GLY	
R532	Y470	PRO	V248	SER	SER	
H533	Y471	GLY	V249	GLY	SER	
V534	E472	GLY		GLN	ALA	
GLY	C473	SER	T252	ASP	LEU	
SER	HIS	G374	Y99	P98	ALA	
ASN	ASN	T375	M258	A100	GLY	
LEU	ALA				GLY	
CYS	GLY	R383		F104	GLY	
ASP	G478		V264	N105	GLY	
SER	N479	K383	G265		GLY	
ARG	Q480	N394	A266		GLY	
THR	E481	F395		L112	ALA	
ALA	W482	Y396	K271		GLY	
LYS	A483	Y397		R116	ARG	
SER	L484	A398	V276		LYS	
GLY	L485	A399	M277	H123	GLU	
GLY	K486	V400	L278	D124	ASP	
LEU	E487	P401	V279	Q125	TRP	
SER	K488	S402	F280	C126	ASN	
VAL	S489	A403	K281	Q127	GLU	
GLU	V490		V282	R128	ILE	
VAL		M410	D283		ASP	
CYS	M493	L411	Y284	W131	PRO	
GLY		Q412		R132	ILE	
PRO	C496	S413	R291	V133	LYS	
ALA	L497	R414	S292	D134	LYS	
LEU	T498	L415	R293		LYS	
SER	V499		Q294	T143	ASP	
GLN	V500	L421		L153	LEU	
	D501	S422	I301		HIS	
	R502				HIS	
M563					ASN	
K564	ALA	Y434	I306	V157	SER	
R565	PRO			S145	ASN	

- Molecule 3: PEPTIDE

Chain L:

Diagram illustrating a 10-slot bus system with 5 red LEDs. The slots are labeled S5, T6, C7, P8, A9, and A10. The LEDs are lit in slots S5, T6, C7, P8, and A9, indicating a specific configuration or state.

- Molecule 3: PEPTIDE

Chain 0:

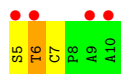
- Molecule 3: PEPTIDE

Chain P: 



● Molecule 3: PEPTIDE

Chain X: 



● Molecule 3: PEPTIDE

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.77Å 120.90Å 249.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.61 – 2.85 46.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (249.61-2.85) 100.0 (46.14-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.235 0.219 , 0.236	Depositor DCC
R_{free} test set	2285 reflections (2.83%)	DCC
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 83232 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21829	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MN, BBK

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	0.95	4/4027 (0.1%)	1.03	4/5443 (0.1%)
1	B	1.19	5/3967 (0.1%)	1.05	6/5361 (0.1%)
1	D	1.18	4/4005 (0.1%)	1.05	8/5413 (0.1%)
1	E	1.12	3/4006 (0.1%)	1.05	7/5415 (0.1%)
1	F	0.84	1/2297 (0.0%)	1.03	2/3104 (0.1%)
2	C	0.90	2/3639 (0.1%)	1.03	3/4909 (0.1%)
3	L	0.64	0/32	0.65	0/44
3	O	0.87	0/32	1.25	0/44
3	P	0.94	0/32	1.33	0/44
3	X	0.68	0/32	0.89	0/44
3	Z	0.90	0/31	0.93	0/42
All	All	1.05	19/22100 (0.1%)	1.04	30/29863 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	C	0	1
All	All	0	2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	LYS	CB-CG	-34.06	0.60	1.52
1	D	202	GLU	C-N	-33.06	0.73	1.33
1	B	84	GLU	CB-CG	-32.47	0.90	1.52
1	E	84	GLU	CB-CG	-30.61	0.94	1.52
1	D	486	LYS	CB-CG	-25.67	0.83	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	LYS	CB-CG-CD	18.38	159.39	111.60
1	B	84	GLU	CA-CB-CG	13.47	143.04	113.40
1	A	294	GLN	CA-CB-CG	11.16	137.95	113.40
1	B	75	LYS	CA-CB-CG	11.01	137.63	113.40
2	C	75	LYS	CB-CG-CD	10.64	139.28	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	127	GLN	Peptide
1	D	332	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3938	0	3863	38	0
1	B	3877	0	3804	96	0
1	D	3916	0	3842	82	0
1	E	3917	0	3843	75	0
1	F	2246	0	2214	88	0
2	C	3560	0	3495	106	0
3	L	32	0	28	3	0
3	O	32	0	28	1	0
3	P	32	0	28	0	0
3	X	32	0	28	7	0
3	Z	31	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	B	15	0	0	1	0
5	D	15	0	0	0	0
5	E	15	0	0	0	0
6	A	25	0	11	0	0
6	B	25	0	11	0	0
6	C	25	0	11	0	0
6	D	25	0	11	0	0
6	E	25	0	11	1	0
6	F	25	0	11	0	0
All	All	21829	0	21267	483	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 483 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:328:MET:SD	1:F:334:GLU:CB	2.07	1.42
1:D:202:GLU:C	1:D:203:GLY:CA	1.92	1.36
1:D:202:GLU:CA	1:D:203:GLY:N	1.92	1.30
1:F:328:MET:SD	1:F:334:GLU:HB2	1.68	1.29
1:B:329:ASP:HB2	1:B:379:ARG:NH2	1.47	1.28

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	A	487/571 (85%)	461 (95%)	24 (5%)	2 (0%)	43 80
1	B	477/571 (84%)	445 (93%)	26 (6%)	6 (1%)	18 51
1	D	483/571 (85%)	449 (93%)	28 (6%)	6 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	483/571 (85%)	457 (95%)	21 (4%)	5 (1%)	22	59
1	F	272/571 (48%)	252 (93%)	15 (6%)	5 (2%)	13	41
2	C	422/571 (74%)	387 (92%)	27 (6%)	8 (2%)	12	39
3	L	4/6 (67%)	1 (25%)	1 (25%)	2 (50%)	0	0
3	O	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
3	P	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
3	X	4/6 (67%)	1 (25%)	2 (50%)	1 (25%)	0	0
3	Z	3/6 (50%)	3 (100%)	0	0	100	100
All	All	2643/3456 (76%)	2461 (93%)	146 (6%)	36 (1%)	16	49

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	A	477	GLY
1	B	132	ARG
1	B	477	GLY
2	C	365	HIS

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	A	425/485 (88%)	386 (91%)	39 (9%)	13	35
1	B	418/485 (86%)	379 (91%)	39 (9%)	13	35
1	D	423/485 (87%)	379 (90%)	44 (10%)	10	27
1	E	423/485 (87%)	384 (91%)	39 (9%)	13	35
1	F	244/485 (50%)	215 (88%)	29 (12%)	8	19
2	C	385/486 (79%)	340 (88%)	45 (12%)	8	20
3	L	4/4 (100%)	4 (100%)	0	100	100
3	O	4/4 (100%)	2 (50%)	2 (50%)	0	0
3	P	4/4 (100%)	3 (75%)	1 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	4/4 (100%)	4 (100%)	0	100	100
3	Z	4/4 (100%)	3 (75%)	1 (25%)	1	2
All	All	2338/2931 (80%)	2099 (90%)	239 (10%)	11	28

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	434	TYR
1	D	199	ASP
1	F	204	LEU
2	C	457	LEU
2	C	528	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	380	ASN
1	D	277	ASN
1	F	145	HIS
2	C	405	ASN
2	C	462	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	BBK	A	1571	-	15,15,15	8.32	3 (20%)	21,21,21	2.50	4 (19%)
6	UDP	A	1572	4	26,26,26	1.33	4 (15%)	36,40,40	1.57	5 (13%)
5	BBK	B	1572	-	15,15,15	8.22	4 (26%)	21,21,21	2.53	3 (14%)
6	UDP	B	1573	4	26,26,26	1.45	5 (19%)	36,40,40	1.65	4 (11%)
6	UDP	C	1571	4	26,26,26	1.34	4 (15%)	36,40,40	1.49	5 (13%)
6	UDP	D	1571	4	26,26,26	1.41	4 (15%)	36,40,40	1.54	3 (8%)
5	BBK	D	1572	-	15,15,15	8.36	4 (26%)	21,21,21	2.14	8 (38%)
5	BBK	E	1571	-	15,15,15	8.59	4 (26%)	21,21,21	1.86	4 (19%)
6	UDP	E	1572	4	26,26,26	1.32	4 (15%)	36,40,40	1.62	3 (8%)
6	UDP	F	1364	4	26,26,26	1.25	4 (15%)	36,40,40	1.58	3 (8%)

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	BBK	A	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	A	1572	4	-	0/14/32/32	0/2/2/2
5	BBK	B	1572	-	-	0/6/26/26	0/1/1/1
6	UDP	B	1573	4	-	0/14/32/32	0/2/2/2
6	UDP	C	1571	4	-	0/14/32/32	0/2/2/2
6	UDP	D	1571	4	-	0/14/32/32	0/2/2/2
5	BBK	D	1572	-	-	0/6/26/26	0/1/1/1
5	BBK	E	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	E	1572	4	-	0/14/32/32	0/2/2/2
6	UDP	F	1364	4	-	0/14/32/32	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1571	BBK	C5-S5	-26.28	1.43	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1571	BBK	C5-S5	-25.58	1.44	1.82
5	D	1572	BBK	C5-S5	-25.45	1.44	1.82
5	B	1572	BBK	C5-S5	-24.98	1.45	1.82
5	E	1571	BBK	C1-S5	-19.94	1.43	1.83

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1571	BBK	C1-S5-C5	9.78	118.98	96.41
5	B	1572	BBK	C1-S5-C5	9.46	118.25	96.41
6	D	1571	UDP	N3-C2-N1	6.57	121.45	115.97
6	B	1573	UDP	N3-C2-N1	6.20	121.15	115.97
6	A	1572	UDP	N3-C2-N1	6.15	121.11	115.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	491/571 (85%)	0.02	14 (2%)	49	59	28, 56, 96, 129	5 (1%)
1	B	482/571 (84%)	0.12	15 (3%)	47	56	32, 65, 115, 151	5 (1%)
1	D	487/571 (85%)	0.16	16 (3%)	44	53	29, 64, 110, 144	5 (1%)
1	E	487/571 (85%)	0.15	16 (3%)	44	53	31, 58, 105, 159	5 (1%)
1	F	276/571 (48%)	0.98	43 (15%)	3	3	59, 112, 167, 187	2 (0%)
2	C	436/571 (76%)	0.70	67 (15%)	3	3	35, 89, 149, 182	5 (1%)
3	L	6/6 (100%)	2.22	4 (66%)	0	0	86, 109, 116, 126	0
3	O	6/6 (100%)	0.70	0	100	100	72, 94, 105, 110	0
3	P	6/6 (100%)	0.52	0	100	100	44, 72, 78, 90	0
3	X	6/6 (100%)	2.88	4 (66%)	0	0	91, 106, 118, 123	0
3	Z	5/6 (83%)	0.54	0	100	100	72, 73, 88, 92	0
All	All	2688/3456 (77%)	0.31	179 (6%)	17	20	28, 67, 136, 187	27 (1%)

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	10	ALA	7.3
1	F	276	TRP	6.9
2	C	500	VAL	6.7
1	F	264	VAL	6.5
2	C	511	GLN	6.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BBK	E	1571	15/15	0.30	4.50	67,86,120,144	0
5	BBK	D	1572	15/15	0.28	3.34	97,106,117,122	0
5	BBK	B	1572	15/15	0.23	2.65	66,81,110,110	0
5	BBK	A	1571	15/15	0.21	1.42	52,76,82,88	0
6	UDP	C	1571	25/25	0.19	-0.30	83,96,111,114	0
6	UDP	D	1571	25/25	0.19	-0.32	64,98,118,128	0
6	UDP	B	1573	25/25	0.17	-0.57	77,89,97,106	0
4	MN	D	1570	1/1	0.14	-0.60	58,58,58,58	0
6	UDP	A	1572	25/25	0.14	-0.90	54,74,89,97	0
6	UDP	E	1572	25/25	0.15	-1.06	69,78,89,97	0
4	MN	B	1571	1/1	0.16	-1.19	63,63,63,63	0
6	UDP	F	1364	25/25	0.17	-1.27	107,134,151,177	0
4	MN	F	1363	1/1	0.10	-1.51	93,93,93,93	0
4	MN	C	1570	1/1	0.14	-1.59	67,67,67,67	0
4	MN	E	1570	1/1	0.13	-1.84	46,46,46,46	0
4	MN	A	1570	1/1	0.09	-2.33	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.