



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:34 AM GMT

PDB ID : 4HSI
Title : Glycoprotein B from Herpes simplex virus type 1, A504P/R505G/Q507G/N511Gmutant, low-pH
Authors : Heldwein, E.E.
Deposited on : 2012-10-30
Resolution : 3.10 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>

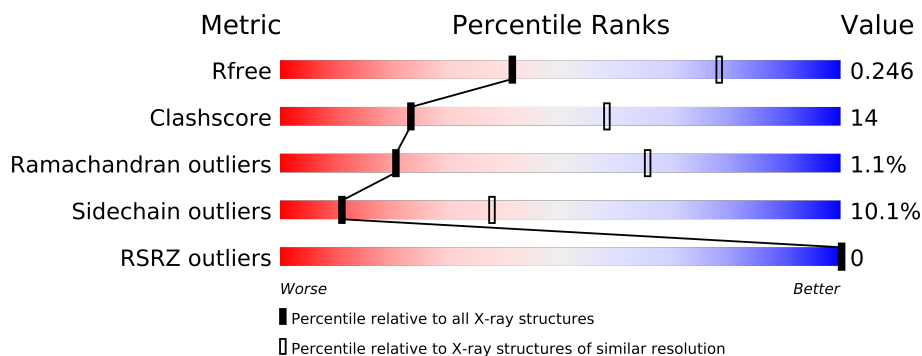
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	703	
1	B	703	
1	C	703	
1	D	703	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19653 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4846	3057	851	916	22			
1	B	606	Total	C	N	O	S	0	0	0
			4891	3085	862	922	22			
1	C	602	Total	C	N	O	S	0	0	0
			4856	3063	854	917	22			
1	D	605	Total	C	N	O	S	0	0	0
			4882	3079	862	919	22			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	30	ALA	-	EXPRESSION TAG	UNP P06437
A	31	ALA	-	EXPRESSION TAG	UNP P06437
A	32	PRO	-	EXPRESSION TAG	UNP P06437
A	33	THR	-	EXPRESSION TAG	UNP P06437
A	34	SER	-	EXPRESSION TAG	UNP P06437
A	35	PRO	-	EXPRESSION TAG	UNP P06437
A	36	GLY	-	EXPRESSION TAG	UNP P06437
A	37	THR	-	EXPRESSION TAG	UNP P06437
A	38	PRO	-	EXPRESSION TAG	UNP P06437
A	39	GLY	-	EXPRESSION TAG	UNP P06437
A	40	VAL	-	EXPRESSION TAG	UNP P06437
A	41	ALA	-	EXPRESSION TAG	UNP P06437
A	42	ALA	-	EXPRESSION TAG	UNP P06437
A	43	ALA	-	EXPRESSION TAG	UNP P06437
A	44	THR	-	EXPRESSION TAG	UNP P06437
A	45	GLN	-	EXPRESSION TAG	UNP P06437
A	46	ALA	-	EXPRESSION TAG	UNP P06437
A	47	ALA	-	EXPRESSION TAG	UNP P06437
A	48	ASN	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	EXPRESSION TAG	UNP P06437
A	50	GLY	-	EXPRESSION TAG	UNP P06437
A	51	PRO	-	EXPRESSION TAG	UNP P06437
A	52	ALA	-	EXPRESSION TAG	UNP P06437
A	53	THR	-	EXPRESSION TAG	UNP P06437
A	54	PRO	-	EXPRESSION TAG	UNP P06437
A	55	ALA	-	EXPRESSION TAG	UNP P06437
A	56	PRO	-	EXPRESSION TAG	UNP P06437
A	57	PRO	-	EXPRESSION TAG	UNP P06437
A	58	PRO	-	EXPRESSION TAG	UNP P06437
A	59	LEU	-	EXPRESSION TAG	UNP P06437
A	60	GLY	-	EXPRESSION TAG	UNP P06437
A	313	SER	THR	CONFLICT	UNP P06437
A	443	LEU	GLN	CONFLICT	UNP P06437
A	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
A	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
A	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
A	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437
B	28	ASP	-	EXPRESSION TAG	UNP P06437
B	29	PRO	-	EXPRESSION TAG	UNP P06437
B	30	ALA	-	EXPRESSION TAG	UNP P06437
B	31	ALA	-	EXPRESSION TAG	UNP P06437
B	32	PRO	-	EXPRESSION TAG	UNP P06437
B	33	THR	-	EXPRESSION TAG	UNP P06437
B	34	SER	-	EXPRESSION TAG	UNP P06437
B	35	PRO	-	EXPRESSION TAG	UNP P06437
B	36	GLY	-	EXPRESSION TAG	UNP P06437
B	37	THR	-	EXPRESSION TAG	UNP P06437
B	38	PRO	-	EXPRESSION TAG	UNP P06437
B	39	GLY	-	EXPRESSION TAG	UNP P06437
B	40	VAL	-	EXPRESSION TAG	UNP P06437
B	41	ALA	-	EXPRESSION TAG	UNP P06437
B	42	ALA	-	EXPRESSION TAG	UNP P06437
B	43	ALA	-	EXPRESSION TAG	UNP P06437
B	44	THR	-	EXPRESSION TAG	UNP P06437
B	45	GLN	-	EXPRESSION TAG	UNP P06437
B	46	ALA	-	EXPRESSION TAG	UNP P06437
B	47	ALA	-	EXPRESSION TAG	UNP P06437
B	48	ASN	-	EXPRESSION TAG	UNP P06437
B	49	GLY	-	EXPRESSION TAG	UNP P06437
B	50	GLY	-	EXPRESSION TAG	UNP P06437
B	51	PRO	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	ALA	-	EXPRESSION TAG	UNP P06437
B	53	THR	-	EXPRESSION TAG	UNP P06437
B	54	PRO	-	EXPRESSION TAG	UNP P06437
B	55	ALA	-	EXPRESSION TAG	UNP P06437
B	56	PRO	-	EXPRESSION TAG	UNP P06437
B	57	PRO	-	EXPRESSION TAG	UNP P06437
B	58	PRO	-	EXPRESSION TAG	UNP P06437
B	59	LEU	-	EXPRESSION TAG	UNP P06437
B	60	GLY	-	EXPRESSION TAG	UNP P06437
B	313	SER	THR	CONFLICT	UNP P06437
B	443	LEU	GLN	CONFLICT	UNP P06437
B	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
B	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
B	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
B	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437
C	28	ASP	-	EXPRESSION TAG	UNP P06437
C	29	PRO	-	EXPRESSION TAG	UNP P06437
C	30	ALA	-	EXPRESSION TAG	UNP P06437
C	31	ALA	-	EXPRESSION TAG	UNP P06437
C	32	PRO	-	EXPRESSION TAG	UNP P06437
C	33	THR	-	EXPRESSION TAG	UNP P06437
C	34	SER	-	EXPRESSION TAG	UNP P06437
C	35	PRO	-	EXPRESSION TAG	UNP P06437
C	36	GLY	-	EXPRESSION TAG	UNP P06437
C	37	THR	-	EXPRESSION TAG	UNP P06437
C	38	PRO	-	EXPRESSION TAG	UNP P06437
C	39	GLY	-	EXPRESSION TAG	UNP P06437
C	40	VAL	-	EXPRESSION TAG	UNP P06437
C	41	ALA	-	EXPRESSION TAG	UNP P06437
C	42	ALA	-	EXPRESSION TAG	UNP P06437
C	43	ALA	-	EXPRESSION TAG	UNP P06437
C	44	THR	-	EXPRESSION TAG	UNP P06437
C	45	GLN	-	EXPRESSION TAG	UNP P06437
C	46	ALA	-	EXPRESSION TAG	UNP P06437
C	47	ALA	-	EXPRESSION TAG	UNP P06437
C	48	ASN	-	EXPRESSION TAG	UNP P06437
C	49	GLY	-	EXPRESSION TAG	UNP P06437
C	50	GLY	-	EXPRESSION TAG	UNP P06437
C	51	PRO	-	EXPRESSION TAG	UNP P06437
C	52	ALA	-	EXPRESSION TAG	UNP P06437
C	53	THR	-	EXPRESSION TAG	UNP P06437
C	54	PRO	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	55	ALA	-	EXPRESSION TAG	UNP P06437
C	56	PRO	-	EXPRESSION TAG	UNP P06437
C	57	PRO	-	EXPRESSION TAG	UNP P06437
C	58	PRO	-	EXPRESSION TAG	UNP P06437
C	59	LEU	-	EXPRESSION TAG	UNP P06437
C	60	GLY	-	EXPRESSION TAG	UNP P06437
C	313	SER	THR	CONFLICT	UNP P06437
C	443	LEU	GLN	CONFLICT	UNP P06437
C	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
C	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
C	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
C	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437
D	28	ASP	-	EXPRESSION TAG	UNP P06437
D	29	PRO	-	EXPRESSION TAG	UNP P06437
D	30	ALA	-	EXPRESSION TAG	UNP P06437
D	31	ALA	-	EXPRESSION TAG	UNP P06437
D	32	PRO	-	EXPRESSION TAG	UNP P06437
D	33	THR	-	EXPRESSION TAG	UNP P06437
D	34	SER	-	EXPRESSION TAG	UNP P06437
D	35	PRO	-	EXPRESSION TAG	UNP P06437
D	36	GLY	-	EXPRESSION TAG	UNP P06437
D	37	THR	-	EXPRESSION TAG	UNP P06437
D	38	PRO	-	EXPRESSION TAG	UNP P06437
D	39	GLY	-	EXPRESSION TAG	UNP P06437
D	40	VAL	-	EXPRESSION TAG	UNP P06437
D	41	ALA	-	EXPRESSION TAG	UNP P06437
D	42	ALA	-	EXPRESSION TAG	UNP P06437
D	43	ALA	-	EXPRESSION TAG	UNP P06437
D	44	THR	-	EXPRESSION TAG	UNP P06437
D	45	GLN	-	EXPRESSION TAG	UNP P06437
D	46	ALA	-	EXPRESSION TAG	UNP P06437
D	47	ALA	-	EXPRESSION TAG	UNP P06437
D	48	ASN	-	EXPRESSION TAG	UNP P06437
D	49	GLY	-	EXPRESSION TAG	UNP P06437
D	50	GLY	-	EXPRESSION TAG	UNP P06437
D	51	PRO	-	EXPRESSION TAG	UNP P06437
D	52	ALA	-	EXPRESSION TAG	UNP P06437
D	53	THR	-	EXPRESSION TAG	UNP P06437
D	54	PRO	-	EXPRESSION TAG	UNP P06437
D	55	ALA	-	EXPRESSION TAG	UNP P06437
D	56	PRO	-	EXPRESSION TAG	UNP P06437
D	57	PRO	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	58	PRO	-	EXPRESSION TAG	UNP P06437
D	59	LEU	-	EXPRESSION TAG	UNP P06437
D	60	GLY	-	EXPRESSION TAG	UNP P06437
D	313	SER	THR	CONFLICT	UNP P06437
D	443	LEU	GLN	CONFLICT	UNP P06437
D	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
D	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
D	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
D	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	30	ALA	-	EXPRESSION TAG	UNP P06437
A	31	ALA	-	EXPRESSION TAG	UNP P06437
A	32	PRO	-	EXPRESSION TAG	UNP P06437
A	33	THR	-	EXPRESSION TAG	UNP P06437
A	34	SER	-	EXPRESSION TAG	UNP P06437
A	35	PRO	-	EXPRESSION TAG	UNP P06437
A	36	GLY	-	EXPRESSION TAG	UNP P06437
A	37	THR	-	EXPRESSION TAG	UNP P06437
A	38	PRO	-	EXPRESSION TAG	UNP P06437
A	39	GLY	-	EXPRESSION TAG	UNP P06437
A	40	VAL	-	EXPRESSION TAG	UNP P06437
A	41	ALA	-	EXPRESSION TAG	UNP P06437
A	42	ALA	-	EXPRESSION TAG	UNP P06437
A	43	ALA	-	EXPRESSION TAG	UNP P06437
A	44	THR	-	EXPRESSION TAG	UNP P06437
A	45	GLN	-	EXPRESSION TAG	UNP P06437
A	46	ALA	-	EXPRESSION TAG	UNP P06437
A	47	ALA	-	EXPRESSION TAG	UNP P06437
A	48	ASN	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

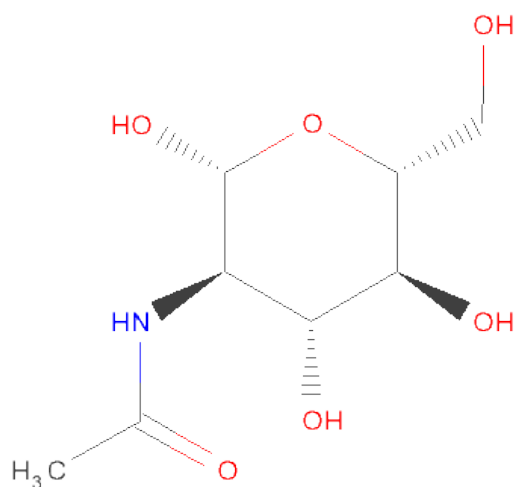
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	EXPRESSION TAG	UNP P06437
A	50	GLY	-	EXPRESSION TAG	UNP P06437
A	51	PRO	-	EXPRESSION TAG	UNP P06437
A	52	ALA	-	EXPRESSION TAG	UNP P06437
A	53	THR	-	EXPRESSION TAG	UNP P06437
A	54	PRO	-	EXPRESSION TAG	UNP P06437
A	55	ALA	-	EXPRESSION TAG	UNP P06437
A	56	PRO	-	EXPRESSION TAG	UNP P06437
A	57	PRO	-	EXPRESSION TAG	UNP P06437
A	58	PRO	-	EXPRESSION TAG	UNP P06437
A	59	LEU	-	EXPRESSION TAG	UNP P06437
A	60	GLY	-	EXPRESSION TAG	UNP P06437
A	313	SER	THR	CONFLICT	UNP P06437
A	443	LEU	GLN	CONFLICT	UNP P06437
A	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
A	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
A	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
A	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437
C	28	ASP	-	EXPRESSION TAG	UNP P06437
C	29	PRO	-	EXPRESSION TAG	UNP P06437
C	30	ALA	-	EXPRESSION TAG	UNP P06437
C	31	ALA	-	EXPRESSION TAG	UNP P06437
C	32	PRO	-	EXPRESSION TAG	UNP P06437
C	33	THR	-	EXPRESSION TAG	UNP P06437
C	34	SER	-	EXPRESSION TAG	UNP P06437
C	35	PRO	-	EXPRESSION TAG	UNP P06437
C	36	GLY	-	EXPRESSION TAG	UNP P06437
C	37	THR	-	EXPRESSION TAG	UNP P06437
C	38	PRO	-	EXPRESSION TAG	UNP P06437
C	39	GLY	-	EXPRESSION TAG	UNP P06437
C	40	VAL	-	EXPRESSION TAG	UNP P06437
C	41	ALA	-	EXPRESSION TAG	UNP P06437
C	42	ALA	-	EXPRESSION TAG	UNP P06437
C	43	ALA	-	EXPRESSION TAG	UNP P06437
C	44	THR	-	EXPRESSION TAG	UNP P06437
C	45	GLN	-	EXPRESSION TAG	UNP P06437
C	46	ALA	-	EXPRESSION TAG	UNP P06437
C	47	ALA	-	EXPRESSION TAG	UNP P06437
C	48	ASN	-	EXPRESSION TAG	UNP P06437
C	49	GLY	-	EXPRESSION TAG	UNP P06437
C	50	GLY	-	EXPRESSION TAG	UNP P06437
C	51	PRO	-	EXPRESSION TAG	UNP P06437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	ALA	-	EXPRESSION TAG	UNP P06437
C	53	THR	-	EXPRESSION TAG	UNP P06437
C	54	PRO	-	EXPRESSION TAG	UNP P06437
C	55	ALA	-	EXPRESSION TAG	UNP P06437
C	56	PRO	-	EXPRESSION TAG	UNP P06437
C	57	PRO	-	EXPRESSION TAG	UNP P06437
C	58	PRO	-	EXPRESSION TAG	UNP P06437
C	59	LEU	-	EXPRESSION TAG	UNP P06437
C	60	GLY	-	EXPRESSION TAG	UNP P06437
C	313	SER	THR	CONFLICT	UNP P06437
C	443	LEU	GLN	CONFLICT	UNP P06437
C	504	PRO	ALA	ENGINEERED MUTATION	UNP P06437
C	505	GLY	ARG	ENGINEERED MUTATION	UNP P06437
C	507	GLY	GLN	ENGINEERED MUTATION	UNP P06437
C	511	GLY	ASN	ENGINEERED MUTATION	UNP P06437

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



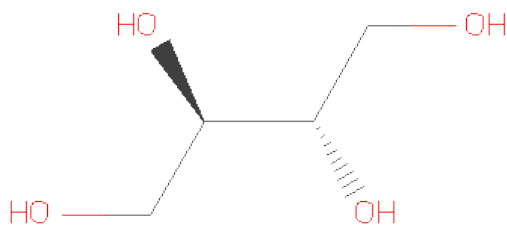
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



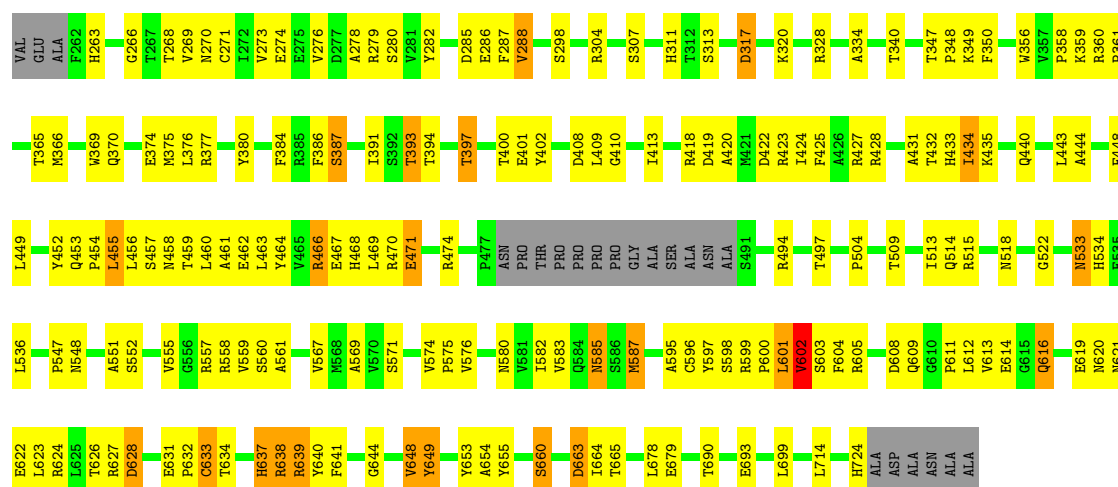
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	1	Total 1	O 1	0	0
6	C	3	Total 3	O 3	0	0
6	D	6	Total 6	O 6	0	0



T690	A595	PRO	L399	D285	F194
E693	C596	PRO	T400	E286	E195
I694	Y597	PRO	E401	F287	E196
	S598	GLY	Y402	V288	F197
L700	B599	ALA	P403		I198
	P600	SER	L404	D283	T201
D720	L601	ALA	S405	F294	R202
	V602	ASN	R406	V295	A203
H724	S603	ALA	Y407	Y296	K204
ALA	F604	SER	D408		
ASP	R605	VAL	L409	F300	C207
ALA	V606	GLU			
ASN	E607	R494	R418	Y303	Y213
ALA	D608		D419	R304	V214
ALA	Q609	I501	A420	E305	R215
		E502		G306	
L612		L506	I424	S307	H224
V613			F425	H308	R225
	Q616		A426	T309	
		L521	Y429	E310	T230
E619	B619	R523	N430	H311	E233
			A431	T312	L234
E622		L531	T432	S313	K235
L623			H433	F319	P236
		E535	I434	K320	A237
	R627			Q321	
P632		N540	Q440		S244
G633		R543	Y441	R328	R245
T634				D329	G246
	H637	N548	A444	L330	V247
R638			N445	T331	H248
R639		S552	F448	T340	
V640		V553	L449		D251
P641		T554	T450	N343	L252
T642		V555	A451	L344	K253
F643		G556	L455	L345	Y254
		R557	L456	R255	P256
Q646		R558		T347	S257
		V559	L460	P348	R258
	Y649	S560	A461	VAL	
		A561	E462	GLU	
	B552		L463		A261
		M568	Y464	W356	F262
L659			V465		H263
S660		S571	R466	K359	R264
	D663	T572	E467		Y265
			H468	K368	G266
S668		D579	L469	W369	T267
		N580	R470	V269	T268
		V581	E471	R377	V269
L673		I582		S378	N270
	L686		R474		C271
B687		S586			T272
V688		M587	N478	S392	V273
		R588	PRO	T393	E274
Y689		I589	THR	T396	
					Y282

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	117.30Å 117.30Å 321.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.91 – 3.10 45.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.8 (45.91-3.10) 75.7 (45.91-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.205 , 0.255 0.201 , 0.246	Depositor DCC
R_{free} test set	3442 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 8.0	EDS
Estimated twinning fraction	0.020 for -h,-k,l 0.459 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 74374 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19653	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7087e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, MRY, NAG

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	0.49	0/4966	0.64	2/6747 (0.0%)
1	B	0.45	0/5013	0.62	0/6809
1	C	0.44	0/4977	0.62	0/6762
1	D	0.46	0/5004	0.62	0/6797
All	All	0.46	0/19960	0.63	2/27115 (0.0%)

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
2	C	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	515	ARG	NE-CZ-NH2	-5.60	117.50	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	NAG	C1

There are no planarity outliers.

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	4846	0	4657	117	1
1	B	4891	0	4703	168	0
1	C	4856	0	4664	151	1
1	D	4882	0	4694	121	0
2	A	28	0	25	0	0
2	C	28	0	25	0	0
3	A	14	0	13	0	0
3	B	28	0	26	1	0
3	C	14	0	13	0	0
3	D	28	0	26	1	0
4	A	8	0	10	0	0
4	C	8	0	10	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
6	A	8	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	6	0	0	0	0
All	All	19653	0	18866	557	2

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 14.

The worst 5 of 557 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:515:ARG:NH2	5:A:805:CL:CL	2.36	0.95
1:C:515:ARG:NH2	5:C:805:CL:CL	2.40	0.91
1:C:614:GLU:HB3	1:C:627:ARG:HH21	1.37	0.87
1:D:116:CYS:HB3	1:D:560:SER:HB3	1.63	0.81
1:B:587:MET:HB3	1:B:653:TYR:HD2	1.48	0.79

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	Distance(Å)	Clash(Å)
1:A:152:GLU:O	1:A:689:TYR:OH[3_555]	2.13	0.07
1:C:152:GLU:O	1:C:689:TYR:OH[3_555]	2.18	0.02

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	597/703 (85%)	529 (89%)	66 (11%)	2 (0%)	50	87
1	B	600/703 (85%)	537 (90%)	54 (9%)	9 (2%)	15	57
1	C	598/703 (85%)	527 (88%)	64 (11%)	7 (1%)	19	62
1	D	599/703 (85%)	537 (90%)	54 (9%)	8 (1%)	18	60
All	All	2394/2812 (85%)	2130 (89%)	238 (10%)	26 (1%)	21	65

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ALA
1	B	413	ILE
1	C	413	ILE
1	D	462	GLU
1	C	465	VAL

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	522/592 (88%)	463 (89%)	59 (11%)	9	32
1	B	528/592 (89%)	466 (88%)	62 (12%)	8	29
1	C	523/592 (88%)	470 (90%)	53 (10%)	11	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	526/592 (89%)	489 (93%)	37 (7%)	21	61
All	All	2099/2368 (89%)	1888 (90%)	211 (10%)	11	38

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	459	THR
1	B	663	ASP
1	D	432	THR
1	B	471	GLU
1	B	616	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	GLN
1	A	658	GLN
1	C	468	HIS
1	D	440	GLN

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 ⓘ

4 carbohydrates are 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
2	NAG	A	801	1,2	12,14,15	0.70	1 (8%)	15,19,21	1.14	2 (13%)
2	NAG	A	802	2	12,14,15	0.74	1 (8%)	15,19,21	1.07	1 (6%)
2	NAG	C	801	1,2	12,14,15	0.75	1 (8%)	15,19,21	1.12	0
2	NAG	C	802	2	12,14,15	0.69	0	15,19,21	1.76	2 (13%)

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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	802	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	O5-C5	-2.30	1.41	1.45
2	C	801	NAG	O5-C5	-2.09	1.41	1.45
2	A	801	NAG	O5-C5	-2.07	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	NAG	O5-C5-C4	4.85	116.81	110.65
2	C	802	NAG	C3-C4-C5	3.80	117.00	110.20
2	A	801	NAG	C3-C4-C5	2.32	114.35	110.20
2	A	801	NAG	O5-C5-C4	2.28	113.55	110.65
2	A	802	NAG	O5-C5-C6	2.25	109.34	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 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$
3	NAG	A	803	1	12,14,15	0.88	1 (8%)	15,19,21	0.96	1 (6%)
4	MRY	A	804	-	7,7,7	0.36	0	8,8,8	0.81	0
3	NAG	B	801	1	12,14,15	0.66	0	15,19,21	1.54	4 (26%)
3	NAG	B	802	1	12,14,15	0.65	0	15,19,21	1.36	2 (13%)
3	NAG	C	803	1	12,14,15	0.51	0	15,19,21	1.09	0
4	MRY	C	804	-	7,7,7	0.30	0	8,8,8	1.09	0
3	NAG	D	801	1	12,14,15	0.58	0	15,19,21	1.01	0
3	NAG	D	802	1	12,14,15	0.62	0	15,19,21	1.14	1 (6%)

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
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	MRY	A	804	-	-	0/8/8/8	0/0/0/0
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1	1/1/5/7	0/6/23/26	0/1/1/1
4	MRY	C	804	-	-	0/8/8/8	0/0/0/0
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	802	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	NAG	O5-C5	-2.47	1.40	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	NAG	C2-N2-C7	-3.25	117.63	123.09
3	B	801	NAG	C3-C2-N2	-3.25	106.82	111.76
3	D	802	NAG	C2-N2-C7	-3.04	117.98	123.09
3	B	801	NAG	C2-N2-C7	3.02	128.16	123.09
3	B	802	NAG	O5-C5-C6	2.26	109.35	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	803	NAG	C1

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	601/703 (85%)	-0.14	0 100 100	1, 37, 84, 140	0
1	B	606/703 (86%)	-0.12	0 100 100	3, 44, 95, 185	0
1	C	602/703 (85%)	-0.12	0 100 100	7, 44, 98, 157	0
1	D	605/703 (86%)	-0.15	0 100 100	2, 39, 78, 147	1 (0%)
All	All	2414/2812 (85%)	-0.13	0 100 100	1, 41, 89, 185	1 (0%)

There are no RSRZ outliers to report.

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 ⓘ

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
2	NAG	C	801	14/15	0.19	0.01	88,88,88,88	0
2	NAG	A	801	14/15	0.18	-0.37	92,92,92,92	0
2	NAG	A	802	14/15	0.16	-	86,86,86,86	0
2	NAG	C	802	14/15	0.17	-	92,92,92,92	0

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	CL	D	803	1/1	0.25	1.94	71,71,71,71	0
4	MRY	A	804	8/8	0.23	1.70	44,44,44,44	0
4	MRY	C	804	8/8	0.23	0.90	34,34,34,34	0
5	CL	B	803	1/1	0.20	-0.25	67,67,67,67	0
3	NAG	A	803	14/15	0.15	-0.39	71,71,71,71	0
3	NAG	B	801	14/15	0.20	-0.43	69,69,69,69	0
3	NAG	B	802	14/15	0.14	-1.09	31,31,31,31	0
3	NAG	D	802	14/15	0.14	-1.18	27,27,27,27	0
3	NAG	C	803	14/15	0.15	-1.39	71,71,71,71	0
3	NAG	D	801	14/15	0.15	-1.65	71,71,71,71	0
5	CL	A	805	1/1	0.13	-1.71	30,30,30,30	0
5	CL	C	805	1/1	0.11	-3.23	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.