



Full wwPDB X-ray Structure Validation 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 full wwPDB 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/ValidationPDFNotes.html>

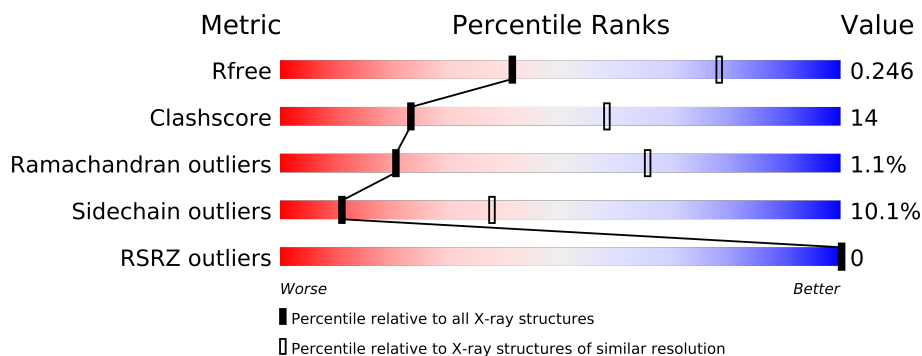
The following versions of software and data (see [references](#)) were used in the production of this report:

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

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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

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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

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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

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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

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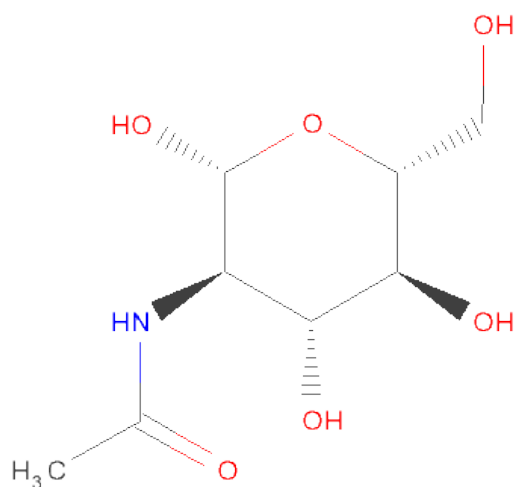
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	EXPRESSION TAG	UNP P06437
A	50	GLY	-	EXPRESSION TAG	UNP P06437
A	51	PRO	-	EXPRESSION TAG	UNP P06437
A	52	ALA	-	EXPRESSION TAG	UNP P06437
A	53	THR	-	EXPRESSION TAG	UNP P06437
A	54	PRO	-	EXPRESSION TAG	UNP P06437
A	55	ALA	-	EXPRESSION TAG	UNP P06437
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

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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: $C_8H_{15}NO_6$).



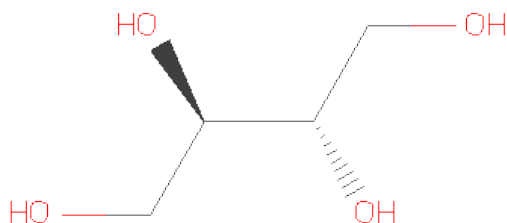
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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.

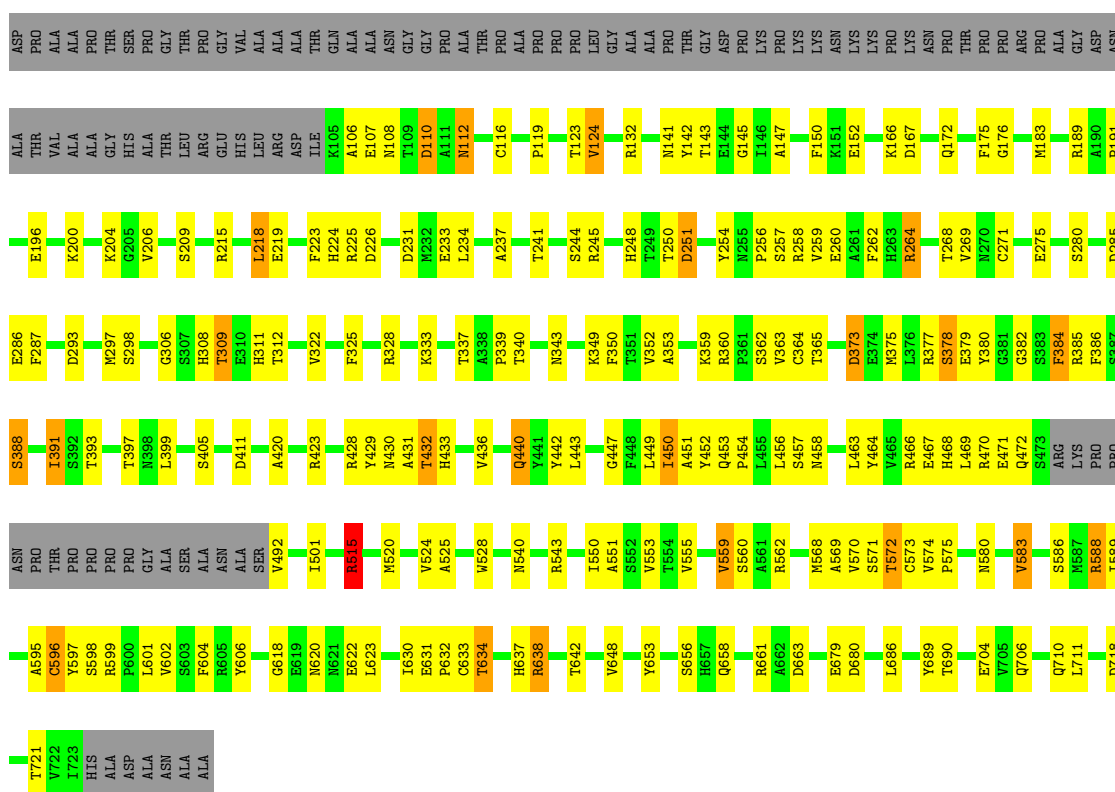
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	1	Total 1	O 1	0	0
6	C	3	Total 3	O 3	0	0
6	D	6	Total 6	O 6	0	0

3 Residue-property plots

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.

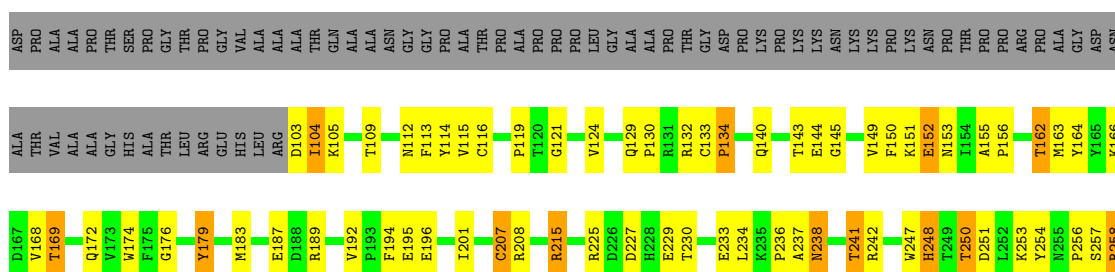
• Molecule 1: Envelope glycoprotein B

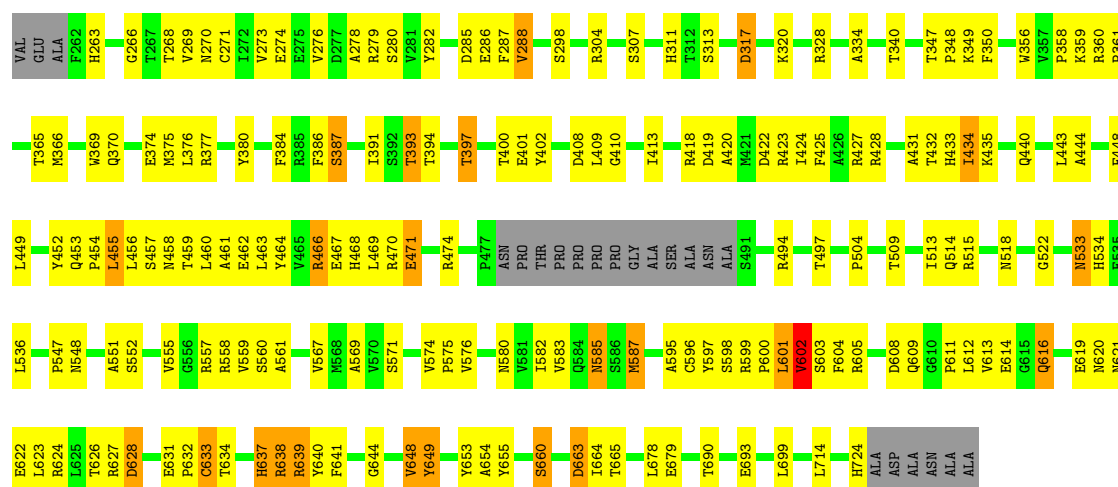
Chain A:



• Molecule 1: Envelope glycoprotein B

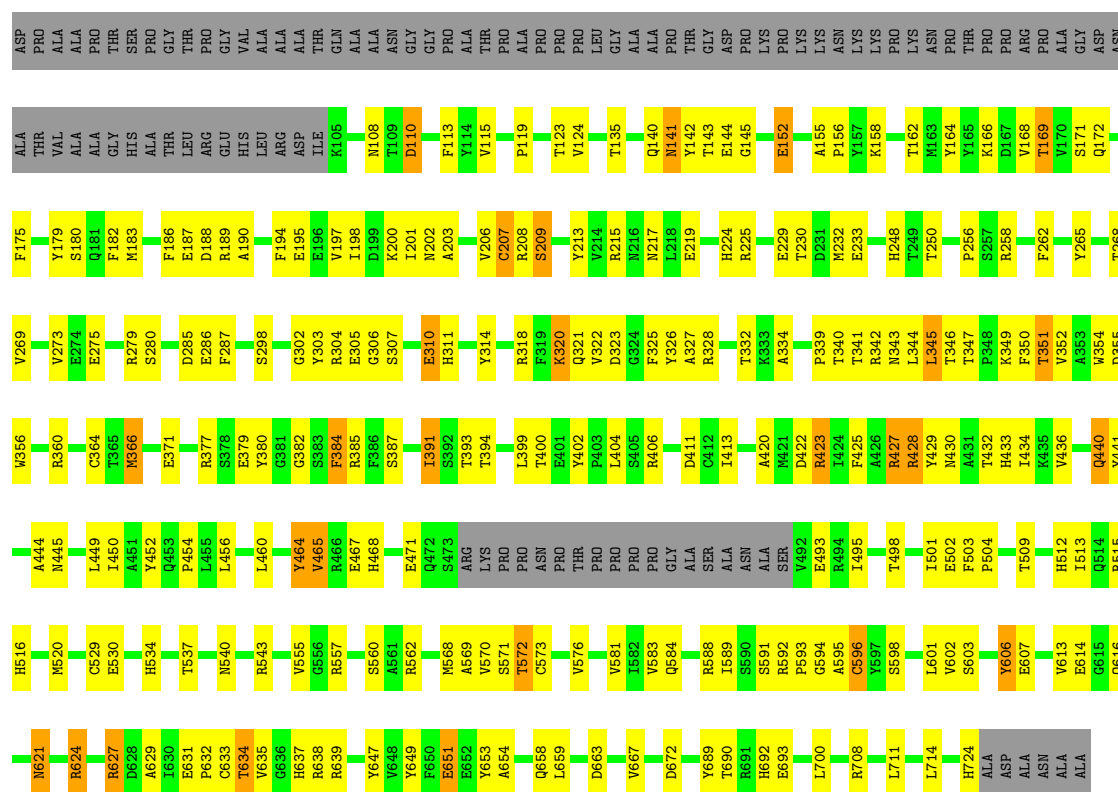
Chain B:





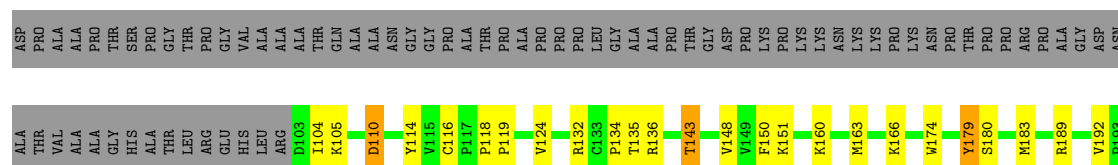
• Molecule 1: Envelope glycoprotein B

Chain C:



• Molecule 1: Envelope glycoprotein B

Chain D:



T690	A595	PRO	PRO	L399	D285	F194
E693	C596	PRO	PRO	T400	D286	E195
I694	Y597	PRO	PRO	E401	E287	E196
	S598	GLY	GLY	Y402	V288	F197
L700	B599	ALA	ALA	P403		I198
	B600	SER	SER	L404	D283	T201
D720	L601	ALA	ALA	S405	F294	R202
	V602	ASN	ASN	R406	V295	A203
H724	S603	ALA	ALA	Y407	Y296	K204
ALA	F604	SER	SER	D408		
ASP	B605	VAL	VAL	L409	F300	C207
ALA	V606	GLU	GLU	R418	Y303	
ASN	B607	R494	R494	D419	R304	Y213
ALA	D608	I501	I501	A420	E305	V214
ALA	Q609	E502	E502		G306	R215
	L612	L506	L506	I424	S307	H224
	V613			F425	H308	R225
	Q616			A426	T309	
	B619	L521	L521	Y429	E310	T230
		R523	R523	N430	H311	E233
		L531	L531	A431	T312	L234
	E622			T432	S313	K235
	L623			H433	F319	P236
		E535	E535	I434	K320	A237
	R627			Q440	Q321	
	P632	N540	N540	Y441	R328	S244
	O633	R543	R543		D329	R245
	T634	N548	N548	A444	L330	G246
	H637			N445	T331	V247
	R638	S552	S552	F448	T340	H248
	R639	V553	V553	L449		
	Y640	T554	T554	T450	N343	D251
	P641	V555	V555	A451	L344	L252
	T642	G556	G556	L455	L345	K253
	F643	R557	R557	L456	T346	Y254
	Q646	R558	R558		T347	R255
		S560	S560	L460	P348	P256
	Y649	A561	A561	A461	R258	S257
				E462	VAL	
		V567	V567	L463	GLU	
		M568	M568	Y464	T351	A261
				V465	W356	F262
		S571	S571	R466	K359	H263
		T572	T572	E467		R264
				H468		Y265
		D579	D579	L469	K368	G266
		N580	N580	R470	W369	T267
		V581	V581	E471		T268
		I582	I582		R377	V269
					S378	N270
						C271
		S586	S586	R474		T272
	B587	M587	M587		S392	V273
	V688	R588	R588	N478	T393	E274
	Y689	I589	I589	PRO		
				THR	Y396	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.

All (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
1:B:471:GLU:OE1	1:B:474:ARG:NH1	2.20	0.75
1:C:304:ARG:NH1	1:C:341:THR:OG1	2.20	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:105:LYS:HG2	1:D:582:ILE:HG12	1.69	0.74
1:A:648:VAL:HA	1:A:658:GLN:HA	1.69	0.74
1:B:548:ASN:OD1	1:B:561:ALA:N	2.20	0.74
1:D:599:ARG:O	1:D:616:GLN:NE2	2.21	0.74
1:B:601:LEU:HB3	1:B:627:ARG:HE	1.51	0.73
1:B:637:HIS:CE1	1:B:653:TYR:H	2.05	0.73
1:C:207:CYS:O	1:C:232:MET:N	2.15	0.73
1:C:346:THR:HA	1:C:351:THR:HA	1.70	0.72
1:C:596:CYS:SG	1:C:633:CYS:N	2.62	0.72
1:D:110:ASP:N	1:D:110:ASP:OD1	2.18	0.71
1:D:607:GLU:OE1	1:D:609:GLN:NE2	2.24	0.71
1:A:468:HIS:NE2	1:A:472:GLN:OE1	2.25	0.70
1:A:112:ASN:N	1:A:112:ASN:OD1	2.25	0.70
1:B:595:ALA:HA	1:B:632:PRO:HA	1.73	0.70
1:A:360:ARG:NH2	1:A:411:ASP:OD1	2.23	0.70
1:C:595:ALA:HA	1:C:632:PRO:HA	1.73	0.69
1:B:585:ASN:N	1:B:585:ASN:OD1	2.25	0.69
1:D:136:ARG:HH12	1:D:523:ARG:HH21	1.38	0.69
1:C:690:THR:HG22	1:C:692:HIS:H	1.58	0.69
1:D:432:THR:HB	1:D:433:HIS:CE1	2.28	0.69
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.75	0.69
1:B:250:THR:O	1:B:270:ASN:ND2	2.26	0.68
1:A:172:GLN:HG3	1:A:183:MET:HB2	1.75	0.68
1:C:406:ARG:O	1:C:493:GLU:N	2.25	0.68
1:B:638:ARG:O	1:B:639:ARG:NE	2.26	0.68
1:D:119:PRO:HA	1:D:571:SER:HB3	1.77	0.67
1:A:391:ILE:HG13	1:A:393:THR:HG23	1.77	0.67
1:B:105:LYS:HG2	1:B:582:ILE:HG12	1.77	0.66
1:C:634:THR:N	1:C:653:TYR:OH	2.25	0.66
1:D:638:ARG:O	1:D:639:ARG:NE	2.27	0.66
1:B:639:ARG:HB3	1:B:641:PHE:CE2	2.30	0.66
1:B:585:ASN:HA	1:B:655:TYR:HB3	1.77	0.66
1:B:463:LEU:O	1:B:467:GLU:N	2.28	0.66
1:A:599:ARG:NH1	1:A:618:GLY:O	2.29	0.66
1:B:163:MET:HB2	1:B:274:GLU:HB2	1.78	0.66
1:D:253:LYS:HA	1:D:268:THR:HG21	1.78	0.65
1:C:342:ARG:NH1	1:C:355:ASP:OD1	2.30	0.65
1:D:637:HIS:HB3	1:D:652:GLU:HA	1.79	0.65
1:B:601:LEU:HB2	1:B:627:ARG:HH21	1.61	0.65
1:B:256:PRO:HD3	1:B:266:GLY:HA3	1.78	0.65
1:D:463:LEU:O	1:D:467:GLU:N	2.21	0.65
1:C:690:THR:HB	1:C:693:GLU:HG3	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:213:TYR:CE2	1:C:215:ARG:HB2	2.32	0.64
1:A:110:ASP:N	1:A:110:ASP:OD1	2.31	0.64
1:A:718:ASP:OD1	1:A:721:THR:N	2.30	0.64
1:C:614:GLU:HB3	1:C:627:ARG:NH2	2.11	0.64
1:A:285:ASP:HB2	1:A:311:HIS:HB3	1.80	0.64
1:A:206:VAL:HG12	1:A:233:GLU:HA	1.80	0.64
1:C:711:LEU:HD23	1:C:714:LEU:HD12	1.80	0.63
1:B:557:ARG:HG3	1:B:559:VAL:HG13	1.79	0.63
1:A:377:ARG:HD3	1:A:386:PHE:CZ	2.32	0.63
1:C:432:THR:HG22	1:C:433:HIS:ND1	2.14	0.63
1:D:461:ALA:O	1:D:464:TYR:N	2.24	0.63
1:B:518:ASN:O	1:B:522:GLY:N	2.32	0.62
1:C:206:VAL:HG12	1:C:233:GLU:HA	1.80	0.62
1:B:616:GLN:HG2	1:B:627:ARG:HA	1.81	0.62
1:D:660:SER:O	1:D:663:ASP:N	2.32	0.62
1:B:144:GLU:HA	1:B:376:LEU:HD23	1.82	0.62
1:A:373:ASP:OD2	1:A:428:ARG:NH1	2.33	0.62
1:C:322:VAL:HG12	1:C:325:PHE:HB2	1.81	0.61
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.01	0.61
1:B:605:ARG:HH11	1:B:612:LEU:HD21	1.65	0.61
1:A:431:ALA:O	1:A:458:ASN:ND2	2.34	0.60
1:B:121:GLY:HA2	1:B:569:ALA:HB1	1.83	0.60
1:A:467:GLU:O	1:A:471:GLU:HG2	2.01	0.60
1:C:436:VAL:HB	1:C:454:PRO:HB2	1.83	0.60
1:D:461:ALA:O	1:D:463:LEU:N	2.34	0.60
1:D:189:ARG:NH2	1:D:293:ASP:OD2	2.35	0.60
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.83	0.60
1:B:637:HIS:CD2	1:B:639:ARG:HG2	2.37	0.60
1:A:259:VAL:HG12	1:A:264:ARG:HE	1.66	0.60
1:B:555:VAL:HG23	1:B:557:ARG:H	1.65	0.60
1:D:557:ARG:HH21	1:D:572:THR:HB	1.66	0.59
1:D:589:ILE:HG13	1:D:596:CYS:HA	1.85	0.59
1:A:456:LEU:HD21	1:A:463:LEU:HB2	1.85	0.59
1:D:248:HIS:HA	1:D:271:CYS:O	2.03	0.59
1:A:604:PHE:HE1	1:A:606:TYR:HE2	1.49	0.59
1:B:456:LEU:HD21	1:B:463:LEU:HB2	1.83	0.59
1:D:150:PHE:HB2	1:D:449:LEU:HB3	1.84	0.59
1:A:256:PRO:HB2	1:A:264:ARG:HG3	1.83	0.59
1:C:143:THR:HG21	1:C:377:ARG:HH21	1.68	0.59
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.84	0.59
1:A:248:HIS:HE1	1:A:251:ASP:HB3	1.68	0.59
1:B:105:LYS:HA	1:B:582:ILE:HA	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:428:ARG:HB3	1:C:429:TYR:CD1	2.38	0.59
1:C:166:LYS:N	1:C:190:ALA:O	2.35	0.59
1:D:471:GLU:OE2	1:D:474:ARG:NH1	2.36	0.59
1:B:587:MET:HB3	1:B:653:TYR:CD2	2.34	0.58
1:C:195:GLU:N	1:C:195:GLU:OE1	2.36	0.58
1:B:397:THR:HG22	1:B:444:ALA:HA	1.85	0.58
1:B:172:GLN:HG2	1:B:183:MET:HB2	1.84	0.58
1:D:163:MET:O	1:D:273:VAL:HA	2.03	0.58
1:C:598:SER:N	1:C:629:ALA:O	2.35	0.58
1:A:583:VAL:HA	1:A:602:VAL:HG12	1.86	0.58
1:B:104:ILE:O	1:B:583:VAL:N	2.34	0.58
1:C:366:MET:HE1	1:C:495:ILE:HB	1.86	0.58
1:A:224:HIS:HB2	1:A:269:VAL:HB	1.84	0.58
1:D:124:VAL:HB	1:D:567:VAL:HG12	1.86	0.58
1:D:166:LYS:HE3	1:D:192:VAL:HG22	1.84	0.58
1:D:603:SER:HA	1:D:613:VAL:O	2.04	0.57
1:C:596:CYS:O	1:C:631:GLU:N	2.31	0.57
1:B:583:VAL:HA	1:B:602:VAL:HG12	1.86	0.57
1:B:113:PHE:O	1:B:576:VAL:N	2.30	0.57
1:C:343:ASN:OD1	1:C:356:TRP:HB2	2.04	0.57
1:C:637:HIS:CG	1:C:653:TYR:HH	2.20	0.57
1:B:663:ASP:OD1	1:B:663:ASP:N	2.36	0.57
1:A:106:ALA:HA	1:A:658:GLN:HE22	1.70	0.57
1:B:614:GLU:HB3	1:B:627:ARG:NH1	2.19	0.57
1:B:248:HIS:HB2	1:B:270:ASN:OD1	2.05	0.57
1:C:589:ILE:HG22	1:C:591:SER:H	1.68	0.57
1:C:543:ARG:HB2	1:C:568:MET:HE1	1.86	0.57
1:D:306:GLY:O	1:D:309:THR:N	2.34	0.56
1:B:115:VAL:HG22	1:B:623:LEU:HB2	1.87	0.56
1:B:614:GLU:HB3	1:B:627:ARG:HH12	1.69	0.56
1:B:514:GLN:HG3	1:B:515:ARG:N	2.21	0.56
1:D:195:GLU:CD	1:D:195:GLU:H	2.09	0.56
1:B:375:MET:SD	1:B:386:PHE:HB3	2.46	0.56
1:B:150:PHE:HB2	1:B:449:LEU:HB3	1.86	0.56
1:C:638:ARG:HG2	1:C:649:TYR:HE1	1.71	0.56
1:B:444:ALA:HB3	1:B:448:PHE:HB2	1.88	0.56
1:C:420:ALA:HA	1:C:423:ARG:HH12	1.70	0.56
1:C:651:GLU:N	1:C:654:ALA:O	2.39	0.56
1:C:285:ASP:HB2	1:C:311:HIS:HB3	1.87	0.56
1:B:460:LEU:HB3	1:B:463:LEU:HD13	1.87	0.56
1:B:431:ALA:O	1:B:458:ASN:ND2	2.39	0.56
1:C:140:GLN:OE1	1:C:141:ASN:N	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ARG:HD3	1:B:254:TYR:CD1	2.41	0.56
1:A:382:GLY:HA2	1:A:399:LEU:HD11	1.86	0.55
1:A:223:PHE:HB2	1:A:226:ASP:HA	1.88	0.55
1:D:311:HIS:HE2	1:D:313:SER:HG	1.46	0.55
1:C:382:GLY:O	1:C:399:LEU:HG	2.06	0.55
1:C:634:THR:O	1:C:637:HIS:HB2	2.07	0.55
1:C:280:SER:HB2	1:C:287:PHE:HB3	1.87	0.55
1:B:599:ARG:HH12	1:B:619:GLU:CD	2.10	0.55
1:C:119:PRO:HG2	1:C:562:ARG:HB2	1.89	0.55
1:A:638:ARG:HH11	1:A:638:ARG:HB2	1.71	0.55
1:C:215:ARG:NH2	1:C:349:LYS:HD3	2.22	0.55
1:C:124:VAL:HA	1:C:569:ALA:HA	1.89	0.55
1:C:637:HIS:CE1	1:C:653:TYR:HH	2.24	0.54
1:D:425:PHE:HZ	1:D:434:ILE:HG12	1.72	0.54
1:B:282:TYR:HE2	1:B:409:LEU:HD12	1.72	0.54
1:D:463:LEU:HB3	1:D:467:GLU:HG2	1.88	0.54
1:D:347:THR:N	1:D:350:PHE:O	2.40	0.54
1:B:152:GLU:HG2	1:B:497:THR:H	1.72	0.54
1:D:460:LEU:HB3	1:D:463:LEU:HD12	1.88	0.54
1:A:175:PHE:CZ	1:A:258:ARG:HA	2.43	0.54
1:C:256:PRO:HG3	1:C:265:TYR:C	2.28	0.54
1:D:425:PHE:CD1	1:D:429:TYR:HB2	2.42	0.54
1:D:105:LYS:HE2	1:D:582:ILE:HD11	1.88	0.54
1:A:377:ARG:HD2	1:A:384:PHE:CG	2.43	0.54
1:C:603:SER:OG	1:C:614:GLU:HA	2.08	0.53
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.90	0.53
1:B:145:GLY:HA3	1:B:452:TYR:OH	2.07	0.53
1:B:587:MET:HG3	1:B:600:PRO:HA	1.90	0.53
1:C:594:GLY:O	1:C:633:CYS:HB2	2.08	0.53
1:D:597:TYR:CE2	1:D:601:LEU:HD21	2.43	0.53
1:A:196:GLU:HG3	1:A:200:LYS:HG3	1.89	0.53
1:A:200:LYS:O	1:A:204:LYS:N	2.28	0.53
1:C:509:THR:O	1:C:513:ILE:HG13	2.09	0.53
1:D:311:HIS:NE2	1:D:313:SER:OG	2.39	0.53
1:C:171:SER:HB2	1:C:182:PHE:HE1	1.74	0.53
1:C:512:HIS:HA	1:C:515:ARG:NH1	2.24	0.53
1:B:374:GLU:OE2	1:B:428:ARG:NH2	2.42	0.53
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.24	0.53
1:A:559:VAL:HG12	1:A:572:THR:HA	1.90	0.53
1:D:285:ASP:N	1:D:285:ASP:OD1	2.37	0.52
1:B:253:LYS:HA	1:B:268:THR:HG21	1.91	0.52
1:A:248:HIS:CE1	1:A:251:ASP:HB3	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:366:MET:CE	1:C:495:ILE:HB	2.40	0.52
1:D:425:PHE:HD1	1:D:429:TYR:HB2	1.73	0.52
1:A:237:ALA:HA	1:A:248:HIS:CD2	2.44	0.52
1:A:123:THR:HB	1:A:570:VAL:O	2.10	0.52
1:C:391:ILE:HG13	1:C:393:THR:HG23	1.90	0.52
1:A:429:TYR:HA	1:A:432:THR:OG1	2.09	0.52
1:C:171:SER:HB2	1:C:182:PHE:CE1	2.45	0.52
1:B:597:TYR:CE2	1:B:601:LEU:HD21	2.45	0.52
1:D:456:LEU:HD11	1:D:460:LEU:HB2	1.91	0.52
1:B:601:LEU:HA	1:B:616:GLN:HA	1.91	0.52
1:C:164:TYR:HB2	1:C:351:THR:HG22	1.92	0.52
1:A:562:ARG:O	1:A:569:ALA:N	2.41	0.52
1:B:225:ARG:HA	1:B:254:TYR:CG	2.45	0.51
1:C:202:ASN:HD21	1:C:327:ALA:HA	1.75	0.51
1:D:235:LYS:NZ	1:D:251:ASP:OD1	2.42	0.51
1:C:224:HIS:CE1	1:C:225:ARG:HG3	2.45	0.51
1:B:174:TRP:HB2	1:B:263:HIS:ND1	2.26	0.51
1:D:189:ARG:HB2	1:D:349:LYS:HD2	1.93	0.51
1:A:286:GLU:HA	1:A:297:MET:O	2.11	0.51
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.92	0.51
1:A:377:ARG:HD2	1:A:384:PHE:CD1	2.46	0.51
1:A:540:ASN:O	1:A:543:ARG:HB3	2.11	0.51
1:A:595:ALA:HA	1:A:632:PRO:HA	1.92	0.51
1:B:113:PHE:O	1:B:575:PRO:HA	2.10	0.50
1:D:690:THR:O	1:D:694:ILE:HG13	2.11	0.50
1:A:166:LYS:HE3	1:A:271:CYS:SG	2.51	0.50
1:A:377:ARG:HB2	1:A:386:PHE:CD2	2.46	0.50
1:D:204:LYS:O	1:D:328:ARG:NH1	2.44	0.50
1:D:586:SER:OG	1:D:588:ARG:HG3	2.11	0.50
1:D:401:GLU:HG3	1:D:441:TYR:O	2.11	0.50
1:C:440:GLN:HG2	1:C:452:TYR:O	2.11	0.50
1:A:245:ARG:NH2	1:A:275:GLU:OE1	2.44	0.50
1:D:256:PRO:HD3	1:D:266:GLY:HA3	1.94	0.50
1:D:595:ALA:HA	1:D:632:PRO:HA	1.94	0.50
1:C:428:ARG:HB3	1:C:429:TYR:HD1	1.76	0.50
1:D:399:LEU:O	1:D:474:ARG:HG2	2.12	0.50
1:B:166:LYS:HA	1:B:271:CYS:HA	1.93	0.50
1:B:462:GLU:H	1:B:462:GLU:CD	2.14	0.50
1:C:164:TYR:HD2	1:C:273:VAL:HG22	1.76	0.50
1:C:326:TYR:CZ	1:C:339:PRO:HB3	2.47	0.50
1:B:558:ARG:NH1	1:B:620:ASN:HB3	2.27	0.50
1:B:317:ASP:OD1	1:B:317:ASP:N	2.39	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:580:ASN:HB3	1:B:605:ARG:O	2.11	0.49
1:B:580:ASN:HD21	1:B:608:ASP:HA	1.77	0.49
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.77	0.49
1:B:585:ASN:O	1:B:654:ALA:HA	2.12	0.49
1:B:176:GLY:N	1:B:179:TYR:O	2.40	0.49
1:A:107:GLU:H	1:A:658:GLN:NE2	2.10	0.49
1:D:124:VAL:HB	1:D:567:VAL:CG1	2.42	0.49
1:C:123:THR:O	1:C:570:VAL:N	2.31	0.49
1:B:552:SER:HA	1:B:559:VAL:HG22	1.95	0.49
1:A:440:GLN:NE2	1:A:442:TYR:OH	2.44	0.49
1:C:502:GLU:HG3	1:C:503:PHE:N	2.28	0.49
1:D:148:VAL:HB	1:D:451:ALA:HB3	1.95	0.49
1:B:638:ARG:HB3	1:B:649:TYR:HE1	1.77	0.49
1:A:257:SER:O	1:A:264:ARG:NH2	2.46	0.49
1:B:587:MET:N	1:B:653:TYR:O	2.45	0.49
1:B:408:ASP:O	1:B:410:GLY:N	2.46	0.49
1:D:114:TYR:O	1:D:623:LEU:N	2.40	0.49
1:A:280:SER:HB2	1:A:287:PHE:CB	2.43	0.49
1:D:237:ALA:N	1:D:246:GLY:O	2.41	0.49
1:B:640:TYR:HA	1:B:648:VAL:O	2.13	0.49
1:D:174:TRP:HB2	1:D:263:HIS:CE1	2.47	0.49
1:A:388:SER:OG	1:A:391:ILE:HG12	2.13	0.49
1:B:628:ASP:OD1	1:B:628:ASP:N	2.46	0.48
1:C:464:TYR:CE2	1:C:468:HIS:HD2	2.31	0.48
1:C:420:ALA:HA	1:C:423:ARG:NH1	2.27	0.48
1:C:318:ARG:HD3	1:C:346:THR:O	2.14	0.48
1:C:145:GLY:HA3	1:C:452:TYR:CZ	2.47	0.48
1:C:621:ASN:HD22	1:C:621:ASN:N	2.11	0.48
1:A:382:GLY:O	1:A:399:LEU:HG	2.13	0.48
1:B:418:ARG:O	1:B:422:ASP:N	2.45	0.48
1:A:433:HIS:CD2	1:A:457:SER:HA	2.48	0.48
1:C:584:GLN:N	1:C:601:LEU:O	2.47	0.48
1:C:402:TYR:N	1:C:441:TYR:O	2.41	0.48
1:B:443:LEU:O	3:B:801:NAG:H81	2.13	0.48
1:B:678:LEU:HD12	1:B:679:GLU:H	1.76	0.48
1:B:435:LYS:HD2	1:B:453:GLN:OE1	2.14	0.48
1:B:103:ASP:N	1:B:103:ASP:OD1	2.46	0.48
1:D:548:ASN:OD1	1:D:561:ALA:N	2.31	0.48
1:D:136:ARG:HH12	1:D:523:ARG:NH2	2.11	0.47
1:A:145:GLY:HA3	1:A:452:TYR:CE1	2.49	0.47
1:A:143:THR:O	1:A:452:TYR:OH	2.32	0.47
1:B:119:PRO:HA	1:B:571:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:402:TYR:HA	1:D:403:PRO:HD3	1.71	0.47
1:D:464:TYR:HE1	1:D:468:HIS:ND1	2.11	0.47
1:C:345:LEU:O	1:C:352:VAL:N	2.46	0.47
1:D:579:ASP:OD1	1:D:580:ASN:N	2.47	0.47
1:A:420:ALA:HA	1:A:423:ARG:NH1	2.29	0.47
1:C:638:ARG:O	1:C:639:ARG:HG2	2.14	0.47
1:A:551:ALA:HB2	1:A:568:MET:HE3	1.96	0.47
1:A:215:ARG:NH2	1:A:349:LYS:HD3	2.29	0.47
1:D:196:GLU:O	1:D:201:ILE:HG13	2.14	0.47
1:B:533:ASN:O	1:B:536:LEU:HB3	2.15	0.47
1:C:168:VAL:O	1:C:187:GLU:HA	2.15	0.47
1:C:304:ARG:NH2	1:C:323:ASP:OD1	2.47	0.47
1:C:200:LYS:HE3	1:C:208:ARG:HH21	1.79	0.47
1:B:624:ARG:NH2	1:B:628:ASP:OD1	2.45	0.47
1:C:637:HIS:CG	1:C:653:TYR:CZ	3.03	0.47
1:B:304:ARG:O	1:B:307:SER:OG	2.22	0.47
1:A:385:ARG:HH11	1:A:385:ARG:HG2	1.79	0.47
1:C:197:VAL:HA	1:C:201:ILE:HD12	1.97	0.47
1:C:215:ARG:HH22	1:C:349:LYS:HD3	1.80	0.47
1:B:377:ARG:NH1	1:B:440:GLN:OE1	2.45	0.47
1:C:440:GLN:N	1:C:452:TYR:O	2.46	0.47
1:B:236:PRO:HA	1:B:247:TRP:CD1	2.50	0.47
1:A:634:THR:N	1:A:653:TYR:OH	2.28	0.47
1:C:647:TYR:O	1:C:658:GLN:HG3	2.15	0.47
1:B:144:GLU:HA	1:B:376:LEU:CD2	2.44	0.47
1:A:453:GLN:NE2	1:A:454:PRO:O	2.47	0.47
1:A:378:SER:O	1:A:385:ARG:N	2.45	0.47
1:B:156:PRO:HG2	1:B:279:ARG:NH2	2.29	0.47
1:D:568:MET:HE2	1:D:568:MET:HB2	1.65	0.47
1:C:659:LEU:HD12	1:C:663:ASP:HB2	1.97	0.47
1:B:143:THR:HB	1:B:377:ARG:HB2	1.97	0.46
1:B:145:GLY:HA2	1:B:455:LEU:HD11	1.97	0.46
1:A:378:SER:HB3	1:A:385:ARG:NH2	2.30	0.46
1:D:688:VAL:HG12	1:D:689:TYR:CD2	2.50	0.46
1:B:603:SER:HA	1:B:613:VAL:O	2.15	0.46
1:A:379:GLU:HB2	1:A:384:PHE:CE1	2.50	0.46
1:C:440:GLN:O	1:C:452:TYR:N	2.40	0.46
1:A:147:ALA:HA	1:A:451:ALA:O	2.16	0.46
1:D:444:ALA:HB3	1:D:448:PHE:HB2	1.97	0.46
1:B:664:ILE:HG22	1:B:665:THR:O	2.14	0.46
1:C:606:TYR:CD1	1:C:606:TYR:N	2.83	0.46
1:D:540:ASN:O	1:D:543:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:572:THR:HG22	1:C:573:CYS:H	1.80	0.46
1:B:215:ARG:NH2	1:B:348:PRO:O	2.47	0.46
1:B:194:PHE:CD2	1:B:320:LYS:HE3	2.50	0.46
1:C:110:ASP:OD1	1:C:110:ASP:N	2.48	0.46
1:D:639:ARG:O	1:D:649:TYR:HD1	1.99	0.46
1:C:215:ARG:HD3	1:C:215:ARG:HA	1.79	0.46
1:A:436:VAL:HG12	1:A:471:GLU:HG3	1.96	0.46
1:A:550:ILE:O	1:A:553:VAL:HG12	2.16	0.46
1:D:643:PHE:N	1:D:646:GLY:O	2.45	0.46
1:A:328:ARG:HH12	1:A:333:LYS:HB3	1.81	0.46
1:C:633:CYS:HA	1:C:653:TYR:CZ	2.51	0.46
1:C:342:ARG:NH2	1:C:354:TRP:HA	2.30	0.46
1:D:552:SER:HA	1:D:559:VAL:HG22	1.96	0.46
1:C:377:ARG:HD2	1:C:384:PHE:CG	2.50	0.46
1:C:360:ARG:NE	1:C:411:ASP:OD1	2.27	0.46
1:C:172:GLN:HG2	1:C:183:MET:HB2	1.98	0.46
1:B:471:GLU:HA	1:B:474:ARG:NH1	2.31	0.46
1:B:358:PRO:HG2	1:B:361:PRO:HG2	1.96	0.46
1:D:286:GLU:HB2	1:D:296:TYR:HA	1.96	0.46
1:D:616:GLN:HB2	1:D:627:ARG:HA	1.97	0.46
1:B:163:MET:O	1:B:273:VAL:HA	2.16	0.46
1:B:580:ASN:O	1:B:604:PHE:HB2	2.16	0.46
1:D:555:VAL:HG12	1:D:557:ARG:H	1.81	0.46
1:C:280:SER:HB2	1:C:287:PHE:CB	2.46	0.46
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.97	0.46
1:D:213:TYR:CE2	1:D:215:ARG:HB2	2.51	0.46
1:D:345:LEU:O	1:D:351:THR:HA	2.15	0.46
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.98	0.46
1:D:639:ARG:HB3	1:D:641:PHE:CE2	2.51	0.45
1:C:325:PHE:HB3	1:C:340:THR:O	2.17	0.45
1:C:302:GLY:HA3	1:C:321:GLN:NE2	2.31	0.45
1:A:440:GLN:HB2	1:A:442:TYR:CE1	2.51	0.45
1:A:633:CYS:HA	1:A:653:TYR:CZ	2.52	0.45
1:B:420:ALA:O	1:B:424:ILE:N	2.38	0.45
1:D:445:ASN:OD1	3:D:801:NAG:H82	2.17	0.45
1:A:501:ILE:HD12	1:A:501:ILE:HA	1.80	0.45
1:B:547:PRO:HB2	1:B:561:ALA:O	2.15	0.45
1:C:467:GLU:O	1:C:471:GLU:HG2	2.16	0.45
1:C:179:TYR:O	1:C:258:ARG:NH2	2.50	0.45
1:D:179:TYR:HD1	1:D:180:SER:N	2.15	0.45
1:A:225:ARG:HD2	1:A:254:TYR:CD1	2.51	0.45
1:C:208:ARG:NH1	1:C:229:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ILE:HD11	1:B:207:CYS:SG	2.56	0.45
1:A:449:LEU:HA	1:A:449:LEU:HD12	1.67	0.45
1:B:432:THR:HB	1:B:433:HIS:CD2	2.51	0.45
1:B:162:THR:HB	1:B:164:TYR:CZ	2.51	0.45
1:A:466:ARG:HH12	1:A:470:ARG:HD3	1.81	0.45
1:A:520:MET:O	1:A:524:VAL:HG23	2.17	0.45
1:D:404:LEU:HD12	1:D:404:LEU:HA	1.75	0.45
1:D:307:SER:HA	1:D:310:GLU:HG2	1.99	0.45
1:A:596:CYS:O	1:A:631:GLU:N	2.40	0.45
1:C:444:ALA:HB2	1:C:450:ILE:HD11	1.97	0.45
1:C:583:VAL:HA	1:C:602:VAL:HG12	1.99	0.45
1:C:436:VAL:HA	1:C:464:TYR:CE1	2.51	0.45
1:C:314:TYR:CD1	1:C:345:LEU:HD11	2.51	0.45
1:A:706:GLN:OE1	1:A:710:GLN:NE2	2.35	0.45
1:B:461:ALA:O	1:B:464:TYR:N	2.50	0.45
1:B:238:ASN:N	1:B:238:ASN:OD1	2.49	0.45
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.83	0.45
1:C:113:PHE:HB2	1:C:576:VAL:HB	1.98	0.45
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.83	0.45
1:B:660:SER:H	1:B:663:ASP:CG	2.20	0.45
1:A:443:LEU:HD11	1:A:447:GLY:HA2	1.98	0.45
1:B:616:GLN:HG2	1:B:627:ARG:HG3	1.98	0.44
1:B:166:LYS:HE3	1:B:207:CYS:SG	2.57	0.44
1:B:509:THR:O	1:B:513:ILE:HG13	2.17	0.44
1:A:377:ARG:HD2	1:A:384:PHE:CD2	2.52	0.44
1:D:449:LEU:HD12	1:D:449:LEU:HA	1.76	0.44
1:C:560:SER:N	1:C:571:SER:O	2.50	0.44
1:B:601:LEU:HD23	1:B:627:ARG:HG2	1.99	0.44
1:C:537:THR:O	1:C:540:ASN:HB2	2.18	0.44
1:D:254:TYR:HB3	1:D:267:THR:O	2.17	0.44
1:C:213:TYR:HE2	1:C:215:ARG:HB2	1.76	0.44
1:B:580:ASN:ND2	1:B:608:ASP:OD1	2.48	0.44
1:C:371:GLU:OE1	1:C:423:ARG:NH2	2.50	0.44
1:D:690:THR:OG1	1:D:693:GLU:HG3	2.18	0.44
1:C:175:PHE:CE2	1:C:258:ARG:HA	2.53	0.44
1:D:225:ARG:HH11	1:D:254:TYR:HD2	1.65	0.44
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.81	0.44
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.98	0.44
1:A:588:ARG:HH21	1:A:633:CYS:HB3	1.81	0.44
1:A:430:ASN:OD1	1:A:430:ASN:N	2.50	0.44
1:B:386:PHE:O	1:B:394:THR:HA	2.18	0.44
1:D:425:PHE:CZ	1:D:430:ASN:HA	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:202:ASN:OD1	1:C:328:ARG:N	2.39	0.44
1:C:360:ARG:HB3	1:C:411:ASP:OD2	2.17	0.44
1:C:303:TYR:CE2	1:C:321:GLN:HB2	2.53	0.44
1:B:464:TYR:O	1:B:468:HIS:ND1	2.44	0.44
1:B:195:GLU:OE1	1:B:196:GLU:N	2.51	0.44
1:C:305:GLU:HB3	1:C:306:GLY:H	1.60	0.44
1:A:436:VAL:O	1:A:454:PRO:HG2	2.18	0.44
1:D:246:GLY:HA2	1:D:273:VAL:O	2.18	0.44
1:B:425:PHE:HZ	1:B:434:ILE:HG13	1.83	0.44
1:A:359:LYS:O	1:A:362:SER:N	2.49	0.44
1:C:207:CYS:SG	1:C:208:ARG:N	2.91	0.44
1:B:558:ARG:HH12	1:B:620:ASN:HB3	1.83	0.44
1:A:442:TYR:O	1:A:450:ILE:N	2.40	0.44
1:D:300:PHE:O	1:D:356:TRP:NE1	2.39	0.44
1:D:282:TYR:OH	1:D:408:ASP:OD2	2.26	0.44
1:C:332:THR:C	1:C:334:ALA:H	2.21	0.44
1:A:325:PHE:O	1:A:339:PRO:HA	2.18	0.44
1:A:375:MET:SD	1:A:386:PHE:HB3	2.57	0.44
1:D:403:PRO:HG2	1:D:406:ARG:CZ	2.48	0.44
1:C:616:GLN:O	1:C:624:ARG:N	2.50	0.44
1:D:471:GLU:CD	1:D:474:ARG:HH11	2.20	0.43
1:D:580:ASN:OD1	1:D:608:ASP:HA	2.18	0.43
1:B:233:GLU:HG2	1:B:234:LEU:H	1.83	0.43
1:C:402:TYR:OH	1:C:406:ARG:HD2	2.18	0.43
1:C:144:GLU:CD	1:C:433:HIS:HE2	2.20	0.43
1:A:218:LEU:HD12	1:A:219:GLU:N	2.33	0.43
1:B:596:CYS:HB2	1:B:633:CYS:HB3	1.60	0.43
1:D:143:THR:OG1	1:D:377:ARG:NH2	2.49	0.43
1:C:164:TYR:CD2	1:C:273:VAL:HG22	2.52	0.43
1:A:468:HIS:O	1:A:472:GLN:HG3	2.17	0.43
1:C:155:ALA:HB1	1:C:158:LYS:NZ	2.33	0.43
1:C:123:THR:HB	1:C:570:VAL:O	2.19	0.43
1:B:461:ALA:O	1:B:464:TYR:HB3	2.18	0.43
1:C:194:PHE:CD1	1:C:320:LYS:HG3	2.54	0.43
1:A:618:GLY:N	1:A:622:GLU:O	2.51	0.43
1:C:427:ARG:HG3	1:C:428:ARG:N	2.34	0.43
1:B:304:ARG:HD2	1:B:356:TRP:CZ3	2.53	0.43
1:D:151:LYS:HD3	1:D:369:TRP:CD1	2.53	0.43
1:C:248:HIS:ND1	1:C:250:THR:O	2.52	0.43
1:B:152:GLU:HA	1:B:366:MET:SD	2.59	0.43
1:D:502:GLU:O	1:D:506:LEU:N	2.50	0.43
1:B:149:VAL:HB	1:B:370:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:278:ALA:HA	1:B:288:VAL:O	2.18	0.43
1:D:580:ASN:HB3	1:D:605:ARG:O	2.18	0.43
1:C:606:TYR:HE1	1:C:613:VAL:HB	1.84	0.43
1:A:466:ARG:NH1	1:A:470:ARG:HD3	2.33	0.43
1:C:449:LEU:HD12	1:C:449:LEU:HA	1.80	0.43
1:B:443:LEU:HD12	1:B:448:PHE:O	2.18	0.43
1:C:169:THR:HA	1:C:186:PHE:O	2.18	0.43
1:C:434:ILE:N	1:C:456:LEU:O	2.50	0.43
1:D:288:VAL:HG12	1:D:294:PHE:HA	2.01	0.43
1:B:456:LEU:HB2	1:B:467:GLU:OE1	2.19	0.43
1:C:425:PHE:O	1:C:429:TYR:N	2.48	0.43
1:B:145:GLY:O	1:B:374:GLU:HA	2.19	0.43
1:D:174:TRP:HB2	1:D:263:HIS:ND1	2.34	0.43
1:B:391:ILE:HG13	1:B:393:THR:OG1	2.19	0.43
1:D:531:LEU:O	1:D:535:GLU:HG2	2.19	0.43
1:C:377:ARG:HD2	1:C:384:PHE:CD1	2.53	0.42
1:B:104:ILE:HG12	1:B:104:ILE:H	1.57	0.42
1:B:452:TYR:O	1:B:454:PRO:HD3	2.19	0.42
1:A:343:ASN:O	1:A:353:ALA:HA	2.20	0.42
1:D:319:PHE:HE1	1:D:343:ASN:HB3	1.83	0.42
1:C:304:ARG:O	1:C:307:SER:OG	2.25	0.42
1:C:144:GLU:OE2	1:C:433:HIS:NE2	2.38	0.42
1:D:605:ARG:CZ	1:D:612:LEU:HD21	2.49	0.42
1:A:306:GLY:O	1:A:309:THR:OG1	2.37	0.42
1:D:329:ASP:OD1	1:D:331:THR:N	2.39	0.42
1:A:515:ARG:CG	1:A:515:ARG:HH11	2.31	0.42
1:A:297:MET:HG2	1:A:298:SER:O	2.18	0.42
1:B:393:THR:HG22	1:B:504:PRO:HB2	2.01	0.42
1:B:621:ASN:OD1	1:B:644:GLY:N	2.34	0.42
1:B:168:VAL:HG22	1:B:269:VAL:HG22	2.01	0.42
1:D:303:TYR:N	1:D:321:GLN:OE1	2.43	0.42
1:A:119:PRO:HB3	1:A:571:SER:N	2.34	0.42
1:D:700:LEU:HA	1:D:700:LEU:HD23	1.88	0.42
1:D:359:LYS:HE2	1:D:409:LEU:HD21	2.01	0.42
1:D:136:ARG:HB3	1:D:136:ARG:HE	1.68	0.42
1:A:191:PRO:HA	1:A:350:PHE:HA	2.02	0.42
1:D:673:LEU:HA	1:D:673:LEU:HD12	1.80	0.42
1:B:401:GLU:HG2	1:B:402:TYR:H	1.85	0.42
1:C:394:THR:N	1:C:504:PRO:O	2.47	0.42
1:A:405:SER:O	1:A:492:VAL:HG12	2.19	0.42
1:C:280:SER:OG	1:C:286:GLU:O	2.22	0.42
1:B:533:ASN:O	1:B:536:LEU:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:420:ALA:O	1:D:424:ILE:HG13	2.19	0.42
1:B:638:ARG:HB3	1:B:649:TYR:CE1	2.55	0.42
1:B:463:LEU:O	1:B:466:ARG:N	2.53	0.42
1:C:194:PHE:CE1	1:C:198:ILE:HD11	2.55	0.42
1:A:124:VAL:HA	1:A:568:MET:O	2.20	0.42
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.81	0.42
1:A:176:GLY:O	1:A:258:ARG:NH2	2.40	0.41
1:B:114:TYR:HA	1:B:574:VAL:O	2.20	0.41
1:B:257:SER:OG	1:B:258:ARG:N	2.53	0.41
1:B:285:ASP:N	1:B:285:ASP:OD1	2.53	0.41
1:A:432:THR:O	1:A:458:ASN:HB2	2.20	0.41
1:C:285:ASP:HA	1:C:298:SER:HB2	2.02	0.41
1:D:304:ARG:O	1:D:307:SER:OG	2.35	0.41
1:A:598:SER:H	1:A:630:ILE:HA	1.85	0.41
1:D:285:ASP:O	1:D:311:HIS:HD2	2.04	0.41
1:B:282:TYR:OH	1:B:408:ASP:OD2	2.30	0.41
1:B:328:ARG:HA	1:B:334:ALA:O	2.20	0.41
1:D:686:LEU:HG	1:D:687:GLU:N	2.35	0.41
1:B:116:CYS:HB3	1:B:560:SER:HB2	2.02	0.41
1:B:347:THR:N	1:B:350:PHE:O	2.50	0.41
1:D:194:PHE:CG	1:D:320:LYS:HD2	2.54	0.41
1:D:401:GLU:OE1	1:D:440:GLN:HA	2.20	0.41
1:B:116:CYS:HB2	1:B:622:GLU:OE1	2.21	0.41
1:B:153:ASN:OD1	1:B:155:ALA:N	2.50	0.41
1:D:224:HIS:HB2	1:D:269:VAL:HB	2.02	0.41
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.88	0.41
1:C:700:LEU:HD23	1:C:700:LEU:HA	1.90	0.41
1:B:466:ARG:HH21	1:B:470:ARG:NH1	2.18	0.41
1:A:258:ARG:NH1	1:A:260:GLU:HG2	2.36	0.41
1:C:194:PHE:CG	1:C:320:LYS:HG3	2.56	0.41
1:A:189:ARG:NH1	1:A:293:ASP:OD2	2.43	0.41
1:C:406:ARG:O	1:C:493:GLU:HG2	2.21	0.41
1:D:192:VAL:HG11	1:D:201:ILE:HD11	2.03	0.41
1:B:152:GLU:O	1:B:152:GLU:HG3	2.20	0.41
1:B:143:THR:CB	1:B:377:ARG:HB2	2.51	0.41
1:A:244:SER:OG	1:A:275:GLU:O	2.27	0.41
1:D:462:GLU:CD	1:D:462:GLU:H	2.24	0.41
1:C:200:LYS:HE3	1:C:208:ARG:NH2	2.36	0.41
1:D:118:PRO:HA	1:D:119:PRO:HD3	1.97	0.41
1:D:347:THR:OG1	1:D:350:PHE:N	2.51	0.41
1:B:377:ARG:HG3	1:B:452:TYR:CE2	2.56	0.41
1:C:209:SER:HB3	1:C:230:THR:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:387:SER:HA	1:B:394:THR:OG1	2.21	0.41
1:C:298:SER:CB	1:C:310:GLU:HG3	2.50	0.41
1:A:543:ARG:HD2	1:A:568:MET:CG	2.50	0.41
1:D:396:THR:O	1:D:444:ALA:HA	2.21	0.41
1:C:347:THR:N	1:C:350:PHE:O	2.53	0.41
1:B:169:THR:HG23	1:B:187:GLU:HG2	2.03	0.41
1:B:467:GLU:HG3	1:B:470:ARG:HH21	1.85	0.41
1:C:188:ASP:OD1	1:C:215:ARG:NH2	2.54	0.41
1:B:145:GLY:HA3	1:B:452:TYR:CE1	2.55	0.41
1:A:215:ARG:HH22	1:A:349:LYS:HD3	1.86	0.41
1:B:419:ASP:O	1:B:423:ARG:HB2	2.21	0.41
1:B:311:HIS:NE2	1:B:313:SER:OG	2.53	0.41
1:A:525:ALA:O	1:A:528:TRP:HB3	2.21	0.41
1:B:151:LYS:HZ3	1:B:369:TRP:HD1	1.67	0.41
1:C:530:GLU:O	1:C:534:HIS:HB2	2.21	0.41
1:B:548:ASN:HA	1:B:561:ALA:HB3	2.02	0.41
1:C:188:ASP:OD1	1:C:189:ARG:N	2.54	0.41
1:B:551:ALA:O	1:B:555:VAL:HG22	2.20	0.41
1:B:678:LEU:HD12	1:B:679:GLU:N	2.36	0.41
1:C:162:THR:HA	1:C:275:GLU:HA	2.03	0.41
1:D:521:LEU:HA	1:D:521:LEU:HD23	1.79	0.41
1:B:631:GLU:OE2	1:B:653:TYR:OH	2.37	0.40
1:A:388:SER:OG	1:A:391:ILE:N	2.55	0.40
1:B:466:ARG:HG3	1:B:467:GLU:N	2.36	0.40
1:B:605:ARG:HB3	1:B:611:PRO:O	2.21	0.40
1:C:379:GLU:HB2	1:C:384:PHE:CE1	2.56	0.40
1:B:360:ARG:HG2	1:B:409:LEU:HD23	2.02	0.40
1:C:516:HIS:O	1:C:520:MET:HG2	2.21	0.40
1:A:589:ILE:HG12	1:A:597:TYR:CE2	2.56	0.40
1:D:198:ILE:HA	1:D:198:ILE:HD13	1.94	0.40
1:C:555:VAL:HG12	1:C:557:ARG:HH12	1.85	0.40
1:D:619:GLU:O	1:D:622:GLU:HB3	2.21	0.40
1:C:464:TYR:CZ	1:C:468:HIS:HD2	2.39	0.40
1:A:259:VAL:HG12	1:A:264:ARG:NE	2.36	0.40
1:D:622:GLU:HG3	1:D:623:LEU:N	2.36	0.40
1:D:368:LYS:HB3	1:D:368:LYS:HE2	1.91	0.40
1:B:208:ARG:HD2	1:B:229:GLU:OE1	2.21	0.40
1:C:342:ARG:CZ	1:C:354:TRP:HA	2.52	0.40
1:A:209:SER:HB2	1:A:224:HIS:HB3	2.03	0.40
1:B:192:VAL:HG11	1:B:201:ILE:HD12	2.04	0.40
1:B:637:HIS:ND1	1:B:637:HIS:O	2.55	0.40
1:B:113:PHE:HB2	1:B:576:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:604:PHE:O	1:D:612:LEU:HA	2.22	0.40
1:C:113:PHE:CD2	1:C:581:VAL:HG21	2.57	0.40
1:D:369:TRP:CH2	1:D:501:ILE:HD11	2.57	0.40
1:C:592:ARG:HA	1:C:593:PRO:HD3	1.98	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	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

All (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
1	B	533	ASN
1	B	699	LEU
1	C	203	ALA
1	C	423	ARG

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Mol	Chain	Res	Type
1	C	464	TYR
1	A	373	ASP
1	D	225	ARG
1	D	244	SER
1	D	426	ALA
1	C	404	LEU
1	D	134	PRO
1	D	431	ALA
1	A	322	VAL
1	B	359	LYS
1	C	422	ASP
1	D	203	ALA
1	B	276	VAL
1	B	602	VAL
1	B	567	VAL
1	B	134	PRO
1	D	104	ILE

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

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	110	ASP
1	A	112	ASN
1	A	124	VAL
1	A	132	ARG

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	142	TYR
1	A	167	ASP
1	A	218	LEU
1	A	231	ASP
1	A	241	THR
1	A	250	THR
1	A	251	ASP
1	A	262	PHE
1	A	264	ARG
1	A	268	THR
1	A	308	HIS
1	A	309	THR
1	A	312	THR
1	A	337	THR
1	A	340	THR
1	A	352	VAL
1	A	363	VAL
1	A	364	CYS
1	A	365	THR
1	A	378	SER
1	A	380	TYR
1	A	384	PHE
1	A	388	SER
1	A	391	ILE
1	A	397	THR
1	A	432	THR
1	A	440	GLN
1	A	450	ILE
1	A	464	TYR
1	A	515	ARG
1	A	555	VAL
1	A	559	VAL
1	A	572	THR
1	A	573	CYS
1	A	580	ASN
1	A	583	VAL
1	A	586	SER
1	A	588	ARG
1	A	596	CYS
1	A	601	LEU
1	A	620	ASN

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Mol	Chain	Res	Type
1	A	634	THR
1	A	637	HIS
1	A	638	ARG
1	A	642	THR
1	A	656	SER
1	A	661	ARG
1	A	663	ASP
1	A	679	GLU
1	A	680	ASP
1	A	686	LEU
1	A	690	THR
1	A	704	GLU
1	B	104	ILE
1	B	109	THR
1	B	112	ASN
1	B	124	VAL
1	B	132	ARG
1	B	140	GLN
1	B	152	GLU
1	B	162	THR
1	B	169	THR
1	B	179	TYR
1	B	207	CYS
1	B	215	ARG
1	B	227	ASP
1	B	230	THR
1	B	238	ASN
1	B	241	THR
1	B	248	HIS
1	B	250	THR
1	B	251	ASP
1	B	258	ARG
1	B	286	GLU
1	B	288	VAL
1	B	298	SER
1	B	317	ASP
1	B	340	THR
1	B	365	THR
1	B	380	TYR
1	B	384	PHE
1	B	387	SER
1	B	393	THR

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Mol	Chain	Res	Type
1	B	397	THR
1	B	400	THR
1	B	427	ARG
1	B	434	ILE
1	B	455	LEU
1	B	457	SER
1	B	459	THR
1	B	466	ARG
1	B	469	LEU
1	B	471	GLU
1	B	494	ARG
1	B	534	HIS
1	B	585	ASN
1	B	587	MET
1	B	598	SER
1	B	601	LEU
1	B	602	VAL
1	B	609	GLN
1	B	616	GLN
1	B	626	THR
1	B	628	ASP
1	B	633	CYS
1	B	634	THR
1	B	637	HIS
1	B	638	ARG
1	B	639	ARG
1	B	648	VAL
1	B	649	TYR
1	B	660	SER
1	B	663	ASP
1	B	714	LEU
1	B	724	HIS
1	C	108	ASN
1	C	110	ASP
1	C	115	VAL
1	C	135	THR
1	C	141	ASN
1	C	142	TYR
1	C	152	GLU
1	C	169	THR
1	C	180	SER
1	C	207	CYS

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Mol	Chain	Res	Type
1	C	209	SER
1	C	217	ASN
1	C	219	GLU
1	C	262	PHE
1	C	268	THR
1	C	310	GLU
1	C	320	LYS
1	C	344	LEU
1	C	345	LEU
1	C	351	THR
1	C	364	CYS
1	C	366	MET
1	C	380	TYR
1	C	384	PHE
1	C	385	ARG
1	C	387	SER
1	C	391	ILE
1	C	400	THR
1	C	427	ARG
1	C	428	ARG
1	C	430	ASN
1	C	440	GLN
1	C	445	ASN
1	C	460	LEU
1	C	465	VAL
1	C	498	THR
1	C	501	ILE
1	C	529	CYS
1	C	572	THR
1	C	588	ARG
1	C	596	CYS
1	C	606	TYR
1	C	607	GLU
1	C	621	ASN
1	C	624	ARG
1	C	627	ARG
1	C	634	THR
1	C	635	VAL
1	C	651	GLU
1	C	667	VAL
1	C	672	ASP
1	C	708	ARG

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Mol	Chain	Res	Type
1	C	724	HIS
1	D	110	ASP
1	D	132	ARG
1	D	135	THR
1	D	143	THR
1	D	160	LYS
1	D	179	TYR
1	D	183	MET
1	D	195	GLU
1	D	207	CYS
1	D	230	THR
1	D	233	GLU
1	D	234	LEU
1	D	248	HIS
1	D	264	ARG
1	D	274	GLU
1	D	286	GLU
1	D	340	THR
1	D	378	SER
1	D	392	SER
1	D	393	THR
1	D	418	ARG
1	D	432	THR
1	D	433	HIS
1	D	455	LEU
1	D	464	TYR
1	D	466	ARG
1	D	469	LEU
1	D	471	GLU
1	D	501	ILE
1	D	553	VAL
1	D	588	ARG
1	D	622	GLU
1	D	634	THR
1	D	659	LEU
1	D	668	SER
1	D	720	ASP
1	D	724	HIS

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
3	A	803	NAG	C3-C4-C5	2.17	114.07	110.20
3	B	801	NAG	O7-C7-N2	2.10	126.29	121.90
3	B	801	NAG	O5-C5-C6	2.05	109.13	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.