



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:02 PM BST

PDB ID : 4HSI  
Title : Glycoprotein B from Herpes simplex virus type 1, A504P/R505G/Q507G/N511G mutant, low-pH  
Authors : Heldwein, E.E.  
Deposited on : 2012-10-30  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

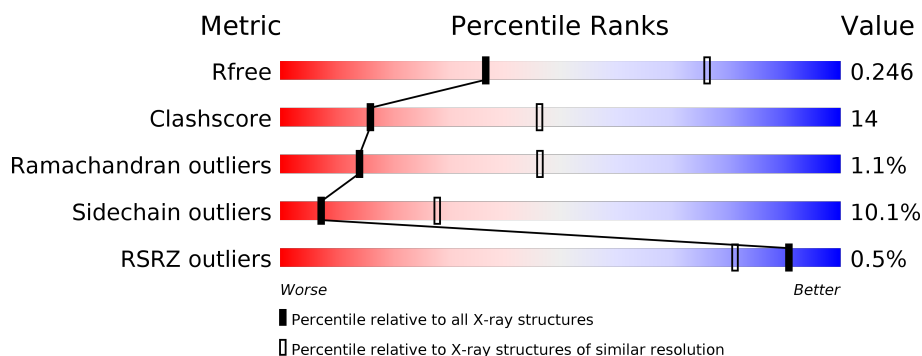
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	703	<div> <div></div> <div>56%26%•15%</div> </div>
1	B	703	<div> <div>%</div> <div>50%31%5%14%</div> </div>
1	C	703	<div> <div>%</div> <div>52%30%•14%</div> </div>
1	D	703	<div> <div></div> <div>57%27%•14%</div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	X	-	-	-
3	NAG	C	803	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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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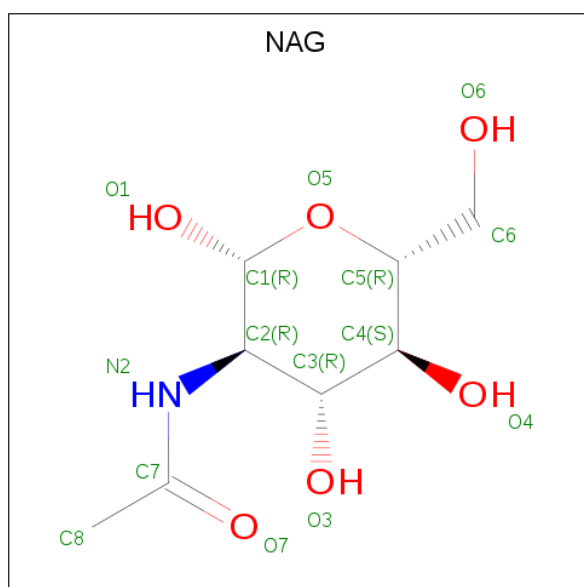
Chain	Residue	Modelled	Actual	Comment	Reference
D	58	PRO	-	expression tag	UNP P06437
D	59	LEU	-	expression tag	UNP P06437
D	60	GLY	-	expression tag	UNP P06437
D	313	SER	THR	conflict	UNP P06437
D	443	LEU	GLN	conflict	UNP P06437
D	504	PRO	ALA	engineered mutation	UNP P06437
D	505	GLY	ARG	engineered mutation	UNP P06437
D	507	GLY	GLN	engineered mutation	UNP P06437
D	511	GLY	ASN	engineered mutation	UNP P06437

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

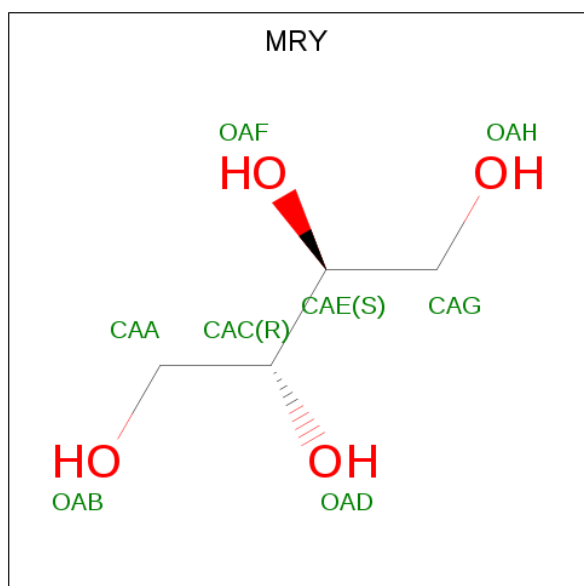
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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		
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		

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

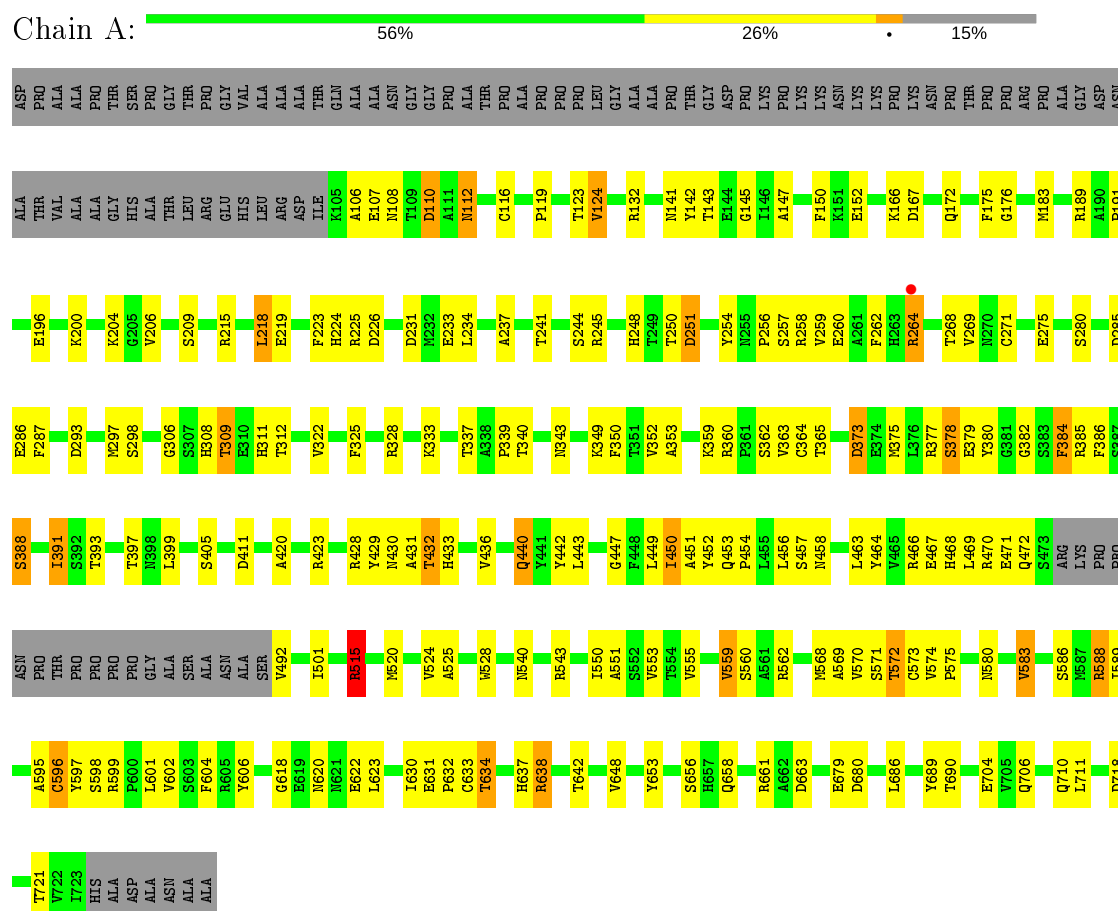
- Molecule 6 is water.

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

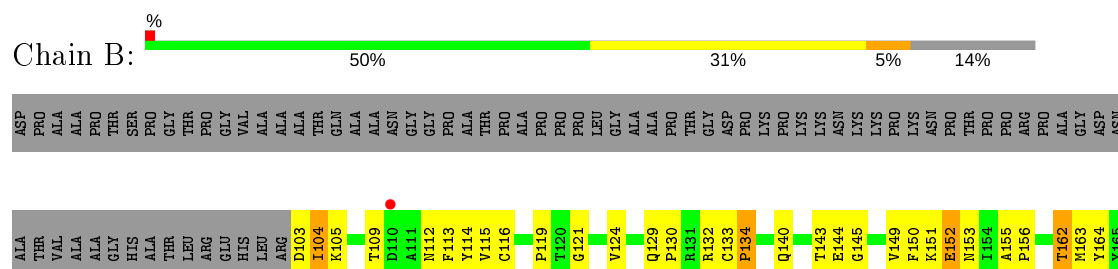
### 3 Residue-property plots

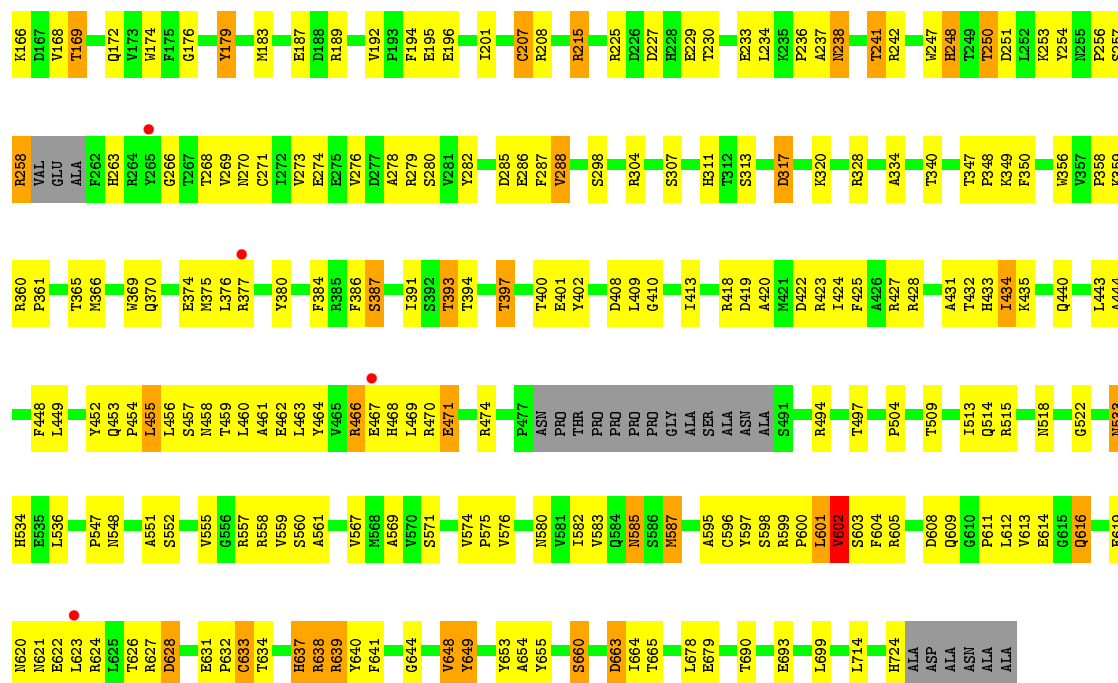
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Envelope glycoprotein B

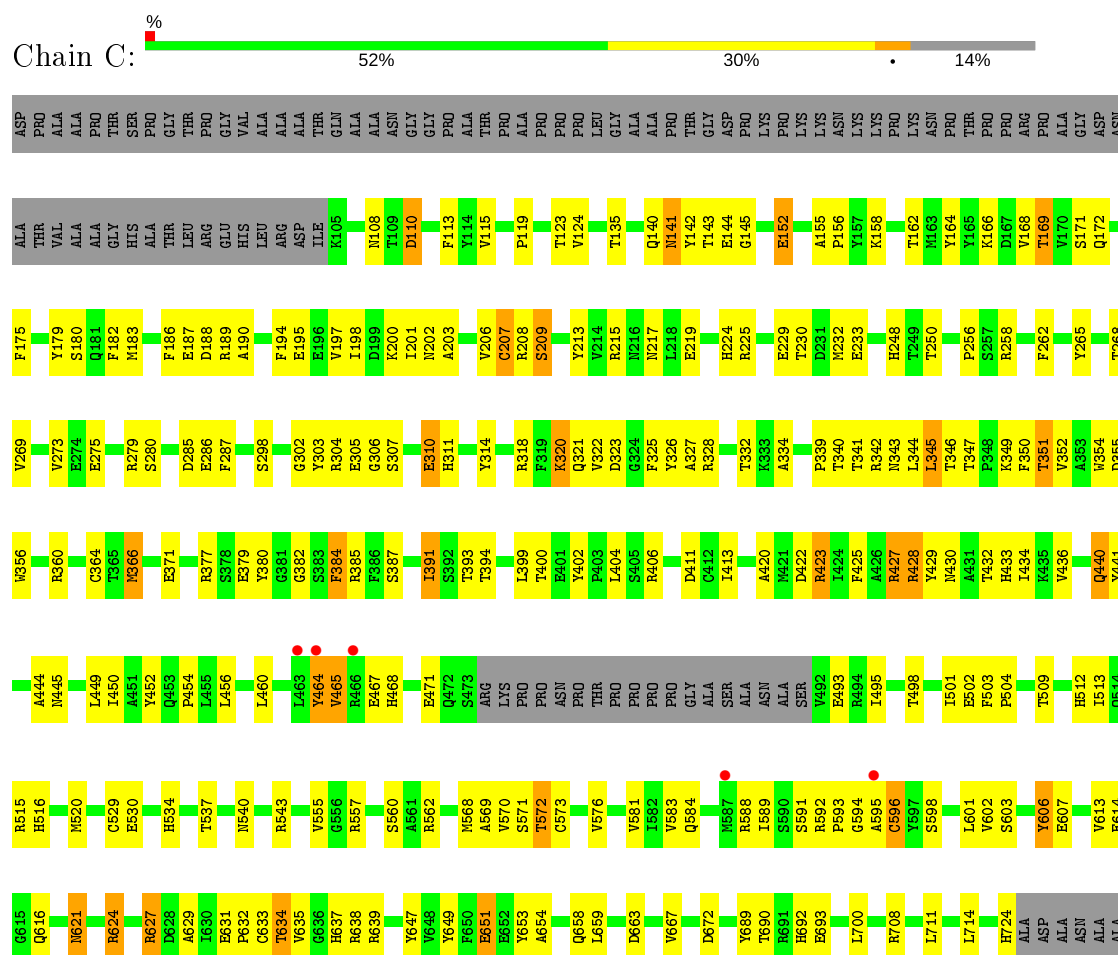


#### • Molecule 1: Envelope glycoprotein B





• Molecule 1: Envelope glycoprotein B



• Molecule 1: Envelope glycoprotein B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.205 , 0.255 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	3774 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.459 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

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

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:463:LEU:O	1:B:467:GLU:N	2.28	0.66
1:B:585:ASN:HA	1:B:655:TYR:HB3	1.77	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
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:A:285:ASP:HB2	1:A:311:HIS:HB3	1.80	0.64
1:C:614:GLU:HB3	1:C:627:ARG:NH2	2.11	0.64
1:A:206:VAL:HG12	1:A:233:GLU:HA	1.80	0.64
1:B:557:ARG:HG3	1:B:559:VAL:HG13	1.79	0.63
1:C:711:LEU:HD23	1:C:714:LEU:HD12	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:150:PHE:HB2	1:A:449:LEU:HB3	1.83	0.60
1:D:189:ARG:NH2	1:D:293:ASP:OD2	2.35	0.60
1:A:259:VAL:HG12	1:A:264:ARG:HE	1.66	0.60
1:B:637:HIS:CD2	1:B:639:ARG:HG2	2.37	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:A:604:PHE:HE1	1:A:606:TYR:HE2	1.49	0.59
1:D:248:HIS:HA	1:D:271:CYS:O	2.03	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:A:248:HIS:HE1	1:A:251:ASP:HB3	1.68	0.59
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.84	0.59
1:B:105:LYS:HA	1:B:582:ILE:HA	1.85	0.59
1:C:166:LYS:N	1:C:190:ALA:O	2.35	0.59
1:C:428:ARG:HB3	1:C:429:TYR:CD1	2.38	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:A:583:VAL:HA	1:A:602:VAL:HG12	1.86	0.58
1:C:598:SER:N	1:C:629:ALA:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:MET:O	1:D:273:VAL:HA	2.03	0.58
1:B:104:ILE:O	1:B:583:VAL:N	2.34	0.58
1:A:224:HIS:HB2	1:A:269:VAL:HB	1.84	0.58
1:C:366:MET:HE1	1:C:495:ILE:HB	1.86	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:B:583:VAL:HA	1:B:602:VAL:HG12	1.86	0.57
1:C:596:CYS:O	1:C:631:GLU:N	2.31	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:B:663:ASP:OD1	1:B:663:ASP:N	2.36	0.57
1:C:637:HIS:CG	1:C:653:TYR:HH	2.20	0.57
1:A:106:ALA:HA	1:A:658:GLN:HE22	1.70	0.57
1:B:248:HIS:HB2	1:B:270:ASN:OD1	2.05	0.57
1:B:614:GLU:HB3	1:B:627:ARG:NH1	2.19	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:B:115:VAL:HG22	1:B:623:LEU:HB2	1.87	0.56
1:D:306:GLY:O	1:D:309:THR:N	2.34	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:431:ALA:O	1:B:458:ASN:ND2	2.39	0.56
1:B:460:LEU:HB3	1:B:463:LEU:HD13	1.87	0.56
1:B:225:ARG:HD3	1:B:254:TYR:CD1	2.41	0.56
1:C:140:GLN:OE1	1:C:141:ASN:N	2.39	0.56
1:A:223:PHE:HB2	1:A:226:ASP:HA	1.88	0.55
1:A:382:GLY:HA2	1:A:399:LEU:HD11	1.86	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:280:SER:HB2	1:C:287:PHE:HB3	1.87	0.55
1:C:634:THR:O	1:C:637:HIS:HB2	2.07	0.55
1:B:599:ARG:HH12	1:B:619:GLU:CD	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:VAL:HA	1:C:569:ALA:HA	1.89	0.55
1:C:215:ARG:NH2	1:C:349:LYS:HD3	2.22	0.55
1:B:282:TYR:HE2	1:B:409:LEU:HD12	1.72	0.54
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:D:347:THR:N	1:D:350:PHE:O	2.40	0.54
1:D:463:LEU:HB3	1:D:467:GLU:HG2	1.88	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:A:377:ARG:HD2	1:A:384:PHE:CG	2.43	0.54
1:D:105:LYS:HE2	1:D:582:ILE:HD11	1.88	0.54
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.90	0.53
1:C:603:SER:OG	1:C:614:GLU:HA	2.08	0.53
1:B:145:GLY:HA3	1:B:452:TYR:OH	2.07	0.53
1:A:196:GLU:HG3	1:A:200:LYS:HG3	1.89	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: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:C:171:SER:HB2	1:C:182:PHE:HE1	1.74	0.53
1:D:311:HIS:NE2	1:D:313:SER:OG	2.39	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:C:512:HIS:HA	1:C:515:ARG:NH1	2.24	0.53
1:A:559:VAL:HG12	1:A:572:THR:HA	1.90	0.53
1:B:253:LYS:HA	1:B:268:THR:HG21	1.91	0.52
1:D:285:ASP:N	1:D:285:ASP:OD1	2.37	0.52
1:A:248:HIS:CE1	1:A:251:ASP:HB3	2.45	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:562:ARG:O	1:A:569:ALA:N	2.41	0.52
1:C:164:TYR:HB2	1:C:351:THR:HG22	1.92	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:C:440:GLN:HG2	1:C:452:TYR:O	2.11	0.50
1:D:204:LYS:O	1:D:328:ARG:NH1	2.44	0.50
1:D:401:GLU:HG3	1:D:441:TYR:O	2.11	0.50
1:D:586:SER:OG	1:D:588:ARG:HG3	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: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:D:399:LEU:O	1:D:474:ARG:HG2	2.12	0.50
1:B:317:ASP:N	1:B:317:ASP:OD1	2.39	0.50
1:B:558:ARG:NH1	1:B:620:ASN:HB3	2.27	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: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:176:GLY:N	1:B:179:TYR:O	2.40	0.49
1:B:585:ASN:O	1:B:654:ALA:HA	2.12	0.49
1:A:107:GLU:H	1:A:658:GLN:NE2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:440:GLN:NE2	1:A:442:TYR:OH	2.44	0.49
1:B:552:SER:HA	1:B:559:VAL:HG22	1.95	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:A:257:SER:O	1:A:264:ARG:NH2	2.46	0.49
1:B:638:ARG:HB3	1:B:649:TYR:HE1	1.77	0.49
1:A:280:SER:HB2	1:A:287:PHE:CB	2.43	0.49
1:B:408:ASP:O	1:B:410:GLY:N	2.46	0.49
1:B:587:MET:N	1:B:653:TYR:O	2.45	0.49
1:D:114:TYR:O	1:D:623:LEU:N	2.40	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:D:237:ALA:N	1:D:246:GLY:O	2.41	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:420:ALA:HA	1:C:423:ARG:NH1	2.27	0.48
1:C:464:TYR:CE2	1:C:468:HIS:HD2	2.31	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:A:433:HIS:CD2	1:A:457:SER:HA	2.48	0.48
1:B:418:ARG:O	1:B:422:ASP:N	2.45	0.48
1:C:584:GLN:N	1:C:601:LEU:O	2.47	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:C:402:TYR:N	1:C:441:TYR:O	2.41	0.48
1:B:435:LYS:HD2	1:B:453:GLN:OE1	2.14	0.48
1:B:103:ASP:OD1	1:B:103:ASP:N	2.46	0.48
1:D:548:ASN:OD1	1:D:561:ALA:N	2.31	0.48
1:A:145:GLY:HA3	1:A:452:TYR:CE1	2.49	0.47
1:D:136:ARG:HH12	1:D:523:ARG:NH2	2.11	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
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:A:420:ALA:HA	1:A:423:ARG:NH1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH2	1:A:349:LYS:HD3	2.29	0.47
1:A:551:ALA:HB2	1:A:568:MET:HE3	1.96	0.47
1:C:638:ARG:O	1:C:639:ARG:HG2	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:D:196:GLU:O	1:D:201:ILE:HG13	2.14	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:304:ARG:NH2	1:C:323:ASP:OD1	2.47	0.47
1:A:385:ARG:HH11	1:A:385:ARG:HG2	1.79	0.47
1:B:304:ARG:O	1:B:307:SER:OG	2.22	0.47
1:C:197:VAL:HA	1:C:201:ILE:HD12	1.97	0.47
1:C:637:HIS:CG	1:C:653:TYR:CZ	3.03	0.47
1:A:634:THR:N	1:A:653:TYR:OH	2.28	0.47
1:B:236:PRO:HA	1:B:247:TRP:CD1	2.50	0.47
1:B:377:ARG:NH1	1:B:440:GLN:OE1	2.45	0.47
1:C:215:ARG:HH22	1:C:349:LYS:HD3	1.80	0.47
1:C:440:GLN:N	1:C:452:TYR:O	2.46	0.47
1:C:647:TYR:O	1:C:658:GLN:HG3	2.15	0.47
1:A:378:SER:O	1:A:385:ARG:N	2.45	0.47
1:A:453:GLN:NE2	1:A:454:PRO:O	2.47	0.47
1:B:156:PRO:HG2	1:B:279:ARG:NH2	2.29	0.47
1:B:144:GLU:HA	1:B:376:LEU:CD2	2.44	0.47
1:C:659:LEU:HD12	1:C:663:ASP:HB2	1.97	0.47
1:D:568:MET:HE2	1:D:568:MET:HB2	1.65	0.47
1:A:378:SER:HB3	1:A:385:ARG:NH2	2.30	0.46
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: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:147:ALA:HA	1:A:451:ALA:O	2.16	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:D:444:ALA:HB3	1:D:448:PHE:HB2	1.97	0.46
1:B:215:ARG:NH2	1:B:348:PRO:O	2.47	0.46
1:B:664:ILE:HG22	1:B:665:THR:O	2.14	0.46
1:C:572:THR:HG22	1:C:573:CYS:H	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH12	1:A:333:LYS:HB3	1.81	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:C:215:ARG:HA	1:C:215:ARG:HD3	1.79	0.46
1:D:639:ARG:O	1:D:649:TYR:HD1	1.99	0.46
1:D:643:PHE:N	1:D:646:GLY:O	2.45	0.46
1:C:342:ARG:NH2	1:C:354:TRP:HA	2.30	0.46
1:C:633:CYS:HA	1:C:653:TYR:CZ	2.51	0.46
1:D:552:SER:HA	1:D:559:VAL:HG22	1.96	0.46
1:C:172:GLN:HG2	1:C:183:MET:HB2	1.98	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:B:358:PRO:HG2	1:B:361:PRO:HG2	1.96	0.46
1:B:471:GLU:HA	1:B:474:ARG:NH1	2.31	0.46
1:D:286:GLU:HB2	1:D:296:TYR:HA	1.96	0.46
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.98	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:C:224:HIS:HB2	1:C:269:VAL:HB	1.97	0.46
1:C:280:SER:HB2	1:C:287:PHE:CB	2.46	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:D:555:VAL:HG12	1:D:557:ARG:H	1.81	0.46
1:D:616:GLN:HB2	1:D:627:ARG:HA	1.97	0.46
1:C:302:GLY:HA3	1:C:321:GLN:NE2	2.31	0.45
1:C:325:PHE:HB3	1:C:340:THR:O	2.17	0.45
1:D:639:ARG:HB3	1:D:641:PHE:CE2	2.51	0.45
1:A:440:GLN:HB2	1:A:442:TYR:CE1	2.51	0.45
1:A:501:ILE:HA	1:A:501:ILE:HD12	1.80	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:225:ARG:HD2	1:A:254:TYR:CD1	2.51	0.45
1:B:547:PRO:HB2	1:B:561:ALA:O	2.15	0.45
1:C:179:TYR:O	1:C:258:ARG:NH2	2.50	0.45
1:C:467:GLU:O	1:C:471:GLU:HG2	2.16	0.45
1:D:179:TYR:HD1	1:D:180:SER:N	2.15	0.45
1:B:201:ILE:HD11	1:B:207:CYS:SG	2.56	0.45
1:C:208:ARG:NH1	1:C:229:GLU:OE2	2.50	0.45
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.67	0.45
1:A:466:ARG:HH12	1:A:470:ARG:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:HB	1:B:164:TYR:CZ	2.51	0.45
1:B:432:THR:HB	1:B:433:HIS:CD2	2.51	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: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:D:307:SER:HA	1:D:310:GLU:HG2	1.99	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:C:314:TYR:CD1	1:C:345:LEU:HD11	2.51	0.45
1:C:436:VAL:HA	1:C:464:TYR:CE1	2.51	0.45
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.83	0.45
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.83	0.45
1:B:238:ASN:OD1	1:B:238:ASN:N	2.49	0.45
1:C:113:PHE:HB2	1:C:576:VAL:HB	1.98	0.45
1:A:443:LEU:HD11	1:A:447:GLY:HA2	1.98	0.45
1:B:660:SER:H	1:B:663:ASP:CG	2.20	0.45
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:B:616:GLN:HG2	1:B:627:ARG:HG3	1.98	0.44
1:A:377:ARG:HD2	1:A:384:PHE:CD2	2.52	0.44
1:C:560:SER:N	1:C:571:SER:O	2.50	0.44
1:D:449:LEU:HD12	1:D:449:LEU:HA	1.76	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:A:234:LEU:HD23	1:A:234:LEU:HA	1.81	0.44
1:B:580:ASN:ND2	1:B:608:ASP:OD1	2.48	0.44
1:C:213:TYR:HE2	1:C:215:ARG:HB2	1.76	0.44
1:C:175:PHE:CE2	1:C:258:ARG:HA	2.53	0.44
1:C:371:GLU:OE1	1:C:423:ARG:NH2	2.50	0.44
1:D:225:ARG:HH11	1:D:254:TYR:HD2	1.65	0.44
1:D:690:THR:OG1	1:D:693:GLU:HG3	2.18	0.44
1:A:430:ASN:OD1	1:A:430:ASN:N	2.50	0.44
1:A:588:ARG:HH21	1:A:633:CYS:HB3	1.81	0.44
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.98	0.44
1:B:195:GLU:OE1	1:B:196:GLU:N	2.51	0.44
1:B:386:PHE:O	1:B:394:THR:HA	2.18	0.44
1:B:464:TYR:O	1:B:468:HIS:ND1	2.44	0.44
1:C:202:ASN:OD1	1:C:328:ARG:N	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:TYR:CE2	1:C:321:GLN:HB2	2.53	0.44
1:C:305:GLU:HB3	1:C:306:GLY:H	1.60	0.44
1:C:360:ARG:HB3	1:C:411:ASP:OD2	2.17	0.44
1:D:425:PHE:CZ	1:D:430:ASN:HA	2.53	0.44
1:A:359:LYS:O	1:A:362:SER:N	2.49	0.44
1:A:436:VAL:O	1:A:454:PRO:HG2	2.18	0.44
1:B:425:PHE:HZ	1:B:434:ILE:HG13	1.83	0.44
1:D:246:GLY:HA2	1:D:273:VAL:O	2.18	0.44
1:A:325:PHE:O	1:A:339:PRO:HA	2.18	0.44
1:A:442:TYR:O	1:A:450:ILE:N	2.40	0.44
1:B:558:ARG:HH12	1:B:620:ASN:HB3	1.83	0.44
1:C:207:CYS:SG	1:C:208:ARG:N	2.91	0.44
1:C:332:THR:C	1:C:334:ALA:H	2.21	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:A:375:MET:SD	1:A:386:PHE:HB3	2.57	0.44
1:C:616:GLN:O	1:C:624:ARG:N	2.50	0.44
1:D:403:PRO:HG2	1:D:406:ARG:CZ	2.48	0.44
1:B:233:GLU:HG2	1:B:234:LEU:H	1.83	0.43
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: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: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:D:143:THR:OG1	1:D:377:ARG:NH2	2.49	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:164:TYR:CD2	1:C:273:VAL:HG22	2.52	0.43
1:B:461:ALA:O	1:B:464:TYR:HB3	2.18	0.43
1:C:123:THR:HB	1:C:570:VAL:O	2.19	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:B:304:ARG:HD2	1:B:356:TRP:CZ3	2.53	0.43
1:C:248:HIS:ND1	1:C:250:THR:O	2.52	0.43
1:C:427:ARG:HG3	1:C:428:ARG:N	2.34	0.43
1:D:151:LYS:HD3	1:D:369:TRP:CD1	2.53	0.43
1:B:278:ALA:HA	1:B:288:VAL:O	2.18	0.43
1:B:152:GLU:HA	1:B:366:MET:SD	2.59	0.43
1:B:149:VAL:HB	1:B:370:GLN:HB2	2.00	0.43
1:D:502:GLU:O	1:D:506:LEU:N	2.50	0.43

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:THR:OG1	1:D:350:PHE:N	2.51	0.41
1:A:543:ARG:HD2	1:A:568:MET:CG	2.50	0.41
1:B:169:THR:HG23	1:B:187:GLU:HG2	2.03	0.41
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:C:347:THR:N	1:C:350:PHE:O	2.53	0.41
1:D:396:THR:O	1:D:444:ALA:HA	2.21	0.41
1:B:311:HIS:NE2	1:B:313:SER:OG	2.53	0.41
1:B:419:ASP:O	1:B:423:ARG:HB2	2.21	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:A:215:ARG:HH22	1:A:349:LYS:HD3	1.86	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:B:145:GLY:HA3	1:B:452:TYR:CE1	2.55	0.41
1:C:530:GLU:O	1:C:534:HIS:HB2	2.21	0.41
1:B:551:ALA:O	1:B:555:VAL:HG22	2.20	0.41
1:B:548:ASN:HA	1:B:561:ALA:HB3	2.02	0.41
1:B:678:LEU:HD12	1:B:679:GLU:N	2.36	0.41
1:C:188:ASP:OD1	1:C:189:ARG:N	2.54	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:A:388:SER:OG	1:A:391:ILE:N	2.55	0.40
1:A:589:ILE:HG12	1:A:597:TYR:CE2	2.56	0.40
1:B:360:ARG:HG2	1:B:409:LEU:HD23	2.02	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:B:631:GLU:OE2	1:B:653:TYR:OH	2.37	0.40
1:C:379:GLU:HB2	1:C:384:PHE:CE1	2.56	0.40
1:C:516:HIS:O	1:C:520:MET:HG2	2.21	0.40
1:C:555:VAL:HG12	1:C:557:ARG:HH12	1.85	0.40
1:D:198:ILE:HA	1:D:198:ILE:HD13	1.94	0.40
1:D:619:GLU:O	1:D:622:GLU:HB3	2.21	0.40
1:A:259:VAL:HG12	1:A:264:ARG:NE	2.36	0.40
1:B:208:ARG:HD2	1:B:229:GLU:OE1	2.21	0.40
1:C:464:TYR:CZ	1:C:468:HIS:HD2	2.39	0.40
1:D:368:LYS:HB3	1:D:368:LYS:HE2	1.91	0.40
1:D:622:GLU:HG3	1:D:623:LEU:N	2.36	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:C:342:ARG:CZ	1:C:354:TRP:HA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:HB2	1:B:576:VAL:HB	2.04	0.40
1:B:637:HIS:O	1:B:637:HIS:ND1	2.55	0.40
1:C:113:PHE:CD2	1:C:581:VAL:HG21	2.57	0.40
1:C:592:ARG:HA	1:C:593:PRO:HD3	1.98	0.40
1:D:369:TRP:CH2	1:D:501:ILE:HD11	2.57	0.40
1:D:604:PHE:O	1:D:612:LEU:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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 [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	597/703 (85%)	529 (89%)	66 (11%)	2 (0%)	41	73
1	B	600/703 (85%)	537 (90%)	54 (9%)	9 (2%)	10	39
1	C	598/703 (85%)	527 (88%)	64 (11%)	7 (1%)	13	44
1	D	599/703 (85%)	537 (90%)	54 (9%)	8 (1%)	12	42
All	All	2394/2812 (85%)	2130 (89%)	238 (10%)	26 (1%)	14	46

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ALA
1	B	413	ILE
1	C	413	ILE

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Mol	Chain	Res	Type
1	D	462	GLU
1	C	465	VAL
1	B	533	ASN
1	B	699	LEU
1	C	203	ALA
1	C	423	ARG
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%)	6	23
1	B	528/592 (89%)	466 (88%)	62 (12%)	5	22
1	C	523/592 (88%)	470 (90%)	53 (10%)	7	28
1	D	526/592 (89%)	489 (93%)	37 (7%)	15	45
All	All	2099/2368 (89%)	1888 (90%)	211 (10%)	7	28

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
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

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Mol	Chain	Res	Type
1	A	588	ARG
1	A	596	CYS
1	A	601	LEU
1	A	620	ASN
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

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Mol	Chain	Res	Type
1	B	380	TYR
1	B	384	PHE
1	B	387	SER
1	B	393	THR
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

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Mol	Chain	Res	Type
1	C	152	GLU
1	C	169	THR
1	C	180	SER
1	C	207	CYS
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

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Mol	Chain	Res	Type
1	C	651	GLU
1	C	667	VAL
1	C	672	ASP
1	C	708	ARG
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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

4 monosaccharides 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	E	1	1,2	14,14,15	0.63	0	17,19,21	1.19	2 (11%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	1.08	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	1.13	1 (5%)
2	NAG	F	2	2	14,14,15	0.56	0	17,19,21	1.82	4 (23%)

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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C1-C2	-4.60	104.02	111.29
2	F	2	NAG	C3-C4-C5	3.79	117.00	110.24
2	E	1	NAG	C4-C3-C2	3.40	116.00	111.02
2	F	1	NAG	C4-C3-C2	2.61	114.84	111.02
2	F	2	NAG	O5-C5-C4	2.46	116.81	110.83
2	E	1	NAG	C3-C4-C5	2.30	114.35	110.24
2	F	2	NAG	C1-C2-N2	2.22	114.29	110.49
2	E	2	NAG	C4-C3-C2	-2.07	107.98	111.02
2	E	2	NAG	C1-O5-C5	2.02	114.93	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1

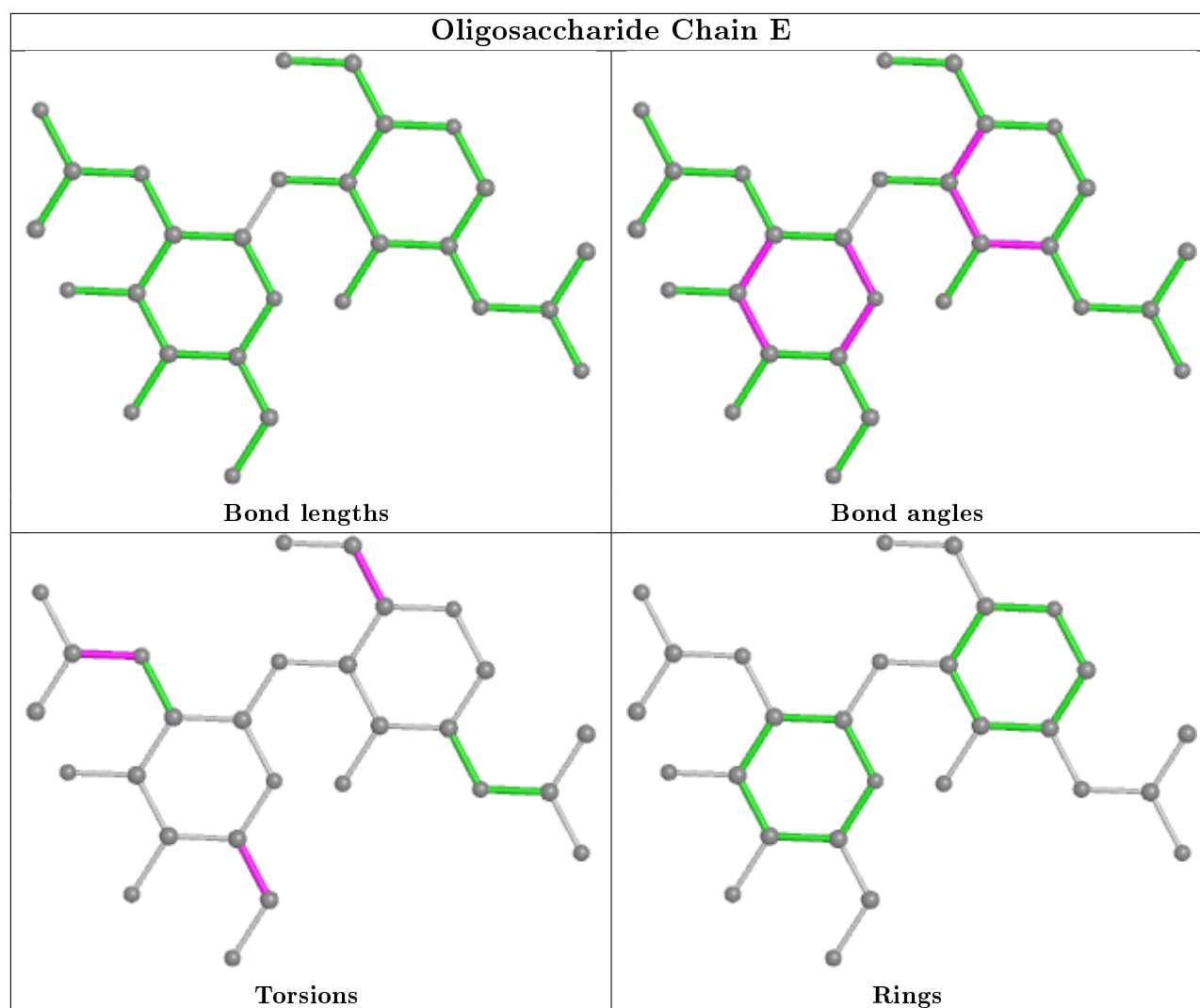
All (7) torsion outliers are listed below:

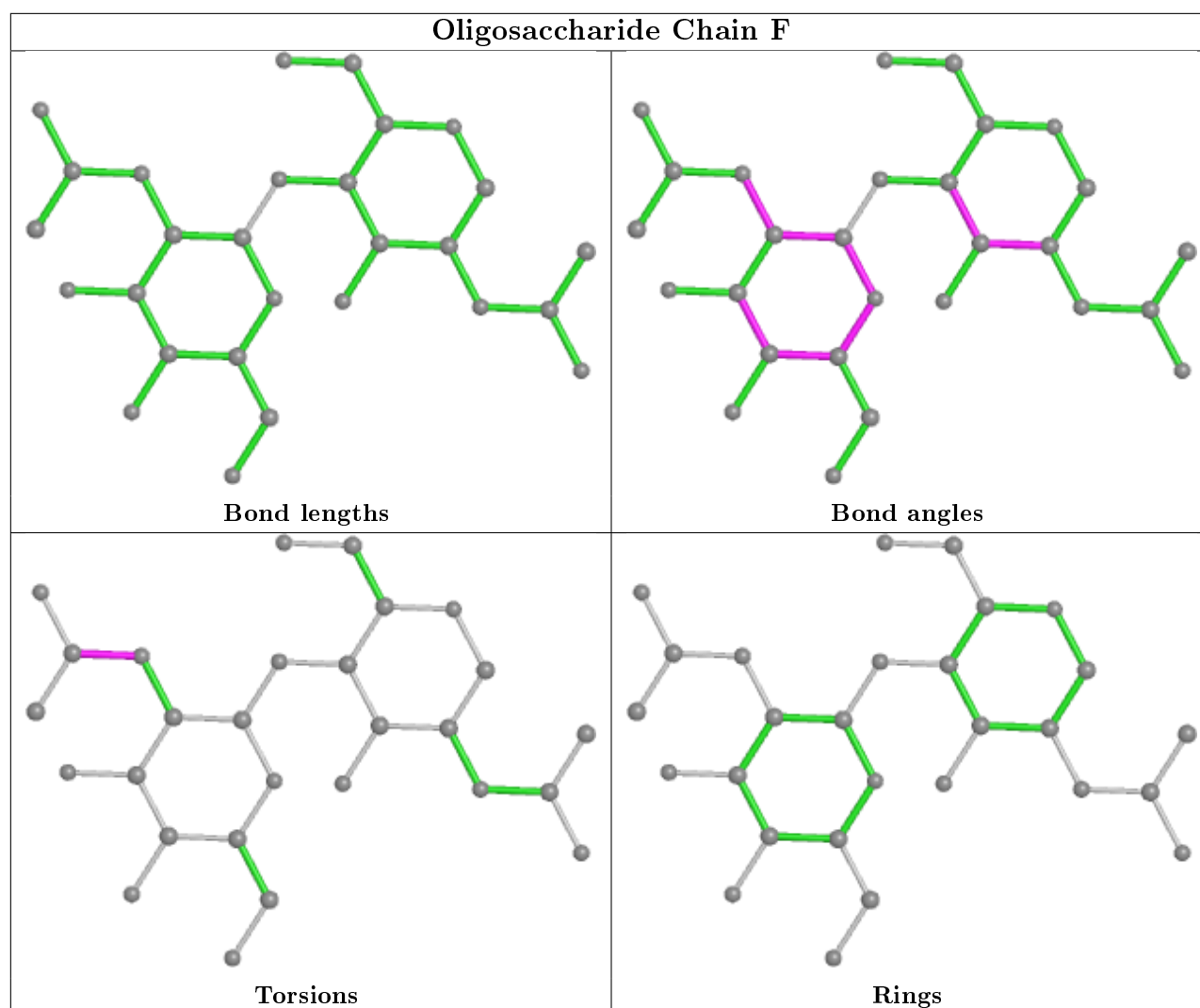
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

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	D	802	1	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
3	NAG	C	803	1	14,14,15	0.46	0	17,19,21	1.67	2 (11%)
3	NAG	D	801	1	14,14,15	0.43	0	17,19,21	1.50	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	801	1	14,14,15	0.55	0	17,19,21	1.77	4 (23%)
3	NAG	A	803	1	14,14,15	0.73	0	17,19,21	1.16	2 (11%)
4	MRY	C	804	-	7,7,7	0.33	0	8,8,8	1.07	0
4	MRY	A	804	-	7,7,7	0.39	0	8,8,8	0.87	0
3	NAG	B	802	1	14,14,15	0.59	0	17,19,21	1.37	1 (5%)

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	D	802	1	-	2/6/23/26	0/1/1/1
3	NAG	C	803	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	D	801	1	-	4/6/23/26	0/1/1/1
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
4	MRY	C	804	-	-	0/8/8/8	-
4	MRY	A	804	-	-	0/8/8/8	-
3	NAG	B	802	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	NAG	O5-C1-C2	-5.40	102.77	111.29
3	D	801	NAG	C1-O5-C5	4.43	118.20	112.19
3	B	801	NAG	C1-O5-C5	4.18	117.85	112.19
3	B	802	NAG	C2-N2-C7	-3.70	117.63	122.90
3	B	801	NAG	C2-N2-C7	3.69	128.16	122.90
3	D	802	NAG	C2-N2-C7	-3.46	117.98	122.90
3	D	801	NAG	O5-C1-C2	2.58	115.36	111.29
3	D	802	NAG	C4-C3-C2	-2.52	107.33	111.02
3	B	801	NAG	O7-C7-N2	2.36	126.29	121.95
3	C	803	NAG	C2-N2-C7	-2.16	119.83	122.90
3	A	803	NAG	C3-C4-C5	2.15	114.07	110.24
3	B	801	NAG	O5-C1-C2	2.09	114.59	111.29
3	A	803	NAG	O5-C1-C2	-2.06	108.03	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	803	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	802	NAG	O7-C7-N2-C2
3	C	803	NAG	C8-C7-N2-C2
3	C	803	NAG	O7-C7-N2-C2
3	D	801	NAG	C8-C7-N2-C2
3	D	801	NAG	O7-C7-N2-C2
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	D	802	NAG	C8-C7-N2-C2
3	B	802	NAG	C8-C7-N2-C2
3	D	801	NAG	O5-C5-C6-O6
3	B	802	NAG	O7-C7-N2-C2
3	D	801	NAG	C4-C5-C6-O6
3	C	803	NAG	C4-C5-C6-O6
3	C	803	NAG	O5-C5-C6-O6
3	A	803	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	NAG	1	0
3	B	801	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	601/703 (85%)	-0.18	1 (0%) 95 90	1, 37, 84, 140	0
1	B	606/703 (86%)	-0.13	5 (0%) 86 72	3, 44, 95, 185	0
1	C	602/703 (85%)	-0.14	5 (0%) 86 72	7, 44, 98, 157	0
1	D	605/703 (86%)	-0.18	1 (0%) 95 90	2, 39, 78, 147	1 (0%)
All	All	2414/2812 (85%)	-0.16	12 (0%) 91 81	1, 41, 89, 185	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	TYR	3.0
1	B	467	GLU	2.8
1	C	464	TYR	2.8
1	A	264	ARG	2.7
1	B	623	LEU	2.7
1	C	595	ALA	2.6
1	B	110	ASP	2.6
1	C	463	LEU	2.5
1	C	466	ARG	2.4
1	C	587	MET	2.2
1	B	377	ARG	2.1
1	D	625	LEU	2.0

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

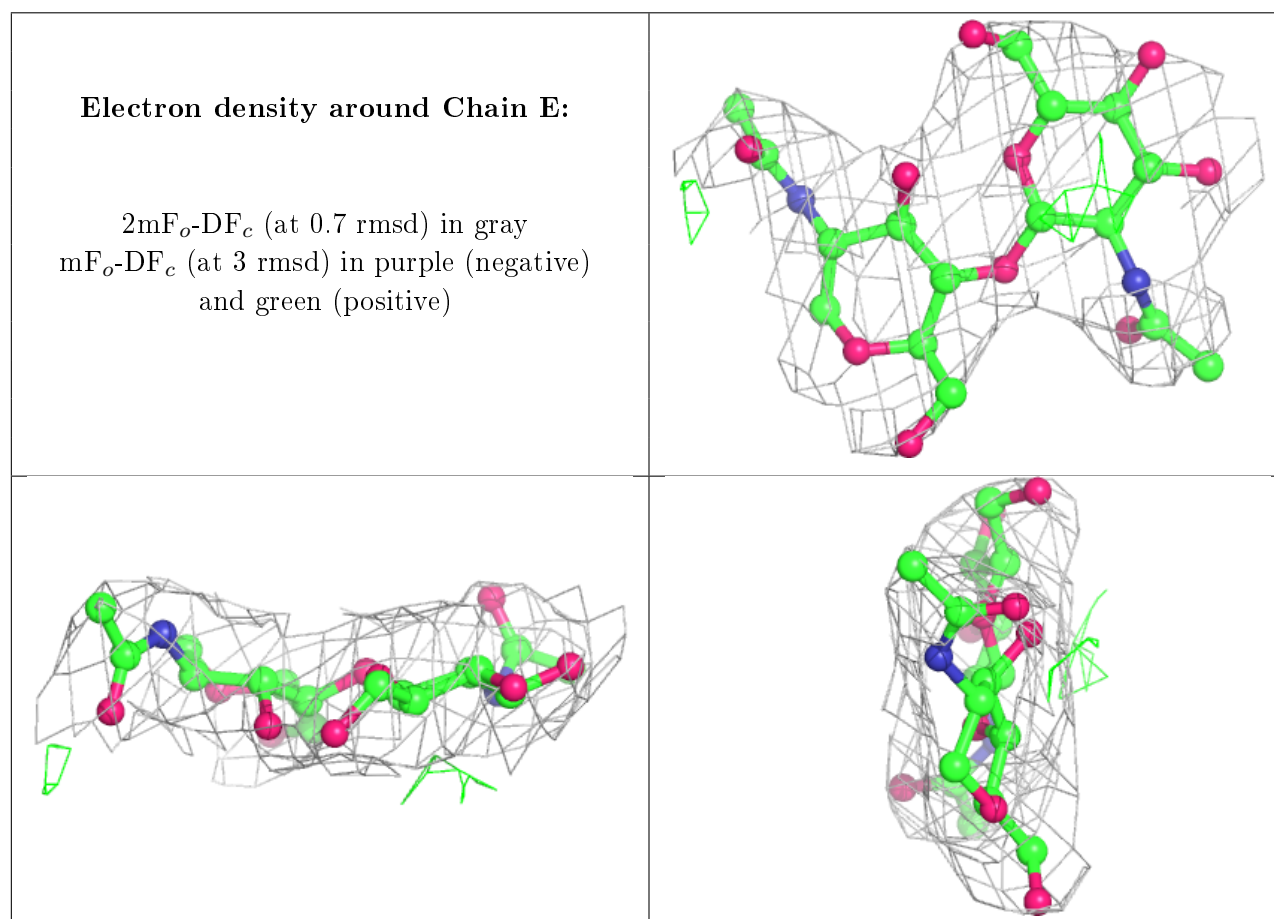
There are no non-standard protein/DNA/RNA residues in this entry.

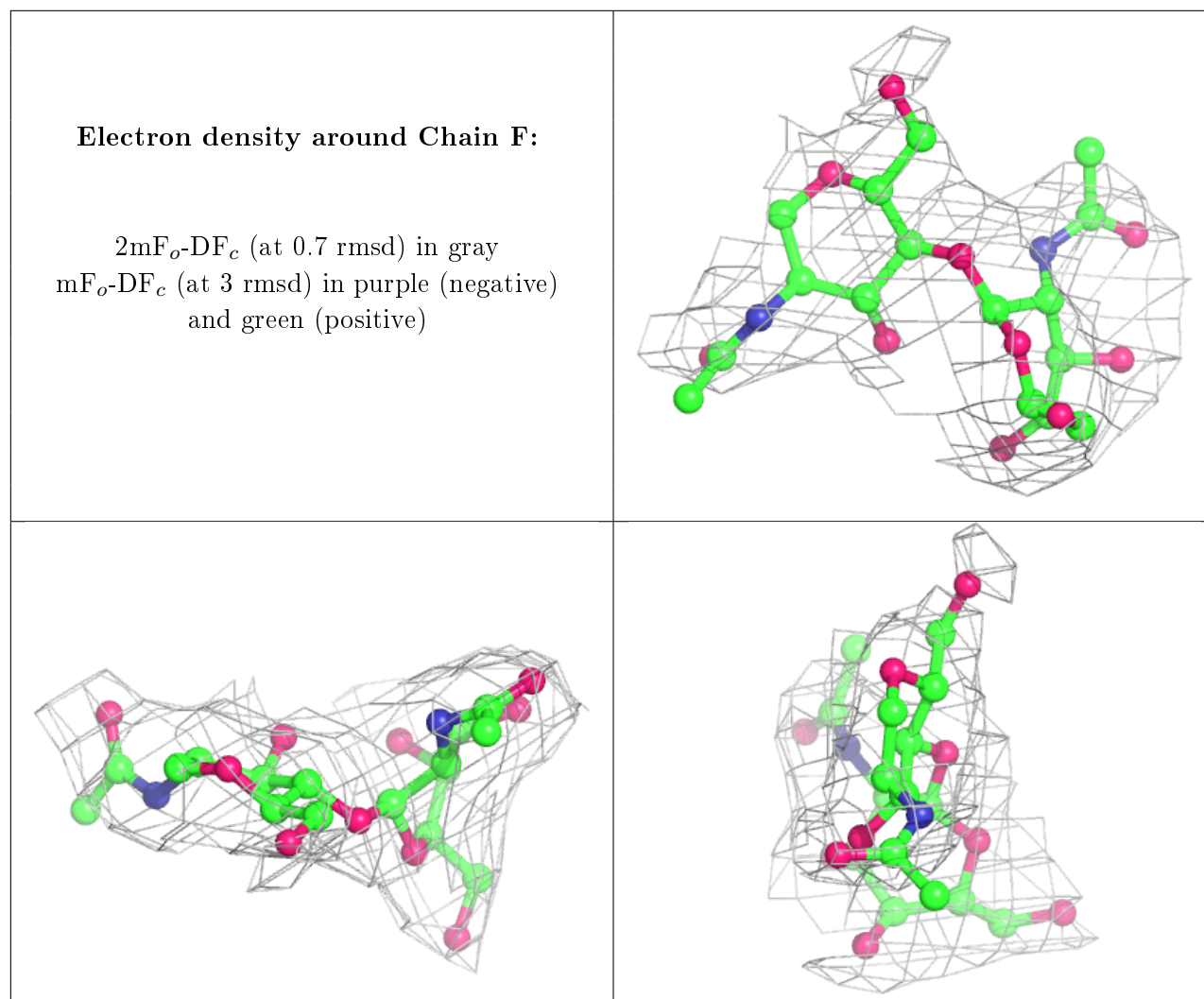
## 6.3 Carbohydrates ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	F	1	14/15	0.90	0.19	88,88,88,88	0
2	NAG	F	2	14/15	0.90	0.17	92,92,92,92	0
2	NAG	E	2	14/15	0.92	0.16	86,86,86,86	0
2	NAG	E	1	14/15	0.93	0.19	92,92,92,92	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	B	803	1/1	0.81	0.20	67,67,67,67	0
3	NAG	A	803	14/15	0.88	0.15	71,71,71,71	0
3	NAG	C	803	14/15	0.88	0.15	71,71,71,71	0
3	NAG	B	801	14/15	0.91	0.19	69,69,69,69	0
4	MRY	C	804	8/8	0.94	0.23	34,34,34,34	0
4	MRY	A	804	8/8	0.94	0.23	44,44,44,44	0
5	CL	D	803	1/1	0.94	0.26	71,71,71,71	0
3	NAG	D	801	14/15	0.94	0.15	71,71,71,71	0
5	CL	A	805	1/1	0.96	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	802	14/15	0.96	0.14	31,31,31,31	0
5	CL	C	805	1/1	0.97	0.12	32,32,32,32	0
3	NAG	D	802	14/15	0.97	0.14	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.