



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 PM GMT

PDB ID : 4P5M  
Title : Structural Basis of Chronic Beryllium Disease: Bridging the Gap Between Allergic Hypersensitivity and Autoimmunity  
Authors : Wang, Y.; Dai, S.; Kappler, J.  
Deposited on : 2014-03-18  
Resolution : 1.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

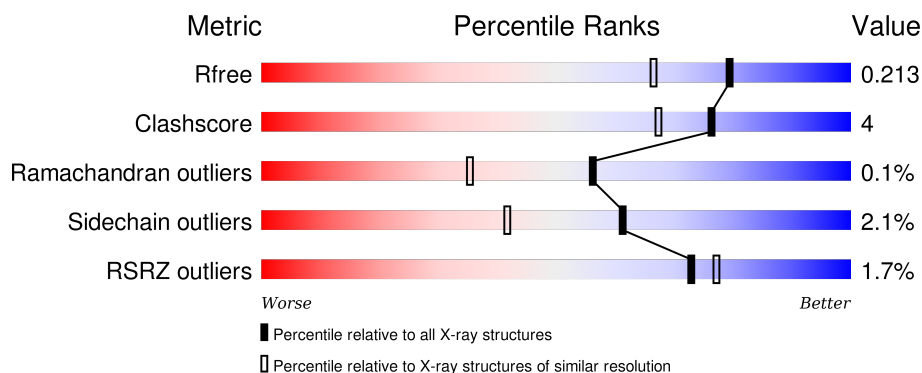
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	183	<div> <div>89%</div> <div>8%</div> <div>...</div> </div>
1	C	183	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	E	183	<div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	G	183	<div> <div>91%</div> <div>7%</div> <div>.</div> </div>
2	B	212	<div> <div>4%</div> <div>85%</div> <div>7%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	212	
2	F	212	
2	H	212	

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
4	NAG	E	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14385 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 HLA class II histocompatibility antigen, DP alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	2	0
			1487	962	240	279	6			
1	C	180	Total	C	N	O	S	0	3	0
			1495	968	240	281	6			
1	E	180	Total	C	N	O	S	0	3	0
			1494	967	240	282	5			
1	G	180	Total	C	N	O	S	0	3	0
			1494	965	240	284	5			

- Molecule 2 is a protein called peptide,HLA class II histocompatibility antigen, DP beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	1	0
			1638	1031	288	311	8			
2	D	199	Total	C	N	O	S	0	2	0
			1646	1035	289	313	9			
2	F	190	Total	C	N	O	S	0	5	0
			1598	1002	278	309	9			
2	H	191	Total	C	N	O	S	0	3	0
			1583	997	273	305	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLY	-	linker	PDB ?
B	-12	GLY	-	linker	PDB ?
B	-11	SER	-	linker	PDB ?
B	-10	LEU	-	linker	PDB ?
B	-9	VAL	-	linker	PDB ?
B	-8	PRO	-	linker	PDB ?
B	-7	ARG	-	linker	PDB ?
B	-6	GLY	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	linker	PDB ?
B	-4	GLY	-	linker	PDB ?
B	-3	GLY	-	linker	PDB ?
B	-2	GLY	-	linker	PDB ?
B	-1	GLY	-	linker	PDB ?
B	3	SER	THR	variant	UNP Q5EP54
D	-13	GLY	-	linker	PDB ?
D	-12	GLY	-	linker	PDB ?
D	-11	SER	-	linker	PDB ?
D	-10	LEU	-	linker	PDB ?
D	-9	VAL	-	linker	PDB ?
D	-8	PRO	-	linker	PDB ?
D	-7	ARG	-	linker	PDB ?
D	-6	GLY	-	linker	PDB ?
D	-5	SER	-	linker	PDB ?
D	-4	GLY	-	linker	PDB ?
D	-3	GLY	-	linker	PDB ?
D	-2	GLY	-	linker	PDB ?
D	-1	GLY	-	linker	PDB ?
D	3	SER	THR	variant	UNP Q5EP54
F	-13	GLY	-	linker	PDB ?
F	-12	GLY	-	linker	PDB ?
F	-11	SER	-	linker	PDB ?
F	-10	LEU	-	linker	PDB ?
F	-9	VAL	-	linker	PDB ?
F	-8	PRO	-	linker	PDB ?
F	-7	ARG	-	linker	PDB ?
F	-6	GLY	-	linker	PDB ?
F	-5	SER	-	linker	PDB ?
F	-4	GLY	-	linker	PDB ?
F	-3	GLY	-	linker	PDB ?
F	-2	GLY	-	linker	PDB ?
F	-1	GLY	-	linker	PDB ?
F	3	SER	THR	variant	UNP Q5EP54
H	-13	GLY	-	linker	PDB ?
H	-12	GLY	-	linker	PDB ?
H	-11	SER	-	linker	PDB ?
H	-10	LEU	-	linker	PDB ?
H	-9	VAL	-	linker	PDB ?
H	-8	PRO	-	linker	PDB ?
H	-7	ARG	-	linker	PDB ?
H	-6	GLY	-	linker	PDB ?

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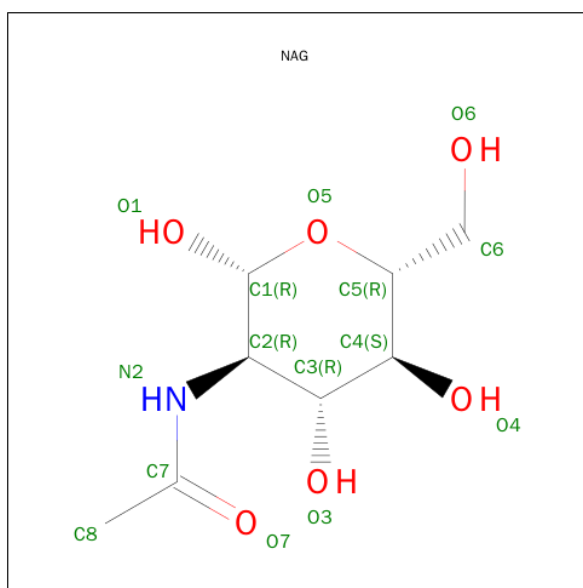
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	SER	-	linker	PDB ?
H	-4	GLY	-	linker	PDB ?
H	-3	GLY	-	linker	PDB ?
H	-2	GLY	-	linker	PDB ?
H	-1	GLY	-	linker	PDB ?
H	3	SER	THR	variant	UNP Q5EP54

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



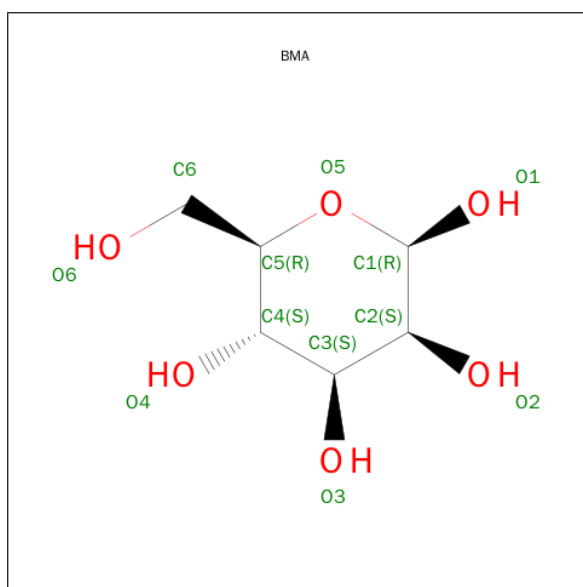
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			11	6	5		
5	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is water.

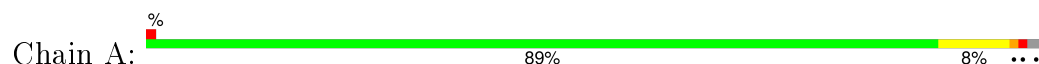
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	205	Total	O	0	0
			205	205		
6	B	192	Total	O	0	0
			192	192		
6	C	225	Total	O	0	0
			225	225		
6	D	195	Total	O	0	0
			195	195		
6	E	222	Total	O	0	0
			222	222		
6	F	207	Total	O	0	0
			207	207		
6	G	200	Total	O	0	0
			200	200		
6	H	214	Total	O	0	0
			214	214		



### 3 Residue-property plots [i](#)

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

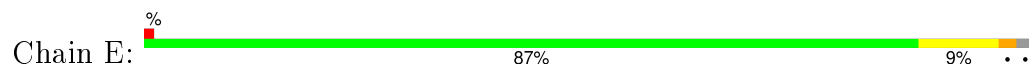
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



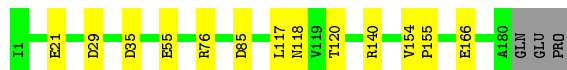
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



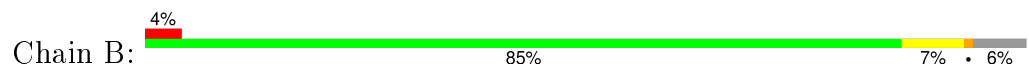
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

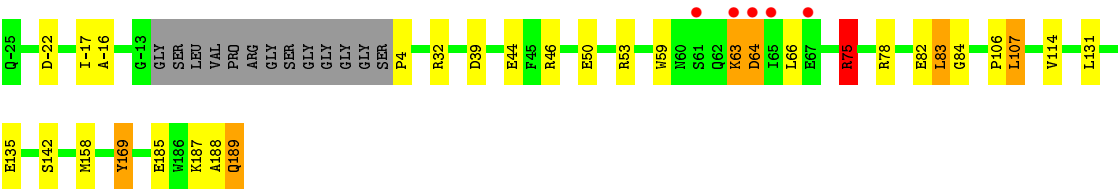


- Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

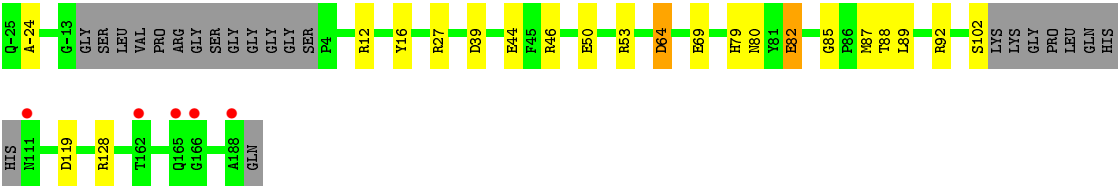
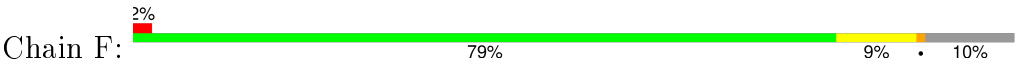


- Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain

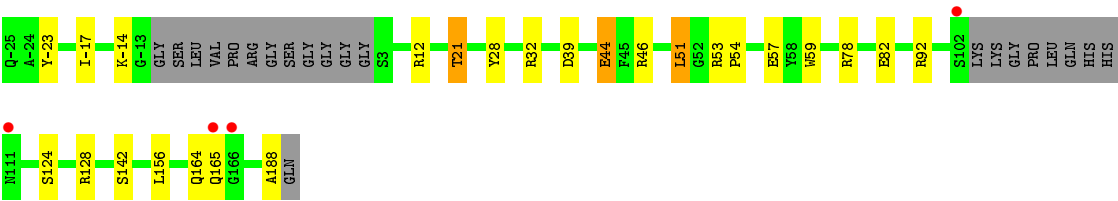
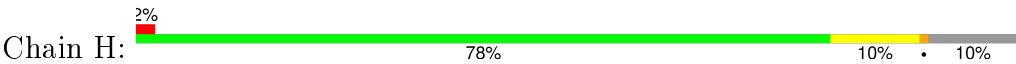




• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain



• Molecule 2: peptide,HLA class II histocompatibility antigen, DP beta 1 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.63Å 130.47Å 107.99Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	47.98 – 1.70 47.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	87.5 (47.98-1.70) 87.5 (47.98-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.168 , 0.204 0.178 , 0.213	Depositor DCC
$R_{free}$ test set	10564 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 207071 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, BMA, 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	1.11	2/1538 (0.1%)	1.09	8/2098 (0.4%)
1	C	1.20	6/1546 (0.4%)	1.06	3/2109 (0.1%)
1	E	1.16	4/1545 (0.3%)	1.08	6/2109 (0.3%)
1	G	1.10	1/1545 (0.1%)	1.03	5/2111 (0.2%)
2	B	1.11	0/1681	1.09	4/2279 (0.2%)
2	D	1.13	2/1689 (0.1%)	1.06	4/2288 (0.2%)
2	F	1.21	3/1635 (0.2%)	1.15	6/2215 (0.3%)
2	H	1.19	5/1625 (0.3%)	1.16	5/2203 (0.2%)
All	All	1.15	23/12804 (0.2%)	1.09	41/17412 (0.2%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	55	GLU	CD-OE2	8.10	1.34	1.25
2	F	82	GLU	CD-OE2	7.80	1.34	1.25
1	E	95	GLU	CD-OE2	7.69	1.34	1.25
1	E	55	GLU	CD-OE1	6.96	1.33	1.25
1	C	40	GLU	CD-OE1	6.87	1.33	1.25
1	C	150	TYR	CG-CD1	6.68	1.47	1.39
2	F	69	GLU	CD-OE2	6.39	1.32	1.25
1	C	150	TYR	CG-CD2	-5.95	1.31	1.39
1	C	166	GLU	CG-CD	5.77	1.60	1.51
1	A	15	THR	CB-CG2	-5.75	1.33	1.52
2	H	44	GLU	CG-CD	5.75	1.60	1.51
2	F	16	TYR	CE1-CZ	-5.71	1.31	1.38
1	C	40	GLU	CD-OE2	5.64	1.31	1.25
1	E	57	GLN	CD-OE1	5.63	1.36	1.24
1	A	43	TRP	CE2-CZ2	-5.62	1.30	1.39
1	G	166	GLU	CD-OE1	5.58	1.31	1.25
2	H	142	SER	CB-OG	-5.56	1.35	1.42
2	D	142	SER	CB-OG	5.55	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	-23	TYR	CE1-CZ	-5.49	1.31	1.38
2	H	12	ARG	CZ-NH1	5.38	1.40	1.33
2	H	124	SER	CB-OG	-5.36	1.35	1.42
1	C	169	GLY	N-CA	-5.32	1.38	1.46
2	D	169	TYR	CE1-CZ	-5.06	1.31	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	12	ARG	NE-CZ-NH2	-12.07	114.27	120.30
2	H	12	ARG	NE-CZ-NH1	11.71	126.15	120.30
2	B	78	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	A	76	ARG	NE-CZ-NH2	9.63	125.11	120.30
1	A	76	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	C	110	ASP	CB-CG-OD1	9.03	126.42	118.30
2	B	78	ARG	NE-CZ-NH1	-8.63	115.98	120.30
2	D	39	ASP	CB-CG-OD2	-8.35	110.78	118.30
2	D	39	ASP	CB-CG-OD1	7.99	125.50	118.30
1	A	73	LEU	CA-CB-CG	-7.65	97.71	115.30
1	E	21	GLU	OE1-CD-OE2	7.40	132.18	123.30
2	F	12	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	60	LEU	CA-CB-CG	-7.07	99.05	115.30
2	D	75	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	G	140	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	F	39	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	117	LEU	CA-CB-CG	6.06	129.23	115.30
1	C	140	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	110	ASP	CB-CG-OD1	5.89	123.60	118.30
1	E	175	LEU	CA-CB-CG	5.82	128.69	115.30
1	E	164	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	G	21	GLU	OE1-CD-OE2	5.69	130.13	123.30
2	F	64[A]	ASP	CB-CG-OD1	5.65	123.38	118.30
2	F	64[B]	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	36	LEU	CB-CG-CD2	5.62	120.55	111.00
2	F	27	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	G	117	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	117	LEU	CB-CA-C	-5.32	100.10	110.20
2	D	32	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	G	29	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	E	117	LEU	CB-CA-C	-5.27	100.18	110.20
2	H	39	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	169	TYR	CB-CG-CD2	-5.26	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	H	128	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	F	128	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	35	ASP	CB-CG-OD1	5.10	122.89	118.30
2	H	39	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	105	LEU	CB-CG-CD2	5.04	119.56	111.00
1	E	175	LEU	CB-CG-CD2	5.03	119.56	111.00
1	E	29	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1487	0	1392	9	1
1	C	1495	0	1401	3	0
1	E	1494	0	1398	11	0
1	G	1494	0	1393	8	0
2	B	1638	0	1553	12	0
2	D	1646	0	1555	20	0
2	F	1598	0	1489	16	1
2	H	1583	0	1495	17	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	25	0	0
4	B	56	0	49	1	0
4	C	28	0	25	0	0
4	D	42	0	37	1	0
4	E	14	0	13	0	0
4	F	42	0	36	1	0
4	G	28	0	25	0	0
4	H	28	0	24	0	0
5	F	11	0	9	1	0
5	H	11	0	10	0	0
6	A	205	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	192	0	0	3	0
6	C	225	0	0	2	0
6	D	195	0	0	8	0
6	E	222	0	0	7	0
6	F	207	0	0	2	0
6	G	200	0	0	5	1
6	H	214	0	0	6	0
All	All	14385	0	11929	93	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 4.

All (93) 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)
2:F:82:GLU:HG3	6:F:377:HOH:O	1.58	1.00
2:F:44:GLU:CD	2:F:46:ARG:HH12	1.69	0.95
2:F:44:GLU:OE2	2:F:46:ARG:NH1	2.04	0.90
2:D:78:ARG:HD2	6:D:473:HOH:O	1.76	0.85
1:G:85[B]:ASP:OD1	6:G:368:HOH:O	1.94	0.85
2:F:44:GLU:OE1	6:F:301:HOH:O	1.94	0.85
1:E:95:GLU:OE1	2:F:119:ASP:OD2	1.95	0.84
2:B:53:ARG:NH1	6:B:421:HOH:O	2.13	0.81
2:F:50[A]:GLU:H	2:F:50[A]:GLU:CD	1.83	0.78
2:F:44:GLU:CG	2:F:46:ARG:NH1	2.47	0.77
2:F:44:GLU:CG	2:F:46:ARG:HH12	1.98	0.76
2:D:4:PRO:N	6:D:462:HOH:O	2.20	0.74
1:E:118:ASN:OD1	6:E:482:HOH:O	2.04	0.73
1:A:15:THR:CG2	2:B:7:TYR:H	2.01	0.72
5:F:201:BMA:O6	4:F:203:NAG:H2	1.91	0.71
2:F:44:GLU:HG3	2:F:46:ARG:NH1	2.08	0.68
1:G:55:GLU:HG2	6:G:498:HOH:O	1.94	0.68
2:D:185[B]:GLU:OE1	6:D:444:HOH:O	2.08	0.68
2:B:-22:ASP:OD1	6:B:482:HOH:O	2.13	0.67
2:B:33:GLU:OE2	2:B:49:THR:HG21	1.94	0.67
2:D:-22:ASP:OD1	6:D:454:HOH:O	2.11	0.66
1:A:118:ASN:OD1	6:A:301:HOH:O	2.13	0.66
1:E:180:ALA:C	6:E:515:HOH:O	2.33	0.65
2:H:44:GLU:HG3	2:H:46:ARG:NH1	2.11	0.65
1:G:118:ASN:OD1	6:G:433:HOH:O	2.13	0.64
1:E:180:ALA:O	6:E:515:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG23	2:B:7:TYR:H	1.62	0.64
1:C:75:GLN:NE2	6:C:449:HOH:O	2.29	0.64
1:E:170:LEU:O	6:E:331:HOH:O	2.16	0.63
2:H:53:ARG:NH1	6:H:304:HOH:O	2.33	0.61
2:B:-14:LYS:HD2	2:B:58:TYR:CE2	2.36	0.60
2:F:44:GLU:OE2	2:F:46:ARG:CZ	2.49	0.60
2:F:44:GLU:OE2	2:F:46:ARG:NH2	2.35	0.60
2:F:88:THR:OG1	2:F:89:LEU:N	2.35	0.60
2:D:50:GLU:OE2	2:D:53:ARG:HG3	2.01	0.59
1:E:147:LYS:NZ	6:E:449:HOH:O	2.33	0.59
2:D:189:GLN:HE21	2:D:189:GLN:HA	1.66	0.59
2:B:44:GLU:OE2	2:B:46:ARG:NH1	2.31	0.59
2:B:78:ARG:HH21	2:B:78:ARG:HG2	1.69	0.58
2:H:21[A]:THR:HG21	6:H:407:HOH:O	2.03	0.57
2:D:83:LEU:C	2:D:83:LEU:HD12	2.25	0.57
2:D:84:GLY:HA3	6:D:369:HOH:O	2.06	0.56
1:G:85[A]:ASP:OD2	2:H:32:ARG:NH2	2.37	0.56
2:H:78:ARG:O	2:H:82[A]:GLU:HG2	2.06	0.56
1:G:120[A]:THR:HG21	6:G:316:HOH:O	2.06	0.55
1:E:33:TYR:CD1	1:E:136[B]:LEU:HD21	2.43	0.54
2:D:114:VAL:HG22	2:D:158:MET:HG2	1.90	0.54
4:B:202:NAG:O5	4:B:204:NAG:H61	2.08	0.53
1:C:38:LYS:NZ	6:C:500:HOH:O	2.42	0.52
2:H:44:GLU:HG3	2:H:46:ARG:HH12	1.75	0.51
1:G:76:ARG:HD2	2:H:51:LEU:HD22	1.92	0.50
2:D:188:ALA:O	2:D:189:GLN:HB2	2.10	0.50
1:E:162:ASP:HB3	1:E:175:LEU:HD22	1.93	0.50
2:H:188:ALA:O	6:H:507:HOH:O	2.19	0.50
2:H:57:GLU:OE1	6:H:301:HOH:O	2.19	0.49
2:H:53:ARG:N	2:H:54:PRO:HD2	2.28	0.49
2:H:82[A]:GLU:OE1	2:H:82[A]:GLU:HA	2.13	0.49
2:H:53:ARG:N	2:H:54:PRO:CD	2.76	0.48
2:H:92:ARG:NH1	6:H:439:HOH:O	2.47	0.48
2:H:156:LEU:HD12	2:H:156:LEU:N	2.29	0.48
2:H:82[A]:GLU:CA	2:H:82[A]:GLU:OE1	2.63	0.47
1:E:166:GLU:OE1	6:E:480:HOH:O	2.20	0.47
2:B:-17:ILE:HD11	2:B:45:PHE:CZ	2.51	0.46
6:D:463:HOH:O	2:F:92:ARG:NE	2.49	0.45
1:A:15:THR:HG23	2:B:6:ASN:HA	1.99	0.44
4:D:202:NAG:H61	4:D:203:NAG:O5	2.17	0.44
2:D:44:GLU:OE1	2:D:46:ARG:NH1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:PRO:HB2	2:D:107:LEU:HD23	2.00	0.44
1:A:38:LYS:O	1:A:39:LYS:HB2	2.17	0.44
1:C:75:GLN:HA	1:C:75:GLN:OE1	2.17	0.44
2:F:79[B]:HIS:HD2	2:F:80:ASN:OD1	2.01	0.43
2:D:-17:ILE:HG22	2:D:-16:ALA:N	2.33	0.43
2:B:128:ARG:HD2	6:H:439:HOH:O	2.17	0.43
1:E:154:VAL:HA	1:E:155:PRO:HD3	1.89	0.43
2:B:-17:ILE:HD11	2:B:45:PHE:HZ	1.84	0.43
2:D:63:LYS:HG2	2:D:64:ASP:N	2.34	0.43
2:H:-17[A]:ILE:HG21	2:H:59:TRP:CE2	2.54	0.42
1:A:15:THR:HB	6:A:412:HOH:O	2.19	0.42
1:A:95:GLU:HG2	6:B:349:HOH:O	2.19	0.42
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.93	0.42
2:H:-17[B]:ILE:HG12	2:H:28:TYR:CZ	2.55	0.42
2:F:-24:ALA:O	2:F:79[B]:HIS:NE2	2.46	0.42
2:D:75:ARG:HH11	2:D:75:ARG:HG2	1.85	0.42
2:D:-17:ILE:CG2	2:D:59:TRP:CZ2	3.03	0.42
2:F:50[B]:GLU:HG2	2:F:53:ARG:CZ	2.50	0.41
1:G:154:VAL:HA	1:G:155:PRO:HD3	1.93	0.41
2:D:63:LYS:HG2	2:D:64:ASP:H	1.86	0.41
2:D:131:LEU:HD13	2:D:169:TYR:CE2	2.56	0.41
1:G:55:GLU:OE2	6:G:301:HOH:O	2.21	0.40
2:D:82:GLU:OE1	6:D:459:HOH:O	2.21	0.40
1:A:101:GLN:O	1:A:155:PRO:HD2	2.21	0.40
1:E:99:LEU:HD22	6:E:521:HOH:O	2.21	0.40
2:D:135:GLU:OE1	6:D:464:HOH:O	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)
6:A:301:HOH:O	6:G:313:HOH:O[2_645]	2.01	0.19
1:A:39:LYS:NZ	2:F:64[A]:ASP:OD2[2_545]	2.19	0.01

## 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	180/183 (98%)	179 (99%)	1 (1%)	0	100	100
1	C	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	E	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	G	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
2	B	196/212 (92%)	193 (98%)	3 (2%)	0	100	100
2	D	197/212 (93%)	195 (99%)	2 (1%)	0	100	100
2	F	189/212 (89%)	185 (98%)	3 (2%)	1 (0%)	34	15
2	H	188/212 (89%)	182 (97%)	6 (3%)	0	100	100
All	All	1493/1580 (94%)	1474 (99%)	18 (1%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	85	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	163/164 (99%)	158 (97%)	5 (3%)	47	25
1	C	164/164 (100%)	162 (99%)	2 (1%)	78	65
1	E	164/164 (100%)	162 (99%)	2 (1%)	78	65
1	G	164/164 (100%)	164 (100%)	0	100	100
2	B	178/185 (96%)	174 (98%)	4 (2%)	60	39
2	D	179/185 (97%)	171 (96%)	8 (4%)	34	13
2	F	174/185 (94%)	172 (99%)	2 (1%)	80	69
2	H	173/185 (94%)	167 (96%)	6 (4%)	43	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1359/1396 (97%)	1330 (98%)	29 (2%)	61 42

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	15	THR
1	A	60	LEU
1	A	76	ARG
1	A	179	GLU
2	B	-14	LYS
2	B	49	THR
2	B	165	GLN
2	B	189	GLN
1	C	158	GLU
1	C	176	LYS
2	D	63	LYS
2	D	64	ASP
2	D	66	LEU
2	D	75	ARG
2	D	83	LEU
2	D	107	LEU
2	D	187	LYS
2	D	189	GLN
1	E	99	LEU
1	E	127	LEU
2	F	87	MET
2	F	102	SER
2	H	-14	LYS
2	H	21[A]	THR
2	H	21[B]	THR
2	H	51	LEU
2	H	164	GLN
2	H	165	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	62	GLN
2	D	189	GLN
2	H	31	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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$
4	NAG	A	202	1,4	14,14,15	0.67	0	15,19,21	1.51	2 (13%)
4	NAG	A	203	4	14,14,15	0.57	0	15,19,21	2.25	4 (26%)
4	NAG	B	201	2,4	14,14,15	1.03	1 (7%)	15,19,21	3.56	8 (53%)
4	NAG	B	202	4	14,14,15	0.70	0	15,19,21	1.96	3 (20%)
4	NAG	B	203	4	14,14,15	0.63	0	15,19,21	1.33	2 (13%)
4	NAG	B	204	4	14,14,15	0.99	1 (7%)	15,19,21	2.65	6 (40%)
4	NAG	C	202	1,4	14,14,15	1.19	1 (7%)	15,19,21	1.68	4 (26%)
4	NAG	C	203	4	14,14,15	0.58	0	15,19,21	2.20	3 (20%)
4	NAG	D	201	2,4	14,14,15	1.12	2 (14%)	15,19,21	2.02	5 (33%)
4	NAG	D	202	4	14,14,15	0.77	0	15,19,21	2.95	9 (60%)
4	NAG	D	203	4	14,14,15	0.66	0	15,19,21	1.72	1 (6%)
4	NAG	E	201	1	14,14,15	0.98	0	15,19,21	1.64	4 (26%)
5	BMA	F	201	4	11,11,12	0.72	0	14,15,17	5.48	10 (71%)
4	NAG	F	202	4	14,14,15	0.77	0	15,19,21	2.01	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	203	4	14,14,15	0.83	0	15,19,21	1.81	5 (33%)
4	NAG	F	204	2,5,4	14,14,15	1.54	2 (14%)	15,19,21	1.78	3 (20%)
4	NAG	G	201	1,4	14,14,15	0.95	0	15,19,21	2.10	4 (26%)
4	NAG	G	202	4	14,14,15	0.56	0	15,19,21	2.16	3 (20%)
5	BMA	H	201	4	11,11,12	2.19	4 (36%)	14,15,17	4.05	8 (57%)
4	NAG	H	202	2,5,4	14,14,15	1.17	2 (14%)	15,19,21	0.99	1 (6%)
4	NAG	H	203	4	14,14,15	1.20	2 (14%)	15,19,21	1.75	3 (20%)

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
4	NAG	A	202	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	203	4	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	4	-	0/6/23/26	0/1/1/1
4	NAG	B	203	4	-	0/6/23/26	0/1/1/1
4	NAG	B	204	4	-	0/6/23/26	0/1/1/1
4	NAG	C	202	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	203	4	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	202	4	-	0/6/23/26	0/1/1/1
4	NAG	D	203	4	-	0/6/23/26	0/1/1/1
4	NAG	E	201	1	-	0/6/23/26	0/1/1/1
5	BMA	F	201	4	-	0/2/19/22	0/1/1/1
4	NAG	F	202	4	-	0/6/23/26	0/1/1/1
4	NAG	F	203	4	-	0/6/23/26	0/1/1/1
4	NAG	F	204	2,5,4	-	0/6/23/26	0/1/1/1
4	NAG	G	201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	202	4	-	0/6/23/26	0/1/1/1
5	BMA	H	201	4	-	0/2/19/22	0/1/1/1
4	NAG	H	202	2,5,4	-	0/6/23/26	0/1/1/1
4	NAG	H	203	4	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	201	BMA	O5-C1	-5.30	1.34	1.43
4	F	204	NAG	O5-C1	-4.05	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	202	NAG	O5-C1	-3.42	1.38	1.43
5	H	201	BMA	C6-C5	-2.84	1.41	1.51
5	H	201	BMA	C4-C5	-2.34	1.48	1.53
5	H	201	BMA	O3-C3	-2.29	1.37	1.43
4	F	204	NAG	C2-N2	-2.27	1.42	1.46
4	C	202	NAG	O3-C3	-2.27	1.37	1.43
4	D	201	NAG	O5-C1	-2.21	1.40	1.43
4	H	202	NAG	C2-N2	-2.14	1.42	1.46
4	B	201	NAG	O5-C1	-2.10	1.40	1.43
4	D	201	NAG	C8-C7	-2.09	1.46	1.50
4	H	203	NAG	C8-C7	2.05	1.54	1.50
4	B	204	NAG	C1-C2	2.37	1.55	1.52
4	H	203	NAG	C1-C2	3.14	1.56	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	201	BMA	O4-C4-C3	-11.06	85.44	110.34
5	H	201	BMA	O4-C4-C3	-9.09	89.86	110.34
5	F	201	BMA	O4-C4-C5	-7.96	88.13	109.24
5	H	201	BMA	O6-C6-C5	-6.37	90.28	111.33
4	B	201	NAG	O5-C5-C6	-5.76	94.88	107.35
5	H	201	BMA	O4-C4-C5	-5.63	94.31	109.24
4	D	203	NAG	C2-N2-C7	-4.97	116.66	123.04
4	G	201	NAG	O3-C3-C2	-4.88	99.46	109.11
4	A	203	NAG	C3-C4-C5	-4.80	101.83	110.20
4	B	204	NAG	O6-C6-C5	-4.76	95.60	111.33
4	B	202	NAG	O6-C6-C5	-4.26	97.25	111.33
4	B	202	NAG	C3-C4-C5	-4.03	103.17	110.20
4	A	202	NAG	C2-N2-C7	-4.02	117.88	123.04
4	B	201	NAG	O7-C7-C8	-3.86	114.97	122.06
4	C	202	NAG	C3-C4-C5	-3.83	103.53	110.20
4	H	203	NAG	O6-C6-C5	-3.76	98.91	111.33
4	F	202	NAG	C4-C3-C2	-3.62	105.59	111.23
4	D	201	NAG	O7-C7-C8	-3.53	115.59	122.06
4	E	201	NAG	O7-C7-C8	-3.51	115.62	122.06
4	A	203	NAG	C1-O5-C5	-3.46	107.86	112.25
4	G	201	NAG	O7-C7-C8	-3.41	115.80	122.06
4	A	203	NAG	C2-N2-C7	-3.37	118.71	123.04
4	F	203	NAG	O4-C4-C3	-3.27	102.97	110.34
4	F	203	NAG	C4-C3-C2	-3.20	106.25	111.23
4	D	202	NAG	O6-C6-C5	-3.18	100.82	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	203	NAG	O4-C4-C5	-3.03	101.20	109.24
4	B	201	NAG	O3-C3-C4	-3.02	103.54	110.34
4	G	202	NAG	O7-C7-C8	-3.02	116.53	122.06
4	C	203	NAG	C2-N2-C7	-2.99	119.20	123.04
4	D	202	NAG	O3-C3-C2	-2.94	103.29	109.11
4	B	203	NAG	C4-C3-C2	-2.91	106.71	111.23
4	E	201	NAG	C3-C4-C5	-2.89	105.16	110.20
4	B	201	NAG	O4-C4-C3	-2.88	103.86	110.34
4	F	204	NAG	O3-C3-C2	-2.62	103.92	109.11
4	H	203	NAG	O5-C5-C6	-2.44	102.07	107.35
4	D	202	NAG	C2-N2-C7	-2.42	119.93	123.04
4	B	204	NAG	C3-C2-N2	-2.38	104.86	110.56
4	D	201	NAG	O4-C4-C3	-2.36	105.02	110.34
4	D	202	NAG	O7-C7-C8	-2.23	117.97	122.06
4	C	202	NAG	O4-C4-C3	-2.20	105.38	110.34
4	B	204	NAG	O4-C4-C5	-2.19	103.43	109.24
4	F	203	NAG	C1-O5-C5	-2.17	109.50	112.25
4	F	202	NAG	C6-C5-C4	-2.16	107.70	113.02
4	C	202	NAG	O6-C6-C5	-2.09	104.43	111.33
4	D	202	NAG	O3-C3-C4	-2.06	105.70	110.34
4	G	202	NAG	O3-C3-C4	-2.01	105.82	110.34
4	B	201	NAG	C8-C7-N2	2.01	119.95	116.11
4	F	202	NAG	O6-C6-C5	2.02	118.01	111.33
4	F	203	NAG	O7-C7-N2	2.08	126.10	121.86
4	F	204	NAG	C1-O5-C5	2.11	114.92	112.25
4	F	203	NAG	O5-C5-C6	2.17	112.06	107.35
4	D	201	NAG	C8-C7-N2	2.18	120.28	116.11
4	D	202	NAG	C3-C4-C5	2.21	114.05	110.20
4	H	202	NAG	O5-C5-C6	2.23	112.17	107.35
4	G	201	NAG	O3-C3-C4	2.23	115.37	110.34
4	A	202	NAG	C4-C3-C2	2.32	114.84	111.23
5	F	201	BMA	O3-C3-C4	2.33	115.59	110.34
4	C	203	NAG	O4-C4-C5	2.44	115.71	109.24
5	F	201	BMA	C6-C5-C4	2.60	119.44	113.02
4	F	202	NAG	O5-C5-C6	2.62	113.02	107.35
4	E	201	NAG	C8-C7-N2	2.65	121.18	116.11
4	C	202	NAG	C4-C3-C2	2.69	115.41	111.23
5	F	201	BMA	O3-C3-C2	2.71	114.90	110.00
4	B	204	NAG	C2-N2-C7	2.74	126.56	123.04
5	F	201	BMA	C2-C3-C4	2.76	115.73	111.04
4	E	201	NAG	O4-C4-C5	2.87	116.85	109.24
4	D	202	NAG	C8-C7-N2	2.92	121.69	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	BMA	O5-C5-C6	3.08	114.02	107.35
4	B	201	NAG	C2-N2-C7	3.12	127.05	123.04
4	G	201	NAG	C2-N2-C7	3.27	127.24	123.04
5	H	201	BMA	C2-C3-C4	3.52	117.02	111.04
5	H	201	BMA	C3-C4-C5	3.64	116.54	110.20
4	B	203	NAG	C1-O5-C5	3.67	116.91	112.25
4	B	202	NAG	C1-O5-C5	3.70	116.94	112.25
4	F	202	NAG	C1-O5-C5	3.77	117.03	112.25
4	D	201	NAG	O5-C5-C6	3.78	115.54	107.35
5	H	201	BMA	C1-O5-C5	3.81	117.08	112.25
4	D	201	NAG	C1-O5-C5	3.93	117.24	112.25
4	D	202	NAG	C4-C3-C2	3.94	117.35	111.23
4	A	203	NAG	O5-C5-C6	4.08	116.17	107.35
5	H	201	BMA	O3-C3-C2	4.24	117.66	110.00
4	B	204	NAG	C4-C3-C2	4.62	118.41	111.23
4	F	204	NAG	C2-N2-C7	5.12	129.61	123.04
4	B	204	NAG	C1-O5-C5	5.17	118.81	112.25
5	F	201	BMA	C3-C4-C5	5.18	119.22	110.20
5	F	201	BMA	C1-C2-C3	5.45	115.99	109.54
4	B	201	NAG	O6-C6-C5	5.85	130.65	111.33
4	G	202	NAG	C1-O5-C5	6.51	120.52	112.25
4	C	203	NAG	C1-O5-C5	6.76	120.83	112.25
5	F	201	BMA	O5-C5-C6	7.13	122.79	107.35
4	D	202	NAG	C1-O5-C5	7.96	122.35	112.25
4	B	201	NAG	C1-O5-C5	8.44	122.96	112.25
5	F	201	BMA	C1-O5-C5	9.78	124.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	NAG	1	0
4	B	204	NAG	1	0
4	D	202	NAG	1	0
4	D	203	NAG	1	0
5	F	201	BMA	1	0
4	F	203	NAG	1	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	180/183 (98%)	-0.23	1 (0%) 90 92	13, 21, 38, 56	0
1	C	180/183 (98%)	-0.35	1 (0%) 90 92	12, 20, 34, 52	0
1	E	180/183 (98%)	-0.29	1 (0%) 90 92	11, 20, 39, 56	0
1	G	180/183 (98%)	-0.26	0 100 100	10, 20, 37, 50	0
2	B	199/212 (93%)	-0.07	8 (4%) 42 46	11, 23, 50, 68	0
2	D	199/212 (93%)	-0.06	5 (2%) 61 65	10, 23, 48, 68	0
2	F	190/212 (89%)	-0.16	5 (2%) 59 64	11, 20, 42, 65	0
2	H	191/212 (90%)	-0.23	4 (2%) 67 71	11, 20, 42, 56	0
All	All	1499/1580 (94%)	-0.20	25 (1%) 73 77	10, 21, 42, 68	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	165	GLN	4.9
2	H	165	GLN	4.7
2	H	166	GLY	4.2
2	F	166	GLY	4.1
2	F	188	ALA	3.5
1	A	158	GLU	3.5
2	H	111	ASN	3.1
1	C	171	ASP	3.0
2	D	63	LYS	2.9
2	D	67	GLU	2.8
2	B	64	ASP	2.8
2	F	162	THR	2.6
2	B	103	LYS	2.6
2	B	105	GLY	2.5
2	B	67	GLU	2.4
2	D	61	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	102	SER	2.3
2	D	65	ILE	2.3
2	B	44	GLU	2.3
1	E	158	GLU	2.2
2	D	64	ASP	2.2
2	B	63	LYS	2.2
2	B	50	GLU	2.1
2	F	111	ASN	2.0
2	B	53	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	E	201	14/15	0.91	0.12	2.71	27,37,51,52	0
4	NAG	A	202	14/15	0.87	0.11	1.50	25,35,46,48	0
4	NAG	C	202	14/15	0.90	0.09	0.69	28,32,45,47	0
4	NAG	B	201	14/15	0.94	0.07	0.33	22,28,41,54	0
4	NAG	G	201	14/15	0.92	0.10	0.09	26,31,43,47	0
4	NAG	D	201	14/15	0.95	0.07	-0.42	24,30,37,47	0
3	NA	C	201	1/1	0.99	0.05	-1.05	32,32,32,32	0
4	NAG	H	202	14/15	0.98	0.06	-1.14	15,17,22,25	0
4	NAG	F	204	14/15	0.97	0.06	-1.76	14,17,24,24	0
4	NAG	H	203	14/15	0.91	0.10	-	24,28,33,41	0
4	NAG	F	203	14/15	0.95	0.11	-	21,28,34,40	0
5	BMA	H	201	11/12	0.92	0.09	-	21,29,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	F	201	11/12	0.94	0.09	-	21,27,35,53	0
4	NAG	D	203	14/15	0.83	0.18	-	41,45,55,65	0
4	NAG	B	203	14/15	0.72	0.33	-	60,72,83,84	0
4	NAG	A	203	14/15	0.84	0.21	-	47,57,74,80	0
4	NAG	B	202	14/15	0.85	0.18	-	36,42,52,62	0
3	NA	A	201	1/1	0.98	0.06	-	31,31,31,31	0
4	NAG	D	202	14/15	0.89	0.18	-	37,54,72,85	0
4	NAG	F	202	14/15	0.79	0.26	-	45,55,77,86	0
4	NAG	G	202	14/15	0.87	0.23	-	50,60,73,74	0
4	NAG	B	204	14/15	0.88	0.18	-	33,48,72,87	0
4	NAG	C	203	14/15	0.78	0.21	-	46,53,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.