



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:50 am GMT

PDB ID : 4EEF
Title : Crystal structure of the designed inhibitor protein F-HB80.4 in complex with the 1918 influenza virus hemagglutinin.
Authors : Dreyfus, C.; Wilson, I.A.
Deposited on : 2012-03-28
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

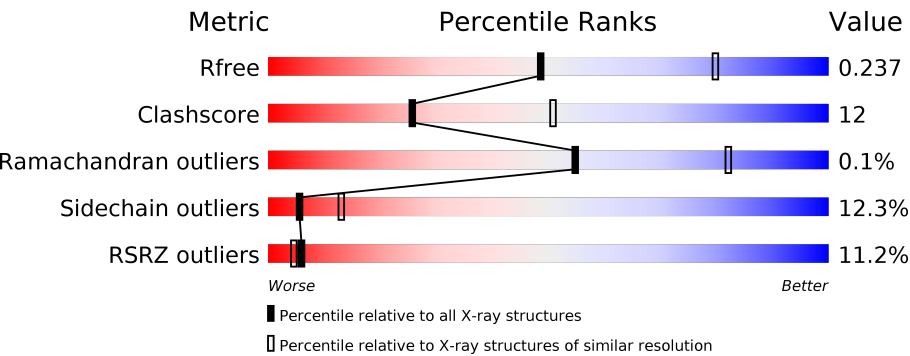
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 ≥ 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	331	<div><div>3%</div><div><div></div><div>74%</div><div>21%</div><div></div><div></div></div><div></div></div>
1	C	331	<div><div>%</div><div><div></div><div>73%</div><div>22%</div><div></div><div></div></div><div></div></div>
1	E	331	<div><div>%</div><div><div></div><div>69%</div><div>25%</div><div></div><div></div></div><div></div></div>
2	B	179	<div><div>22%</div><div><div></div><div>61%</div><div>29%</div><div>6%</div><div></div></div><div></div></div>
2	D	179	<div><div>15%</div><div><div></div><div>61%</div><div>32%</div><div></div><div></div></div><div></div></div>
2	F	179	<div><div>24%</div><div><div></div><div>47%</div><div>42%</div><div>6%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	74	<div><div><div></div><div></div><div></div><div></div></div><div>15%46%14%•39%</div></div>
3	H	74	<div><div><div></div><div></div><div></div><div></div></div><div>19%55%7%•36%</div></div>
3	I	74	<div><div><div></div><div></div><div></div><div></div></div><div>39%49%15%36%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12880 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	8	2	0
			2529	1594	434	490	11			
1	C	323	Total	C	N	O	S	6	1	0
			2510	1583	431	485	11			
1	E	323	Total	C	N	O	S	0	1	0
			2512	1583	432	486	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	THR	CONFLICT	UNP Q9WFX3
A	9	PRO	ASN	CONFLICT	UNP Q9WFX3
A	10	GLY	ALA	CONFLICT	UNP Q9WFX3
C	8	ASP	THR	CONFLICT	UNP Q9WFX3
C	9	PRO	ASN	CONFLICT	UNP Q9WFX3
C	10	GLY	ALA	CONFLICT	UNP Q9WFX3
E	8	ASP	THR	CONFLICT	UNP Q9WFX3
E	9	PRO	ASN	CONFLICT	UNP Q9WFX3
E	10	GLY	ALA	CONFLICT	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1394	871	239	278	6			
2	D	173	Total	C	N	O	S	5	1	0
			1399	874	240	279	6			
2	F	171	Total	C	N	O	S	0	1	0
			1382	863	238	275	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
B	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
B	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3
D	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
D	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
D	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3
F	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
F	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
F	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3

- Molecule 3 is a protein called F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	45	Total	C	N	O	0	0	0
			301	195	49	57			
3	H	47	Total	C	N	O	0	0	0
			303	195	53	55			
3	I	47	Total	C	N	O	0	0	0
			294	187	53	54			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	13	Total	O	0	0
			13	13		
5	C	37	Total	O	0	0
			37	37		
5	D	7	Total	O	0	0
			7	7		

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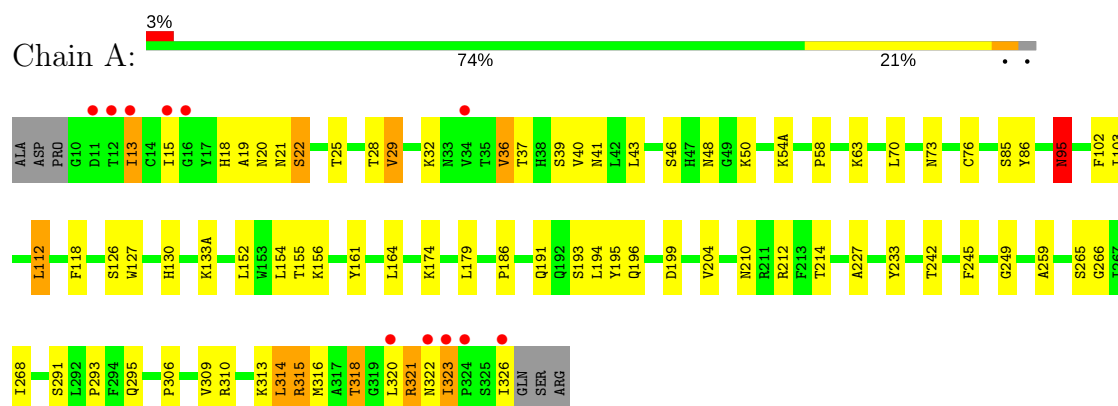
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	23	Total 23	O 23	0	0
5	F	9	Total 9	O 9	0	0

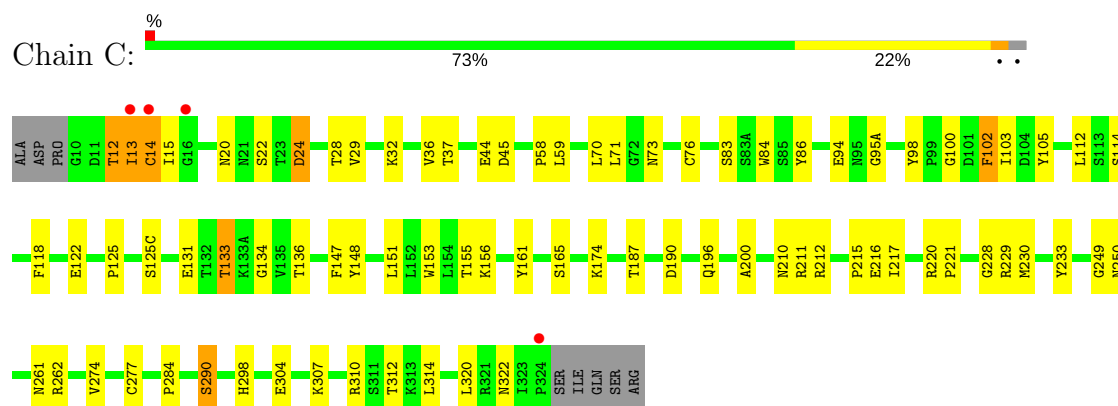
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

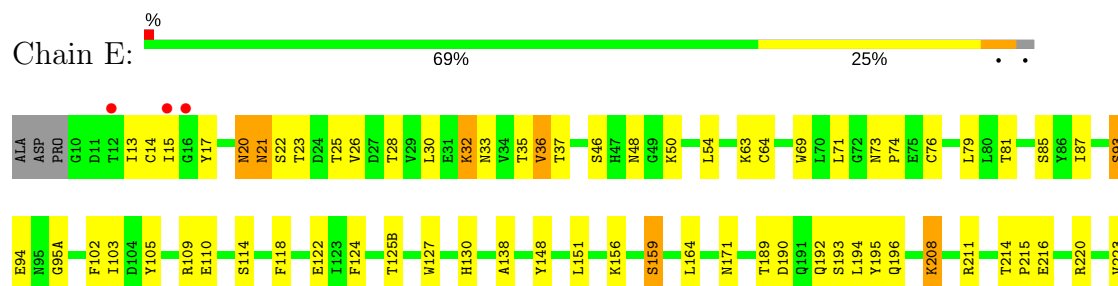
- Molecule 1: Hemagglutinin HA1 chain

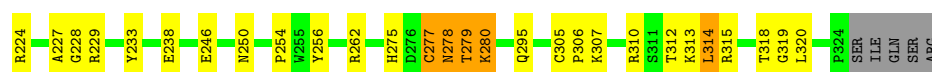


- Molecule 1: Hemagglutinin HA1 chain

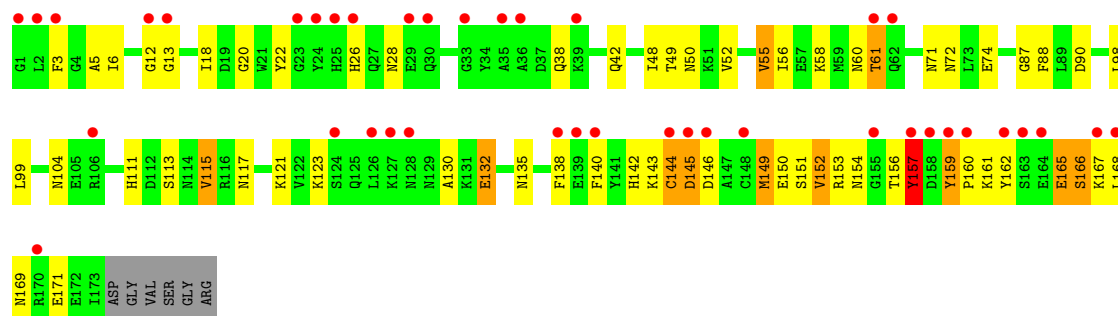


- Molecule 1: Hemagglutinin HA1 chain

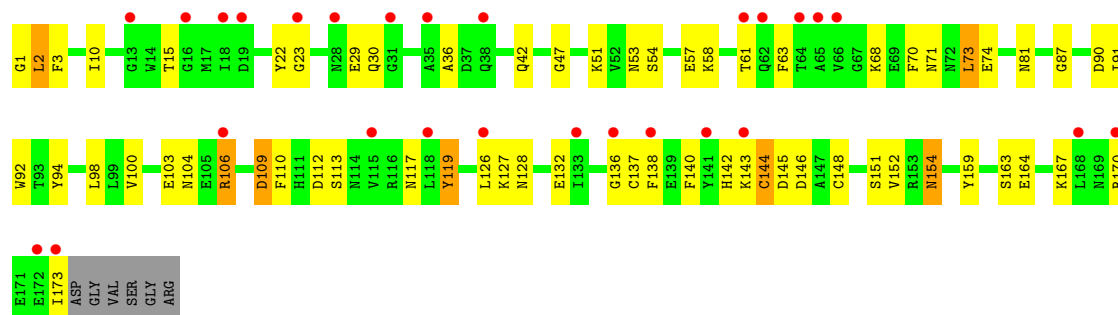




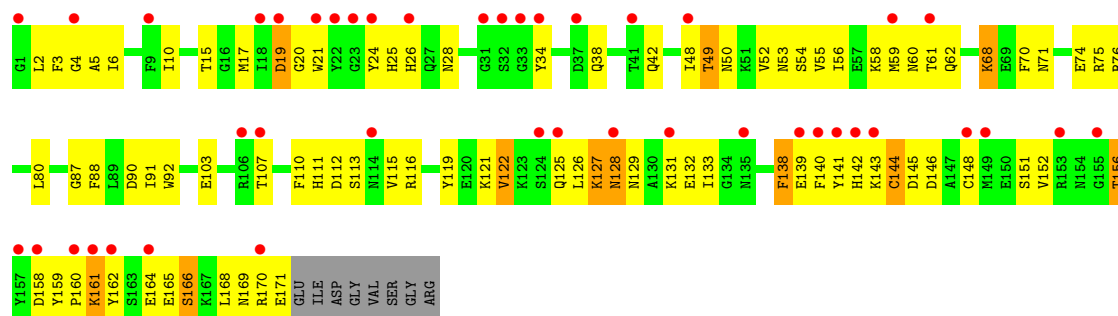
• Molecule 2: Hemagglutinin HA2 chain



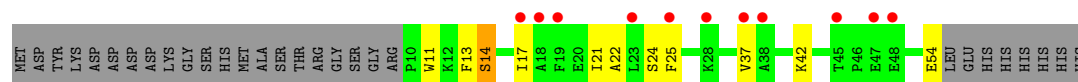
• Molecule 2: Hemagglutinin HA2 chain



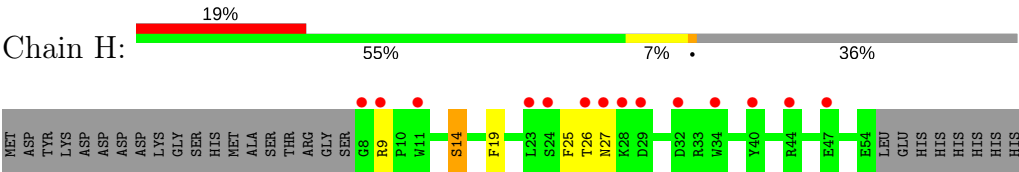
• Molecule 2: Hemagglutinin HA2 chain



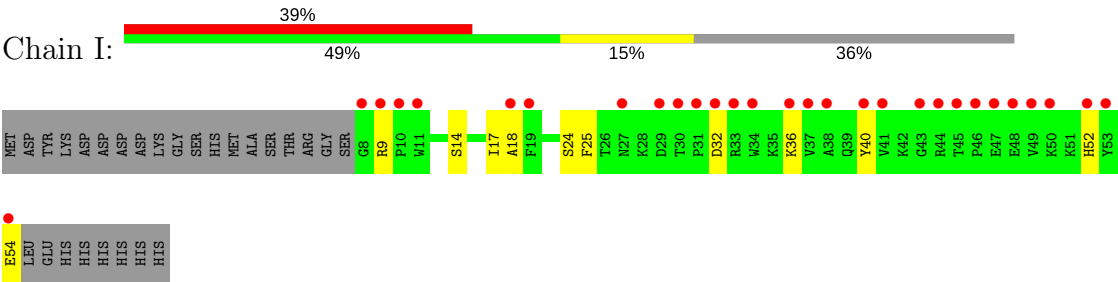
• Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



● Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



● Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.33Å 126.15Å 243.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.70 43.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.67-2.70) 90.2 (43.67-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.229 , 0.285 0.232 , 0.237	Depositor DCC
R_{free} test set	2952 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12880	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2596	0.67	0/3536
1	C	0.50	0/2577	0.66	0/3510
1	E	0.48	0/2576	0.64	0/3509
2	B	0.42	0/1421	0.65	1/1913 (0.1%)
2	D	0.39	0/1429	0.58	0/1924
2	F	0.38	0/1412	0.61	0/1901
3	G	0.38	0/308	0.63	0/421
3	H	0.30	0/309	0.60	0/423
3	I	0.29	0/299	0.54	0/409
All	All	0.45	0/12927	0.64	1/17546 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	F	0	2
3	G	0	1
3	H	0	3
3	I	0	1
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	MET	CG-SD-CE	6.58	110.73	100.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ASN	Peptide
2	B	157	TYR	Peptide
2	F	144	CYS	Peptide
2	F	168	LEU	Peptide
3	G	42	LYS	Peptide

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	2529	0	2453	46	0
1	C	2510	0	2435	52	0
1	E	2512	0	2431	71	0
2	B	1394	0	1312	59	0
2	D	1399	0	1318	51	0
2	F	1382	0	1300	75	0
3	G	301	0	212	9	0
3	H	303	0	217	1	0
3	I	294	0	203	8	0
4	A	39	0	34	0	0
4	C	39	0	34	0	0
4	E	39	0	34	1	0
5	A	50	0	0	0	0
5	B	13	0	0	0	0
5	C	37	0	0	1	0
5	D	7	0	0	0	0
5	E	23	0	0	2	0
5	F	9	0	0	1	0
All	All	12880	0	11983	294	0

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 12.

The worst 5 of 294 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:E:307:LYS:HD2	2:F:59:MET:CE	1.70	1.19
1:E:307:LYS:CD	2:F:59:MET:CE	2.25	1.13
2:D:70:PHE:HA	2:D:74:GLU:OE1	1.51	1.10
1:E:307:LYS:HD2	2:F:59:MET:HE3	1.12	1.10
3:G:14:SER:HA	3:G:17:ILE:HD12	1.32	1.10

There are no symmetry-related clashes.

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	325/331 (98%)	316 (97%)	9 (3%)	0	100	100
1	C	322/331 (97%)	314 (98%)	8 (2%)	0	100	100
1	E	322/331 (97%)	309 (96%)	13 (4%)	0	100	100
2	B	171/179 (96%)	160 (94%)	11 (6%)	0	100	100
2	D	172/179 (96%)	162 (94%)	10 (6%)	0	100	100
2	F	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
3	G	43/74 (58%)	39 (91%)	4 (9%)	0	100	100
3	H	45/74 (61%)	41 (91%)	3 (7%)	1 (2%)	8	20
3	I	45/74 (61%)	40 (89%)	5 (11%)	0	100	100
All	All	1615/1752 (92%)	1538 (95%)	76 (5%)	1 (0%)	55	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	26	THR

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	282/285 (99%)	251 (89%)	31 (11%)	7	17
1	C	279/285 (98%)	256 (92%)	23 (8%)	13	30
1	E	279/285 (98%)	246 (88%)	33 (12%)	6	14
2	B	148/152 (97%)	127 (86%)	21 (14%)	4	9
2	D	149/152 (98%)	127 (85%)	22 (15%)	3	9
2	F	147/152 (97%)	122 (83%)	25 (17%)	2	6
3	G	18/66 (27%)	13 (72%)	5 (28%)	0	1
3	H	17/66 (26%)	15 (88%)	2 (12%)	6	14
3	I	15/66 (23%)	14 (93%)	1 (7%)	19	42
All	All	1334/1509 (88%)	1171 (88%)	163 (12%)	5	13

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	307	LYS
2	D	140	PHE
2	F	161	LYS
2	D	2	LEU
2	D	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	210	ASN
1	C	261	ASN
1	E	250	ASN
2	B	169	ASN
1	E	20	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 ⓘ

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	401	1,4	14,14,15	0.48	0	15,19,21	2.25	4 (26%)
4	NAG	A	402	4	14,14,15	0.60	0	15,19,21	1.79	3 (20%)
4	BMA	A	403	4	11,11,12	0.60	0	13,15,17	0.89	0
4	NAG	C	401	1,4	14,14,15	0.69	0	15,19,21	2.47	5 (33%)
4	NAG	C	402	4	14,14,15	0.75	1 (7%)	15,19,21	1.54	3 (20%)
4	BMA	C	403	4	11,11,12	0.67	0	13,15,17	1.01	0
4	NAG	E	401	1,4	14,14,15	0.48	0	15,19,21	1.31	3 (20%)
4	NAG	E	402	4	14,14,15	0.72	0	15,19,21	1.38	2 (13%)
4	BMA	E	403	4	11,11,12	0.60	0	13,15,17	0.49	0

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	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	402	4	-	0/6/23/26	0/1/1/1
4	BMA	A	403	4	-	0/2/19/22	0/1/1/1
4	NAG	C	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	402	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	C	403	4	-	0/2/19/22	0/1/1/1
4	NAG	E	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	402	4	-	0/6/23/26	0/1/1/1
4	BMA	E	403	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	NAG	O5-C1	-2.16	1.40	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	NAG	O5-C1-C2	-4.16	105.68	111.47
4	E	402	NAG	C2-N2-C7	-3.65	117.61	122.94
4	C	401	NAG	C6-C5-C4	-2.71	106.65	113.00
4	E	401	NAG	C6-C5-C4	-2.61	106.89	113.00
4	C	401	NAG	O7-C7-C8	-2.57	117.37	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	NAG	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/331 (98%)	-0.10	11 (3%) 46 45	25, 53, 103, 161	0
1	C	323/331 (97%)	-0.19	4 (1%) 79 80	30, 58, 97, 120	0
1	E	323/331 (97%)	-0.05	3 (0%) 84 85	34, 62, 106, 155	0
2	B	173/179 (96%)	1.17	40 (23%) 1 1	36, 105, 151, 174	0
2	D	173/179 (96%)	0.86	27 (15%) 2 2	28, 102, 129, 153	0
2	F	171/179 (95%)	1.40	43 (25%) 1 0	28, 121, 172, 183	0
3	G	45/74 (60%)	1.26	11 (24%) 1 1	63, 121, 145, 159	0
3	H	47/74 (63%)	1.42	14 (29%) 1 0	100, 125, 158, 186	0
3	I	47/74 (63%)	2.73	29 (61%) 0 0	111, 156, 179, 208	0
All	All	1627/1752 (92%)	0.45	182 (11%) 6 4	25, 74, 153, 208	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	27	ASN	11.8
3	I	8	GLY	11.5
2	B	138	PHE	7.6
3	I	43	GLY	7.4
2	F	149	MET	7.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	401	14/15	0.93	0.17	-0.14	48,60,67,72	0
4	NAG	E	401	14/15	0.95	0.16	-0.24	38,50,64,74	0
4	NAG	C	401	14/15	0.96	0.12	-1.18	27,47,62,74	0
4	NAG	C	402	14/15	0.95	0.14	-	67,76,88,95	0
4	BMA	E	403	11/12	0.84	0.18	-	97,99,109,109	0
4	BMA	C	403	11/12	0.67	0.24	-	98,102,104,105	0
4	NAG	E	402	14/15	0.89	0.15	-	72,78,85,92	0
4	BMA	A	403	11/12	0.78	0.21	-	89,94,107,110	0
4	NAG	A	402	14/15	0.92	0.13	-	51,65,82,82	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.