Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2017 – 11:29 AM EDT

PDB ID	:	5VJK
Title	:	Crystal structure of H7 hemagglutinin mutant (V186K, K193T, G228S) from the influenza virus A/Shanghai/2/2013 (H7N9)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2017-04-19
Resolution	:	2.59 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) 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	:	rb-20029077
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)	:	rb-20029077

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 2.59 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.
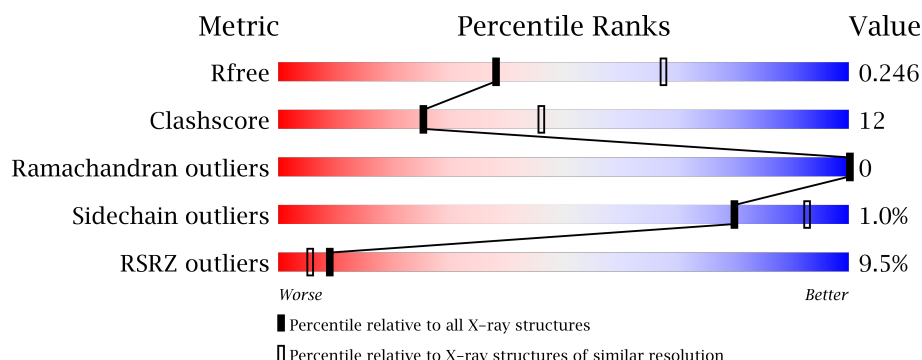
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 <=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	325	3% / 73% / 22% / · ·
2	B	183	20% / 72% / 18% / · / 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3904 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2406	1494	435	462	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP R4NN21
A	8	ASP	-	expression tag	UNP R4NN21
A	9	PRO	-	expression tag	UNP R4NN21
A	10	GLY	-	expression tag	UNP R4NN21
A	186	LYS	VAL	engineered mutation	UNP R4NN21
A	193	THR	LYS	engineered mutation	UNP R4NN21
A	228	SER	GLY	engineered mutation	UNP R4NN21

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1360	841	235	277	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP R4NN21
B	178	GLY	-	expression tag	UNP R4NN21
B	179	ARG	-	expression tag	UNP R4NN21
B	180	LEU	-	expression tag	UNP R4NN21
B	181	VAL	-	expression tag	UNP R4NN21
B	182	PRO	-	expression tag	UNP R4NN21
B	183	ARG	-	expression tag	UNP R4NN21

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
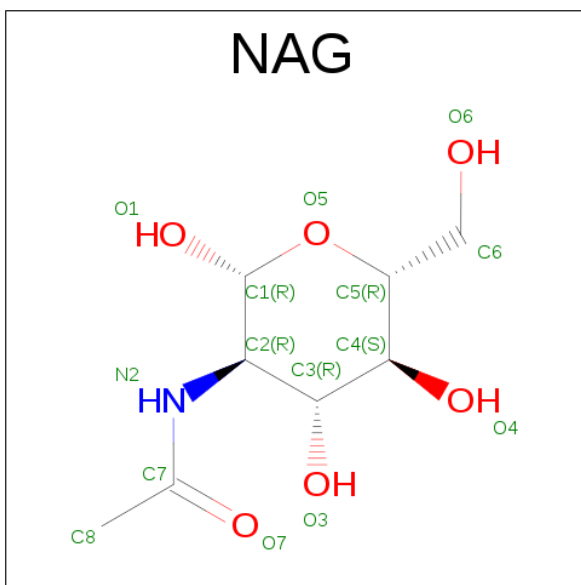
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
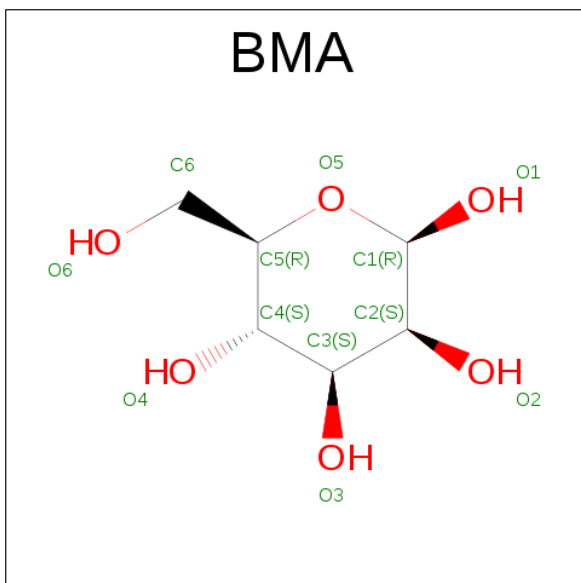
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 11	C 6	O 5	0	0

- Molecule 5 is water.

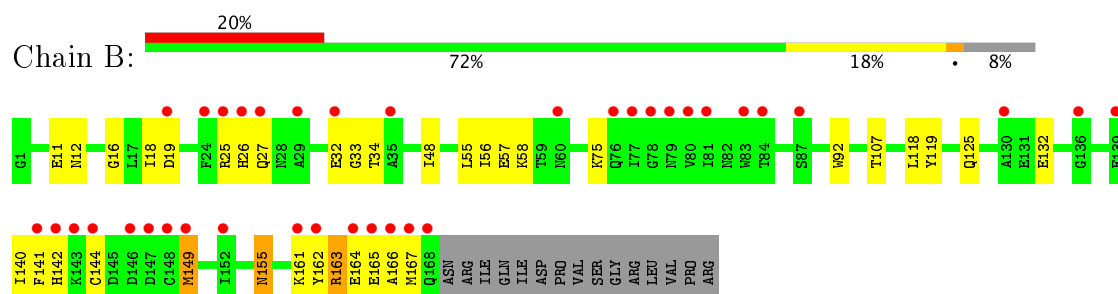| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total 48	O 48	0	0
5	B	23	Total 23	O 23	0	0

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
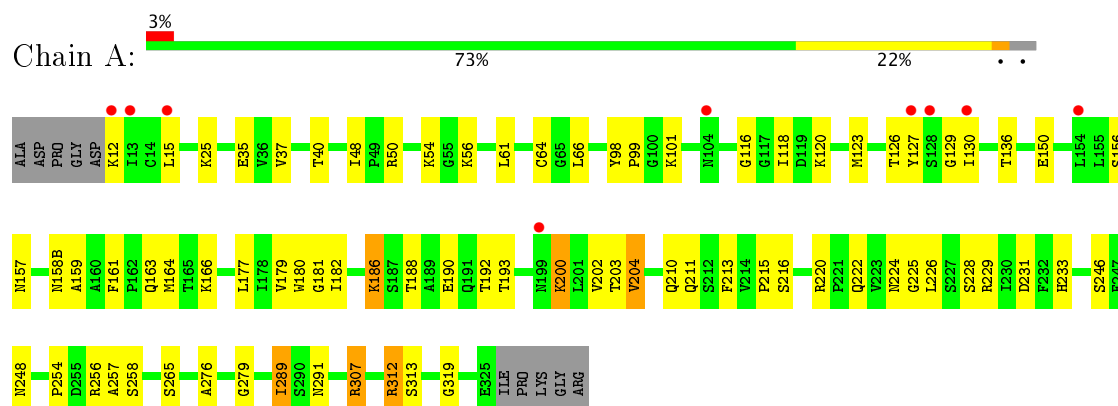
- Molecule 2: Hemagglutinin HA2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	115.44Å 115.44Å 294.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 2.59 49.77 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.77-2.59) 99.2 (49.77-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.203 , 0.251 0.198 , 0.246	Depositor DCC
R_{free} test set	1210 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.022 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.011 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3904	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.58	0/2452	0.91	6/3314 (0.2%)
2	B	0.57	0/1384	0.90	5/1865 (0.3%)
All	All	0.58	0/3836	0.91	11/5179 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	ILE	CG1-CB-CG2	-7.60	94.68	111.40
2	B	163	ARG	CA-CB-CG	7.36	129.58	113.40
2	B	55	LEU	CA-CB-CG	-7.06	99.06	115.30
2	B	149	MET	CG-SD-CE	6.74	110.98	100.20
1	A	200	LYS	CB-CG-CD	6.50	128.50	111.60
1	A	204	VAL	CG1-CB-CG2	-6.15	101.06	110.90
2	B	57	GLU	CA-CB-CG	-6.10	99.97	113.40
1	A	66	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	A	164	MET	CA-CB-CG	5.72	123.03	113.30
2	B	149	MET	CA-CB-CG	5.48	122.62	113.30
1	A	312	ARG	CD-NE-CZ	5.08	130.72	123.60

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	2406	0	2365	61	0
2	B	1360	0	1261	35	0
3	A	28	0	26	2	0
3	B	28	0	24	1	0
4	B	11	0	10	0	0
5	A	48	0	0	0	0
5	B	23	0	0	0	0
All	All	3904	0	3686	90	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.

All (90) 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:B:163:ARG:HG3	2:B:167:MET:HE1	1.47	0.96
1:A:291:ASN:HB3	2:B:56:ILE:HG23	1.56	0.88
1:A:220:ARG:HD3	1:A:229:ARG:HG3	1.63	0.78
2:B:25:ARG:HE	2:B:34:THR:HG21	1.49	0.78
2:B:25:ARG:HG3	2:B:34:THR:HG22	1.64	0.77
1:A:48:ILE:HD12	1:A:289:ILE:HD12	1.69	0.73
2:B:25:ARG:HE	2:B:34:THR:CG2	2.02	0.72
1:A:12:LYS:HA	2:B:140:ILE:HG13	1.72	0.71
1:A:126:THR:O	1:A:166:LYS:NZ	2.26	0.68
1:A:179:VAL:O	1:A:254:PRO:HB3	1.96	0.64
1:A:123:MET:HE3	1:A:257:ALA:HB2	1.78	0.64
2:B:26:HIS:HB2	2:B:149:MET:SD	2.39	0.62
1:A:150:GLU:OE1	1:A:256:ARG:HD3	1.99	0.62
1:A:161:PHE:HB3	1:A:248:ASN:O	1.99	0.61
1:A:291:ASN:HB3	2:B:56:ILE:CG2	2.29	0.61
2:B:11:GLU:HG3	2:B:12:ASN:N	2.17	0.60
1:A:12:LYS:N	2:B:27:GLN:O	2.36	0.59
2:B:25:ARG:NE	2:B:34:THR:HG21	2.17	0.58
1:A:188:THR:O	1:A:192:THR:HG23	2.04	0.58
1:A:123:MET:CE	1:A:257:ALA:HB2	2.35	0.55
1:A:54:LYS:HB2	1:A:276:ALA:O	2.06	0.55
2:B:25:ARG:CG	2:B:34:THR:HG22	2.33	0.55
1:A:222:GLN:OE1	1:A:225:GLY:HA2	2.06	0.54
1:A:15:LEU:CD2	2:B:118:LEU:HG	2.37	0.54
1:A:186:LYS:HE2	1:A:190:GLU:OE2	2.07	0.54
2:B:119:TYR:OH	2:B:132:GLU:OE2	2.23	0.54
2:B:144:CYS:SG	2:B:149:MET:HE2	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:HIS:CE1	2:B:162:TYR:CD2	2.97	0.53
2:B:141:PHE:O	2:B:166:ALA:HA	2.10	0.52
1:A:129:GLY:C	1:A:157:ASN:HD21	2.13	0.52
1:A:216:SER:O	1:A:220:ARG:NH2	2.43	0.52
1:A:163:GLN:OE1	1:A:248:ASN:HB3	2.10	0.51
2:B:140:ILE:O	2:B:140:ILE:HD12	2.10	0.51
1:A:202:VAL:CG2	1:A:213:PHE:HB2	2.40	0.51
1:A:202:VAL:HG22	1:A:213:PHE:HB2	1.91	0.51
2:B:164:GLU:HG2	2:B:165:GLU:N	2.26	0.51
1:A:98:TYR:HD2	1:A:136:THR:HG21	1.74	0.51
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.46	0.50
1:A:186:LYS:CE	1:A:190:GLU:OE2	2.59	0.50
1:A:40:THR:HB	3:A:502:NAG:H62	1.93	0.50
1:A:202:VAL:HG23	1:A:213:PHE:HD2	1.76	0.50
1:A:118:ILE:HD12	1:A:120:LYS:HE3	1.94	0.49
1:A:213:PHE:CE1	1:A:233:HIS:CD2	3.01	0.49
1:A:210:GLN:O	1:A:211:GLN:HG3	2.13	0.48
1:A:158(B):ASN:ND2	1:A:193:THR:HA	2.29	0.48
1:A:182:ILE:HD11	1:A:202:VAL:HG21	1.95	0.48
1:A:228:SER:O	1:A:229:ARG:HG2	2.14	0.48
1:A:116:GLY:HA2	1:A:265:SER:HB3	1.94	0.48
2:B:19:ASP:N	2:B:19:ASP:OD1	2.45	0.47
2:B:26:HIS:C	2:B:26:HIS:CD2	2.87	0.47
1:A:37:VAL:HG22	1:A:319:GLY:HA3	1.96	0.47
1:A:25:LYS:HG2	1:A:35:GLU:HG3	1.95	0.47
1:A:224:ASN:O	1:A:226:LEU:HD12	2.14	0.47
1:A:200:LYS:O	1:A:215:PRO:HD2	2.14	0.47
2:B:11:GLU:CG	2:B:12:ASN:N	2.78	0.46
2:B:125:GLN:OE1	2:B:155:ASN:HA	2.15	0.46
2:B:58:LYS:HB2	2:B:58:LYS:HE2	1.59	0.46
1:A:202:VAL:HA	1:A:246:SER:O	2.15	0.46
1:A:156:SER:HB3	1:A:159:ALA:HB3	1.98	0.46
1:A:307:ARG:HG2	2:B:92:TRP:CE2	2.50	0.46
2:B:161:LYS:HG2	2:B:162:TYR:CE1	2.51	0.46
2:B:144:CYS:SG	2:B:149:MET:CE	3.04	0.45
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.99	0.45
2:B:25:ARG:NE	2:B:34:THR:CG2	2.76	0.45
1:A:61:LEU:HB3	1:A:64:CYS:O	2.16	0.44
1:A:127:TYR:CB	1:A:130:ILE:HD11	2.48	0.44
1:A:181:GLY:HA2	1:A:231:ASP:O	2.16	0.44
2:B:11:GLU:OE1	2:B:12:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:CD1	1:A:202:VAL:HG21	2.48	0.43
1:A:177:LEU:HB3	1:A:258:SER:HB2	1.99	0.43
2:B:75:LYS:HD2	3:B:201:NAG:H81	2.00	0.43
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.00	0.43
2:B:32:GLU:OE2	2:B:32:GLU:N	2.52	0.42
1:A:180:TRP:CZ2	1:A:204:VAL:HG21	2.54	0.42
1:A:312:ARG:HG3	1:A:313:SER:N	2.33	0.42
2:B:56:ILE:O	2:B:56:ILE:HG22	2.20	0.42
1:A:98:TYR:CZ	1:A:226:LEU:HD22	2.54	0.41
1:A:200:LYS:HE2	1:A:248:ASN:O	2.20	0.41
1:A:101:LYS:HB2	1:A:101:LYS:HE3	1.79	0.41
1:A:56:LYS:NZ	1:A:279:GLY:O	2.43	0.41
2:B:16:GLY:O	2:B:18:ILE:HG13	2.19	0.41
1:A:180:TRP:CH2	1:A:204:VAL:HG11	2.55	0.41
1:A:222:GLN:HG3	1:A:225:GLY:C	2.40	0.41
1:A:40:THR:CB	3:A:502:NAG:H62	2.51	0.41
1:A:127:TYR:HB3	1:A:130:ILE:HD11	2.03	0.41
1:A:166:LYS:HD3	1:A:166:LYS:HA	1.77	0.41
1:A:228:SER:C	1:A:229:ARG:HG2	2.41	0.41
1:A:231:ASP:HB3	1:A:233:HIS:HE1	1.86	0.41
1:A:203:THR:OG1	1:A:246:SER:HB3	2.22	0.40
1:A:289:ILE:HD13	1:A:289:ILE:HG21	1.89	0.40

There are no symmetry-related clashes.

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	313/325 (96%)	304 (97%)	9 (3%)	0	100	100
2	B	166/183 (91%)	161 (97%)	5 (3%)	0	100	100
All	All	479/508 (94%)	465 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	265/272 (97%)	262 (99%)	3 (1%)	78	92
2	B	143/157 (91%)	142 (99%)	1 (1%)	87	96
All	All	408/429 (95%)	404 (99%)	4 (1%)	80	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	186	LYS
1	A	307	ARG
2	B	155	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	157	ASN
1	A	158(B)	ASN
1	A	199	ASN
1	A	233	HIS
1	A	276(A)	ASN
1	A	291	ASN
2	B	26	HIS
2	B	155	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#|Z| > 2$
3	NAG	A	501	1	14,14,15	0.70	0	15,19,21	0.96	1 (6%)
3	NAG	A	502	1	14,14,15	1.21	1 (7%)	15,19,21	1.19	1 (6%)
3	NAG	B	201	3,2	14,14,15	0.94	1 (7%)	15,19,21	1.40	2 (13%)
3	NAG	B	202	3,4	14,14,15	0.64	1 (7%)	15,19,21	0.74	0
4	BMA	B	203	3	11,11,12	0.64	0	13,15,17	0.85	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
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	201	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	202	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	203	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	NAG	O5-C1	-3.23	1.38	1.43
3	B	202	NAG	O5-C1	-2.13	1.40	1.43
3	A	502	NAG	O5-C1	4.43	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	NAG	O4-C4-C3	-2.75	104.38	110.36
3	A	501	NAG	C1-O5-C5	3.13	116.48	112.17
3	B	201	NAG	C1-O5-C5	3.67	117.23	112.17
3	A	502	NAG	C1-O5-C5	4.14	117.88	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	2	0
3	B	201	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 (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	315/325 (96%)	0.18	9 (2%)	52	45	41, 72, 109, 155	0
2	B	168/183 (91%)	1.13	37 (22%)	1	0	40, 97, 154, 175	0
All	All	483/508 (95%)	0.51	46 (9%)	9	5	40, 79, 142, 175	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	143	LYS	6.0
2	B	60	ASN	4.9
2	B	27	GLN	4.7
2	B	168	GLN	4.7
2	B	24	PHE	4.3
2	B	141	PHE	4.3
2	B	166	ALA	4.2
2	B	152	ILE	3.8
1	A	15	LEU	3.3
1	A	12	LYS	3.3
2	B	80	VAL	3.3
2	B	81	ILE	3.3
2	B	161	LYS	3.2
2	B	35	ALA	3.1
2	B	139	GLU	3.0
2	B	84	THR	3.0
2	B	142	HIS	2.9
2	B	29	ALA	2.8
2	B	32	GLU	2.8
2	B	83	TRP	2.7
1	A	13	ILE	2.7
2	B	136	GLY	2.7
2	B	77	ILE	2.7
2	B	167	MET	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	146	ASP	2.5
2	B	78	GLY	2.4
2	B	79	ASN	2.4
1	A	127	TYR	2.3
1	A	128	SER	2.3
2	B	144	CYS	2.3
2	B	162	TYR	2.3
2	B	25	ARG	2.2
2	B	19	ASP	2.2
2	B	130	ALA	2.2
2	B	148	CYS	2.2
2	B	165	GLU	2.2
2	B	26	HIS	2.2
2	B	149	MET	2.2
2	B	147	ASP	2.1
2	B	76	GLN	2.1
1	A	199	ASN	2.1
2	B	164	GLU	2.1
1	A	104	ASN	2.1
2	B	87	SER	2.0
1	A	130	ILE	2.0
1	A	154	LEU	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, 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($\mathring{A}^2$)	Q<0.9
3	NAG	B	201	14/15	0.90	0.18	-1.55	79,93,110,125	0
3	NAG	B	202	14/15	0.82	0.22	-	124,127,141,153	0
4	BMA	B	203	11/12	0.75	0.35	-	154,170,176,178	0
3	NAG	A	501	14/15	0.79	0.26	-	121,126,135,141	0
3	NAG	A	502	14/15	0.82	0.20	-	104,134,139,140	0

6.5 Other polymers (i)

There are no such residues in this entry.