



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:40 AM GMT

PDB ID : 1KEN
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH AN AN-
TIBODY THAT PREVENTS THE HEMAGGLUTININ LOW PH FUSO-
GENIC TRANSITION
Authors : Barbey-Martin, C.; Gigant, B.; Bizebard, T.; Calder, L.J.; Wharto, S.A.;
Skehel, J.J.; Knossow, M.
Deposited on : 2001-11-16
Resolution : 3.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

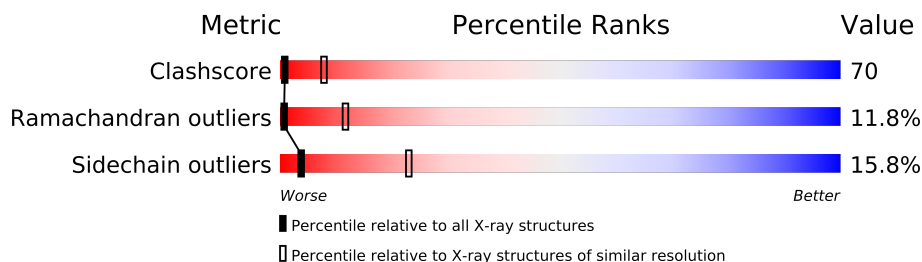
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	
3	L	213	
3	U	213	
4	H	221	
4	T	221	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18492 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	C	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	E	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			

- Molecule 2 is a protein called hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	D	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	F	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

- Molecule 3 is a protein called influenza virus infectivity neutralizing antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			
3	U	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			

- Molecule 4 is a protein called influenza virus infectivity neutralizing antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1720	1102	272	340	6			
4	T	219	Total	C	N	O	S	0	0	0
			1700	1092	267	335	6			

- Molecule 5 is a polymer of unknown type called SUGAR (NAG-NAG-MAN).

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

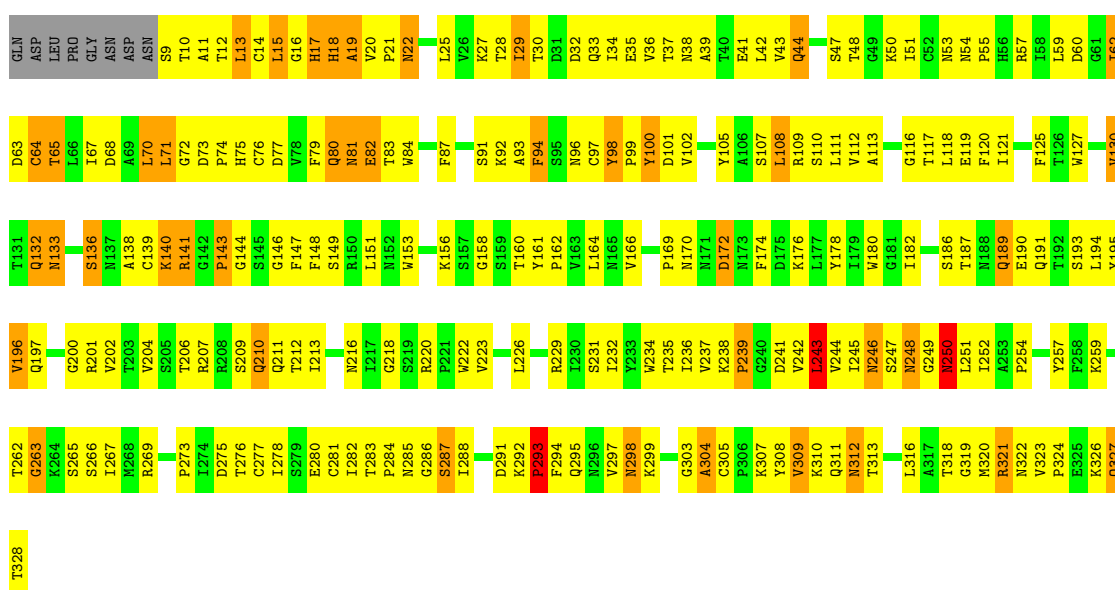
3 Residue-property plots

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

Note EDS was not executed.

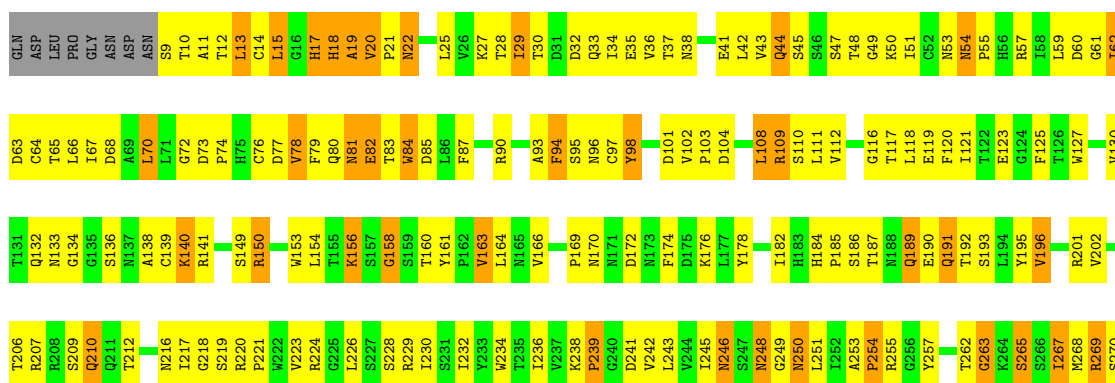
• Molecule 1: hemagglutinin HA1

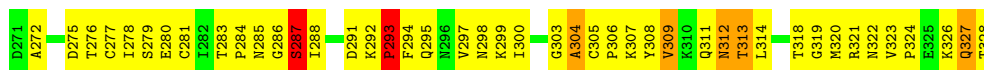
Chain A:



• Molecule 1: hemagglutinin HA1

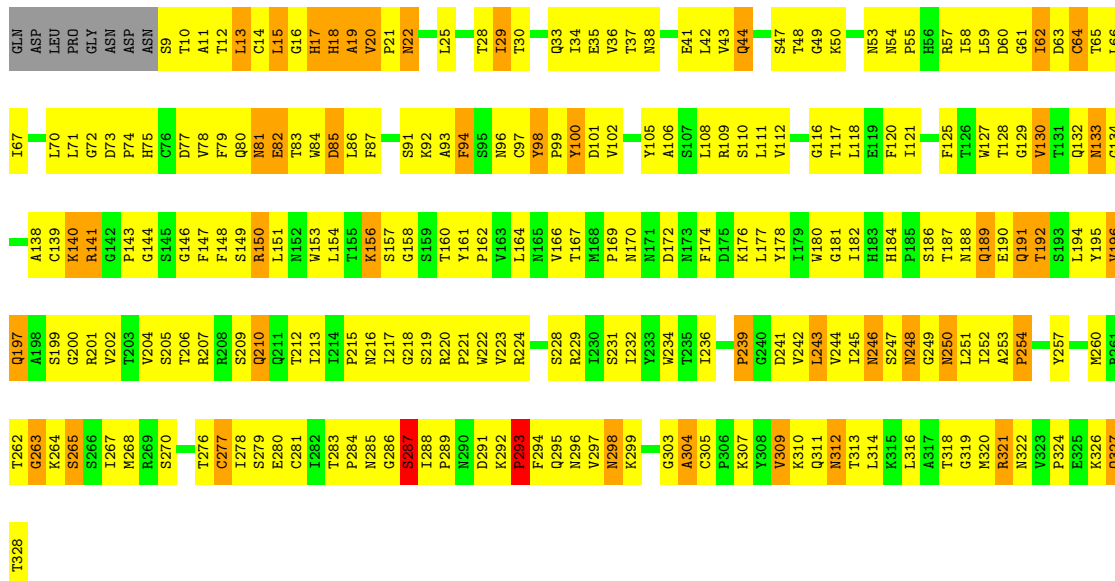
Chain C:





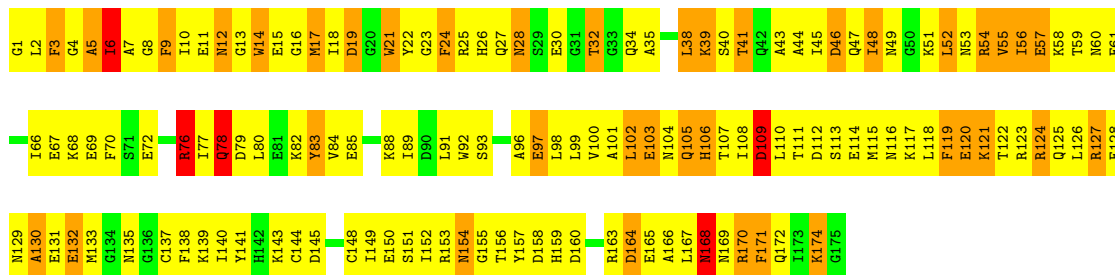
• Molecule 1: hemagglutinin HA1

Chain E:



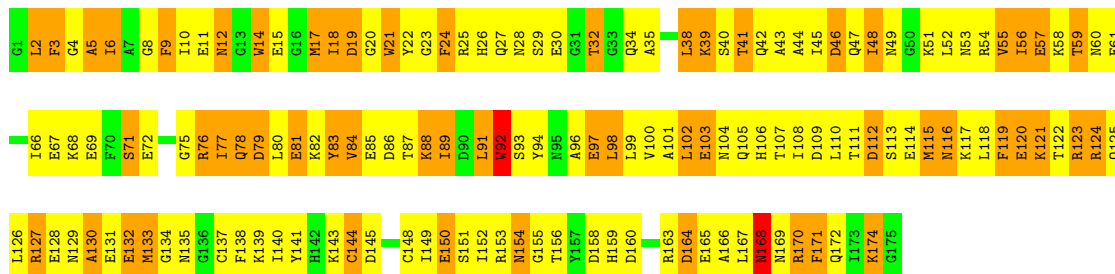
• Molecule 2: hemagglutinin HA2

Chain B:



• Molecule 2: hemagglutinin HA2

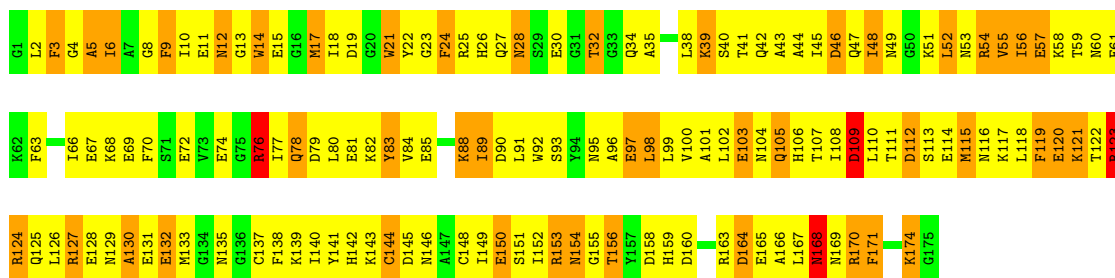
Chain D:



• Molecule 2: hemagglutinin HA2

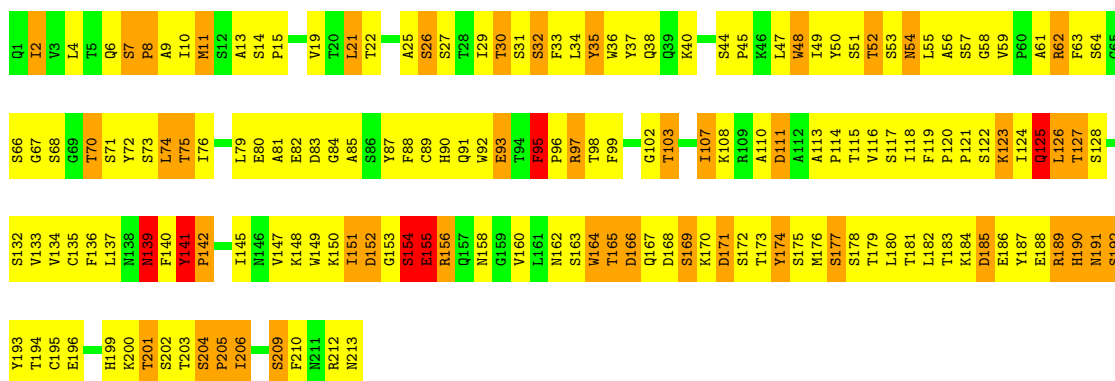
Chain F:





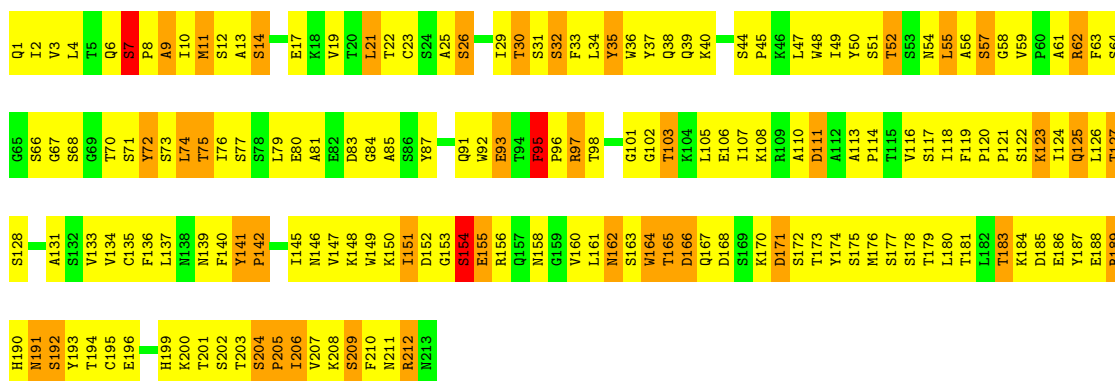
• Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain L:



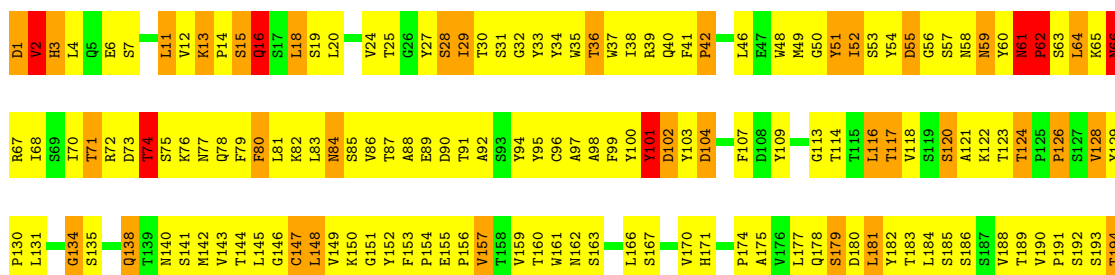
• Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain U:



• Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

Chain H:



W195	P196	S197	E198	T199	V200	T201	C202	H203	V204	A205	H206	P207	A208	S209	S210	T211	K212	T213	D214	K215	K216	I217	V218	P219	R220	D221
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

Chain T:

D1	V2	H3	L4	Q5	E6	S7	L11	V12	K13	P14	S15	Q16	S17	L18	S19	L20	T21	C22	Y23	V24	T25	G26	Y27	S28	I29	T30	S31	G32	Y33	Y34	W35	T36	W37	I38	R39	Q40	F41	P42	G43	N44	K45	L46	E47	W48	M49	G50	Y51	I52	S53	Y54	D55	G56	S57	N58	N59	Y60	M61	P62
S63	L64	K65	N66	R67	I68	S69	I70	T71	D72	T73	T74	S75	K76	N77	F78	R80	L81	K82	L83	N84	S85	V86	T87	A88	E89	D90	T91	A92	S93	Y94	Y95	C96	A97	A98	F99	Y100	Y101	D102	Y103	D104	F107	D108	Y109	W110	T114	T115	L116	T117	V118	S119	S120	A121	K122	T123	T124	P125		
P126	Y129	P130	L131	G134	S135	Q138	T139	N140	S141	M142	V143	T144	L145	G146	G147	L148	V149	K150	G151	Y152	F153	P154	E155	P156	V157	T158	V159	T160	W161	M162	S163	L166	V170	H171	D172	T173	P174	A175	V176	L177	Q178	S179	D180	L181	Y182	T183	L184	S185	S186	S187	V188	T189	V190	P191				
S192	S193	T194	W195	P196	S197	E198	T199	V200	T201	C202	N203	H206	P207	A208	S209	D214	K215	K216	I217	V218	P219	ARG	ASP																																			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.04Å 315.59Å 97.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.50	Depositor
% Data completeness (in resolution range)	91.8 (25.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.255 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18492	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN

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	0.71	0/2528	0.91	3/3443 (0.1%)
1	C	0.77	1/2528 (0.0%)	0.96	2/3443 (0.1%)
1	E	0.71	0/2528	0.93	2/3443 (0.1%)
2	B	0.74	0/1445	0.86	0/1939
2	D	0.77	1/1445 (0.1%)	0.89	3/1939 (0.2%)
2	F	0.73	0/1445	0.84	0/1939
3	L	0.82	2/1679 (0.1%)	1.05	7/2281 (0.3%)
3	U	0.76	0/1679	0.97	3/2281 (0.1%)
4	H	0.85	2/1774 (0.1%)	1.00	2/2431 (0.1%)
4	T	0.78	1/1754 (0.1%)	1.00	2/2406 (0.1%)
All	All	0.76	7/18805 (0.0%)	0.95	24/25545 (0.1%)

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
3	L	0	1
3	U	0	1
4	H	0	1
4	T	0	2
5	A	1	0
5	C	1	0
5	E	1	0
All	All	3	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	ASP	CB-CG	7.47	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	155	GLU	CB-CG	7.10	1.65	1.52
3	L	155	GLU	CG-CD	6.60	1.61	1.51
4	H	61	ASN	CB-CG	5.86	1.64	1.51
2	D	92	TRP	CB-CG	-5.42	1.40	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	64	LEU	CA-CB-CG	-10.84	90.37	115.30
3	L	111	ASP	N-CA-C	-9.85	84.40	111.00
4	H	64	LEU	CA-CB-CG	-7.90	97.13	115.30
3	U	111	ASP	N-CA-C	-7.69	90.24	111.00
2	D	79	ASP	CB-CG-OD2	7.20	124.78	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	452	MAN	C1
5	C	452	MAN	C1
5	E	452	MAN	C1

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	101	TYR	Sidechain
3	L	141	TYR	Sidechain
4	T	33	TYR	Sidechain
4	T	95	TYR	Sidechain
3	U	72	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2472	0	2424	336	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2472	0	2424	328	0
1	E	2472	0	2424	334	0
2	B	1421	0	1346	259	0
2	D	1421	0	1346	273	0
2	F	1421	0	1346	276	0
3	L	1638	0	1578	232	0
3	U	1638	0	1578	260	0
4	H	1720	0	1639	264	0
4	T	1700	0	1622	276	0
5	A	39	0	34	3	0
5	C	39	0	34	4	0
5	E	39	0	34	0	0
All	All	18492	0	17829	2549	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 70.

The worst 5 of 2549 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:PRO:HA	1:A:141:ARG:HH12	1.11	1.16
3:U:199:HIS:HB3	3:U:201:THR:HG22	1.28	1.11
3:U:134:VAL:HG22	3:U:179:THR:HG23	1.30	1.11
1:C:77:ASP:O	1:C:80:GLN:HG2	1.47	1.10
1:C:96:ASN:HD21	1:C:140:LYS:HE2	1.10	1.10

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	318/328 (97%)	247 (78%)	43 (14%)	28 (9%)	1	19
1	C	318/328 (97%)	241 (76%)	53 (17%)	24 (8%)	2	24
1	E	318/328 (97%)	250 (79%)	41 (13%)	27 (8%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	173/175 (99%)	96 (56%)	44 (25%)	33 (19%)	0	3
2	D	173/175 (99%)	89 (51%)	48 (28%)	36 (21%)	0	2
2	F	173/175 (99%)	89 (51%)	49 (28%)	35 (20%)	0	2
3	L	211/213 (99%)	141 (67%)	46 (22%)	24 (11%)	1	12
3	U	211/213 (99%)	139 (66%)	51 (24%)	21 (10%)	1	15
4	H	219/221 (99%)	158 (72%)	38 (17%)	23 (10%)	1	14
4	T	217/221 (98%)	147 (68%)	47 (22%)	23 (11%)	1	14
All	All	2331/2377 (98%)	1597 (68%)	460 (20%)	274 (12%)	1	12

5 of 274 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	81	ASN
1	A	210	GLN
1	A	263	GLY
1	A	287	SER

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	282/289 (98%)	252 (89%)	30 (11%)	10	45
1	C	282/289 (98%)	249 (88%)	33 (12%)	8	38
1	E	282/289 (98%)	248 (88%)	34 (12%)	7	36
2	B	149/149 (100%)	120 (80%)	29 (20%)	2	12
2	D	149/149 (100%)	116 (78%)	33 (22%)	1	8
2	F	149/149 (100%)	118 (79%)	31 (21%)	2	10
3	L	187/187 (100%)	147 (79%)	40 (21%)	1	9
3	U	187/187 (100%)	152 (81%)	35 (19%)	2	13
4	H	196/196 (100%)	163 (83%)	33 (17%)	3	19
4	T	194/196 (99%)	167 (86%)	27 (14%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2057/2080 (99%)	1732 (84%)	325 (16%)	4 23

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	239	PRO
2	F	123	ARG
4	T	16	GLN
1	E	250	ASN
2	F	21	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	28	ASN
1	E	80	GLN
4	T	58	ASN
2	D	49	ASN
2	D	154	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

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
5	NAG	A	450	1,5	12,14,15	0.76	0	15,19,21	1.26	2 (13%)
5	NAG	A	451	5	12,14,15	0.58	0	15,19,21	0.85	1 (6%)
5	MAN	A	452	5	10,11,12	0.95	1 (10%)	11,15,17	1.02	1 (9%)
5	NAG	C	450	1,5	12,14,15	0.64	0	15,19,21	0.86	1 (6%)
5	NAG	C	451	5	12,14,15	0.73	0	15,19,21	0.86	1 (6%)
5	MAN	C	452	5	10,11,12	1.05	0	11,15,17	1.16	1 (9%)
5	NAG	E	450	1,5	12,14,15	0.69	0	15,19,21	1.09	1 (6%)
5	NAG	E	451	5	12,14,15	0.96	0	15,19,21	1.03	1 (6%)
5	MAN	E	452	5	10,11,12	0.85	0	11,15,17	1.19	1 (9%)

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
5	NAG	A	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	451	5	-	0/6/23/26	0/1/1/1
5	MAN	A	452	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	C	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	451	5	-	0/6/23/26	0/1/1/1
5	MAN	C	452	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	E	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	451	5	-	0/6/23/26	0/1/1/1
5	MAN	E	452	5	1/1/4/5	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)
5	A	452	MAN	C4-C5	2.11	1.57	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	450	NAG	C2-N2-C7	-3.28	117.58	123.09
5	C	452	MAN	C6-C5-C4	2.92	120.06	113.00
5	E	452	MAN	C6-C5-C4	2.74	119.61	113.00
5	A	452	MAN	C6-C5-C4	2.42	118.84	113.00
5	E	451	NAG	C2-N2-C7	-2.26	119.29	123.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	452	MAN	C1
5	A	452	MAN	C1
5	C	452	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.