



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 AM GMT

PDB ID : 2VIS  
Title : INFLUENZA VIRUS HEMAGGLUTININ, (ESCAPE) MUTANT WITH  
THR 131 REPLACED BY ILE, COMPLEXED WITH A NEUTRALIZING  
ANTIBODY  
Authors : Bizebard, T.; Fleury, D.; Gigant, B.; Wharton, S.A.; Skehel, J.J.; Knossow, M.  
Deposited on : 1997-12-22  
Resolution : 3.25 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

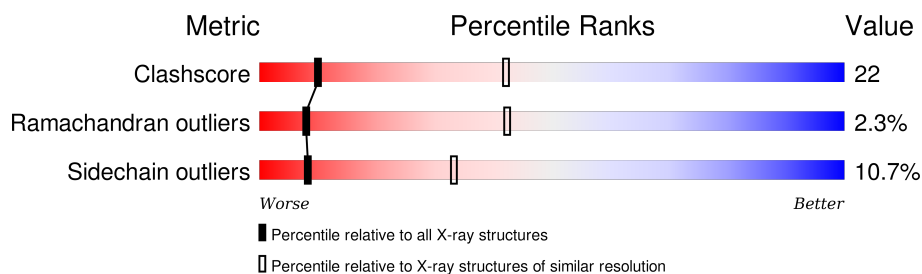
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	210	
2	B	221	
3	C	282	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5354 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 IMMUNOGLOBULIN (IGG1, LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1589	994	266	323	6			

- Molecule 2 is a protein called IMMUNOGLOBULIN (IGG1, LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1672	1065	270	328	9			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLN	LYS	CONFLICT	GB 4096752
B	5	LYS	GLN	CONFLICT	GB 4096752
B	28	LEU	SER	CONFLICT	GB 4096752
B	30	ILE	THR	CONFLICT	GB 4096752
B	32	ASN	TYR	CONFLICT	GB 4096752
B	63	LEU	HIS	CONFLICT	GB 4096752
B	69	ILE	PHE	CONFLICT	GB 4096752
B	83	LYS	ASN	CONFLICT	GB 4096752
B	92	MET	LEU	CONFLICT	GB 4096752
B	98	ASP	-	INSERTION	GB 4096752
B	99	PHE	-	INSERTION	GB 4096752
B	100	TYR	-	INSERTION	GB 4096752
B	102	TYR	HIS	CONFLICT	GB 4096752
B	103	ASP	GLY	CONFLICT	GB 4096752
B	105	PHE	-	INSERTION	GB 4096752
B	106	TYR	-	INSERTION	GB 4096752
B	107	TYR	-	INSERTION	GB 4096752
B	108	ALA	-	INSERTION	GB 4096752
B	109	MET	-	INSERTION	GB 4096752
B	110	ASP	-	INSERTION	GB 4096752

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Chain	Residue	Modelled	Actual	Comment	Reference
B	117	SER	LEU	CONFLICT	GB 4096752
B	122	SER	ALA	CONFLICT	GB 4096752
B	135	PRO	SER	CONFLICT	GB 4096752

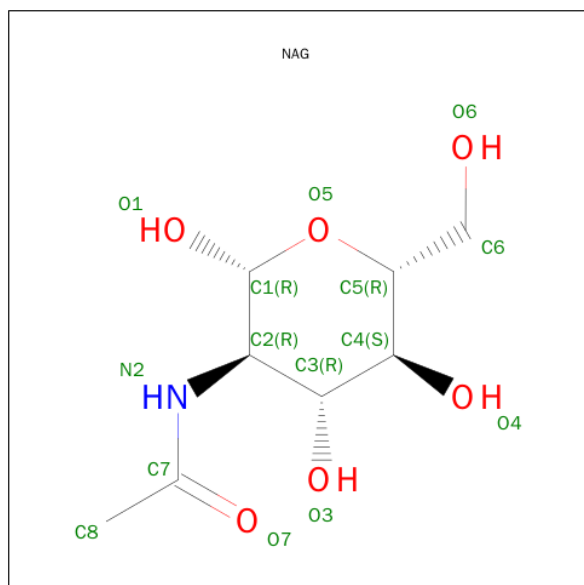
- Molecule 3 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2076	1306	363	396	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	131	ILE	THR	ENGINEERED	UNP P03437

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

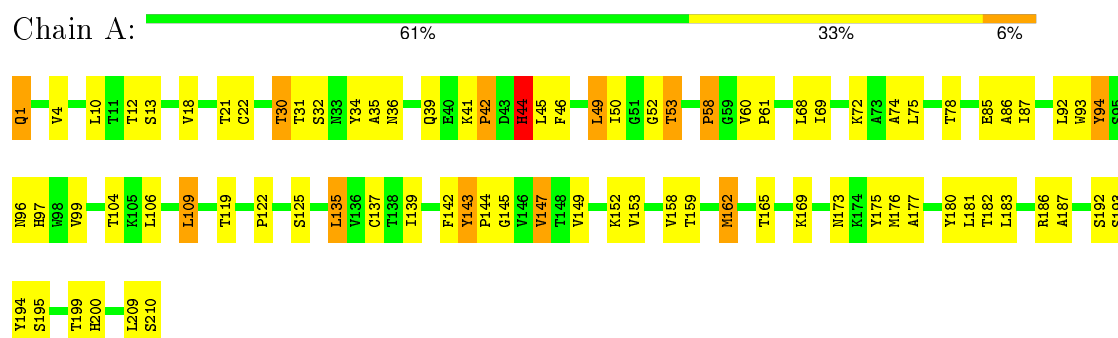
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Zn 2	0	0
5	C	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

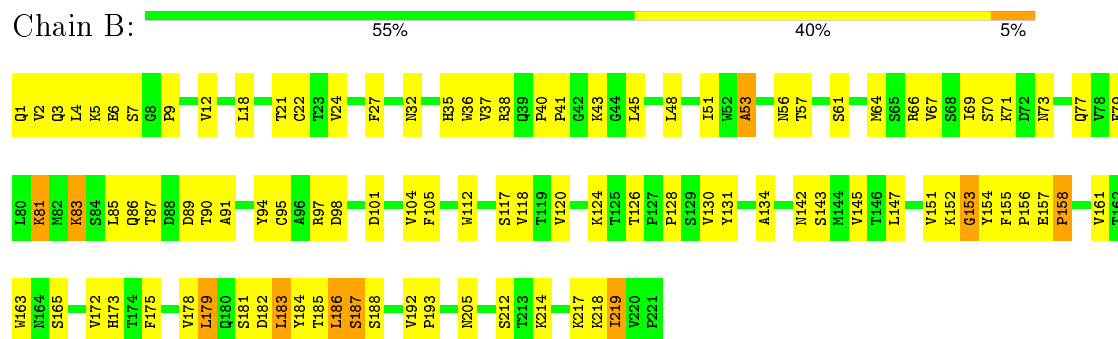
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

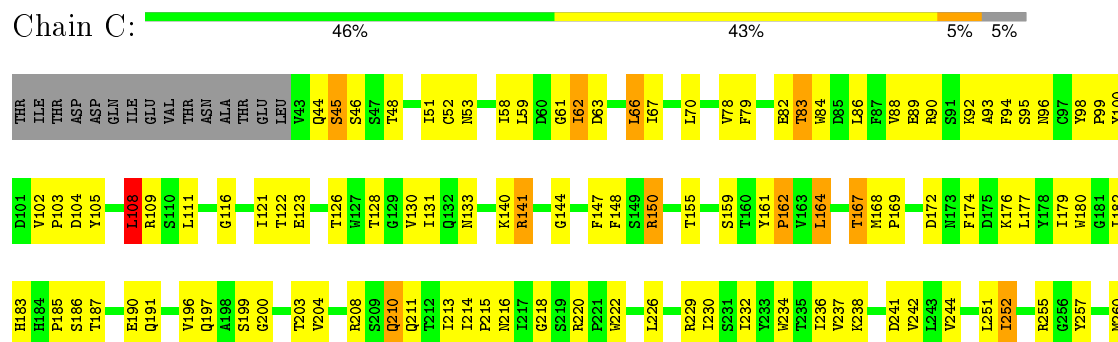
#### • Molecule 1: IMMUNOGLOBULIN (IGG1, LAMBDA)



#### • Molecule 2: IMMUNOGLOBULIN (IGG1, LAMBDA)



#### • Molecule 3: HEMAGGLUTININ



K261	K262	G263	K264	S265	S266	K267	K268		K274	D275	T276	G277	K278		K282	T283	P284	K285	K286	S287	K288	P289		K290	D291	K292		K295	K296	S297	K298	K299	K300	T301	Y302		K303	K304	C305	P306	S307	Y308	Y309
------	------	------	------	------	------	------	------	--	------	------	------	------	------	--	------	------	------	------	------	------	------	------	--	------	------	------	--	------	------	------	------	------	------	------	------	--	------	------	------	------	------	------	------

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.50 Å 85.50 Å 515.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 3.25	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.25)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.188 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: ZN, 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	0/1627	0.85	3/2224 (0.1%)
2	B	0.61	0/1718	0.86	1/2351 (0.0%)
3	C	0.60	0/2128	0.87	2/2897 (0.1%)
All	All	0.60	0/5473	0.86	6/7472 (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
1	A	0	2
2	B	0	1
3	C	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	153	GLY	N-CA-C	6.29	128.82	113.10
1	A	135	LEU	CA-CB-CG	5.89	128.85	115.30
3	C	108	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	45	LEU	N-CA-C	-5.21	96.94	111.00
3	C	252	ILE	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Sidechain
1	A	94	TYR	Sidechain
2	B	53	ALA	Mainchain
3	C	302	TYR	Sidechain

## 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	1589	0	1532	67	0
2	B	1672	0	1635	75	0
3	C	2076	0	2020	97	0
4	C	14	0	13	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
All	All	5354	0	5200	232	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 22.

All (232) 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:134:ALA:HB2	2:B:219:ILE:HD11	1.50	0.89
3:C:283:THR:HG23	3:C:285:ASN:H	1.38	0.89
2:B:1:GLN:HE21	2:B:3:GLN:HB2	1.42	0.84
1:A:44:HIS:HB2	2:B:94:TYR:OH	1.80	0.82
3:C:45:SER:HB3	3:C:296:ASN:OD1	1.80	0.81
2:B:40:PRO:HG2	2:B:43:LYS:HB2	1.62	0.79
2:B:131:TYR:CE2	2:B:152:LYS:HE3	2.18	0.78
3:C:148:PHE:HE2	3:C:230:ILE:HD11	1.49	0.78
1:A:93:TRP:CH2	1:A:96:ASN:HA	2.19	0.78
1:A:39:GLN:HB2	1:A:49:LEU:HD22	1.65	0.77
3:C:283:THR:HG22	3:C:286:GLY:O	1.85	0.77
2:B:131:TYR:HE2	2:B:152:LYS:HE3	1.51	0.75
3:C:283:THR:HG23	3:C:285:ASN:N	2.03	0.74
3:C:298:ASN:HD22	3:C:300:ILE:H	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:LEU:HB2	2:B:85:LEU:HD11	1.70	0.71
2:B:66:ARG:HA	2:B:83:LYS:HE3	1.72	0.71
3:C:121:ILE:HG13	3:C:257:TYR:CE1	2.26	0.71
1:A:147:VAL:HG12	1:A:200:HIS:HB2	1.71	0.71
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.73	0.71
2:B:1:GLN:NE2	2:B:3:GLN:HB2	2.06	0.70
1:A:152:LYS:HB2	1:A:195:SER:OG	1.92	0.70
1:A:142:PHE:CE2	1:A:147:VAL:HG22	2.27	0.70
2:B:143:SER:O	2:B:193:PRO:HA	1.94	0.68
2:B:53:ALA:HB3	3:C:131:ILE:HG12	1.75	0.68
1:A:49:LEU:HD12	1:A:60:VAL:HG22	1.75	0.68
1:A:12:THR:HB	1:A:18:VAL:HG11	1.77	0.67
3:C:103:PRO:O	3:C:104:ASP:HB3	1.95	0.66
1:A:50:ILE:HD12	1:A:75:LEU:HD13	1.78	0.66
3:C:148:PHE:HE2	3:C:230:ILE:CD1	2.08	0.65
3:C:111:LEU:HD11	3:C:236:ILE:HD11	1.79	0.65
2:B:6:GLU:HA	2:B:21:THR:O	1.96	0.65
2:B:40:PRO:HG2	2:B:43:LYS:CB	2.26	0.65
1:A:192:SER:O	1:A:210:SER:HA	1.97	0.65
2:B:51:ILE:HA	2:B:57:THR:HG22	1.78	0.65
2:B:77:GLN:HB3	2:B:79:PHE:CE1	2.32	0.64
2:B:124:LYS:O	2:B:126:THR:HG23	1.96	0.64
3:C:186:SER:HA	3:C:218:GLY:O	1.98	0.63
3:C:284:PRO:HD3	3:C:300:ILE:O	1.97	0.63
3:C:298:ASN:ND2	3:C:300:ILE:H	1.97	0.62
3:C:148:PHE:CE2	3:C:230:ILE:HD11	2.33	0.62
3:C:52:CYS:HB3	3:C:277:CYS:O	1.99	0.61
3:C:59:LEU:HD22	3:C:82:GLU:HG2	1.81	0.61
3:C:59:LEU:CD2	3:C:82:GLU:HG2	2.30	0.61
3:C:214:ILE:HD12	3:C:215:PRO:O	2.00	0.61
3:C:82:GLU:HG3	3:C:83:THR:H	1.66	0.61
3:C:46:SER:O	3:C:288:ILE:HG22	2.00	0.60
1:A:153:VAL:HG22	1:A:194:TYR:CD1	2.36	0.60
2:B:186:LEU:HD23	2:B:187:SER:N	2.16	0.60
2:B:71:LYS:HE3	2:B:73:ASN:HD21	1.66	0.60
1:A:169:LYS:HZ2	1:A:175:TYR:HE1	1.51	0.58
3:C:94:PHE:HD2	3:C:95:SER:O	1.85	0.58
3:C:237:VAL:CG1	3:C:241:ASP:HB3	2.33	0.58
2:B:12:VAL:O	2:B:120:VAL:HA	2.02	0.58
3:C:89:GLU:CD	3:C:109:ARG:HH12	2.07	0.58
3:C:238:LYS:O	3:C:241:ASP:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:HB3	1:A:209:LEU:HD22	1.85	0.58
2:B:87:THR:O	2:B:90:THR:HG22	2.04	0.58
1:A:139:ILE:HD11	1:A:149:VAL:HG21	1.85	0.57
3:C:108:LEU:HB2	3:C:234:TRP:NE1	2.19	0.57
3:C:44:GLN:OE1	3:C:289:PRO:HG2	2.04	0.57
3:C:176:LYS:HE2	3:C:257:TYR:CE2	2.40	0.57
1:A:153:VAL:HG23	1:A:158:VAL:HG22	1.85	0.57
2:B:86:GLN:HA	2:B:86:GLN:OE1	2.05	0.56
2:B:36:TRP:HD1	2:B:69:ILE:HD13	1.70	0.56
2:B:35:HIS:CD2	2:B:98:ASP:HB2	2.39	0.56
3:C:222:TRP:HA	3:C:226:LEU:O	2.05	0.56
1:A:153:VAL:HG22	1:A:194:TYR:CE1	2.40	0.56
1:A:193:SER:HA	1:A:209:LEU:O	2.06	0.55
1:A:69:ILE:HG22	1:A:69:ILE:O	2.06	0.55
2:B:71:LYS:HE3	2:B:73:ASN:ND2	2.22	0.55
2:B:130:VAL:O	2:B:217:LYS:HE3	2.07	0.55
1:A:78:THR:HG22	1:A:78:THR:O	2.05	0.55
1:A:162:MET:HA	1:A:180:TYR:O	2.06	0.55
3:C:53:ASN:OD1	3:C:276:THR:HA	2.08	0.54
2:B:64:MET:HA	2:B:67:VAL:HG22	1.88	0.54
1:A:153:VAL:HG23	1:A:158:VAL:CG2	2.38	0.54
3:C:295:GLN:HB3	3:C:306:PRO:HB2	1.89	0.54
3:C:180:TRP:CE2	3:C:204:VAL:HG21	2.43	0.54
3:C:123:GLU:HB3	3:C:168:MET:HE1	1.89	0.53
2:B:155:PHE:CE1	2:B:156:PRO:HB3	2.43	0.53
1:A:1:GLN:O	1:A:99:VAL:HG21	2.08	0.53
3:C:237:VAL:HG13	3:C:241:ASP:HB3	1.91	0.53
3:C:89:GLU:HG3	3:C:267:ILE:HD11	1.89	0.53
2:B:1:GLN:HG2	2:B:2:VAL:O	2.08	0.53
1:A:4:VAL:HG13	1:A:22:CYS:SG	2.49	0.53
3:C:162:PRO:HG2	3:C:164:LEU:HD13	1.91	0.53
1:A:87:ILE:HD12	1:A:87:ILE:N	2.25	0.52
3:C:130:VAL:HG13	3:C:162:PRO:HD2	1.92	0.52
3:C:183:HIS:HB2	3:C:252:ILE:HD11	1.91	0.52
3:C:200:GLY:O	3:C:215:PRO:HD2	2.09	0.52
1:A:49:LEU:HA	1:A:60:VAL:HG21	1.92	0.52
3:C:172:ASP:HB3	3:C:174:PHE:CE1	2.45	0.52
1:A:12:THR:HB	1:A:18:VAL:CG1	2.41	0.51
3:C:242:VAL:HG12	3:C:244:VAL:HG23	1.93	0.51
3:C:86:LEU:HA	3:C:266:SER:O	2.10	0.51
2:B:128:PRO:CB	2:B:154:TYR:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ASP:HB2	2:B:120:VAL:HG21	1.93	0.50
2:B:134:ALA:CB	2:B:219:ILE:HD11	2.34	0.50
3:C:180:TRP:HH2	3:C:213:ILE:HD13	1.76	0.50
3:C:167:THR:HB	3:C:244:VAL:HG22	1.94	0.50
1:A:53:THR:HG21	1:A:68:LEU:CD2	2.42	0.49
2:B:90:THR:HA	2:B:118:VAL:O	2.13	0.49
1:A:1:GLN:NE2	1:A:97:HIS:HB3	2.27	0.49
1:A:21:THR:HB	1:A:72:LYS:HD2	1.95	0.49
1:A:147:VAL:CG1	1:A:200:HIS:HB2	2.42	0.49
2:B:4:LEU:HG	2:B:24:VAL:HG12	1.95	0.49
2:B:41:PRO:O	2:B:43:LYS:HD2	2.12	0.48
2:B:157:GLU:OE1	2:B:158:PRO:HA	2.13	0.48
3:C:213:ILE:N	3:C:213:ILE:HD12	2.28	0.48
1:A:30:THR:OG1	1:A:31:THR:N	2.47	0.48
3:C:82:GLU:HG3	3:C:83:THR:N	2.26	0.48
1:A:177:ALA:O	2:B:175:PHE:CE1	2.67	0.48
3:C:267:ILE:HG13	3:C:268:MET:N	2.29	0.48
3:C:84:TRP:CE2	3:C:116:GLY:HA2	2.49	0.47
3:C:102:VAL:HG22	3:C:232:ILE:HB	1.94	0.47
2:B:37:VAL:CG1	2:B:45:LEU:HD22	2.44	0.47
3:C:88:VAL:HA	3:C:268:MET:O	2.14	0.47
1:A:119:THR:O	1:A:137:CYS:HA	2.14	0.47
1:A:49:LEU:O	1:A:60:VAL:HG21	2.15	0.47
2:B:64:MET:HA	2:B:67:VAL:CG2	2.44	0.47
1:A:139:ILE:HD11	1:A:149:VAL:CG2	2.44	0.46
3:C:216:ASN:HD22	3:C:220:ARG:NH2	2.13	0.46
3:C:291:ASP:OD1	3:C:292:LYS:HG3	2.15	0.46
1:A:46:PHE:CZ	2:B:45:LEU:HD21	2.50	0.46
2:B:181:SER:OG	2:B:182:ASP:N	2.45	0.46
3:C:176:LYS:HE2	3:C:257:TYR:CD2	2.51	0.46
2:B:145:VAL:CG1	2:B:192:VAL:HG23	2.45	0.46
2:B:85:LEU:HD23	2:B:89:ASP:OD2	2.16	0.46
3:C:51:ILE:CG2	3:C:58:ILE:HD13	2.45	0.46
2:B:179:LEU:HD13	2:B:184:TYR:CD1	2.51	0.46
1:A:169:LYS:HD2	1:A:175:TYR:CZ	2.51	0.46
3:C:295:GLN:O	3:C:308:TYR:HA	2.15	0.46
3:C:301:THR:HB	3:C:305:CYS:SG	2.55	0.46
3:C:100:TYR:CB	3:C:230:ILE:HG13	2.46	0.46
2:B:61:SER:O	2:B:64:MET:HG2	2.15	0.46
2:B:27:PHE:CE2	2:B:97:ARG:HD3	2.51	0.46
3:C:94:PHE:CD2	3:C:95:SER:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:C	2:B:186:LEU:HD23	2.37	0.45
3:C:99:PRO:HB2	3:C:229:ARG:HD3	1.98	0.45
2:B:172:VAL:HG13	2:B:172:VAL:O	2.16	0.45
2:B:12:VAL:HG21	2:B:85:LEU:HD13	1.99	0.45
2:B:48:LEU:HD23	2:B:48:LEU:HA	1.78	0.45
1:A:85:GLU:HG3	1:A:106:LEU:O	2.16	0.45
3:C:111:LEU:HD21	3:C:260:MET:CE	2.46	0.45
3:C:98:TYR:HA	3:C:99:PRO:HD3	1.88	0.45
3:C:122:THR:HG22	3:C:123:GLU:N	2.32	0.45
2:B:40:PRO:HA	2:B:91:ALA:CB	2.47	0.45
1:A:53:THR:HG21	1:A:68:LEU:HD22	1.98	0.45
3:C:180:TRP:HH2	3:C:213:ILE:CD1	2.30	0.44
1:A:85:GLU:O	1:A:86:ALA:HB2	2.17	0.44
2:B:214:LYS:HB3	2:B:214:LYS:HE2	1.66	0.44
1:A:52:GLY:O	1:A:53:THR:HB	2.17	0.44
3:C:90:ARG:HH22	3:C:274:ILE:HG13	1.83	0.44
2:B:105:PHE:CZ	3:C:190:GLU:HG3	2.53	0.44
2:B:81:LYS:HZ1	2:B:83:LYS:HB3	1.82	0.44
3:C:150:ARG:HD2	3:C:150:ARG:N	2.33	0.44
3:C:140:LYS:NZ	3:C:144:GLY:HA2	2.33	0.44
1:A:34:TYR:O	1:A:35:ALA:C	2.55	0.44
3:C:262:THR:O	3:C:264:LYS:N	2.51	0.44
3:C:177:LEU:HG	3:C:177:LEU:O	2.17	0.44
1:A:35:ALA:HA	1:A:92:LEU:HD23	2.00	0.44
1:A:135:LEU:HB2	1:A:181:LEU:HB3	1.97	0.44
1:A:93:TRP:CZ3	1:A:96:ASN:HA	2.51	0.44
2:B:37:VAL:HG21	2:B:112:TRP:CH2	2.52	0.44
1:A:152:LYS:HB2	1:A:195:SER:HG	1.83	0.44
1:A:153:VAL:HG13	1:A:194:TYR:CE1	2.53	0.44
1:A:169:LYS:NZ	1:A:175:TYR:CE1	2.84	0.44
3:C:123:GLU:HB3	3:C:168:MET:CE	2.48	0.44
1:A:4:VAL:CG1	1:A:22:CYS:SG	3.06	0.44
3:C:141:ARG:NH1	3:C:147:PHE:O	2.46	0.44
1:A:39:GLN:HB2	1:A:49:LEU:CD2	2.41	0.43
3:C:86:LEU:HD12	3:C:266:SER:O	2.18	0.43
3:C:203:THR:HA	3:C:211:GLN:O	2.19	0.43
3:C:89:GLU:CG	3:C:267:ILE:HD11	2.48	0.43
1:A:69:ILE:HD12	1:A:74:ALA:HB3	1.99	0.43
2:B:9:PRO:HG3	2:B:18:LEU:HD12	2.00	0.43
2:B:128:PRO:HB3	2:B:154:TYR:CD2	2.53	0.43
2:B:161:VAL:HG11	2:B:188:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HG3	1:A:187:ALA:N	2.34	0.43
3:C:295:GLN:CB	3:C:306:PRO:HB2	2.47	0.43
3:C:168:MET:HA	3:C:169:PRO:HD2	1.87	0.43
1:A:176:MET:HB3	1:A:176:MET:HE2	1.75	0.43
3:C:283:THR:HG22	3:C:286:GLY:N	2.34	0.43
1:A:44:HIS:HB2	2:B:94:TYR:HH	1.80	0.43
2:B:155:PHE:CD1	2:B:156:PRO:N	2.86	0.43
3:C:103:PRO:O	3:C:104:ASP:CB	2.63	0.43
3:C:177:LEU:HB2	3:C:260:MET:SD	2.59	0.43
1:A:165:THR:HG22	2:B:178:VAL:CG1	2.49	0.43
1:A:122:PRO:HB3	1:A:209:LEU:CD2	2.49	0.42
1:A:94:TYR:O	1:A:97:HIS:HB2	2.19	0.42
1:A:87:ILE:HA	1:A:104:THR:O	2.19	0.42
2:B:56:ASN:N	2:B:56:ASN:OD1	2.52	0.42
3:C:185:PRO:HG3	3:C:191:GLN:OE1	2.20	0.42
2:B:27:PHE:HD1	2:B:32:ASN:HD22	1.65	0.42
3:C:70:LEU:HD21	3:C:179:ILE:HD11	2.02	0.42
3:C:282:ILE:O	3:C:301:THR:HA	2.19	0.42
2:B:128:PRO:HB2	2:B:151:VAL:HG13	2.01	0.42
1:A:60:VAL:HA	1:A:61:PRO:HD3	1.82	0.42
3:C:180:TRP:CD2	3:C:204:VAL:HG21	2.54	0.42
3:C:180:TRP:CH2	3:C:213:ILE:HD13	2.53	0.42
1:A:4:VAL:HG23	1:A:99:VAL:HG12	2.02	0.42
2:B:70:SER:OG	2:B:79:PHE:HB2	2.20	0.42
3:C:67:ILE:HD12	3:C:108:LEU:CD1	2.50	0.42
3:C:102:VAL:O	3:C:105:TYR:HB2	2.20	0.42
2:B:27:PHE:CE1	2:B:32:ASN:HB2	2.55	0.42
2:B:163:TRP:HZ2	2:B:188:SER:O	2.03	0.42
2:B:155:PHE:C	2:B:155:PHE:CD1	2.93	0.41
1:A:169:LYS:HE3	1:A:173:ASN:HA	2.02	0.41
3:C:51:ILE:O	3:C:274:ILE:HA	2.21	0.41
3:C:105:TYR:C	3:C:105:TYR:CD1	2.94	0.41
3:C:62:ILE:HB	3:C:63:ASP:H	1.66	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.87	0.41
3:C:62:ILE:HG23	3:C:62:ILE:HD12	1.72	0.41
1:A:153:VAL:HG22	1:A:194:TYR:HD1	1.85	0.41
3:C:174:PHE:HZ	3:C:257:TYR:OH	2.04	0.41
3:C:111:LEU:HD23	3:C:111:LEU:C	2.41	0.41
1:A:169:LYS:NZ	1:A:175:TYR:HE1	2.16	0.41
3:C:264:LYS:HE2	3:C:264:LYS:HB2	1.90	0.41
2:B:101:ASP:OD2	2:B:104:VAL:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ASP:C	2:B:183:LEU:HG	2.40	0.41
1:A:41:LYS:HB3	1:A:42:PRO:HD2	2.02	0.41
2:B:35:HIS:O	2:B:95:CYS:HA	2.21	0.40
3:C:61:GLY:HA2	3:C:79:PHE:CZ	2.57	0.40
2:B:5:LYS:O	2:B:22:CYS:HA	2.20	0.40
3:C:66:LEU:HD12	3:C:267:ILE:HD13	2.03	0.40
3:C:108:LEU:HB2	3:C:234:TRP:HE1	1.83	0.40
3:C:58:ILE:HG12	3:C:86:LEU:HD23	2.03	0.40
2:B:179:LEU:HD12	2:B:179:LEU:HA	1.86	0.40
1:A:49:LEU:HA	1:A:60:VAL:CG2	2.51	0.40
1:A:143:TYR:CD1	1:A:144:PRO:HA	2.56	0.40
2:B:66:ARG:HA	2:B:83:LYS:CE	2.48	0.40
2:B:163:TRP:CD1	2:B:172:VAL:HG22	2.55	0.40

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	208/210 (99%)	180 (86%)	23 (11%)	5 (2%)	7	41
2	B	219/221 (99%)	186 (85%)	30 (14%)	3 (1%)	14	54
3	C	265/282 (94%)	232 (88%)	25 (9%)	8 (3%)	5	35
All	All	692/713 (97%)	598 (86%)	78 (11%)	16 (2%)	8	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	173	HIS
2	B	212	SER
3	C	210	GLN
3	C	263	GLY

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Mol	Chain	Res	Type
1	A	44	HIS
1	A	109	LEU
2	B	153	GLY
3	C	96	ASN
3	C	133	ASN
3	C	304	ALA
1	A	53	THR
3	C	93	ALA
1	A	58	PRO
3	C	62	ILE
1	A	145	GLY
3	C	196	VAL

### 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	178/178 (100%)	160 (90%)	18 (10%)	9	36
2	B	192/192 (100%)	175 (91%)	17 (9%)	12	43
3	C	236/250 (94%)	206 (87%)	30 (13%)	5	25
All	All	606/620 (98%)	541 (89%)	65 (11%)	8	33

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	LEU
1	A	13	SER
1	A	30	THR
1	A	32	SER
1	A	36	ASN
1	A	42	PRO
1	A	44	HIS
1	A	49	LEU
1	A	58	PRO

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Mol	Chain	Res	Type
1	A	109	LEU
1	A	125	SER
1	A	147	VAL
1	A	159	THR
1	A	162	MET
1	A	182	THR
1	A	183	LEU
1	A	199	THR
2	B	7	SER
2	B	38	ARG
2	B	81	LYS
2	B	83	LYS
2	B	117	SER
2	B	142	ASN
2	B	147	LEU
2	B	158	PRO
2	B	165	SER
2	B	179	LEU
2	B	183	LEU
2	B	185	THR
2	B	186	LEU
2	B	187	SER
2	B	205	ASN
2	B	218	LYS
2	B	219	ILE
3	C	45	SER
3	C	48	THR
3	C	66	LEU
3	C	78	VAL
3	C	83	THR
3	C	92	LYS
3	C	108	LEU
3	C	126	THR
3	C	128	THR
3	C	141	ARG
3	C	150	ARG
3	C	155	THR
3	C	159	SER
3	C	161	TYR
3	C	162	PRO
3	C	164	LEU
3	C	167	THR

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Mol	Chain	Res	Type
3	C	182	ILE
3	C	187	THR
3	C	197	GLN
3	C	199	SER
3	C	208	ARG
3	C	210	GLN
3	C	251	LEU
3	C	255	ARG
3	C	264	LYS
3	C	267	ILE
3	C	275	ASP
3	C	277	CYS
3	C	278	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	36	ASN
1	A	54	ASN
1	A	96	ASN
2	B	3	GLN
2	B	142	ASN
3	C	80	GLN
3	C	210	GLN
3	C	216	ASN
3	C	298	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	C	4	3	14,14,15	1.59	5 (35%)	15,19,21	2.64	5 (33%)

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	C	4	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4	NAG	O5-C1	-2.83	1.39	1.43
4	C	4	NAG	C1-C2	-2.04	1.49	1.52
4	C	4	NAG	C4-C5	2.07	1.57	1.53
4	C	4	NAG	C6-C5	2.19	1.59	1.51
4	C	4	NAG	C4-C3	2.80	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4	NAG	O5-C5-C6	-4.00	98.69	107.35
4	C	4	NAG	C4-C3-C2	-2.35	107.57	111.23
4	C	4	NAG	O6-C6-C5	2.53	119.70	111.33
4	C	4	NAG	C6-C5-C4	5.22	125.88	113.02
4	C	4	NAG	C1-O5-C5	6.35	120.31	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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