



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:56 AM UTC

PDB ID : 2VIR / pdb_00002vir
Title : INFLUENZA VIRUS HEMAGGLUTININ 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

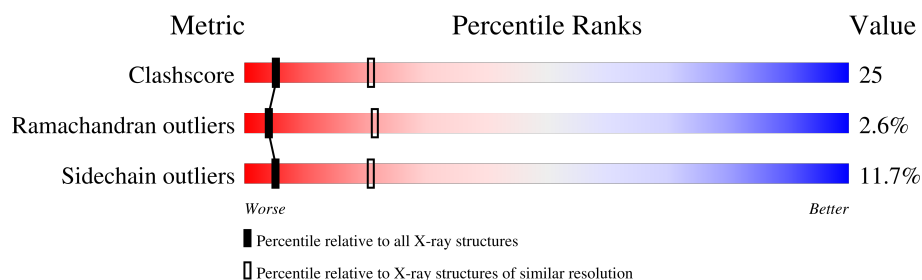
1 Overall quality at a glance

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	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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 4 unique types of molecules in this entry. The entry contains 5339 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
			2075	1304	360	400	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	ASP	ASN	conflict	UNP P03437
C	81	ASP	ASN	modified residue	UNP P03437
C	165	ASP	ASN	modified residue	UNP P03437
C	285	ASP	ASN	modified residue	UNP P03437

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

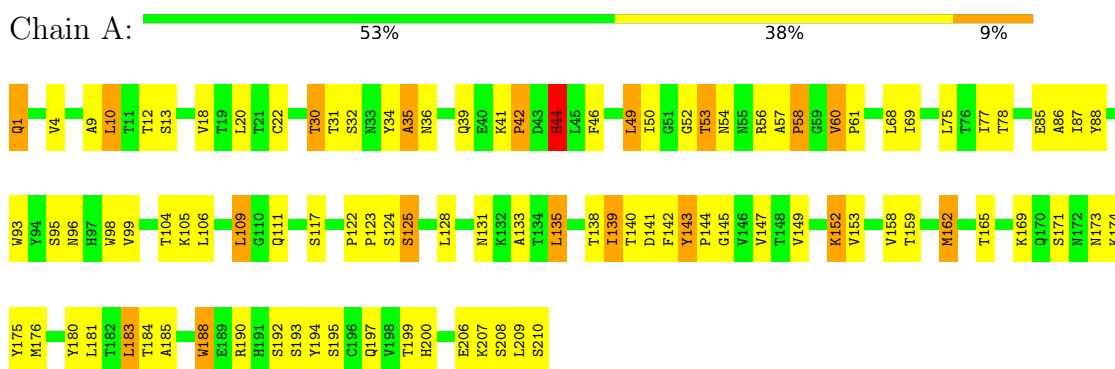
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	C	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

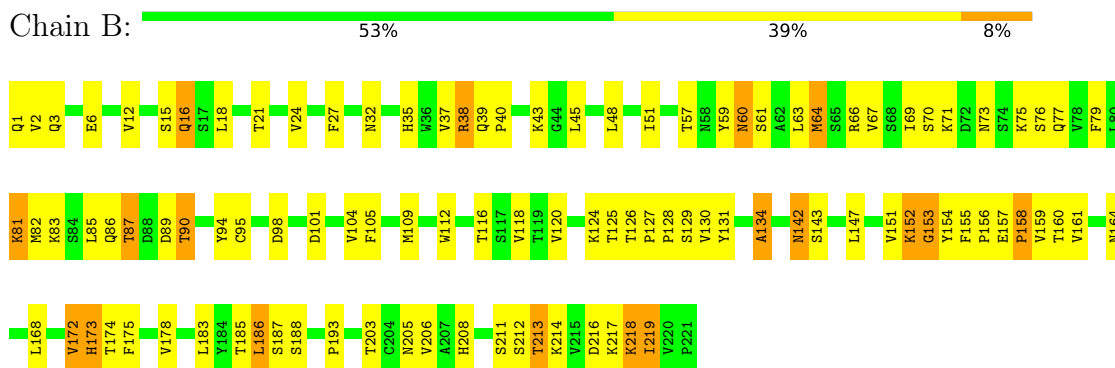
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

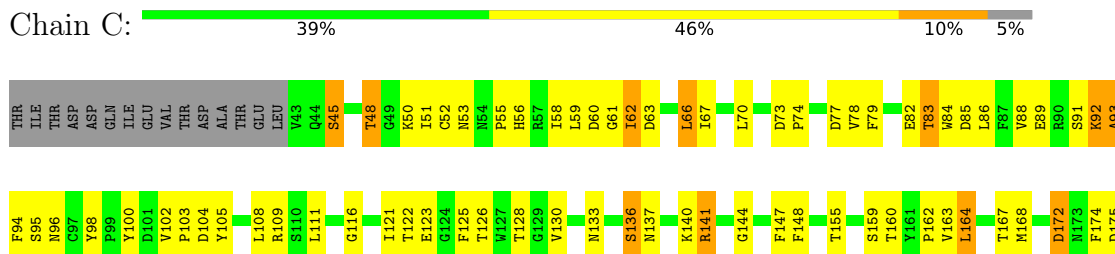
• Molecule 1: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 2: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 3: HEMAGGLUTININ



K176	L177	Y178	I179	W180	G181	I182	H183	H184	P185	S186	T187	M188	Q189	E190	Q191	T192		Y195	V196	Q197	A198	S199	G200	R201	V202	I203	V204	S205	T206	R207	R208	S209	Q210		I213	I214	P215	N216	I217	G218	S219	R220	P221	W222		L226	S227		I230	S231	I232		I236	V237	K238	P239	G240	D241	V242
L243	V244		S247	N248	G249	N250	L251	I252	A253	P254	R255	G256	Y257		M260		G263	G264	S265	S266	I267	M268		D275	T276	C277	I278	S279	E280	C281	I282	T283	P284	D285	G286	S287	I288	P289	N290	D291	K292		Q295	N296	V297	N298	K299	I300		A304	C305	P306		V309					

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.50Å 85.50Å 515.00Å 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}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.198 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5339	wwPDB-VP
Average B, all atoms (Å ²)	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

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	0.77	1/1627 (0.1%)	1.21	13/2224 (0.6%)
2	B	0.74	0/1718	1.24	14/2351 (0.6%)
3	C	0.80	1/2127 (0.0%)	1.25	20/2896 (0.7%)
All	All	0.77	2/5472 (0.0%)	1.24	47/7471 (0.6%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	237	VAL	CA-CB	-5.33	1.47	1.54
1	A	138	THR	CA-CB	5.30	1.60	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	48	THR	N-CA-C	-10.20	100.16	111.07
3	C	160	THR	N-CA-C	9.38	122.94	108.96
2	B	208	HIS	CA-C-N	9.02	131.12	119.84
2	B	208	HIS	C-N-CA	9.02	131.12	119.84
2	B	134	ALA	CA-C-N	8.32	130.24	119.84
2	B	134	ALA	C-N-CA	8.32	130.24	119.84
3	C	85	ASP	N-CA-C	-8.05	103.05	113.12
2	B	127	PRO	CA-C-N	7.84	128.45	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	PRO	C-N-CA	7.84	128.45	119.99
3	C	136	SER	N-CA-C	6.79	119.40	109.07
3	C	98	TYR	CA-C-N	6.65	128.15	119.84
3	C	98	TYR	C-N-CA	6.65	128.15	119.84
3	C	253	ALA	N-CA-C	6.63	119.06	109.84
1	A	131	ASN	N-CA-C	6.40	120.48	111.52
1	A	117	SER	N-CA-C	-6.36	98.16	108.52
3	C	305	CYS	N-CA-C	6.34	120.14	110.50
1	A	95	SER	N-CA-C	6.26	118.84	111.02
1	A	207	LYS	N-CA-C	-6.19	99.93	109.52
3	C	206	THR	N-CA-C	-6.19	100.40	109.18
2	B	159	VAL	N-CA-C	-6.14	100.57	109.29
2	B	16	GLN	N-CA-C	-6.10	97.81	110.80
1	A	57	ALA	CA-C-N	6.01	127.36	119.84
1	A	57	ALA	C-N-CA	6.01	127.36	119.84
2	B	153	GLY	N-CA-C	6.00	127.40	113.18
1	A	171	SER	N-CA-C	-5.88	104.79	111.14
1	A	60	VAL	CA-C-N	5.85	125.81	119.78
1	A	60	VAL	C-N-CA	5.85	125.81	119.78
3	C	172	ASP	N-CA-C	5.82	117.84	110.33
2	B	216	ASP	N-CA-C	-5.80	99.94	109.40
2	B	129	SER	N-CA-C	-5.71	100.36	109.96
3	C	213	ILE	CA-C-N	-5.64	118.42	123.33
3	C	213	ILE	C-N-CA	-5.64	118.42	123.33
3	C	73	ASP	N-CA-C	-5.59	101.28	109.50
1	A	139	ILE	CB-CA-C	-5.54	104.26	110.96
3	C	243	LEU	N-CA-C	-5.45	101.59	110.20
3	C	227	SER	N-CA-C	-5.42	105.89	112.88
2	B	206	VAL	N-CA-C	5.39	114.13	106.53
1	A	140	THR	N-CA-C	5.38	117.16	109.14
2	B	90	THR	N-CA-C	-5.32	101.77	109.59
3	C	264	LYS	N-CA-C	-5.28	107.21	113.97
3	C	77	ASP	N-CA-C	-5.25	105.67	111.71
3	C	205	SER	N-CA-C	5.22	118.58	110.17
1	A	141	ASP	N-CA-C	5.17	118.73	111.90
2	B	64	MET	N-CA-C	5.09	117.48	111.33
3	C	280	GLU	N-CA-C	5.04	119.56	113.41
3	C	232	ILE	N-CA-C	5.03	115.98	108.54
1	A	77	ILE	N-CA-C	-5.02	100.55	108.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	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	73	0
2	B	1672	0	1635	81	0
3	C	2075	0	2011	112	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
All	All	5339	0	5178	258	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 25.

All (258) 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	1.40	1.03
1:A:147:VAL:HG12	1:A:200:HIS:HB2	1.47	0.97
3:C:283:THR:HG23	3:C:285:ASP:H	1.33	0.93
2:B:40:PRO:HG2	2:B:43:LYS:HB2	1.51	0.91
3:C:45:SER:HB3	3:C:296:ASN:OD1	1.81	0.81
1:A:44:HIS:HB2	2:B:94:TYR:OH	1.84	0.78
2:B:131:TYR:CE2	2:B:152:LYS:HE3	2.22	0.75
1:A:93:TRP:CH2	1:A:96:ASN:HA	2.21	0.74
1:A:153:VAL:HG23	1:A:158:VAL:HG22	1.68	0.74
2:B:51:ILE:HA	2:B:57:THR:HG22	1.68	0.73
3:C:148:PHE:HE2	3:C:230:ILE:HD11	1.51	0.73
2:B:174:THR:HG23	2:B:188:SER:HB2	1.70	0.72
2:B:40:PRO:HG2	2:B:43:LYS:CB	2.19	0.72
1:A:152:LYS:HB2	1:A:195:SER:OG	1.89	0.71
1:A:39:GLN:HB2	1:A:49:LEU:HD22	1.73	0.70
3:C:283:THR:HG23	3:C:285:ASP:N	2.07	0.69
3:C:214:ILE:HD12	3:C:215:PRO:O	1.92	0.69
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG23	1:A:158:VAL:CG2	2.23	0.68
1:A:49:LEU:HD12	1:A:60:VAL:HG22	1.74	0.68
3:C:111:LEU:HD21	3:C:260:MET:CE	2.23	0.68
1:A:162:MET:HA	1:A:180:TYR:O	1.94	0.68
1:A:12:THR:HB	1:A:18:VAL:HG11	1.74	0.68
2:B:1:GLN:HE21	2:B:3:GLN:HB2	1.59	0.67
3:C:298:ASN:HD22	3:C:300:ILE:H	1.41	0.67
2:B:18:LEU:HB2	2:B:85:LEU:HD11	1.77	0.67
3:C:185:PRO:HG3	3:C:191:GLN:OE1	1.96	0.66
3:C:103:PRO:O	3:C:104:ASP:HB3	1.94	0.66
2:B:64:MET:HA	2:B:67:VAL:HG22	1.78	0.66
2:B:6:GLU:HA	2:B:21:THR:O	1.97	0.64
2:B:186:LEU:HD23	2:B:187:SER:N	2.13	0.64
3:C:52:CYS:HB3	3:C:277:CYS:O	1.97	0.64
3:C:213:ILE:HD12	3:C:213:ILE:N	2.14	0.63
1:A:46:PHE:CZ	2:B:45:LEU:HD21	2.34	0.63
1:A:153:VAL:HG13	1:A:194:TYR:CE1	2.34	0.63
3:C:237:VAL:HG13	3:C:241:ASP:HB3	1.82	0.62
2:B:155:PHE:CE1	2:B:156:PRO:HB3	2.35	0.62
2:B:143:SER:O	2:B:193:PRO:HA	2.00	0.61
3:C:82:GLU:HG3	3:C:83:THR:H	1.65	0.61
1:A:46:PHE:CE2	2:B:45:LEU:HD11	2.36	0.61
2:B:1:GLN:NE2	2:B:3:GLN:HB2	2.16	0.61
1:A:192:SER:O	1:A:210:SER:HA	2.00	0.60
3:C:283:THR:HG22	3:C:286:GLY:O	2.02	0.60
2:B:131:TYR:HE2	2:B:152:LYS:HE3	1.62	0.60
3:C:283:THR:HG22	3:C:286:GLY:H	1.67	0.60
2:B:87:THR:O	2:B:90:THR:HG22	2.03	0.59
3:C:298:ASN:ND2	3:C:300:ILE:H	2.00	0.59
3:C:242:VAL:HG12	3:C:244:VAL:HG23	1.85	0.59
2:B:134:ALA:CB	2:B:219:ILE:HD11	2.25	0.58
1:A:135:LEU:HB2	1:A:181:LEU:HB3	1.84	0.58
3:C:237:VAL:CG1	3:C:241:ASP:HB3	2.33	0.58
3:C:125:PHE:CE1	3:C:168:MET:HE2	2.39	0.58
3:C:180:TRP:CE2	3:C:204:VAL:HG21	2.39	0.57
1:A:153:VAL:HG22	1:A:194:TYR:CE1	2.40	0.57
3:C:61:GLY:HA2	3:C:79:PHE:CZ	2.40	0.57
3:C:111:LEU:HD21	3:C:260:MET:HE3	1.85	0.57
1:A:139:ILE:HD11	1:A:149:VAL:CG2	2.35	0.57
2:B:59:TYR:HE1	2:B:69:ILE:HG13	1.70	0.56
3:C:89:GLU:CD	3:C:109:ARG:HH12	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:VAL:HG22	3:C:232:ILE:HB	1.85	0.56
2:B:64:MET:HA	2:B:67:VAL:CG2	2.36	0.56
2:B:85:LEU:HD23	2:B:89:ASP:OD2	2.06	0.56
1:A:195:SER:HB3	1:A:208:SER:HB3	1.88	0.55
2:B:105:PHE:CZ	3:C:190:GLU:HG3	2.41	0.55
2:B:66:ARG:HA	2:B:83:LYS:HE3	1.88	0.55
3:C:186:SER:HA	3:C:218:GLY:O	2.06	0.55
1:A:176:MET:HE2	2:B:173:HIS:HD1	1.72	0.55
2:B:12:VAL:HG21	2:B:85:LEU:HD13	1.88	0.55
3:C:53:ASN:OD1	3:C:276:THR:HA	2.06	0.55
2:B:61:SER:O	2:B:64:MET:HG2	2.06	0.54
3:C:58:ILE:HD11	3:C:282:ILE:HD13	1.88	0.54
3:C:84:TRP:CE2	3:C:116:GLY:HA2	2.42	0.54
3:C:51:ILE:CG2	3:C:58:ILE:HD13	2.38	0.54
3:C:172:ASP:HB3	3:C:174:PHE:CE1	2.42	0.54
3:C:121:ILE:HG13	3:C:257:TYR:CE1	2.43	0.54
3:C:176:LYS:HE2	3:C:257:TYR:CE2	2.43	0.54
1:A:1:GLN:O	1:A:99:VAL:HG21	2.08	0.53
1:A:87:ILE:N	1:A:87:ILE:HD12	2.23	0.53
3:C:86:LEU:HD12	3:C:266:SER:O	2.08	0.53
3:C:140:LYS:HE3	3:C:144:GLY:HA2	1.89	0.53
2:B:128:PRO:CB	2:B:154:TYR:HB3	2.39	0.53
1:A:142:PHE:HD1	1:A:142:PHE:H	1.55	0.53
3:C:103:PRO:O	3:C:104:ASP:CB	2.57	0.53
3:C:178:TYR:CD2	3:C:243:LEU:HD22	2.44	0.53
1:A:87:ILE:HA	1:A:104:THR:O	2.09	0.53
3:C:284:PRO:HD3	3:C:300:ILE:O	2.09	0.52
2:B:164:ASN:HB2	2:B:168:LEU:HD13	1.91	0.52
1:A:153:VAL:HG22	1:A:194:TYR:CD1	2.44	0.52
1:A:139:ILE:HD11	1:A:149:VAL:HG22	1.91	0.52
1:A:41:LYS:HE3	1:A:42:PRO:HD2	1.92	0.52
1:A:49:LEU:O	1:A:60:VAL:HG21	2.10	0.52
2:B:90:THR:HA	2:B:118:VAL:O	2.10	0.52
3:C:148:PHE:HE2	3:C:230:ILE:CD1	2.19	0.52
3:C:283:THR:HG22	3:C:286:GLY:N	2.24	0.52
1:A:56:ARG:HD2	1:A:60:VAL:HG12	1.91	0.52
1:A:169:LYS:HZ3	1:A:175:TYR:HE1	1.56	0.52
2:B:63:LEU:N	2:B:63:LEU:HD12	2.25	0.52
3:C:299:LYS:HG2	3:C:300:ILE:HD12	1.92	0.52
2:B:12:VAL:CG2	2:B:85:LEU:HD13	2.39	0.51
2:B:35:HIS:CD2	2:B:98:ASP:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD23	2:B:186:LEU:C	2.34	0.51
2:B:77:GLN:HB3	2:B:79:PHE:CE1	2.46	0.51
2:B:128:PRO:HB3	2:B:154:TYR:CD2	2.46	0.51
1:A:169:LYS:HE3	1:A:173:ASN:HA	1.93	0.51
2:B:27:PHE:HD2	2:B:32:ASN:HD22	1.57	0.51
3:C:192:THR:HG22	3:C:196:VAL:O	2.11	0.51
2:B:1:GLN:HG2	2:B:2:VAL:O	2.10	0.51
1:A:86:ALA:HB3	1:A:88:TYR:CE1	2.46	0.50
1:A:30:THR:OG1	1:A:31:THR:N	2.45	0.50
2:B:71:LYS:HE3	2:B:73:ASN:HD21	1.76	0.50
3:C:184:HIS:HB3	3:C:220:ARG:HH12	1.77	0.50
3:C:122:THR:HG22	3:C:123:GLU:N	2.26	0.50
3:C:183:HIS:HB2	3:C:252:ILE:HD11	1.93	0.50
1:A:142:PHE:CE2	1:A:147:VAL:HG22	2.47	0.50
3:C:111:LEU:HD11	3:C:236:ILE:HD11	1.94	0.50
2:B:24:VAL:HB	2:B:27:PHE:CE1	2.47	0.49
2:B:157:GLU:OE1	2:B:158:PRO:HA	2.12	0.49
1:A:10:LEU:O	1:A:106:LEU:HD12	2.11	0.49
2:B:211:SER:O	2:B:213:THR:N	2.45	0.49
2:B:126:THR:O	2:B:154:TYR:HA	2.12	0.49
3:C:66:LEU:HD12	3:C:267:ILE:HD13	1.94	0.49
3:C:177:LEU:O	3:C:177:LEU:HG	2.12	0.49
3:C:267:ILE:HG13	3:C:268:MET:N	2.28	0.49
2:B:89:ASP:HB2	2:B:120:VAL:HG21	1.93	0.49
1:A:98:TRP:CE2	2:B:109:MET:HE2	2.47	0.49
2:B:125:THR:HG22	2:B:211:SER:HB3	1.93	0.49
1:A:9:ALA:HB2	1:A:105:LYS:HB3	1.95	0.49
1:A:34:TYR:O	1:A:35:ALA:C	2.56	0.49
1:A:54:ASN:N	1:A:54:ASN:ND2	2.61	0.49
3:C:88:VAL:HA	3:C:268:MET:O	2.13	0.49
3:C:195:TYR:CE2	3:C:250:ASN:ND2	2.81	0.49
3:C:299:LYS:HZ3	3:C:300:ILE:HD11	1.77	0.49
1:A:12:THR:HB	1:A:18:VAL:CG1	2.41	0.48
3:C:213:ILE:HD12	3:C:213:ILE:H	1.77	0.48
2:B:86:GLN:HA	2:B:86:GLN:OE1	2.12	0.48
3:C:111:LEU:HD21	3:C:260:MET:HE1	1.95	0.48
3:C:148:PHE:CE2	3:C:230:ILE:HD11	2.40	0.48
3:C:177:LEU:HB2	3:C:260:MET:SD	2.54	0.48
3:C:206:THR:HA	3:C:242:VAL:O	2.13	0.48
3:C:51:ILE:HG22	3:C:58:ILE:HD13	1.94	0.48
2:B:203:THR:HG23	2:B:218:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:GLU:HG3	3:C:83:THR:N	2.28	0.47
3:C:164:LEU:HD12	3:C:164:LEU:HA	1.66	0.47
1:A:4:VAL:HG13	1:A:22:CYS:SG	2.53	0.47
3:C:50:LYS:HD3	3:C:275:ASP:CG	2.39	0.47
3:C:94:PHE:HD2	3:C:95:SER:O	1.97	0.47
1:A:9:ALA:CB	1:A:105:LYS:HB3	2.45	0.47
2:B:70:SER:OG	2:B:79:PHE:HB2	2.14	0.47
2:B:81:LYS:HZ1	2:B:83:LYS:HB3	1.79	0.47
3:C:86:LEU:HA	3:C:266:SER:O	2.14	0.47
3:C:102:VAL:O	3:C:105:TYR:HB2	2.14	0.47
2:B:38:ARG:HG2	2:B:48:LEU:HD21	1.96	0.47
2:B:160:THR:HG22	2:B:160:THR:O	2.15	0.47
3:C:238:LYS:O	3:C:241:ASP:HB2	2.15	0.46
1:A:123:PRO:HG2	1:A:128:LEU:HD11	1.97	0.46
2:B:60:ASN:OD1	2:B:60:ASN:C	2.58	0.46
3:C:200:GLY:O	3:C:215:PRO:HD2	2.15	0.46
2:B:59:TYR:CE1	2:B:69:ILE:HG13	2.51	0.46
2:B:51:ILE:CA	2:B:57:THR:HG22	2.44	0.46
3:C:60:ASP:CG	3:C:62:ILE:HD13	2.41	0.46
3:C:222:TRP:HA	3:C:226:LEU:O	2.15	0.46
3:C:216:ASN:O	3:C:216:ASN:ND2	2.49	0.46
1:A:174:LYS:C	1:A:175:TYR:CD1	2.94	0.46
2:B:124:LYS:O	2:B:126:THR:HG23	2.15	0.46
1:A:85:GLU:HG3	1:A:106:LEU:O	2.16	0.46
3:C:184:HIS:ND1	3:C:216:ASN:N	2.58	0.46
1:A:53:THR:HG21	1:A:68:LEU:CD2	2.46	0.45
1:A:193:SER:HA	1:A:209:LEU:O	2.15	0.45
2:B:37:VAL:CG1	2:B:45:LEU:HD22	2.46	0.45
3:C:100:TYR:CB	3:C:230:ILE:HG13	2.46	0.45
1:A:165:THR:HG22	2:B:178:VAL:CG1	2.47	0.45
1:A:124:SER:O	1:A:125:SER:C	2.59	0.45
3:C:299:LYS:HG2	3:C:300:ILE:CD1	2.46	0.45
1:A:169:LYS:NZ	1:A:175:TYR:HE1	2.14	0.45
3:C:59:LEU:HD22	3:C:82:GLU:HG2	1.97	0.45
3:C:299:LYS:NZ	3:C:300:ILE:HD11	2.32	0.45
3:C:130:VAL:CG1	3:C:162:PRO:HD2	2.47	0.45
3:C:281:CYS:HB3	3:C:288:ILE:O	2.16	0.45
1:A:50:ILE:HD12	1:A:75:LEU:HD13	1.99	0.45
1:A:128:LEU:HD21	1:A:133:ALA:HB2	1.98	0.45
1:A:78:THR:O	1:A:78:THR:HG22	2.17	0.44
2:B:63:LEU:N	2:B:63:LEU:CD1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:LYS:HB2	3:C:264:LYS:HE2	1.76	0.44
3:C:180:TRP:CD2	3:C:204:VAL:HG21	2.53	0.44
1:A:93:TRP:CZ3	1:A:96:ASN:HA	2.51	0.44
3:C:56:HIS:HE1	3:C:280:GLU:O	2.00	0.44
1:A:111:GLN:HG3	1:A:143:TYR:CD2	2.53	0.44
3:C:62:ILE:HD12	3:C:62:ILE:HG23	1.78	0.44
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.85	0.44
1:A:54:ASN:N	1:A:54:ASN:HD22	2.14	0.44
2:B:12:VAL:O	2:B:120:VAL:HA	2.17	0.44
3:C:140:LYS:NZ	3:C:144:GLY:HA2	2.33	0.44
3:C:141:ARG:NH1	3:C:147:PHE:O	2.48	0.44
3:C:178:TYR:CG	3:C:243:LEU:HD22	2.52	0.44
2:B:51:ILE:HG23	2:B:51:ILE:O	2.18	0.44
3:C:187:THR:HG22	3:C:188:ASN:N	2.33	0.44
2:B:15:SER:O	2:B:16:GLN:HG2	2.17	0.44
1:A:143:TYR:CD1	1:A:144:PRO:HA	2.52	0.43
1:A:169:LYS:NZ	1:A:175:TYR:CE1	2.85	0.43
3:C:94:PHE:CD2	3:C:95:SER:O	2.71	0.43
3:C:140:LYS:CE	3:C:144:GLY:HA2	2.48	0.43
1:A:183:LEU:HD13	1:A:188:TRP:HB2	2.00	0.43
1:A:184:THR:O	1:A:185:ALA:C	2.60	0.43
2:B:12:VAL:HG21	2:B:85:LEU:CD1	2.48	0.43
3:C:187:THR:HG22	3:C:189:GLN:H	1.82	0.43
1:A:197:GLN:HG2	1:A:206:GLU:HB3	1.99	0.43
3:C:74:PRO:HG3	3:C:141:ARG:NH1	2.33	0.43
1:A:53:THR:HG21	1:A:68:LEU:HD21	2.00	0.43
2:B:1:GLN:NE2	2:B:3:GLN:NE2	2.67	0.43
3:C:182:ILE:HD13	3:C:202:VAL:HG23	1.99	0.43
3:C:289:PRO:HB2	3:C:291:ASP:OD2	2.18	0.43
1:A:122:PRO:HB3	1:A:209:LEU:HD22	1.99	0.43
2:B:128:PRO:HB2	2:B:151:VAL:HG13	2.01	0.43
3:C:70:LEU:HD21	3:C:179:ILE:HD11	2.01	0.43
3:C:185:PRO:O	3:C:217:ILE:HA	2.19	0.43
3:C:283:THR:CG2	3:C:286:GLY:H	2.30	0.43
1:A:174:LYS:O	1:A:175:TYR:CD1	2.72	0.43
3:C:214:ILE:HD12	3:C:214:ILE:C	2.44	0.43
2:B:101:ASP:OD2	2:B:104:VAL:N	2.48	0.42
3:C:163:VAL:O	3:C:163:VAL:HG12	2.19	0.42
3:C:178:TYR:CD1	3:C:256:GLY:O	2.72	0.42
3:C:295:GLN:HB3	3:C:306:PRO:HB2	2.01	0.42
1:A:60:VAL:HA	1:A:61:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:HIS:HB3	3:C:220:ARG:NH1	2.35	0.42
3:C:291:ASP:OD1	3:C:292:LYS:HG3	2.18	0.42
1:A:4:VAL:CG1	1:A:22:CYS:SG	3.08	0.42
2:B:37:VAL:HG21	2:B:112:TRP:CH2	2.54	0.42
2:B:64:MET:HE3	2:B:64:MET:HB2	1.95	0.42
1:A:85:GLU:O	1:A:86:ALA:HB2	2.20	0.42
3:C:247:SER:OG	3:C:248:ASN:N	2.51	0.42
1:A:49:LEU:HA	1:A:60:VAL:HG21	2.02	0.42
3:C:89:GLU:HG3	3:C:267:ILE:HD11	2.01	0.42
3:C:175:ASP:OD1	3:C:239:PRO:HD3	2.19	0.42
2:B:38:ARG:NH2	2:B:82:MET:HE1	2.35	0.41
3:C:59:LEU:CD2	3:C:82:GLU:HG2	2.51	0.41
3:C:275:ASP:HB3	3:C:277:CYS:SG	2.61	0.41
1:A:41:LYS:HB3	1:A:42:PRO:HD2	2.01	0.41
3:C:91:SER:O	3:C:92:LYS:C	2.64	0.41
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.03	0.41
1:A:153:VAL:HG22	1:A:194:TYR:HE1	1.86	0.41
2:B:142:ASN:ND2	2:B:143:SER:H	2.19	0.41
3:C:63:ASP:O	3:C:93:ALA:HA	2.20	0.41
3:C:84:TRP:CZ2	3:C:116:GLY:HA2	2.56	0.41
3:C:105:TYR:CD1	3:C:105:TYR:C	2.99	0.41
3:C:180:TRP:HH2	3:C:213:ILE:HD13	1.85	0.41
2:B:172:VAL:O	2:B:173:HIS:C	2.64	0.41
3:C:288:ILE:O	3:C:288:ILE:HG13	2.20	0.41
1:A:69:ILE:O	1:A:69:ILE:HG22	2.20	0.40
2:B:35:HIS:O	2:B:95:CYS:HA	2.21	0.40
3:C:136:SER:OG	3:C:137:ASN:N	2.53	0.40
2:B:75:LYS:O	2:B:76:SER:HB2	2.20	0.40
2:B:130:VAL:O	2:B:217:LYS:HE3	2.21	0.40
2:B:128:PRO:CA	2:B:154:TYR:HB3	2.52	0.40
2:B:155:PHE:CD1	2:B:155:PHE:C	2.99	0.40
2:B:214:LYS:HE2	2:B:214:LYS:HB3	1.61	0.40
1:A:52:GLY:O	1:A:53:THR:HB	2.21	0.40
1:A:176:MET:HB2	2:B:175:PHE:CE1	2.57	0.40
3:C:180:TRP:NE1	3:C:204:VAL:HG11	2.37	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%)	183 (88%)	19 (9%)	6 (3%)	3	20
2	B	219/221 (99%)	189 (86%)	26 (12%)	4 (2%)	6	29
3	C	265/282 (94%)	232 (88%)	25 (9%)	8 (3%)	3	19
All	All	692/713 (97%)	604 (87%)	70 (10%)	18 (3%)	4	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	87	THR
2	B	173	HIS
2	B	212	SER
3	C	210	GLN
2	B	153	GLY
3	C	133	ASN
3	C	263	GLY
3	C	304	ALA
1	A	44	HIS
1	A	53	THR
1	A	58	PRO
1	A	109	LEU
1	A	145	GLY
3	C	93	ALA
3	C	96	ASN
1	A	35	ALA
3	C	62	ILE
3	C	196	VAL

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	178/178 (100%)	157 (88%)	21 (12%)	5	21
2	B	192/192 (100%)	175 (91%)	17 (9%)	9	30
3	C	236/250 (94%)	203 (86%)	33 (14%)	3	15
All	All	606/620 (98%)	535 (88%)	71 (12%)	5	21

All (71) 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	20	LEU
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
1	A	109	LEU
1	A	125	SER
1	A	135	LEU
1	A	152	LYS
1	A	159	THR
1	A	162	MET
1	A	183	LEU
1	A	188	TRP
1	A	190	ARG
1	A	199	THR
2	B	38	ARG
2	B	60	ASN
2	B	81	LYS
2	B	116	THR
2	B	142	ASN
2	B	147	LEU
2	B	152	LYS
2	B	158	PRO
2	B	161	VAL
2	B	172	VAL

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Mol	Chain	Res	Type
2	B	183	LEU
2	B	185	THR
2	B	186	LEU
2	B	205	ASN
2	B	213	THR
2	B	218	LYS
2	B	219	ILE
3	C	45	SER
3	C	48	THR
3	C	55	PRO
3	C	66	LEU
3	C	67	ILE
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	155	THR
3	C	159	SER
3	C	164	LEU
3	C	167	THR
3	C	179	ILE
3	C	182	ILE
3	C	188	ASN
3	C	197	GLN
3	C	199	SER
3	C	207	ARG
3	C	208	ARG
3	C	210	GLN
3	C	214	ILE
3	C	230	ILE
3	C	251	LEU
3	C	255	ARG
3	C	264	LYS
3	C	267	ILE
3	C	275	ASP
3	C	278	ILE
3	C	283	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	54	ASN
1	A	81	GLN
2	B	3	GLN
2	B	142	ASN
2	B	180	GLN
3	C	80	GLN
3	C	189	GLN
3	C	210	GLN
3	C	216	ASN
3	C	298	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.