



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 AM UTC

PDB ID : 2VIS / pdb_00002vis
Title : INFLUENZA VIRUS HEMAGGLUTININ, (ESCAPE) MUTANT WITH THR 131 REPLACED BY ILE, COMPLEXED WITH A NEUTRALIZING ANTIBODY
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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

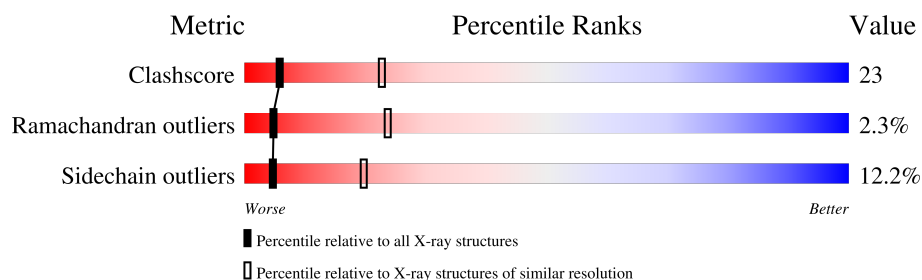
1 Overall quality at a glance

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 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			

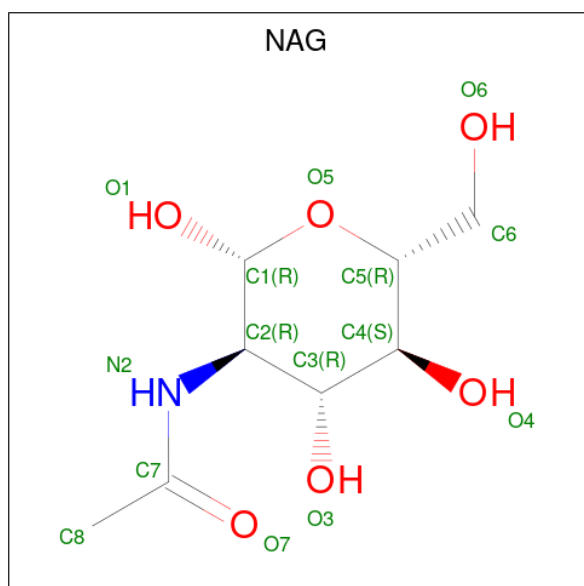
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	131	ILE	THR	engineered mutation	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		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



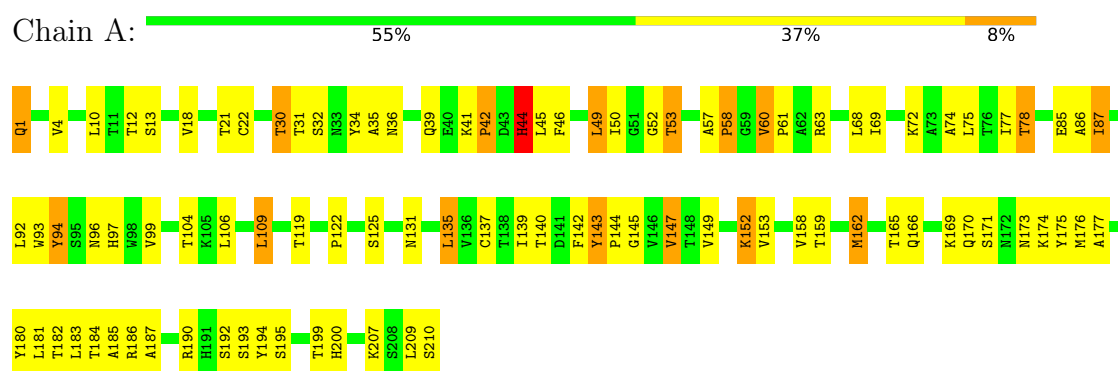
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

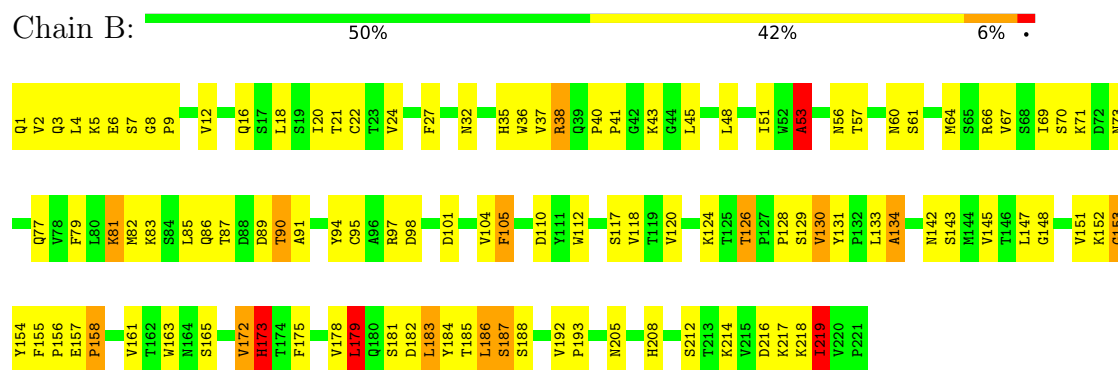
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

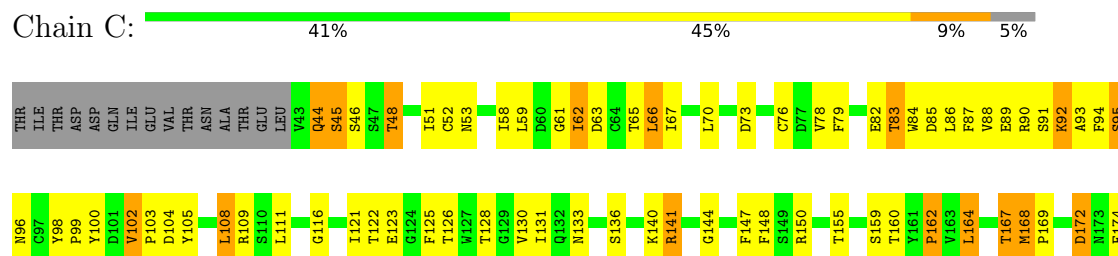
• Molecule 1: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 2: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 3: HEMAGGLUTININ



D175	K176	L177	Y178	I179	W180	G181	I182	H183	H184	P185	S186	T187	E190	Q191	V196	Q197	A198	S199	G200	T203	V204	S205	T206	R207	R208	S209	Q210	Q211	T212	I213	I214	P215	N216	I217	G218	S219	R220	P221	W222	L226	R229	I230	S231	I232	Y233	W234	T235	I236	V237	K238	D241	V242	L243
V244	N250	L251	I252	A253	P254	R255	G256	Y257	M260	R261	T262	G263	K264	S265	S266	I267	M268	I274	D275	T276	Q277	L278	S279	E280	C281	I282	T283	P284	N285	G286	S287	I288	P289	N290	D291	K292	Q295	N296	V297	N298	K299	I300	T301	Y302	G303	A304	C305	P306	K307	Y308	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}	0.11	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 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, 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	0.72	0/1627	1.19	10/2224 (0.4%)
2	B	0.78	3/1718 (0.2%)	1.22	17/2351 (0.7%)
3	C	0.78	0/2128	1.29	23/2897 (0.8%)
All	All	0.76	3/5473 (0.1%)	1.24	50/7472 (0.7%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	219	ILE	CA-CB	6.15	1.60	1.53
2	B	53	ALA	N-CA	-5.74	1.38	1.46
2	B	173	HIS	CD2-NE2	5.42	1.43	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	85	ASP	N-CA-C	-9.50	101.25	113.12
3	C	160	THR	N-CA-C	9.39	122.95	108.96
2	B	134	ALA	CA-C-N	7.68	127.22	119.24
2	B	134	ALA	C-N-CA	7.68	127.22	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	73	ASP	N-CA-C	-7.43	98.58	109.50
2	B	216	ASP	N-CA-C	-7.39	97.90	109.72
1	A	131	ASN	N-CA-C	7.04	121.11	111.54
2	B	16	GLN	N-CA-C	-6.97	98.39	107.73
3	C	136	SER	N-CA-C	6.93	119.60	109.07
3	C	305	CYS	N-CA-C	6.74	120.41	110.10
3	C	48	THR	N-CA-C	-6.73	103.87	111.07
2	B	208	HIS	CA-C-N	6.71	128.23	119.84
2	B	208	HIS	C-N-CA	6.71	128.23	119.84
2	B	153	GLY	N-CA-C	6.60	128.82	113.18
3	C	280	GLU	N-CA-C	6.58	121.53	112.90
3	C	253	ALA	N-CA-C	6.55	118.95	109.84
2	B	110	ASP	N-CA-C	6.43	119.53	111.24
3	C	184	HIS	CB-CA-C	-6.28	103.93	110.33
3	C	172	ASP	N-CA-C	6.26	117.95	110.19
3	C	206	THR	N-CA-C	-6.14	100.06	109.65
1	A	60	VAL	CA-C-N	6.05	126.01	119.78
1	A	60	VAL	C-N-CA	6.05	126.01	119.78
2	B	8	GLY	CA-C-N	5.93	127.25	119.84
2	B	8	GLY	C-N-CA	5.93	127.25	119.84
3	C	76	CYS	N-CA-C	-5.92	104.72	112.41
3	C	252	ILE	N-CA-C	-5.91	97.05	109.34
2	B	105	PHE	N-CA-C	5.72	117.60	110.91
1	A	63	ARG	N-CA-C	5.69	119.70	112.87
2	B	90	THR	N-CA-C	-5.64	101.49	109.96
1	A	57	ALA	CA-C-N	5.59	126.83	119.84
1	A	57	ALA	C-N-CA	5.59	126.83	119.84
2	B	130	VAL	N-CA-C	5.57	115.61	107.37
1	A	166	GLN	N-CA-C	-5.54	102.22	110.20
2	B	179	LEU	N-CA-C	5.46	116.24	108.54
1	A	207	LYS	N-CA-C	-5.21	101.27	109.50
2	B	129	SER	N-CA-C	-5.21	100.82	109.46
3	C	250	ASN	N-CA-C	5.19	121.85	110.80
3	C	48	THR	CB-CA-C	-5.18	102.74	110.88
3	C	168	MET	CA-C-N	5.17	125.33	119.90
3	C	168	MET	C-N-CA	5.17	125.33	119.90
2	B	126	THR	CA-C-N	5.16	123.42	119.66
2	B	126	THR	C-N-CA	5.16	123.42	119.66
1	A	45	LEU	N-CA-C	-5.15	96.94	107.70
3	C	213	ILE	CA-C-N	-5.14	118.86	123.33
3	C	213	ILE	C-N-CA	-5.14	118.86	123.33
3	C	65	THR	N-CA-C	-5.13	102.40	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	VAL	CB-CA-C	-5.11	106.23	111.08
3	C	44	GLN	N-CA-C	-5.06	100.92	108.96
3	C	95	SER	N-CA-C	-5.03	103.41	110.35
1	A	140	THR	N-CA-C	5.02	116.62	109.14

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	69	0
2	B	1672	0	1635	80	0
3	C	2076	0	2020	102	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	C	14	0	13	0	0
All	All	5354	0	5200	244	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 23.

All (244) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:53:ALA:HB3	3:C:131:ILE:HG12	1.75	0.68
2:B:143:SER:O	2:B:193:PRO:HA	1.94	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
1:A:169:LYS:HZ2	1:A:175:TYR:HE1	1.43	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:89:GLU:CD	3:C:109:ARG:HH12	2.07	0.63
2:B:38:ARG:NH2	2:B:82:MET:HE1	2.15	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:153:VAL:HG22	1:A:194:TYR:CD1	2.36	0.60
3:C:46:SER:O	3:C:288:ILE:HG22	2.00	0.60
1:A:170:GLN:HG2	1:A:176:MET:HE3	1.83	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
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
1:A:176:MET:HE2	2:B:173:HIS:HD1	1.69	0.58
2:B:12:VAL:O	2:B:120:VAL:HA	2.02	0.58
1:A:122:PRO:HB3	1:A:209:LEU:HD22	1.85	0.58
3:C:238:LYS:O	3:C:241:ASP:HB2	2.04	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:36:TRP:HD1	2:B:69:ILE:HD13	1.70	0.56
2:B:86:GLN:HA	2:B:86:GLN:OE1	2.05	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:O	1:A:69:ILE:HG22	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:180:TRP:CE2	3:C:204:VAL:HG21	2.43	0.54
3:C:295:GLN:HB3	3:C:306:PRO:HB2	1.89	0.54
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:89:GLU:HG3	3:C:267:ILE:HD11	1.89	0.53
3:C:237:VAL:HG13	3:C:241:ASP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG13	1:A:22:CYS:SG	2.49	0.53
2:B:1:GLN:HG2	2:B:2:VAL:O	2.08	0.53
3:C:162:PRO:HG2	3:C:164:LEU:HD13	1.91	0.53
1:A:87:ILE:N	1:A:87:ILE:HD12	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
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
2:B:186:LEU:HD23	2:B:186:LEU:C	2.37	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
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
2:B:90:THR:HA	2:B:118:VAL:O	2.13	0.49
1:A:34:TYR:O	1:A:35:ALA:C	2.55	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
1:A:30:THR:OG1	1:A:31:THR:N	2.47	0.48
3:C:213:ILE:HD12	3:C:213:ILE:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:PHE:C	2:B:155:PHE:CD1	2.93	0.46
2:B:181:SER:OG	2:B:182:ASP:N	2.45	0.46
2:B:145:VAL:CG1	2:B:192:VAL:HG23	2.45	0.46
3:C:176:LYS:HE2	3:C:257:TYR:CD2	2.51	0.46
2:B:85:LEU:HD23	2:B:89:ASP:OD2	2.16	0.46
2:B:179:LEU:HD13	2:B:184:TYR:CD1	2.51	0.46
3:C:51:ILE:CG2	3:C:58:ILE:HD13	2.45	0.46
1:A:169:LYS:HD2	1:A:175:TYR:CZ	2.51	0.46
3:C:105:TYR:C	3:C:105:TYR:CD1	2.94	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
2:B:27:PHE:CE2	2:B:97:ARG:HD3	2.51	0.46
2:B:61:SER:O	2:B:64:MET:HG2	2.15	0.46
3:C:100:TYR:CB	3:C:230:ILE:HG13	2.46	0.46
3:C:111:LEU:HD23	3:C:111:LEU:C	2.41	0.46
3:C:94:PHE:CD2	3:C:95:SER:O	2.68	0.46
3:C:99:PRO:HB2	3:C:229:ARG:HD3	1.98	0.45
1:A:85:GLU:HG3	1:A:106:LEU: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
2:B:182:ASP:C	2:B:183:LEU:HG	2.40	0.45
3:C:98:TYR:HA	3:C:99:PRO:HD3	1.88	0.45
3:C:111:LEU:HD21	3:C:260:MET:CE	2.46	0.45
3:C:122:THR:HG22	3:C:123:GLU:N	2.32	0.45
1:A:53:THR:HG21	1:A:68:LEU:HD22	1.98	0.45
2:B:40:PRO:HA	2:B:91:ALA:CB	2.47	0.45
2:B:214:LYS:HB3	2:B:214:LYS:HE2	1.66	0.44
3:C:180:TRP:HH2	3:C:213:ILE:CD1	2.30	0.44
1:A:52:GLY:O	1:A:53:THR:HB	2.17	0.44
1:A:85:GLU:O	1:A:86:ALA:HB2	2.17	0.44
1:A:152:LYS:HB2	1:A:195:SER:HG	1.82	0.44
2:B:105:PHE:CZ	3:C:190:GLU:HG3	2.53	0.44
3:C:90:ARG:HH22	3:C:274:ILE:HG13	1.83	0.44
3:C:140:LYS:NZ	3:C:144:GLY:HA2	2.33	0.44
3:C:150:ARG:HD2	3:C:150:ARG:N	2.33	0.44
3:C:262:THR:O	3:C:264:LYS:N	2.51	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
3:C:177:LEU:O	3:C:177:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:172:VAL:O	2:B:172:VAL:HG13	2.16	0.44
1:A:4:VAL:CG1	1:A:22:CYS:SG	3.06	0.44
1:A:153:VAL:HG13	1:A:194:TYR:CE1	2.53	0.44
3:C:123:GLU:HB3	3:C:168:MET:CE	2.48	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
2:B:81:LYS:HZ1	2:B:83:LYS:HB3	1.83	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
2:B:172:VAL:O	2:B:173:HIS:C	2.60	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
3:C:168:MET:HA	3:C:169:PRO:HD2	1.87	0.43
3:C:295:GLN:CB	3:C:306:PRO:HB2	2.47	0.43
2:B:155:PHE:CD1	2:B:156:PRO:N	2.86	0.43
3:C:283:THR:HG22	3:C:286:GLY:N	2.34	0.43
1:A:186:ARG:HG3	1:A:187:ALA:N	2.34	0.43
3:C:111:LEU:HD21	3:C:260:MET:HE3	1.99	0.43
3:C:103:PRO:O	3:C:104:ASP:CB	2.63	0.43
1:A:165:THR:HG22	2:B:178:VAL:CG1	2.49	0.43
3:C:177:LEU:HB2	3:C:260:MET:SD	2.59	0.43
1:A:87:ILE:HA	1:A:104:THR:O	2.19	0.42
1:A:94:TYR:O	1:A:97:HIS:HB2	2.19	0.42
1:A:122:PRO:HB3	1:A:209:LEU:CD2	2.49	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:44:GLN:CD	3:C:289:PRO:HG2	2.44	0.42
3:C:70:LEU:HD21	3:C:179:ILE:HD11	2.02	0.42
2:B:133:LEU:HB2	2:B:148:GLY:C	2.45	0.42
3:C:257:TYR:CD1	3:C:257:TYR:C	2.97	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
3:C:91:SER:O	3:C:92:LYS:C	2.63	0.42
1:A:4:VAL:HG23	1:A:99:VAL:HG12	2.02	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: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
2:B:70:SER:OG	2:B:79:PHE:HB2	2.20	0.42
2:B:27:PHE:CE1	2:B:32:ASN:HB2	2.55	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:163:TRP:HZ2	2:B:188:SER:O	2.03	0.42
1:A:184:THR:O	1:A:185:ALA:C	2.62	0.41
2:B:60:ASN:OD1	2:B:60:ASN:C	2.62	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: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
3:C:125:PHE:CZ	3:C:168:MET:HE2	2.55	0.41
1:A:153:VAL:HG22	1:A:194:TYR:HD1	1.85	0.41
1:A:171:SER:C	1:A:173:ASN:H	2.27	0.41
3:C:174:PHE:HZ	3:C:257:TYR:OH	2.04	0.41
2:B:101:ASP:OD2	2:B:104:VAL:N	2.50	0.41
3:C:264:LYS:HB2	3:C:264:LYS:HE2	1.90	0.41
1:A:41:LYS:HB3	1:A:42:PRO:HD2	2.02	0.41
2:B:5:LYS:O	2:B:22:CYS:HA	2.20	0.40
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
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
1:A:174:LYS:C	1:A:175:TYR:CD1	2.99	0.40
2:B:64:MET:HE3	2:B:64:MET:HB2	1.90	0.40
2:B:179:LEU:HD12	2:B:179:LEU:HA	1.86	0.40
3:C:58:ILE:HG12	3:C:86:LEU:HD23	2.03	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
1:A:169:LYS:NZ	1:A:175:TYR:HE1	2.16	0.40
3:C:87:PHE:CD1	3:C:87:PHE:C	2.99	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%)	4	23
2	B	219/221 (99%)	186 (85%)	30 (14%)	3 (1%)	9	33
3	C	265/282 (94%)	232 (88%)	25 (9%)	8 (3%)	3	19
All	All	692/713 (97%)	598 (86%)	78 (11%)	16 (2%)	5	24

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
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 [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%)	154 (86%)	24 (14%)	4	16
2	B	192/192 (100%)	174 (91%)	18 (9%)	8	29
3	C	236/250 (94%)	204 (86%)	32 (14%)	3	16
All	All	606/620 (98%)	532 (88%)	74 (12%)	5	20

All (74) 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
1	A	77	ILE
1	A	78	THR
1	A	87	ILE
1	A	109	LEU
1	A	125	SER
1	A	135	LEU
1	A	147	VAL
1	A	152	LYS
1	A	159	THR
1	A	162	MET
1	A	182	THR
1	A	183	LEU
1	A	190	ARG
1	A	199	THR
2	B	7	SER
2	B	20	ILE
2	B	38	ARG
2	B	81	LYS
2	B	117	SER
2	B	142	ASN
2	B	147	LEU
2	B	158	PRO

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Mol	Chain	Res	Type
2	B	165	SER
2	B	172	VAL
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	155	THR
3	C	159	SER
3	C	162	PRO
3	C	164	LEU
3	C	167	THR
3	C	179	ILE
3	C	182	ILE
3	C	187	THR
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	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
3	C	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	36	ASN
1	A	54	ASN
1	A	170	GLN
2	B	3	GLN
2	B	73	ASN
2	B	142	ASN
3	C	54	ASN
3	C	80	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 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
5	NAG	C	4	3	14,14,15	1.62	4 (28%)	17,19,21	2.63	6 (35%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4	NAG	C4-C3	2.86	1.59	1.52
5	C	4	NAG	O5-C1	-2.80	1.39	1.43
5	C	4	NAG	C6-C5	2.36	1.59	1.51
5	C	4	NAG	C4-C5	2.09	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	NAG	C1-O5-C5	6.06	120.31	112.19
5	C	4	NAG	C6-C5-C4	5.24	125.88	113.02
5	C	4	NAG	O5-C5-C6	-4.61	98.69	107.66
5	C	4	NAG	C1-C2-N2	3.31	115.65	110.43
5	C	4	NAG	O6-C6-C5	2.46	119.70	111.33
5	C	4	NAG	C4-C3-C2	-2.35	107.57	111.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	4	NAG	O5-C5-C6-O6

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

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.