



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:48 PM UTC

PDB ID : 1DBM / pdb_00001dbm
Title : MOLECULAR BASIS OF CROSS-REACTIVITY AND THE LIMITS OF ANTIBODY-ANTIGEN COMPLEMENTARITY
Authors : Arevalo, J.H.; Wilson, I.A.
Deposited on : 1993-08-24
Resolution : 2.70 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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

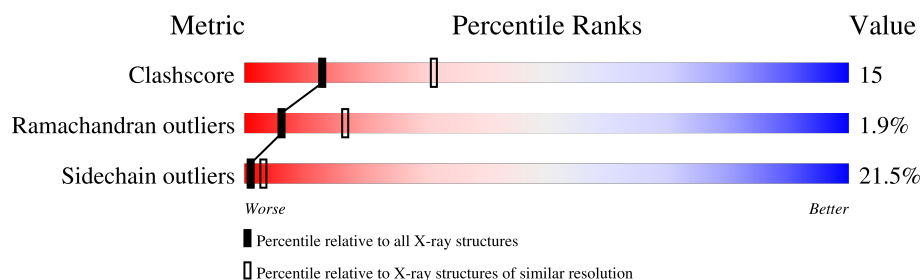
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	L	216	
2	H	219	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3385 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 IGG1-KAPPA DB3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1679	1051	286	335	7			

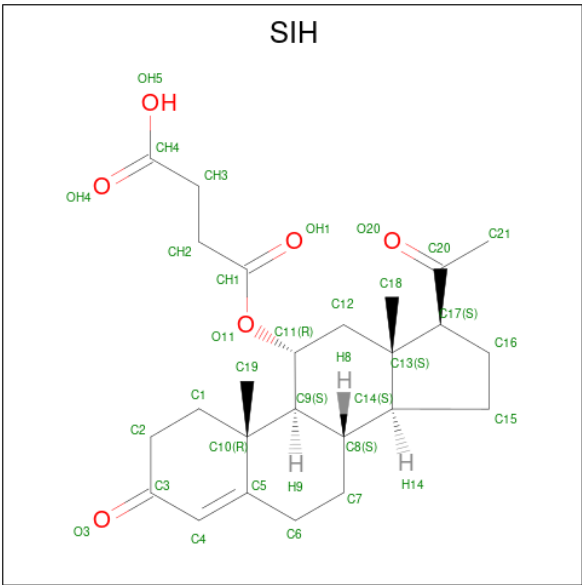
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	ILE	conflict	GB 1589925
L	7	ILE	SER	conflict	GB 1589925
L	14	ASN	SER	conflict	GB 1589925
L	27B	LEU	VAL	conflict	GB 1589925
L	27C	ILE	VAL	conflict	GB 1589925
L	34	HIS	GLU	conflict	GB 1589925
L	36	TYR	PHE	conflict	GB 1589925
L	48	MET	ILE	conflict	GB 1589925
L	56	TYR	SER	conflict	GB 1589925
L	85	ILE	VAL	conflict	GB 1589925
L	87	PHE	TYR	conflict	GB 1589925
L	89	SER	PHE	conflict	GB 1589925
L	91	SER	ALA	conflict	GB 1589925
L	96	PRO	TRP	conflict	GB 1589925

- Molecule 2 is a protein called IGG1-KAPPA DB3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1675	1071	270	328	6			

- Molecule 3 is PROGESTERONE-11-ALPHA-OL-HEMISUCCINATE (CCD ID: SIH) (formula: C₂₅H₃₄O₆).



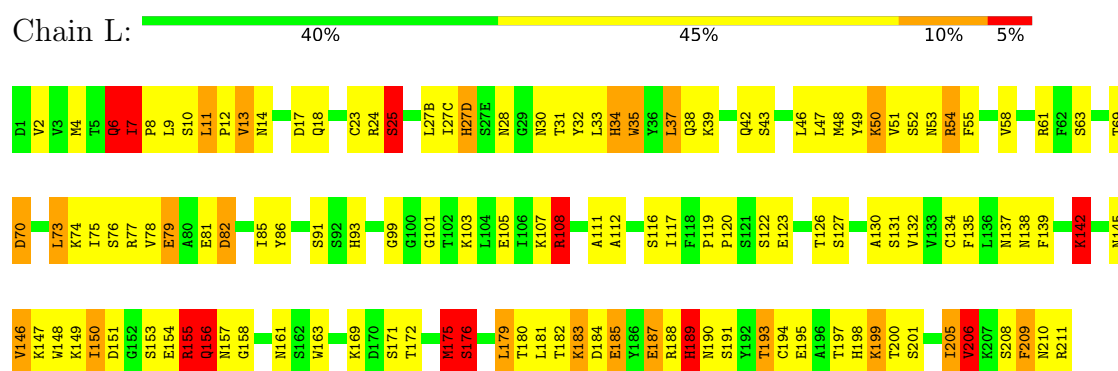
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			31	25	6		

3 Residue-property plots

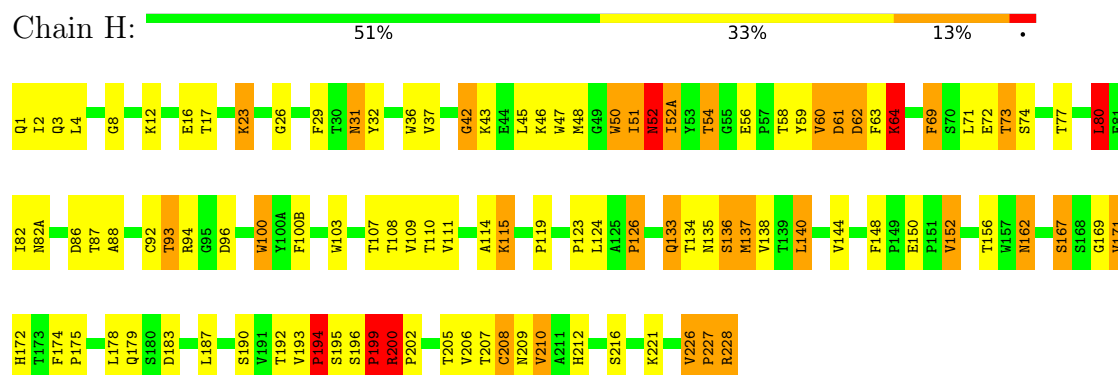
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG1-KAPPA DB3 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA DB3 FAB (HEAVY CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.76Å 134.76Å 124.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3385	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	L	1.21	9/1719 (0.5%)	2.11	61/2331 (2.6%)
2	H	1.25	8/1723 (0.5%)	2.19	75/2358 (3.2%)
All	All	1.23	17/3442 (0.5%)	2.15	136/4689 (2.9%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	189	HIS	CD2-NE2	-7.64	1.29	1.37
2	H	212	HIS	CD2-NE2	-7.56	1.29	1.37
1	L	198	HIS	CD2-NE2	-7.43	1.29	1.37
2	H	210	VAL	CA-CB	7.43	1.62	1.54
2	H	171	VAL	CA-CB	6.69	1.62	1.54
1	L	205	ILE	CA-CB	6.55	1.61	1.53
2	H	172	HIS	CD2-NE2	-6.49	1.30	1.37
2	H	134	THR	CA-CB	6.46	1.64	1.53
1	L	34	HIS	CD2-NE2	-6.45	1.30	1.37
1	L	93	HIS	CD2-NE2	-6.28	1.30	1.37
1	L	27(D)	HIS	CD2-NE2	-6.04	1.31	1.37
2	H	172	HIS	CG-ND1	-5.80	1.31	1.38
2	H	227	PRO	CA-CB	-5.63	1.46	1.53
1	L	35	TRP	CG-CD2	-5.53	1.33	1.43
1	L	206	VAL	CA-CB	5.32	1.62	1.55
1	L	189	HIS	CG-ND1	-5.24	1.32	1.38
2	H	16	GLU	CA-CB	-5.22	1.45	1.53

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	L	137	ASN	OD1-CG-ND2	-9.24	113.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ASP	CA-CB-CG	8.98	121.58	112.60
2	H	52	ASN	OD1-CG-ND2	-8.87	113.73	122.60
2	H	226	VAL	CB-CA-C	8.87	118.03	109.33
1	L	27(D)	HIS	CB-CG-CD2	-8.79	119.77	131.20
2	H	62	ASP	N-CA-C	-8.70	102.57	113.01
2	H	100	TRP	N-CA-C	8.57	123.32	112.86
2	H	226	VAL	N-CA-CB	-8.43	102.62	111.64
2	H	148	PHE	O-C-N	-7.95	115.63	121.83
2	H	94	ARG	CB-CG-CD	-7.91	93.11	111.30
2	H	227	PRO	N-CA-C	7.89	123.66	111.11
1	L	123	GLU	CA-CB-CG	7.81	129.72	114.10
1	L	91	SER	N-CA-C	-7.70	101.21	110.44
1	L	35	TRP	CE2-CD2-CE3	7.69	126.49	118.80
1	L	189	HIS	N-CA-C	7.69	120.90	108.76
2	H	72	GLU	CB-CG-CD	7.60	125.52	112.60
2	H	4	LEU	N-CA-C	-7.44	96.77	108.90
1	L	70	ASP	CA-CB-CG	-7.35	105.25	112.60
2	H	172	HIS	CB-CG-CD2	-7.35	121.65	131.20
1	L	156	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	L	148	TRP	CG-CD2-CE3	7.15	141.05	133.90
2	H	60	VAL	N-CA-C	-7.07	96.81	106.85
1	L	38	GLN	OE1-CD-NE2	-7.06	115.54	122.60
2	H	50	TRP	CE2-CD2-CE3	7.02	125.82	118.80
2	H	47	TRP	CG-CD2-CE3	7.00	140.90	133.90
1	L	7	ILE	CA-CB-CG2	-6.90	98.77	110.50
2	H	209	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	L	184	ASP	N-CA-CB	-6.83	99.44	109.82
2	H	8	GLY	CA-C-N	6.83	126.75	119.85
2	H	8	GLY	C-N-CA	6.83	126.75	119.85
2	H	72	GLU	CA-C-O	6.81	129.53	120.89
2	H	179	GLN	N-CA-C	-6.76	95.84	107.61
1	L	27(D)	HIS	CB-CG-ND1	6.74	132.81	122.70
2	H	228	ARG	N-CA-C	-6.72	92.17	111.00
2	H	115	LYS	N-CA-C	-6.71	99.75	110.14
2	H	194	PRO	CA-C-O	-6.66	114.06	121.32
1	L	2	VAL	N-CA-C	-6.66	100.94	109.80
2	H	1	GLN	N-CA-C	-6.66	92.37	111.00
1	L	138	ASN	CA-CB-CG	-6.55	106.05	112.60
1	L	132	VAL	N-CA-C	-6.50	98.85	109.12
1	L	184	ASP	CA-CB-CG	6.45	119.05	112.60
1	L	75	ILE	N-CA-C	-6.44	98.95	109.12
2	H	109	VAL	N-CA-C	-6.44	99.12	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	146	VAL	CB-CA-C	-6.43	102.63	110.99
1	L	25	SER	N-CA-C	6.41	120.14	109.95
2	H	1	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	L	158	GLY	N-CA-C	-6.24	107.09	115.21
2	H	54	THR	N-CA-C	6.24	118.89	111.71
1	L	190	ASN	OD1-CG-ND2	-6.19	116.41	122.60
2	H	29	PHE	CA-CB-CG	6.14	119.94	113.80
2	H	152	VAL	O-C-N	-6.14	116.23	123.05
1	L	175	MET	CA-C-O	-6.10	113.97	121.11
2	H	37	VAL	O-C-N	-6.09	116.93	123.14
2	H	103	TRP	CG-CD2-CE3	6.09	139.99	133.90
1	L	209	PHE	CA-CB-CG	6.08	119.88	113.80
2	H	193	VAL	CA-CB-CG1	-6.04	100.13	110.40
1	L	131	SER	N-CA-C	-6.00	99.42	109.07
1	L	198	HIS	CB-CG-CD2	-6.00	123.41	131.20
2	H	162	ASN	OD1-CG-ND2	-5.98	116.62	122.60
2	H	193	VAL	CA-C-N	5.98	126.33	119.93
2	H	193	VAL	C-N-CA	5.98	126.33	119.93
2	H	23	LYS	CB-CG-CD	5.97	125.03	111.30
2	H	114	ALA	N-CA-C	-5.97	102.50	110.55
1	L	7	ILE	CA-CB-CG1	5.95	120.51	110.40
2	H	1	GLN	CG-CD-NE2	5.89	125.24	116.40
2	H	172	HIS	CB-CA-C	-5.89	102.82	111.77
2	H	42	GLY	O-C-N	5.85	128.51	122.54
1	L	142	LYS	N-CA-C	5.81	123.17	110.80
1	L	175	MET	CA-CB-CG	5.80	125.69	114.10
2	H	227	PRO	CA-C-O	5.80	127.92	121.43
1	L	194	CYS	N-CA-C	-5.76	100.59	109.76
2	H	82	ILE	N-CA-C	-5.72	100.24	108.48
1	L	73	LEU	N-CA-C	-5.72	99.86	109.07
1	L	179	LEU	CA-C-O	-5.69	114.57	121.05
1	L	34	HIS	CB-CG-CD2	-5.67	123.83	131.20
2	H	199	PRO	CA-N-CD	-5.65	104.09	112.00
1	L	108	ARG	CB-CG-CD	5.64	124.27	111.30
1	L	43	SER	CA-C-N	5.63	125.58	119.78
1	L	43	SER	C-N-CA	5.63	125.58	119.78
2	H	174	PHE	CA-CB-CG	-5.63	108.17	113.80
1	L	79	GLU	CA-CB-CG	5.63	125.35	114.10
1	L	145	ASN	OD1-CG-ND2	-5.59	117.01	122.60
2	H	193	VAL	CA-CB-CG2	5.58	119.89	110.40
2	H	100	TRP	CG-CD2-CE3	5.57	139.47	133.90
1	L	138	ASN	N-CA-C	5.53	119.02	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	93	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	L	153	SER	N-CA-C	5.49	118.00	109.60
2	H	226	VAL	O-C-N	-5.48	118.24	121.69
2	H	64	LYS	N-CA-C	5.46	118.38	109.59
2	H	47	TRP	CE2-CD2-CG	-5.46	100.65	107.20
2	H	50	TRP	CE2-CD2-CG	-5.46	100.65	107.20
2	H	107	THR	N-CA-C	-5.45	98.37	107.80
2	H	32	TYR	O-C-N	-5.45	116.10	122.96
1	L	193	THR	CA-C-O	5.45	126.98	120.28
1	L	156	GLN	CB-CG-CD	5.44	121.85	112.60
1	L	6	GLN	CG-CD-NE2	5.41	124.52	116.40
2	H	80	LEU	O-C-N	-5.39	116.89	123.30
1	L	27(C)	ILE	N-CA-C	-5.38	100.83	108.58
2	H	126	PRO	N-CA-C	5.38	123.56	112.47
2	H	92	CYS	N-CA-C	-5.38	100.93	109.59
1	L	53	ASN	N-CA-C	5.36	117.46	108.73
2	H	73	THR	N-CA-C	5.33	117.84	111.71
1	L	176	SER	CA-CB-OG	5.32	121.74	111.10
1	L	199	LYS	CB-CA-C	-5.31	99.85	110.42
1	L	12	PRO	CA-C-O	-5.30	115.56	121.23
1	L	155	ARG	CA-CB-CG	-5.30	103.50	114.10
1	L	185	GLU	CA-CB-CG	5.28	124.66	114.10
1	L	156	GLN	CA-CB-CG	5.28	124.65	114.10
2	H	31	ASN	OD1-CG-ND2	-5.28	117.32	122.60
2	H	216	SER	N-CA-CB	-5.28	103.89	111.70
1	L	14	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	H	16	GLU	CB-CG-CD	-5.24	103.70	112.60
1	L	154	GLU	CA-CB-CG	5.23	124.56	114.10
2	H	175	PRO	CA-N-CD	-5.22	104.69	112.00
2	H	52	ASN	CA-CB-CG	5.22	117.82	112.60
2	H	51	ILE	CB-CA-C	5.22	116.36	110.41
2	H	152	VAL	CA-C-O	-5.21	115.02	120.76
1	L	14	ASN	N-CA-C	-5.21	100.82	109.46
1	L	148	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	L	139	PHE	N-CA-C	5.19	118.02	109.72
2	H	47	TRP	CB-CG-CD1	-5.19	119.12	126.90
2	H	150	GLU	CB-CG-CD	-5.17	103.81	112.60
2	H	50	TRP	NE1-CE2-CD2	5.12	114.06	107.40
1	L	197	THR	CA-C-O	-5.11	114.70	120.32
2	H	150	GLU	N-CA-C	-5.10	103.72	110.40
1	L	82	ASP	CA-CB-CG	5.09	117.69	112.60
2	H	96	ASP	N-CA-CB	-5.07	102.74	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	58	THR	N-CA-C	-5.07	100.91	109.07
2	H	86	ASP	N-CA-C	5.07	119.31	113.18
2	H	135	ASN	CA-CB-CG	-5.05	107.55	112.60
2	H	100	TRP	CE2-CD2-CG	-5.05	101.14	107.20
2	H	169	GLY	CA-C-O	-5.04	114.11	119.55
2	H	200	ARG	CA-C-O	-5.02	115.11	120.23
1	L	148	TRP	CB-CG-CD1	-5.00	119.40	126.90
2	H	47	TRP	CG-CD1-NE1	-5.00	103.70	110.20

There are no chirality outliers.

There are no planarity outliers.

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	L	1679	0	1625	59	0
2	H	1675	0	1633	41	0
3	H	31	0	33	7	0
All	All	3385	0	3291	101	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 15.

All (101) 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)
1:L:149:LYS:HB3	1:L:193:THR:HG23	1.46	0.97
2:H:64:LYS:HZ2	2:H:64:LYS:HA	1.40	0.85
2:H:194:PRO:HB2	2:H:199:PRO:HD2	1.62	0.82
2:H:52(A):ILE:HD12	2:H:71:LEU:HD11	1.61	0.81
2:H:200:ARG:HH11	2:H:200:ARG:HB3	1.51	0.76
1:L:120:PRO:HG2	1:L:130:ALA:HB1	1.71	0.72
2:H:167:SER:O	2:H:171:VAL:HG12	1.91	0.70
1:L:195:GLU:HG3	1:L:206:VAL:HB	1.76	0.67
2:H:23:LYS:HG2	2:H:77:THR:OG1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:ILE:HG22	1:L:8:PRO:HA	1.78	0.66
1:L:163:TRP:CD1	1:L:175:MET:HG2	2.32	0.65
1:L:27(B):LEU:O	1:L:31:THR:HA	1.97	0.63
1:L:48:MET:SD	1:L:54:ARG:HG3	2.39	0.63
1:L:61:ARG:HB2	1:L:76:SER:OG	1.98	0.62
1:L:183:LYS:O	1:L:187:GLU:HG2	2.00	0.62
1:L:34:HIS:HD2	1:L:49:TYR:HA	1.65	0.61
2:H:140:LEU:HD23	2:H:206:VAL:HG11	1.83	0.61
1:L:135:PHE:HD1	1:L:176:SER:HB2	1.68	0.58
1:L:181:LEU:HD23	1:L:185:GLU:HG3	1.86	0.57
2:H:17:THR:HG22	2:H:82(A):ASN:HA	1.85	0.57
1:L:27(B):LEU:HB3	1:L:31:THR:HG23	1.87	0.57
2:H:133:GLN:NE2	2:H:136:SER:N	2.54	0.56
1:L:135:PHE:CD1	1:L:176:SER:HB2	2.41	0.56
1:L:18:GLN:HA	1:L:76:SER:O	2.06	0.56
2:H:50:TRP:CH2	3:H:229:SIH:HH21	2.41	0.56
2:H:93:THR:HG21	2:H:100(B):PHE:HB3	1.88	0.55
1:L:189:HIS:O	1:L:211:ARG:HD3	2.07	0.54
2:H:200:ARG:HB3	2:H:200:ARG:NH1	2.20	0.54
1:L:147:LYS:HB3	1:L:195:GLU:HB3	1.90	0.54
2:H:171:VAL:HA	2:H:190:SER:O	2.08	0.54
1:L:191:SER:HA	1:L:210:ASN:HA	1.91	0.53
2:H:87:THR:HG23	2:H:110:THR:HA	1.90	0.53
1:L:17:ASP:O	1:L:78:VAL:HG23	2.07	0.53
1:L:77:ARG:O	1:L:77:ARG:HG3	2.08	0.53
2:H:59:TYR:CD1	2:H:64:LYS:HE2	2.45	0.52
2:H:64:LYS:HZ2	2:H:64:LYS:CA	2.19	0.52
2:H:42:GLY:C	2:H:43:LYS:HD2	2.35	0.51
1:L:6:GLN:O	1:L:7:ILE:HD13	2.10	0.51
1:L:149:LYS:HB3	1:L:193:THR:CG2	2.32	0.51
1:L:108:ARG:NH2	1:L:111:ALA:HB2	2.25	0.50
2:H:208:CYS:SG	2:H:208:CYS:O	2.68	0.50
2:H:36:TRP:CE3	2:H:80:LEU:HD12	2.46	0.50
2:H:136:SER:O	2:H:137:MET:HG2	2.11	0.49
1:L:193:THR:HB	1:L:208:SER:OG	2.13	0.49
2:H:46:LYS:HD3	2:H:63:PHE:CE1	2.47	0.49
1:L:55:PHE:O	1:L:58:VAL:HG12	2.13	0.49
1:L:150:ILE:HG13	1:L:179:LEU:HD21	1.95	0.48
1:L:108:ARG:HH21	1:L:111:ALA:HB2	1.78	0.48
1:L:116:SER:O	1:L:134:CYS:HA	2.13	0.48
2:H:60:VAL:O	2:H:62:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:TYR:O	1:L:101:GLY:HA2	2.13	0.48
1:L:119:PRO:HB3	1:L:209:PHE:CE1	2.49	0.47
1:L:120:PRO:CG	1:L:130:ALA:HB1	2.42	0.47
2:H:119:PRO:HB2	2:H:144:VAL:HG12	1.96	0.47
1:L:4:MET:HE1	1:L:33:LEU:HD21	1.95	0.47
1:L:187:GLU:HA	1:L:211:ARG:CZ	2.44	0.47
1:L:27(D):HIS:NE2	3:H:229:SIH:O3	2.47	0.47
2:H:50:TRP:HH2	3:H:229:SIH:HH21	1.80	0.47
1:L:181:LEU:HB3	1:L:185:GLU:HG3	1.97	0.47
1:L:63:SER:HB2	1:L:74:LYS:HE2	1.97	0.46
1:L:6:GLN:NE2	1:L:99:GLY:HA3	2.31	0.46
1:L:155:ARG:HH11	1:L:155:ARG:HG3	1.80	0.46
1:L:28:ASN:HD21	1:L:30:ASN:HB2	1.81	0.46
2:H:12:LYS:O	2:H:111:VAL:HA	2.16	0.46
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.50	0.45
2:H:88:ALA:O	2:H:108:THR:HA	2.17	0.45
2:H:69:PHE:N	2:H:69:PHE:CD1	2.85	0.45
1:L:103:LYS:NZ	1:L:142:LYS:HZ2	2.15	0.45
1:L:4:MET:CE	1:L:23:CYS:SG	3.05	0.45
2:H:52:ASN:HD21	2:H:54:THR:HG23	1.81	0.45
2:H:133:GLN:NE2	2:H:136:SER:H	2.15	0.45
1:L:155:ARG:HD2	1:L:179:LEU:HD11	1.99	0.44
2:H:162:ASN:ND2	2:H:207:THR:H	2.16	0.44
1:L:27(D):HIS:ND1	1:L:28:ASN:OD1	2.50	0.44
2:H:2:ILE:HG23	2:H:26:GLY:HA3	2.00	0.44
1:L:25:SER:OG	1:L:69:THR:HA	2.18	0.44
1:L:146:VAL:O	1:L:146:VAL:HG23	2.18	0.44
2:H:50:TRP:CE2	3:H:229:SIH:H183	2.54	0.43
2:H:69:PHE:N	2:H:69:PHE:HD1	2.16	0.43
2:H:100:TRP:CZ2	3:H:229:SIH:H12	2.53	0.43
2:H:133:GLN:HE22	2:H:136:SER:H	1.66	0.43
1:L:4:MET:HB3	1:L:4:MET:HE3	1.77	0.43
2:H:200:ARG:HD2	2:H:202:PRO:HA	2.00	0.43
1:L:156:GLN:HG3	1:L:157:ASN:N	2.34	0.43
1:L:11:LEU:HD22	1:L:13:VAL:HG23	2.00	0.43
2:H:123:PRO:HD3	2:H:221:LYS:HE2	2.01	0.43
1:L:112:ALA:HB2	1:L:200:THR:HB	2.00	0.43
3:H:229:SIH:HH21	3:H:229:SIH:H11	1.83	0.42
1:L:6:GLN:NE2	1:L:101:GLY:H	2.16	0.42
1:L:37:LEU:HD11	1:L:39:LYS:HG3	2.00	0.42
2:H:52(A):ILE:CD1	2:H:71:LEU:HD11	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:THR:HB	1:L:185:GLU:HB3	2.02	0.42
2:H:46:LYS:HD3	2:H:63:PHE:HE1	1.85	0.42
1:L:161:ASN:ND2	1:L:175:MET:HE1	2.35	0.41
2:H:52:ASN:ND2	2:H:54:THR:OG1	2.53	0.41
1:L:32:TYR:CD1	1:L:50:LYS:HD3	2.55	0.41
1:L:108:ARG:CG	1:L:171:SER:HB2	2.51	0.41
1:L:6:GLN:HE22	1:L:99:GLY:HA3	1.86	0.40
2:H:100:TRP:CE2	3:H:229:SIH:H9	2.57	0.40
1:L:27(B):LEU:CD2	1:L:33:LEU:HD23	2.52	0.40
1:L:85:ILE:HD13	1:L:103:LYS:HB2	2.03	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	L	214/216 (99%)	194 (91%)	16 (8%)	4 (2%)	6	17
2	H	217/219 (99%)	191 (88%)	22 (10%)	4 (2%)	6	18
All	All	431/435 (99%)	385 (89%)	38 (9%)	8 (2%)	6	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	151	ASP
2	H	61	ASP
2	H	136	SER
1	L	142	LYS
1	L	199	LYS
2	H	199	PRO
2	H	126	PRO
1	L	51	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	L	194/194 (100%)	151 (78%)	43 (22%)	1	3
2	H	188/188 (100%)	149 (79%)	39 (21%)	1	3
All	All	382/382 (100%)	300 (78%)	82 (22%)	1	3

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	7	ILE
1	L	9	LEU
1	L	10	SER
1	L	11	LEU
1	L	13	VAL
1	L	24	ARG
1	L	25	SER
1	L	35	TRP
1	L	37	LEU
1	L	42	GLN
1	L	46	LEU
1	L	47	LEU
1	L	50	LYS
1	L	52	SER
1	L	54	ARG
1	L	70	ASP
1	L	73	LEU
1	L	79	GLU
1	L	81	GLU
1	L	82	ASP
1	L	105	GLU
1	L	107	LYS
1	L	108	ARG
1	L	117	ILE
1	L	122	SER
1	L	126	THR

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Mol	Chain	Res	Type
1	L	127	SER
1	L	150	ILE
1	L	155	ARG
1	L	156	GLN
1	L	169	LYS
1	L	172	THR
1	L	175	MET
1	L	176	SER
1	L	180	THR
1	L	183	LYS
1	L	187	GLU
1	L	188	ARG
1	L	189	HIS
1	L	201	SER
1	L	205	ILE
1	L	206	VAL
2	H	3	GLN
2	H	31	ASN
2	H	45	LEU
2	H	48	MET
2	H	51	ILE
2	H	52	ASN
2	H	52(A)	ILE
2	H	56	GLU
2	H	61	ASP
2	H	64	LYS
2	H	69	PHE
2	H	73	THR
2	H	74	SER
2	H	80	LEU
2	H	93	THR
2	H	115	LYS
2	H	124	LEU
2	H	133	GLN
2	H	137	MET
2	H	138	VAL
2	H	140	LEU
2	H	152	VAL
2	H	156	THR
2	H	167	SER
2	H	178	LEU
2	H	183	ASP

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Mol	Chain	Res	Type
2	H	187	LEU
2	H	192	THR
2	H	194	PRO
2	H	195	SER
2	H	196	SER
2	H	199	PRO
2	H	200	ARG
2	H	205	THR
2	H	208	CYS
2	H	210	VAL
2	H	226	VAL
2	H	227	PRO
2	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	28	ASN
1	L	34	HIS
1	L	189	HIS
1	L	210	ASN
2	H	35	ASN
2	H	133	GLN
2	H	162	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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SIH	H	229	-	34,34,34	2.19	9 (26%)	50,53,53	2.49	22 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIH	H	229	-	-	10/13/74/74	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	SIH	C9-C11	6.63	1.62	1.53
3	H	229	SIH	C6-C5	-4.97	1.42	1.50
3	H	229	SIH	C4-C3	-4.45	1.36	1.45
3	H	229	SIH	C13-C14	-4.09	1.47	1.55
3	H	229	SIH	C13-C17	-3.29	1.50	1.56
3	H	229	SIH	C4-C5	3.27	1.39	1.34
3	H	229	SIH	O11-CH1	-2.25	1.27	1.34
3	H	229	SIH	C7-C8	-2.09	1.49	1.53
3	H	229	SIH	C7-C6	-2.01	1.48	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	SIH	C17-C13-C14	7.48	107.55	99.72
3	H	229	SIH	O11-CH1-CH2	6.23	124.97	111.48
3	H	229	SIH	C5-C4-C3	-4.38	116.89	123.67
3	H	229	SIH	C1-C2-C3	-3.91	103.64	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	SIH	C16-C17-C13	-3.80	100.81	104.21
3	H	229	SIH	OH1-CH1-CH2	-3.74	109.17	123.78
3	H	229	SIH	C15-C14-C8	3.72	125.03	119.10
3	H	229	SIH	C13-C14-C8	-3.55	109.37	114.41
3	H	229	SIH	C12-C13-C14	3.55	111.05	106.96
3	H	229	SIH	C10-C9-C8	-3.34	108.42	113.64
3	H	229	SIH	C1-C10-C9	2.93	113.76	109.34
3	H	229	SIH	C19-C10-C1	-2.89	105.03	109.43
3	H	229	SIH	C6-C7-C8	-2.88	106.59	111.64
3	H	229	SIH	C18-C13-C12	-2.84	106.58	110.77
3	H	229	SIH	C18-C13-C14	-2.70	106.78	111.68
3	H	229	SIH	C11-O11-CH1	2.41	122.39	117.81
3	H	229	SIH	OH4-CH4-CH3	-2.35	115.65	123.09
3	H	229	SIH	C13-C17-C20	2.26	118.09	114.95
3	H	229	SIH	C7-C6-C5	-2.25	107.80	111.93
3	H	229	SIH	CH3-CH2-CH1	-2.11	107.17	113.44
3	H	229	SIH	C7-C8-C14	-2.04	108.69	112.08
3	H	229	SIH	C6-C5-C10	-2.01	113.22	116.76

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	229	SIH	OH1-CH1-O11-C11
3	H	229	SIH	CH2-CH1-O11-C11
3	H	229	SIH	CH1-CH2-CH3-CH4
3	H	229	SIH	C16-C17-C20-C21
3	H	229	SIH	C16-C17-C20-O20
3	H	229	SIH	CH2-CH3-CH4-OH4
3	H	229	SIH	CH2-CH3-CH4-OH5
3	H	229	SIH	C13-C17-C20-O20
3	H	229	SIH	C13-C17-C20-C21
3	H	229	SIH	O11-CH1-CH2-CH3

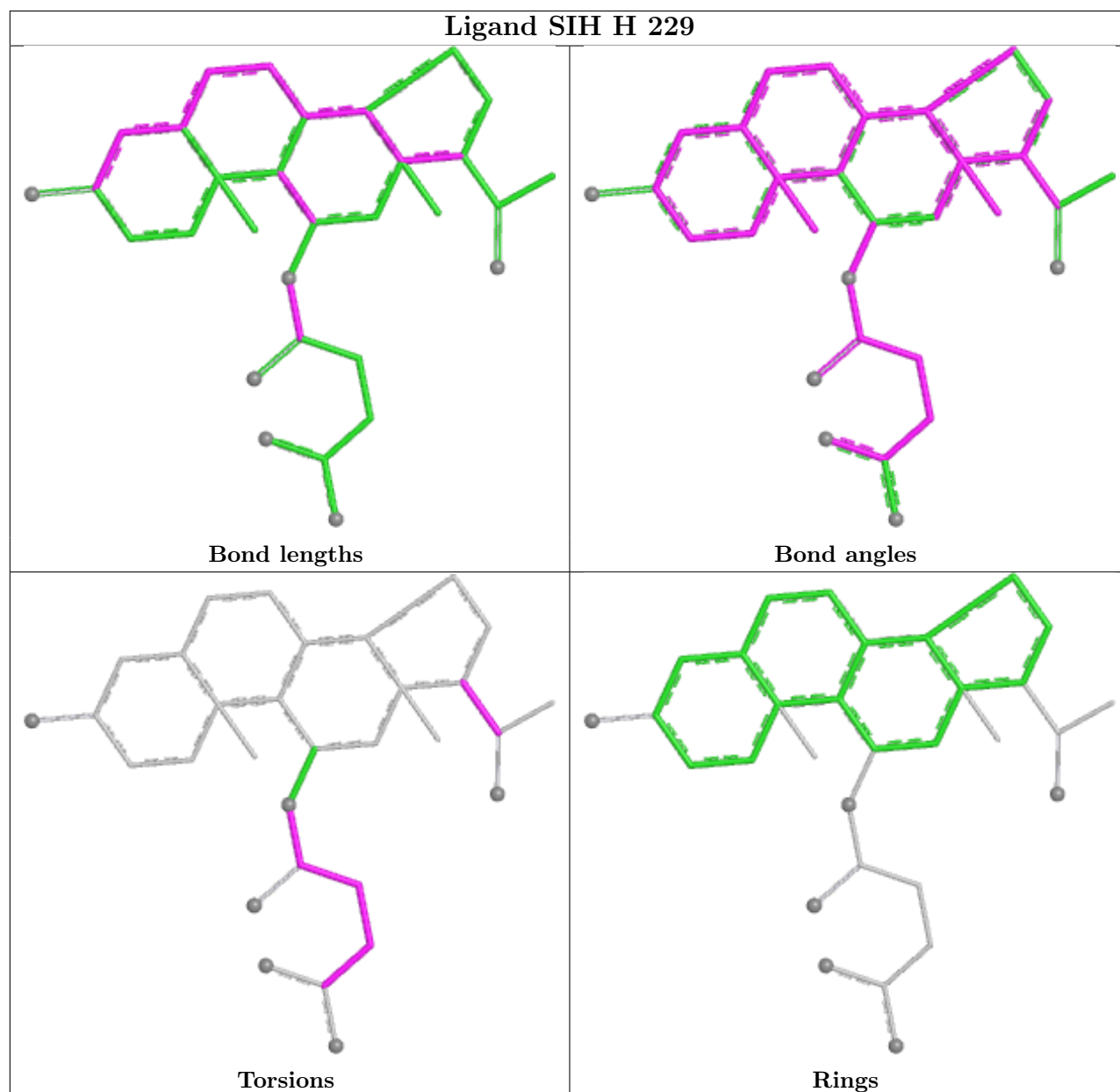
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	SIH	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.