Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 02:54 PM EDT

PDB ID	:	1DBM
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 (i) 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 (1)) were used in the production of this report:

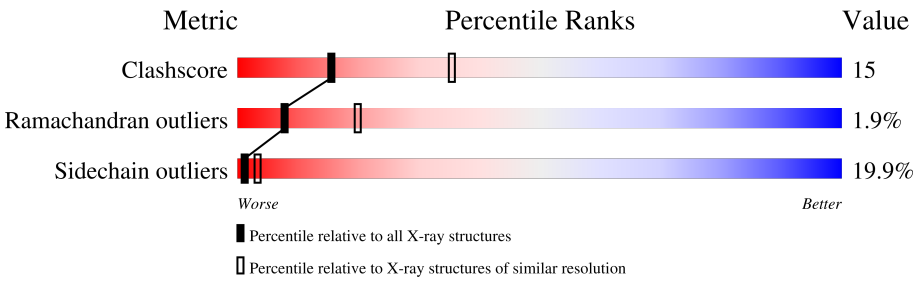
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	50% 37% 12% •
2	H	219	58% 30% 11% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	L	216	1679	1051	286	335	7	0	0	0

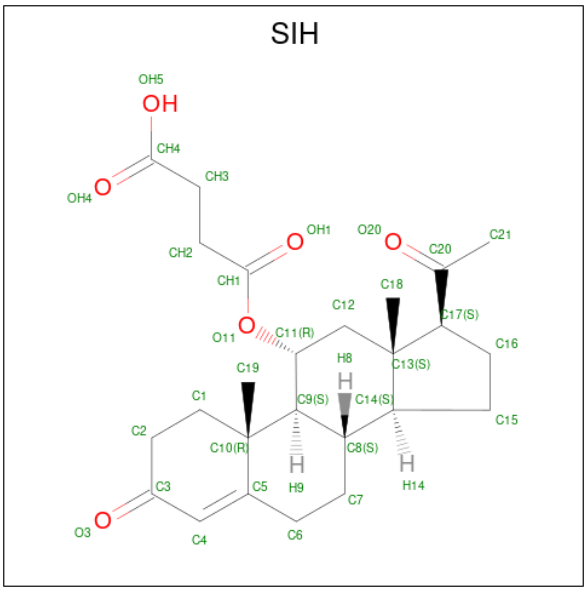
There are 14 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	S			
2	H	219	1675	1071	270	328	6	0	0	0

- Molecule 3 is PROGESTERONE-11-ALPHA-OL-HEMISUCCINATE (three-letter code: SIH) (formula: $C_{25}H_{34}O_6$).



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

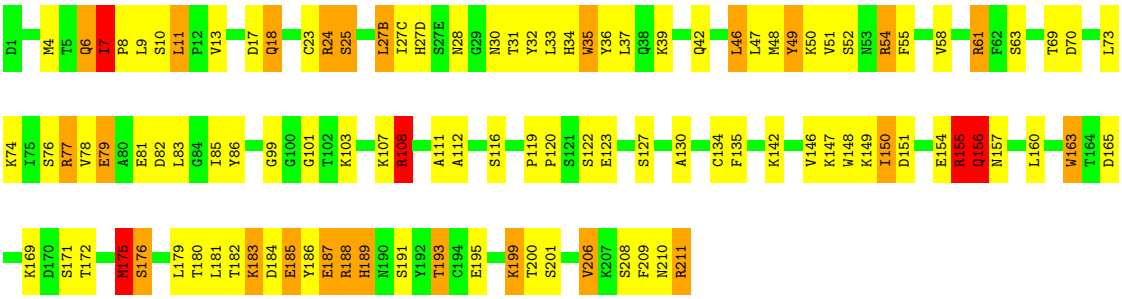
3 Residue-property plots (i)

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.

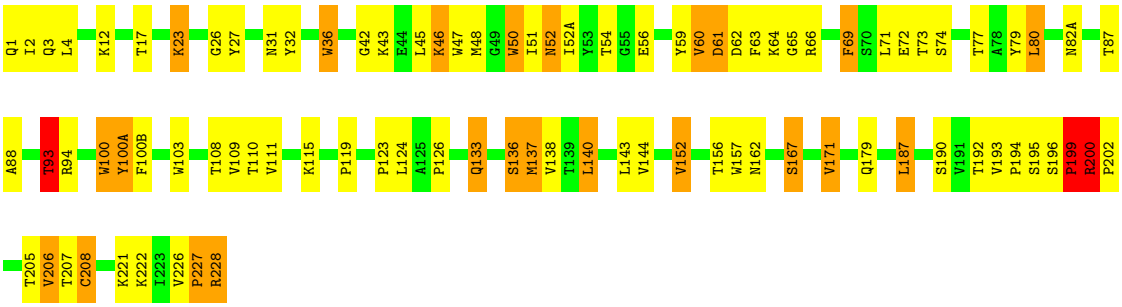
• Molecule 1: IGG1-KAPPA DB3 FAB (LIGHT CHAIN)

Chain L: 50% 37% 12% •



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

Chain H: 58% 30% 11% •



4 Data and refinement statistics (i)

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	0.94	1/1719 (0.1%)	1.80	36/2331 (1.5%)
2	H	1.02	0/1723	1.91	51/2358 (2.2%)
All	All	0.98	1/3442 (0.0%)	1.86	87/4689 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	35	TRP	CG-CD2	-5.79	1.33	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	100(A)	TYR	CB-CG-CD2	-11.68	113.99	121.00
1	L	108	ARG	NE-CZ-NH1	10.58	125.59	120.30
2	H	47	TRP	CD1-CG-CD2	9.51	113.91	106.30
2	H	100	TRP	CD1-CG-CD2	9.24	113.69	106.30
2	H	100(A)	TYR	CB-CG-CD1	9.02	126.41	121.00
2	H	200	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	H	103	TRP	CD1-CG-CD2	8.32	112.96	106.30
2	H	47	TRP	CE2-CD2-CG	-8.31	100.65	107.30
2	H	50	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	L	148	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	L	148	TRP	CG-CD2-CE3	7.94	141.05	133.90
1	L	148	TRP	CE2-CD2-CG	-7.93	100.96	107.30
2	H	47	TRP	CG-CD2-CE3	7.78	140.90	133.90
2	H	100	TRP	CE2-CD2-CG	-7.69	101.14	107.30
2	H	66	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	H	157	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	L	24	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	L	163	TRP	CD1-CG-CD2	7.42	112.24	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	123	GLU	CA-CB-CG	7.42	129.72	113.40
2	H	103	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	L	175	MET	CA-CB-CG	7.29	125.69	113.30
2	H	157	TRP	CE2-CD2-CG	-7.22	101.52	107.30
2	H	193	VAL	CA-CB-CG1	-7.18	100.13	110.90
1	L	77	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	L	46	LEU	CA-CB-CG	7.12	131.67	115.30
2	H	94	ARG	CB-CG-CD	-7.11	93.11	111.60
2	H	36	TRP	CD1-CG-CD2	6.99	111.89	106.30
2	H	228	ARG	N-CA-C	-6.97	92.17	111.00
2	H	1	GLN	N-CA-C	-6.90	92.37	111.00
1	L	163	TRP	CE2-CD2-CG	-6.87	101.80	107.30
2	H	103	TRP	CG-CD2-CE3	6.76	139.99	133.90
2	H	50	TRP	NE1-CE2-CD2	6.76	114.06	107.30
2	H	187	LEU	CA-CB-CG	6.74	130.79	115.30
1	L	49	TYR	CB-CG-CD1	-6.73	116.96	121.00
2	H	206	VAL	CG1-CB-CG2	-6.69	100.19	110.90
2	H	36	TRP	CE2-CD2-CG	-6.66	101.97	107.30
2	H	50	TRP	CD1-CG-CD2	6.66	111.62	106.30
2	H	227	PRO	CA-C-N	-6.52	102.86	117.20
1	L	186	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	L	35	TRP	CE2-CD2-CE3	6.49	126.49	118.70
2	H	47	TRP	CG-CD1-NE1	-6.40	103.70	110.10
2	H	66	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	L	184	ASP	N-CA-CB	-6.20	99.44	110.60
2	H	100	TRP	CG-CD2-CE3	6.19	139.47	133.90
1	L	108	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	H	109	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	L	35	TRP	CD1-CG-CD2	6.08	111.16	106.30
1	L	7	ILE	CA-CB-CG2	-6.07	98.77	110.90
2	H	47	TRP	CB-CG-CD1	-6.06	119.12	127.00
1	L	160	LEU	CA-CB-CG	5.99	129.09	115.30
2	H	193	VAL	CA-CB-CG2	5.99	119.89	110.90
2	H	50	TRP	CE2-CD2-CE3	5.93	125.82	118.70
2	H	93	THR	CA-CB-CG2	-5.92	104.11	112.40
2	H	100	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	L	83	LEU	CA-CB-CG	5.88	128.82	115.30
1	L	148	TRP	CB-CG-CD1	-5.85	119.40	127.00
1	L	193	THR	CA-C-N	-5.83	104.38	117.20
2	H	72	GLU	CA-C-N	-5.76	104.52	117.20
1	L	77	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	H	27	TYR	CB-CG-CD1	-5.68	117.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	103	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	L	211	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	L	35	TRP	CE2-CD2-CG	-5.63	102.80	107.30
2	H	179	GLN	N-CA-C	-5.62	95.84	111.00
1	L	188	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	61	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	L	79	GLU	CA-CB-CG	5.43	125.35	113.40
2	H	171	VAL	CG1-CB-CG2	-5.30	102.43	110.90
2	H	199	PRO	CA-N-CD	-5.29	104.09	111.50
1	L	199	LYS	CB-CA-C	-5.27	99.85	110.40
2	H	4	LEU	N-CA-C	-5.27	96.77	111.00
2	H	60	VAL	N-CA-C	-5.25	96.81	111.00
2	H	152	VAL	CA-C-N	5.24	128.72	117.20
2	H	23	LYS	CB-CG-CD	5.17	125.03	111.60
2	H	143	LEU	CA-CB-CG	5.16	127.17	115.30
1	L	36	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	L	148	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	L	185	GLU	CA-CB-CG	5.12	124.66	113.40
1	L	156	GLN	CA-CB-CG	5.11	124.65	113.40
2	H	228	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	H	79	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	L	154	GLU	CA-CB-CG	5.07	124.56	113.40
1	L	155	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	H	32	TYR	CB-CG-CD1	-5.05	117.97	121.00
2	H	199	PRO	CA-C-N	5.03	128.26	117.20
2	H	157	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	L	7	ILE	CA-CB-CG1	5.00	120.51	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	56	0
2	H	1675	0	1633	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	31	0	33	7	0
All	All	3385	0	3291	99	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 (99) 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: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
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
2:H:64:LYS:HZ2	2:H:65:GLY:H	1.46	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:4:MET:HE1	1:L:23:CYS:SG	2.44	0.57
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:64:LYS:HZ2	2:H:64:LYS:HA	1.71	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
2:H:64:LYS:HA	2:H:64:LYS:NZ	2.23	0.54
1:L:147:LYS:HB3	1:L:195:GLU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:6:GLN:O	1:L:7:ILE:HD13	2.10	0.51
2:H:208:CYS:SG	2:H:208:CYS:O	2.68	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: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
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: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
2:H:42:GLY:C	2:H:43:LYS:HD2	2.35	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
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:4:MET:CE	1:L:23:CYS:SG	3.05	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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%)	8 20
2	H	217/219 (99%)	191 (88%)	22 (10%)	4 (2%)	8 21
All	All	431/435 (99%)	385 (89%)	38 (9%)	8 (2%)	8 20

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 (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	L	194/194 (100%)	154 (79%)	40 (21%)	1 3
2	H	188/188 (100%)	152 (81%)	36 (19%)	1 4
All	All	382/382 (100%)	306 (80%)	76 (20%)	1 3

All (76) 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	18	GLN
1	L	24	ARG
1	L	25	SER

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Mol	Chain	Res	Type
1	L	27(B)	LEU
1	L	27(C)	ILE
1	L	35	TRP
1	L	42	GLN
1	L	46	LEU
1	L	47	LEU
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	107	LYS
1	L	108	ARG
1	L	122	SER
1	L	127	SER
1	L	150	ILE
1	L	155	ARG
1	L	156	GLN
1	L	165	ASP
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	206	VAL
2	H	3	GLN
2	H	31	ASN
2	H	45	LEU
2	H	46	LYS
2	H	48	MET
2	H	51	ILE
2	H	52	ASN
2	H	56	GLU
2	H	61	ASP
2	H	69	PHE

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Mol	Chain	Res	Type
2	H	73	THR
2	H	74	SER
2	H	80	LEU
2	H	93	THR
2	H	100(A)	TYR
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	187	LEU
2	H	192	THR
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	222	LYS
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	34	HIS
1	L	210	ASN
2	H	31	ASN
2	H	35	ASN
2	H	133	GLN
2	H	162	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	2.14	8 (23%)	52,53,53	2.46	22 (42%)

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	-	-	11/13/74/74	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	SIH	C9-C11	6.56	1.62	1.53
3	H	229	SIH	C6-C5	-4.76	1.42	1.50
3	H	229	SIH	C4-C3	-4.30	1.36	1.45
3	H	229	SIH	C13-C14	-3.95	1.47	1.55
3	H	229	SIH	C13-C17	-3.23	1.50	1.56
3	H	229	SIH	C4-C5	3.12	1.39	1.34
3	H	229	SIH	O11-CH1	-2.28	1.27	1.34
3	H	229	SIH	C7-C8	-2.01	1.49	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	229	SIH	C17-C13-C14	7.34	107.55	99.72
3	H	229	SIH	O11-CH1-CH2	6.25	124.97	111.50
3	H	229	SIH	C5-C4-C3	-4.20	116.89	123.67
3	H	229	SIH	C16-C17-C13	-3.81	100.81	104.21
3	H	229	SIH	OH1-CH1-CH2	-3.73	109.17	123.73
3	H	229	SIH	C1-C2-C3	-3.73	103.64	111.62
3	H	229	SIH	C15-C14-C8	3.61	125.03	119.08
3	H	229	SIH	C12-C13-C14	3.57	111.05	106.94
3	H	229	SIH	C13-C14-C8	-3.38	109.37	114.38
3	H	229	SIH	C10-C9-C8	-3.25	108.42	113.63
3	H	229	SIH	C10-C9-C11	-3.24	109.91	114.75
3	H	229	SIH	C1-C10-C9	2.82	113.76	109.38
3	H	229	SIH	C6-C7-C8	-2.82	106.59	111.69
3	H	229	SIH	C18-C13-C12	-2.80	106.58	110.76
3	H	229	SIH	C19-C10-C1	-2.78	105.03	109.43
3	H	229	SIH	C18-C13-C14	-2.65	106.78	111.71
3	H	229	SIH	C11-O11-CH1	2.35	122.39	117.83
3	H	229	SIH	OH4-CH4-CH3	-2.31	115.65	123.08
3	H	229	SIH	C13-C17-C20	2.21	118.09	114.98
3	H	229	SIH	C7-C6-C5	-2.20	107.80	111.93
3	H	229	SIH	CH3-CH2-CH1	-2.15	107.17	113.43
3	H	229	SIH	C16-C17-C20	2.02	117.31	114.23

There are no chirality outliers.

All (11) 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	O11-CH1-CH2-CH3
3	H	229	SIH	C13-C17-C20-C21
3	H	229	SIH	OH1-CH1-CH2-CH3

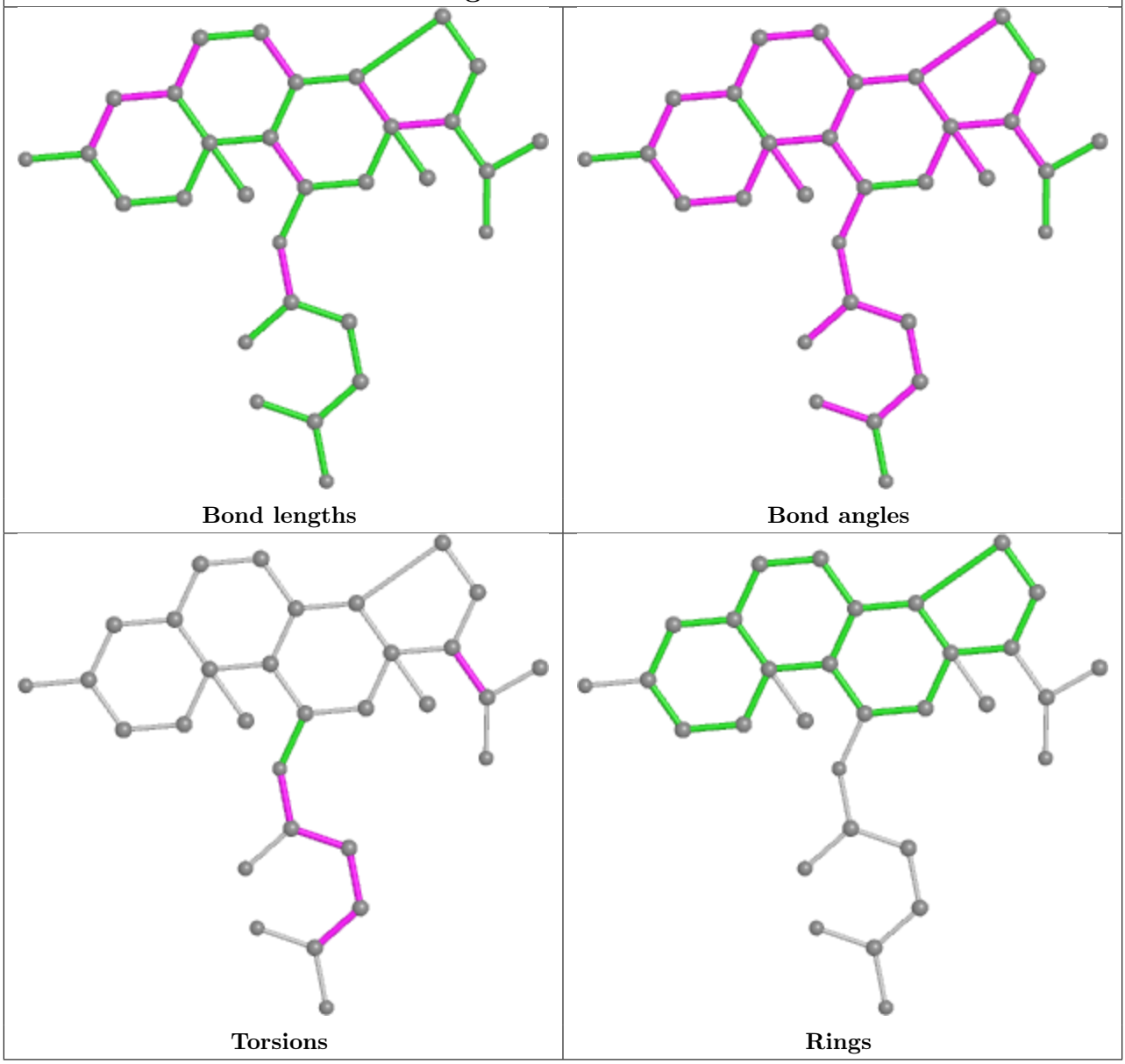
There are no ring outliers.

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 then 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.

Ligand SIH H 229



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.