



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 2DBL / pdb_00002dbl
Title : MOLECULAR BASIS OF CROSS-REACTIVITY AND THE LIMITS OF ANTIBODY-ANTIGEN COMPLEMENTARITY
Authors : Arevalo, J.H.; Wilson, I.A.
Deposited on : 1994-02-08
Resolution : 2.90 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)
Xtrriage (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

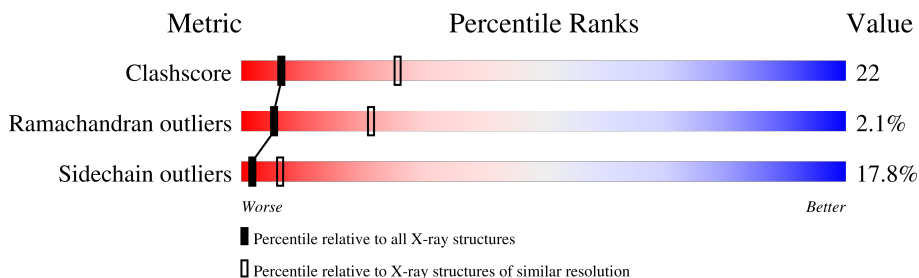
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

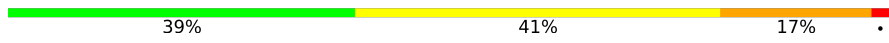

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	 39% 41% 17% •
2	H	219	 47% 38% 13% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3380 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	1677	1051	286	333	7	0	0	0

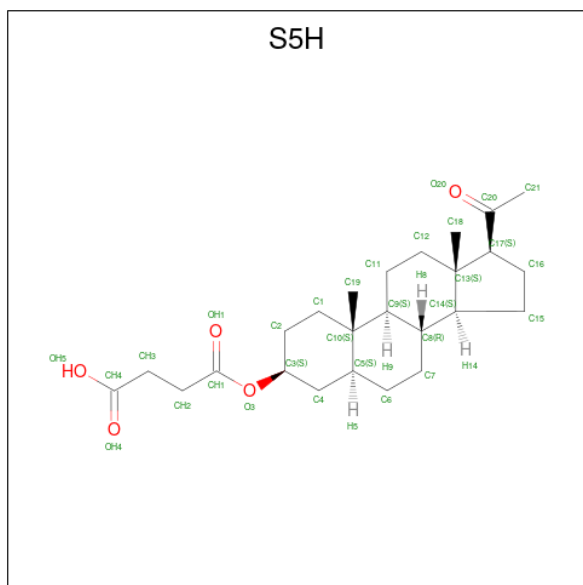
There are 14 discrepancies between the modelled and reference sequences:

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	1673	1071	270	326	6	0	0	0

- Molecule 3 is 5-ALPHA-PREGNANE-3-BETA-OL-HEMISUCCINATE (CCD ID: S5H) (formula: C₂₅H₃₈O₅).



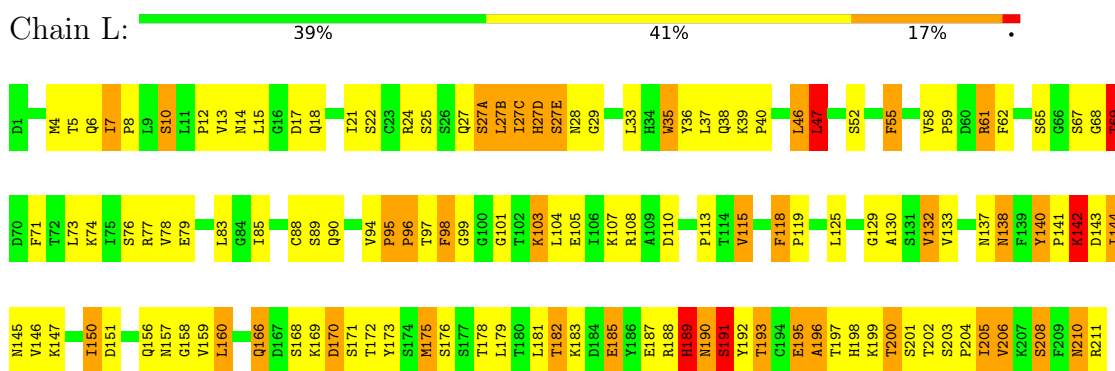
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	C O	0	0
			30	25 5		

3 Residue-property plots [i](#)

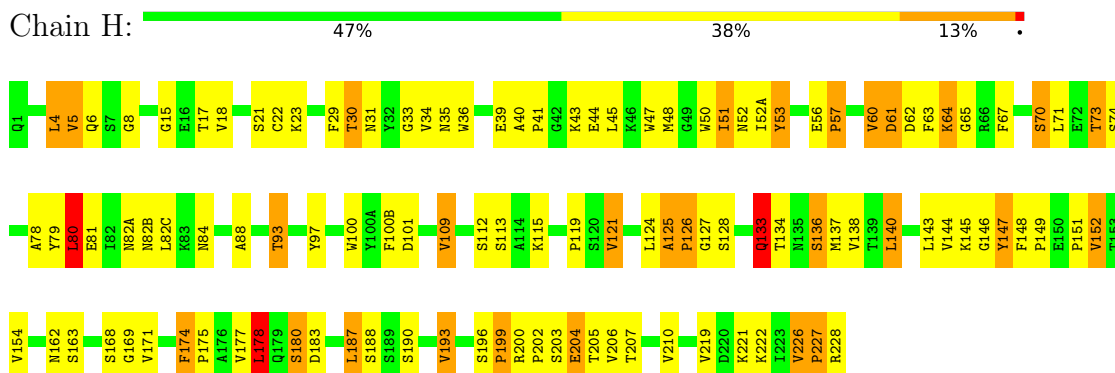
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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



4 Data and refinement statistics

Xtrriage (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 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3380	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: S5H

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	0.93	0/1717	1.55	40/2330 (1.7%)
2	H	1.02	1/1721 (0.1%)	1.43	35/2357 (1.5%)
All	All	0.97	1/3438 (0.0%)	1.49	75/4687 (1.6%)

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	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	5	VAL	CA-CB	5.41	1.61	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	PRO	N-CA-C	10.56	127.71	111.34
1	L	52	SER	N-CA-C	9.96	125.36	112.41
1	L	201	SER	N-CA-C	9.06	124.78	108.48
1	L	96	PRO	N-CA-C	-8.50	97.15	110.50
2	H	73	THR	N-CA-C	8.30	121.38	111.33
2	H	128	SER	N-CA-C	8.28	123.39	111.56
2	H	134	THR	N-CA-C	-8.13	102.11	110.97
1	L	113	PRO	N-CA-C	8.05	123.67	110.55
2	H	4	LEU	N-CA-C	-7.92	96.33	109.07
1	L	98	PHE	N-CA-C	-7.91	96.86	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	45	LEU	N-CA-C	-7.36	97.99	109.25
1	L	158	GLY	N-CA-C	-7.28	104.69	114.95
1	L	188	ARG	N-CA-C	-7.17	103.20	112.23
2	H	128	SER	O-C-N	-7.12	114.62	122.67
1	L	73	LEU	N-CA-C	-7.05	98.11	109.96
2	H	101	ASP	N-CA-C	7.01	122.09	112.90
1	L	35	TRP	N-CA-C	6.84	120.20	108.02
2	H	147	TYR	N-CA-C	6.82	120.47	110.59
2	H	125	ALA	N-CA-C	-6.63	101.77	110.39
1	L	21	ILE	N-CA-C	-6.61	98.94	108.53
2	H	8	GLY	CA-C-N	6.57	126.92	119.83
2	H	8	GLY	C-N-CA	6.57	126.92	119.83
1	L	138	ASN	N-CA-C	6.56	120.42	111.17
1	L	185	GLU	N-CA-C	-6.52	104.17	111.28
2	H	126	PRO	N-CA-C	6.51	125.89	112.47
1	L	190	ASN	N-CA-C	-6.47	100.41	110.17
2	H	29	PHE	N-CA-C	6.36	119.02	111.33
1	L	137	ASN	N-CA-C	6.18	119.61	109.72
1	L	76	SER	N-CA-C	6.14	118.51	111.02
1	L	69	THR	N-CA-C	6.12	122.33	114.56
1	L	150	ILE	CB-CA-C	6.08	118.89	110.99
2	H	60	VAL	N-CA-C	-6.04	99.69	108.87
1	L	115	VAL	N-CA-C	6.02	117.06	107.98
1	L	150	ILE	N-CA-CB	-6.00	104.34	111.90
1	L	118	PHE	CA-C-N	5.95	126.51	120.38
1	L	118	PHE	C-N-CA	5.95	126.51	120.38
2	H	146	GLY	N-CA-C	5.92	124.08	115.32
1	L	193	THR	N-CA-C	5.92	119.12	109.06
1	L	191	SER	N-CA-C	5.91	123.40	110.80
2	H	109	VAL	N-CA-C	-5.91	99.89	108.17
2	H	97	TYR	N-CA-C	5.90	119.58	112.38
1	L	27(A)	SER	N-CA-C	-5.87	100.11	109.96
1	L	101	GLY	N-CA-C	-5.83	99.37	113.18
2	H	140	LEU	N-CA-C	-5.80	101.34	109.69
2	H	80	LEU	N-CA-C	-5.77	99.02	108.76
1	L	97	THR	CB-CA-C	5.70	119.81	109.37
2	H	169	GLY	N-CA-C	-5.70	108.30	115.08
2	H	152	VAL	N-CA-C	-5.64	99.66	108.86
1	L	208	SER	N-CA-C	5.58	117.56	109.07
2	H	163	SER	N-CA-C	5.53	119.06	111.54
2	H	53	TYR	CA-CB-CG	5.51	123.82	113.90
1	L	132	VAL	N-CA-C	-5.48	100.55	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	129	GLY	N-CA-C	-5.46	104.26	112.89
1	L	178	THR	N-CA-C	5.45	118.41	107.41
1	L	61	ARG	N-CA-C	-5.44	105.51	111.82
1	L	46	LEU	N-CA-C	-5.44	101.61	110.20
2	H	178	LEU	N-CA-C	5.43	118.33	109.59
2	H	174	PHE	CA-C-N	5.40	125.66	119.83
2	H	174	PHE	C-N-CA	5.40	125.66	119.83
2	H	227	PRO	CA-C-N	5.37	131.37	121.70
2	H	227	PRO	C-N-CA	5.37	131.37	121.70
1	L	142	LYS	N-CA-C	5.36	122.21	110.80
1	L	115	VAL	CB-CA-C	-5.32	105.49	111.23
2	H	136	SER	N-CA-C	5.29	118.89	111.90
2	H	133	GLN	N-CA-C	-5.27	102.25	110.10
2	H	205	THR	N-CA-C	5.24	118.09	109.76
1	L	205	ILE	N-CA-C	-5.20	100.26	107.80
1	L	189	HIS	N-CA-C	5.15	117.01	109.24
2	H	121	VAL	CB-CA-C	-5.14	106.35	111.80
2	H	193	VAL	CA-C-N	5.11	125.01	119.85
2	H	193	VAL	C-N-CA	5.11	125.01	119.85
1	L	47	LEU	N-CA-C	-5.08	106.17	112.93
1	L	55	PHE	N-CA-C	-5.06	103.72	110.55
1	L	196	ALA	N-CA-C	5.01	117.49	107.62
1	L	195	GLU	N-CA-C	5.01	116.55	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	140	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	L	1677	0	1625	80	0
2	H	1673	0	1633	70	0
3	L	30	0	37	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3380	0	3295	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (145) 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:H:17:THR:HG22	2:H:82(A):ASN:HA	1.46	0.98
2:H:39:GLU:O	2:H:88:ALA:HB1	1.76	0.85
2:H:36:TRP:CE3	2:H:80:LEU:HD12	2.17	0.80
1:L:193:THR:HB	1:L:208:SER:HB3	1.65	0.78
2:H:70:SER:HB2	2:H:79:TYR:HB2	1.65	0.77
2:H:127:GLY:HA2	2:H:228:ARG:HG2	1.67	0.77
1:L:14:ASN:HB3	1:L:17:ASP:OD2	1.86	0.75
2:H:196:SER:HB3	2:H:199:PRO:HD3	1.72	0.72
1:L:47:LEU:O	1:L:58:VAL:HG21	1.91	0.70
1:L:13:VAL:HG21	1:L:78:VAL:HG21	1.75	0.68
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.76	0.67
1:L:130:ALA:HB3	1:L:181:LEU:O	1.95	0.67
1:L:85:ILE:HG12	1:L:103:LYS:HG3	1.77	0.66
1:L:144:ILE:HG23	1:L:175:MET:HE2	1.78	0.66
1:L:183:LYS:HD3	1:L:187:GLU:OE2	1.97	0.65
2:H:52(A):ILE:HD12	2:H:71:LEU:HD11	1.80	0.63
1:L:7:ILE:HG22	1:L:8:PRO:HA	1.80	0.63
2:H:187:LEU:C	2:H:187:LEU:HD23	2.24	0.62
1:L:159:VAL:HG12	1:L:160:LEU:N	2.15	0.62
1:L:89:SER:OG	1:L:98:PHE:CD2	2.51	0.62
2:H:48:MET:HG2	2:H:63:PHE:CD2	2.37	0.59
2:H:18:VAL:HG23	2:H:82(C):LEU:HD21	1.84	0.59
1:L:12:PRO:HA	1:L:105:GLU:HG3	1.85	0.58
2:H:154:VAL:HG22	2:H:210:VAL:HG22	1.86	0.58
2:H:52(A):ILE:CD1	2:H:71:LEU:HD11	2.34	0.58
3:L:212:S5H:H162	2:H:35:ASN:HD21	1.69	0.58
1:L:47:LEU:HD11	1:L:62:PHE:CD2	2.39	0.57
1:L:166:GLN:HG3	1:L:173:TYR:CE1	2.40	0.57
1:L:195:GLU:HG2	1:L:206:VAL:HG12	1.87	0.56
1:L:90:GLN:O	1:L:96:PRO:HA	2.06	0.56
2:H:93:THR:HG21	2:H:100(B):PHE:HB3	1.87	0.56
2:H:133:GLN:HB2	2:H:136:SER:N	2.21	0.56
1:L:17:ASP:O	1:L:78:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HG12	2:H:71:LEU:HD13	1.89	0.55
2:H:51:ILE:HD11	2:H:71:LEU:HD22	1.89	0.55
1:L:10:SER:HB2	1:L:142:LYS:NZ	2.22	0.55
1:L:190:ASN:OD1	1:L:210:ASN:HB3	2.06	0.55
2:H:64:LYS:HZ2	2:H:64:LYS:HA	1.73	0.54
2:H:6:GLN:HA	2:H:21:SER:O	2.08	0.54
1:L:115:VAL:HG13	1:L:115:VAL:O	2.07	0.53
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.89	0.53
1:L:110:ASP:HB3	1:L:200:THR:CG2	2.38	0.53
1:L:176:SER:HB3	2:H:174:PHE:CE2	2.43	0.53
3:L:212:S5H:H3	2:H:100:TRP:CZ3	2.43	0.53
2:H:17:THR:HG22	2:H:82(A):ASN:CA	2.31	0.52
1:L:14:ASN:HB2	1:L:107:LYS:HE2	1.92	0.52
1:L:108:ARG:HG3	1:L:140:TYR:CD2	2.44	0.52
2:H:147:TYR:CE2	2:H:152:VAL:HG23	2.45	0.52
1:L:144:ILE:HD13	1:L:145:ASN:N	2.25	0.52
1:L:67:SER:O	1:L:69:THR:N	2.43	0.52
1:L:18:GLN:H	1:L:18:GLN:CD	2.18	0.51
2:H:30:THR:HA	2:H:52(A):ILE:CG2	2.41	0.51
2:H:34:VAL:HB	2:H:51:ILE:HG23	1.92	0.51
2:H:144:VAL:HG11	2:H:152:VAL:HG11	1.91	0.51
2:H:127:GLY:CA	2:H:228:ARG:HG2	2.38	0.51
1:L:18:GLN:HB2	1:L:74:LYS:HZ3	1.74	0.51
2:H:61:ASP:HA	2:H:64:LYS:HG2	1.93	0.51
2:H:5:VAL:HG12	2:H:23:LYS:O	2.11	0.51
1:L:145:ASN:HB3	1:L:197:THR:OG1	2.11	0.51
1:L:198:HIS:O	1:L:199:LYS:C	2.53	0.50
2:H:187:LEU:HD23	2:H:188:SER:N	2.26	0.50
1:L:27(E):SER:C	1:L:29:GLY:H	2.20	0.49
2:H:171:VAL:HA	2:H:190:SER:O	2.13	0.49
2:H:133:GLN:HB2	2:H:136:SER:H	1.78	0.49
1:L:159:VAL:CG1	1:L:160:LEU:N	2.76	0.49
1:L:196:ALA:HB3	1:L:205:ILE:HB	1.94	0.49
1:L:182:THR:HG23	1:L:185:GLU:HB2	1.93	0.48
2:H:121:VAL:HG21	2:H:219:VAL:HB	1.94	0.48
2:H:207:THR:HG23	2:H:222:LYS:HA	1.93	0.48
3:L:212:S5H:H211	2:H:33:GLY:N	2.29	0.48
2:H:5:VAL:HG13	2:H:23:LYS:HB3	1.94	0.48
2:H:15:GLY:HA2	2:H:82(B):ASN:HA	1.93	0.48
2:H:143:LEU:CD2	2:H:145:LYS:HB2	2.43	0.48
1:L:27(D):HIS:HD1	1:L:28:ASN:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ASN:OD1	2:H:53:TYR:HB2	2.14	0.48
2:H:226:VAL:HG13	2:H:227:PRO:HD2	1.96	0.48
1:L:190:ASN:OD1	1:L:191:SER:N	2.47	0.47
2:H:127:GLY:HA2	2:H:228:ARG:CG	2.41	0.47
2:H:148:PHE:CD1	2:H:149:PRO:HG3	2.50	0.47
1:L:140:TYR:CG	1:L:141:PRO:HA	2.49	0.47
2:H:121:VAL:O	2:H:221:LYS:HG3	2.14	0.47
1:L:160:LEU:HG	2:H:177:VAL:HG11	1.96	0.47
1:L:27(C):ILE:HG22	1:L:27(C):ILE:O	2.15	0.47
2:H:22:CYS:HB3	2:H:78:ALA:HB3	1.96	0.47
1:L:144:ILE:HD13	1:L:144:ILE:C	2.40	0.46
1:L:189:HIS:CD2	1:L:189:HIS:N	2.83	0.46
1:L:133:VAL:HG21	2:H:143:LEU:HD12	1.98	0.46
1:L:7:ILE:CB	1:L:8:PRO:HA	2.46	0.46
1:L:119:PRO:HD2	2:H:228:ARG:NH2	2.31	0.46
2:H:70:SER:CB	2:H:79:TYR:HB2	2.40	0.46
1:L:36:TYR:CD1	1:L:46:LEU:HA	2.52	0.45
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.76	0.45
2:H:18:VAL:O	2:H:81:GLU:HA	2.17	0.45
1:L:202:THR:OG1	1:L:203:SER:N	2.50	0.45
3:L:212:S5H:H211	2:H:33:GLY:H	1.82	0.45
1:L:10:SER:HB2	1:L:142:LYS:HZ1	1.82	0.44
2:H:196:SER:HB3	2:H:199:PRO:CD	2.45	0.44
1:L:110:ASP:HB3	1:L:200:THR:HG22	2.00	0.44
2:H:124:LEU:HD11	2:H:143:LEU:HB2	2.00	0.44
1:L:203:SER:HB2	1:L:204:PRO:CD	2.48	0.44
1:L:46:LEU:HD23	1:L:55:PHE:CD1	2.52	0.44
1:L:47:LEU:HD22	1:L:58:VAL:HG22	1.99	0.44
1:L:4:MET:HB2	1:L:99:GLY:HA3	1.99	0.44
1:L:144:ILE:CG2	1:L:175:MET:HE2	2.46	0.44
1:L:7:ILE:CG2	1:L:8:PRO:HA	2.46	0.43
2:H:125:ALA:HB1	2:H:126:PRO:HD2	2.00	0.43
2:H:4:LEU:HD23	2:H:22:CYS:SG	2.59	0.43
1:L:94:VAL:HG23	3:L:212:S5H:H42	2.01	0.43
1:L:27(B):LEU:HD22	1:L:71:PHE:CE2	2.54	0.43
1:L:141:PRO:HG2	1:L:199:LYS:HD3	2.00	0.43
1:L:170:ASP:O	1:L:172:THR:N	2.52	0.43
1:L:39:LYS:HB3	1:L:40:PRO:HD2	2.00	0.43
1:L:37:LEU:HD12	1:L:38:GLN:N	2.34	0.42
1:L:125:LEU:HD23	1:L:125:LEU:HA	1.83	0.42
2:H:67:PHE:CD1	2:H:67:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:212:S5H:H183	2:H:50:TRP:CE2	2.54	0.42
1:L:14:ASN:O	1:L:15:LEU:C	2.62	0.42
2:H:47:TRP:HZ2	2:H:50:TRP:HB2	1.85	0.42
2:H:202:PRO:O	2:H:203:SER:C	2.61	0.42
1:L:36:TYR:HD1	1:L:46:LEU:HA	1.85	0.42
2:H:177:VAL:HG12	2:H:178:LEU:N	2.35	0.42
1:L:6:GLN:HB2	1:L:22:SER:O	2.20	0.42
1:L:27(B):LEU:HD22	1:L:71:PHE:HE2	1.85	0.41
1:L:159:VAL:CG1	1:L:160:LEU:H	2.33	0.41
1:L:78:VAL:HG12	1:L:79:GLU:N	2.34	0.41
1:L:27(B):LEU:HD11	1:L:90:GLN:HG2	2.02	0.41
1:L:85:ILE:HG12	1:L:103:LYS:CG	2.49	0.41
1:L:150:ILE:O	1:L:151:ASP:HB2	2.20	0.41
2:H:187:LEU:C	2:H:187:LEU:CD2	2.92	0.41
2:H:199:PRO:O	2:H:204:GLU:N	2.46	0.41
1:L:27(E):SER:C	1:L:29:GLY:N	2.78	0.41
1:L:190:ASN:HA	1:L:211:ARG:HB3	2.01	0.41
2:H:41:PRO:C	2:H:43:LYS:H	2.27	0.41
2:H:180:SER:O	2:H:183:ASP:HB2	2.20	0.41
1:L:202:THR:H	1:L:202:THR:HG23	1.69	0.41
1:L:193:THR:CB	1:L:208:SER:HB3	2.44	0.41
2:H:73:THR:O	2:H:74:SER:C	2.64	0.41
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.55	0.40
1:L:95:PRO:HB2	2:H:47:TRP:HE3	1.85	0.40
2:H:162:ASN:HD21	2:H:206:VAL:HA	1.85	0.40
2:H:36:TRP:CZ3	2:H:80:LEU:HB2	2.56	0.40
2:H:56:GLU:HA	2:H:57:PRO:HD3	1.91	0.40
1:L:59:PRO:C	1:L:61:ARG:H	2.29	0.40
1:L:115:VAL:HG11	1:L:205:ILE:HG22	2.03	0.40
1:L:150:ILE:HG13	1:L:192:TYR:CE2	2.56	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%)	188 (88%)	20 (9%)	6 (3%)	4	15
2	H	217/219 (99%)	190 (88%)	24 (11%)	3 (1%)	9	30
All	All	431/435 (99%)	378 (88%)	44 (10%)	9 (2%)	5	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	171	SER
1	L	68	GLY
1	L	168	SER
1	L	191	SER
2	H	57	PRO
1	L	200	THR
2	H	61	ASP
1	L	142	LYS
2	H	65	GLY

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%)	156 (80%)	38 (20%)	1	5
2	H	188/188 (100%)	158 (84%)	30 (16%)	2	8
All	All	382/382 (100%)	314 (82%)	68 (18%)	2	6

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	ILE
1	L	10	SER
1	L	24	ARG

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Mol	Chain	Res	Type
1	L	25	SER
1	L	27	GLN
1	L	27(A)	SER
1	L	27(B)	LEU
1	L	27(C)	ILE
1	L	27(D)	HIS
1	L	27(E)	SER
1	L	33	LEU
1	L	47	LEU
1	L	65	SER
1	L	69	THR
1	L	77	ARG
1	L	83	LEU
1	L	95	PRO
1	L	103	LYS
1	L	104	LEU
1	L	132	VAL
1	L	138	ASN
1	L	143	ASP
1	L	144	ILE
1	L	146	VAL
1	L	147	LYS
1	L	156	GLN
1	L	157	ASN
1	L	160	LEU
1	L	166	GLN
1	L	169	LYS
1	L	170	ASP
1	L	175	MET
1	L	179	LEU
1	L	182	THR
1	L	189	HIS
1	L	206	VAL
1	L	210	ASN
2	H	30	THR
2	H	31	ASN
2	H	44	GLU
2	H	51	ILE
2	H	60	VAL
2	H	62	ASP
2	H	64	LYS
2	H	70	SER

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Mol	Chain	Res	Type
2	H	80	LEU
2	H	84	ASN
2	H	93	THR
2	H	109	VAL
2	H	112	SER
2	H	113	SER
2	H	115	LYS
2	H	133	GLN
2	H	137	MET
2	H	138	VAL
2	H	140	LEU
2	H	151	PRO
2	H	168	SER
2	H	175	PRO
2	H	178	LEU
2	H	180	SER
2	H	187	LEU
2	H	193	VAL
2	H	199	PRO
2	H	200	ARG
2	H	204	GLU
2	H	226	VAL

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	28	ASN
1	L	156	GLN
2	H	3	GLN
2	H	31	ASN
2	H	35	ASN
2	H	82(B)	ASN
2	H	135	ASN
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 [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](#)

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	S5H	L	212	-	33,33,33	1.45	5 (15%)	51,51,51	1.91	15 (29%)

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	S5H	L	212	-	-	7/13/71/71	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	212	S5H	C13-C14	-4.37	1.46	1.55
3	L	212	S5H	O3-CH1	-2.92	1.26	1.34
3	L	212	S5H	C1-C10	2.90	1.59	1.54
3	L	212	S5H	C13-C17	-2.24	1.52	1.56
3	L	212	S5H	C4-C3	2.01	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	212	S5H	C17-C13-C14	6.19	106.19	99.72
3	L	212	S5H	O3-CH1-CH2	3.90	119.93	111.48
3	L	212	S5H	C2-C1-C10	3.27	118.26	112.74
3	L	212	S5H	C1-C2-C3	3.10	115.39	110.33
3	L	212	S5H	C13-C14-C8	-3.04	110.10	114.41
3	L	212	S5H	C3-O3-CH1	2.68	124.20	117.80
3	L	212	S5H	C4-C3-C2	-2.60	108.28	111.53
3	L	212	S5H	OH4-CH4-CH3	-2.40	115.49	123.09
3	L	212	S5H	C10-C9-C8	-2.37	110.02	112.43
3	L	212	S5H	C1-C10-C9	-2.34	107.71	111.34
3	L	212	S5H	C16-C17-C13	-2.29	102.16	104.21
3	L	212	S5H	C18-C13-C12	-2.21	107.35	110.61
3	L	212	S5H	C14-C8-C9	-2.14	106.29	109.09
3	L	212	S5H	C7-C8-C14	-2.13	108.54	112.08
3	L	212	S5H	C4-C5-C10	-2.04	110.49	112.66

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	212	S5H	C2-C3-O3-CH1
3	L	212	S5H	CH2-CH1-O3-C3
3	L	212	S5H	OH1-CH1-O3-C3
3	L	212	S5H	C16-C17-C20-O20
3	L	212	S5H	C16-C17-C20-C21
3	L	212	S5H	C13-C17-C20-C21
3	L	212	S5H	O3-CH1-CH2-CH3

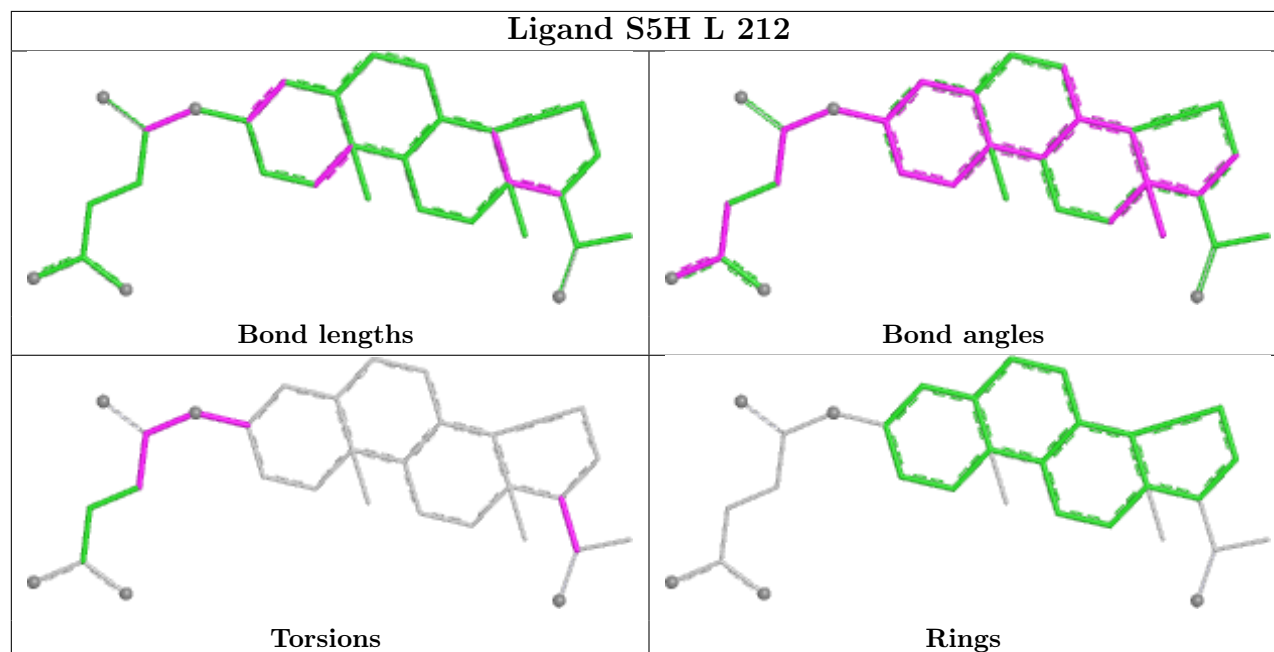
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	212	S5H	6	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 [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

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.