



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:03 PM UTC

PDB ID : 1DBJ / pdb_00001dbj
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

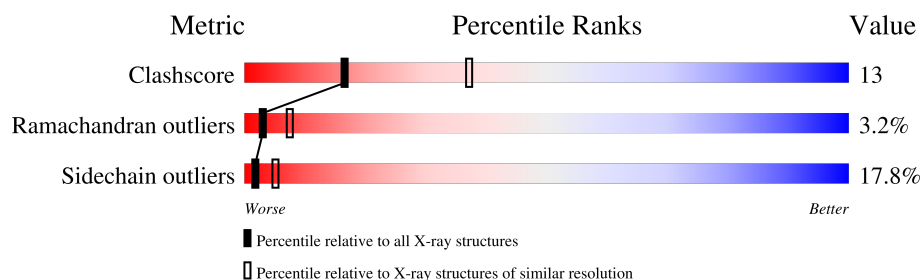
1 Overall quality at a glance

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	43% 40% 16% .
2	H	219	46% 39% 11% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3376 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			

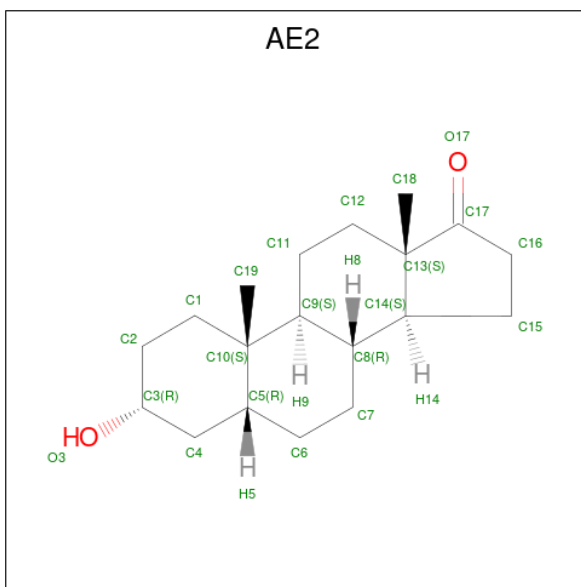
There are 14 discrepancies between the modelled and reference sequences:

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 AETIOCHOLANOLONE (CCD ID: AE2) (formula: C₁₉H₃₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is water.

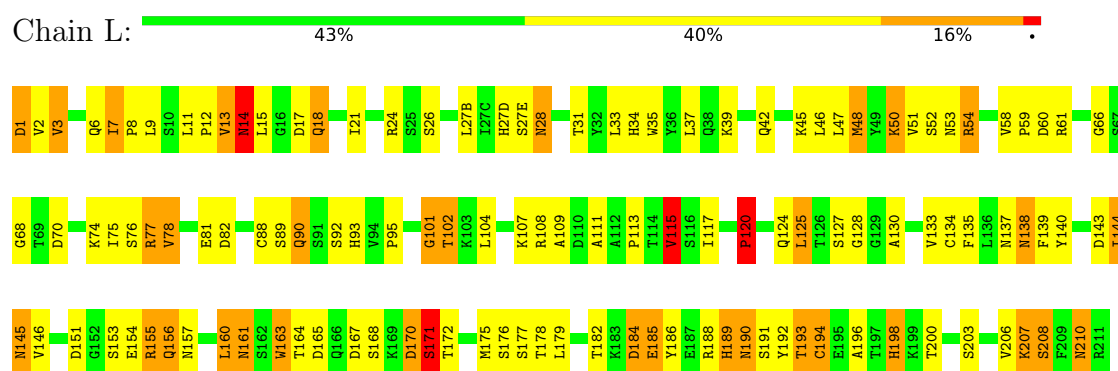
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

3 Residue-property plots

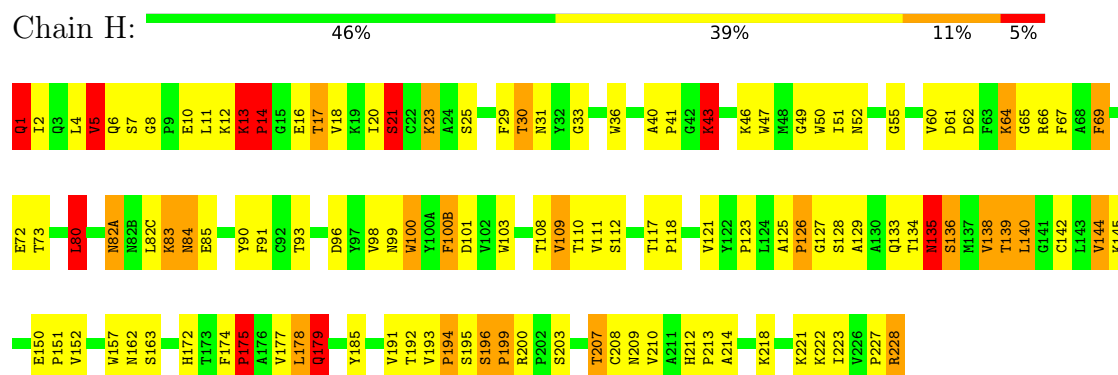
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 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}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3376	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: AE2

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	1.26	8/1719 (0.5%)	2.09	64/2331 (2.7%)
2	H	1.39	13/1723 (0.8%)	2.18	86/2358 (3.6%)
All	All	1.33	21/3442 (0.6%)	2.14	150/4689 (3.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	144	VAL	CA-CB	8.50	1.64	1.53
2	H	212	HIS	CD2-NE2	-7.92	1.29	1.37
2	H	5	VAL	CA-CB	7.23	1.63	1.54
2	H	208	CYS	CA-CB	-7.08	1.43	1.53
1	L	115	VAL	CA-CB	6.33	1.61	1.54
1	L	93	HIS	CD2-NE2	-6.25	1.30	1.37
1	L	198	HIS	CD2-NE2	-6.06	1.31	1.37
1	L	189	HIS	CD2-NE2	-6.04	1.31	1.37
2	H	199	PRO	C-O	-5.97	1.16	1.24
2	H	172	HIS	CD2-NE2	-5.96	1.31	1.37
1	L	34	HIS	CD2-NE2	-5.70	1.31	1.37
1	L	186	TYR	CA-CB	5.60	1.62	1.53
1	L	7	ILE	CA-CB	5.56	1.61	1.54
2	H	195	SER	CA-CB	-5.56	1.43	1.53
2	H	98	VAL	CA-CB	5.50	1.61	1.54
2	H	199	PRO	CA-CB	-5.39	1.46	1.53
2	H	196	SER	CA-CB	-5.29	1.45	1.53
1	L	12	PRO	CA-CB	-5.28	1.46	1.53
2	H	157	TRP	CG-CD2	-5.27	1.34	1.43
2	H	110	THR	CA-CB	-5.15	1.45	1.53
2	H	194	PRO	CA-C	5.11	1.59	1.52

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	200	THR	N-CA-C	11.49	123.89	111.36
2	H	69	PHE	CA-CB-CG	9.99	123.79	113.80
2	H	101	ASP	N-CA-C	9.89	125.54	113.38
2	H	99	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	L	138	ASN	N-CA-C	9.21	124.18	111.74
2	H	135	ASN	OD1-CG-ND2	-9.05	113.55	122.60
1	L	170	ASP	CA-CB-CG	9.05	121.65	112.60
1	L	60	ASP	CA-CB-CG	8.37	120.97	112.60
2	H	31	ASN	CB-CG-ND2	8.12	128.59	116.40
2	H	4	LEU	N-CA-C	-8.11	95.19	108.41
1	L	14	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	L	165	ASP	CA-CB-CG	7.74	120.33	112.60
2	H	150	GLU	CA-C-O	-7.68	112.73	120.64
2	H	209	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	H	193	VAL	CA-C-N	7.49	127.25	119.76
2	H	193	VAL	C-N-CA	7.49	127.25	119.76
2	H	134	THR	N-CA-C	-7.24	103.11	112.23
1	L	82	ASP	N-CA-C	-7.20	104.10	113.17
2	H	228	ARG	N-CA-C	-7.18	90.89	111.00
2	H	83	LYS	O-C-N	-7.16	112.70	122.23
2	H	31	ASN	OD1-CG-ND2	-7.14	115.45	122.60
1	L	156	GLN	CG-CD-NE2	7.01	126.92	116.40
2	H	179	GLN	N-CA-CB	-6.96	98.92	110.47
1	L	124	GLN	OE1-CD-NE2	-6.93	115.67	122.60
2	H	99	ASN	CB-CG-ND2	6.87	126.70	116.40
1	L	208	SER	N-CA-C	6.84	119.26	108.79
2	H	31	ASN	N-CA-C	6.83	122.80	113.37
1	L	190	ASN	CA-CB-CG	6.82	119.42	112.60
1	L	101	GLY	CA-C-O	-6.79	116.79	122.29
2	H	195	SER	N-CA-C	6.79	120.66	112.38
2	H	100	TRP	N-CA-C	6.76	125.20	110.80
1	L	70	ASP	CA-CB-CG	6.71	119.31	112.60
1	L	185	GLU	N-CA-C	-6.68	103.25	111.40
2	H	83	LYS	N-CA-CB	-6.65	101.20	110.38
2	H	49	GLY	CA-C-O	-6.64	115.80	121.04
2	H	6	GLN	N-CA-C	6.63	120.70	110.42
1	L	35	TRP	CD2-CE2-CZ2	-6.60	115.80	122.40
1	L	184	ASP	CA-CB-CG	6.55	119.15	112.60
1	L	127	SER	O-C-N	-6.51	115.13	122.23
2	H	66	ARG	N-CA-C	6.50	120.31	112.38
1	L	48	MET	CA-CB-CG	6.46	127.03	114.10
2	H	227	PRO	CA-C-O	6.43	128.33	121.32
2	H	100(B)	PHE	CA-CB-CG	6.38	120.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	61	ASP	CA-CB-CG	6.37	118.97	112.60
2	H	80	LEU	CA-CB-CG	6.31	138.37	116.30
2	H	172	HIS	O-C-N	-6.27	115.99	123.27
1	L	124	GLN	N-CA-C	-6.27	104.55	111.82
2	H	84	ASN	CA-CB-CG	-6.26	106.34	112.60
1	L	54	ARG	N-CA-C	6.25	119.42	109.24
2	H	46	LYS	N-CA-C	6.25	119.42	109.24
2	H	82(A)	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	L	167	ASP	CA-CB-CG	6.19	118.79	112.60
1	L	163	TRP	CG-CD2-CE3	6.17	140.07	133.90
1	L	186	TYR	O-C-N	-6.12	115.67	122.03
1	L	3	VAL	O-C-N	6.06	129.15	122.66
2	H	55	GLY	N-CA-C	-6.06	106.15	114.64
2	H	175	PRO	O-C-N	6.04	130.80	122.64
2	H	200	ARG	N-CA-C	-6.04	101.20	110.32
2	H	13	LYS	CA-C-N	6.03	127.38	119.84
2	H	13	LYS	C-N-CA	6.03	127.38	119.84
1	L	125	LEU	CA-C-O	-5.99	114.07	120.42
1	L	161	ASN	OD1-CG-ND2	-5.95	116.65	122.60
2	H	172	HIS	CB-CG-CD2	-5.94	123.48	131.20
2	H	227	PRO	O-C-N	5.90	130.05	122.85
1	L	45	LYS	CA-CB-CG	5.90	125.90	114.10
2	H	90	TYR	CA-C-O	-5.88	114.02	120.43
1	L	2	VAL	N-CA-C	-5.84	98.22	107.15
2	H	30	THR	N-CA-C	-5.79	105.71	112.89
1	L	138	ASN	OD1-CG-ND2	-5.78	116.82	122.60
2	H	199	PRO	N-CD-CG	5.76	111.85	103.20
2	H	101	ASP	CA-CB-CG	5.76	118.36	112.60
2	H	96	ASP	O-C-N	-5.75	116.46	123.19
2	H	91	PHE	CA-CB-CG	5.75	119.55	113.80
2	H	194	PRO	O-C-N	-5.74	116.21	123.10
1	L	163	TRP	CB-CG-CD1	-5.74	118.30	126.90
1	L	156	GLN	O-C-N	-5.70	115.08	122.09
2	H	96	ASP	N-CA-CB	-5.70	101.11	110.52
1	L	144	ILE	N-CA-C	-5.70	100.02	107.88
2	H	136	SER	N-CA-C	5.70	122.94	110.80
2	H	33	GLY	O-C-N	-5.69	115.30	122.70
1	L	77	ARG	N-CA-C	-5.68	95.68	107.67
1	L	14	ASN	CA-CB-CG	5.63	118.23	112.60
2	H	67	PHE	CA-CB-CG	-5.61	108.19	113.80
2	H	72	GLU	CB-CG-CD	5.61	122.14	112.60
1	L	42	GLN	OE1-CD-NE2	-5.61	117.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	43	LYS	N-CA-C	-5.60	101.23	109.18
1	L	120	PRO	CA-C-O	5.54	127.99	121.56
1	L	134	CYS	O-C-N	-5.53	116.72	123.19
2	H	209	ASN	CA-CB-CG	5.50	118.10	112.60
1	L	184	ASP	N-CA-CB	5.49	119.08	110.46
2	H	103	TRP	CG-CD2-CE3	5.47	139.37	133.90
2	H	67	PHE	CA-C-O	-5.45	114.75	120.80
2	H	199	PRO	N-CA-CB	5.45	108.97	103.25
2	H	212	HIS	CB-CG-CD2	-5.44	124.12	131.20
2	H	199	PRO	CA-N-CD	-5.43	104.39	112.00
2	H	138	VAL	CA-CB-CG1	-5.42	101.18	110.40
2	H	100	TRP	CG-CD2-CE3	5.41	139.31	133.90
2	H	29	PHE	N-CA-C	5.40	117.92	111.71
2	H	1	GLN	N-CA-C	-5.38	95.95	111.00
1	L	60	ASP	N-CA-C	5.37	122.23	110.80
1	L	75	ILE	O-C-N	-5.37	117.07	123.03
2	H	50	TRP	O-C-N	-5.36	117.69	123.42
2	H	11	LEU	O-C-N	-5.33	116.08	123.12
2	H	21	SER	CA-CB-OG	5.33	121.76	111.10
1	L	171	SER	N-CA-C	5.33	122.14	110.80
2	H	139	THR	N-CA-C	-5.32	99.74	108.41
1	L	128	GLY	O-C-N	-5.32	115.79	122.70
1	L	160	LEU	CA-CB-CG	5.32	134.91	116.30
1	L	163	TRP	CE2-CD2-CG	-5.31	100.83	107.20
2	H	162	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	H	179	GLN	CB-CA-C	5.30	119.44	110.79
2	H	129	ALA	N-CA-C	-5.30	99.11	108.23
2	H	177	VAL	CA-CB-CG1	5.30	119.41	110.40
2	H	36	TRP	CE2-CD2-CG	-5.29	100.86	107.20
1	L	140	TYR	O-C-N	-5.27	116.68	122.06
2	H	108	THR	CA-C-O	-5.27	115.06	120.54
2	H	163	SER	N-CA-CB	-5.27	103.99	111.84
2	H	214	ALA	N-CA-C	5.25	118.47	111.75
1	L	157	ASN	OD1-CG-ND2	-5.25	117.36	122.60
1	L	1	ASP	CA-CB-CG	-5.24	107.36	112.60
1	L	179	LEU	N-CA-C	-5.24	101.24	109.25
1	L	92	SER	N-CA-C	-5.22	107.29	113.97
1	L	210	ASN	O-C-N	5.22	129.43	123.27
2	H	218	LYS	CB-CG-CD	-5.21	99.32	111.30
2	H	203	SER	N-CA-C	5.20	116.64	111.07
1	L	14	ASN	N-CA-C	-5.20	101.29	109.25
1	L	156	GLN	OE1-CD-NE2	-5.20	117.40	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	110	THR	CA-CB-OG1	-5.18	101.83	109.60
1	L	66	GLY	O-C-N	-5.16	117.59	122.65
1	L	188	ARG	N-CA-C	-5.16	106.30	112.59
2	H	98	VAL	N-CA-C	5.12	116.58	111.00
1	L	34	HIS	O-C-N	-5.11	116.95	123.24
2	H	47	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	L	35	TRP	CA-CB-CG	5.10	123.29	113.60
2	H	177	VAL	CA-CB-CG2	-5.10	101.74	110.40
2	H	55	GLY	O-C-N	-5.09	116.62	122.42
1	L	154	GLU	N-CA-CB	-5.09	102.95	111.20
2	H	46	LYS	O-C-N	-5.08	117.52	123.27
1	L	137	ASN	CA-C-N	5.08	129.35	122.19
1	L	137	ASN	C-N-CA	5.08	129.35	122.19
2	H	8	GLY	CA-C-N	5.07	124.97	119.85
2	H	8	GLY	C-N-CA	5.07	124.97	119.85
1	L	139	PHE	N-CA-C	5.07	118.27	110.42
1	L	7	ILE	CB-CG1-CD1	-5.06	103.18	113.80
1	L	157	ASN	CB-CG-ND2	5.04	123.97	116.40
2	H	52	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	H	192	THR	O-C-N	-5.03	116.48	123.12
1	L	11	LEU	CA-C-N	5.02	124.78	119.76
1	L	11	LEU	C-N-CA	5.02	124.78	119.76
2	H	177	VAL	N-CA-C	-5.00	98.93	109.34

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	44	0
2	H	1675	0	1633	43	0
3	H	21	0	30	0	0
4	H	1	0	0	0	0
All	All	3376	0	3288	86	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 13.

All (86) 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:194:PRO:O	2:H:199:PRO:HD2	1.56	1.03
1:L:14:ASN:OD1	1:L:107:LYS:HD3	1.94	0.68
2:H:93:THR:HG21	2:H:100(B):PHE:HB3	1.77	0.67
1:L:113:PRO:HG3	1:L:144:ILE:HD11	1.77	0.66
1:L:133:VAL:HG13	1:L:178:THR:HG22	1.78	0.66
2:H:51:ILE:HD11	2:H:69:PHE:HB3	1.77	0.65
2:H:93:THR:CG2	2:H:100(B):PHE:HB3	2.26	0.64
1:L:108:ARG:HG2	1:L:171:SER:HB2	1.80	0.64
2:H:12:LYS:O	2:H:111:VAL:HA	2.00	0.61
1:L:61:ARG:HB2	1:L:76:SER:HB2	1.83	0.60
1:L:193:THR:HB	1:L:208:SER:OG	2.03	0.58
1:L:155:ARG:HH21	1:L:185:GLU:HG2	1.67	0.58
2:H:83:LYS:HD3	2:H:85:GLU:H	1.68	0.58
2:H:194:PRO:O	2:H:199:PRO:CD	2.42	0.57
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.87	0.57
2:H:83:LYS:NZ	2:H:85:GLU:HB3	2.20	0.56
2:H:83:LYS:HZ3	2:H:85:GLU:HB3	1.71	0.55
1:L:151:ASP:HA	1:L:191:SER:OG	2.07	0.55
2:H:18:VAL:HG12	2:H:82(C):LEU:HD21	1.88	0.55
1:L:108:ARG:HH12	1:L:111:ALA:HB2	1.72	0.55
2:H:207:THR:HG23	2:H:222:LYS:HD3	1.89	0.55
1:L:6:GLN:NE2	1:L:101:GLY:H	2.04	0.55
2:H:5:VAL:HG13	2:H:23:LYS:HB2	1.89	0.54
2:H:14:PRO:HD3	2:H:111:VAL:HG12	1.90	0.54
1:L:27(B):LEU:HD11	1:L:90:GLN:HG3	1.90	0.54
1:L:8:PRO:O	1:L:102:THR:HB	2.08	0.54
1:L:6:GLN:CD	1:L:88:CYS:SG	2.91	0.53
1:L:50:LYS:HB2	1:L:53:ASN:HD22	1.73	0.52
2:H:178:LEU:HA	2:H:185:TYR:HA	1.92	0.52
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.92	0.52
2:H:5:VAL:HG22	2:H:23:LYS:HD2	1.92	0.51
1:L:108:ARG:HD3	1:L:109:ALA:O	2.10	0.51
2:H:13:LYS:O	2:H:16:GLU:HG3	2.11	0.50
1:L:117:ILE:HD13	1:L:194:CYS:HB3	1.93	0.50
1:L:182:THR:HG23	1:L:185:GLU:H	1.77	0.50
2:H:13:LYS:N	2:H:13:LYS:HE3	2.27	0.49
2:H:140:LEU:HG	2:H:223:ILE:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:PRO:HG3	2:H:84:ASN:OD1	2.13	0.49
1:L:120:PRO:HG2	1:L:130:ALA:HB1	1.94	0.49
2:H:21:SER:HB2	2:H:23:LYS:NZ	2.28	0.49
2:H:17:THR:OG1	2:H:82(A):ASN:HA	2.13	0.48
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.94	0.48
1:L:144:ILE:HD12	1:L:198:HIS:HB2	1.95	0.48
2:H:64:LYS:HD2	2:H:65:GLY:H	1.79	0.48
1:L:115:VAL:HG22	1:L:207:LYS:HZ2	1.79	0.48
2:H:151:PRO:O	2:H:213:PRO:HD2	2.15	0.47
1:L:7:ILE:HG22	1:L:8:PRO:HA	1.97	0.47
1:L:143:ASP:O	1:L:198:HIS:HD2	1.98	0.47
2:H:83:LYS:HD3	2:H:84:ASN:N	2.30	0.47
2:H:179:GLN:HE21	2:H:179:GLN:HB3	1.62	0.47
2:H:194:PRO:C	2:H:199:PRO:HD2	2.34	0.47
1:L:161:ASN:HB2	1:L:163:TRP:CH2	2.50	0.46
2:H:69:PHE:CE1	2:H:80:LEU:HD23	2.50	0.46
2:H:139:THR:HA	2:H:191:VAL:O	2.15	0.46
1:L:7:ILE:CG2	1:L:8:PRO:HA	2.46	0.46
2:H:41:PRO:O	2:H:43:LYS:HD2	2.17	0.45
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.17	0.45
2:H:60:VAL:HG12	2:H:62:ASP:H	1.82	0.44
1:L:37:LEU:HD21	1:L:39:LYS:HE3	1.99	0.44
1:L:48:MET:HB2	1:L:48:MET:HE2	1.74	0.44
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.75	0.44
1:L:145:ASN:O	1:L:196:ALA:HA	2.18	0.44
1:L:135:PHE:HD1	1:L:176:SER:HB3	1.83	0.44
1:L:18:GLN:OE1	1:L:74:LYS:HE2	2.17	0.44
2:H:20:ILE:HD12	2:H:80:LEU:HD12	1.99	0.44
1:L:117:ILE:O	1:L:117:ILE:HG23	2.19	0.43
2:H:83:LYS:HD2	2:H:85:GLU:HG2	2.00	0.43
1:L:48:MET:SD	1:L:54:ARG:HG2	2.57	0.43
1:L:54:ARG:HH11	1:L:54:ARG:HD2	1.69	0.43
2:H:13:LYS:HA	2:H:112:SER:O	2.19	0.43
1:L:27(D):HIS:ND1	1:L:28:ASN:OD1	2.51	0.43
2:H:5:VAL:O	2:H:23:LYS:HD2	2.18	0.43
2:H:126:PRO:O	2:H:128:SER:N	2.52	0.42
1:L:3:VAL:HB	1:L:26:SER:HB3	2.02	0.42
2:H:117:THR:HA	2:H:118:PRO:HD2	1.82	0.42
1:L:6:GLN:CG	1:L:88:CYS:SG	3.08	0.41
1:L:13:VAL:HG11	1:L:78:VAL:HG21	2.03	0.41
1:L:33:LEU:HD22	1:L:89:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ASP:O	1:L:172:THR:HG23	2.21	0.41
1:L:146:VAL:HG11	1:L:161:ASN:ND2	2.36	0.41
2:H:1:GLN:OE1	2:H:1:GLN:N	2.47	0.41
2:H:10:GLU:HB2	2:H:109:VAL:HG13	2.03	0.41
1:L:164:THR:HG23	2:H:174:PHE:CD1	2.56	0.41
2:H:121:VAL:HG12	2:H:221:LYS:HG3	2.03	0.40
2:H:83:LYS:HD2	2:H:85:GLU:OE2	2.21	0.40
2:H:125:ALA:O	2:H:228:ARG:NH1	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	L	214/216 (99%)	191 (89%)	16 (8%)	7 (3%)	3	7
2	H	217/219 (99%)	188 (87%)	22 (10%)	7 (3%)	3	7
All	All	431/435 (99%)	379 (88%)	38 (9%)	14 (3%)	3	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	GLY
1	L	27(E)	SER
1	L	28	ASN
1	L	153	SER
1	L	171	SER
2	H	14	PRO
2	H	136	SER
1	L	17	ASP
1	L	68	GLY
2	H	7	SER

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Mol	Chain	Res	Type
2	H	100	TRP
2	H	135	ASN
2	H	175	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%)	157 (81%)	37 (19%)	1	4
2	H	188/188 (100%)	157 (84%)	31 (16%)	2	6
All	All	382/382 (100%)	314 (82%)	68 (18%)	2	5

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

Mol	Chain	Res	Type
1	L	1	ASP
1	L	9	LEU
1	L	13	VAL
1	L	14	ASN
1	L	15	LEU
1	L	18	GLN
1	L	24	ARG
1	L	31	THR
1	L	46	LEU
1	L	50	LYS
1	L	52	SER
1	L	77	ARG
1	L	78	VAL
1	L	81	GLU
1	L	90	GLN
1	L	95	PRO
1	L	102	THR
1	L	104	LEU
1	L	115	VAL

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Mol	Chain	Res	Type
1	L	120	PRO
1	L	125	LEU
1	L	138	ASN
1	L	145	ASN
1	L	155	ARG
1	L	156	GLN
1	L	160	LEU
1	L	168	SER
1	L	175	MET
1	L	177	SER
1	L	184	ASP
1	L	190	ASN
1	L	193	THR
1	L	194	CYS
1	L	203	SER
1	L	206	VAL
1	L	207	LYS
1	L	210	ASN
2	H	1	GLN
2	H	2	ILE
2	H	5	VAL
2	H	13	LYS
2	H	14	PRO
2	H	17	THR
2	H	21	SER
2	H	23	LYS
2	H	25	SER
2	H	30	THR
2	H	43	LYS
2	H	64	LYS
2	H	73	THR
2	H	80	LEU
2	H	109	VAL
2	H	123	PRO
2	H	126	PRO
2	H	133	GLN
2	H	135	ASN
2	H	138	VAL
2	H	140	LEU
2	H	142	CYS
2	H	144	VAL
2	H	145	LYS

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Mol	Chain	Res	Type
2	H	152	VAL
2	H	175	PRO
2	H	178	LEU
2	H	179	GLN
2	H	196	SER
2	H	207	THR
2	H	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	34	HIS
1	L	53	ASN
1	L	161	ASN
2	H	135	ASN
2	H	179	GLN

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](#)

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	AE2	H	229	-	24,24,24	1.28	4 (16%)	39,39,39	1.72	10 (25%)

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	AE2	H	229	-	-	-	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	AE2	C4-C3	2.89	1.57	1.52
3	H	229	AE2	C13-C17	-2.43	1.49	1.52
3	H	229	AE2	C11-C9	-2.37	1.49	1.53
3	H	229	AE2	C12-C13	-2.06	1.50	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	AE2	C15-C14-C8	5.00	127.08	119.10
3	H	229	AE2	C19-C10-C1	-3.90	102.10	108.31
3	H	229	AE2	C5-C4-C3	-3.13	107.98	112.71
3	H	229	AE2	C19-C10-C9	2.88	115.05	111.18
3	H	229	AE2	C12-C13-C17	-2.58	113.06	116.71
3	H	229	AE2	C4-C5-C10	-2.57	109.92	112.66
3	H	229	AE2	C10-C9-C8	-2.35	110.04	112.43
3	H	229	AE2	C18-C13-C14	2.28	116.27	112.99
3	H	229	AE2	C4-C5-C6	-2.22	107.88	111.73
3	H	229	AE2	C13-C14-C8	-2.19	110.83	113.13

There are no chirality outliers.

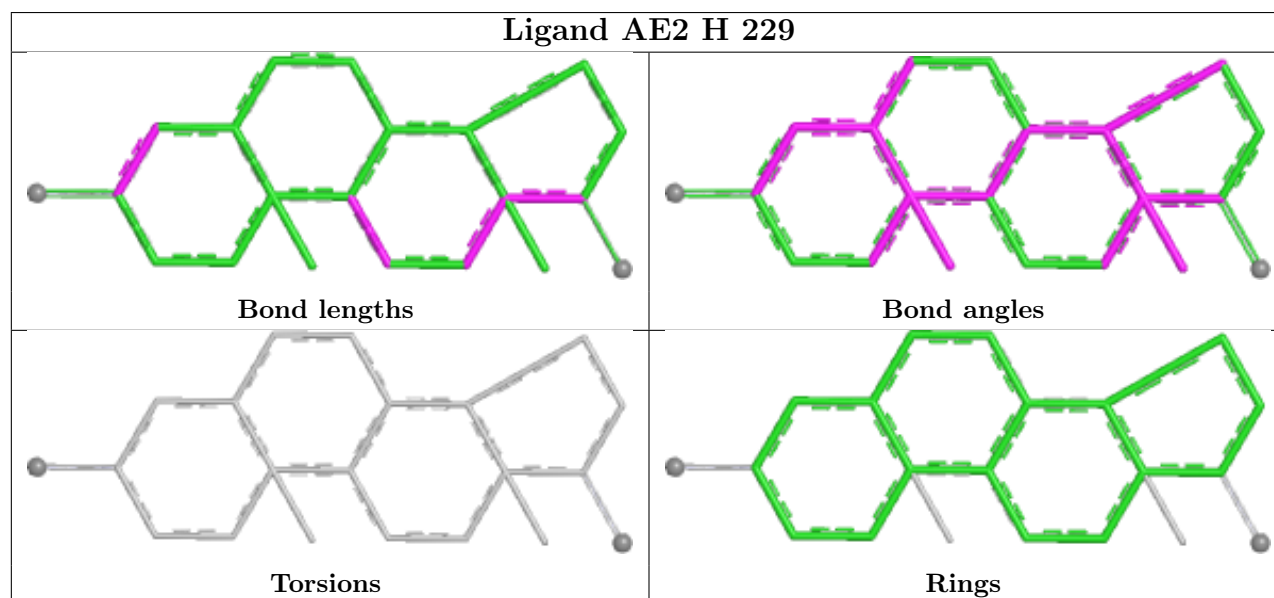
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.