



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 1DBB / pdb_00001dbb
Title : THREE-DIMENSIONAL STRUCTURE OF AN ANTI-STEROID FAB' AND
PROGESTERONE-FAB' COMPLEX
Authors : Arevalo, J.H.; Wilson, I.A.
Deposited on : 1992-11-11
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

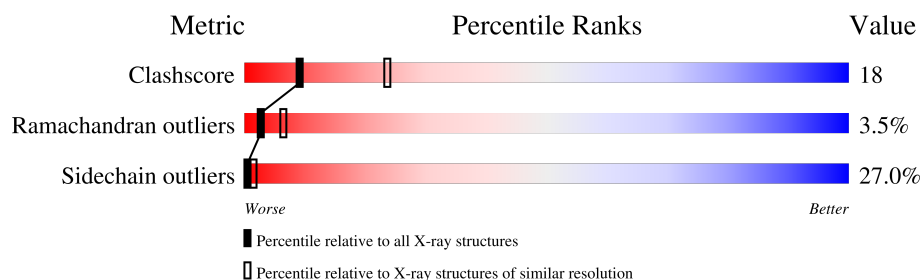
1 Overall quality at a glance

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 3377 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			

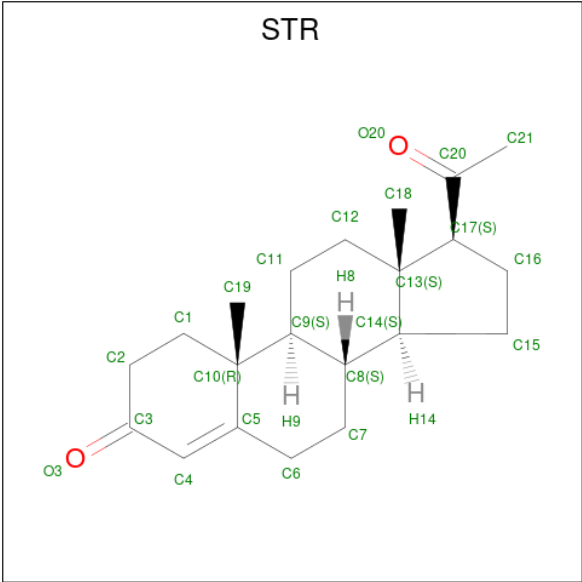
There are 14 discrepancies between the modelled and reference sequences:

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 (CCD ID: STR) (formula: $C_{21}H_{30}O_2$).



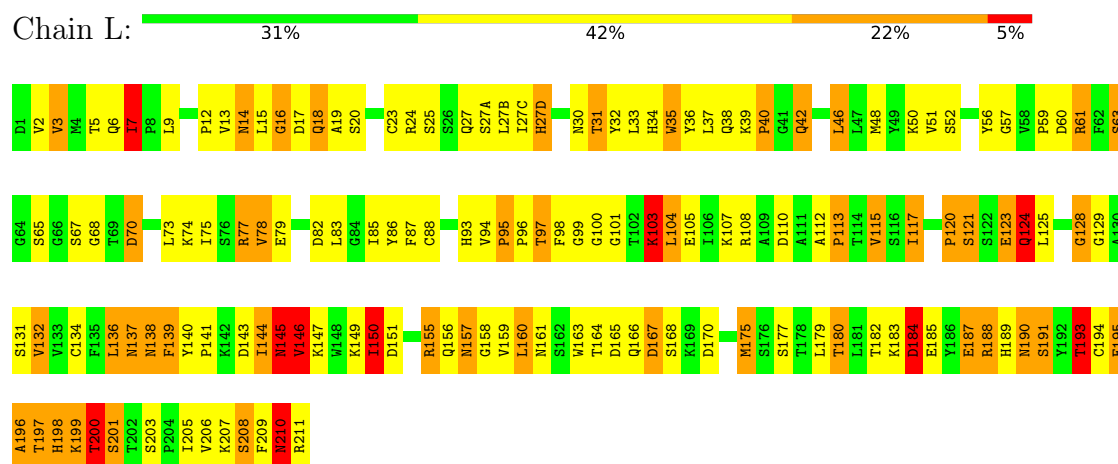
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			23	21	2		

3 Residue-property plots

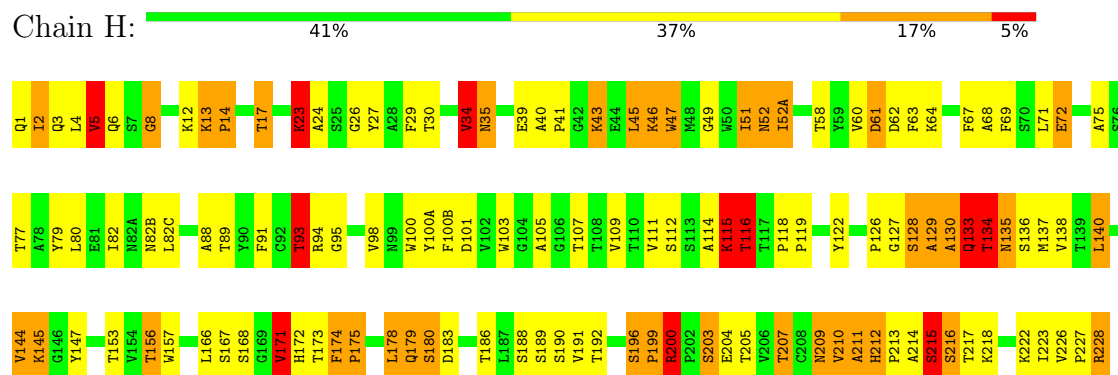
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3377	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	10/1719 (0.6%)	2.23	74/2331 (3.2%)
2	H	1.29	9/1723 (0.5%)	2.17	77/2358 (3.3%)
All	All	1.27	19/3442 (0.6%)	2.20	151/4689 (3.2%)

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
2	H	0	3
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	34	VAL	CA-CB	8.63	1.64	1.53
1	L	7	ILE	CA-CB	8.26	1.64	1.54
2	H	172	HIS	CD2-NE2	-7.85	1.29	1.37
1	L	198	HIS	CD2-NE2	-7.64	1.29	1.37
2	H	116	THR	CA-CB	7.12	1.64	1.53
1	L	34	HIS	CD2-NE2	-6.65	1.30	1.37
2	H	226	VAL	CA-CB	6.64	1.59	1.54
2	H	212	HIS	CD2-NE2	-6.58	1.30	1.37
1	L	193	THR	CA-CB	6.46	1.64	1.53
1	L	93	HIS	CD2-NE2	-6.39	1.30	1.37
2	H	5	VAL	CA-CB	6.28	1.62	1.54
1	L	189	HIS	CD2-NE2	-6.23	1.30	1.37
2	H	210	VAL	CA-CB	6.00	1.61	1.54
1	L	94	VAL	CA-CB	5.81	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	172	HIS	CG-ND1	-5.48	1.32	1.38
1	L	198	HIS	CG-ND1	-5.42	1.32	1.38
1	L	27(D)	HIS	CD2-NE2	-5.40	1.31	1.37
1	L	63	SER	C-N	-5.17	1.26	1.33
2	H	144	VAL	CA-CB	5.07	1.59	1.53

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	184	ASP	CA-CB-CG	-13.19	99.41	112.60
1	L	121	SER	N-CA-C	10.62	124.03	110.33
1	L	3	VAL	N-CA-CB	-10.47	99.11	110.53
2	H	60	VAL	N-CA-C	-10.36	98.50	110.21
2	H	45	LEU	N-CA-C	-9.99	92.64	108.63
2	H	209	ASN	CA-CB-CG	9.56	122.16	112.60
1	L	157	ASN	OD1-CG-ND2	-9.09	113.51	122.60
2	H	227	PRO	O-C-N	9.01	133.85	122.85
1	L	156	GLN	O-C-N	-8.84	112.45	122.09
1	L	170	ASP	CA-CB-CG	8.57	121.17	112.60
2	H	62	ASP	N-CA-C	8.11	120.12	111.28
2	H	3	GLN	OE1-CD-NE2	-7.98	114.62	122.60
1	L	189	HIS	CB-CG-CD2	-7.95	120.86	131.20
1	L	27	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	L	163	TRP	CA-C-O	-7.76	112.63	121.40
1	L	138	ASN	OD1-CG-ND2	-7.72	114.88	122.60
2	H	157	TRP	CE2-CD2-CE3	7.62	126.42	118.80
1	L	95	PRO	N-CD-CG	-7.60	94.68	103.80
2	H	129	ALA	N-CA-C	-7.59	99.80	110.50
1	L	137	ASN	OD1-CG-ND2	-7.54	115.06	122.60
2	H	172	HIS	CB-CG-CD2	-7.53	121.42	131.20
1	L	14	ASN	CA-CB-CG	7.52	120.12	112.60
2	H	128	SER	CA-C-O	7.45	131.17	120.51
1	L	70	ASP	CA-C-O	-7.37	112.14	120.32
1	L	27(D)	HIS	CB-CG-CD2	-7.34	121.66	131.20
1	L	157	ASN	CA-CB-CG	7.30	119.90	112.60
1	L	144	ILE	CB-CA-C	-7.25	99.40	111.29
1	L	146	VAL	N-CA-C	7.16	118.11	106.72
1	L	14	ASN	OD1-CG-ND2	-7.13	115.47	122.60
2	H	58	THR	CA-CB-OG1	-7.10	98.94	109.60
2	H	100	TRP	N-CA-C	7.08	121.29	111.74
1	L	185	GLU	N-CA-C	-7.05	102.73	111.75
1	L	167	ASP	CA-CB-CG	6.99	119.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	144	ILE	N-CA-CB	6.96	122.70	111.23
1	L	136	LEU	N-CA-C	-6.91	97.47	108.73
1	L	110	ASP	N-CA-C	6.90	119.87	110.35
1	L	151	ASP	N-CA-C	-6.86	101.12	111.34
2	H	8	GLY	CA-C-N	6.80	126.78	119.78
2	H	8	GLY	C-N-CA	6.80	126.78	119.78
1	L	67	SER	N-CA-C	6.79	120.36	108.75
1	L	27(C)	ILE	N-CA-C	-6.72	98.65	108.87
1	L	137	ASN	N-CA-C	6.70	119.60	109.41
2	H	153	THR	N-CA-CB	-6.67	100.29	110.77
1	L	197	THR	CA-CB-OG1	-6.66	99.61	109.60
2	H	203	SER	CA-CB-OG	6.57	124.24	111.10
2	H	115	LYS	N-CA-C	-6.57	99.96	110.14
2	H	35	ASN	CA-CB-CG	6.49	119.09	112.60
2	H	101	ASP	N-CA-C	6.48	122.14	113.72
1	L	145	ASN	CA-CB-CG	6.44	119.04	112.60
1	L	201	SER	N-CA-C	-6.42	97.79	108.32
1	L	103	LYS	CA-CB-CG	6.40	126.89	114.10
1	L	128	GLY	N-CA-C	-6.38	104.36	112.65
2	H	35	ASN	O-C-N	-6.38	115.95	123.22
2	H	175	PRO	O-C-N	6.36	131.22	122.64
2	H	103	TRP	CG-CD2-CE3	6.35	140.25	133.90
1	L	132	VAL	N-CA-C	-6.35	99.34	108.48
1	L	180	THR	CA-CB-OG1	-6.33	100.11	109.60
1	L	196	ALA	O-C-N	-6.33	115.85	123.13
2	H	216	SER	N-CA-CB	-6.33	102.29	111.91
1	L	184	ASP	CA-C-O	-6.33	112.20	118.97
1	L	124	GLN	O-C-N	6.28	128.54	122.07
1	L	124	GLN	CA-C-N	6.26	128.58	120.44
1	L	124	GLN	C-N-CA	6.26	128.58	120.44
1	L	198	HIS	CB-CG-CD2	-6.26	123.06	131.20
2	H	172	HIS	CB-CG-ND1	6.22	132.04	122.70
1	L	210	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	L	14	ASN	N-CA-C	-6.20	99.17	109.46
2	H	211	ALA	O-C-N	-6.16	115.97	123.30
2	H	61	ASP	CA-CB-CG	6.12	118.72	112.60
1	L	60	ASP	CA-CB-CG	6.05	118.66	112.60
2	H	13	LYS	CA-C-O	-6.04	114.42	120.64
1	L	40	PRO	O-C-N	6.03	130.33	123.03
2	H	145	LYS	N-CA-C	6.03	119.23	109.40
2	H	91	PHE	CA-CB-CG	5.97	119.77	113.80
2	H	228	ARG	N-CA-C	-5.93	94.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	94	VAL	CA-C-O	5.92	123.02	119.94
2	H	13	LYS	N-CA-C	-5.92	101.60	110.24
2	H	199	PRO	CA-N-CD	-5.92	103.72	112.00
1	L	35	TRP	CD2-CE2-CZ2	-5.87	116.53	122.40
2	H	153	THR	CB-CA-C	5.80	119.43	110.14
1	L	139	PHE	N-CA-C	5.80	119.13	110.14
2	H	93	THR	CA-CB-OG1	5.73	118.20	109.60
2	H	35	ASN	OD1-CG-ND2	-5.72	116.88	122.60
2	H	34	VAL	CB-CA-C	5.72	119.14	111.19
2	H	114	ALA	N-CA-C	5.71	117.90	110.43
1	L	18	GLN	N-CA-C	-5.69	102.05	110.48
2	H	178	LEU	N-CA-C	5.67	118.47	107.71
2	H	23	LYS	N-CA-C	5.67	117.75	108.52
2	H	128	SER	N-CA-C	5.66	122.86	110.80
2	H	174	PHE	CA-C-N	5.66	126.91	119.84
2	H	174	PHE	C-N-CA	5.66	126.91	119.84
2	H	171	VAL	CG1-CB-CG2	-5.62	98.43	110.80
1	L	120	PRO	O-C-N	5.62	129.39	123.10
2	H	199	PRO	O-C-N	-5.62	115.06	122.64
2	H	179	GLN	OE1-CD-NE2	-5.60	117.00	122.60
2	H	180	SER	N-CA-C	5.60	122.72	110.80
1	L	96	PRO	N-CA-C	-5.57	102.45	111.03
2	H	47	TRP	CG-CD2-CE3	5.57	139.47	133.90
1	L	134	CYS	N-CA-C	-5.55	99.36	108.41
1	L	124	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	L	194	CYS	N-CA-C	-5.55	100.64	109.96
2	H	200	ARG	O-C-N	-5.52	113.28	121.12
2	H	105	ALA	N-CA-C	5.50	122.52	110.80
2	H	226	VAL	CA-C-N	5.46	125.78	119.93
2	H	226	VAL	C-N-CA	5.46	125.78	119.93
2	H	179	GLN	N-CA-C	-5.45	101.31	109.15
2	H	175	PRO	N-CD-CG	-5.43	95.06	103.20
1	L	120	PRO	N-CA-C	5.42	118.99	110.80
1	L	105	GLU	N-CA-C	5.42	116.91	110.19
2	H	174	PHE	CA-CB-CG	-5.42	108.38	113.80
2	H	68	ALA	N-CA-C	5.41	118.57	107.69
1	L	155	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	L	42	GLN	CB-CG-CD	-5.34	103.51	112.60
1	L	14	ASN	CB-CG-ND2	5.34	124.41	116.40
2	H	207	THR	CA-C-O	-5.32	114.95	120.70
1	L	27(D)	HIS	CB-CG-ND1	5.32	130.68	122.70
1	L	115	VAL	N-CA-C	5.31	117.43	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	23	CYS	CA-C-O	-5.31	114.91	121.06
1	L	137	ASN	CB-CG-ND2	5.29	124.34	116.40
2	H	118	PRO	CA-C-O	-5.28	112.90	120.56
1	L	200	THR	N-CA-C	5.28	122.04	110.80
1	L	2	VAL	N-CA-C	-5.26	100.81	108.17
2	H	3	GLN	CG-CD-NE2	5.25	124.28	116.40
1	L	16	GLY	O-C-N	-5.25	115.88	122.70
2	H	58	THR	CA-CB-CG2	5.24	119.41	110.50
2	H	29	PHE	CA-CB-CG	5.24	119.04	113.80
1	L	57	GLY	N-CA-C	-5.21	100.82	113.18
2	H	144	VAL	CB-CA-C	5.20	118.59	111.88
2	H	100	TRP	N-CA-CB	-5.20	104.28	112.13
2	H	2	ILE	N-CA-C	-5.20	99.63	107.73
2	H	4	LEU	O-C-N	-5.19	117.16	123.13
1	L	138	ASN	CB-CG-ND2	5.16	124.14	116.40
2	H	6	GLN	N-CA-C	5.16	117.73	110.14
2	H	47	TRP	CE2-CD2-CG	-5.16	101.01	107.20
2	H	173	THR	N-CA-C	-5.16	101.29	109.96
2	H	228	ARG	CA-CB-CG	5.16	124.42	114.10
2	H	189	SER	CA-C-O	-5.13	115.60	121.40
2	H	144	VAL	N-CA-CB	-5.12	105.82	111.66
1	L	190	ASN	N-CA-C	-5.11	101.92	109.94
2	H	200	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	L	198	HIS	CB-CG-ND1	5.07	130.31	122.70
2	H	100(A)	TYR	CA-CB-CG	5.07	123.03	113.90
2	H	94	ARG	N-CA-C	-5.07	101.86	109.15
1	L	97	THR	O-C-N	5.05	129.75	123.19
2	H	77	THR	CA-C-O	-5.04	115.21	120.80
2	H	13	LYS	CA-C-N	5.04	126.13	119.84
2	H	13	LYS	C-N-CA	5.04	126.13	119.84
2	H	95	GLY	CA-C-O	5.04	125.50	120.92
1	L	87	PHE	O-C-N	-5.03	116.83	123.21
1	L	113	PRO	N-CA-C	5.01	118.42	110.21
1	L	189	HIS	CB-CG-ND1	5.00	130.21	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	130	ALA	Peptide
2	H	134	THR	Peptide
2	H	200	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	L	150	ILE	Peptide

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	71	0
2	H	1675	0	1633	56	0
3	H	23	0	29	0	0
All	All	3377	0	3287	122	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 18.

All (122) 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:150:ILE:HD12	1:L:155:ARG:HG3	1.30	1.06
2:H:93:THR:HG21	2:H:100(B):PHE:HB3	1.53	0.88
1:L:149:LYS:HB2	1:L:193:THR:HG23	1.61	0.80
2:H:34:VAL:HG13	2:H:51:ILE:HG23	1.66	0.76
1:L:193:THR:HB	1:L:208:SER:OG	1.87	0.74
1:L:196:ALA:HB3	1:L:205:ILE:HG23	1.70	0.74
1:L:12:PRO:HB2	1:L:107:LYS:HB2	1.72	0.71
1:L:13:VAL:HG11	1:L:78:VAL:HG11	1.75	0.69
1:L:199:LYS:H	1:L:199:LYS:HD3	1.58	0.68
2:H:130:ALA:O	2:H:134:THR:N	2.26	0.68
2:H:156:THR:HG23	2:H:209:ASN:HB2	1.77	0.67
1:L:27(B):LEU:O	1:L:31:THR:HA	1.97	0.64
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.80	0.64
1:L:144:ILE:HG22	1:L:198:HIS:CD2	2.34	0.63
1:L:107:LYS:HA	1:L:140:TYR:OH	2.02	0.60
1:L:123:GLU:HG3	2:H:122:TYR:CD1	2.36	0.60
1:L:128:GLY:HA2	1:L:183:LYS:HE2	1.84	0.60
2:H:136:SER:O	2:H:137:MET:SD	2.60	0.59
1:L:144:ILE:HD11	1:L:175:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ASN:OD1	1:L:177:SER:HB3	2.03	0.59
1:L:86:TYR:O	1:L:101:GLY:HA2	2.03	0.58
1:L:85:ILE:HD12	1:L:103:LYS:HE3	1.85	0.58
1:L:83:LEU:HD23	1:L:104:LEU:O	2.02	0.58
2:H:47:TRP:HE1	2:H:100(B):PHE:HZ	1.51	0.58
2:H:196:SER:O	2:H:203:SER:HB3	2.04	0.58
1:L:164:THR:HG23	2:H:174:PHE:HD1	1.69	0.57
1:L:155:ARG:NH2	1:L:157:ASN:HB3	2.19	0.57
1:L:63:SER:O	1:L:73:LEU:HD12	2.04	0.57
1:L:144:ILE:HG22	1:L:198:HIS:HB2	1.87	0.57
1:L:129:GLY:H	1:L:183:LYS:H	1.53	0.56
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.87	0.56
1:L:187:GLU:HA	1:L:211:ARG:NE	2.20	0.56
1:L:187:GLU:HA	1:L:211:ARG:CZ	2.35	0.56
1:L:95:PRO:O	1:L:97:THR:HG23	2.06	0.56
2:H:49:GLY:HA3	2:H:69:PHE:HE2	1.71	0.56
2:H:179:GLN:HE22	2:H:186:THR:HG21	1.71	0.56
2:H:5:VAL:HG13	2:H:23:LYS:HG2	1.87	0.56
1:L:124:GLN:HG2	2:H:122:TYR:CD2	2.42	0.55
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.41	0.55
2:H:171:VAL:HA	2:H:190:SER:O	2.07	0.55
1:L:143:ASP:HB2	1:L:199:LYS:NZ	2.23	0.54
2:H:93:THR:CG2	2:H:100(B):PHE:HB3	2.33	0.54
1:L:184:ASP:O	1:L:188:ARG:HG3	2.08	0.54
1:L:112:ALA:HB2	1:L:200:THR:HB	1.90	0.53
1:L:14:ASN:HB2	1:L:17:ASP:CG	2.33	0.53
2:H:212:HIS:ND1	2:H:215:SER:HB3	2.24	0.53
1:L:157:ASN:OD1	1:L:158:GLY:N	2.43	0.52
2:H:8:GLY:O	2:H:107:THR:HG23	2.10	0.52
2:H:52(A):ILE:HD12	2:H:71:LEU:HD11	1.91	0.52
1:L:199:LYS:HD3	1:L:199:LYS:N	2.24	0.51
2:H:69:PHE:HA	2:H:79:TYR:O	2.11	0.51
1:L:145:ASN:HD22	1:L:145:ASN:N	2.07	0.51
2:H:12:LYS:O	2:H:111:VAL:HA	2.10	0.51
1:L:164:THR:HG23	2:H:174:PHE:CD1	2.45	0.51
2:H:166:LEU:HD23	2:H:191:VAL:HG21	1.93	0.51
1:L:143:ASP:HB2	1:L:199:LYS:HZ3	1.75	0.51
2:H:2:ILE:HD12	2:H:26:GLY:O	2.11	0.50
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.46	0.50
2:H:207:THR:HG23	2:H:222:LYS:HD2	1.93	0.50
2:H:49:GLY:HA3	2:H:69:PHE:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:VAL:HG12	2:H:52(A):ILE:HD11	1.95	0.49
1:L:27(A):SER:HA	1:L:68:GLY:O	2.13	0.49
1:L:38:GLN:NE2	1:L:42:GLN:O	2.46	0.49
1:L:6:GLN:O	1:L:7:ILE:HD12	2.13	0.49
2:H:39:GLU:O	2:H:88:ALA:HB1	2.13	0.49
1:L:158:GLY:O	1:L:160:LEU:HD23	2.13	0.48
1:L:190:ASN:HB3	1:L:210:ASN:OD1	2.13	0.48
2:H:17:THR:HA	2:H:82:ILE:O	2.14	0.48
2:H:211:ALA:HB2	2:H:218:LYS:HD3	1.95	0.48
1:L:36:TYR:CE1	1:L:46:LEU:HD23	2.48	0.48
1:L:83:LEU:HD12	1:L:83:LEU:H	1.78	0.48
1:L:121:SER:O	1:L:125:LEU:HD23	2.14	0.47
2:H:82(C):LEU:HD22	2:H:82(C):LEU:H	1.79	0.47
1:L:98:PHE:HB2	2:H:45:LEU:O	2.15	0.47
2:H:180:SER:O	2:H:183:ASP:HB2	2.14	0.47
1:L:27(D):HIS:N	1:L:30:ASN:O	2.48	0.46
1:L:85:ILE:HG23	1:L:103:LYS:HE3	1.97	0.46
1:L:150:ILE:HD12	1:L:155:ARG:CG	2.23	0.46
2:H:2:ILE:CG2	2:H:27:TYR:HB3	2.45	0.46
2:H:72:GLU:O	2:H:75:ALA:HB3	2.16	0.46
2:H:115:LYS:HD3	2:H:116:THR:H	1.81	0.46
1:L:184:ASP:HA	1:L:187:GLU:H	1.81	0.45
1:L:79:GLU:HB2	1:L:82:ASP:OD1	2.16	0.45
2:H:133:GLN:HE21	2:H:133:GLN:HB2	1.59	0.45
2:H:136:SER:C	2:H:137:MET:SD	3.00	0.45
1:L:48:MET:HB2	1:L:48:MET:HE2	1.67	0.44
2:H:41:PRO:O	2:H:43:LYS:HD2	2.16	0.44
2:H:130:ALA:O	2:H:134:THR:HG23	2.18	0.44
1:L:39:LYS:HB3	1:L:40:PRO:HD2	1.99	0.43
2:H:82(B):ASN:N	2:H:82(B):ASN:HD22	2.16	0.43
1:L:85:ILE:CD1	1:L:103:LYS:HG3	2.48	0.43
2:H:5:VAL:HG13	2:H:23:LYS:CG	2.47	0.43
1:L:14:ASN:O	1:L:17:ASP:HB2	2.18	0.43
1:L:48:MET:HE3	1:L:73:LEU:CD1	2.49	0.43
2:H:179:GLN:NE2	2:H:186:THR:HG21	2.33	0.43
2:H:46:LYS:HD3	2:H:47:TRP:N	2.34	0.43
1:L:6:GLN:HG3	1:L:99:GLY:O	2.19	0.43
1:L:61:ARG:O	1:L:75:ILE:HA	2.19	0.43
2:H:14:PRO:HA	2:H:82(C):LEU:O	2.19	0.42
2:H:127:GLY:O	2:H:129:ALA:N	2.52	0.42
2:H:52:ASN:C	2:H:52:ASN:OD1	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:ILE:CG2	1:L:198:HIS:CD2	3.02	0.42
1:L:16:GLY:O	1:L:77:ARG:NH1	2.53	0.42
2:H:140:LEU:HG	2:H:223:ILE:HG21	2.02	0.42
2:H:167:SER:O	2:H:171:VAL:HG12	2.19	0.42
1:L:199:LYS:O	1:L:201:SER:N	2.53	0.41
2:H:133:GLN:O	2:H:135:ASN:N	2.53	0.41
1:L:120:PRO:HB3	1:L:131:SER:O	2.20	0.41
1:L:144:ILE:HD13	1:L:144:ILE:HG21	1.84	0.41
2:H:213:PRO:C	2:H:215:SER:H	2.27	0.41
1:L:117:ILE:HD12	1:L:209:PHE:HD1	1.84	0.41
1:L:149:LYS:N	1:L:193:THR:O	2.54	0.41
1:L:75:ILE:HD12	1:L:75:ILE:N	2.35	0.41
1:L:146:VAL:HA	1:L:195:GLU:O	2.20	0.41
1:L:18:GLN:HG2	1:L:19:ALA:N	2.35	0.41
1:L:113:PRO:HB3	1:L:139:PHE:CD2	2.55	0.41
2:H:133:GLN:C	2:H:135:ASN:N	2.78	0.41
1:L:32:TYR:CD1	1:L:32:TYR:N	2.89	0.41
2:H:63:PHE:O	2:H:67:PHE:HB2	2.21	0.41
2:H:13:LYS:HD3	2:H:112:SER:O	2.20	0.41
1:L:61:ARG:HD2	1:L:77:ARG:O	2.22	0.40
1:L:184:ASP:CG	1:L:187:GLU:HB2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	213/216 (99%)	169 (79%)	36 (17%)	8 (4%)	2	5
2	H	217/219 (99%)	184 (85%)	26 (12%)	7 (3%)	3	7
All	All	430/435 (99%)	353 (82%)	62 (14%)	15 (4%)	3	6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	159	VAL
1	L	191	SER
1	L	200	THR
2	H	128	SER
2	H	133	GLN
1	L	100	GLY
1	L	187	GLU
2	H	175	PRO
1	L	167	ASP
2	H	214	ALA
2	H	215	SER
2	H	135	ASN
1	L	138	ASN
2	H	14	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%)	136 (70%)	58 (30%)	0	1
2	H	188/188 (100%)	143 (76%)	45 (24%)	1	2
All	All	382/382 (100%)	279 (73%)	103 (27%)	0	1

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	5	THR
1	L	7	ILE
1	L	9	LEU
1	L	15	LEU
1	L	20	SER
1	L	24	ARG
1	L	25	SER

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Mol	Chain	Res	Type
1	L	31	THR
1	L	33	LEU
1	L	37	LEU
1	L	46	LEU
1	L	50	LYS
1	L	52	SER
1	L	56	TYR
1	L	59	PRO
1	L	61	ARG
1	L	65	SER
1	L	70	ASP
1	L	74	LYS
1	L	77	ARG
1	L	78	VAL
1	L	103	LYS
1	L	104	LEU
1	L	108	ARG
1	L	115	VAL
1	L	117	ILE
1	L	123	GLU
1	L	124	GLN
1	L	132	VAL
1	L	136	LEU
1	L	137	ASN
1	L	141	PRO
1	L	145	ASN
1	L	146	VAL
1	L	147	LYS
1	L	150	ILE
1	L	160	LEU
1	L	165	ASP
1	L	166	GLN
1	L	168	SER
1	L	175	MET
1	L	179	LEU
1	L	180	THR
1	L	182	THR
1	L	184	ASP
1	L	188	ARG
1	L	191	SER
1	L	193	THR
1	L	195	GLU

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Mol	Chain	Res	Type
1	L	197	THR
1	L	199	LYS
1	L	200	THR
1	L	203	SER
1	L	206	VAL
1	L	207	LYS
1	L	208	SER
1	L	210	ASN
2	H	1	GLN
2	H	5	VAL
2	H	17	THR
2	H	23	LYS
2	H	30	THR
2	H	34	VAL
2	H	35	ASN
2	H	43	LYS
2	H	46	LYS
2	H	51	ILE
2	H	52	ASN
2	H	52(A)	ILE
2	H	61	ASP
2	H	64	LYS
2	H	72	GLU
2	H	80	LEU
2	H	89	THR
2	H	93	THR
2	H	98	VAL
2	H	109	VAL
2	H	115	LYS
2	H	116	THR
2	H	126	PRO
2	H	133	GLN
2	H	134	THR
2	H	138	VAL
2	H	140	LEU
2	H	144	VAL
2	H	145	LYS
2	H	156	THR
2	H	168	SER
2	H	171	VAL
2	H	178	LEU
2	H	188	SER

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Mol	Chain	Res	Type
2	H	192	THR
2	H	196	SER
2	H	199	PRO
2	H	200	ARG
2	H	204	GLU
2	H	205	THR
2	H	210	VAL
2	H	215	SER
2	H	216	SER
2	H	217	THR
2	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	14	ASN
1	L	34	HIS
1	L	145	ASN
1	L	156	GLN
1	L	166	GLN
2	H	6	GLN
2	H	35	ASN
2	H	82(B)	ASN
2	H	133	GLN

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	STR	H	229	-	26,26,26	2.16	11 (42%)	42,42,42	2.38	16 (38%)

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	STR	H	229	-	-	0/4/62/62	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	STR	C4-C5	4.91	1.41	1.34
3	H	229	STR	C4-C3	-4.57	1.36	1.45
3	H	229	STR	C7-C6	-3.11	1.46	1.53
3	H	229	STR	C12-C11	-2.93	1.47	1.53
3	H	229	STR	C11-C9	-2.89	1.49	1.53
3	H	229	STR	C12-C13	2.84	1.59	1.54
3	H	229	STR	C13-C14	-2.76	1.49	1.55
3	H	229	STR	C10-C9	-2.62	1.51	1.56
3	H	229	STR	C13-C17	-2.61	1.51	1.56
3	H	229	STR	C7-C8	-2.48	1.49	1.53
3	H	229	STR	C17-C20	-2.21	1.48	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	STR	C15-C14-C8	7.54	131.13	119.10
3	H	229	STR	C17-C13-C14	7.11	107.15	99.72
3	H	229	STR	C13-C17-C20	4.65	121.42	114.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	STR	C19-C10-C9	3.13	115.17	111.66
3	H	229	STR	C13-C14-C8	-3.09	110.02	114.41
3	H	229	STR	C1-C2-C3	-3.01	105.47	111.60
3	H	229	STR	C15-C14-C13	-2.86	100.48	103.84
3	H	229	STR	C11-C12-C13	2.72	117.32	112.74
3	H	229	STR	C10-C9-C8	-2.69	108.78	112.71
3	H	229	STR	C12-C11-C9	-2.37	109.10	113.14
3	H	229	STR	C18-C13-C14	-2.29	107.52	111.68
3	H	229	STR	C6-C5-C10	-2.27	112.74	116.76
3	H	229	STR	C7-C8-C14	-2.25	108.34	112.08
3	H	229	STR	C5-C4-C3	-2.23	120.23	123.67
3	H	229	STR	C11-C9-C10	-2.21	110.36	113.08
3	H	229	STR	O20-C20-C21	-2.01	117.61	121.17

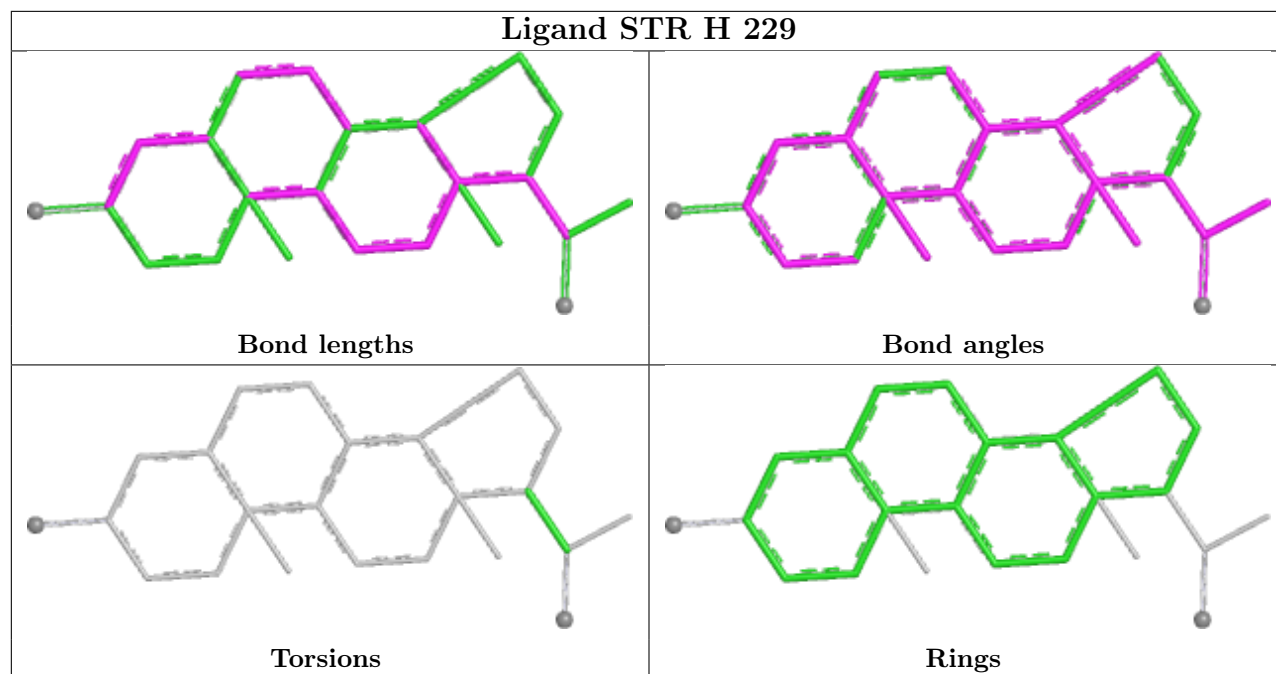
There are no chirality outliers.

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.