



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:17 PM UTC

PDB ID : 1EAP / pdb_00001eap
Title : CRYSTAL STRUCTURE OF A CATALYTIC ANTIBODY WITH A SERINE
PROTEASE ACTIVE SITE
Authors : Zhou, G.W.; Guo, J.; Huang, W.; Scanlan, T.S.; Fletterick, R.J.
Deposited on : 1994-08-10
Resolution : 2.40 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

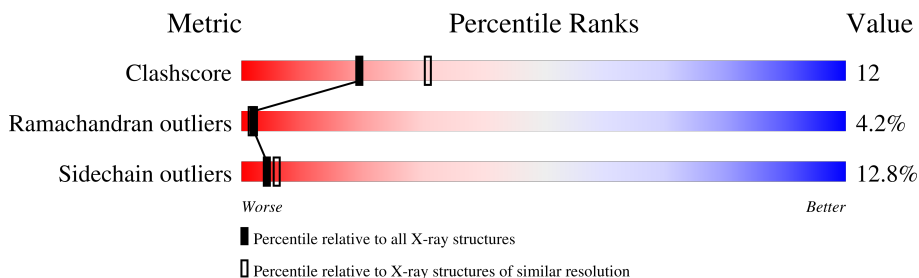
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	A	213	
2	B	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3287 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 IGG2B-KAPPA 17E8 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1655	1037	282	330	6			

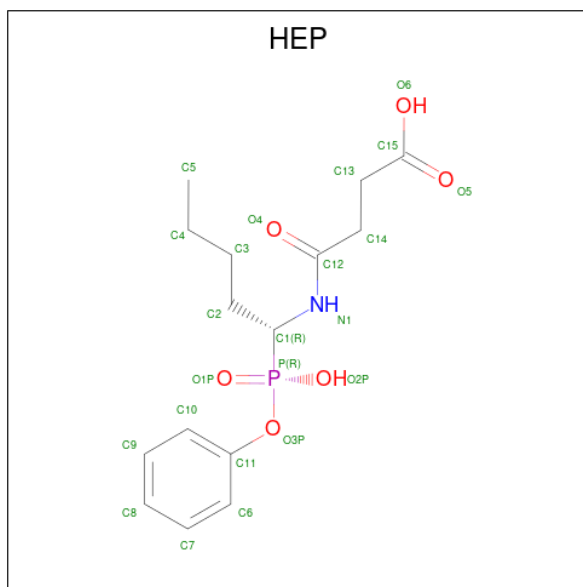
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	LEU	MET	conflict	GB 12002896
A	22	THR	ALA	conflict	GB 12002896
A	26	SER	ASN	conflict	GB 12002896
A	30	LYS	ASN	conflict	GB 12002896
A	34	GLY	ALA	conflict	GB 12002896
A	55	LEU	GLN	conflict	GB 12002896
A	63	ARG	SER	conflict	GB 12002896
A	80	GLY	PRO	conflict	GB 12002896
A	81	GLY	GLU	conflict	GB 12002896
A	92	TYR	ASP	conflict	GB 12002896
A	156	ALA	GLN	conflict	GB 12002896
A	157	GLN	ASN	conflict	GB 12002896
A	187	GLU	GLY	conflict	GB 12002896

- Molecule 2 is a protein called IGG2B-KAPPA 17E8 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1609	1015	260	327	7			

- Molecule 3 is PHENYL[1-(N-SUCCINYLAMINO)PENTYL]PHOSPHONATE (CCD ID: HEP) (formula: C₁₅H₂₂NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			23	15	1	6	1		

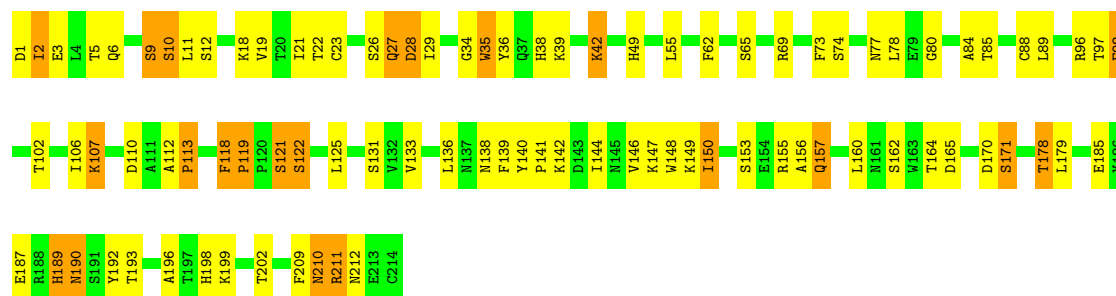
3 Residue-property plots [i](#)

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.

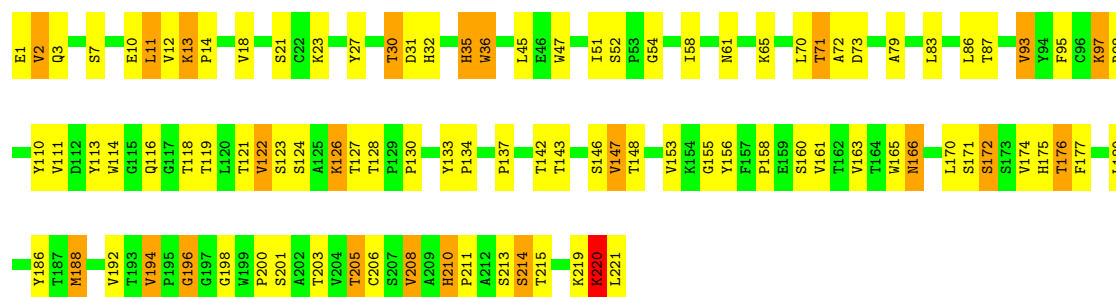
• Molecule 1: IGG2B-KAPPA 17E8 FAB (LIGHT CHAIN)

Chain A: 



• Molecule 2: IGG2B-KAPPA 17E8 FAB (HEAVY CHAIN)

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.41Å 78.06Å 81.94Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3287	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: HEP

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	A	0.95	3/1693 (0.2%)	1.79	37/2291 (1.6%)
2	B	1.02	7/1650 (0.4%)	1.89	41/2251 (1.8%)
All	All	0.99	10/3343 (0.3%)	1.84	78/4542 (1.7%)

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
2	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	198	HIS	CD2-NE2	-6.77	1.30	1.37
2	B	208	VAL	CA-CB	6.60	1.63	1.54
2	B	175	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	49	HIS	CD2-NE2	-6.38	1.30	1.37
2	B	210	HIS	CD2-NE2	-6.18	1.31	1.37
2	B	35	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	189	HIS	CD2-NE2	-6.06	1.31	1.37
2	B	32	HIS	CG-ND1	-5.55	1.32	1.38
2	B	175	HIS	CG-ND1	-5.11	1.32	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	SER	N-CA-C	-8.27	95.93	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ASP	CA-CB-CG	8.24	120.84	112.60
2	B	27	TYR	O-C-N	-7.57	114.89	122.99
2	B	73	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	190	ASN	N-CA-C	6.91	125.53	110.80
1	A	189	HIS	N-CA-C	6.91	125.52	110.80
2	B	128	THR	CA-C-N	6.71	124.49	119.66
2	B	128	THR	C-N-CA	6.71	124.49	119.66
2	B	95	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	210	ASN	CA-CB-CG	6.50	119.11	112.60
2	B	214	SER	N-CA-C	-6.44	97.07	110.80
2	B	210	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	34	GLY	O-C-N	-6.39	118.04	123.60
1	A	198	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	98	PHE	CA-CB-CG	6.33	120.13	113.80
2	B	12	VAL	N-CA-C	6.30	117.43	108.42
2	B	177	PHE	CA-CB-CG	-6.26	107.53	113.80
2	B	133	TYR	CA-C-N	6.24	126.00	119.76
2	B	133	TYR	C-N-CA	6.24	126.00	119.76
1	A	157	GLN	OE1-CD-NE2	-6.03	116.57	122.60
2	B	122	VAL	N-CA-C	6.02	116.48	107.51
2	B	52	SER	O-C-N	-6.00	114.42	121.32
2	B	110	TYR	N-CA-C	5.92	117.82	111.36
1	A	2	ILE	N-CA-C	-5.84	100.64	108.35
1	A	49	HIS	CA-CB-CG	5.83	119.63	113.80
1	A	62	PHE	N-CA-C	-5.79	101.05	110.20
2	B	165	TRP	CG-CD2-CE3	5.78	139.68	133.90
2	B	13	LYS	CG-CD-CE	-5.76	98.04	111.30
1	A	189	HIS	O-C-N	-5.75	114.95	122.59
1	A	198	HIS	CB-CG-ND1	5.72	131.28	122.70
1	A	27	GLN	N-CA-C	-5.70	101.09	109.81
1	A	80	GLY	N-CA-C	-5.63	99.83	113.18
2	B	127	THR	CA-CB-OG1	-5.62	101.17	109.60
2	B	176	THR	CA-CB-OG1	-5.59	101.21	109.60
2	B	36	TRP	CG-CD2-CE3	5.58	139.48	133.90
1	A	178	THR	CA-CB-OG1	-5.57	101.25	109.60
2	B	196	GLY	N-CA-C	-5.54	106.15	112.79
2	B	13	LYS	N-CA-C	5.52	116.84	109.83
2	B	61	ASN	CA-C-O	-5.51	114.64	120.92
1	A	28	ASP	N-CA-C	-5.51	101.00	109.76
1	A	119	PRO	N-CA-C	5.50	117.41	110.70
1	A	78	LEU	N-CA-C	-5.50	101.51	109.59
2	B	118	THR	O-C-N	-5.46	116.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	GLN	CA-CB-CG	5.45	124.99	114.10
1	A	156	ALA	O-C-N	-5.42	115.74	122.25
1	A	211	ARG	N-CA-C	5.42	118.43	110.30
2	B	71	THR	N-CA-CB	-5.42	102.61	111.66
1	A	38	HIS	CB-CG-CD2	-5.40	124.17	131.20
1	A	171	SER	N-CA-C	5.40	119.44	112.86
2	B	166	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	142	LYS	CA-CB-CG	5.30	124.69	114.10
1	A	121	SER	N-CA-C	5.28	122.06	110.80
1	A	112	ALA	CA-C-N	5.24	125.41	119.90
1	A	112	ALA	C-N-CA	5.24	125.41	119.90
2	B	71	THR	CA-CB-OG1	-5.24	101.74	109.60
2	B	165	TRP	CE2-CD2-CG	-5.22	100.94	107.20
2	B	93	VAL	N-CA-C	-5.21	100.87	108.17
1	A	118	PHE	CA-C-N	5.21	125.74	120.38
1	A	118	PHE	C-N-CA	5.21	125.74	120.38
1	A	98	PHE	CB-CA-C	-5.20	101.22	109.80
1	A	49	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	B	210	HIS	CB-CG-ND1	5.18	130.47	122.70
2	B	23	LYS	CA-CB-CG	5.15	124.40	114.10
2	B	32	HIS	CB-CG-CD2	-5.14	124.52	131.20
2	B	137	PRO	N-CA-C	5.09	122.97	112.47
2	B	3	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	148	TRP	CE2-CD2-CG	-5.09	101.10	107.20
2	B	61	ASN	N-CA-C	-5.08	102.53	110.10
2	B	114	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	35	TRP	CB-CG-CD1	-5.06	119.31	126.90
2	B	206	CYS	N-CA-C	-5.06	101.91	109.95
2	B	220	LYS	O-C-N	5.05	128.31	122.09
1	A	189	HIS	CB-CG-CD2	-5.05	124.64	131.20
2	B	12	VAL	CA-C-N	5.04	127.64	120.49
2	B	12	VAL	C-N-CA	5.04	127.64	120.49
1	A	113	PRO	N-CA-C	5.02	118.38	110.80
2	B	31	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	35	TRP	CG-CD2-CE3	5.00	138.90	133.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	194	VAL	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	A	1655	0	1609	39	0
2	B	1609	0	1561	37	0
3	B	23	0	20	4	0
All	All	3287	0	3190	75	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 12.

All (75) 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:B:153:VAL:HG11	2:B:161:VAL:HG11	1.75	0.68
1:A:39:LYS:HB2	1:A:42:LYS:HD2	1.74	0.68
2:B:147:VAL:HG23	2:B:194:VAL:HG23	1.76	0.68
1:A:136:LEU:HD23	1:A:144:ILE:HD13	1.76	0.67
2:B:203:THR:HG22	2:B:220:LYS:HB2	1.77	0.66
2:B:174:VAL:HG22	2:B:192:VAL:HG12	1.79	0.64
1:A:122:SER:HA	1:A:125:LEU:HD23	1.81	0.61
2:B:130:PRO:HD2	2:B:215:THR:HG21	1.83	0.61
2:B:11:LEU:HG	2:B:121:THR:HG23	1.83	0.60
2:B:134:PRO:HD3	2:B:219:LYS:HG2	1.85	0.58
1:A:85:THR:HA	1:A:102:THR:O	2.05	0.55
1:A:6:GLN:HG3	1:A:23:CYS:SG	2.45	0.55
1:A:162:SER:HB3	2:B:180:LEU:HD11	1.87	0.55
2:B:158:PRO:O	2:B:210:HIS:HE1	1.90	0.54
1:A:187:GLU:HA	1:A:211:ARG:NH1	2.22	0.54
1:A:190:ASN:O	1:A:211:ARG:HB2	2.09	0.53
2:B:18:VAL:HG12	2:B:83:LEU:HB2	1.90	0.53
1:A:36:TYR:HE1	1:A:89:LEU:HD23	1.74	0.53
1:A:190:ASN:HA	1:A:211:ARG:HB2	1.90	0.53
1:A:192:TYR:HE2	1:A:211:ARG:HD3	1.74	0.52
1:A:149:LYS:HB2	1:A:193:THR:HB	1.91	0.52
2:B:30:THR:HG22	2:B:54:GLY:HA2	1.92	0.52
1:A:107:LYS:HA	1:A:140:TYR:OH	2.10	0.51
2:B:51:ILE:HG13	2:B:58:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ASN:HB3	2:B:170:LEU:H	1.77	0.50
2:B:126:LYS:HB2	2:B:126:LYS:HZ3	1.76	0.50
1:A:6:GLN:HB2	1:A:23:CYS:SG	2.52	0.50
2:B:205:THR:HA	2:B:220:LYS:HA	1.94	0.49
1:A:2:ILE:O	1:A:97:THR:HG21	2.13	0.49
1:A:133:VAL:HG22	1:A:178:THR:OG1	2.13	0.49
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.95	0.48
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.47	0.48
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.48	0.48
1:A:36:TYR:CE1	1:A:89:LEU:HD23	2.49	0.48
2:B:156:TYR:CE1	2:B:186:TYR:HB2	2.50	0.47
1:A:89:LEU:HD11	1:A:96:ARG:HB3	1.96	0.47
1:A:21:ILE:HD12	1:A:73:PHE:HD2	1.79	0.46
2:B:146:SER:HA	2:B:196:GLY:C	2.40	0.46
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.15	0.46
2:B:220:LYS:HG2	2:B:221:LEU:H	1.80	0.46
1:A:27:GLN:O	1:A:69:ARG:HG2	2.16	0.46
1:A:96:ARG:HG3	3:B:222:HEP:H10	1.98	0.46
2:B:97:LYS:NZ	3:B:222:HEP:O1P	2.49	0.46
3:B:222:HEP:H6	3:B:222:HEP:H21	1.98	0.45
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.82	0.45
2:B:72:ALA:HA	2:B:79:ALA:HA	1.99	0.45
1:A:160:LEU:HG	2:B:180:LEU:HD13	1.99	0.45
2:B:14:PRO:HD3	2:B:123:SER:C	2.42	0.45
2:B:65:LYS:HB2	2:B:65:LYS:HE2	1.79	0.45
1:A:36:TYR:OH	3:B:222:HEP:H7	2.17	0.45
2:B:148:THR:HA	2:B:192:VAL:O	2.17	0.45
2:B:35:HIS:HB3	2:B:47:TRP:HE1	1.82	0.44
1:A:21:ILE:HB	1:A:73:PHE:HB3	1.98	0.44
1:A:12:SER:HB3	1:A:107:LYS:HB2	2.00	0.44
1:A:118:PHE:HA	1:A:119:PRO:HD2	1.75	0.43
1:A:106:ILE:HD11	1:A:171:SER:OG	2.17	0.43
1:A:136:LEU:HD21	1:A:196:ALA:HB2	2.01	0.43
2:B:163:VAL:HG23	2:B:188:MET:HE1	2.00	0.43
1:A:131:SER:HB3	1:A:178:THR:HG23	2.01	0.43
2:B:2:VAL:HG13	2:B:113:TYR:CE1	2.54	0.43
2:B:93:VAL:HG22	2:B:119:THR:HG22	2.01	0.42
1:A:150:ILE:HD11	1:A:155:ARG:HD2	2.01	0.42
1:A:113:PRO:HB3	1:A:139:PHE:CD2	2.55	0.42
2:B:2:VAL:HG21	2:B:98:ARG:NH1	2.35	0.42
2:B:36:TRP:CD1	2:B:70:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:HB2	2:B:126:LYS:NZ	2.36	0.41
2:B:111:VAL:HG13	2:B:113:TYR:CE2	2.55	0.41
2:B:219:LYS:HD3	2:B:219:LYS:HA	1.85	0.41
1:A:89:LEU:HD22	1:A:98:PHE:CE2	2.56	0.41
1:A:110:ASP:OD1	1:A:141:PRO:HD3	2.21	0.41
1:A:190:ASN:HA	1:A:211:ARG:CB	2.52	0.40
2:B:86:LEU:HB3	2:B:122:VAL:HG21	2.03	0.40
2:B:87:THR:O	2:B:122:VAL:HG11	2.20	0.40
1:A:39:LYS:HG2	1:A:84:ALA:HB2	2.03	0.40
2:B:2:VAL:HG21	2:B:98:ARG:HH11	1.87	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	A	211/213 (99%)	185 (88%)	18 (8%)	8 (4%)	2	2
2	B	214/216 (99%)	185 (86%)	19 (9%)	10 (5%)	2	1
All	All	425/429 (99%)	370 (87%)	37 (9%)	18 (4%)	2	2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
2	B	160	SER
2	B	213	SER
1	A	10	SER
1	A	150	ILE
2	B	172	SER
2	B	205	THR
2	B	211	PRO

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Mol	Chain	Res	Type
2	B	214	SER
1	A	138	ASN
1	A	170	ASP
1	A	199	LYS
2	B	201	SER
1	A	122	SER
1	A	212	ASN
2	B	155	GLY
2	B	198	GLY
2	B	200	PRO

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	A	186/186 (100%)	160 (86%)	26 (14%)	3	4
2	B	182/182 (100%)	161 (88%)	21 (12%)	5	8
All	All	368/368 (100%)	321 (87%)	47 (13%)	4	6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	THR
1	A	9	SER
1	A	10	SER
1	A	11	LEU
1	A	18	LYS
1	A	19	VAL
1	A	22	THR
1	A	26	SER
1	A	28	ASP
1	A	42	LYS
1	A	55	LEU
1	A	65	SER

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Mol	Chain	Res	Type
1	A	74	SER
1	A	77	ASN
1	A	107	LYS
1	A	146	VAL
1	A	147	LYS
1	A	153	SER
1	A	157	GLN
1	A	164	THR
1	A	165	ASP
1	A	179	LEU
1	A	185	GLU
1	A	202	THR
1	A	210	ASN
2	B	1	GLU
2	B	2	VAL
2	B	7	SER
2	B	10	GLU
2	B	11	LEU
2	B	21	SER
2	B	30	THR
2	B	45	LEU
2	B	71	THR
2	B	97	LYS
2	B	124	SER
2	B	126	LYS
2	B	142	THR
2	B	143	THR
2	B	147	VAL
2	B	171	SER
2	B	172	SER
2	B	176	THR
2	B	188	MET
2	B	208	VAL
2	B	220	LYS

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	137	ASN
1	A	138	ASN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	212	ASN
2	B	35	HIS
2	B	74	GLN
2	B	82	GLN
2	B	182	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	HEP	B	222	-	22,23,23	2.33	3 (13%)	23,30,30	1.68	4 (17%)

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	HEP	B	222	-	-	9/24/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	222	HEP	P-C1	-8.36	1.73	1.84
3	B	222	HEP	P-O3P	5.39	1.64	1.58
3	B	222	HEP	P-O2P	-3.01	1.49	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	222	HEP	C14-C12-N1	-4.21	108.44	115.86
3	B	222	HEP	O1P-P-C1	-4.06	108.66	114.19
3	B	222	HEP	O3P-P-O1P	-3.12	108.12	114.81
3	B	222	HEP	O2P-P-O1P	2.45	117.54	111.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	222	HEP	C2-C1-P-O1P
3	B	222	HEP	N1-C1-P-O1P
3	B	222	HEP	O4-C12-N1-C1
3	B	222	HEP	C15-C13-C14-C12
3	B	222	HEP	C2-C3-C4-C5
3	B	222	HEP	C14-C13-C15-O5
3	B	222	HEP	C14-C13-C15-O6
3	B	222	HEP	N1-C1-P-O3P
3	B	222	HEP	C2-C1-P-O3P

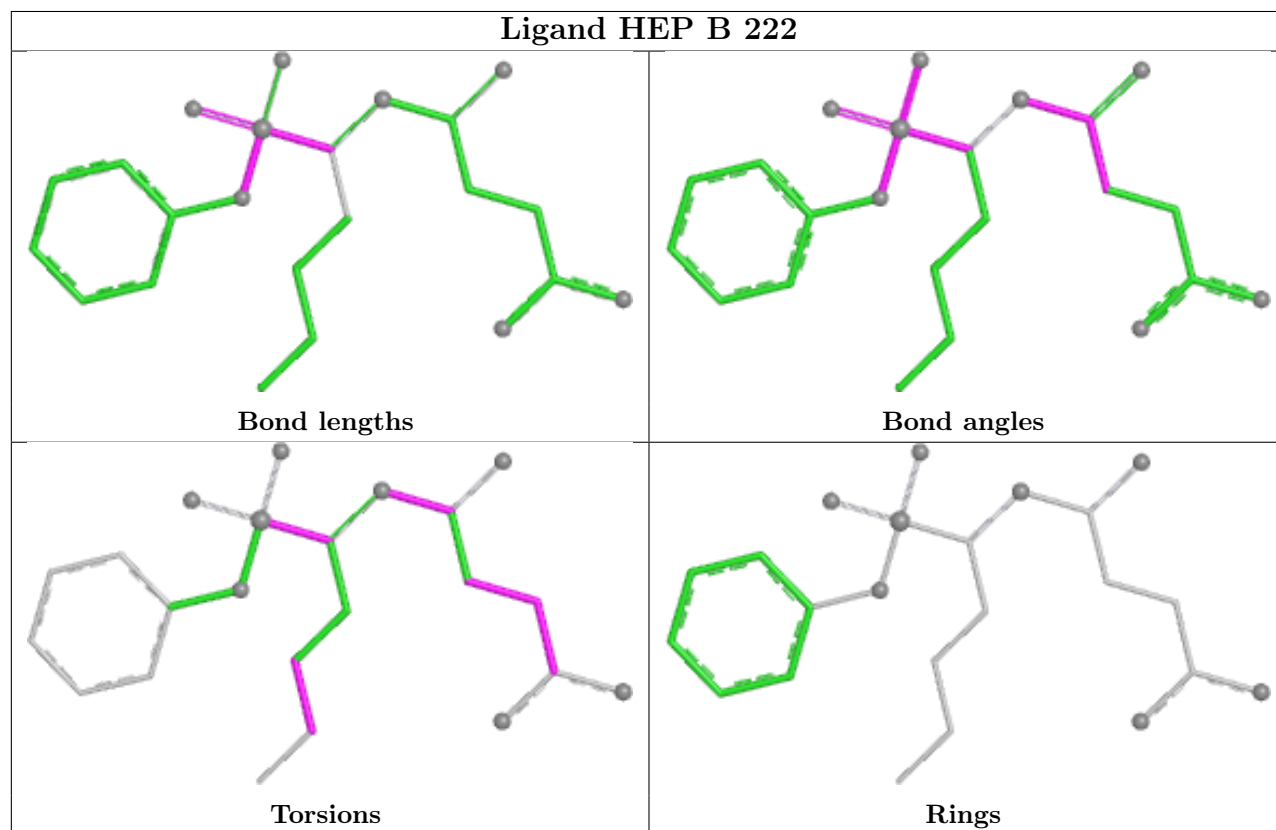
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	222	HEP	4	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.