



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:07 AM UTC

PDB ID : 1DBA / pdb_00001dba
Title : THREE-DIMENSIONAL STRUCTURE OF AN ANTI-STEROID FAB' AND
PROGESTERONE-FAB' COMPLEX
Authors : Arevalo, J.H.; Wilson, I.A.
Deposited on : 1992-11-10
Resolution : 2.80 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
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

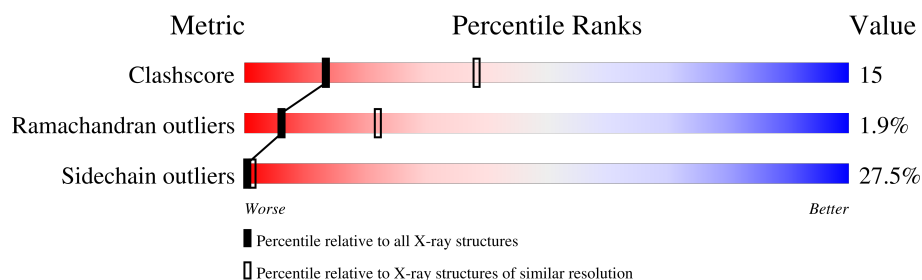
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	40% 37% 22% .
2	H	219	47% 40% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EOH	H	230	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3360 atoms, of which 1 is hydrogen 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			

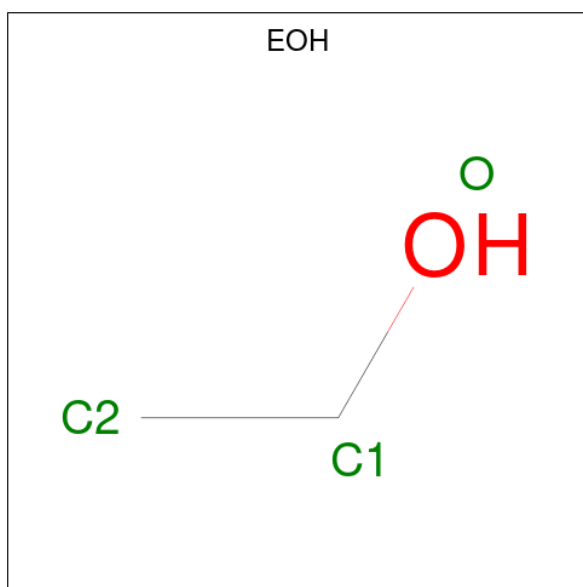
There are 14 discrepancies between the modelled and reference sequences:

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 ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



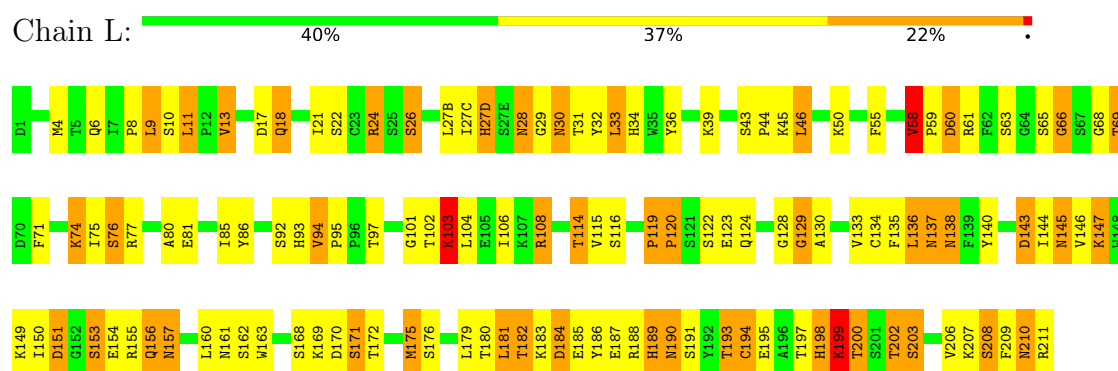
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	H	0	0
			3	2	1		
3	H	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots

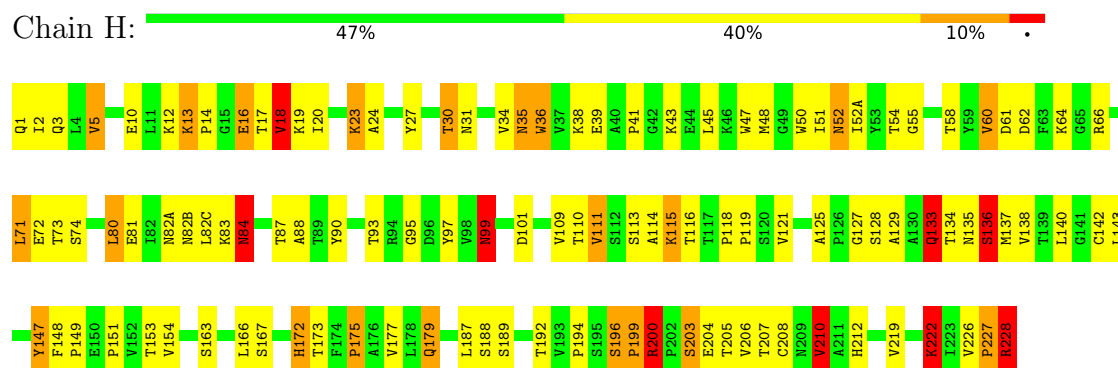
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3360	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: EOH

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	1.21	10/1719 (0.6%)	2.00	59/2331 (2.5%)
2	H	1.26	10/1723 (0.6%)	2.04	50/2358 (2.1%)
All	All	1.24	20/3442 (0.6%)	2.02	109/4689 (2.3%)

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	H	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	30	THR	CA-CB	7.07	1.66	1.53
2	H	212	HIS	CD2-NE2	-7.00	1.30	1.37
2	H	5	VAL	CA-CB	6.81	1.62	1.54
1	L	34	HIS	CD2-NE2	-6.67	1.30	1.37
1	L	198	HIS	CD2-NE2	-6.48	1.30	1.37
2	H	210	VAL	CA-CB	6.48	1.61	1.54
1	L	114	THR	CA-CB	6.24	1.61	1.53
1	L	58	VAL	CA-CB	6.13	1.62	1.54
2	H	99	ASN	CA-CB	-6.07	1.42	1.53
2	H	111	VAL	CA-CB	5.95	1.62	1.54
1	L	93	HIS	CD2-NE2	-5.92	1.31	1.37
2	H	172	HIS	CG-ND1	-5.84	1.31	1.38
1	L	163	TRP	CG-CD2	-5.83	1.33	1.43
2	H	172	HIS	CD2-NE2	-5.67	1.31	1.37
1	L	202	THR	CA-CB	5.63	1.62	1.53
2	H	118	PRO	CA-CB	-5.56	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	34	HIS	CG-ND1	-5.49	1.32	1.38
1	L	27(D)	HIS	CD2-NE2	-5.41	1.31	1.37
1	L	94	VAL	CA-CB	5.35	1.61	1.54
2	H	134	THR	CA-CB	5.03	1.61	1.53

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	99	ASN	N-CA-C	9.58	124.77	113.18
2	H	222	LYS	CA-CB-CG	9.43	132.97	114.10
2	H	228	ARG	N-CA-C	-9.07	85.59	111.00
2	H	93	THR	CA-CB-OG1	-8.16	97.36	109.60
2	H	60	VAL	N-CA-C	-8.08	98.46	109.37
1	L	190	ASN	N-CA-C	8.06	123.53	111.04
1	L	69	THR	CA-CB-OG1	-8.00	97.61	109.60
1	L	66	GLY	CA-C-O	-7.92	114.33	122.01
1	L	202	THR	N-CA-C	-7.65	102.59	112.23
2	H	45	LEU	N-CA-C	-7.61	98.40	109.59
2	H	133	GLN	O-C-N	7.38	131.89	122.81
2	H	134	THR	N-CA-C	-7.25	102.99	111.03
2	H	227	PRO	N-CA-C	7.23	122.67	110.95
1	L	145	ASN	CA-CB-CG	7.15	119.75	112.60
1	L	140	TYR	O-C-N	-7.08	116.32	121.84
1	L	80	ALA	CA-C-N	7.07	130.07	120.38
1	L	80	ALA	C-N-CA	7.07	130.07	120.38
1	L	45	LYS	CA-CB-CG	-7.05	100.00	114.10
2	H	200	ARG	NE-CZ-NH2	-6.77	113.11	119.20
2	H	200	ARG	NE-CZ-NH1	6.77	128.27	121.50
2	H	200	ARG	CG-CD-NE	-6.70	97.25	112.00
2	H	196	SER	N-CA-C	-6.64	103.45	112.35
2	H	47	TRP	CG-CD2-CE3	6.64	140.54	133.90
2	H	52	ASN	OD1-CG-ND2	-6.62	115.98	122.60
2	H	2	ILE	N-CA-C	-6.51	98.48	107.99
1	L	138	ASN	OD1-CG-ND2	-6.49	116.11	122.60
2	H	199	PRO	CA-N-CD	-6.47	102.94	112.00
1	L	60	ASP	N-CA-C	6.46	124.56	110.80
2	H	212	HIS	CA-C-N	6.37	126.58	119.32
2	H	212	HIS	C-N-CA	6.37	126.58	119.32
2	H	55	GLY	O-C-N	-6.29	115.51	122.55
1	L	133	VAL	CG1-CB-CG2	-6.28	96.97	110.80
1	L	194	CYS	N-CA-C	-6.22	100.37	110.20
1	L	28	ASN	OD1-CG-ND2	-6.21	116.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	189	HIS	CB-CG-CD2	-6.20	123.15	131.20
2	H	147	TYR	N-CA-C	6.16	119.57	109.72
2	H	99	ASN	CA-CB-CG	-6.13	106.47	112.60
1	L	163	TRP	CE2-CD2-CE3	6.12	124.92	118.80
1	L	119	PRO	N-CA-C	6.08	118.12	110.70
2	H	93	THR	CA-CB-CG2	6.06	120.81	110.50
2	H	172	HIS	CA-C-O	-6.00	113.88	120.24
2	H	66	ARG	CA-C-O	-6.00	112.26	119.27
1	L	129	GLY	O-C-N	-5.97	118.39	123.23
1	L	77	ARG	N-CA-C	-5.93	96.00	107.44
1	L	153	SER	N-CA-C	5.87	119.33	110.64
1	L	17	ASP	N-CA-C	5.86	117.62	110.41
1	L	103	LYS	CA-CB-CG	5.86	125.81	114.10
1	L	186	TYR	O-C-N	5.86	128.18	122.09
1	L	119	PRO	CA-C-N	5.85	127.16	119.84
1	L	119	PRO	C-N-CA	5.85	127.16	119.84
1	L	34	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	H	187	LEU	O-C-N	-5.82	115.63	122.96
1	L	45	LYS	O-C-N	-5.81	116.51	123.31
2	H	166	LEU	N-CA-C	-5.80	98.83	108.34
2	H	101	ASP	N-CA-C	5.78	120.46	113.41
2	H	194	PRO	CA-N-CD	-5.77	103.93	112.00
1	L	75	ILE	N-CA-C	-5.76	101.61	109.55
1	L	209	PHE	CA-CB-CG	5.71	119.51	113.80
2	H	23	LYS	CA-CB-CG	5.68	125.46	114.10
1	L	24	ARG	N-CA-C	5.64	117.85	108.99
2	H	203	SER	N-CA-CB	-5.57	101.14	110.39
1	L	156	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	L	198	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	L	199	LYS	N-CA-C	5.51	122.53	110.80
2	H	82(B)	ASN	CA-CB-CG	5.51	118.11	112.60
1	L	210	ASN	OD1-CG-ND2	-5.50	117.09	122.60
1	L	13	VAL	O-C-N	-5.49	116.94	123.04
1	L	198	HIS	O-C-N	-5.47	116.71	123.44
1	L	69	THR	CA-CB-CG2	5.45	119.76	110.50
1	L	189	HIS	CA-CB-CG	-5.44	108.36	113.80
2	H	62	ASP	O-C-N	5.41	127.72	122.09
2	H	36	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	L	182	THR	CA-C-O	-5.39	114.90	121.05
2	H	200	ARG	O-C-N	-5.38	115.50	121.53
1	L	162	SER	N-CA-C	-5.37	101.13	109.24
2	H	133	GLN	N-CA-C	5.36	117.64	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	18	VAL	CA-CB-CG1	-5.34	101.32	110.40
2	H	18	VAL	CB-CA-C	-5.28	102.37	110.50
1	L	21	ILE	N-CA-C	-5.27	100.80	109.12
2	H	175	PRO	N-CA-C	5.26	119.13	111.03
1	L	69	THR	N-CA-CB	-5.25	102.82	111.01
2	H	137	MET	CG-SD-CE	-5.24	89.37	100.90
1	L	151	ASP	N-CA-C	-5.23	97.67	108.18
2	H	111	VAL	CA-C-O	5.23	125.55	120.27
1	L	9	LEU	O-C-N	-5.21	116.67	122.09
1	L	106	ILE	CA-C-N	5.20	128.23	120.95
1	L	106	ILE	C-N-CA	5.20	128.23	120.95
1	L	137	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	L	34	HIS	CB-CG-ND1	5.17	130.46	122.70
2	H	110	THR	CA-C-N	-5.15	115.66	122.98
2	H	110	THR	C-N-CA	-5.15	115.66	122.98
1	L	11	LEU	CA-C-N	5.15	126.56	120.23
1	L	11	LEU	C-N-CA	5.15	126.56	120.23
2	H	20	ILE	CA-C-O	-5.15	114.87	120.84
1	L	182	THR	N-CA-C	-5.12	102.11	110.20
1	L	4	MET	O-C-N	-5.11	117.50	123.27
1	L	114	THR	N-CA-C	-5.10	100.20	108.41
2	H	179	GLN	N-CA-C	-5.10	98.36	107.28
1	L	203	SER	O-C-N	-5.08	115.94	121.53
2	H	134	THR	N-CA-CB	5.08	117.34	109.98
2	H	58	THR	N-CA-C	-5.07	100.43	109.06
1	L	93	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	L	27(D)	HIS	CB-CG-CD2	-5.06	124.62	131.20
2	H	84	ASN	N-CA-C	5.06	121.57	110.80
1	L	145	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	L	26	SER	CA-CB-OG	5.04	121.17	111.10
2	H	72	GLU	N-CA-C	-5.01	101.47	108.54
1	L	76	SER	N-CA-CB	-5.00	103.94	110.59
2	H	227	PRO	O-C-N	5.00	128.43	122.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	200	ARG	Peptide
2	H	227	PRO	Peptide,Mainchain

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	60	0
2	H	1675	0	1633	41	0
3	H	5	1	4	0	0
All	All	3359	1	3262	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (97) 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:187:GLU:HA	1:L:211:ARG:HH21	1.28	0.95
1:L:187:GLU:HA	1:L:211:ARG:NH2	1.94	0.82
2:H:10:GLU:HG3	2:H:18:VAL:HG11	1.62	0.81
1:L:150:ILE:HD12	1:L:155:ARG:HD2	1.65	0.78
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.66	0.77
1:L:119:PRO:HG2	2:H:228:ARG:HE	1.49	0.77
1:L:145:ASN:HB3	1:L:197:THR:HB	1.67	0.77
2:H:133:GLN:OE1	2:H:136:SER:HA	1.95	0.66
1:L:18:GLN:HB2	1:L:74:LYS:HZ3	1.59	0.66
2:H:35:ASN:HD21	2:H:95:GLY:HA3	1.59	0.66
1:L:124:GLN:HG2	1:L:129:GLY:O	1.97	0.65
1:L:108:ARG:HG3	1:L:171:SER:HB2	1.80	0.63
1:L:27(B):LEU:O	1:L:31:THR:HA	1.98	0.63
2:H:16:GLU:O	2:H:82(C):LEU:HB2	1.99	0.62
2:H:12:LYS:HG3	2:H:13:LYS:HZ3	1.65	0.61
2:H:125:ALA:H	2:H:228:ARG:HH12	1.49	0.60
2:H:206:VAL:H	2:H:222:LYS:HZ1	1.50	0.59
1:L:115:VAL:HG13	1:L:207:LYS:HG3	1.83	0.59
2:H:52(A):ILE:HD12	2:H:71:LEU:HD21	1.84	0.59
2:H:41:PRO:O	2:H:43:LYS:HG2	2.03	0.58
2:H:36:TRP:HB3	2:H:48:MET:HE3	1.85	0.58
2:H:115:LYS:HD3	2:H:116:THR:H	1.69	0.57
1:L:193:THR:HG23	1:L:208:SER:HB3	1.86	0.57
2:H:35:ASN:ND2	2:H:95:GLY:HA3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:LEU:HD22	2:H:73:THR:OG1	2.05	0.56
1:L:155:ARG:HH12	1:L:157:ASN:HD22	1.53	0.56
1:L:182:THR:OG1	1:L:185:GLU:HB2	2.06	0.55
2:H:154:VAL:HG11	2:H:189:SER:HB2	1.88	0.55
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.71	0.55
1:L:181:LEU:HD23	1:L:185:GLU:HB3	1.89	0.55
2:H:52:ASN:ND2	2:H:97:TYR:OH	2.41	0.54
1:L:30:ASN:HD22	1:L:31:THR:H	1.55	0.54
1:L:27(C):ILE:HD13	1:L:68:GLY:HA2	1.90	0.53
2:H:125:ALA:H	2:H:228:ARG:NH1	2.05	0.53
1:L:190:ASN:HB3	1:L:210:ASN:OD1	2.09	0.53
1:L:189:HIS:O	1:L:211:ARG:HD2	2.09	0.53
2:H:18:VAL:HG22	2:H:82(C):LEU:HD21	1.92	0.52
2:H:14:PRO:HG3	2:H:84:ASN:OD1	2.10	0.52
1:L:146:VAL:HA	1:L:195:GLU:O	2.11	0.51
1:L:195:GLU:HB2	1:L:206:VAL:HG22	1.91	0.51
2:H:10:GLU:HG3	2:H:18:VAL:CG1	2.38	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.51
1:L:155:ARG:HH12	1:L:157:ASN:ND2	2.08	0.51
1:L:27(B):LEU:HD12	1:L:71:PHE:CE1	2.46	0.50
1:L:143:ASP:O	1:L:198:HIS:HD2	1.94	0.50
1:L:138:ASN:OD1	2:H:172:HIS:HE1	1.95	0.50
2:H:18:VAL:O	2:H:81:GLU:HA	2.11	0.50
2:H:133:GLN:HG2	2:H:135:ASN:N	2.27	0.50
2:H:12:LYS:HG3	2:H:13:LYS:NZ	2.25	0.50
1:L:95:PRO:O	1:L:97:THR:HG23	2.12	0.49
1:L:135:PHE:HB3	1:L:137:ASN:ND2	2.28	0.49
1:L:32:TYR:HB2	1:L:92:SER:N	2.28	0.49
1:L:55:PHE:O	1:L:58:VAL:HG13	2.13	0.49
1:L:150:ILE:HG22	1:L:153:SER:O	2.14	0.48
1:L:18:GLN:CB	1:L:74:LYS:HZ3	2.26	0.48
1:L:33:LEU:HD13	1:L:71:PHE:CD1	2.49	0.47
1:L:136:LEU:HD21	1:L:146:VAL:HG11	1.95	0.47
1:L:86:TYR:O	1:L:101:GLY:HA2	2.14	0.47
2:H:127:GLY:O	2:H:129:ALA:N	2.48	0.47
1:L:195:GLU:HG3	1:L:206:VAL:HG23	1.96	0.47
1:L:50:LYS:HG3	2:H:99:ASN:HD21	1.80	0.46
1:L:85:ILE:CD1	1:L:103:LYS:HG2	2.45	0.46
1:L:128:GLY:HA2	1:L:183:LYS:HB2	1.98	0.46
1:L:190:ASN:HA	1:L:211:ARG:HB3	1.98	0.46
2:H:38:LYS:HG3	2:H:90:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:THR:O	2:H:210:VAL:HA	2.15	0.46
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.51	0.46
1:L:27(D):HIS:HB3	1:L:28:ASN:OD1	2.16	0.45
1:L:151:ASP:HA	1:L:191:SER:OG	2.16	0.45
1:L:155:ARG:HH12	1:L:157:ASN:HB3	1.81	0.45
2:H:87:THR:HA	2:H:109:VAL:O	2.17	0.45
1:L:160:LEU:HD21	2:H:177:VAL:HB	1.98	0.44
2:H:34:VAL:HG23	2:H:52(A):ILE:HD11	1.99	0.44
2:H:17:THR:HG22	2:H:82(A):ASN:HA	1.99	0.44
2:H:13:LYS:CE	2:H:16:GLU:HB2	2.48	0.43
2:H:222:LYS:HD3	2:H:226:VAL:HG12	2.00	0.43
2:H:200:ARG:HE	2:H:200:ARG:HB3	1.44	0.43
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.60	0.43
1:L:161:ASN:OD1	1:L:175:MET:SD	2.76	0.43
2:H:39:GLU:O	2:H:88:ALA:HB1	2.18	0.43
1:L:27(D):HIS:O	1:L:29:GLY:N	2.50	0.43
1:L:120:PRO:HG2	1:L:130:ALA:HB1	2.00	0.43
1:L:144:ILE:HG23	1:L:175:MET:HE2	2.01	0.43
1:L:146:VAL:HG13	1:L:175:MET:HE3	2.01	0.42
1:L:30:ASN:HD22	1:L:31:THR:N	2.17	0.42
2:H:173:THR:HA	2:H:189:SER:HA	2.02	0.42
1:L:149:LYS:HD2	1:L:195:GLU:OE1	2.21	0.41
1:L:155:ARG:NH1	1:L:157:ASN:HB3	2.35	0.41
1:L:115:VAL:HG23	1:L:134:CYS:SG	2.60	0.41
1:L:183:LYS:O	1:L:184:ASP:C	2.64	0.41
1:L:147:LYS:HZ3	1:L:195:GLU:HG2	1.86	0.41
1:L:8:PRO:O	1:L:102:THR:HG23	2.21	0.40
1:L:193:THR:CG2	1:L:206:VAL:HG13	2.51	0.40
2:H:48:MET:HE1	2:H:80:LEU:HD11	2.03	0.40
1:L:170:ASP:O	1:L:172:THR:HG23	2.21	0.40
1:L:36:TYR:CE1	1:L:46:LEU:HD23	2.57	0.40
2:H:114:ALA:HB3	2:H:148:PHE:CG	2.56	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	214/216 (99%)	187 (87%)	24 (11%)	3 (1%)	9	30
2	H	217/219 (99%)	193 (89%)	19 (9%)	5 (2%)	5	18
All	All	431/435 (99%)	380 (88%)	43 (10%)	8 (2%)	6	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	128	SER
1	L	199	LYS
1	L	200	THR
2	H	136	SER
2	H	84	ASN
1	L	171	SER
2	H	61	ASP
2	H	199	PRO

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%)	139 (72%)	55 (28%)	0	1
2	H	188/188 (100%)	138 (73%)	50 (27%)	0	2
All	All	382/382 (100%)	277 (72%)	105 (28%)	0	1

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	9	LEU
1	L	10	SER
1	L	11	LEU

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Mol	Chain	Res	Type
1	L	13	VAL
1	L	18	GLN
1	L	22	SER
1	L	24	ARG
1	L	26	SER
1	L	30	ASN
1	L	33	LEU
1	L	39	LYS
1	L	43	SER
1	L	44	PRO
1	L	46	LEU
1	L	58	VAL
1	L	60	ASP
1	L	61	ARG
1	L	63	SER
1	L	65	SER
1	L	69	THR
1	L	74	LYS
1	L	76	SER
1	L	81	GLU
1	L	94	VAL
1	L	103	LYS
1	L	104	LEU
1	L	108	ARG
1	L	114	THR
1	L	116	SER
1	L	120	PRO
1	L	122	SER
1	L	123	GLU
1	L	136	LEU
1	L	143	ASP
1	L	147	LYS
1	L	154	GLU
1	L	156	GLN
1	L	157	ASN
1	L	168	SER
1	L	169	LYS
1	L	175	MET
1	L	176	SER
1	L	179	LEU
1	L	180	THR
1	L	181	LEU

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Mol	Chain	Res	Type
1	L	184	ASP
1	L	188	ARG
1	L	193	THR
1	L	194	CYS
1	L	199	LYS
1	L	200	THR
1	L	202	THR
1	L	203	SER
1	L	208	SER
2	H	1	GLN
2	H	3	GLN
2	H	5	VAL
2	H	13	LYS
2	H	16	GLU
2	H	18	VAL
2	H	19	LYS
2	H	23	LYS
2	H	30	THR
2	H	31	ASN
2	H	35	ASN
2	H	50	TRP
2	H	51	ILE
2	H	54	THR
2	H	60	VAL
2	H	64	LYS
2	H	71	LEU
2	H	74	SER
2	H	80	LEU
2	H	83	LYS
2	H	99	ASN
2	H	111	VAL
2	H	113	SER
2	H	115	LYS
2	H	121	VAL
2	H	133	GLN
2	H	136	SER
2	H	138	VAL
2	H	140	LEU
2	H	142	CYS
2	H	143	LEU
2	H	149	PRO
2	H	151	PRO

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Mol	Chain	Res	Type
2	H	163	SER
2	H	167	SER
2	H	175	PRO
2	H	179	GLN
2	H	188	SER
2	H	192	THR
2	H	196	SER
2	H	200	ARG
2	H	203	SER
2	H	204	GLU
2	H	205	THR
2	H	207	THR
2	H	208	CYS
2	H	210	VAL
2	H	219	VAL
2	H	222	LYS
2	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	30	ASN
1	L	93	HIS
1	L	124	GLN
1	L	137	ASN
1	L	157	ASN
1	L	161	ASN
2	H	35	ASN
2	H	52	ASN
2	H	82(B)	ASN
2	H	99	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	EOH	H	229	-	1,1,2	0.83	0	-		
3	EOH	H	230	-	2,2,2	7.89	1 (50%)	1,1,1	7.04	1 (100%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	230	EOH	O-C1	11.13	2.42	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	230	EOH	O-C1-C2	-7.04	33.16	113.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.