



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:56 PM GMT

PDB ID : 1DBA
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

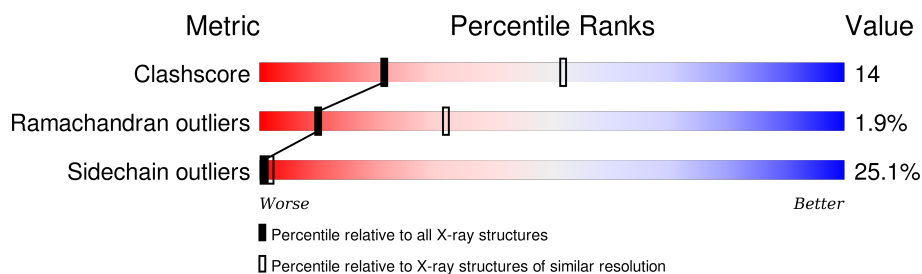
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	
2	H	219	

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			

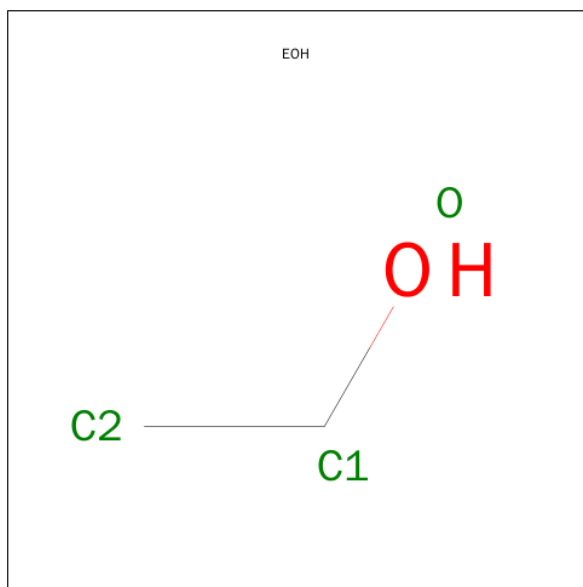
There are 14 discrepancies between the modelled and reference sequences:

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 (three-letter code: EOH) (formula: C₂H₆O).



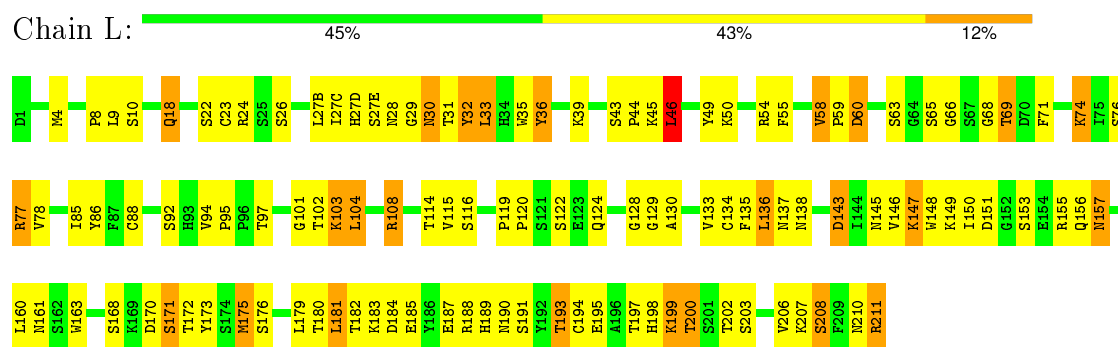
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	H	0	0
			3	2	1		
3	H	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots

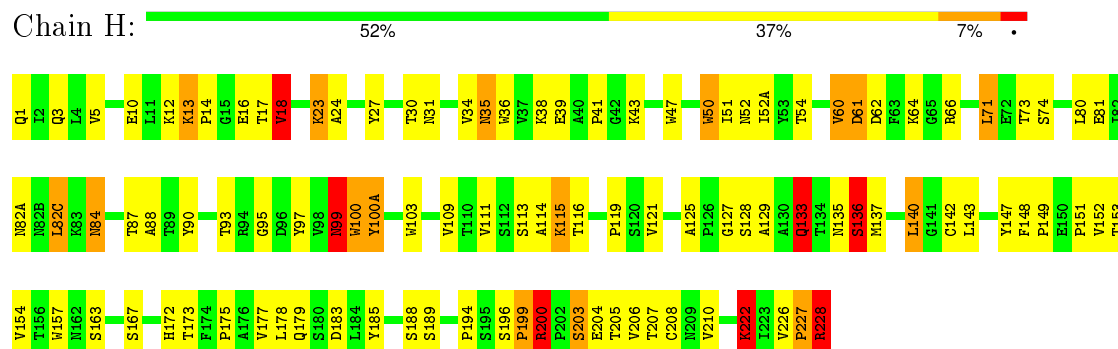
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be 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

5.1 Standard geometry

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	0.96	1/1719 (0.1%)	1.70	26/2331 (1.1%)
2	H	1.02	0/1723	1.87	43/2358 (1.8%)
All	All	0.99	1/3442 (0.0%)	1.79	69/4689 (1.5%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	163	TRP	CG-CD2	-6.11	1.33	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	200	ARG	NE-CZ-NH1	15.94	128.27	120.30
2	H	200	ARG	NE-CZ-NH2	-14.39	113.11	120.30
2	H	66	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	L	49	TYR	CB-CG-CD1	-10.15	114.91	121.00
2	H	228	ARG	N-CA-C	-9.41	85.59	111.00
2	H	222	LYS	CA-CB-CG	8.89	132.97	113.40
2	H	100	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	L	133	VAL	CG1-CB-CG2	-8.70	96.97	110.90
2	H	100(A)	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	L	77	ARG	NE-CZ-NH1	8.43	124.51	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	103	TRP	CD1-CG-CD2	8.39	113.01	106.30
2	H	36	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	L	35	TRP	CD1-CG-CD2	7.74	112.50	106.30
2	H	47	TRP	CD1-CG-CD2	7.74	112.49	106.30
2	H	47	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	H	47	TRP	CG-CD2-CE3	7.38	140.54	133.90
2	H	157	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	L	54	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	H	100	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	L	77	ARG	NE-CZ-NH2	-7.20	116.70	120.30
2	H	103	TRP	CE2-CD2-CG	-7.18	101.55	107.30
2	H	227	PRO	CA-C-N	-7.18	101.41	117.20
2	H	36	TRP	CE2-CD2-CG	-7.02	101.69	107.30
2	H	200	ARG	CG-CD-NE	-6.93	97.25	111.80
2	H	140	LEU	CA-CB-CG	6.89	131.14	115.30
1	L	163	TRP	CD1-CG-CD2	6.83	111.77	106.30
2	H	66	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	H	137	MET	CG-SD-CE	-6.77	89.37	100.20
1	L	35	TRP	CE2-CD2-CG	-6.70	101.94	107.30
2	H	152	VAL	CG1-CB-CG2	-6.63	100.28	110.90
1	L	211	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	L	148	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	L	173	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	L	148	TRP	CD1-CG-CD2	6.45	111.46	106.30
2	H	178	LEU	CA-CB-CG	-6.43	100.51	115.30
2	H	157	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	L	36	TYR	CB-CG-CD2	-6.41	117.16	121.00
2	H	18	VAL	CA-CB-CG1	-6.39	101.32	110.90
2	H	203	SER	N-CA-CB	-6.24	101.14	110.50
1	L	46	LEU	CA-CB-CG	6.12	129.38	115.30
2	H	199	PRO	CA-N-CD	-6.11	102.94	111.50
1	L	45	LYS	CA-CB-CG	-6.09	100.00	113.40
2	H	50	TRP	CE2-CD2-CG	-6.01	102.49	107.30
2	H	36	TRP	CG-CD2-CE3	6.01	139.31	133.90
2	H	93	THR	CA-CB-CG2	6.00	120.81	112.40
2	H	50	TRP	CD1-CG-CD2	5.93	111.05	106.30
1	L	104	LEU	CA-CB-CG	5.82	128.69	115.30
1	L	32	TYR	CB-CG-CD1	-5.79	117.53	121.00
2	H	47	TRP	CB-CG-CD1	-5.78	119.48	127.00
2	H	133	GLN	O-C-N	5.74	131.89	122.70
1	L	103	LYS	CA-CB-CG	5.64	125.81	113.40
1	L	77	ARG	N-CA-C	-5.55	96.00	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	THR	CA-CB-OG1	-5.54	97.36	109.00
2	H	23	LYS	CA-CB-CG	5.48	125.46	113.40
1	L	148	TRP	CG-CD2-CE3	5.46	138.81	133.90
1	L	69	THR	CA-CB-OG1	-5.42	97.61	109.00
2	H	194	PRO	CA-N-CD	-5.41	103.93	111.50
2	H	100(A)	TYR	CB-CG-CD1	5.40	124.24	121.00
2	H	36	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	L	69	THR	CA-CB-CG2	5.25	119.76	112.40
2	H	103	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	H	185	TYR	CB-CG-CD1	-5.21	117.87	121.00
2	H	60	VAL	CG1-CB-CG2	-5.19	102.59	110.90
1	L	163	TRP	CE2-CD2-CE3	5.18	124.92	118.70
2	H	99	ASN	N-CA-C	5.10	124.77	111.00
1	L	78	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	L	60	ASP	N-CA-C	5.02	124.56	111.00
1	L	163	TRP	CE2-CD2-CG	-5.01	103.29	107.30
2	H	60	VAL	CA-CB-CG2	-5.00	103.39	110.90

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	Mainchain,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	58	0
2	H	1675	0	1633	40	0
3	H	5	1	4	1	0
All	All	3359	1	3262	94	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 14.

All (94) 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
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
1:L:18:GLN:HB2	1:L:74:LYS:HZ3	1.63	0.62
2:H:16:GLU:O	2:H:82(C):LEU:HB2	1.99	0.62
2:H:125:ALA:H	2:H:228:ARG:HH12	1.49	0.60
2:H:12:LYS:HG3	2:H:13:LYS:HZ3	1.66	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: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
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:181:LEU:HD23	1:L:185:GLU:HB3	1.89	0.55
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.71	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
2:H:125:ALA:H	2:H:228:ARG:NH1	2.05	0.53
1:L:27(C):ILE:HD13	1:L:68:GLY:HA2	1.90	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
2:H:10:GLU:HG3	2:H:18:VAL:CG1	2.38	0.51
1:L:195:GLU:HB2	1:L:206:VAL:HG22	1.91	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:18:VAL:O	2:H:81:GLU:HA	2.11	0.50
1:L:138:ASN:OD1	2:H:172:HIS:HE1	1.95	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
2:H:100:TRP:HE3	3:H:230:EOH:HO	1.61	0.48
1:L:150:ILE:HG22	1:L:153:SER:O	2.14	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
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:155:ARG:HH12	1:L:157:ASN:HB3	1.81	0.45
1:L:151:ASP:HA	1:L:191:SER:OG	2.16	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
1:L:4:MET:HE2	1:L:88:CYS:SG	2.57	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:HB3	2:H:200:ARG:HE	1.44	0.43
1:L:161:ASN:OD1	1:L:175:MET:SD	2.76	0.43
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:VAL:HG22	1:L:175:MET:HE3	2.03	0.41
1:L:115:VAL:HG23	1:L:134:CYS:SG	2.60	0.41
1:L:147:LYS:HZ3	1:L:195:GLU:HG2	1.86	0.41
1:L:193:THR:CG2	1:L:206:VAL:HG13	2.51	0.40
1:L:8:PRO:O	1:L:102:THR:HG23	2.21	0.40
1:L:170:ASP:O	1:L:172:THR:HG23	2.21	0.40
2:H:114:ALA:HB3	2:H:148:PHE:CG	2.56	0.40
1:L:36:TYR:CE1	1:L:46:LEU:HD23	2.57	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%)	14	42
2	H	217/219 (99%)	193 (89%)	19 (9%)	5 (2%)	8	26
All	All	431/435 (99%)	380 (88%)	43 (10%)	8 (2%)	10	32

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	146 (75%)	48 (25%)	1	2
2	H	188/188 (100%)	140 (74%)	48 (26%)	1	2
All	All	382/382 (100%)	286 (75%)	96 (25%)	1	2

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LEU
1	L	10	SER
1	L	18	GLN
1	L	22	SER
1	L	23	CYS
1	L	24	ARG
1	L	26	SER
1	L	27(E)	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	63	SER
1	L	65	SER
1	L	69	THR
1	L	74	LYS
1	L	76	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	77	ARG
1	L	94	VAL
1	L	104	LEU
1	L	108	ARG
1	L	114	THR
1	L	116	SER
1	L	122	SER
1	L	136	LEU
1	L	143	ASP
1	L	147	LYS
1	L	156	GLN
1	L	157	ASN
1	L	168	SER
1	L	175	MET
1	L	176	SER
1	L	179	LEU
1	L	180	THR
1	L	181	LEU
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	18	VAL
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	61	ASP
2	H	62	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	64	LYS
2	H	71	LEU
2	H	74	SER
2	H	80	LEU
2	H	82(C)	LEU
2	H	99	ASN
2	H	100(A)	TYR
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	140	LEU
2	H	142	CYS
2	H	143	LEU
2	H	149	PRO
2	H	151	PRO
2	H	163	SER
2	H	167	SER
2	H	175	PRO
2	H	179	GLN
2	H	183	ASP
2	H	188	SER
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	222	LYS
2	H	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	30	ASN
1	L	157	ASN
1	L	161	ASN
2	H	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	52	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	0,1,2	0.00	-	0,0,1	0.00	-
3	EOH	H	230	-	2,2,2	6.84	1 (50%)	1,1,1	6.40	1 (100%)

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	EOH	H	229	-	-	0/0/0/0	0/0/0/0
3	EOH	H	230	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	230	EOH	O-C1	9.64	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	-6.40	33.16	114.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	230	EOH	1	0

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.