



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:05 AM UTC

PDB ID : 2AJZ / pdb_00002ajz
Title : Crystal Structure of Cocaine catalytic Antibody 7A1 Fab' in Complex with ecgonine methyl ester
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2005-08-02
Resolution : 2.30 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

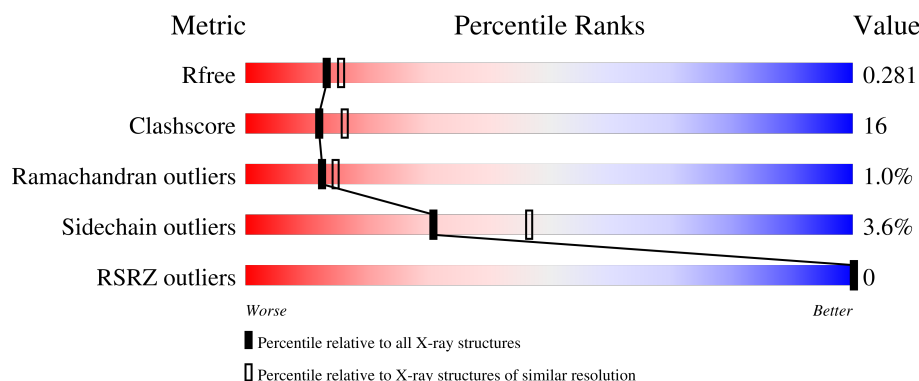
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

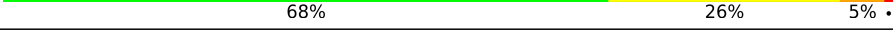
The reported resolution of this entry is 2.30 Å.

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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	216	 69% 29% 2%
1	L	216	 64% 32% 4%
2	B	219	 64% 34% 2%
2	H	219	 68% 26% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7037 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.

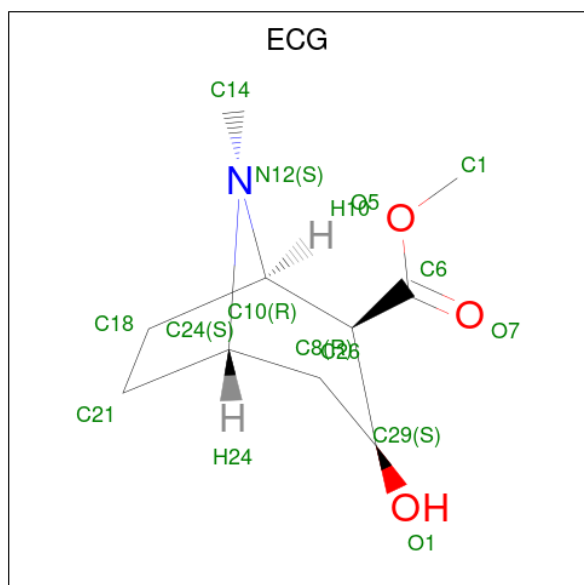
- Molecule 1 is a protein called Antibody 7A1 Fab'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1692	1056	285	345	6			
1	A	216	Total	C	N	O	S	0	0	0
			1692	1056	285	345	6			

- Molecule 2 is a protein called Antibody 7A1 Fab'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1681	1069	274	332	6			
2	B	219	Total	C	N	O	S	0	0	0
			1681	1069	274	332	6			

- Molecule 3 is 3-HYDROXY-8-METHYL-8-AZA-BICYCLO[3.2.1]OCTANE-2-CARBOXYLIC ACID METHYL ESTER (CCD ID: ECG) (formula: C₁₀H₁₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			14	10	1	3		
3	A	1	Total	C	N	O	0	0
			14	10	1	3		

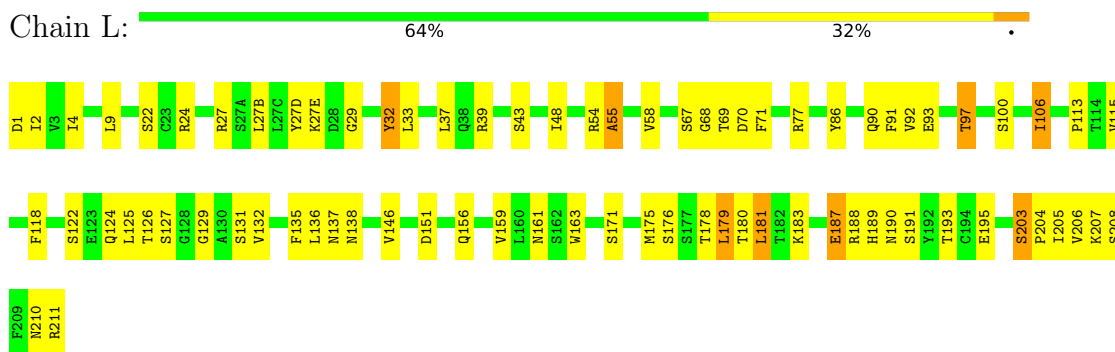
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	51	Total	O	0	0
			51	51		
4	H	74	Total	O	0	0
			74	74		
4	A	64	Total	O	0	0
			64	64		
4	B	74	Total	O	0	0
			74	74		

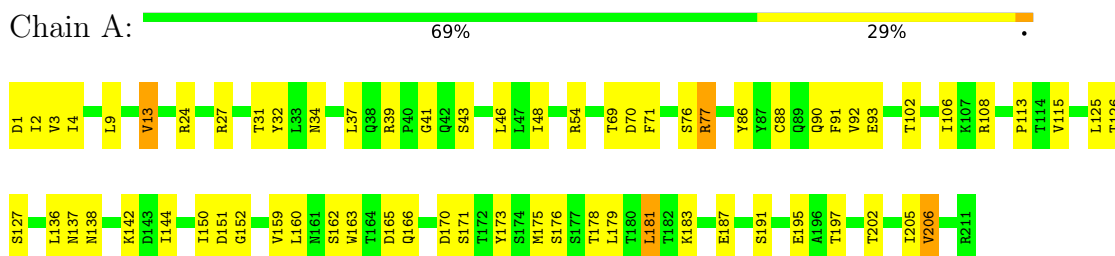
3 Residue-property plots

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 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.

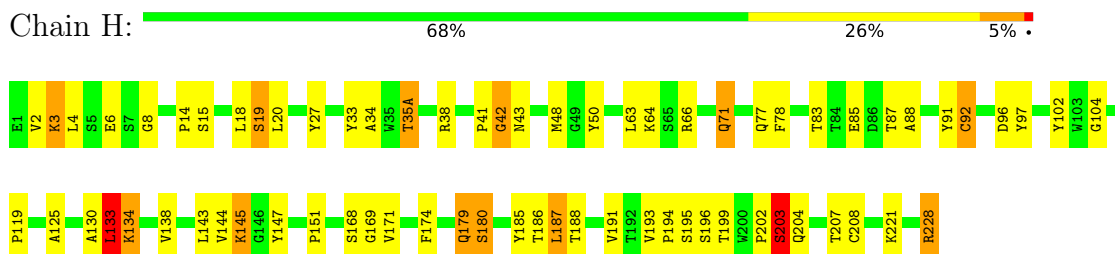
• Molecule 1: Antibody 7A1 Fab'



• Molecule 1: Antibody 7A1 Fab'

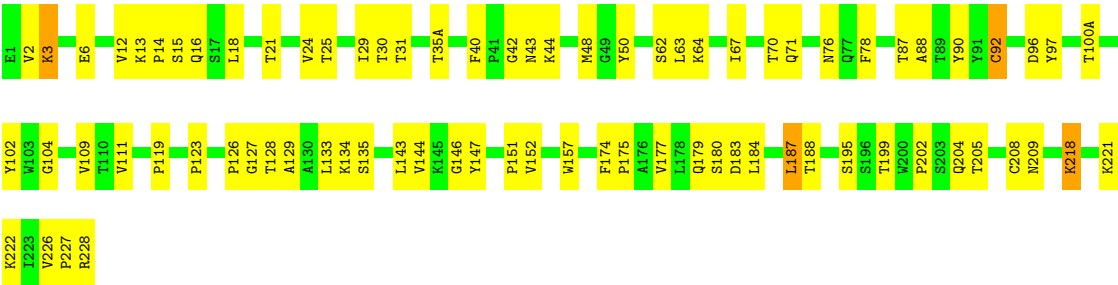


• Molecule 2: Antibody 7A1 Fab'



• Molecule 2: Antibody 7A1 Fab'





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.93Å 78.49Å 130.33Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.2 (50.00-2.30) 86.2 (50.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.285 0.237 , 0.281	Depositor DCC
R_{free} test set	2019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.148 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/1728	0.98	7/2341 (0.3%)
1	L	0.52	0/1728	1.02	12/2341 (0.5%)
2	B	0.59	0/1727	1.06	10/2367 (0.4%)
2	H	0.60	0/1727	1.07	12/2367 (0.5%)
All	All	0.56	0/6910	1.03	41/9416 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	156	GLN	OE1-CD-NE2	-9.73	112.87	122.60
2	H	71	GLN	OE1-CD-NE2	-9.51	113.09	122.60
2	H	42	GLY	N-CA-C	-8.33	103.60	114.85
2	H	64	LYS	CB-CA-C	-7.25	108.22	116.63
1	L	137	ASN	N-CA-C	6.84	121.19	110.17
2	B	42	GLY	N-CA-C	-6.73	105.31	115.00
1	L	203	SER	CA-C-N	6.72	126.96	119.90
1	L	203	SER	C-N-CA	6.72	126.96	119.90
2	B	128	THR	N-CA-C	-6.64	100.86	108.49
2	H	180	SER	N-CA-C	-6.61	104.52	112.58
1	A	115	VAL	N-CA-C	6.58	117.76	108.36
2	H	71	GLN	CG-CD-NE2	6.46	126.10	116.40
2	B	127	GLY	N-CA-C	6.45	121.03	112.77
1	L	156	GLN	CG-CD-NE2	6.43	126.04	116.40
2	B	35(A)	THR	N-CA-C	6.19	120.02	110.42
1	A	13	VAL	N-CA-C	6.19	116.80	110.05
2	B	129	ALA	N-CA-C	6.16	118.82	109.95
2	H	35(A)	THR	N-CA-C	6.01	119.46	110.14
2	H	174	PHE	CA-C-N	5.96	126.27	119.83
2	H	174	PHE	C-N-CA	5.96	126.27	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	41	PRO	N-CA-C	-5.96	101.14	110.50
1	L	97	THR	N-CA-C	5.73	118.79	110.42
2	B	43	ASN	N-CA-C	5.73	122.43	113.72
1	A	137	ASN	N-CA-C	5.69	118.96	110.14
1	A	206	VAL	N-CA-C	5.62	115.96	107.80
2	B	92	CYS	N-CA-C	-5.59	100.77	109.72
1	L	32	TYR	N-CA-C	5.45	118.26	108.17
2	B	174	PHE	CA-C-N	5.37	125.38	119.90
2	B	174	PHE	C-N-CA	5.37	125.38	119.90
1	A	43	SER	CA-C-N	-5.28	115.13	120.31
1	A	43	SER	C-N-CA	-5.28	115.13	120.31
1	L	115	VAL	N-CA-C	5.18	116.75	108.87
2	H	145	LYS	N-CA-C	5.12	117.76	109.06
2	H	92	CYS	N-CA-C	-5.09	101.86	109.95
2	H	19	SER	N-CA-C	5.07	116.84	108.13
1	L	138	ASN	N-CA-C	5.05	117.33	111.02
1	L	22	SER	N-CA-C	5.05	117.71	109.59
2	B	30	THR	N-CA-C	-5.04	107.41	113.21
1	A	126	THR	N-CA-C	-5.03	107.20	113.19
1	L	171	SER	CB-CA-C	-5.02	103.50	111.48
1	L	55	ALA	N-CA-C	-5.01	103.87	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1692	0	1629	43	0
1	L	1692	0	1629	55	0
2	B	1681	0	1654	57	0
2	H	1681	0	1654	59	0
3	A	14	0	17	2	0
3	L	14	0	17	3	0
4	A	64	0	0	1	0
4	B	74	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	74	0	0	6	0
4	L	51	0	0	3	0
All	All	7037	0	6600	208	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 16.

All (208) 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:119:PRO:HB3	2:B:147:TYR:HB3	1.45	0.96
2:B:3:LYS:NZ	2:B:3:LYS:HB3	1.83	0.92
2:B:126:PRO:O	2:B:228:ARG:HG3	1.76	0.85
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.59	0.85
1:L:4:ILE:HD11	1:L:90:GLN:HB3	1.61	0.81
2:H:133:LEU:H	2:H:133:LEU:HD23	1.52	0.74
2:B:3:LYS:HB3	2:B:3:LYS:HZ3	1.51	0.74
1:L:181:LEU:HD12	1:L:181:LEU:N	2.03	0.73
2:B:70:THR:HB	4:B:240:HOH:O	1.88	0.73
1:A:183:LYS:O	1:A:187:GLU:HG2	1.89	0.73
2:H:63:LEU:O	2:H:66:ARG:HG2	1.91	0.71
2:H:125:ALA:HB3	2:H:228:ARG:HD2	1.73	0.70
2:B:199:THR:O	2:B:204:GLN:HB2	1.92	0.70
1:L:55:ALA:HB3	1:L:58:VAL:HG21	1.73	0.70
1:L:2:ILE:HG12	1:L:27:ARG:HD3	1.72	0.69
2:H:134:LYS:HD2	2:H:195:SER:HB3	1.73	0.69
2:B:134:LYS:HE2	2:B:135:SER:H	1.56	0.69
1:L:93:GLU:HA	3:L:301:ECG:H13	1.75	0.68
2:H:2:VAL:HB	2:H:102:TYR:CE1	2.29	0.67
2:B:13:LYS:HB2	2:B:16:GLN:NE2	2.10	0.66
1:L:183:LYS:O	1:L:187:GLU:HG2	1.96	0.66
1:L:179:LEU:HD22	1:L:181:LEU:HD11	1.78	0.65
2:B:18:LEU:HD13	2:B:109:VAL:HG11	1.77	0.65
1:A:4:ILE:HD11	1:A:90:GLN:HB3	1.79	0.65
3:A:302:ECG:H212	2:B:97:TYR:CZ	2.31	0.65
2:B:187:LEU:C	2:B:187:LEU:HD23	2.22	0.65
1:L:118:PHE:HD2	2:H:125:ALA:O	1.80	0.64
1:L:122:SER:O	1:L:126:THR:HG23	1.97	0.64
1:L:113:PRO:HG2	1:L:205:ILE:HD12	1.77	0.64
1:L:146:VAL:HG11	1:L:175:MET:HE1	1.81	0.63
2:H:35(A):THR:HG21	4:H:229:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ARG:HG3	1:L:69:THR:O	1.99	0.62
1:A:24:ARG:HD3	1:A:70:ASP:OD1	2.00	0.62
2:B:119:PRO:CB	2:B:147:TYR:HB3	2.24	0.62
3:A:302:ECG:H261	2:B:97:TYR:O	2.00	0.61
1:L:179:LEU:HD22	1:L:181:LEU:CD1	2.32	0.60
2:B:143:LEU:HD13	2:B:188:THR:HG22	1.83	0.60
2:H:204:GLN:NE2	4:H:290:HOH:O	2.35	0.59
1:L:180:THR:C	1:L:181:LEU:HD12	2.28	0.59
2:H:171:VAL:HG22	2:H:191:VAL:HG23	1.82	0.59
1:L:146:VAL:CG1	1:L:175:MET:HE1	2.33	0.58
2:B:134:LYS:CE	2:B:195:SER:HB2	2.32	0.58
1:A:175:MET:HG2	1:A:176:SER:H	1.69	0.58
1:L:151:ASP:HA	1:L:191:SER:HB3	1.84	0.57
1:A:175:MET:HG2	1:A:176:SER:N	2.18	0.57
2:B:202:PRO:HG3	2:B:227:PRO:HG2	1.87	0.57
2:B:50:TYR:C	2:B:50:TYR:CD1	2.82	0.57
2:B:144:VAL:HB	2:B:187:LEU:HD22	1.87	0.57
1:A:34:ASN:O	1:A:88:CYS:HA	2.05	0.57
2:B:3:LYS:HB3	2:B:3:LYS:HZ2	1.65	0.57
2:B:134:LYS:HE3	2:B:195:SER:HB2	1.86	0.57
2:H:50:TYR:C	2:H:50:TYR:CD1	2.83	0.56
2:B:48:MET:HE1	2:B:90:TYR:HE2	1.70	0.56
3:L:301:ECG:H212	2:H:97:TYR:CZ	2.40	0.56
2:B:6:GLU:HG3	2:B:92:CYS:SG	2.46	0.56
2:H:83:THR:OG1	2:H:85:GLU:HB2	2.05	0.56
1:A:163:TRP:NE1	1:A:175:MET:HE2	2.21	0.56
1:L:24:ARG:HD3	1:L:70:ASP:OD1	2.06	0.56
1:L:135:PHE:C	1:L:136:LEU:HD12	2.31	0.56
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.05	0.55
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.42	0.55
2:H:133:LEU:HD23	2:H:133:LEU:N	2.18	0.55
2:H:2:VAL:HB	2:H:102:TYR:CD1	2.43	0.54
1:A:160:LEU:HD13	2:B:177:VAL:HG11	1.90	0.54
1:L:131:SER:OG	1:L:180:THR:HG22	2.06	0.54
2:H:207:THR:HG23	2:H:221:LYS:C	2.33	0.54
2:H:96:ASP:HB2	4:H:278:HOH:O	2.07	0.54
2:H:169:GLY:O	2:H:191:VAL:HA	2.08	0.54
2:H:87:THR:O	2:H:88:ALA:HB2	2.06	0.54
2:H:133:LEU:H	2:H:133:LEU:CD2	2.20	0.54
2:H:179:GLN:O	2:H:180:SER:HB2	2.07	0.54
1:L:39:ARG:HD2	4:L:315:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:THR:HG22	2:H:208:CYS:N	2.23	0.54
2:H:3:LYS:HZ3	2:H:3:LYS:HB3	1.74	0.53
2:H:194:PRO:HB2	2:H:199:THR:HG23	1.91	0.53
2:H:187:LEU:C	2:H:187:LEU:HD23	2.33	0.53
2:B:29:ILE:C	2:B:31:THR:H	2.15	0.53
2:H:138:VAL:HG12	2:H:193:VAL:O	2.08	0.53
1:A:163:TRP:HE1	1:A:175:MET:HE2	1.74	0.53
2:B:146:GLY:HA2	2:B:184:LEU:HB3	1.91	0.53
1:L:92:VAL:HG23	1:L:93:GLU:HG2	1.91	0.52
1:A:46:LEU:HD22	2:B:100(A):THR:H	1.74	0.52
1:A:2:ILE:HG13	1:A:93:GLU:OE2	2.08	0.52
1:L:178:THR:HG22	1:L:180:THR:HG23	1.91	0.52
1:L:124:GLN:O	1:L:127:SER:HB2	2.10	0.52
1:L:188:ARG:NH2	4:L:345:HOH:O	2.43	0.51
1:L:32:TYR:HB3	1:L:91:PHE:HB3	1.91	0.51
1:A:76:SER:O	1:A:77:ARG:C	2.53	0.51
2:H:168:SER:HB3	4:H:237:HOH:O	2.10	0.51
2:H:34:ALA:O	2:H:35(A):THR:HG23	2.11	0.51
1:A:144:ILE:CG2	1:A:175:MET:HE3	2.41	0.51
1:A:113:PRO:HG2	1:A:205:ILE:HD12	1.93	0.50
2:H:3:LYS:NZ	2:H:3:LYS:CB	2.74	0.50
2:H:3:LYS:NZ	4:H:286:HOH:O	2.43	0.50
2:B:2:VAL:HB	2:B:102:TYR:CE1	2.47	0.50
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.94	0.50
2:B:2:VAL:HB	2:B:102:TYR:CD1	2.47	0.50
1:L:136:LEU:HD12	1:L:136:LEU:N	2.27	0.50
1:L:181:LEU:N	1:L:181:LEU:CD1	2.73	0.49
1:A:144:ILE:HG23	1:A:175:MET:HE3	1.93	0.49
1:A:160:LEU:HD13	2:B:177:VAL:CG1	2.42	0.49
2:B:25:THR:HG23	4:B:241:HOH:O	2.12	0.49
2:H:130:ALA:HB3	4:H:287:HOH:O	2.12	0.49
1:L:125:LEU:O	1:L:183:LYS:HD2	2.13	0.49
1:L:131:SER:CB	1:L:180:THR:HG22	2.43	0.49
1:A:13:VAL:HG23	1:A:106:ILE:HD13	1.95	0.49
2:B:205:THR:HA	4:B:246:HOH:O	2.13	0.49
1:A:163:TRP:HE1	1:A:175:MET:CE	2.26	0.48
1:L:39:ARG:NE	4:L:328:HOH:O	2.46	0.48
1:L:2:ILE:CG1	1:L:27:ARG:HD3	2.42	0.48
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.78	0.48
2:H:144:VAL:HB	2:H:187:LEU:CD2	2.43	0.48
2:B:123:PRO:HD3	2:B:221:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:MET:HG2	1:L:176:SER:N	2.29	0.47
1:L:125:LEU:C	1:L:127:SER:H	2.22	0.47
2:B:179:GLN:O	2:B:180:SER:HB2	2.13	0.47
1:A:27:ARG:NH1	1:A:93:GLU:OE1	2.47	0.47
2:B:157:TRP:CZ3	2:B:208:CYS:HB3	2.49	0.47
2:H:143:LEU:HD13	2:H:188:THR:HG22	1.95	0.47
1:A:4:ILE:HD11	1:A:90:GLN:CB	2.44	0.47
1:A:31:THR:HG21	1:A:71:PHE:HE2	1.80	0.47
1:A:151:ASP:HA	1:A:191:SER:HB3	1.95	0.47
2:B:143:LEU:HD13	2:B:188:THR:CG2	2.43	0.47
1:A:136:LEU:HD12	1:A:136:LEU:N	2.30	0.47
2:B:40:PHE:HD2	2:B:44:LYS:HD3	1.79	0.47
2:H:119:PRO:CB	2:H:147:TYR:HB3	2.39	0.47
2:B:18:LEU:CD1	2:B:109:VAL:HG11	2.45	0.47
2:B:119:PRO:HB3	2:B:147:TYR:CB	2.31	0.47
2:H:228:ARG:H	2:H:228:ARG:HG2	1.37	0.47
1:A:92:VAL:HG23	1:A:93:GLU:HG2	1.97	0.46
2:B:14:PRO:O	2:B:15:SER:OG	2.23	0.46
2:H:125:ALA:HB3	2:H:228:ARG:CD	2.44	0.46
1:L:195:GLU:HG3	1:L:206:VAL:HG12	1.96	0.46
2:B:12:VAL:O	2:B:111:VAL:HA	2.16	0.46
1:A:195:GLU:HG3	1:A:206:VAL:HG12	1.97	0.46
2:B:13:LYS:HG3	4:B:239:HOH:O	2.14	0.45
1:L:124:GLN:HG2	1:L:129:GLY:O	2.15	0.45
1:A:125:LEU:C	1:A:127:SER:H	2.24	0.45
2:H:143:LEU:HD13	2:H:188:THR:CG2	2.47	0.45
2:H:3:LYS:HB3	2:H:3:LYS:NZ	2.30	0.45
2:H:34:ALA:O	2:H:35(A):THR:CG2	2.65	0.45
1:A:2:ILE:HG22	1:A:3:VAL:N	2.31	0.45
2:H:3:LYS:C	2:H:4:LEU:HD12	2.42	0.45
1:A:39:ARG:HG3	1:A:39:ARG:NH1	2.31	0.45
1:A:166:GLN:HB2	1:A:173:TYR:CE1	2.52	0.45
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.57	0.45
2:B:62:SER:C	2:B:64:LYS:H	2.25	0.45
2:H:202:PRO:O	2:H:203:SER:C	2.58	0.45
2:B:63:LEU:HD13	2:B:67:ILE:HD12	1.98	0.45
2:B:209:ASN:HB3	2:B:218:LYS:HE2	1.98	0.45
1:A:48:ILE:HD13	1:A:54:ARG:HA	1.99	0.45
1:A:32:TYR:HB3	1:A:91:PHE:HB3	2.00	0.44
2:H:71:GLN:HA	2:H:78:PHE:HA	2.00	0.44
2:B:205:THR:HB	2:B:222:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:SER:HG	2:H:91:TYR:HE1	1.66	0.44
1:L:106:ILE:HD13	1:L:106:ILE:HA	1.85	0.44
1:A:37:LEU:HD13	1:A:86:TYR:CZ	2.53	0.44
2:B:40:PHE:CD2	2:B:44:LYS:HD3	2.53	0.44
1:L:190:ASN:O	1:L:210:ASN:HA	2.18	0.43
2:H:144:VAL:HB	2:H:187:LEU:HD23	2.00	0.43
2:H:14:PRO:O	2:H:15:SER:CB	2.66	0.43
1:L:27(B):LEU:HA	1:L:92:VAL:HG11	1.99	0.43
1:A:108:ARG:HD2	1:A:171:SER:HB2	2.00	0.43
1:L:48:ILE:HD13	1:L:54:ARG:HA	1.99	0.43
1:L:193:THR:OG1	1:L:208:SER:HB3	2.18	0.43
2:H:145:LYS:HG3	2:H:186:THR:OG1	2.18	0.43
1:L:55:ALA:HB3	1:L:58:VAL:CG2	2.45	0.43
2:B:6:GLU:HA	2:B:21:THR:O	2.19	0.43
1:A:24:ARG:HG3	1:A:69:THR:O	2.19	0.43
2:B:3:LYS:O	2:B:24:VAL:HA	2.19	0.43
2:B:183:ASP:O	2:B:183:ASP:CG	2.61	0.43
2:H:38:ARG:HD3	2:H:48:MET:SD	2.58	0.43
2:H:179:GLN:O	2:H:180:SER:CB	2.67	0.43
1:L:27(D):TYR:CE2	3:L:301:ECG:H181	2.53	0.42
1:L:161:ASN:HB2	1:L:163:TRP:CH2	2.53	0.42
1:A:142:LYS:HB3	1:A:173:TYR:CE2	2.54	0.42
2:B:96:ASP:OD1	2:B:96:ASP:C	2.62	0.42
1:L:203:SER:HA	1:L:204:PRO:HD3	1.72	0.42
2:H:42:GLY:O	2:H:43:ASN:HB2	2.20	0.42
2:B:222:LYS:HE3	2:B:226:VAL:HG12	2.02	0.42
1:L:2:ILE:HG12	1:L:27:ARG:CD	2.48	0.42
1:L:189:HIS:O	1:L:211:ARG:NE	2.39	0.42
1:L:206:VAL:O	1:L:206:VAL:HG23	2.20	0.42
1:L:118:PHE:O	1:L:132:VAL:HG13	2.19	0.42
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.20	0.42
1:L:27(D):TYR:O	1:L:29:GLY:N	2.45	0.41
1:L:159:VAL:HA	1:L:178:THR:O	2.20	0.41
2:H:207:THR:HG23	2:H:221:LYS:O	2.20	0.41
2:B:87:THR:O	2:B:88:ALA:HB2	2.20	0.41
1:A:9:LEU:HD13	1:A:102:THR:HG21	2.01	0.41
1:A:150:ILE:O	1:A:151:ASP:HB2	2.19	0.41
1:A:181:LEU:HD12	1:A:181:LEU:N	2.35	0.41
2:H:18:LEU:HD12	2:H:19:SER:H	1.86	0.41
2:H:27:TYR:OH	2:H:33:TYR:HE2	2.04	0.41
2:B:29:ILE:HG12	2:B:76:ASN:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:OG	2:B:175:PRO:HD2	2.20	0.41
2:B:187:LEU:C	2:B:187:LEU:CD2	2.92	0.41
2:H:130:ALA:HB1	2:H:133:LEU:HD23	2.03	0.41
2:H:202:PRO:O	2:H:203:SER:O	2.38	0.41
1:A:41:GLY:N	4:A:316:HOH:O	2.52	0.41
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.56	0.41
1:L:193:THR:HG23	1:L:207:LYS:O	2.20	0.41
1:L:67:SER:OG	1:L:68:GLY:N	2.51	0.41
2:H:147:TYR:CZ	2:H:185:TYR:HB3	2.55	0.41
2:H:187:LEU:HD23	2:H:187:LEU:O	2.21	0.41
1:A:159:VAL:HA	1:A:178:THR:O	2.21	0.41
1:A:108:ARG:HD2	1:A:170:ASP:O	2.21	0.40
2:B:71:GLN:HA	2:B:78:PHE:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/216 (99%)	203 (95%)	8 (4%)	3 (1%)	9	9
1	L	214/216 (99%)	202 (94%)	11 (5%)	1 (0%)	24	31
2	B	217/219 (99%)	201 (93%)	15 (7%)	1 (0%)	24	31
2	H	217/219 (99%)	201 (93%)	12 (6%)	4 (2%)	6	6
All	All	862/870 (99%)	807 (94%)	46 (5%)	9 (1%)	12	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	133	LEU
2	B	133	LEU

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Mol	Chain	Res	Type
2	H	203	SER
2	H	134	LYS
1	A	77	ARG
1	L	27(E)	LYS
1	A	138	ASN
2	H	179	GLN
1	A	152	GLY

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	A	195/195 (100%)	189 (97%)	6 (3%)	35	52
1	L	195/195 (100%)	186 (95%)	9 (5%)	24	36
2	B	195/195 (100%)	190 (97%)	5 (3%)	40	59
2	H	195/195 (100%)	187 (96%)	8 (4%)	27	41
All	All	780/780 (100%)	752 (96%)	28 (4%)	31	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	9	LEU
1	L	77	ARG
1	L	97	THR
1	L	100	SER
1	L	106	ILE
1	L	179	LEU
1	L	181	LEU
1	L	187	GLU
2	H	3	LYS
2	H	77	GLN
2	H	133	LEU
2	H	151	PRO
2	H	187	LEU

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Mol	Chain	Res	Type
2	H	196	SER
2	H	203	SER
2	H	228	ARG
1	A	1	ASP
1	A	165	ASP
1	A	179	LEU
1	A	181	LEU
1	A	197	THR
1	A	202	THR
2	B	3	LYS
2	B	151	PRO
2	B	152	VAL
2	B	187	LEU
2	B	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	45	GLN
1	L	89	GLN
1	L	137	ASN
1	L	138	ASN
1	L	145	ASN
1	L	157	ASN
2	H	71	GLN
2	H	77	GLN
2	H	82(A)	ASN
2	H	179	GLN
1	A	190	ASN
2	B	16	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 [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	ECG	A	302	-	15,15,15	2.52	7 (46%)	20,22,22	1.71	5 (25%)
3	ECG	L	301	-	15,15,15	2.67	7 (46%)	20,22,22	1.73	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ECG	A	302	-	-	0/6/31/31	0/3/2/2
3	ECG	L	301	-	-	0/6/31/31	0/3/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	301	ECG	C8-C29	5.82	1.63	1.54
3	A	302	ECG	C8-C29	5.44	1.62	1.54
3	L	301	ECG	C8-C10	4.00	1.59	1.54
3	A	302	ECG	C8-C10	3.95	1.59	1.54
3	L	301	ECG	C26-C29	3.55	1.59	1.52
3	L	301	ECG	C8-C6	3.31	1.56	1.51
3	L	301	ECG	C14-N12	3.17	1.51	1.47
3	A	302	ECG	C14-N12	3.11	1.51	1.47
3	A	302	ECG	C26-C29	3.07	1.58	1.52
3	A	302	ECG	C8-C6	3.02	1.56	1.51
3	A	302	ECG	O5-C6	2.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	301	ECG	C26-C24	2.86	1.58	1.53
3	L	301	ECG	O5-C6	2.85	1.40	1.33
3	A	302	ECG	C26-C24	2.77	1.58	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	ECG	C24-N12-C10	3.74	104.49	101.14
3	A	302	ECG	C29-C8-C6	3.54	115.92	109.30
3	L	301	ECG	C18-C10-N12	-3.49	101.58	105.18
3	A	302	ECG	C24-N12-C10	3.45	104.24	101.14
3	A	302	ECG	C18-C10-N12	-3.32	101.76	105.18
3	L	301	ECG	C29-C8-C6	3.23	115.33	109.30
3	A	302	ECG	O7-C6-C8	-2.32	120.70	125.01
3	A	302	ECG	C10-C8-C6	-2.29	104.79	112.04
3	L	301	ECG	O7-C6-C8	-2.14	121.04	125.01
3	L	301	ECG	C10-C8-C6	-2.11	105.35	112.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	ECG	2	0
3	L	301	ECG	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/216 (100%)	-1.48	0 100 100	22, 36, 48, 64	0
1	L	216/216 (100%)	-1.48	0 100 100	21, 39, 51, 57	0
2	B	219/219 (100%)	-1.45	0 100 100	15, 32, 51, 71	0
2	H	219/219 (100%)	-1.45	0 100 100	18, 33, 55, 77	0
All	All	870/870 (100%)	-1.47	0 100 100	15, 35, 51, 77	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ECG	L	301	14/14	0.99	0.04	58,59,60,61	0
3	ECG	A	302	14/14	0.99	0.05	57,59,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.