



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:58 PM UTC

PDB ID : 1OSP / pdb_00001osp
Title : CRYSTAL STRUCTURE OF OUTER SURFACE PROTEIN A OF BORRELIA BURGDORFERI COMPLEXED WITH A MURINE MONOCLONAL ANTIBODY FAB
Authors : Li, H.; Lawson, C.L.
Deposited on : 1996-11-23
Resolution : 1.95 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
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

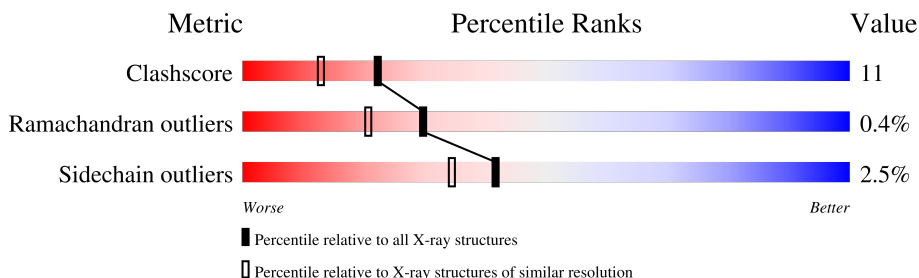
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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	214	 73% 25% •
2	H	218	 67% 28% 5%
3	O	257	 82% 15% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7418 atoms, of which 1881 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 FAB 184.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	29	0	0
			2057	1036	392	278	344	7			

- Molecule 2 is a protein called FAB 184.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	218	Total	C	H	N	O	S	49	0	0
			2015	1048	364	264	332	7			

- Molecule 3 is a protein called OUTER SURFACE PROTEIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	O	251	Total	C	H	N	O	S	0	0	0
			2362	1170	469	313	408	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	ALA	CYS	conflict	UNP P14013
O	39	LYS	ASN	variant	UNP P14013
O	84	CYS	SER	engineered mutation	UNP P14013
O	149	GLY	GLU	variant	UNP P14013
O	164	GLY	SER	variant	UNP P14013

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	119	Total	H	O	0	0
			357	238	119		
4	H	99	Total	H	O	0	0
			297	198	99		

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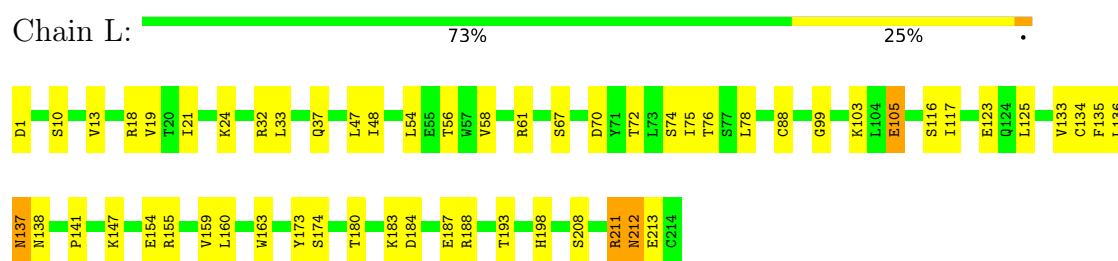
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	110	Total 330	H 220	O 110	0	0

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.

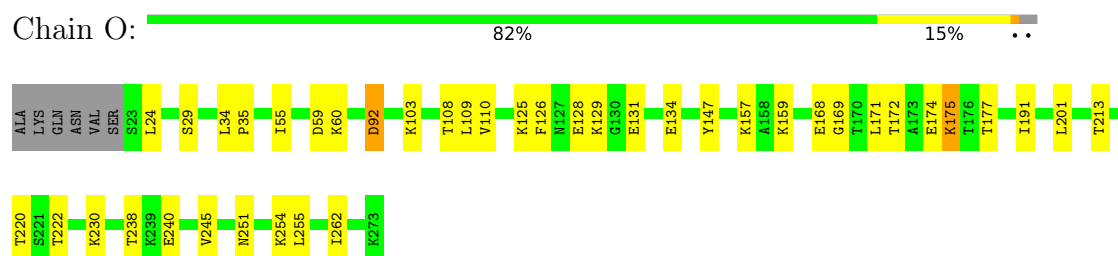
• Molecule 1: FAB 184.1



• Molecule 2: FAB 184.1



• Molecule 3: OUTER SURFACE PROTEIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.10Å 91.70Å 100.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.95)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.229 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7418	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.90	3/1704 (0.2%)	1.06	10/2315 (0.4%)
2	H	0.65	1/1698 (0.1%)	1.13	14/2323 (0.6%)
3	O	0.45	0/1902	0.87	4/2550 (0.2%)
All	All	0.68	4/5304 (0.1%)	1.02	28/7188 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	213	GLU	C-N	24.39	1.67	1.33
2	H	133	PRO	C-N	17.63	1.59	1.33
1	L	211	ARG	C-N	-16.00	1.15	1.33
1	L	212	ASN	C-N	-11.08	1.15	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	PRO	O-C-N	22.15	149.87	122.85
1	L	211	ARG	O-C-N	-13.19	105.24	122.39
1	L	58	VAL	N-CA-C	7.76	116.55	108.95
2	H	150	LYS	N-CA-C	7.64	121.94	109.72
3	O	110	VAL	N-CA-C	-7.58	105.76	111.90
1	L	56	THR	N-CA-C	7.48	120.32	111.71
1	L	212	ASN	O-C-N	-6.78	114.25	122.65
3	O	29	SER	N-CA-C	6.72	119.07	108.79
1	L	32	ARG	N-CA-C	-6.34	101.86	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	137	ASN	N-CA-C	6.29	120.07	109.76
2	H	133	PRO	CA-C-N	-6.13	109.39	121.41
2	H	133	PRO	C-N-CA	-6.13	109.39	121.41
1	L	159	VAL	N-CA-C	5.93	116.41	108.11
2	H	8	GLY	CA-C-N	5.88	125.79	119.85
2	H	8	GLY	C-N-CA	5.88	125.79	119.85
2	H	35	ASP	N-CA-C	5.67	118.85	110.46
1	L	138	ASN	N-CA-C	5.65	118.08	111.02
2	H	199	THR	N-CA-C	5.53	118.03	110.24
2	H	127	SER	N-CA-C	-5.52	99.52	108.52
2	H	206	HIS	CA-C-N	5.40	125.47	119.32
2	H	206	HIS	C-N-CA	5.40	125.47	119.32
2	H	108	ALA	N-CA-C	5.37	118.29	111.69
2	H	111	GLY	N-CA-C	-5.27	104.56	112.89
2	H	153	PHE	N-CA-C	5.24	121.39	109.81
1	L	67	SER	N-CA-C	5.13	121.73	110.80
3	O	92	ASP	N-CA-C	5.12	117.52	111.33
1	L	99	GLY	N-CA-C	-5.03	104.75	112.85
3	O	238	THR	N-CA-C	5.02	117.16	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	211	ARG	Mainchain
1	L	212	ASN	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	1665	392	1589	33	3
2	H	1651	364	1598	54	0
3	O	1893	469	1965	22	6
4	H	99	198	0	2	1
4	L	119	238	0	2	6
4	O	110	220	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5537	1881	5152	105	8

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 11.

All (105) 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:H:170:VAL:HG22	2:H:188:VAL:HG22	1.39	1.04
3:O:159:LYS:HG2	3:O:168:GLU:HG2	1.53	0.88
1:L:18:ARG:NH2	1:L:76:THR:HG22	1.93	0.84
2:H:2:VAL:HG13	2:H:27:GLU:HB3	1.59	0.84
2:H:159:VAL:HG23	2:H:184:MET:HE1	1.60	0.82
3:O:24:LEU:HG	3:O:55:ILE:HD12	1.62	0.80
2:H:195:TRP:HZ2	2:H:218:GLU:HB2	1.52	0.74
3:O:220:THR:OG1	3:O:222:THR:HG22	1.87	0.73
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.69	0.71
1:L:13:VAL:HB	1:L:78:LEU:HD22	1.71	0.70
2:H:24:VAL:HG11	2:H:29:ILE:CG2	2.24	0.67
3:O:129:LYS:NZ	3:O:131:GLU:HB2	2.11	0.66
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.78	0.66
2:H:195:TRP:CZ2	2:H:218:GLU:HB2	2.32	0.64
3:O:174:GLU:HG3	3:O:175:LYS:HD3	1.80	0.64
2:H:24:VAL:HG11	2:H:29:ILE:HG23	1.81	0.63
2:H:3:GLN:HB2	2:H:25:THR:OG1	2.00	0.62
1:L:160:LEU:HD11	2:H:176:LEU:HB2	1.81	0.61
2:H:97:ARG:HD2	2:H:98:SER:O	2.03	0.58
1:L:18:ARG:HH12	1:L:74:SER:HB3	1.69	0.58
2:H:65:SER:HB2	2:H:82:LEU:HD11	1.85	0.58
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.86	0.57
3:O:169:GLY:HA3	3:O:177:THR:O	2.05	0.57
1:L:141:PRO:O	1:L:198:HIS:HE1	1.89	0.56
1:L:117:ILE:HG13	1:L:134:CYS:SG	2.46	0.56
1:L:193:THR:OG1	1:L:208:SER:HB3	2.05	0.55
3:O:129:LYS:HZ2	3:O:131:GLU:HB2	1.71	0.55
2:H:195:TRP:HB3	2:H:196:PRO:HD3	1.89	0.55
2:H:2:VAL:CG1	2:H:27:GLU:HB3	2.34	0.54
3:O:157:LYS:HE2	3:O:159:LYS:HE3	1.89	0.54
3:O:254:LYS:HG2	3:O:255:LEU:N	2.23	0.54
1:L:116:SER:O	1:L:134:CYS:HA	2.09	0.53
2:H:24:VAL:HG13	2:H:76:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:GLU:HG3	1:L:173:TYR:OH	2.09	0.53
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.91	0.53
2:H:161:TRP:CG	2:H:188:VAL:HG21	2.44	0.53
1:L:180:THR:HG21	2:H:150:LYS:NZ	2.24	0.52
2:H:162:ASN:O	2:H:200:VAL:HA	2.10	0.51
1:L:13:VAL:HG11	1:L:19:VAL:HG22	1.92	0.51
3:O:109:LEU:HD13	3:O:126:PHE:CZ	2.45	0.51
2:H:2:VAL:HG13	2:H:27:GLU:CB	2.37	0.51
2:H:123:THR:HG23	2:H:154:PRO:HG2	1.93	0.50
2:H:194:THR:O	2:H:198:GLN:HB2	2.12	0.50
1:L:37:GLN:HB2	1:L:47:LEU:HD12	1.94	0.49
2:H:204:VAL:O	2:H:212:THR:HA	2.12	0.49
2:H:34:TRP:CH2	2:H:97:ARG:HG3	2.47	0.49
2:H:133:PRO:HD3	2:H:145:LEU:HD23	1.93	0.49
1:L:21:ILE:O	1:L:72:THR:HA	2.12	0.49
1:L:1:ASP:HA	4:L:278:HOH:O	2.13	0.49
2:H:161:TRP:CE2	2:H:188:VAL:HG23	2.48	0.49
3:O:172:THR:OG1	3:O:174:GLU:HG2	2.13	0.48
3:O:103:LYS:HD2	3:O:108:THR:HB	1.96	0.48
1:L:123:GLU:HB2	4:L:330:HOH:O	2.13	0.47
2:H:159:VAL:CG2	2:H:184:MET:HE1	2.37	0.47
1:L:135:PHE:C	1:L:136:LEU:HD12	2.40	0.47
2:H:11:LEU:HD22	2:H:154:PRO:HG3	1.97	0.46
2:H:86:VAL:HG23	2:H:88:GLU:H	1.80	0.46
2:H:12:VAL:O	2:H:118:VAL:HA	2.15	0.46
2:H:60:ASN:HB3	2:H:63:LEU:HG	1.97	0.46
2:H:156:SER:HA	4:H:262:HOH:O	2.16	0.46
1:L:24:LYS:HG2	1:L:70:ASP:CG	2.41	0.46
2:H:112:GLU:HG2	2:H:113:GLY:N	2.30	0.46
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.98	0.46
1:L:137:ASN:HD22	1:L:174:SER:HB3	1.81	0.46
3:O:129:LYS:HZ1	3:O:131:GLU:HB2	1.81	0.45
1:L:125:LEU:O	1:L:183:LYS:HD2	2.16	0.45
2:H:161:TRP:CD2	2:H:188:VAL:HG21	2.52	0.45
3:O:125:LYS:HB3	3:O:134:GLU:HB2	1.98	0.45
2:H:38:ARG:HD3	2:H:46:GLU:OE1	2.16	0.45
3:O:201:LEU:HD23	3:O:201:LEU:C	2.42	0.45
3:O:175:LYS:HB2	3:O:191:ILE:O	2.17	0.45
1:L:48:ILE:HG12	1:L:54:LEU:HD23	1.99	0.45
2:H:155:GLU:O	2:H:156:SER:HB2	2.17	0.45
1:L:18:ARG:NH1	1:L:18:ARG:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:240:GLU:HA	4:O:366:HOH:O	2.17	0.44
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.98	0.44
2:H:82:LEU:HG	2:H:85:VAL:HG12	1.99	0.44
2:H:16:GLN:O	2:H:85:VAL:HG22	2.18	0.44
2:H:184:MET:HG2	2:H:185:SER:N	2.33	0.43
1:L:183:LYS:O	1:L:187:GLU:HG3	2.18	0.43
2:H:133:PRO:HG3	4:H:281:HOH:O	2.18	0.43
1:L:18:ARG:HG3	1:L:18:ARG:HH11	1.83	0.43
2:H:153:PHE:O	2:H:154:PRO:C	2.58	0.43
2:H:153:PHE:O	2:H:182:TYR:CD2	2.72	0.43
2:H:99:ARG:NH2	3:O:92:ASP:OD2	2.51	0.43
2:H:171:HIS:O	2:H:186:SER:HA	2.19	0.43
1:L:10:SER:HA	1:L:103:LYS:O	2.19	0.43
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.19	0.43
3:O:34:LEU:HB3	3:O:35:PRO:HD2	2.01	0.42
2:H:12:VAL:HG13	2:H:118:VAL:HG22	2.01	0.42
1:L:155:ARG:HH11	1:L:155:ARG:HG3	1.84	0.42
1:L:184:ASP:O	1:L:188:ARG:HG3	2.19	0.42
3:O:59:ASP:O	3:O:60:LYS:HB2	2.19	0.42
1:L:180:THR:HG21	2:H:150:LYS:HZ3	1.84	0.42
2:H:64:LYS:NZ	2:H:86:VAL:HG21	2.35	0.42
3:O:245:VAL:HG21	3:O:262:ILE:HD11	2.02	0.42
2:H:50:TYR:CD1	2:H:50:TYR:C	2.97	0.41
2:H:153:PHE:O	2:H:182:TYR:HD2	2.04	0.41
2:H:195:TRP:CD1	2:H:195:TRP:C	2.99	0.41
1:L:147:LYS:HE3	1:L:154:GLU:CD	2.46	0.41
2:H:170:VAL:HG22	2:H:188:VAL:CG2	2.30	0.41
2:H:143:VAL:O	2:H:189:THR:HA	2.20	0.41
1:L:133:VAL:HG12	1:L:134:CYS:N	2.36	0.40
3:O:147:TYR:CD1	3:O:171:LEU:HD22	2.56	0.40
2:H:195:TRP:O	2:H:196:PRO:C	2.63	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:230:LYS:HZ3	4:L:275:HOH:H1[3_446]	0.65	0.95
3:O:254:LYS:HZ1	4:L:258:HOH:H2[3_446]	0.66	0.94
1:L:188:ARG:HH12	4:L:281:HOH:H1[4_456]	1.09	0.51
1:L:61:ARG:HH22	4:H:306:HOH:H1[4_556]	1.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:254:LYS:HZ1	4:L:258:HOH:O[3_446]	1.27	0.33
3:O:230:LYS:HZ3	4:L:275:HOH:O[3_446]	1.55	0.05
1:L:163:TRP:H	3:O:251:ASN:OD1[3_456]	1.57	0.03
3:O:254:LYS:NZ	4:L:258:HOH:O[3_446]	2.17	0.03

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	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
2	H	216/218 (99%)	204 (94%)	9 (4%)	3 (1%)	9	3
3	O	249/257 (97%)	245 (98%)	4 (2%)	0	100	100
All	All	677/689 (98%)	650 (96%)	24 (4%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	153	PHE
2	H	156	SER
2	H	195	TRP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	192/192 (100%)	191 (100%)	1 (0%)	81 82
2	H	190/190 (100%)	179 (94%)	11 (6%)	18 7
3	O	220/225 (98%)	217 (99%)	3 (1%)	59 56
All	All	602/607 (99%)	587 (98%)	15 (2%)	42 34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	105	GLU
2	H	2	VAL
2	H	4	LEU
2	H	30	THR
2	H	35	ASP
2	H	41	PRO
2	H	52	ARG
2	H	99	ARG
2	H	112	GLU
2	H	139	THR
2	H	155	GLU
2	H	184	MET
3	O	128	GLU
3	O	175	LYS
3	O	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
1	L	138	ASN
1	L	190	ASN
1	L	198	HIS
2	H	43	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	213:GLU	C	214:CYS	N	1.67
1	L	211:ARG	C	212:ASN	N	1.15
1	L	212:ASN	C	213:GLU	N	1.15

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.