



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 PM UTC

PDB ID : 1AQK / pdb_00001aqq
Title : THREE-DIMENSIONAL STRUCTURE OF A HUMAN FAB WITH HIGH AFFINITY FOR TETANUS TOXOID
Authors : Faber, C.; Fan, Z.; Edmundson, A.B.
Deposited on : 1997-07-30
Resolution : 1.84 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

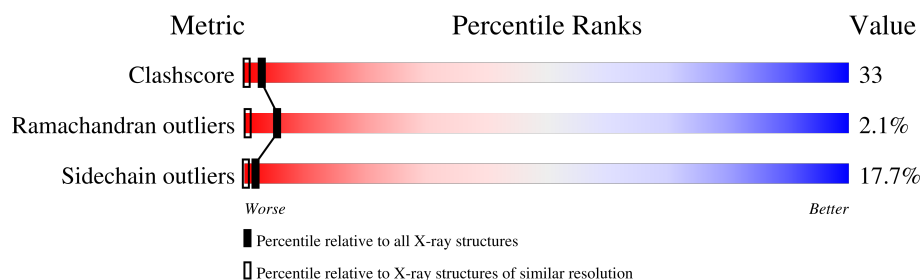
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)

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	
2	H	226	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3597 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 FAB B7-15A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1597	995	272	325	5			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	17	ARG	LYS	conflict	UNP P01842
L	18	VAL	ILE	conflict	UNP P01842
L	23	THR	SER	conflict	UNP P01842
L	25	SER	THR	conflict	UNP P01842
L	26	ASN	SER	conflict	UNP P01842
L	33	PHE	HIS	conflict	UNP P01842
L	34	THR	HIS	conflict	UNP P01842
L	40	HIS	GLN	conflict	UNP P01842
L	41	LEU	VAL	conflict	UNP P01842
L	51	PHE	TYR	conflict	UNP P01842
L	53	ASN	ASP	conflict	UNP P01842
L	54	THR	ASN	conflict	UNP P01842
L	64	PHE	ILE	conflict	UNP P01842
L	81	GLN	ARG	conflict	UNP P01842
L	93	TYR	PHE	conflict	UNP P01842
L	?	-	GLY	deletion	UNP P01842
L	99	ALA	TRP	conflict	UNP P01842
L	100	ARG	VAL	conflict	UNP P01842
L	104	GLY	ALA	conflict	UNP P01842
L	106	ARG	LYS	conflict	UNP P01842
L	160	ASN	THR	conflict	UNP P01842
L	167	LYS	THR	conflict	UNP P01842
L	213	ALA	THR	conflict	UNP P01842

- Molecule 2 is a protein called FAB B7-15A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1711	1088	289	327	7			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	30	ASN	SER	conflict	UNP P01857
H	33	ALA	GLY	conflict	UNP P01857
H	34	ILE	MET	conflict	UNP P01857
H	50	PHE	ALA	conflict	UNP P01857
H	52	SER	TRP	conflict	UNP P01857
H	57	LYS	ASN	conflict	UNP P01857
H	58	ASN	LYS	conflict	UNP P01857
H	80	PHE	TYR	conflict	UNP P01857
H	81	LEU	MET	conflict	UNP P01857
H	88	PRO	ALA	conflict	UNP P01857
H	93	ILE	VAL	conflict	UNP P01857
H	99	VAL	-	insertion	UNP P01857
H	100	LEU	-	insertion	UNP P01857
H	101	PHE	GLU	conflict	UNP P01857
H	102	GLN	GLY	conflict	UNP P01857
H	103	GLN	ARG	conflict	UNP P01857
H	104	LEU	TRP	conflict	UNP P01857
H	106	LEU	ARG	conflict	UNP P01857
H	?	-	THR	deletion	UNP P01857
H	?	-	THR	deletion	UNP P01857
H	?	-	VAL	deletion	UNP P01857
H	?	-	THR	deletion	UNP P01857
H	?	-	THR	deletion	UNP P01857
H	?	-	ILE	deletion	UNP P01857
H	?	-	GLY	deletion	UNP P01857
H	108	ALA	TYR	conflict	UNP P01857
H	109	PRO	TYR	conflict	UNP P01857
H	112	ILE	TYR	conflict	UNP P01857
H	118	MET	LEU	conflict	UNP P01857
H	158	GLN	GLU	conflict	UNP P01857
H	220	LYS	ARG	conflict	UNP P01857

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	128	Total	O	0	0
			128	128		

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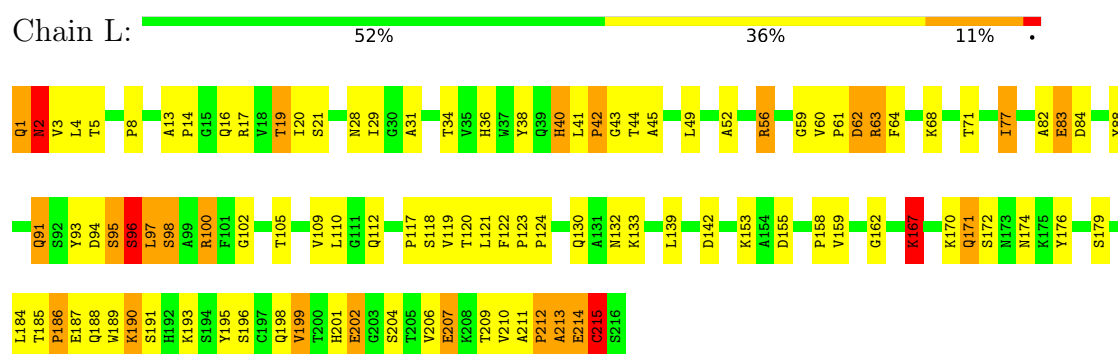
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	161	Total 161	O 161	0	0

3 Residue-property plots [i](#)

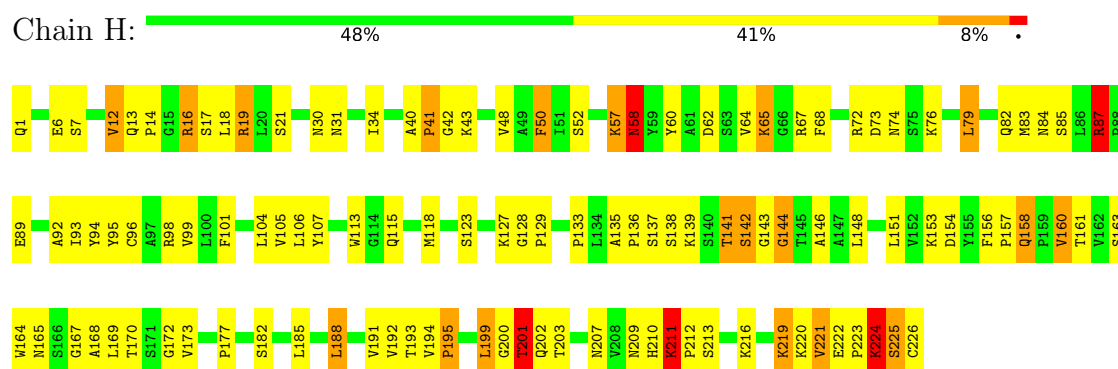
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: FAB B7-15A2



• Molecule 2: FAB B7-15A2



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	40.70 Å 78.60 Å 74.60 Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	20.00 – 1.84	Depositor
% Data completeness (in resolution range)	81.0 (20.00-1.84)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E, X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: PCA

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	1.38	3/1629 (0.2%)	1.85	36/2225 (1.6%)
2	H	1.39	3/1747 (0.2%)	1.83	32/2380 (1.3%)
All	All	1.38	6/3376 (0.2%)	1.84	68/4605 (1.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	87	ARG	CA-C	-6.21	1.46	1.52
2	H	211	LYS	CA-C	-5.30	1.47	1.52
1	L	120	THR	C-N	5.08	1.40	1.33
1	L	207	GLU	C-O	-5.08	1.18	1.23
2	H	211	LYS	CA-CB	-5.03	1.49	1.54
1	L	124	PRO	CA-C	-5.02	1.46	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	143	GLY	N-CA-C	-10.93	96.60	115.61
2	H	41	PRO	N-CA-CB	10.44	111.65	103.30
2	H	143	GLY	CA-C-N	9.92	133.82	123.30
2	H	143	GLY	C-N-CA	9.92	133.82	123.30
2	H	144	GLY	N-CA-C	-9.82	103.07	113.58
1	L	34	THR	N-CA-CB	-9.69	95.69	110.42
1	L	96	SER	N-CA-C	-8.24	105.23	114.62
2	H	41	PRO	CB-CA-C	8.05	120.33	111.56
1	L	61	PRO	CA-C-N	7.59	130.78	120.38
1	L	61	PRO	C-N-CA	7.59	130.78	120.38
1	L	167	LYS	N-CA-C	-7.33	99.39	110.39
2	H	79	LEU	N-CA-CB	7.25	122.94	111.20
1	L	59	GLY	N-CA-C	-7.05	106.04	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	105	THR	CA-C-N	-6.81	113.32	122.72
1	L	105	THR	C-N-CA	-6.81	113.32	122.72
2	H	113	TRP	CA-C-N	-6.75	115.59	122.27
2	H	113	TRP	C-N-CA	-6.75	115.59	122.27
1	L	98	SER	N-CA-C	-6.73	98.24	109.07
1	L	62	ASP	CB-CA-C	-6.62	99.42	110.68
2	H	199	LEU	CA-C-N	-6.54	108.58	121.41
2	H	199	LEU	C-N-CA	-6.54	108.58	121.41
2	H	60	TYR	N-CA-C	6.53	119.82	109.50
2	H	48	VAL	N-CA-C	6.49	117.14	111.56
1	L	179	SER	CB-CA-C	-6.34	95.49	109.56
1	L	142	ASP	N-CA-C	6.28	120.19	111.90
1	L	8	PRO	CA-C-N	-6.26	110.91	121.75
1	L	8	PRO	C-N-CA	-6.26	110.91	121.75
2	H	95	TYR	CB-CA-C	-6.11	97.30	109.33
2	H	153	LYS	N-CA-C	6.09	119.63	109.95
1	L	40	HIS	N-CA-C	6.04	119.34	108.48
2	H	67	ARG	NE-CZ-NH2	5.96	124.57	119.20
2	H	199	LEU	O-C-N	-5.89	115.86	122.75
1	L	124	PRO	CB-CA-C	-5.88	103.54	111.12
1	L	19	THR	N-CA-CB	-5.85	100.42	111.00
1	L	5	THR	N-CA-CB	-5.79	100.97	110.52
1	L	31	ALA	CA-C-N	-5.71	114.53	122.86
1	L	31	ALA	C-N-CA	-5.71	114.53	122.86
1	L	62	ASP	N-CA-CB	-5.68	101.54	110.06
2	H	93	ILE	CB-CA-C	-5.66	103.90	110.91
1	L	142	ASP	CA-CB-CG	-5.64	106.96	112.60
1	L	202	GLU	CB-CA-C	-5.62	103.44	112.09
2	H	58	ASN	CA-CB-CG	-5.62	106.98	112.60
1	L	174	ASN	CA-CB-CG	-5.56	107.04	112.60
2	H	96	CYS	N-CA-CB	5.50	119.55	110.69
2	H	129	PRO	CB-CA-C	-5.48	102.23	110.17
2	H	58	ASN	N-CA-C	5.42	116.52	108.60
1	L	45	ALA	CA-C-N	-5.38	114.08	120.11
1	L	45	ALA	C-N-CA	-5.38	114.08	120.11
2	H	177	PRO	N-CA-CB	5.33	107.99	103.35
2	H	221	VAL	N-CA-CB	5.32	118.48	111.25
1	L	212	PRO	N-CA-CB	5.29	108.03	103.27
1	L	184	LEU	CB-CA-C	-5.29	99.83	110.30
2	H	160	VAL	N-CA-C	-5.27	100.78	108.99
2	H	168	ALA	N-CA-C	5.24	117.74	111.71
2	H	201	THR	N-CA-C	-5.21	107.09	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	71	THR	CA-C-N	-5.21	114.41	122.59
1	L	71	THR	C-N-CA	-5.21	114.41	122.59
1	L	118	SER	N-CA-C	-5.18	100.80	109.24
2	H	195	PRO	N-CA-CB	5.17	107.77	103.17
1	L	186	PRO	N-CA-CB	5.16	108.64	103.48
2	H	95	TYR	CA-C-O	-5.15	115.29	121.11
2	H	133	PRO	N-CA-CB	5.12	108.12	103.15
1	L	2	ASN	CA-CB-CG	-5.10	107.50	112.60
1	L	102	GLY	N-CA-C	-5.08	104.83	112.60
2	H	93	ILE	N-CA-C	-5.08	101.27	108.58
1	L	88	TYR	CA-C-O	-5.06	114.71	120.32
1	L	117	PRO	CB-CA-C	-5.05	103.41	110.63
2	H	195	PRO	CB-CA-C	-5.04	105.15	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1597	0	1541	97	0
2	H	1711	0	1685	128	0
3	H	161	0	0	26	0
3	L	128	0	0	18	0
All	All	3597	0	3226	213	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 33.

All (213) 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:2:ASN:H	1:L:100:ARG:NH2	1.51	1.07
2:H:224:LYS:HZ2	2:H:224:LYS:N	1.52	1.06
2:H:50:PHE:HE1	2:H:57:LYS:HE2	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:PHE:HB2	2:H:105:VAL:HG11	1.47	0.96
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.13	0.96
2:H:138:SER:HA	2:H:141:THR:CG2	2.03	0.88
2:H:101:PHE:CB	2:H:105:VAL:HG11	2.03	0.87
2:H:50:PHE:CE1	2:H:57:LYS:HE2	2.11	0.85
2:H:19:ARG:HG2	2:H:19:ARG:HH11	1.41	0.85
1:L:56:ARG:HD2	3:L:289:HOH:O	1.79	0.82
2:H:224:LYS:N	2:H:224:LYS:NZ	2.30	0.80
2:H:41:PRO:HA	3:H:317:HOH:O	1.81	0.80
1:L:2:ASN:H	1:L:100:ARG:HH22	1.30	0.78
2:H:72:ARG:NE	2:H:74:ASN:HD21	1.81	0.77
1:L:41:LEU:HD23	1:L:43:GLY:H	1.49	0.77
2:H:72:ARG:HE	2:H:74:ASN:ND2	1.85	0.74
1:L:210:VAL:HG12	2:H:139:LYS:HD2	1.70	0.74
2:H:224:LYS:HZ2	2:H:224:LYS:CA	2.02	0.73
1:L:97:LEU:CD2	2:H:106:LEU:HD22	2.18	0.73
1:L:36:HIS:HD2	1:L:52:ALA:H	1.36	0.72
1:L:82:ALA:HB3	1:L:83:GLU:OE1	1.90	0.72
1:L:212:PRO:O	1:L:213:ALA:C	2.32	0.71
2:H:161:THR:HG22	3:H:344:HOH:O	1.89	0.71
2:H:57:LYS:HG2	2:H:58:ASN:N	2.04	0.71
2:H:224:LYS:H	2:H:224:LYS:CE	2.04	0.70
1:L:2:ASN:N	1:L:100:ARG:NH2	2.34	0.69
2:H:194:VAL:HB	2:H:195:PRO:HD2	1.75	0.69
1:L:13:ALA:HB1	1:L:14:PRO:HD2	1.74	0.68
1:L:36:HIS:CD2	1:L:52:ALA:H	2.10	0.68
2:H:52:SER:N	3:H:311:HOH:O	2.26	0.68
1:L:155:ASP:OD1	1:L:193:LYS:HG2	1.94	0.68
1:L:41:LEU:HD23	1:L:43:GLY:N	2.08	0.67
2:H:19:ARG:HG2	2:H:19:ARG:NH1	2.05	0.67
1:L:130:GLN:HG2	3:L:294:HOH:O	1.93	0.67
2:H:139:LYS:O	2:H:139:LYS:HG2	1.95	0.66
2:H:219:LYS:NZ	3:H:324:HOH:O	2.28	0.66
2:H:115:GLN:CD	2:H:115:GLN:H	2.04	0.66
2:H:138:SER:HA	2:H:141:THR:HG22	1.77	0.66
2:H:193:THR:HB	3:H:379:HOH:O	1.95	0.66
2:H:68:PHE:CE2	2:H:83:MET:HE3	2.30	0.65
1:L:162:GLY:HA3	3:L:271:HOH:O	1.96	0.65
2:H:173:VAL:HG22	2:H:192:VAL:HG22	1.78	0.65
2:H:137:SER:O	2:H:141:THR:N	2.28	0.65
1:L:215:CYS:N	3:L:329:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:CYS:N	3:H:335:HOH:O	2.30	0.65
2:H:19:ARG:NE	3:H:385:HOH:O	2.30	0.65
2:H:224:LYS:HZ2	2:H:224:LYS:H	1.44	0.65
1:L:121:LEU:O	2:H:139:LYS:NZ	2.30	0.65
2:H:158:GLN:NE2	3:H:271:HOH:O	2.29	0.64
2:H:224:LYS:HB2	3:H:375:HOH:O	1.98	0.64
1:L:212:PRO:O	1:L:214:GLU:N	2.31	0.64
2:H:40:ALA:C	3:H:304:HOH:O	2.40	0.64
2:H:211:LYS:HA	2:H:211:LYS:NZ	2.12	0.64
2:H:225:SER:N	3:H:375:HOH:O	2.28	0.64
2:H:87:ARG:HD3	3:H:302:HOH:O	1.96	0.64
1:L:2:ASN:HA	3:L:276:HOH:O	1.99	0.63
1:L:130:GLN:O	1:L:130:GLN:NE2	2.31	0.63
1:L:199:VAL:N	3:L:280:HOH:O	2.32	0.63
1:L:94:ASP:OD2	1:L:100:ARG:NE	2.30	0.63
1:L:13:ALA:H	1:L:16:GLN:CD	2.06	0.62
1:L:214:GLU:O	1:L:214:GLU:HG2	1.99	0.62
1:L:123:PRO:HD3	2:H:139:LYS:HZ3	1.64	0.62
2:H:224:LYS:HZ2	2:H:224:LYS:C	2.08	0.62
2:H:224:LYS:NZ	2:H:224:LYS:H	1.96	0.62
2:H:200:GLY:HA2	3:H:383:HOH:O	1.99	0.62
1:L:110:LEU:HD13	1:L:110:LEU:N	2.14	0.61
1:L:186:PRO:O	1:L:190:LYS:HG3	2.00	0.61
1:L:96:SER:HA	3:L:306:HOH:O	2.00	0.61
2:H:19:ARG:HH11	2:H:19:ARG:CG	2.12	0.60
2:H:68:PHE:CZ	2:H:83:MET:HE2	2.36	0.60
1:L:119:VAL:HG21	1:L:199:VAL:HG21	1.83	0.60
2:H:57:LYS:HB2	3:H:266:HOH:O	2.01	0.60
2:H:73:ASP:OD2	2:H:76:LYS:HD2	2.01	0.60
2:H:137:SER:O	2:H:141:THR:HB	2.02	0.60
1:L:13:ALA:HB1	1:L:14:PRO:CD	2.32	0.59
2:H:141:THR:HG23	2:H:142:SER:N	2.16	0.59
2:H:101:PHE:HB3	2:H:105:VAL:HG11	1.83	0.58
2:H:137:SER:C	2:H:141:THR:HB	2.27	0.58
2:H:148:LEU:C	2:H:148:LEU:HD12	2.29	0.58
1:L:56:ARG:HH11	1:L:62:ASP:HA	1.69	0.58
2:H:199:LEU:O	2:H:201:THR:N	2.37	0.58
1:L:97:LEU:HD22	2:H:106:LEU:HD22	1.84	0.58
2:H:92:ALA:O	2:H:118:MET:HE3	2.03	0.58
1:L:213:ALA:C	1:L:215:CYS:H	2.10	0.57
1:L:63:ARG:NH2	1:L:84:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:PHE:CE2	1:L:77:ILE:HD13	2.39	0.57
1:L:56:ARG:NH1	1:L:62:ASP:HA	2.19	0.57
1:L:122:PHE:HA	2:H:139:LYS:HZ2	1.69	0.57
1:L:82:ALA:HA	3:L:318:HOH:O	2.04	0.57
1:L:3:VAL:HG22	1:L:4:LEU:H	1.68	0.57
1:L:122:PHE:HA	2:H:139:LYS:NZ	2.19	0.57
2:H:135:ALA:HB1	2:H:136:PRO:HD2	1.86	0.57
1:L:170:LYS:HE2	1:L:176:TYR:CZ	2.40	0.56
1:L:170:LYS:HE2	1:L:176:TYR:OH	2.05	0.56
1:L:41:LEU:CD2	1:L:43:GLY:H	2.16	0.56
2:H:209:ASN:ND2	3:H:314:HOH:O	2.37	0.56
1:L:109:VAL:O	1:L:112:GLN:NE2	2.32	0.56
2:H:58:ASN:C	2:H:58:ASN:HD22	2.14	0.56
1:L:210:VAL:CG1	2:H:139:LYS:HD2	2.36	0.55
1:L:20:ILE:HA	3:L:274:HOH:O	2.06	0.55
1:L:3:VAL:HG22	1:L:4:LEU:N	2.22	0.55
2:H:13:GLN:HB3	2:H:14:PRO:HD2	1.90	0.54
2:H:57:LYS:HG2	2:H:58:ASN:H	1.71	0.54
2:H:138:SER:HA	2:H:141:THR:CB	2.37	0.54
1:L:17:ARG:NH2	3:L:328:HOH:O	2.24	0.54
1:L:42:PRO:C	1:L:44:THR:H	2.16	0.54
2:H:157:PRO:O	2:H:210:HIS:HE1	1.91	0.54
2:H:164:TRP:O	2:H:165:ASN:C	2.49	0.54
2:H:209:ASN:HD22	2:H:216:LYS:CD	2.21	0.54
1:L:158:PRO:HB3	3:L:252:HOH:O	2.08	0.54
1:L:123:PRO:HD3	2:H:139:LYS:NZ	2.23	0.53
1:L:41:LEU:HD23	1:L:41:LEU:O	2.07	0.53
1:L:21:SER:N	3:L:274:HOH:O	2.29	0.53
1:L:40:HIS:HE1	1:L:44:THR:O	1.92	0.52
1:L:63:ARG:HH22	1:L:84:ASP:CG	2.16	0.52
2:H:6:GLU:HA	2:H:21:SER:O	2.10	0.52
1:L:96:SER:O	1:L:97:LEU:HB2	2.10	0.52
2:H:19:ARG:HD3	2:H:82:GLN:OE1	2.11	0.51
2:H:50:PHE:CZ	2:H:57:LYS:HD3	2.46	0.51
2:H:138:SER:HA	2:H:141:THR:HB	1.93	0.51
2:H:146:ALA:N	2:H:194:VAL:O	2.29	0.51
1:L:41:LEU:HD23	1:L:41:LEU:C	2.36	0.51
2:H:17:SER:OG	2:H:84:ASN:ND2	2.43	0.51
2:H:211:LYS:HZ1	2:H:211:LYS:C	2.17	0.51
2:H:210:HIS:HD2	2:H:213:SER:OG	1.94	0.50
2:H:211:LYS:HB2	2:H:212:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:GLY:N	3:H:317:HOH:O	2.10	0.50
2:H:209:ASN:HD22	2:H:216:LYS:HD2	1.76	0.50
1:L:56:ARG:HD3	1:L:60:VAL:HG12	1.94	0.49
1:L:199:VAL:HG13	3:L:280:HOH:O	2.11	0.49
1:L:56:ARG:HG3	1:L:60:VAL:CG1	2.43	0.49
2:H:16:ARG:NH2	3:H:261:HOH:O	2.44	0.49
1:L:13:ALA:O	1:L:16:GLN:HG2	2.13	0.49
1:L:213:ALA:HA	3:L:329:HOH:O	2.13	0.49
1:L:214:GLU:O	1:L:215:CYS:O	2.30	0.48
1:L:187:GLU:OE1	1:L:187:GLU:N	2.44	0.48
2:H:68:PHE:CE2	2:H:83:MET:CE	2.97	0.48
1:L:211:ALA:HB3	1:L:214:GLU:OE1	2.14	0.48
2:H:83:MET:HE1	2:H:94:TYR:CZ	2.49	0.47
2:H:211:LYS:HA	2:H:211:LYS:HZ2	1.76	0.47
1:L:3:VAL:HG23	3:L:292:HOH:O	2.14	0.47
1:L:28:ASN:O	1:L:29:ILE:C	2.57	0.47
1:L:167:LYS:HD2	3:L:279:HOH:O	2.13	0.47
2:H:199:LEU:C	2:H:201:THR:H	2.22	0.47
2:H:156:PHE:HB2	2:H:185:LEU:HD23	1.96	0.47
2:H:211:LYS:HB3	2:H:211:LYS:HE3	1.43	0.47
2:H:172:GLY:HA3	3:H:379:HOH:O	2.14	0.47
2:H:209:ASN:ND2	2:H:216:LYS:HD2	2.30	0.47
1:L:40:HIS:CE1	1:L:42:PRO:HA	2.49	0.47
2:H:82:GLN:HE21	2:H:84:ASN:ND2	2.12	0.47
2:H:173:VAL:HG22	2:H:192:VAL:CG2	2.43	0.47
1:L:119:VAL:CG2	1:L:199:VAL:HG21	2.45	0.47
1:L:119:VAL:HG21	1:L:199:VAL:CG2	2.45	0.47
2:H:104:LEU:HB3	3:H:362:HOH:O	2.15	0.47
1:L:2:ASN:O	1:L:100:ARG:NH1	2.48	0.46
2:H:57:LYS:HD3	3:H:311:HOH:O	2.15	0.46
1:L:206:VAL:HG22	1:L:207:GLU:N	2.30	0.46
1:L:199:VAL:HG23	1:L:199:VAL:O	2.14	0.46
1:L:38:TYR:OH	1:L:91:GLN:NE2	2.49	0.46
2:H:68:PHE:CZ	2:H:83:MET:CE	2.98	0.46
1:L:110:LEU:HA	1:L:110:LEU:HD12	1.53	0.46
2:H:188:LEU:C	2:H:188:LEU:HD12	2.41	0.46
2:H:211:LYS:NZ	2:H:211:LYS:CA	2.77	0.46
2:H:64:VAL:O	2:H:65:LYS:C	2.57	0.45
2:H:209:ASN:ND2	2:H:216:LYS:CE	2.80	0.45
1:L:112:GLN:HB3	3:L:256:HOH:O	2.15	0.45
2:H:101:PHE:HB2	2:H:105:VAL:CG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:GLU:OE1	1:L:83:GLU:N	2.50	0.45
2:H:220:LYS:HD3	3:H:368:HOH:O	2.16	0.45
2:H:30:ASN:HB2	3:H:336:HOH:O	2.17	0.44
2:H:142:SER:C	2:H:144:GLY:H	2.06	0.44
1:L:112:GLN:N	1:L:112:GLN:CD	2.76	0.44
1:L:198:GLN:HA	3:L:280:HOH:O	2.16	0.44
2:H:163:SER:OG	2:H:207:ASN:HB2	2.18	0.43
2:H:7:SER:HB3	3:H:316:HOH:O	2.18	0.43
1:L:19:THR:O	1:L:19:THR:HG22	2.18	0.43
2:H:167:GLY:O	2:H:170:THR:HG23	2.18	0.43
1:L:201:HIS:O	1:L:202:GLU:C	2.59	0.43
2:H:82:GLN:HE21	2:H:84:ASN:HD21	1.67	0.42
1:L:16:GLN:HG3	1:L:17:ARG:N	2.34	0.42
2:H:138:SER:HA	2:H:141:THR:HG21	1.92	0.42
2:H:199:LEU:C	2:H:201:THR:N	2.77	0.42
1:L:209:THR:HG22	1:L:210:VAL:N	2.35	0.42
1:L:195:TYR:O	1:L:209:THR:HG23	2.20	0.42
2:H:98:ARG:HG2	2:H:99:VAL:O	2.20	0.42
2:H:31:ASN:HD22	2:H:31:ASN:HA	1.66	0.42
1:L:139:LEU:CD1	2:H:191:VAL:HG21	2.50	0.42
2:H:12:VAL:HG21	2:H:18:LEU:HD22	2.01	0.42
2:H:127:LYS:NZ	2:H:128:GLY:O	2.53	0.42
1:L:63:ARG:H	1:L:63:ARG:HG3	1.63	0.41
2:H:58:ASN:C	2:H:58:ASN:ND2	2.76	0.41
1:L:132:ASN:O	1:L:133:LYS:HG2	2.20	0.41
2:H:57:LYS:C	3:H:311:HOH:O	2.62	0.41
2:H:216:LYS:HA	3:H:372:HOH:O	2.19	0.41
2:H:201:THR:O	2:H:201:THR:HG23	2.20	0.41
2:H:209:ASN:ND2	2:H:216:LYS:CD	2.84	0.41
1:L:171:GLN:HE21	1:L:171:GLN:HB2	1.64	0.41
1:L:199:VAL:HG22	1:L:206:VAL:HG13	2.03	0.41
1:L:1:PCA:HA	1:L:100:ARG:HH21	1.86	0.41
1:L:214:GLU:O	1:L:215:CYS:C	2.64	0.41
1:L:42:PRO:C	1:L:44:THR:N	2.79	0.41
2:H:115:GLN:CD	2:H:115:GLN:N	2.77	0.41
2:H:136:PRO:HG2	2:H:223:PRO:HB3	2.01	0.41
2:H:6:GLU:OE1	2:H:115:GLN:NE2	2.53	0.40
2:H:192:VAL:HG12	2:H:193:THR:N	2.35	0.40
2:H:138:SER:CA	2:H:141:THR:HB	2.52	0.40
1:L:93:TYR:CZ	2:H:107:TYR:HA	2.55	0.40
1:L:139:LEU:HD13	2:H:191:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:GLN:O	1:L:189:TRP:C	2.62	0.40
2:H:225:SER:C	3:H:335:HOH:O	2.61	0.40
2:H:173:VAL:HA	2:H:192:VAL:HG22	2.04	0.40
2:H:62:ASP:HA	2:H:65:LYS:HE3	2.04	0.40
2:H:85:SER:O	2:H:85:SER:OG	2.33	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	L	214/216 (99%)	194 (91%)	14 (6%)	6 (3%)	4	0
2	H	224/226 (99%)	208 (93%)	13 (6%)	3 (1%)	9	2
All	All	438/442 (99%)	402 (92%)	27 (6%)	9 (2%)	5	0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	213	ALA
1	L	215	CYS
1	L	97	LEU
2	H	142	SER
1	L	95	SER
1	L	2	ASN
2	H	154	ASP
2	H	224	LYS
1	L	42	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	109/177 (62%)	85 (78%)	24 (22%)	1	0
2	H	191/191 (100%)	162 (85%)	29 (15%)	3	0
All	All	300/368 (82%)	247 (82%)	53 (18%)	2	0

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	49	LEU
1	L	56	ARG
1	L	63	ARG
1	L	68	LYS
1	L	77	ILE
1	L	83	GLU
1	L	91	GLN
1	L	95	SER
1	L	96	SER
1	L	98	SER
1	L	100	ARG
1	L	153	LYS
1	L	159	VAL
1	L	167	LYS
1	L	171	GLN
1	L	172	SER
1	L	185	THR
1	L	190	LYS
1	L	191	SER
1	L	196	SER
1	L	199	VAL
1	L	204	SER
1	L	214	GLU
1	L	215	CYS
2	H	12	VAL
2	H	16	ARG
2	H	19	ARG

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Mol	Chain	Res	Type
2	H	34	ILE
2	H	43	LYS
2	H	50	PHE
2	H	57	LYS
2	H	58	ASN
2	H	65	LYS
2	H	79	LEU
2	H	87	ARG
2	H	89	GLU
2	H	123	SER
2	H	141	THR
2	H	151	LEU
2	H	158	GLN
2	H	160	VAL
2	H	169	LEU
2	H	182	SER
2	H	188	LEU
2	H	201	THR
2	H	202	GLN
2	H	203	THR
2	H	211	LYS
2	H	219	LYS
2	H	221	VAL
2	H	222	GLU
2	H	224	LYS
2	H	225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	36	HIS
1	L	91	GLN
1	L	160	ASN
1	L	171	GLN
1	L	174	ASN
1	L	192	HIS
1	L	201	HIS
2	H	3	GLN
2	H	31	ASN
2	H	58	ASN
2	H	74	ASN
2	H	77	ASN

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Mol	Chain	Res	Type
2	H	84	ASN
2	H	202	GLN
2	H	209	ASN
2	H	210	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	PCA	H	1	2	7,8,9	2.15	2 (28%)	9,10,12	1.43	2 (22%)
1	PCA	L	1	1	7,8,9	2.29	1 (14%)	9,10,12	1.12	0

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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
1	PCA	L	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	PCA	CD-N	5.78	1.48	1.34
2	H	1	PCA	CD-N	5.13	1.47	1.34
2	H	1	PCA	CA-N	-2.01	1.44	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	OE-CD-CG	-2.68	121.93	126.72
2	H	1	PCA	OE-CD-N	-2.08	120.46	124.96

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
1	L	1	PCA	1	0

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](#)

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.