



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:25 PM UTC

PDB ID : 1GHF / pdb_00001ghf
Title : ANTI-ANTI-IDIOTYPE GH1002 FAB FRAGMENT
Authors : Ban, N.; Day, J.; Wang, X.; Ferrone, S.; McPherson, A.
Deposited on : 1995-11-30
Resolution : 2.70 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

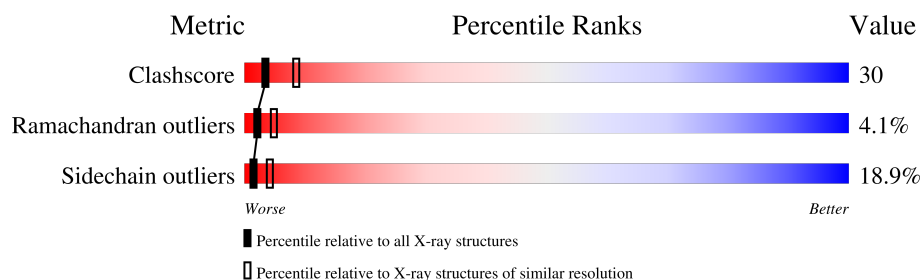
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	211	39% 43% 16% .
2	H	212	41% 41% 17% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3273 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 ANTI-ANTI-IDIOtype GH1002 FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1646	1018	278	344	6			

- Molecule 2 is a protein called ANTI-ANTI-IDIOtype GH1002 FAB FRAGMENT.

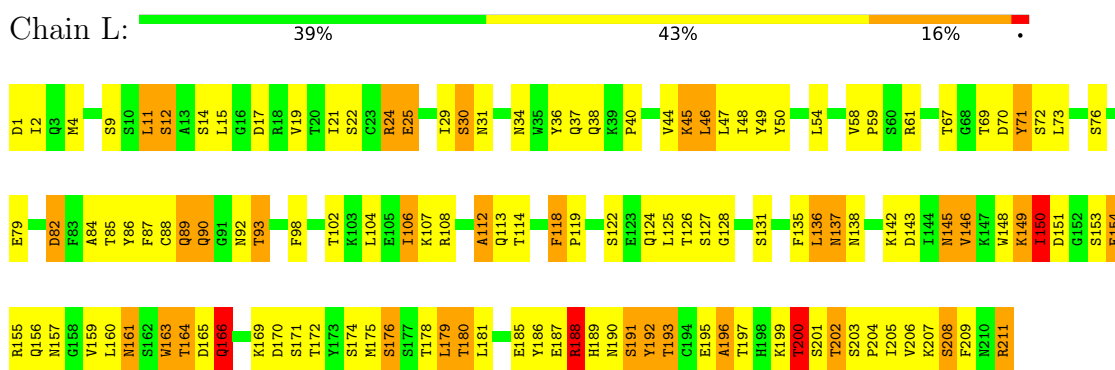
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	44	0	0
			1627	1041	263	315	8			

3 Residue-property plots

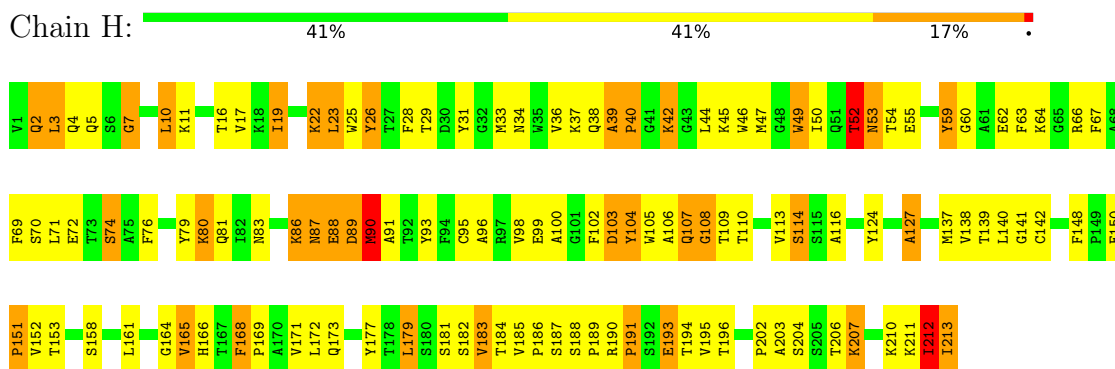
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ANTI-ANTI-IDIOTYPE GH1002 FAB FRAGMENT



• Molecule 2: ANTI-ANTI-IDIOTYPE GH1002 FAB FRAGMENT



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.40 Å 150.40 Å 43.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3273	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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	0.99	2/1679 (0.1%)	1.44	27/2276 (1.2%)
2	H	0.99	2/1673 (0.1%)	1.41	28/2283 (1.2%)
All	All	0.99	4/3352 (0.1%)	1.43	55/4559 (1.2%)

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	1
2	H	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	90	MET	SD-CE	7.04	1.97	1.79
1	L	191	SER	CA-C	6.31	1.61	1.52
1	L	190	ASN	CA-C	5.18	1.59	1.52
2	H	22	LYS	CA-C	5.00	1.58	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	118	PHE	CA-C-N	13.11	129.10	119.66
1	L	118	PHE	C-N-CA	13.11	129.10	119.66
2	H	23	LEU	N-CA-C	11.62	125.67	109.18
1	L	76	SER	N-CA-C	11.02	127.33	112.90
1	L	202	THR	N-CA-C	-10.32	101.24	114.04
2	H	39	ALA	CA-C-N	10.15	132.53	119.84
2	H	39	ALA	C-N-CA	10.15	132.53	119.84
2	H	193	GLU	N-CA-C	-9.41	98.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	192	TYR	N-CA-C	9.24	122.99	108.67
1	L	208	SER	N-CA-C	9.00	120.54	108.38
1	L	171	SER	N-CA-C	8.56	123.29	111.74
2	H	60	GLY	N-CA-C	-8.34	101.61	111.36
2	H	100	ALA	N-CA-C	-7.96	94.72	108.56
1	L	161	ASN	N-CA-C	-7.77	99.03	110.52
1	L	209	PHE	N-CA-C	-7.49	97.23	108.99
1	L	170	ASP	N-CA-C	7.47	122.52	112.88
2	H	168	PHE	N-CA-C	7.10	119.87	110.08
2	H	114	SER	N-CA-C	6.98	125.67	110.80
1	L	112	ALA	N-CA-C	-6.88	101.65	110.53
2	H	49	TRP	CB-CA-C	-6.75	97.55	110.24
1	L	137	ASN	N-CA-C	6.64	120.34	109.85
2	H	212	ILE	N-CA-C	6.63	117.42	107.80
2	H	87	ASN	N-CA-C	-6.50	103.89	110.97
2	H	124	TYR	N-CA-C	-6.48	100.36	110.14
1	L	146	VAL	N-CA-C	6.47	116.89	108.35
1	L	196	ALA	N-CA-C	6.28	119.56	107.44
2	H	89	ASP	N-CA-C	6.26	120.65	112.89
2	H	59	TYR	N-CA-C	6.25	119.66	109.59
1	L	176	SER	N-CA-C	-6.19	100.10	109.95
2	H	164	GLY	N-CA-C	-6.10	106.10	114.64
1	L	143	ASP	N-CA-C	5.89	118.25	109.59
2	H	19	ILE	CB-CA-C	-5.82	103.69	110.91
2	H	116	ALA	N-CA-C	-5.79	100.45	109.72
2	H	127	ALA	N-CA-C	5.75	114.92	108.25
1	L	73	LEU	N-CA-C	-5.68	99.93	109.07
2	H	25	TRP	N-CA-C	5.66	120.24	108.53
2	H	204	SER	N-CA-C	5.65	119.80	113.02
1	L	142	LYS	N-CA-C	5.64	118.97	111.75
2	H	153	THR	N-CA-C	-5.62	100.01	109.07
1	L	193	THR	N-CA-C	5.48	118.17	109.24
1	L	150	ILE	N-CA-C	5.32	120.40	109.34
2	H	183	VAL	N-CA-C	-5.29	100.24	108.86
1	L	114	THR	N-CA-C	-5.24	98.72	107.99
2	H	137	MET	N-CA-C	-5.23	102.32	110.42
2	H	187	SER	N-CA-C	5.21	119.12	112.34
1	L	12	SER	N-CA-C	5.21	117.13	108.02
1	L	163	TRP	N-CA-C	5.20	117.96	109.59
1	L	30	SER	CA-C-N	-5.12	114.45	122.79
1	L	30	SER	C-N-CA	-5.12	114.45	122.79
1	L	149	LYS	N-CA-C	5.10	118.33	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	108	GLY	N-CA-C	-5.10	106.26	112.68
2	H	188	SER	N-CA-C	5.09	121.05	109.81
1	L	21	ILE	CB-CA-C	-5.08	103.26	110.83
2	H	52	THR	N-CA-C	5.07	117.71	111.82
2	H	152	VAL	N-CA-C	-5.04	101.24	108.89

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	104	TYR	Sidechain
2	H	26	TYR	Sidechain
2	H	49	TRP	Mainchain
1	L	71	TYR	Sidechain

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	1646	0	1569	93	0
2	H	1627	0	1594	102	0
All	All	3273	0	3163	190	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 30.

All (190) 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:16:THR:HG22	2:H:83:ASN:HA	1.37	1.04
2:H:70:SER:HB2	2:H:79:TYR:HB2	1.39	1.02
2:H:5:GLN:NE2	2:H:95:CYS:SG	2.35	0.99
2:H:80:LYS:HZ2	2:H:80:LYS:HB3	1.28	0.94
2:H:80:LYS:HB3	2:H:80:LYS:NZ	1.85	0.89
2:H:7:GLY:HA3	2:H:109:THR:HG23	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:MET:HE1	2:H:95:CYS:HB2	1.54	0.86
1:L:148:TRP:CZ3	1:L:179:LEU:HB2	2.13	0.84
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.61	0.83
2:H:186:PRO:O	2:H:189:PRO:HD2	1.83	0.79
1:L:14:SER:O	1:L:17:ASP:HB2	1.83	0.78
2:H:138:VAL:HG12	2:H:185:VAL:O	1.83	0.77
1:L:148:TRP:O	1:L:154:GLU:HA	1.85	0.77
1:L:9:SER:O	1:L:102:THR:HA	1.88	0.74
2:H:19:ILE:HB	2:H:80:LYS:NZ	2.03	0.73
1:L:25:GLU:OE1	1:L:29:ILE:HB	1.88	0.73
2:H:2:GLN:NE2	2:H:3:LEU:HD12	2.03	0.73
1:L:188:ARG:HH11	1:L:188:ARG:HG3	1.54	0.72
2:H:47:MET:HA	2:H:63:PHE:CD2	2.24	0.72
2:H:190:ARG:HB3	2:H:191:PRO:HD3	1.72	0.72
2:H:42:LYS:HB3	2:H:42:LYS:NZ	2.05	0.71
1:L:148:TRP:HE1	1:L:159:VAL:HG11	1.56	0.70
2:H:5:GLN:HG2	2:H:106:ALA:HB1	1.72	0.70
2:H:3:LEU:HD23	2:H:23:LEU:HD21	1.73	0.69
1:L:159:VAL:O	1:L:160:LEU:HD13	1.92	0.69
2:H:107:GLN:HE21	2:H:107:GLN:H	1.41	0.68
2:H:19:ILE:HB	2:H:80:LYS:HZ3	1.60	0.67
2:H:23:LEU:HD13	2:H:28:PHE:HE1	1.60	0.67
1:L:38:GLN:O	1:L:84:ALA:HB1	1.96	0.66
1:L:113:GLN:HG3	1:L:136:LEU:HB3	1.77	0.66
2:H:11:LYS:O	2:H:113:VAL:HA	1.94	0.66
1:L:149:LYS:HA	1:L:153:SER:O	1.95	0.66
1:L:36:TYR:OH	1:L:89:GLN:NE2	2.29	0.65
1:L:131:SER:HA	1:L:180:THR:HA	1.78	0.65
1:L:90:GLN:HG2	1:L:92:ASN:H	1.61	0.65
2:H:3:LEU:CD2	2:H:23:LEU:HD21	2.27	0.65
2:H:28:PHE:HE2	2:H:71:LEU:HD11	1.62	0.65
2:H:34:ASN:HD22	2:H:46:TRP:HE1	1.43	0.64
2:H:55:GLU:HG2	2:H:71:LEU:HD23	1.79	0.64
1:L:136:LEU:C	1:L:137:ASN:HD22	2.06	0.64
1:L:155:ARG:HD2	1:L:155:ARG:N	2.14	0.63
2:H:39:ALA:HB1	2:H:40:PRO:HD2	1.81	0.63
1:L:149:LYS:O	1:L:151:ASP:N	2.33	0.62
2:H:96:ALA:HA	2:H:104:TYR:O	2.00	0.62
2:H:213:ILE:H	2:H:213:ILE:HD13	1.63	0.61
1:L:29:ILE:HG22	1:L:29:ILE:O	1.99	0.61
2:H:33:MET:CE	2:H:95:CYS:HB2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:SER:OG	1:L:180:THR:HB	2.01	0.60
1:L:148:TRP:CD1	1:L:159:VAL:HG21	2.38	0.59
2:H:38:GLN:HB2	2:H:44:LEU:HD23	1.84	0.59
1:L:29:ILE:HD12	1:L:90:GLN:HG3	1.85	0.59
2:H:3:LEU:HD12	2:H:3:LEU:H	1.68	0.59
2:H:7:GLY:HA3	2:H:109:THR:CG2	2.29	0.58
1:L:106:ILE:H	1:L:166:GLN:HE22	1.50	0.58
2:H:189:PRO:O	2:H:193:GLU:HB2	2.03	0.58
2:H:37:LYS:O	2:H:45:LYS:HG2	2.03	0.58
2:H:39:ALA:O	2:H:42:LYS:HB2	2.02	0.58
1:L:153:SER:HB3	1:L:155:ARG:HE	1.70	0.57
2:H:23:LEU:CD2	2:H:26:TYR:HE1	2.17	0.57
1:L:36:TYR:CD1	1:L:46:LEU:HA	2.39	0.56
2:H:2:GLN:NE2	2:H:3:LEU:H	2.02	0.56
2:H:5:GLN:HG3	2:H:108:GLY:H	1.70	0.56
2:H:3:LEU:HD12	2:H:3:LEU:N	2.21	0.56
2:H:66:ARG:NH1	2:H:86:LYS:HE3	2.21	0.56
2:H:38:GLN:O	2:H:91:ALA:HB1	2.06	0.56
1:L:153:SER:HB3	1:L:155:ARG:NE	2.21	0.56
1:L:150:ILE:HG12	1:L:153:SER:HB2	1.87	0.55
1:L:160:LEU:HD21	2:H:173:GLN:OE1	2.06	0.55
1:L:25:GLU:CD	1:L:29:ILE:HB	2.31	0.55
1:L:138:ASN:HA	1:L:172:THR:OG1	2.05	0.55
2:H:34:ASN:ND2	2:H:46:TRP:HE1	2.02	0.55
2:H:3:LEU:HD13	2:H:105:TRP:O	2.07	0.55
2:H:16:THR:CG2	2:H:83:ASN:HA	2.24	0.55
2:H:34:ASN:HD22	2:H:46:TRP:NE1	2.06	0.54
1:L:24:ARG:HA	1:L:69:THR:O	2.07	0.54
2:H:22:LYS:C	2:H:23:LEU:HD12	2.31	0.54
1:L:44:VAL:HG12	1:L:45:LYS:N	2.22	0.54
1:L:148:TRP:NE1	1:L:159:VAL:HG21	2.23	0.54
1:L:155:ARG:O	1:L:159:VAL:HG23	2.07	0.54
1:L:160:LEU:HD12	2:H:171:VAL:HG21	1.90	0.53
1:L:188:ARG:HG3	1:L:188:ARG:NH1	2.22	0.53
1:L:150:ILE:HG22	1:L:192:TYR:HA	1.91	0.52
1:L:196:ALA:O	1:L:205:ILE:HG22	2.08	0.52
2:H:33:MET:HE3	2:H:34:ASN:N	2.24	0.52
1:L:211:ARG:HH11	1:L:211:ARG:HG3	1.74	0.52
2:H:5:GLN:H	2:H:107:GLN:NE2	2.09	0.51
2:H:165:VAL:HA	2:H:182:SER:O	2.11	0.51
1:L:34:ASN:OD1	1:L:49:TYR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ILE:HA	1:L:193:THR:HG23	1.93	0.51
1:L:164:THR:HG23	1:L:165:ASP:N	2.25	0.51
1:L:29:ILE:O	1:L:29:ILE:CG2	2.59	0.50
2:H:23:LEU:HD23	2:H:26:TYR:HE1	1.76	0.50
2:H:190:ARG:HG2	2:H:190:ARG:HH11	1.76	0.50
1:L:4:MET:HE1	1:L:25:GLU:HG2	1.93	0.50
2:H:29:THR:HA	2:H:52:THR:HB	1.93	0.50
1:L:178:THR:HG22	1:L:180:THR:HG22	1.94	0.49
1:L:150:ILE:CG1	1:L:153:SER:HB2	2.43	0.49
1:L:25:GLU:OE2	1:L:29:ILE:HG21	2.12	0.49
1:L:113:GLN:H	1:L:113:GLN:CD	2.21	0.49
1:L:36:TYR:HD1	1:L:46:LEU:HA	1.77	0.49
1:L:146:VAL:HB	1:L:195:GLU:O	2.13	0.49
2:H:39:ALA:CB	2:H:40:PRO:HD2	2.41	0.49
2:H:42:LYS:HB3	2:H:42:LYS:HZ2	1.77	0.49
2:H:34:ASN:O	2:H:95:CYS:HA	2.13	0.49
1:L:118:PHE:HE2	1:L:135:PHE:HD2	1.61	0.48
1:L:29:ILE:O	1:L:30:SER:C	2.56	0.48
1:L:192:TYR:CD1	1:L:192:TYR:N	2.82	0.48
2:H:19:ILE:HD12	2:H:80:LYS:NZ	2.29	0.48
2:H:31:TYR:C	2:H:52:THR:HG1	2.21	0.48
2:H:166:HIS:O	2:H:181:SER:HA	2.14	0.48
1:L:124:GLN:O	1:L:127:SER:HB2	2.13	0.48
1:L:187:GLU:HA	1:L:187:GLU:OE1	2.14	0.48
2:H:168:PHE:HA	2:H:169:PRO:HD3	1.72	0.48
2:H:140:LEU:HD12	2:H:212:ILE:HG21	1.96	0.48
2:H:36:VAL:HG11	2:H:44:LEU:HD22	1.95	0.48
2:H:190:ARG:HG2	2:H:190:ARG:NH1	2.29	0.47
1:L:145:ASN:OD1	1:L:197:THR:HB	2.14	0.47
2:H:47:MET:HA	2:H:63:PHE:CE2	2.50	0.47
1:L:30:SER:OG	1:L:31:ASN:N	2.46	0.46
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.48	0.46
1:L:11:LEU:HD23	1:L:12:SER:N	2.30	0.46
1:L:59:PRO:HB2	1:L:61:ARG:HG3	1.98	0.46
2:H:90:MET:SD	2:H:113:VAL:HB	2.55	0.46
1:L:44:VAL:HG12	1:L:45:LYS:H	1.81	0.46
2:H:4:GLN:HA	2:H:107:GLN:HE22	1.81	0.46
2:H:107:GLN:HE21	2:H:107:GLN:N	2.10	0.46
1:L:207:LYS:HD2	1:L:207:LYS:HA	1.80	0.45
2:H:17:VAL:O	2:H:81:GLN:HB2	2.16	0.45
2:H:23:LEU:HD13	2:H:28:PHE:CE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:LEU:HA	2:H:161:LEU:HD23	1.49	0.45
1:L:15:LEU:C	1:L:17:ASP:H	2.24	0.45
2:H:28:PHE:CE2	2:H:71:LEU:HD11	2.45	0.45
2:H:140:LEU:O	2:H:182:SER:HA	2.16	0.45
2:H:59:TYR:CE1	2:H:69:PHE:CE2	3.05	0.45
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.99	0.45
1:L:155:ARG:HG2	1:L:155:ARG:HH11	1.82	0.45
1:L:199:LYS:O	1:L:201:SER:N	2.49	0.45
2:H:93:TYR:O	2:H:108:GLY:HA2	2.17	0.45
1:L:185:GLU:O	1:L:189:HIS:ND1	2.50	0.44
1:L:2:ILE:HD13	1:L:29:ILE:HD11	1.99	0.44
2:H:196:THR:HG22	2:H:211:LYS:HA	1.98	0.44
1:L:122:SER:O	1:L:125:LEU:HB2	2.18	0.44
2:H:206:THR:C	2:H:207:LYS:HG3	2.42	0.44
1:L:138:ASN:OD1	2:H:166:HIS:CE1	2.70	0.44
2:H:23:LEU:HD12	2:H:23:LEU:N	2.32	0.44
1:L:163:TRP:O	2:H:169:PRO:HG2	2.17	0.44
1:L:70:ASP:C	1:L:71:TYR:CD1	2.95	0.44
2:H:190:ARG:HD3	2:H:191:PRO:N	2.32	0.44
2:H:202:PRO:O	2:H:203:ALA:C	2.60	0.44
1:L:211:ARG:HG3	1:L:211:ARG:NH1	2.33	0.44
2:H:107:GLN:HG2	2:H:108:GLY:O	2.18	0.43
2:H:172:LEU:HD13	2:H:177:TYR:CD1	2.53	0.43
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.19	0.43
2:H:3:LEU:HD11	2:H:104:TYR:CB	2.49	0.43
2:H:139:THR:HG23	2:H:183:VAL:O	2.19	0.43
2:H:5:GLN:HG3	2:H:108:GLY:N	2.34	0.43
1:L:112:ALA:HB2	1:L:200:THR:OG1	2.18	0.42
2:H:138:VAL:HG11	2:H:190:ARG:HB2	2.00	0.42
1:L:125:LEU:HD23	1:L:125:LEU:HA	1.88	0.42
2:H:10:LEU:HD11	2:H:148:PHE:CZ	2.54	0.42
1:L:24:ARG:O	1:L:24:ARG:HG2	2.18	0.42
1:L:38:GLN:HB2	1:L:87:PHE:HE2	1.84	0.42
1:L:92:ASN:O	1:L:93:THR:HG23	2.20	0.42
1:L:148:TRP:CH2	1:L:179:LEU:HB2	2.54	0.42
2:H:150:GLU:HA	2:H:151:PRO:HA	1.67	0.42
1:L:106:ILE:N	1:L:166:GLN:HE22	2.17	0.42
2:H:53:ASN:HD22	2:H:54:THR:HG23	1.85	0.42
1:L:193:THR:HA	1:L:208:SER:OG	2.19	0.41
2:H:67:PHE:CD1	2:H:67:PHE:N	2.88	0.41
1:L:90:GLN:HE21	1:L:90:GLN:HB3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:ARG:CB	2:H:191:PRO:HD3	2.45	0.41
1:L:137:ASN:ND2	1:L:174:SER:HB3	2.35	0.41
1:L:186:TYR:HA	1:L:192:TYR:OH	2.21	0.41
2:H:87:ASN:O	2:H:89:ASP:N	2.53	0.41
2:H:102:PHE:N	2:H:102:PHE:CD1	2.88	0.41
1:L:49:TYR:O	1:L:50:TYR:C	2.63	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.70	0.41
2:H:172:LEU:HD12	2:H:172:LEU:HA	1.78	0.41
1:L:88:CYS:O	1:L:98:PHE:HA	2.20	0.41
1:L:86:TYR:CD1	1:L:86:TYR:N	2.89	0.41
2:H:33:MET:HB2	2:H:50:ILE:CG2	2.51	0.41
2:H:53:ASN:HD22	2:H:54:THR:N	2.19	0.41
2:H:127:ALA:HB3	2:H:213:ILE:HG13	2.03	0.41
1:L:202:THR:O	1:L:204:PRO:HD3	2.20	0.40
2:H:141:GLY:HA2	2:H:181:SER:O	2.21	0.40
1:L:36:TYR:HH	2:H:102:PHE:H	1.68	0.40
1:L:148:TRP:NE1	1:L:159:VAL:HG11	2.31	0.40
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.95	0.40
1:L:150:ILE:HD11	1:L:155:ARG:NH1	2.37	0.40
2:H:179:LEU:HD12	2:H:179:LEU:C	2.46	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	209/211 (99%)	172 (82%)	28 (13%)	9 (4%)	2	4
2	H	210/212 (99%)	171 (81%)	31 (15%)	8 (4%)	2	5
All	All	419/423 (99%)	343 (82%)	59 (14%)	17 (4%)	2	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	150	ILE
1	L	200	THR
2	H	40	PRO
2	H	88	GLU
1	L	166	GLN
1	L	188	ARG
2	H	7	GLY
2	H	103	ASP
2	H	191	PRO
1	L	191	SER
2	H	76	PHE
1	L	40	PRO
2	H	74	SER
1	L	82	ASP
1	L	126	THR
1	L	128	GLY
2	H	151	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	190/190 (100%)	151 (80%)	39 (20%)	1	3
2	H	181/181 (100%)	150 (83%)	31 (17%)	2	6
All	All	371/371 (100%)	301 (81%)	70 (19%)	1	4

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	11	LEU
1	L	19	VAL
1	L	22	SER
1	L	24	ARG
1	L	25	GLU
1	L	45	LYS

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Mol	Chain	Res	Type
1	L	46	LEU
1	L	48	ILE
1	L	54	LEU
1	L	67	THR
1	L	72	SER
1	L	79	GLU
1	L	82	ASP
1	L	85	THR
1	L	89	GLN
1	L	90	GLN
1	L	93	THR
1	L	104	LEU
1	L	106	ILE
1	L	107	LYS
1	L	108	ARG
1	L	136	LEU
1	L	145	ASN
1	L	154	GLU
1	L	156	GLN
1	L	157	ASN
1	L	164	THR
1	L	166	GLN
1	L	169	LYS
1	L	176	SER
1	L	179	LEU
1	L	180	THR
1	L	181	LEU
1	L	188	ARG
1	L	200	THR
1	L	203	SER
1	L	206	VAL
1	L	211	ARG
2	H	2	GLN
2	H	3	LEU
2	H	10	LEU
2	H	42	LYS
2	H	52	THR
2	H	53	ASN
2	H	62	GLU
2	H	64	LYS
2	H	72	GLU
2	H	74	SER

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Mol	Chain	Res	Type
2	H	80	LYS
2	H	86	LYS
2	H	88	GLU
2	H	90	MET
2	H	98	VAL
2	H	99	GLU
2	H	103	ASP
2	H	107	GLN
2	H	110	THR
2	H	114	SER
2	H	142	CYS
2	H	158	SER
2	H	165	VAL
2	H	179	LEU
2	H	184	THR
2	H	194	THR
2	H	195	VAL
2	H	207	LYS
2	H	210	LYS
2	H	212	ILE
2	H	213	ILE

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	6	GLN
1	L	27	GLN
1	L	31	ASN
1	L	37	GLN
1	L	89	GLN
1	L	124	GLN
1	L	137	ASN
1	L	166	GLN
1	L	190	ASN
1	L	210	ASN
2	H	2	GLN
2	H	34	ASN
2	H	53	ASN
2	H	81	GLN
2	H	107	GLN
2	H	198	ASN

5.3.3 RNA [i](#)

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](#)

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.