



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:54 PM UTC

PDB ID : 1FPT / pdb_00001fpt
Title : THREE-DIMENSIONAL STRUCTURE OF THE COMPLEX BETWEEN
THE FAB FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE
1 POLIOVIRUS AND ITS VIRAL EPITOPE
Authors : Wien, M.W.; Hogle, J.M.
Deposited on : 1995-01-26
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

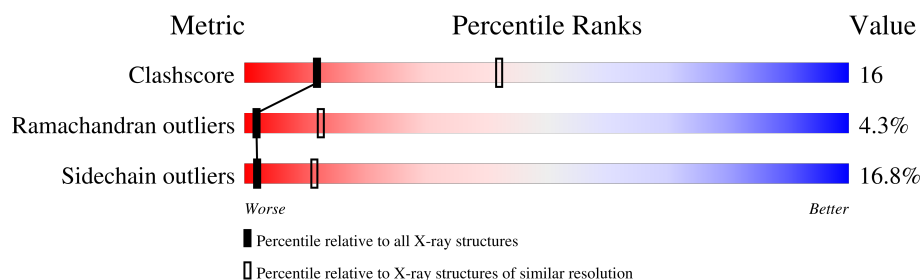
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	P	18	6% 39% 6% 11% 39%
2	L	219	38% 41% 18% .
3	H	220	36% 40% 17% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3465 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 FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE 1 POLIOVIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	0	0	0
			83	47	15	21			

- Molecule 2 is a protein called IGG2A-KAPPA C3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1691	1061	283	341	6			

- Molecule 3 is a protein called IGG2A-KAPPA C3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	0	0
			1652	1045	269	332	6			

- Molecule 4 is water.

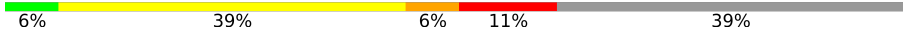
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	2	Total	O	0	0
			2	2		
4	L	17	Total	O	0	0
			17	17		
4	H	20	Total	O	0	0
			20	20		

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.

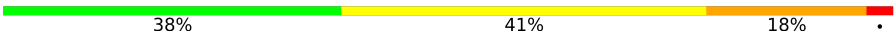
Note EDS was not executed.

- Molecule 1: FAB FRAGMENT OF AN NEUTRALIZING ANTIBODY FOR TYPE 1 POLIOVIRUS

Chain P: 

CYS VAL THR ILE MET THR VAL D93 A94 P95 A96 S97 T98 T99 N100 K101 D102 K103

- Molecule 2: IGG2A-KAPPA C3 FAB (LIGHT CHAIN)

Chain L: 

D1 V2 V3 N4 T5 D6 V7 P8 L9 S10 D82 L11 P12 V13 S14 L15 G16 D17 Q18 A19 S22 C23 Q27 S27A L27B V27C H27D S27E N28 Q29 K30 T31 Y32 L33 H34 K35 V36 L37 Q38 Q42 S43 P44 K45 Y49 K50 V51 S52 S53 S56 G66 S67 G68 T69 Y70 F71

T72 L73 K74 V75 R76 V77 F78 A80 E81 D82 L83 Y86 F87 C88 S89 S91 T92 H93 T97 F98 T102 K103 L104 E105 L106 K107 R108 A109 D110 A111 A112 P113 T114 V115 S116 T117 F118 P119 P120 S121 S122 Q124 S127 G128 S131 V132 V133 C134 F135 L136 N137 N138 F139

K142 D143 I144 V145 V146 K147 W148 D149 L150 D151 G152 S153 E154 V155 Q156 N157 G158 V159 L160 M161 S162 W163 T164 D165 Q166 D167 S168 K169 S171 S174 M175 L179 K183 D184 E185 Y186 E187 R188 H189 N190 Y192 C194 E195 A196 T197 H198 K199 F200 K207 S208 F209 N210

R211 N212 E213 C213A

- Molecule 3: IGG2A-KAPPA C3 FAB (HEAVY CHAIN)

Chain H: 

Q1 V2 Q3 L4 Q5 D6 S7 E10 L11 S12 V12 R13 P14 G15 T16 S17 V18 K19 A24 A27 Y28 A29 F29 T30 N31 Y32 L33 S34 Q35 V36 L37 K38 T39 R40 P41 T42 G42 Q43 G44 L45 E46 W47 I48 G49 V50 S51 N52 T57 D58 Y59 N62 F63 T63 K64 A67 T68 L69 S137 T70

K73 S74 S75 S76 M80 Q81 L82 S82A P151 S152 S82B V12 T153 L154 T155 T156 W157 N162 S163 L166 S167 S168 G169 V171 H172 T173 F174 P175 A176 V177 L178 Q179 S180 D181 L182 Y183 S186 S187 S188 V189 T190 K191 T192 S193 S194 T196 V196 P197 S198 Q203 S204 T205 T206 C208 T209 H212 P213 L214 A214

V219	D220	K221	K222	I223	E226	P227	R228
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.78Å 129.78Å 143.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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	P	1.52	0/83	3.58	17/110 (15.5%)
2	L	1.44	19/1731 (1.1%)	2.40	100/2351 (4.3%)
3	H	1.42	13/1693 (0.8%)	2.45	132/2314 (5.7%)
All	All	1.43	32/3507 (0.9%)	2.46	249/4775 (5.2%)

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	P	0	1
2	L	0	1
3	H	0	2
All	All	0	4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	34	HIS	CD2-NE2	-8.27	1.28	1.37
2	L	34	HIS	CG-ND1	-7.90	1.29	1.38
3	H	123	PRO	CA-CB	-7.72	1.45	1.54
3	H	212	HIS	CD2-NE2	-7.55	1.29	1.37
3	H	172	HIS	CD2-NE2	-7.34	1.29	1.37
2	L	27(D)	HIS	CD2-NE2	-7.01	1.30	1.37
3	H	134	THR	CA-CB	6.63	1.64	1.53
2	L	119	PRO	CA-CB	-6.44	1.48	1.53
2	L	27(D)	HIS	CG-ND1	-6.28	1.31	1.38
3	H	175	PRO	CA-CB	-6.20	1.45	1.53
2	L	189	HIS	CD2-NE2	-6.04	1.31	1.37
3	H	186	SER	CA-CB	-5.95	1.44	1.53
2	L	49	TYR	CA-C	-5.91	1.47	1.52
3	H	110	THR	CA-CB	5.76	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	171	VAL	CA-CB	-5.62	1.46	1.54
2	L	132	VAL	CA-CB	5.58	1.60	1.53
3	H	212	HIS	CG-ND1	-5.52	1.32	1.38
2	L	93	HIS	CD2-NE2	-5.50	1.31	1.37
2	L	35	TRP	CG-CD2	-5.44	1.33	1.43
2	L	188	ARG	NE-CZ	5.44	1.39	1.33
2	L	189	HIS	CG-ND1	-5.36	1.32	1.38
3	H	109	LEU	CA-CB	-5.36	1.45	1.53
2	L	198	HIS	CA-C	5.29	1.59	1.52
2	L	160	LEU	CB-CG	-5.28	1.42	1.53
3	H	119	PRO	CA-CB	-5.13	1.47	1.53
2	L	34	HIS	CE1-NE2	-5.11	1.27	1.32
2	L	77	ARG	CA-C	-5.11	1.47	1.53
3	H	227	PRO	CA-CB	-5.10	1.46	1.53
3	H	82	LEU	CA-CB	-5.06	1.46	1.53
2	L	5	THR	CA-CB	-5.04	1.45	1.53
2	L	200	THR	CA-CB	-5.02	1.45	1.53
2	L	213	GLU	CA-CB	5.02	1.61	1.53

All (249) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	GLN	OE1-CD-NE2	-11.80	110.80	122.60
1	P	94	ASN	O-C-N	-11.76	107.80	121.32
2	L	138	ASN	OD1-CG-ND2	-11.36	111.24	122.60
1	P	100	ASN	OD1-CG-ND2	-10.65	111.95	122.60
2	L	210	ASN	OD1-CG-ND2	-10.32	112.28	122.60
1	P	94	ASN	OD1-CG-ND2	-10.11	112.49	122.60
2	L	137	ASN	N-CA-C	9.78	124.94	110.46
3	H	6	GLN	N-CA-C	9.69	125.44	110.42
1	P	96	ALA	N-CA-C	9.53	124.00	109.23
3	H	142	CYS	CA-CB-SG	-9.46	92.64	114.40
2	L	119	PRO	N-CA-C	9.43	119.52	110.47
2	L	38	GLN	OE1-CD-NE2	-9.37	113.23	122.60
2	L	195	GLU	CA-C-O	9.34	130.30	120.30
2	L	187	GLU	N-CA-C	9.33	123.76	112.38
3	H	1	GLN	OE1-CD-NE2	-9.20	113.40	122.60
3	H	138	VAL	N-CA-C	8.93	120.61	108.11
2	L	212	ASN	CA-C-N	8.92	132.43	120.65
2	L	212	ASN	C-N-CA	8.92	132.43	120.65
3	H	186	SER	CA-CB-OG	-8.83	93.45	111.10
1	P	98	THR	CA-CB-OG1	-8.81	96.39	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	205	ILE	N-CA-C	8.65	120.68	107.78
3	H	10	GLU	N-CA-C	8.60	123.30	108.76
3	H	141	GLY	N-CA-C	8.50	123.52	111.19
2	L	49	TYR	CA-C-O	-8.49	107.51	120.16
2	L	171	SER	N-CA-C	8.47	123.29	113.38
3	H	179	GLN	OE1-CD-NE2	-8.46	114.14	122.60
2	L	97	THR	CA-CB-OG1	-8.39	97.01	109.60
3	H	197	PRO	CA-C-N	8.35	131.30	120.44
3	H	197	PRO	C-N-CA	8.35	131.30	120.44
3	H	6	GLN	OE1-CD-NE2	-8.28	114.32	122.60
3	H	50	VAL	CB-CA-C	-8.24	97.26	110.28
2	L	27(D)	HIS	CA-CB-CG	8.11	121.91	113.80
2	L	127	SER	N-CA-C	8.01	122.12	109.39
2	L	13	VAL	O-C-N	-8.00	114.44	123.00
2	L	5	THR	N-CA-C	7.93	121.52	107.80
2	L	210	ASN	N-CA-C	7.92	121.87	108.02
3	H	24	ALA	N-CA-C	7.90	121.53	108.96
3	H	3	GLN	CG-CD-NE2	7.87	128.21	116.40
3	H	100	ASP	CA-CB-CG	7.84	120.44	112.60
3	H	147	TYR	N-CA-C	7.65	121.37	109.52
3	H	82(C)	LEU	N-CA-C	7.61	121.23	110.50
2	L	27	GLN	CA-CB-CG	-7.58	98.94	114.10
2	L	195	GLU	N-CA-C	7.57	120.75	108.41
3	H	45	LEU	O-C-N	-7.56	114.59	123.06
2	L	156	GLN	OE1-CD-NE2	-7.55	115.05	122.60
3	H	81	GLN	CA-CB-CG	-7.54	99.02	114.10
2	L	183	LYS	CG-CD-CE	-7.53	93.99	111.30
3	H	174	PHE	CA-CB-CG	-7.50	106.30	113.80
3	H	156	THR	CA-CB-OG1	-7.46	98.41	109.60
3	H	148	PHE	O-C-N	-7.34	114.57	122.06
3	H	156	THR	CA-CB-CG2	7.31	122.92	110.50
1	P	99	THR	CA-CB-OG1	-7.29	98.66	109.60
3	H	162	ASN	OD1-CG-ND2	-7.28	115.32	122.60
2	L	108	ARG	N-CA-C	7.28	119.72	110.33
3	H	43	GLN	N-CA-CB	-7.27	99.07	111.21
2	L	210	ASN	CB-CG-ND2	7.25	127.28	116.40
3	H	62	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	L	138	ASN	CB-CG-ND2	7.18	127.17	116.40
1	P	103	LYS	CB-CG-CD	-7.14	94.89	111.30
3	H	151	PRO	N-CA-C	7.11	130.58	112.10
3	H	172	HIS	CB-CG-CD2	-7.11	121.96	131.20
3	H	12	VAL	N-CA-C	7.08	118.03	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	31	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	P	95	PRO	N-CA-C	7.02	126.92	112.47
2	L	142	LYS	N-CA-C	7.00	121.44	112.34
2	L	117	ILE	CB-CA-C	-6.98	101.99	111.63
3	H	183	TYR	N-CA-C	6.98	121.69	109.96
3	H	203	GLN	CA-C-O	-6.97	110.54	120.51
3	H	179	GLN	O-C-N	-6.91	113.40	122.59
2	L	148	TRP	CG-CD2-CE3	6.89	140.79	133.90
2	L	208	SER	CA-CB-OG	6.86	124.81	111.10
2	L	159	VAL	N-CA-C	-6.79	99.98	109.21
1	P	94	ASN	CB-CG-ND2	6.76	126.55	116.40
2	L	53	ASN	OD1-CG-ND2	-6.76	115.84	122.60
3	H	3	GLN	CA-CB-CG	6.72	127.54	114.10
2	L	27(C)	VAL	N-CA-C	6.71	116.90	107.37
3	H	95	ASP	CA-CB-CG	6.71	119.31	112.60
2	L	213	GLU	CB-CG-CD	6.67	123.94	112.60
1	P	94	ASN	CA-CB-CG	6.67	119.27	112.60
2	L	110	ASP	N-CA-C	6.66	124.97	110.80
3	H	39	GLN	OE1-CD-NE2	-6.63	115.97	122.60
3	H	135	GLY	O-C-N	6.63	131.32	122.70
3	H	194	SER	N-CA-C	6.63	121.65	107.67
3	H	6	GLN	CG-CD-NE2	6.61	126.32	116.40
3	H	209	ASN	OD1-CG-ND2	-6.60	116.00	122.60
2	L	93	HIS	CB-CG-CD2	-6.57	122.66	131.20
3	H	43	GLN	OE1-CD-NE2	-6.55	116.05	122.60
2	L	105	GLU	O-C-N	-6.54	115.61	123.13
2	L	154	GLU	CB-CG-CD	6.53	123.70	112.60
2	L	131	SER	O-C-N	-6.53	115.64	123.27
2	L	17	ASP	N-CA-C	6.45	118.85	110.53
3	H	58	ASP	O-C-N	-6.45	114.81	123.19
3	H	15	GLY	CA-C-O	6.44	125.96	119.27
3	H	68	THR	CA-C-O	6.42	128.34	120.25
2	L	87	PHE	CA-CB-CG	-6.42	107.39	113.80
3	H	156	THR	CA-C-O	6.41	128.43	120.54
1	P	101	LYS	CA-C-O	6.39	127.32	120.10
2	L	56	SER	N-CA-C	6.39	119.03	110.35
2	L	139	PHE	CA-CB-CG	6.38	120.18	113.80
3	H	67	ALA	O-C-N	-6.36	115.06	122.95
3	H	213	PRO	N-CA-C	-6.35	104.89	113.40
2	L	190	ASN	CA-CB-CG	6.34	118.94	112.60
2	L	186	TYR	N-CA-C	-6.33	104.00	111.03
3	H	36	TRP	O-C-N	-6.30	116.04	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	191	VAL	O-C-N	-6.30	114.70	122.57
3	H	67	ALA	N-CA-C	6.29	119.47	110.10
1	P	95	PRO	N-CD-CG	6.26	112.59	103.20
3	H	43	GLN	N-CA-C	6.26	117.38	108.74
2	L	161	ASN	N-CA-C	6.25	119.70	109.76
2	L	112	ALA	CA-C-N	6.25	126.22	119.78
2	L	112	ALA	C-N-CA	6.25	126.22	119.78
3	H	82(B)	SER	N-CA-C	6.22	118.80	111.02
2	L	139	PHE	N-CA-C	6.22	120.00	110.36
1	P	98	THR	CA-CB-CG2	6.21	121.06	110.50
3	H	119	PRO	N-CA-CB	6.21	109.08	103.19
2	L	114	THR	CA-C-O	6.19	128.72	121.11
3	H	70	THR	O-C-N	-6.17	115.86	123.33
3	H	112	SER	CA-C-O	6.14	127.62	120.75
2	L	5	THR	CB-CA-C	-6.13	101.67	110.62
2	L	163	TRP	CG-CD2-CE3	6.13	140.03	133.90
2	L	185	GLU	CB-CG-CD	6.10	122.98	112.60
3	H	101	ASP	N-CA-C	6.09	123.78	110.80
3	H	48	ILE	CA-C-O	-6.07	114.82	120.34
2	L	146	VAL	N-CA-C	6.05	116.58	108.11
2	L	42	GLN	O-C-N	-6.05	114.55	122.59
2	L	161	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	L	135	PHE	CA-CB-CG	6.04	119.84	113.80
2	L	162	SER	O-C-N	-6.02	116.14	123.30
2	L	148	TRP	CB-CG-CD1	-6.01	117.88	126.90
2	L	207	LYS	N-CA-C	-6.00	100.83	110.14
2	L	112	ALA	N-CA-C	6.00	119.20	110.14
2	L	131	SER	CA-CB-OG	6.00	123.09	111.10
3	H	85	ASP	N-CA-C	5.99	119.85	112.54
2	L	51	VAL	CG1-CB-CG2	-5.97	97.67	110.80
2	L	27(E)	SER	N-CA-C	5.93	123.42	110.80
3	H	100(J)	GLY	N-CA-C	5.89	118.05	112.04
3	H	52	ASN	CA-CB-CG	5.88	118.48	112.60
3	H	73	LYS	CA-CB-CG	-5.88	102.35	114.10
3	H	103	TRP	O-C-N	-5.87	116.35	123.10
3	H	76	SER	N-CA-C	5.86	123.28	110.80
3	H	82(C)	LEU	CD1-CG-CD2	-5.85	97.93	110.80
2	L	199	LYS	CG-CD-CE	-5.84	97.88	111.30
3	H	125	ALA	N-CA-C	5.83	119.13	110.32
3	H	16	THR	CA-CB-OG1	-5.83	100.86	109.60
1	P	99	THR	CA-CB-CG2	5.79	120.34	110.50
3	H	116	THR	N-CA-CB	5.78	118.49	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	194	SER	CB-CA-C	-5.75	103.62	111.95
3	H	172	HIS	CB-CG-ND1	5.74	131.31	122.70
3	H	205	ILE	CA-C-O	5.73	125.92	120.25
2	L	74	LYS	N-CA-C	5.72	118.80	109.24
3	H	62	ASN	CB-CG-ND2	5.72	124.97	116.40
3	H	204	SER	CB-CA-C	-5.72	99.04	110.42
3	H	128	CYS	N-CA-C	5.71	122.97	110.80
3	H	157	TRP	CA-C-O	5.71	126.41	120.30
2	L	193	THR	N-CA-C	5.69	117.71	108.26
3	H	137	SER	N-CA-C	5.69	119.18	110.36
3	H	89	VAL	O-C-N	-5.68	116.72	123.03
2	L	154	GLU	N-CA-C	5.67	118.41	109.96
2	L	97	THR	N-CA-CB	-5.67	101.38	111.08
2	L	148	TRP	CE2-CD2-CG	-5.64	100.43	107.20
3	H	29	PHE	CA-CB-CG	5.63	119.43	113.80
3	H	43	GLN	CA-CB-CG	5.60	125.29	114.10
3	H	168	SER	O-C-N	-5.59	116.41	122.79
3	H	191	VAL	N-CA-CB	-5.59	102.01	111.23
2	L	153	SER	N-CA-C	5.56	118.62	109.72
3	H	163	SER	N-CA-CB	-5.56	103.79	112.41
2	L	9	LEU	CA-C-O	5.56	126.36	119.97
3	H	29	PHE	N-CA-C	5.55	122.62	110.80
3	H	177	VAL	N-CA-C	5.54	116.47	110.21
3	H	43	GLN	CG-CD-NE2	5.54	124.71	116.40
3	H	107	THR	O-C-N	-5.53	116.91	123.22
3	H	134	THR	CA-C-N	5.52	132.23	121.41
3	H	134	THR	C-N-CA	5.52	132.23	121.41
2	L	124	GLN	OE1-CD-NE2	-5.51	117.08	122.60
2	L	170	ASP	CA-CB-CG	5.50	118.10	112.60
3	H	37	ILE	O-C-N	-5.50	117.53	123.14
2	L	30	LYS	N-CA-C	5.50	117.48	108.52
3	H	104	GLY	O-C-N	-5.48	118.44	122.71
2	L	212	ASN	OD1-CG-ND2	-5.46	117.14	122.60
3	H	203	GLN	CB-CG-CD	-5.46	103.32	112.60
2	L	14	SER	CA-C-O	-5.46	114.84	121.28
3	H	178	LEU	CA-C-O	-5.45	114.48	120.70
2	L	6	GLN	N-CA-C	5.45	118.36	109.59
3	H	19	LYS	O-C-N	-5.45	115.93	123.01
3	H	114	ALA	N-CA-C	5.45	117.36	110.33
3	H	11	LEU	CA-C-O	5.43	126.35	120.43
2	L	212	ASN	CA-CB-CG	-5.42	107.17	112.60
3	H	209	ASN	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	GLN	CG-CD-NE2	5.40	124.50	116.40
3	H	157	TRP	CE2-CD2-CG	-5.39	100.73	107.20
3	H	43	GLN	O-C-N	-5.39	116.62	122.92
3	H	181	ASP	CA-CB-CG	-5.37	107.23	112.60
3	H	206	THR	CA-C-O	5.37	126.28	120.32
2	L	93	HIS	CB-CG-ND1	5.34	130.71	122.70
3	H	47	TRP	CE2-CD2-CG	-5.33	100.80	107.20
2	L	167	ASP	N-CA-C	5.30	118.12	110.28
3	H	5	GLN	N-CA-CB	-5.29	102.80	110.84
3	H	10	GLU	CA-CB-CG	-5.28	103.54	114.10
2	L	51	VAL	CB-CA-C	-5.27	102.64	111.29
2	L	51	VAL	N-CA-CB	5.26	119.90	111.23
3	H	204	SER	N-CA-C	5.25	121.97	110.80
2	L	88	CYS	O-C-N	-5.24	117.06	123.19
3	H	96	PHE	CA-C-O	-5.23	115.44	121.19
2	L	97	THR	CA-CB-CG2	5.22	119.37	110.50
2	L	213	GLU	N-CA-CB	-5.21	102.30	109.91
3	H	63	PHE	CA-CB-CG	-5.19	108.61	113.80
3	H	5	GLN	N-CA-C	5.18	117.24	108.02
1	P	95	PRO	CA-CB-CG	5.17	114.33	104.50
2	L	49	TYR	N-CA-C	5.17	119.21	112.13
3	H	85	ASP	CA-CB-CG	-5.17	107.43	112.60
2	L	146	VAL	O-C-N	5.16	128.83	123.26
3	H	219	VAL	N-CA-C	5.15	115.54	108.12
3	H	193	SER	CA-C-N	-5.15	113.91	122.92
3	H	193	SER	C-N-CA	-5.15	113.91	122.92
2	L	115	VAL	O-C-N	-5.14	117.42	122.67
3	H	157	TRP	CB-CG-CD1	-5.14	119.19	126.90
3	H	228	ARG	N-CA-C	5.14	125.38	111.00
2	L	22	SER	CA-CB-OG	5.13	121.36	111.10
2	L	27(C)	VAL	O-C-N	-5.12	114.50	122.70
2	L	163	TRP	O-C-N	-5.12	116.71	123.21
2	L	163	TRP	CE2-CD2-CG	-5.12	101.05	107.20
3	H	108	THR	CA-CB-OG1	-5.12	101.92	109.60
2	L	32	TYR	N-CA-C	5.12	116.93	109.71
3	H	142	CYS	N-CA-C	5.11	116.75	108.26
3	H	134	THR	N-CA-C	5.11	121.69	110.80
2	L	135	PHE	O-C-N	-5.10	116.37	123.01
2	L	195	GLU	O-C-N	-5.09	117.37	123.27
3	H	69	LEU	O-C-N	-5.08	117.27	123.16
3	H	212	HIS	CB-CG-CD2	-5.08	124.60	131.20
3	H	50	VAL	N-CA-CB	5.08	119.80	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	48	ILE	N-CA-C	-5.07	107.86	112.12
2	L	81	GLU	CA-CB-CG	5.07	124.23	114.10
1	P	101	LYS	CB-CA-C	-5.06	101.27	110.63
2	L	134	CYS	N-CA-C	5.06	117.15	108.90
3	H	18	VAL	CG1-CB-CG2	-5.06	99.68	110.80
2	L	148	TRP	CB-CA-C	-5.05	101.19	109.53
3	H	47	TRP	CD1-CG-CD2	5.05	114.38	106.30
3	H	36	TRP	CE2-CD2-CG	-5.04	101.15	107.20
2	L	164	THR	CA-CB-CG2	5.04	119.07	110.50
3	H	48	ILE	O-C-N	-5.04	116.83	121.97
3	H	172	HIS	CB-CA-C	-5.04	105.10	111.70
2	L	50	LYS	CA-CB-CG	-5.04	104.03	114.10
2	L	120	PRO	N-CA-CB	5.03	107.65	103.17
1	P	97	SER	CA-C-O	5.03	125.83	120.20
3	H	156	THR	CA-C-N	-5.03	115.91	123.00
3	H	156	THR	C-N-CA	-5.03	115.91	123.00
3	H	130	ASP	N-CA-C	5.02	121.50	110.80
3	H	52	ASN	OD1-CG-ND2	-5.01	117.59	122.60
3	H	57	THR	N-CA-C	5.00	117.13	109.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	ARG	Peptide
3	H	59	TYR	Sidechain
2	L	32	TYR	Sidechain
1	P	94	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	P	83	0	76	1	0
2	L	1691	0	1636	57	0
3	H	1652	0	1609	50	0
4	H	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	17	0	0	0	0
4	P	2	0	0	0	0
All	All	3465	0	3321	102	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 (102) 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:L:27(D):HIS:HB2	2:L:92:THR:HG23	1.38	1.04
2:L:147:LYS:HE3	2:L:154:GLU:HG2	1.51	0.93
2:L:134:CYS:HG	2:L:194:CYS:HG	0.89	0.83
2:L:113:PRO:HG3	2:L:144:ILE:HD11	1.61	0.80
2:L:118:PHE:CZ	3:H:140:LEU:HA	2.22	0.73
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.70	0.73
2:L:83:LEU:HD11	2:L:166:GLN:HG2	1.71	0.73
2:L:37:LEU:HD23	2:L:45:LYS:HE2	1.74	0.70
2:L:118:PHE:HZ	3:H:140:LEU:HA	1.56	0.68
2:L:27(B):LEU:HD12	2:L:71:PHE:CE1	2.31	0.66
3:H:156:THR:HG22	3:H:209:ASN:OD1	1.96	0.66
3:H:142:CYS:HG	3:H:208:CYS:CB	2.09	0.65
3:H:119:PRO:HD3	3:H:212:HIS:CD2	2.31	0.65
3:H:48:ILE:HD13	3:H:80:MET:HE1	1.79	0.64
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.78	0.64
2:L:151:ASP:HA	2:L:191:SER:HB2	1.79	0.64
2:L:4:MET:HE1	2:L:27(B):LEU:HD11	1.80	0.63
2:L:183:LYS:O	2:L:186:TYR:HB3	1.99	0.63
2:L:136:LEU:HD12	2:L:144:ILE:HD13	1.80	0.62
2:L:11:LEU:HD23	2:L:104:LEU:HD23	1.81	0.61
2:L:145:ASN:O	2:L:196:ALA:HA	2.01	0.60
3:H:27:TYR:CE1	3:H:29:PHE:HA	2.37	0.59
3:H:138:VAL:HG23	3:H:193:SER:HA	1.83	0.59
3:H:204:SER:O	3:H:205:ILE:HG13	2.03	0.59
3:H:142:CYS:HB3	3:H:154:LEU:HD11	1.86	0.58
2:L:144:ILE:HG13	2:L:198:HIS:HD2	1.68	0.57
3:H:32:TYR:CD2	3:H:96:PHE:HA	2.40	0.57
3:H:47:TRP:HZ2	3:H:50:VAL:HG22	1.70	0.56
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.88	0.55
3:H:12:VAL:HG21	3:H:109:LEU:HD21	1.89	0.55
3:H:162:ASN:HD21	3:H:205:ILE:HG13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:THR:HG21	2:L:71:PHE:CE2	2.44	0.53
3:H:40:ARG:HG2	3:H:41:PRO:HD3	1.92	0.51
2:L:44:PRO:HG2	3:H:103:TRP:CZ3	2.46	0.51
2:L:136:LEU:HD21	2:L:146:VAL:HG21	1.92	0.51
3:H:40:ARG:HH21	3:H:85:ASP:HA	1.76	0.51
2:L:23:CYS:SG	2:L:88:CYS:CB	3.00	0.50
3:H:27:TYR:OH	3:H:34:ILE:HD11	2.11	0.50
3:H:136:SER:O	3:H:193:SER:HB3	2.11	0.50
2:L:187:GLU:HA	2:L:211:ARG:HD2	1.93	0.50
2:L:198:HIS:ND1	2:L:200:THR:OG1	2.45	0.50
3:H:138:VAL:CG2	3:H:193:SER:HA	2.41	0.50
1:P:93:ASP:O	1:P:95:PRO:HD3	2.12	0.50
2:L:117:ILE:HD11	2:L:207:LYS:HB3	1.92	0.50
3:H:138:VAL:HB	3:H:191:VAL:HG12	1.94	0.49
2:L:193:THR:OG1	2:L:208:SER:HB3	2.13	0.49
3:H:151:PRO:O	3:H:213:PRO:HD2	2.13	0.49
3:H:181:ASP:O	3:H:182:LEU:HD23	2.14	0.48
3:H:13:ARG:HG3	3:H:16:THR:OG1	2.13	0.48
2:L:135:PHE:CD2	3:H:188:SER:HB3	2.49	0.48
3:H:11:LEU:HD12	3:H:149:PRO:HG3	1.96	0.47
2:L:163:TRP:NE1	2:L:175:MET:SD	2.87	0.47
3:H:18:VAL:O	3:H:81:GLN:HA	2.14	0.47
2:L:156:GLN:NE2	2:L:156:GLN:HA	2.29	0.47
2:L:149:LYS:HG2	2:L:154:GLU:HA	1.97	0.46
3:H:16:THR:HG22	3:H:17:SER:N	2.29	0.46
3:H:40:ARG:O	3:H:43:GLN:HB3	2.15	0.46
2:L:13:VAL:HG12	2:L:78:VAL:HG11	1.97	0.46
2:L:150:ILE:HG12	2:L:192:TYR:CD1	2.50	0.46
2:L:149:LYS:HA	2:L:153:SER:O	2.16	0.46
2:L:2:VAL:HG12	2:L:4:MET:HE2	1.98	0.46
3:H:203:GLN:O	3:H:204:SER:HB2	2.16	0.46
2:L:27(C):VAL:HG22	2:L:31:THR:OG1	2.17	0.45
2:L:147:LYS:HE3	2:L:154:GLU:CG	2.33	0.45
3:H:180:SER:O	3:H:181:ASP:HB2	2.17	0.45
2:L:16:GLY:O	2:L:77:ARG:HB3	2.17	0.45
2:L:67:SER:O	2:L:69:THR:N	2.50	0.44
2:L:86:TYR:CD1	2:L:86:TYR:N	2.84	0.44
2:L:112:ALA:HB2	2:L:200:THR:CG2	2.45	0.44
2:L:18:GLN:HG2	2:L:19:ALA:N	2.32	0.44
2:L:139:PHE:CE1	2:L:174:SER:HA	2.53	0.44
3:H:142:CYS:CB	3:H:154:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:128:CYS:SG	3:H:129:GLY:N	2.90	0.44
3:H:162:ASN:HB2	3:H:166:LEU:HB2	1.99	0.43
2:L:27(D):HIS:O	2:L:28:ASN:N	2.51	0.43
2:L:80:ALA:HB1	2:L:168:SER:O	2.18	0.43
3:H:103:TRP:N	3:H:103:TRP:CD1	2.85	0.43
2:L:117:ILE:HD11	2:L:207:LYS:C	2.43	0.43
3:H:192:THR:O	3:H:195:THR:HG22	2.19	0.43
2:L:118:PHE:CE2	3:H:140:LEU:HA	2.54	0.43
2:L:108:ARG:NH2	2:L:111:ALA:HB2	2.34	0.43
3:H:222:LYS:HE3	3:H:226:GLU:HG2	2.01	0.43
2:L:2:VAL:HG22	2:L:27:GLN:HB2	2.01	0.43
2:L:199:LYS:O	2:L:199:LYS:HG2	2.16	0.42
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.19	0.42
2:L:164:THR:HG22	2:L:165:ASP:N	2.34	0.42
2:L:185:GLU:HG2	2:L:189:HIS:HE1	1.84	0.42
3:H:47:TRP:CZ2	3:H:50:VAL:HG22	2.53	0.42
3:H:191:VAL:HG21	3:H:205:ILE:HD11	2.01	0.42
3:H:191:VAL:HG21	3:H:205:ILE:CD1	2.49	0.42
2:L:89:SER:HB3	2:L:98:PHE:CD2	2.55	0.42
2:L:210:ASN:O	2:L:212:ASN:N	2.53	0.41
3:H:94:ARG:HE	3:H:101:ASP:HB3	1.84	0.41
2:L:117:ILE:CD1	2:L:207:LYS:HB3	2.50	0.41
3:H:138:VAL:O	3:H:190:THR:HA	2.20	0.41
2:L:66:GLY:HA3	2:L:71:PHE:HA	2.02	0.41
2:L:8:PRO:HG2	2:L:102:THR:HG23	2.02	0.41
2:L:135:PHE:CE2	3:H:188:SER:HB3	2.57	0.40
3:H:40:ARG:NH2	3:H:85:ASP:HA	2.36	0.40
3:H:126:PRO:HD3	3:H:140:LEU:HB3	2.04	0.40
3:H:16:THR:O	3:H:82(C):LEU:HB2	2.22	0.40
3:H:38:LYS:HD2	3:H:90:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	9/18 (50%)	6 (67%)	1 (11%)	2 (22%)	0	0
2	L	217/219 (99%)	189 (87%)	20 (9%)	8 (4%)	2	15
3	H	218/220 (99%)	189 (87%)	20 (9%)	9 (4%)	2	13
All	All	444/457 (97%)	384 (86%)	41 (9%)	19 (4%)	2	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	27(E)	SER
2	L	68	GLY
2	L	211	ARG
3	H	135	GLY
3	H	193	SER
2	L	2	VAL
2	L	51	VAL
3	H	76	SER
3	H	84	SER
3	H	101	ASP
1	P	95	PRO
3	H	134	THR
3	H	179	GLN
2	L	138	ASN
2	L	198	HIS
3	H	29	PHE
1	P	94	ASN
3	H	214	ALA
2	L	128	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	P	10/17 (59%)	8 (80%)	2 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	196/197 (100%)	172 (88%)	24 (12%)	5	21
3	H	187/187 (100%)	147 (79%)	40 (21%)	1	6
All	All	393/401 (98%)	327 (83%)	66 (17%)	2	11

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	94	ASN
1	P	98	THR
2	L	15	LEU
2	L	42	GLN
2	L	53	ASN
2	L	56	SER
2	L	72	THR
2	L	77	ARG
2	L	81	GLU
2	L	91	SER
2	L	107	LYS
2	L	117	ILE
2	L	122	SER
2	L	132	VAL
2	L	136	LEU
2	L	144	ILE
2	L	156	GLN
2	L	157	ASN
2	L	165	ASP
2	L	170	ASP
2	L	179	LEU
2	L	190	ASN
2	L	197	THR
2	L	200	THR
2	L	208	SER
2	L	211	ARG
3	H	7	SER
3	H	11	LEU
3	H	12	VAL
3	H	13	ARG
3	H	34	ILE
3	H	43	GLN
3	H	50	VAL
3	H	64	LYS

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Mol	Chain	Res	Type
3	H	68	THR
3	H	74	SER
3	H	82	LEU
3	H	82(A)	SER
3	H	82(B)	SER
3	H	82(C)	LEU
3	H	101	ASP
3	H	105	GLN
3	H	110	THR
3	H	113	SER
3	H	115	LYS
3	H	127	VAL
3	H	133	THR
3	H	139	THR
3	H	140	LEU
3	H	142	CYS
3	H	150	GLU
3	H	151	PRO
3	H	152	VAL
3	H	156	THR
3	H	163	SER
3	H	166	LEU
3	H	172	HIS
3	H	177	VAL
3	H	179	GLN
3	H	180	SER
3	H	190	THR
3	H	191	VAL
3	H	192	THR
3	H	198	SER
3	H	205	ILE
3	H	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	100	ASN
2	L	27	GLN
3	H	179	GLN
3	H	212	HIS

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.