



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:22 PM UTC

PDB ID : 1ACY / pdb_00001acy
Title : CRYSTAL STRUCTURE OF THE PRINCIPAL NEUTRALIZING SITE OF HIV-1
Authors : Ghiara, J.B.; Wilson, I.A.
Deposited on : 1994-02-10
Resolution : 3.00 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

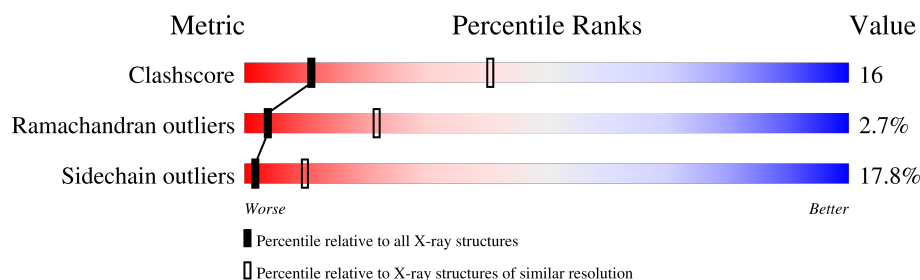
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	L	215	44% 39% 16% .
2	H	221	42% 40% 14% .
3	P	24	17% 21% . 58%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3441 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 IGG1-KAPPA 59.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1662	1031	282	341	8			

- Molecule 2 is a protein called IGG1-KAPPA 59.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1700	1077	283	330	10			

- Molecule 3 is a protein called HIV-1 GP120 (MN ISOLATE).

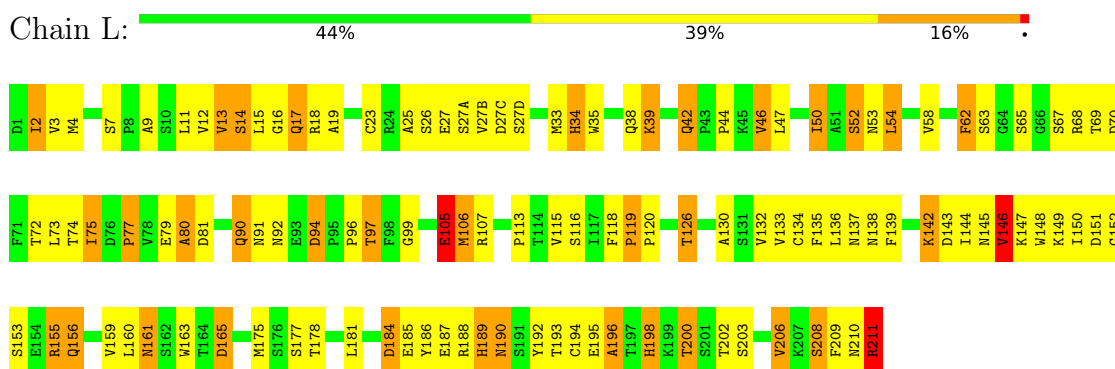
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			79	52	15	12			

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: IGG1-KAPPA 59.1 FAB (LIGHT CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 154.00Å 121.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3441	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	1.31	7/1700 (0.4%)	2.13	71/2310 (3.1%)
2	H	1.39	15/1746 (0.9%)	2.26	86/2385 (3.6%)
3	P	1.31	1/82 (1.2%)	2.12	3/110 (2.7%)
All	All	1.35	23/3528 (0.7%)	2.20	160/4805 (3.3%)

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	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	35(B)	HIS	CD2-NE2	-8.37	1.28	1.37
2	H	35(B)	HIS	CA-CB	-7.64	1.42	1.53
1	L	46	VAL	CA-CB	-7.57	1.46	1.54
1	L	34	HIS	CD2-NE2	-7.23	1.29	1.37
1	L	189	HIS	CD2-NE2	-6.84	1.30	1.37
1	L	3	VAL	CA-CB	-6.73	1.46	1.54
2	H	172	HIS	CD2-NE2	-6.40	1.30	1.37
2	H	97	HIS	CD2-NE2	-6.18	1.31	1.37
2	H	212	HIS	CD2-NE2	-6.17	1.31	1.37
3	P	315	HIS	CD2-NE2	-6.05	1.31	1.37
2	H	212	HIS	CG-ND1	-5.76	1.31	1.38
2	H	47	TRP	CG-CD2	-5.74	1.33	1.43
1	L	198	HIS	CD2-NE2	-5.61	1.31	1.37
2	H	191	VAL	CA-CB	-5.61	1.47	1.54
2	H	172	HIS	CG-ND1	-5.54	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	119	PRO	CA-CB	-5.49	1.47	1.54
1	L	75	ILE	CA-CB	-5.49	1.47	1.54
2	H	20	LEU	CA-CB	-5.43	1.45	1.53
1	L	34	HIS	CG-ND1	-5.41	1.32	1.38
2	H	151	PRO	CA-CB	-5.22	1.44	1.53
2	H	97	HIS	CG-ND1	-5.16	1.32	1.38
2	H	116	THR	CA-CB	5.05	1.60	1.53
2	H	121	VAL	CA-CB	-5.05	1.48	1.54

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	193	VAL	N-CA-CB	-10.77	100.11	111.64
1	L	53	ASN	CA-CB-CG	-9.75	102.85	112.60
2	H	193	VAL	CB-CA-C	9.62	118.76	109.33
1	L	3	VAL	N-CA-CB	-9.57	100.28	110.72
2	H	199	ARG	N-CA-C	-9.51	94.19	109.40
2	H	196	SER	CA-C-N	9.28	129.03	119.56
2	H	196	SER	C-N-CA	9.28	129.03	119.56
2	H	35(B)	HIS	CB-CG-CD2	-9.21	119.23	131.20
1	L	105	GLU	N-CA-C	-9.09	95.18	109.72
1	L	190	ASN	OD1-CG-ND2	-9.05	113.55	122.60
2	H	40	ALA	CA-C-O	-9.02	110.78	120.17
1	L	211	ARG	NE-CZ-NH2	-8.85	111.24	119.20
2	H	135	ASN	CA-CB-CG	8.71	121.31	112.60
1	L	142	LYS	N-CA-C	8.48	121.66	111.82
1	L	106	MET	N-CA-C	8.05	121.70	109.23
1	L	198	HIS	CB-CG-CD2	-7.95	120.86	131.20
2	H	63	ILE	CA-CB-CG1	-7.70	97.32	110.40
2	H	175	PRO	CA-N-CD	-7.69	101.23	112.00
1	L	106	MET	CB-CG-SD	-7.67	89.69	112.70
2	H	100(A)	THR	CA-CB-OG1	-7.63	98.16	109.60
2	H	96	ASN	OD1-CG-ND2	-7.46	115.14	122.60
2	H	193	VAL	O-C-N	-7.42	117.02	121.69
2	H	8	GLY	CA-C-N	7.34	127.10	119.76
2	H	8	GLY	C-N-CA	7.34	127.10	119.76
2	H	69	ILE	N-CA-CB	-7.31	102.66	111.21
1	L	113	PRO	N-CA-C	7.30	121.97	110.50
1	L	165	ASP	N-CA-C	-7.29	99.67	110.46
1	L	70	ASP	CA-CB-CG	-7.18	105.42	112.60
2	H	86	ASP	CA-CB-CG	-7.08	105.53	112.60
2	H	217	THR	N-CA-C	-7.06	98.19	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	184	ASP	CA-CB-CG	7.04	119.64	112.60
3	P	325	TYR	O-C-N	6.92	129.45	122.12
2	H	191	VAL	CB-CA-C	-6.88	99.40	110.28
2	H	16	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	L	34	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	L	75	ILE	N-CA-C	-6.80	97.83	107.75
2	H	126	PRO	N-CA-C	-6.79	100.58	111.03
2	H	140	LEU	CD1-CG-CD2	-6.66	96.16	110.80
1	L	137	ASN	CA-CB-CG	6.65	119.25	112.60
1	L	47	LEU	N-CA-C	-6.65	103.21	112.12
2	H	107	THR	N-CA-C	-6.62	100.67	110.46
1	L	73	LEU	N-CA-C	-6.56	99.00	109.76
1	L	42	GLN	N-CA-C	-6.53	98.05	109.48
1	L	62	PHE	CA-CB-CG	-6.52	107.28	113.80
1	L	189	HIS	CB-CG-CD2	-6.52	122.72	131.20
2	H	196	SER	O-C-N	-6.52	113.82	121.32
1	L	105	GLU	CA-CB-CG	6.47	127.04	114.10
2	H	40	ALA	CA-C-N	6.46	126.49	119.90
2	H	40	ALA	C-N-CA	6.46	126.49	119.90
1	L	106	MET	N-CA-CB	-6.44	99.55	111.53
1	L	198	HIS	CA-CB-CG	6.43	120.23	113.80
2	H	47	TRP	CE2-CD2-CE3	6.43	125.23	118.80
2	H	129	ALA	N-CA-C	6.43	117.92	107.32
1	L	198	HIS	CB-CG-ND1	6.39	132.29	122.70
2	H	148	PHE	CA-C-O	-6.38	112.75	119.13
2	H	4	LEU	CD1-CG-CD2	-6.37	96.78	110.80
2	H	30	THR	N-CA-C	6.36	120.65	113.02
2	H	199	ARG	CB-CA-C	6.35	118.00	109.42
1	L	190	ASN	N-CA-C	6.33	120.27	112.54
2	H	100(A)	THR	CA-CB-CG2	6.33	121.26	110.50
2	H	47	TRP	CD2-CE2-CZ2	-6.32	116.08	122.40
2	H	206	THR	CA-CB-OG1	-6.25	100.23	109.60
2	H	180	SER	CA-C-O	6.24	129.44	120.51
1	L	210	ASN	CA-C-O	-6.22	113.96	121.05
2	H	178	LEU	N-CA-C	6.19	120.36	109.96
2	H	35(A)	TRP	CE2-CD2-CE3	6.18	124.98	118.80
1	L	52	SER	CA-C-O	6.17	125.58	118.55
2	H	96	ASN	N-CA-C	-6.11	97.76	108.20
1	L	94	ASP	N-CA-C	6.08	117.55	109.83
1	L	52	SER	N-CA-CB	-6.01	103.01	111.00
1	L	107	ARG	N-CA-C	6.01	119.03	109.24
2	H	147	TYR	CA-C-O	-5.99	114.11	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	46	VAL	CB-CA-C	-5.97	103.04	111.28
1	L	3	VAL	CB-CA-C	5.93	118.26	110.91
2	H	103	TRP	O-C-N	-5.92	116.14	123.36
2	H	128	SER	N-CA-C	5.91	123.39	110.80
1	L	17	GLN	N-CA-C	5.85	118.43	110.35
2	H	63	ILE	CA-CB-CG2	5.85	120.44	110.50
2	H	171	VAL	N-CA-CB	-5.85	102.25	110.26
2	H	38	ARG	CA-CB-CG	5.82	125.74	114.10
2	H	173	THR	CB-CA-C	5.80	119.09	110.62
1	L	13	VAL	O-C-N	-5.79	116.95	123.03
2	H	38	ARG	O-C-N	-5.79	115.67	123.19
1	L	19	ALA	N-CA-C	-5.78	100.47	109.72
1	L	133	VAL	N-CA-C	5.70	116.48	108.17
2	H	153	THR	CA-CB-OG1	-5.70	101.06	109.60
1	L	9	ALA	N-CA-C	-5.69	105.06	112.23
2	H	173	THR	N-CA-CB	-5.69	102.02	110.90
2	H	24	VAL	N-CA-C	-5.68	102.24	109.80
2	H	194	PRO	CA-C-O	-5.64	114.91	121.34
2	H	31	ARG	N-CA-C	-5.64	102.05	110.23
2	H	100(A)	THR	N-CA-CB	-5.62	103.98	113.15
1	L	34	HIS	CB-CG-ND1	5.57	131.05	122.70
1	L	38	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	H	150	GLU	N-CA-C	-5.50	102.28	110.20
1	L	130	ALA	N-CA-C	5.50	117.31	107.80
2	H	48	MET	O-C-N	5.49	128.84	122.25
2	H	35(B)	HIS	CB-CA-C	-5.48	100.61	110.36
2	H	157	TRP	CB-CG-CD1	-5.48	118.68	126.90
3	P	315	HIS	N-CA-C	-5.47	95.68	111.00
2	H	24	VAL	CB-CA-C	-5.45	103.75	111.28
2	H	148	PHE	CB-CA-C	-5.45	101.62	109.63
1	L	146	VAL	CB-CA-C	-5.44	102.52	110.62
2	H	35(B)	HIS	CB-CG-ND1	5.42	130.83	122.70
2	H	96	ASN	CB-CG-ND2	5.41	124.52	116.40
2	H	38	ARG	N-CA-CB	-5.41	101.83	111.08
1	L	39	LYS	N-CA-C	-5.39	102.64	110.08
2	H	69	ILE	O-C-N	-5.38	115.87	122.97
1	L	92	ASN	N-CA-C	-5.38	106.85	113.41
1	L	138	ASN	N-CA-C	5.38	118.54	111.28
1	L	161	ASN	N-CA-C	5.36	117.64	108.90
1	L	119	PRO	CA-C-N	5.36	125.30	119.78
1	L	119	PRO	C-N-CA	5.36	125.30	119.78
2	H	46	GLU	CA-C-O	5.36	126.27	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	35(B)	HIS	CA-C-O	-5.35	114.93	121.78
2	H	137	MET	O-C-N	-5.35	116.24	123.19
1	L	97	THR	CA-CB-CG2	5.34	119.57	110.50
2	H	162	ASN	N-CA-C	-5.32	104.04	111.39
2	H	82(A)	ILE	CA-CB-CG2	5.31	119.53	110.50
2	H	94	ARG	CD-NE-CZ	-5.29	116.99	124.40
2	H	198	PRO	N-CA-CB	5.28	108.76	103.48
1	L	105	GLU	CA-C-O	5.25	127.05	121.11
1	L	81	ASP	N-CA-CB	-5.24	102.14	110.22
2	H	206	THR	CA-CB-CG2	5.24	119.41	110.50
1	L	107	ARG	O-C-N	5.23	129.18	123.27
1	L	126	THR	CA-CB-OG1	-5.23	101.76	109.60
1	L	63	SER	N-CA-C	5.23	116.93	108.41
3	P	315	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	L	80	ALA	N-CA-C	5.16	121.80	110.80
1	L	35	TRP	CB-CG-CD1	-5.16	119.16	126.90
2	H	97	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	L	63	SER	CA-C-O	5.15	125.81	120.30
2	H	61	PRO	N-CA-C	-5.15	103.02	111.15
2	H	47	TRP	CA-C-N	-5.14	113.32	122.42
2	H	47	TRP	C-N-CA	-5.14	113.32	122.42
2	H	1	GLN	CA-C-O	-5.12	112.10	120.80
1	L	67	SER	N-CA-C	5.11	116.61	108.79
1	L	190	ASN	CA-CB-CG	5.10	117.70	112.60
1	L	90	GLN	CA-CB-CG	5.09	124.29	114.10
2	H	62	SER	N-CA-C	-5.09	99.95	110.80
1	L	148	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	L	211	ARG	N-CA-C	5.09	125.24	111.00
2	H	78	PHE	CA-CB-CG	5.08	118.88	113.80
1	L	47	LEU	CB-CA-C	-5.08	102.83	111.26
2	H	211	ALA	CA-C-N	-5.08	116.92	123.16
2	H	211	ALA	C-N-CA	-5.08	116.92	123.16
1	L	155	ARG	CA-C-O	5.08	127.27	121.58
2	H	96	ASN	CA-CB-CG	-5.06	107.54	112.60
2	H	151	PRO	CA-N-CD	-5.06	104.42	111.50
1	L	163	TRP	CE2-CD2-CG	-5.05	101.13	107.20
1	L	196	ALA	CA-C-O	-5.05	114.93	120.69
2	H	45	LEU	CA-C-O	-5.05	115.51	121.16
1	L	99	GLY	N-CA-C	-5.04	104.74	112.85
1	L	190	ASN	O-C-N	-5.03	115.69	122.43
2	H	68	THR	CA-C-N	-5.02	116.47	122.90
2	H	68	THR	C-N-CA	-5.02	116.47	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	39	LYS	O-C-N	-5.02	116.00	121.53
1	L	189	HIS	CA-CB-CG	5.02	118.82	113.80
2	H	139	THR	N-CA-C	-5.01	101.54	109.76
1	L	126	THR	N-CA-CB	-5.00	102.49	109.94

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	199	ARG	Mainchain
1	L	211	ARG	Sidechain

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	1662	0	1586	55	0
2	H	1700	0	1672	61	0
3	P	79	0	73	2	0
All	All	3441	0	3331	111	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 (111) 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:127:GLY:HA2	2:H:226:ARG:HD3	1.55	0.88
2:H:196:SER:OG	2:H:198:PRO:HD2	1.79	0.82
1:L:147:LYS:HB2	1:L:195:GLU:HB2	1.66	0.78
2:H:199:ARG:HD2	2:H:200:PRO:HA	1.67	0.74
1:L:187:GLU:HA	1:L:211:ARG:NH2	2.03	0.74
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.69	0.74
2:H:35:CYS:HA	2:H:52:CYS:HA	1.69	0.74
1:L:187:GLU:HA	1:L:211:ARG:HH22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:PRO:O	2:H:203:GLU:HB2	1.91	0.71
1:L:190:ASN:HA	1:L:211:ARG:HG3	1.72	0.69
1:L:184:ASP:HA	1:L:187:GLU:HB2	1.74	0.69
1:L:34:HIS:HE2	2:H:100(A):THR:HG22	1.59	0.67
1:L:190:ASN:HA	1:L:211:ARG:CG	2.26	0.66
2:H:138:VAL:HG23	2:H:193:VAL:HG12	1.77	0.65
1:L:139:PHE:HE1	1:L:142:LYS:HA	1.63	0.63
1:L:33:MET:C	1:L:33:MET:SD	2.82	0.62
1:L:106:MET:C	1:L:106:MET:SD	2.83	0.61
2:H:96:ASN:ND2	2:H:99:TYR:H	1.98	0.61
2:H:196:SER:O	2:H:202:SER:HB2	2.01	0.60
1:L:54:LEU:CD2	1:L:58:VAL:HB	2.33	0.59
1:L:115:VAL:HA	1:L:135:PHE:O	2.03	0.59
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.66	0.59
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.39	0.58
1:L:187:GLU:CA	1:L:211:ARG:HH22	2.16	0.58
2:H:93:SER:HB2	2:H:102:VAL:O	2.04	0.57
3:P:319:GLY:O	3:P:322:ARG:HB2	2.05	0.57
1:L:12:VAL:HA	1:L:105:GLU:O	2.05	0.56
2:H:32:THR:HA	2:H:53:TYR:CD2	2.40	0.56
2:H:143:LEU:CD1	2:H:145:LYS:HB2	2.36	0.56
2:H:63:ILE:HG23	2:H:67:SER:CB	2.36	0.55
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.21	0.55
2:H:96:ASN:HB3	2:H:100:GLU:HB2	1.87	0.55
2:H:114:ALA:HB3	2:H:148:PHE:CE2	2.42	0.55
1:L:136:LEU:HD21	1:L:146:VAL:HG13	1.89	0.55
1:L:186:TYR:HA	1:L:192:TYR:OH	2.07	0.55
2:H:140:LEU:CD2	2:H:199:ARG:HG3	2.36	0.55
1:L:54:LEU:HD21	1:L:58:VAL:HB	1.89	0.55
1:L:16:GLY:HA2	1:L:77:PRO:HB2	1.89	0.54
2:H:87:THR:HG23	2:H:110:THR:HA	1.90	0.54
1:L:91:ASN:HB3	2:H:100(A):THR:CG2	2.39	0.53
1:L:34:HIS:CD2	2:H:100(B):TYR:HB3	2.43	0.53
2:H:198:PRO:O	2:H:203:GLU:N	2.40	0.52
2:H:122:TYR:HD2	2:H:143:LEU:HD12	1.75	0.51
1:L:144:ILE:HD11	1:L:196:ALA:HB1	1.93	0.51
1:L:14:SER:O	1:L:17:GLN:HB2	2.10	0.51
1:L:136:LEU:HD12	1:L:136:LEU:N	2.26	0.51
1:L:90:GLN:NE2	1:L:96:PRO:HA	2.25	0.50
1:L:15:LEU:HD23	1:L:79:GLU:HA	1.94	0.50
1:L:65:SER:OG	1:L:72:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:HD21	1:L:146:VAL:CG1	2.41	0.50
1:L:186:TYR:OH	1:L:211:ARG:OXT	2.23	0.50
2:H:34:TYR:HA	2:H:95:GLU:O	2.13	0.49
2:H:11:VAL:HA	2:H:110:THR:O	2.13	0.49
2:H:122:TYR:HB2	2:H:143:LEU:HB3	1.95	0.48
1:L:34:HIS:NE2	2:H:100(A):THR:HG22	2.25	0.48
1:L:160:LEU:HD11	2:H:179:GLN:NE2	2.29	0.48
2:H:13:LYS:HB2	2:H:16:GLN:NE2	2.28	0.48
1:L:147:LYS:O	1:L:194:CYS:HA	2.13	0.48
1:L:25:ALA:O	1:L:69:THR:HG22	2.14	0.48
1:L:4:MET:HE3	1:L:23:CYS:SG	2.53	0.48
2:H:67:SER:HA	2:H:81:GLN:O	2.14	0.48
1:L:193:THR:OG1	1:L:208:SER:HB3	2.14	0.48
2:H:143:LEU:HD11	2:H:145:LYS:HB2	1.94	0.48
1:L:185:GLU:O	1:L:189:HIS:HD2	1.97	0.47
2:H:162:ASN:HB2	2:H:166:LEU:HG	1.96	0.47
2:H:34:TYR:CD2	2:H:94:ARG:HD3	2.49	0.47
2:H:171:VAL:HA	2:H:190:SER:O	2.15	0.47
2:H:221:LYS:HD2	2:H:221:LYS:HA	1.74	0.47
1:L:160:LEU:O	1:L:177:SER:HA	2.15	0.47
1:L:187:GLU:C	1:L:211:ARG:HH12	2.22	0.47
2:H:13:LYS:NZ	2:H:16:GLN:HE22	2.12	0.47
2:H:38:ARG:HA	2:H:89:MET:O	2.15	0.47
2:H:37:ILE:HD13	2:H:103:TRP:CH2	2.50	0.46
1:L:94:ASP:HB3	2:H:58:TYR:CE2	2.50	0.46
1:L:2:ILE:O	1:L:97:THR:HG21	2.15	0.46
2:H:35(A):TRP:CH2	2:H:94:ARG:HG3	2.51	0.46
2:H:19:SER:HA	2:H:80:ILE:O	2.15	0.46
2:H:10:ALA:HB1	2:H:149:PRO:HG2	1.98	0.46
2:H:13:LYS:HZ3	2:H:13:LYS:H	1.64	0.46
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.73	0.46
1:L:150:ILE:HA	1:L:192:TYR:HA	1.97	0.46
2:H:196:SER:CB	2:H:198:PRO:CD	2.94	0.46
2:H:196:SER:OG	2:H:198:PRO:CD	2.59	0.46
1:L:153:SER:HB2	1:L:155:ARG:HH21	1.81	0.45
1:L:161:ASN:ND2	1:L:175:MET:HE1	2.31	0.45
2:H:18:LEU:O	2:H:81:GLN:HA	2.17	0.45
2:H:119:PRO:HD2	2:H:217:THR:HG21	1.98	0.45
1:L:159:VAL:HA	1:L:178:THR:O	2.16	0.45
2:H:24:VAL:HG12	2:H:25:SER:N	2.32	0.44
3:P:321:GLY:HA2	3:P:324:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.53	0.43
1:L:153:SER:HB2	1:L:155:ARG:NH2	2.33	0.43
2:H:140:LEU:HD21	2:H:199:ARG:HG3	2.00	0.43
1:L:181:LEU:HD11	1:L:192:TYR:CE1	2.53	0.43
1:L:116:SER:O	1:L:134:CYS:HA	2.18	0.43
1:L:181:LEU:HD11	1:L:192:TYR:HE1	1.84	0.42
2:H:196:SER:CB	2:H:198:PRO:HD2	2.48	0.42
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.54	0.42
1:L:211:ARG:HG2	1:L:211:ARG:HH11	1.83	0.42
2:H:136:SER:O	2:H:194:PRO:HA	2.19	0.42
2:H:143:LEU:C	2:H:143:LEU:HD13	2.45	0.42
1:L:50:ILE:O	1:L:50:ILE:HG22	2.19	0.42
2:H:154:VAL:HA	2:H:209:ASN:O	2.19	0.42
2:H:90:TYR:O	2:H:106:GLY:HA2	2.19	0.41
2:H:2:VAL:HG21	2:H:94:ARG:NH2	2.35	0.41
2:H:63:ILE:HG23	2:H:67:SER:HB2	2.02	0.41
1:L:195:GLU:HG2	1:L:206:VAL:HG13	2.02	0.41
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.84	0.41
2:H:24:VAL:HB	2:H:76:ASN:ND2	2.36	0.41
1:L:198:HIS:NE2	1:L:200:THR:OG1	2.54	0.41
2:H:53:TYR:CG	2:H:54:GLU:N	2.88	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	213/215 (99%)	191 (90%)	15 (7%)	7 (3%)	3	17
2	H	219/221 (99%)	200 (91%)	15 (7%)	4 (2%)	6	31
3	P	8/24 (33%)	6 (75%)	1 (12%)	1 (12%)	0	1
All	All	440/460 (96%)	397 (90%)	31 (7%)	12 (3%)	4	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	151	ASP
2	H	62	SER
2	H	53	TYR
3	P	322	ARG
1	L	156	GLN
2	H	180	SER
2	H	196	SER
1	L	2	ILE
1	L	68	ARG
1	L	80	ALA
1	L	152	GLY
1	L	50	ILE

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	189/189 (100%)	155 (82%)	34 (18%)	2	10
2	H	198/198 (100%)	162 (82%)	36 (18%)	2	9
3	P	7/20 (35%)	7 (100%)	0	100	100
All	All	394/407 (97%)	324 (82%)	70 (18%)	2	10

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

Mol	Chain	Res	Type
1	L	7	SER
1	L	11	LEU
1	L	13	VAL
1	L	14	SER
1	L	18	ARG
1	L	26	SER
1	L	27	GLU
1	L	27(A)	SER
1	L	27(B)	VAL

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Mol	Chain	Res	Type
1	L	27(C)	ASP
1	L	27(D)	SER
1	L	39	LYS
1	L	42	GLN
1	L	46	VAL
1	L	52	SER
1	L	54	LEU
1	L	74	THR
1	L	77	PRO
1	L	105	GLU
1	L	120	PRO
1	L	126	THR
1	L	132	VAL
1	L	143	ASP
1	L	145	ASN
1	L	146	VAL
1	L	149	LYS
1	L	156	GLN
1	L	165	ASP
1	L	188	ARG
1	L	200	THR
1	L	202	THR
1	L	203	SER
1	L	206	VAL
1	L	208	SER
2	H	2	VAL
2	H	13	LYS
2	H	19	SER
2	H	38	ARG
2	H	54	GLU
2	H	63	ILE
2	H	68	THR
2	H	73	THR
2	H	78	PHE
2	H	79	PHE
2	H	82	LEU
2	H	82(A)	ILE
2	H	82(B)	SER
2	H	82(C)	VAL
2	H	94	ARG
2	H	96	ASN
2	H	105	GLN

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Mol	Chain	Res	Type
2	H	107	THR
2	H	113	SER
2	H	128	SER
2	H	134	THR
2	H	138	VAL
2	H	150	GLU
2	H	151	PRO
2	H	153	THR
2	H	168	SER
2	H	188	SER
2	H	192	THR
2	H	193	VAL
2	H	199	ARG
2	H	204	THR
2	H	206	THR
2	H	210	VAL
2	H	216	SER
2	H	218	LYS
2	H	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	38	GLN
1	L	92	ASN
1	L	210	ASN
2	H	5	GLN
2	H	16	GLN
2	H	39	GLN
2	H	96	ASN
2	H	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.