



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1ACY
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

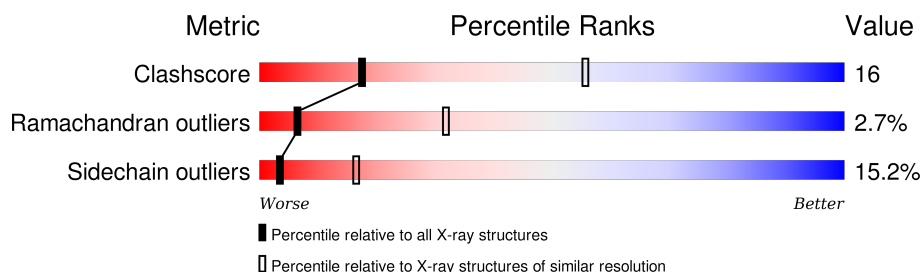
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	
2	H	221	
3	P	24	

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.70 Å 154.00 Å 121.90 Å 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	1.03	0/1700	1.85	36/2310 (1.6%)
2	H	1.10	2/1746 (0.1%)	1.90	44/2385 (1.8%)
3	P	0.99	0/82	1.68	1/110 (0.9%)
All	All	1.07	2/3528 (0.1%)	1.87	81/4805 (1.7%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	47	TRP	CG-CD2	-6.02	1.33	1.43
2	H	35(B)	HIS	CA-CB	-5.32	1.42	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	ARG	NE-CZ-NH2	-18.13	111.24	120.30
2	H	38	ARG	NE-CZ-NH1	12.27	126.44	120.30
1	L	211	ARG	NE-CZ-NH1	11.98	126.29	120.30
2	H	47	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	L	163	TRP	CD1-CG-CD2	8.72	113.28	106.30
1	L	148	TRP	CD1-CG-CD2	8.64	113.21	106.30
2	H	199	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	L	35	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	L	148	TRP	CE2-CD2-CG	-7.76	101.09	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	163	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	L	106	MET	CB-CG-SD	-7.57	89.69	112.40
2	H	66	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	H	175	PRO	CA-N-CD	-7.33	101.23	111.50
2	H	47	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	H	63	ILE	CA-CB-CG1	-7.20	97.32	111.00
2	H	35(A)	TRP	CD1-CG-CD2	7.15	112.02	106.30
2	H	147	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	L	61	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	L	155	ARG	CA-C-N	-6.88	102.07	117.20
1	L	35	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	L	11	LEU	CA-CB-CG	6.83	131.02	115.30
2	H	71	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	H	38	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	L	186	TYR	CB-CG-CD2	-6.67	117.00	121.00
2	H	36	TRP	CE2-CD2-CG	-6.67	101.97	107.30
2	H	103	TRP	CD1-CG-CD2	6.66	111.63	106.30
2	H	199	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	H	103	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	L	133	VAL	CG1-CB-CG2	-6.48	100.53	110.90
2	H	36	TRP	CD1-CG-CD2	6.48	111.48	106.30
2	H	157	TRP	CB-CG-CD1	-6.40	118.68	127.00
2	H	100(A)	THR	CA-CB-CG2	6.33	121.26	112.40
2	H	191	VAL	CB-CA-C	-6.32	99.40	111.40
2	H	66	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	H	199	ARG	N-CA-C	-6.23	94.19	111.00
1	L	105	GLU	CA-CB-CG	6.20	127.04	113.40
1	L	106	MET	N-CA-CB	-6.14	99.55	110.60
1	L	35	TRP	CB-CG-CD1	-6.03	119.16	127.00
2	H	22	CYS	CA-CB-SG	-5.96	103.28	114.00
2	H	98	MET	CA-CB-CG	5.90	123.33	113.30
1	L	88	CYS	CA-CB-SG	-5.88	103.41	114.00
1	L	105	GLU	N-CA-C	-5.86	95.18	111.00
2	H	35(A)	TRP	CE2-CD2-CG	-5.85	102.62	107.30
2	H	89	MET	CG-SD-CE	-5.83	90.87	100.20
1	L	24	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	H	100(B)	TYR	CB-CG-CD2	-5.77	117.54	121.00
2	H	180	SER	CA-C-N	-5.73	104.59	117.20
1	L	188	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	L	87	TYR	CB-CG-CD2	-5.70	117.58	121.00
3	P	315	HIS	N-CA-C	-5.67	95.68	111.00
1	L	68	ARG	NE-CZ-NH1	5.64	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	35	TRP	CG-CD1-NE1	-5.61	104.49	110.10
2	H	38	ARG	CA-CB-CG	5.61	125.74	113.40
2	H	157	TRP	CE2-CD2-CG	-5.60	102.82	107.30
1	L	108	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	H	47	TRP	CE2-CD2-CE3	5.44	125.23	118.70
1	L	148	TRP	CG-CD1-NE1	-5.39	104.71	110.10
2	H	36	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	H	40	ALA	CA-C-N	5.32	132.01	117.10
2	H	62	SER	N-CA-CB	5.32	118.48	110.50
1	L	211	ARG	N-CA-C	5.27	125.24	111.00
1	L	100	ALA	N-CA-CB	-5.25	102.75	110.10
2	H	35(A)	TRP	CE2-CD2-CE3	5.23	124.98	118.70
2	H	47	TRP	CD2-CE2-CZ2	-5.18	116.08	122.30
2	H	193	VAL	N-CA-CB	-5.17	100.11	111.50
1	L	192	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	H	100(A)	THR	CA-CB-OG1	-5.16	98.16	109.00
1	L	108	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	L	97	THR	CA-CB-CG2	5.12	119.57	112.40
2	H	35	CYS	CA-CB-SG	5.12	123.22	114.00
2	H	36	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	L	3	VAL	N-CA-CB	-5.10	100.28	111.50
2	H	103	TRP	CA-C-N	5.10	126.39	116.20
2	H	157	TRP	CD1-CG-CD2	5.09	110.38	106.30
1	L	49	TYR	CA-C-N	-5.08	106.03	117.20
1	L	60	ALA	CA-C-N	-5.07	106.04	117.20
2	H	52	CYS	CA-CB-SG	-5.07	104.87	114.00
1	L	107	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	H	151	PRO	CA-N-CD	-5.06	104.42	111.50
1	L	35	TRP	CG-CD2-CE3	5.05	138.44	133.90
2	H	206	THR	CA-CB-CG2	5.00	119.41	112.40

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 ⓘ

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	53	0
2	H	1700	0	1672	60	0
3	P	79	0	73	2	0
All	All	3441	0	3331	108	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 (108) 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
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.69	0.74
1:L:187:GLU:HA	1:L:211:ARG:NH2	2.03	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
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
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
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.66	0.59
1:L:115:VAL:HA	1:L:135:PHE:O	2.03	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
1:L:106:MET:SD	1:L:106:MET:C	2.83	0.57
1:L:33:MET:SD	1:L:33:MET:C	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:LEU:CD1	2:H:145:LYS:HB2	2.36	0.56
2:H:32:THR:HA	2:H:53:TYR:CD2	2.40	0.56
2:H:63:ILE:HG23	2:H:67:SER:CB	2.36	0.55
2:H:96:ASN:HB3	2:H:100:GLU:HB2	1.87	0.55
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.21	0.55
2:H:114:ALA:HB3	2:H:148:PHE:CE2	2.42	0.55
1:L:186:TYR:HA	1:L:192:TYR:OH	2.07	0.55
1:L:136:LEU:HD21	1:L:146:VAL:HG13	1.89	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:N	1:L:136:LEU:HD12	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:136:LEU:HD21	1:L:146:VAL:CG1	2.41	0.50
1:L:65:SER:OG	1:L:72:THR:HB	2.12	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
2:H:13:LYS:HB2	2:H:16:GLN:NE2	2.28	0.48
1:L:160:LEU:HD11	2:H:179:GLN:NE2	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:35(A):TRP:CH2	2:H:94:ARG:HG3	2.51	0.46
1:L:2:ILE:O	1:L:97:THR:HG21	2.15	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:196:SER:CB	2:H:198:PRO:CD	2.94	0.46
1:L:150:ILE:HA	1:L:192:TYR:HA	1.97	0.46
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.73	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
2:H:119:PRO:HD2	2:H:217:THR:HG21	1.98	0.45
2:H:18:LEU:O	2:H:81:GLN:HA	2.17	0.45
1:L:159:VAL:HA	1:L:178:THR:O	2.16	0.45
2:H:13:LYS:HZ3	2:H:13:LYS:H	1.65	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
2:H:140:LEU:HD21	2:H:199:ARG:HG3	2.00	0.43
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
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
2:H:196:SER:CB	2:H:198:PRO:HD2	2.48	0.42
1:L:181:LEU:HD11	1:L:192:TYR:HE1	1.84	0.42
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.83	0.42
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.54	0.42
2:H:136:SER:O	2:H:194:PRO:HA	2.19	0.42
1:L:187:GLU:C	1:L:211:ARG:HH12	2.22	0.42
2:H:154:VAL:HA	2:H:209:ASN:O	2.19	0.42
1:L:50:ILE:O	1:L:50:ILE:HG22	2.19	0.42
2:H:90:TYR:O	2:H:106:GLY:HA2	2.19	0.41
2:H:63:ILE:HG23	2:H:67:SER:HB2	2.02	0.41
2:H:2:VAL:HG21	2:H:94:ARG:NH2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	213/215 (99%)	191 (90%)	15 (7%)	7 (3%)	5	26
2	H	219/221 (99%)	200 (91%)	15 (7%)	4 (2%)	11	45
3	P	8/24 (33%)	6 (75%)	1 (12%)	1 (12%)	0	1
All	All	440/460 (96%)	397 (90%)	31 (7%)	12 (3%)	6	32

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%)	161 (85%)	28 (15%)	4	17
2	H	198/198 (100%)	167 (84%)	31 (16%)	3	15
3	P	7/20 (35%)	6 (86%)	1 (14%)	4	19
All	All	394/407 (97%)	334 (85%)	60 (15%)	3	16

All (60) 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	39	LYS
1	L	42	GLN
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	132	VAL
1	L	143	ASP
1	L	145	ASN
1	L	146	VAL
1	L	149	LYS
1	L	155	ARG
1	L	156	GLN
1	L	165	ASP
1	L	200	THR
1	L	202	THR
1	L	203	SER

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Mol	Chain	Res	Type
1	L	206	VAL
1	L	211	ARG
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	64	LYS
2	H	73	THR
2	H	78	PHE
2	H	79	PHE
2	H	82	LEU
2	H	82(A)	ILE
2	H	94	ARG
2	H	96	ASN
2	H	105	GLN
2	H	107	THR
2	H	113	SER
2	H	128	SER
2	H	134	THR
2	H	138	VAL
2	H	149	PRO
2	H	150	GLU
2	H	151	PRO
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	210	VAL
2	H	219	VAL
3	P	324	PHE

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

Mol	Chain	Res	Type
1	L	42	GLN
1	L	189	HIS
2	H	16	GLN
2	H	96	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.