Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 06:43 PM EDT

PDB ID	:	1GGI
Title	:	CRYSTAL STRUCTURE OF AN HIV-1 NEUTRALIZING ANTIBODY 50.1 IN COMPLEX WITH ITS V3 LOOP PEPTIDE ANTIGEN
Authors	:	Stanfield, R.L.; Rini, J.M.; Wilson, I.A.
Deposited on	:	1993-04-02
Resolution	:	2.80 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:

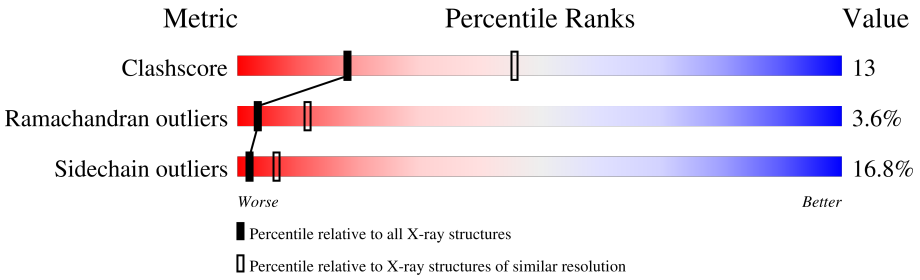
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	218	52% 38% 7% ••
1	M	218	55% 37% 5% ••
2	H	222	48% 35% 12% • •
2	J	222	53% 35% 7% • •
3	P	16	31% 25% 44%
3	Q	16	38% 12% 6% 44%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6712 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 IGG2A 50.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1662	1031	283	343	5			
1	M	215	Total	C	N	O	S	0	0	0
			1662	1031	283	343	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	LEU	MET	conflict	EMBL AJ131289
L	7	SER	THR	conflict	EMBL AJ131289
L	9	GLY	ALA	conflict	EMBL AJ131289
L	27A	SER	ASN	conflict	EMBL AJ131289
L	27C	ASP	ARG	conflict	EMBL AJ131289
L	28	ASP	TYR	conflict	EMBL AJ131289
L	33	LEU	MET	conflict	EMBL AJ131289
L	40	PRO	ALA	conflict	EMBL AJ131289
L	51	SER	ALA	conflict	EMBL AJ131289
L	55	ILE	GLU	conflict	EMBL AJ131289
L	60	ASP	ALA	conflict	EMBL AJ131289
L	87	TYR	PHE	conflict	EMBL AJ131289
L	90	GLN	ARG	conflict	EMBL AJ131289
L	94	ASP	VAL	conflict	EMBL AJ131289
L	96	LEU	TRP	conflict	EMBL AJ131289
L	100	ALA	GLY	conflict	EMBL AJ131289
M	4	LEU	MET	conflict	EMBL AJ131289
M	7	SER	THR	conflict	EMBL AJ131289
M	9	GLY	ALA	conflict	EMBL AJ131289
M	27A	SER	ASN	conflict	EMBL AJ131289
M	27C	ASP	ARG	conflict	EMBL AJ131289
M	28	ASP	TYR	conflict	EMBL AJ131289
M	33	LEU	MET	conflict	EMBL AJ131289
M	40	PRO	ALA	conflict	EMBL AJ131289
M	51	SER	ALA	conflict	EMBL AJ131289

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Chain	Residue	Modelled	Actual	Comment	Reference
M	55	ILE	GLU	conflict	EMBL AJ131289
M	60	ASP	ALA	conflict	EMBL AJ131289
M	87	TYR	PHE	conflict	EMBL AJ131289
M	90	GLN	ARG	conflict	EMBL AJ131289
M	94	ASP	VAL	conflict	EMBL AJ131289
M	96	LEU	TRP	conflict	EMBL AJ131289
M	100	ALA	GLY	conflict	EMBL AJ131289

- Molecule 2 is a protein called IGG2A 50.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1627	1032	266	323	6			
2	J	215	Total	C	N	O	S	0	0	0
			1627	1032	266	323	6			

- Molecule 3 is a protein called HIV-1 V3 LOOP PEPTIDE ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			67	42	15	9	1			
3	Q	9	Total	C	N	O	S	0	0	0
			67	42	15	9	1			

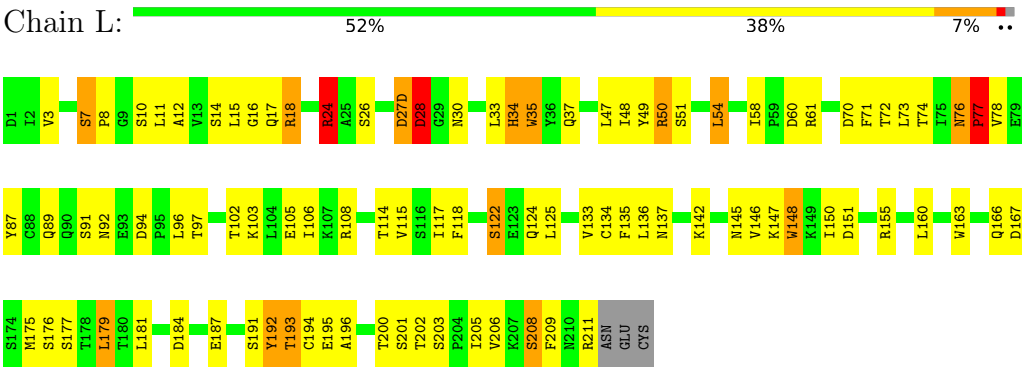
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

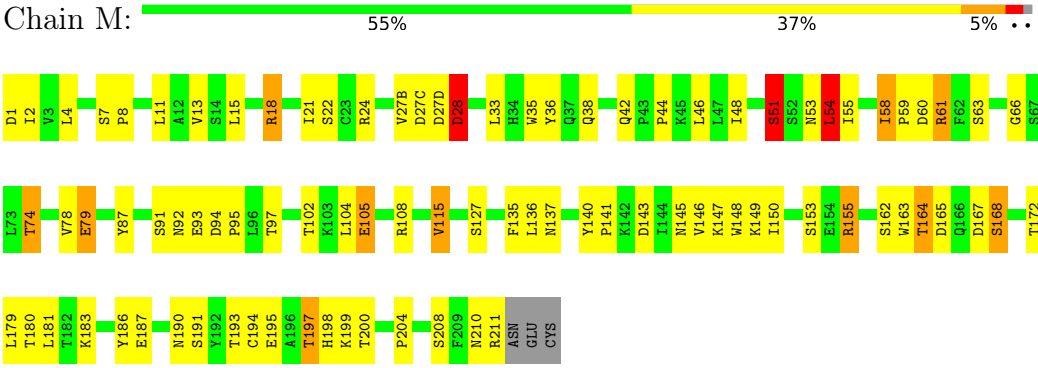
• Molecule 1: IGG2A 50.1 FAB (LIGHT CHAIN)

Chain L:



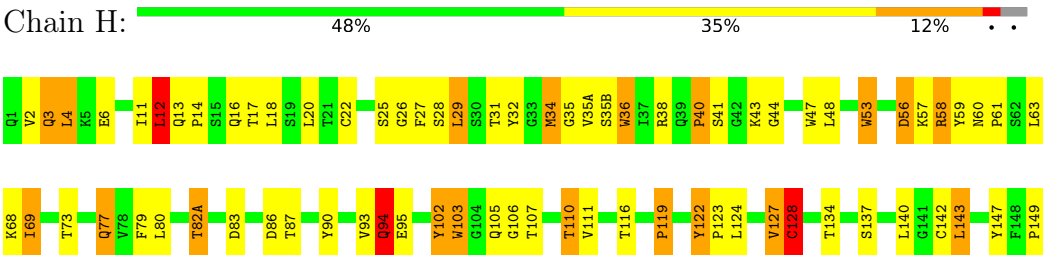
• Molecule 1: IGG2A 50.1 FAB (LIGHT CHAIN)

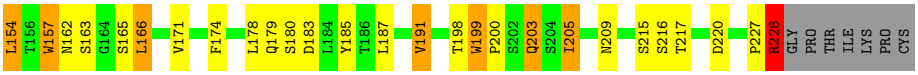
Chain M:



• Molecule 2: IGG2A 50.1 FAB (HEAVY CHAIN)

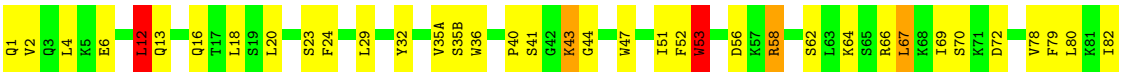
Chain H:

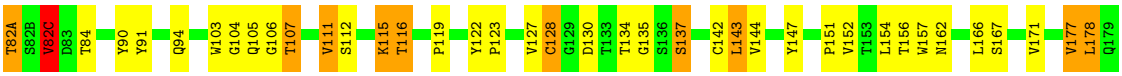




• Molecule 2: IGG2A 50.1 FAB (HEAVY CHAIN)

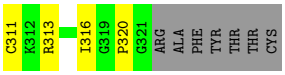
Chain J:





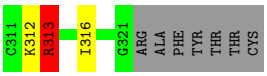
• Molecule 3: HIV-1 V3 LOOP PEPTIDE ANTIGEN

Chain P:



• Molecule 3: HIV-1 V3 LOOP PEPTIDE ANTIGEN

Chain Q:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.33Å 52.57Å 82.04Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6712	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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	0.94	0/1698	1.82	30/2309 (1.3%)
1	M	0.96	0/1698	1.87	33/2309 (1.4%)
2	H	1.00	0/1669	1.92	47/2281 (2.1%)
2	J	0.99	1/1669 (0.1%)	1.95	44/2281 (1.9%)
3	P	1.31	0/68	1.83	0/89
3	Q	1.17	0/68	2.21	1/89 (1.1%)
All	All	0.98	1/6870 (0.0%)	1.89	155/9358 (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	2
1	M	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	199	TRP	CG-CD2	-5.80	1.33	1.43

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	199	TRP	CD1-CG-CD2	11.43	115.44	106.30
2	H	122	TYR	CB-CG-CD2	-10.26	114.84	121.00
2	J	122	TYR	CB-CG-CD2	-9.96	115.03	121.00
1	M	155	ARG	NE-CZ-NH2	-9.37	115.62	120.30
2	J	103	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	M	155	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	L	163	TRP	CD1-CG-CD2	9.16	113.62	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	313	ARG	NE-CZ-NH1	8.91	124.76	120.30
2	H	66	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	J	178	LEU	CA-CB-CG	8.79	135.51	115.30
2	J	199	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	M	24	ARG	NE-CZ-NH1	8.71	124.66	120.30
2	H	36	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	M	163	TRP	CD1-CG-CD2	8.28	112.93	106.30
1	M	148	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	J	53	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	L	28	ASP	CA-C-N	-8.12	99.96	116.20
2	H	228	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	H	58	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	M	54	LEU	CA-CB-CG	8.07	133.86	115.30
2	H	199	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	L	50	ARG	NE-CZ-NH2	-7.99	116.31	120.30
2	J	47	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	L	28	ASP	CA-CB-CG	-7.81	96.21	113.40
2	H	36	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	L	160	LEU	CA-CB-CG	7.71	133.04	115.30
2	H	157	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	L	49	TYR	CB-CG-CD2	-7.64	116.42	121.00
2	J	107	THR	N-CA-CB	7.41	124.38	110.30
2	J	178	LEU	N-CA-C	7.38	130.92	111.00
1	L	163	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	M	163	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	J	53	TRP	CE2-CD2-CG	-7.35	101.42	107.30
2	H	66	ARG	NE-CZ-NH2	-7.29	116.65	120.30
2	J	103	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	H	56	ASP	CA-CB-CG	7.27	129.40	113.40
2	H	53	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	M	68	ARG	NE-CZ-NH2	-7.20	116.70	120.30
2	H	4	LEU	CA-CB-CG	7.19	131.84	115.30
1	M	148	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	M	173	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	M	87	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	H	32	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	L	35	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	L	24	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	M	27(C)	ASP	O-C-N	-7.08	111.38	122.70
1	L	27(D)	ASP	CA-C-N	-6.97	101.86	117.20
2	J	228	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	L	148	TRP	CG-CD2-CE3	6.90	140.11	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	53	TRP	CD1-CG-CD2	6.84	111.77	106.30
2	H	47	TRP	CD1-CG-CD2	6.82	111.76	106.30
1	L	148	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	M	27(C)	ASP	CA-C-N	6.81	132.17	117.20
1	L	87	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	M	93	GLU	CA-CB-CG	6.78	128.32	113.40
2	J	177	VAL	CG1-CB-CG2	6.76	121.72	110.90
2	H	127	VAL	CA-CB-CG2	-6.75	100.77	110.90
2	J	107	THR	CB-CA-C	-6.71	93.48	111.60
2	J	67	LEU	CA-CB-CG	6.70	130.72	115.30
2	J	199	TRP	CG-CD1-NE1	-6.70	103.40	110.10
2	J	143	LEU	CA-CB-CG	6.70	130.71	115.30
2	H	53	TRP	CG-CD2-CE3	6.68	139.91	133.90
2	H	157	TRP	CE2-CD2-CG	-6.65	101.98	107.30
2	J	157	TRP	CD1-CG-CD2	6.64	111.62	106.30
2	H	199	TRP	CE2-CD2-CG	-6.62	102.00	107.30
2	J	47	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	L	35	TRP	CE2-CD2-CG	-6.59	102.03	107.30
2	J	103	TRP	CG-CD1-NE1	-6.49	103.61	110.10
2	J	157	TRP	CE2-CD2-CG	-6.42	102.16	107.30
2	H	179	GLN	CA-CB-CG	6.39	127.45	113.40
1	M	36	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	M	53	ASN	CB-CG-ND2	6.33	131.90	116.70
1	M	35	TRP	CD1-CG-CD2	6.33	111.36	106.30
2	J	94	GLN	O-C-N	-6.33	112.58	122.70
1	L	163	TRP	CB-CA-C	-6.31	97.78	110.40
2	H	12	LEU	CA-CB-CG	6.31	129.81	115.30
2	J	36	TRP	CD1-CG-CD2	6.28	111.32	106.30
1	M	68	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	L	26	SER	CA-CB-OG	6.24	128.06	111.20
2	H	47	TRP	CE2-CD2-CG	-6.22	102.32	107.30
2	H	127	VAL	CA-CB-CG1	6.22	120.23	110.90
1	L	96	LEU	CB-CG-CD1	-6.18	100.50	111.00
1	L	163	TRP	CG-CD1-NE1	-6.13	103.97	110.10
2	H	69	ILE	CB-CA-C	-6.12	99.36	111.60
2	J	36	TRP	CE2-CD2-CG	-6.11	102.41	107.30
2	H	103	TRP	CE2-CD2-CG	-6.09	102.43	107.30
2	H	128	CYS	CA-C-N	-6.06	104.08	116.20
1	L	77	PRO	O-C-N	-6.04	113.03	122.70
2	H	199	TRP	CG-CD1-NE1	-6.04	104.06	110.10
2	J	53	TRP	CB-CG-CD1	-6.03	119.16	127.00
1	L	3	VAL	CA-CB-CG2	-6.01	101.89	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	82(A)	THR	CA-C-N	5.98	130.36	117.20
2	H	14	PRO	CA-C-N	-5.97	104.06	117.20
2	H	18	LEU	CA-CB-CG	5.95	128.99	115.30
1	L	24	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	L	148	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	M	35	TRP	CE2-CD2-CG	-5.89	102.59	107.30
2	H	103	TRP	CD1-CG-CD2	5.84	110.97	106.30
2	H	191	VAL	CG1-CB-CG2	-5.83	101.57	110.90
2	J	82(A)	THR	CA-CB-CG2	5.82	120.54	112.40
2	J	94	GLN	CA-C-N	5.81	129.97	117.20
2	H	53	TRP	CB-CG-CD1	-5.80	119.46	127.00
2	J	53	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	M	168	SER	N-CA-C	5.77	126.58	111.00
2	H	157	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	L	27(D)	ASP	C-N-CA	5.75	136.07	121.70
2	H	36	TRP	CG-CD1-NE1	-5.71	104.39	110.10
2	H	12	LEU	CB-CA-C	-5.69	99.39	110.20
2	H	94	GLN	OE1-CD-NE2	-5.69	108.82	121.90
2	J	32	TYR	CB-CG-CD2	-5.69	117.59	121.00
2	J	82(C)	VAL	N-CA-CB	-5.67	99.02	111.50
1	M	197	THR	CA-CB-CG2	5.67	120.34	112.40
1	M	194	CYS	CA-CB-SG	-5.66	103.81	114.00
2	J	200	PRO	N-CA-C	5.65	126.78	112.10
1	L	148	TRP	CD1-CG-CD2	5.63	110.80	106.30
2	H	56	ASP	CA-C-N	-5.58	104.91	117.20
2	J	47	TRP	CG-CD1-NE1	-5.57	104.53	110.10
2	J	111	VAL	CA-C-N	-5.57	104.95	117.20
1	M	105	GLU	CA-CB-CG	5.56	125.64	113.40
2	H	41	SER	N-CA-CB	5.54	118.81	110.50
2	J	53	TRP	CG-CD1-NE1	-5.54	104.56	110.10
2	J	66	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	H	171	VAL	CA-CB-CG2	-5.50	102.66	110.90
2	H	154	LEU	CA-CB-CG	5.49	127.93	115.30
1	M	66	GLY	O-C-N	-5.49	113.92	122.70
2	H	94	GLN	CG-CD-NE2	5.49	129.87	116.70
1	L	108	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	M	61	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	L	76	ASN	CB-CG-ND2	5.43	129.74	116.70
2	H	157	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	M	51	SER	CB-CA-C	-5.38	99.88	110.10
2	J	12	LEU	CA-CB-CG	5.38	127.67	115.30
2	H	102	TYR	CB-CG-CD1	-5.37	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	35(A)	VAL	CG1-CB-CG2	-5.34	102.35	110.90
1	M	164	THR	CA-CB-CG2	5.34	119.87	112.40
2	J	91	TYR	CB-CG-CD2	-5.32	117.81	121.00
2	J	128	CYS	N-CA-C	5.31	125.34	111.00
1	L	50	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	L	35	TRP	CG-CD1-NE1	-5.27	104.83	110.10
2	J	216	SER	CA-C-N	-5.23	105.70	117.20
2	H	157	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	M	115	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	M	92	ASN	CB-CG-ND2	5.12	129.00	116.70
1	M	172	THR	OG1-CB-CG2	-5.11	98.25	110.00
2	H	127	VAL	C-N-CA	5.10	134.46	121.70
2	J	177	VAL	CA-CB-CG2	-5.10	103.25	110.90
2	J	135	GLY	CA-C-O	5.09	129.76	120.60
2	J	178	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	M	4	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	L	96	LEU	CA-CB-CG	5.06	126.93	115.30
1	L	3	VAL	CA-CB-CG1	5.03	118.44	110.90
1	M	180	THR	CA-C-N	-5.03	106.14	117.20
2	H	111	VAL	CG1-CB-CG2	-5.02	102.86	110.90
2	J	142	CYS	CA-CB-SG	-5.02	104.96	114.00
1	M	190	ASN	CB-CG-ND2	5.01	128.73	116.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	192	TYR	Sidechain
1	L	203	SER	Peptide
1	M	186	TYR	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	1592	48	0
1	M	1662	0	1592	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1627	0	1601	52	0
2	J	1627	0	1601	41	0
3	P	67	0	72	1	0
3	Q	67	0	72	3	0
All	All	6712	0	6530	177	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 13.

All (177) 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:119:PRO:HB3	2:H:147:TYR:HB3	1.44	0.98
1:M:150:ILE:HD11	1:M:179:LEU:HD21	1.64	0.79
1:L:7:SER:HB3	1:L:24:ARG:HH22	1.50	0.76
2:H:6:GLU:HB2	2:H:107:THR:HG23	1.69	0.72
1:L:115:VAL:HG22	1:L:136:LEU:HG	1.72	0.71
2:H:40:PRO:HB2	2:H:43:LYS:HB3	1.73	0.71
2:J:119:PRO:HB3	2:J:147:TYR:HB3	1.73	0.70
2:J:72:ASP:HB2	2:J:79:PHE:HE2	1.56	0.70
1:L:196:ALA:HB3	1:L:205:ILE:HG23	1.74	0.69
1:L:14:SER:O	1:L:17:GLN:HG2	1.93	0.68
2:H:127:VAL:HG22	2:H:228:ARG:HD3	1.75	0.68
2:J:212:HIS:HB3	2:J:217:THR:OG1	1.96	0.66
1:L:18:ARG:HG2	1:L:76:ASN:HB2	1.78	0.66
1:L:135:PHE:HB3	1:L:137:ASN:ND2	2.11	0.66
1:M:59:PRO:HG3	1:M:61:ARG:HH21	1.60	0.65
1:M:149:LYS:HB2	1:M:193:THR:HB	1.81	0.63
2:J:12:LEU:HD12	2:J:111:VAL:HG12	1.81	0.63
1:L:61:ARG:HD2	1:L:77:PRO:HD2	1.80	0.62
1:M:48:ILE:HG22	1:M:54:LEU:CB	2.29	0.62
1:M:61:ARG:NH1	1:M:79:GLU:HB2	2.14	0.62
1:L:122:SER:HA	1:L:125:LEU:HD12	1.82	0.61
1:L:16:GLY:HA2	1:L:77:PRO:HB2	1.83	0.61
1:M:46:LEU:HG	1:M:55:ILE:HD11	1.82	0.61
2:J:40:PRO:HG2	2:J:43:LYS:HB3	1.83	0.61
2:J:72:ASP:HB2	2:J:79:PHE:CE2	2.36	0.61
2:J:211:ALA:HB1	2:J:218:LYS:HE3	1.83	0.60
1:L:136:LEU:HD22	1:L:175:MET:HE1	1.84	0.60
2:H:87:THR:HG23	2:H:110:THR:HA	1.84	0.60
1:L:124:GLN:HG3	2:H:122:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:135:PHE:HB3	1:M:137:ASN:ND2	2.18	0.59
2:H:29:LEU:HD23	2:H:34:MET:HB3	1.84	0.58
2:J:16:GLN:O	2:J:82(C):VAL:HB	2.03	0.58
1:M:135:PHE:HB3	1:M:137:ASN:HD21	1.70	0.57
2:J:35(A):VAL:HG11	2:J:78:VAL:HG21	1.85	0.57
1:L:83:VAL:HG21	1:L:106:ILE:HG12	1.85	0.57
1:M:61:ARG:HH11	1:M:79:GLU:HB2	1.68	0.57
2:J:51:ILE:HB	2:J:69:ILE:HD13	1.86	0.57
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.39	0.57
1:L:187:GLU:HA	1:L:211:ARG:NH1	2.21	0.56
1:L:115:VAL:HA	1:L:135:PHE:O	2.05	0.56
2:H:43:LYS:HE2	2:H:44:GLY:N	2.21	0.56
2:H:60:ASN:HB3	2:H:63:LEU:HB2	1.86	0.56
2:H:67:LEU:O	2:H:68:LYS:HG3	2.06	0.56
1:L:33:LEU:HD22	1:L:71:PHE:CB	2.37	0.55
1:L:150:ILE:HD11	1:L:179:LEU:HD11	1.89	0.55
1:L:133:VAL:HG21	2:H:143:LEU:HD23	1.88	0.55
2:J:67:LEU:HD12	2:J:82:ILE:HG12	1.89	0.55
2:H:90:TYR:O	2:H:106:GLY:HA2	2.07	0.55
2:H:20:LEU:HB3	2:H:36:TRP:CH2	2.41	0.55
2:H:2:VAL:HG22	2:H:26:GLY:HA3	1.88	0.54
2:H:40:PRO:HG2	2:H:43:LYS:HD3	1.89	0.54
1:M:46:LEU:HG	1:M:55:ILE:CD1	2.37	0.54
2:J:167:SER:O	2:J:171:VAL:HB	2.07	0.54
1:M:150:ILE:HD13	1:M:181:LEU:HD21	1.88	0.54
1:M:27(D):ASP:O	1:M:28:ASP:HB2	2.06	0.54
1:L:118:PHE:CD1	2:H:124:LEU:HB3	2.42	0.54
1:M:21:ILE:HG12	1:M:102:THR:HG21	1.88	0.54
1:L:117:ILE:HD13	1:L:209:PHE:HD2	1.73	0.54
2:H:17:THR:HG22	2:H:82(A):THR:HA	1.92	0.52
1:M:63:SER:HB2	1:M:74:THR:HG23	1.92	0.51
1:M:95:PRO:O	1:M:97:THR:HG23	2.09	0.51
2:H:59:TYR:OH	2:H:68:LYS:HA	2.11	0.51
2:J:84:THR:HA	2:J:111:VAL:HG23	1.93	0.51
2:H:12:LEU:HD12	2:H:16:GLN:NE2	2.26	0.50
3:Q:313:ARG:HG3	3:Q:313:ARG:HH11	1.75	0.50
2:H:27:PHE:HD2	2:H:34:MET:HG3	1.77	0.50
1:M:140:TYR:CG	1:M:141:PRO:HA	2.46	0.50
1:M:18:ARG:HH11	1:M:18:ARG:HB2	1.77	0.50
1:L:146:VAL:HA	1:L:195:GLU:O	2.12	0.49
1:L:48:ILE:CD1	1:L:54:LEU:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:GLN:OE1	3:P:316:ILE:HD13	2.12	0.49
2:H:2:VAL:HG13	2:H:25:SER:O	2.12	0.49
2:H:34:MET:O	2:H:53:TRP:HE3	1.95	0.49
2:J:13:GLN:N	2:J:16:GLN:NE2	2.59	0.49
2:J:12:LEU:HB2	2:J:16:GLN:NE2	2.28	0.49
2:J:13:GLN:HA	2:J:112:SER:O	2.12	0.49
2:H:11:ILE:HD11	2:H:149:PRO:HG3	1.94	0.49
2:J:12:LEU:HD21	2:J:18:LEU:HD12	1.94	0.49
1:L:142:LYS:HG2	1:L:173:TYR:CE2	2.47	0.49
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.78	0.48
2:J:115:LYS:HZ2	2:J:116:THR:H	1.59	0.48
2:J:115:LYS:NZ	2:J:115:LYS:HA	2.28	0.48
1:L:15:LEU:HD21	1:L:80:ALA:HB2	1.94	0.48
1:L:35:TRP:CE3	1:L:73:LEU:HD22	2.48	0.48
2:J:90:TYR:O	2:J:106:GLY:HA2	2.14	0.48
2:H:142:CYS:HB2	2:H:157:TRP:CH2	2.49	0.48
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.96	0.48
1:L:34:HIS:HD2	1:L:50:ARG:H	1.59	0.47
1:M:48:ILE:HG22	1:M:54:LEU:HB3	1.95	0.47
1:L:148:TRP:HZ2	1:L:177:SER:O	1.98	0.47
1:M:2:ILE:HG21	1:M:27(B):VAL:HG12	1.97	0.47
1:L:34:HIS:HE1	1:L:91:SER:OG	1.97	0.47
1:L:150:ILE:HD12	1:L:155:ARG:HG2	1.97	0.47
1:M:48:ILE:HD13	1:M:48:ILE:HG21	1.68	0.47
1:M:147:LYS:HB2	1:M:195:GLU:HB3	1.97	0.46
2:J:52:PHE:HB3	2:J:53:TRP:CE3	2.50	0.46
2:H:3:GLN:HB3	2:H:25:SER:OG	2.15	0.46
2:J:12:LEU:HD12	2:J:111:VAL:CG1	2.45	0.46
1:M:115:VAL:HA	1:M:135:PHE:O	2.16	0.46
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.98	0.46
2:H:77:GLN:HB3	2:H:79:PHE:CZ	2.51	0.46
2:H:140:LEU:CD1	2:H:205:ILE:HG13	2.45	0.46
1:L:8:PRO:O	1:L:102:THR:HG23	2.15	0.46
2:J:166:LEU:HD13	2:J:191:VAL:HG21	1.98	0.45
1:M:55:ILE:HB	1:M:58:ILE:HD13	1.96	0.45
2:H:4:LEU:HD12	2:H:22:CYS:SG	2.57	0.45
2:J:162:ASN:HD21	2:J:205:ILE:HD13	1.80	0.45
1:M:27(B):VAL:HG22	1:M:68:ARG:O	2.17	0.45
1:L:193:THR:HB	1:L:208:SER:OG	2.17	0.45
2:H:83:ASP:O	2:H:86:ASP:HB2	2.16	0.45
2:H:11:ILE:HD11	2:H:149:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ILE:HG21	1:M:27(B):VAL:CG1	2.47	0.45
1:M:91:SER:HB3	3:Q:316:ILE:HD12	1.98	0.44
1:M:149:LYS:HA	1:M:153:SER:O	2.17	0.44
2:H:93:VAL:HG13	2:H:103:TRP:CD1	2.53	0.44
2:J:52:PHE:CD1	2:J:56:ASP:HB2	2.52	0.44
1:L:118:PHE:CE2	1:L:135:PHE:HD2	2.35	0.44
1:M:183:LYS:HE3	1:M:187:GLU:OE1	2.18	0.44
2:J:115:LYS:HZ2	2:J:115:LYS:HA	1.81	0.44
2:H:199:TRP:CB	2:H:205:ILE:HD11	2.48	0.44
2:H:38:ARG:HB2	2:H:48:LEU:HD11	1.99	0.44
2:J:43:LYS:HE2	2:J:44:GLY:H	1.83	0.43
2:J:69:ILE:HG12	2:J:70:SER:N	2.32	0.43
2:H:63:LEU:O	2:H:67:LEU:HG	2.17	0.43
2:H:178:LEU:HA	2:H:185:TYR:HA	2.00	0.43
2:J:211:ALA:O	2:J:213:PRO:HD3	2.18	0.43
1:L:124:GLN:HG3	2:H:122:TYR:CZ	2.52	0.43
2:H:34:MET:HE3	2:H:35:GLY:H	1.82	0.43
2:H:199:TRP:CZ2	2:H:227:PRO:HB3	2.53	0.43
1:M:48:ILE:HG22	1:M:54:LEU:HB2	2.00	0.43
1:M:193:THR:HG23	1:M:208:SER:HB3	2.00	0.43
2:H:162:ASN:HB3	2:H:165:SER:HB2	2.00	0.43
1:L:48:ILE:HD11	1:L:54:LEU:HD12	2.01	0.43
1:L:18:ARG:HD3	1:L:74:THR:HG23	2.00	0.43
2:H:61:PRO:HA	2:H:64:LYS:HB2	2.00	0.43
2:H:200:PRO:HB3	2:H:227:PRO:HG3	2.01	0.43
1:M:191:SER:HB3	1:M:210:ASN:OD1	2.18	0.43
1:L:12:ALA:HA	1:L:105:GLU:O	2.18	0.42
1:L:27(D):ASP:O	1:L:28:ASP:HB2	2.19	0.42
1:L:196:ALA:HB3	1:L:205:ILE:CG2	2.46	0.42
1:M:51:SER:HG	1:M:71:PHE:HD2	1.66	0.42
1:M:143:ASP:O	1:M:198:HIS:HD2	2.02	0.42
2:J:137:SER:HB2	2:J:192:THR:HG22	2.01	0.42
1:L:7:SER:H	1:L:24:ARG:NH2	2.18	0.42
1:L:48:ILE:HD13	1:L:54:LEU:HA	2.02	0.42
1:L:176:SER:HB2	2:H:174:PHE:CG	2.54	0.42
2:H:154:LEU:HA	2:H:209:ASN:O	2.19	0.42
2:H:166:LEU:HD23	2:H:191:VAL:HG21	2.02	0.42
2:H:198:THR:HG23	2:H:203:GLN:HB3	2.02	0.42
2:J:156:THR:OG1	2:J:209:ASN:HB2	2.20	0.42
1:M:7:SER:HA	1:M:8:PRO:HA	1.86	0.42
1:M:11:LEU:HD23	1:M:104:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:80:LEU:HD12	2:J:80:LEU:HA	1.77	0.41
1:M:146:VAL:HA	1:M:195:GLU:O	2.20	0.41
2:J:1:GLN:HB2	2:J:2:VAL:H	1.70	0.41
2:J:12:LEU:CD1	2:J:82(C):VAL:HG11	2.50	0.41
1:L:136:LEU:N	1:L:136:LEU:HD12	2.36	0.41
2:H:94:GLN:HG2	2:H:102:TYR:HB2	2.01	0.41
1:M:38:GLN:HG3	1:M:44:PRO:HG3	2.02	0.41
2:J:24:PHE:HE1	2:J:78:VAL:HG13	1.86	0.41
2:J:18:LEU:HG	2:J:20:LEU:HD13	2.03	0.41
1:L:192:TYR:HB2	1:L:209:PHE:CE2	2.55	0.41
2:H:6:GLU:HB2	2:H:107:THR:CG2	2.44	0.41
1:M:136:LEU:HD13	1:M:175:MET:HE2	2.03	0.41
1:M:155:ARG:HD3	1:M:155:ARG:HA	1.95	0.41
2:J:29:LEU:HA	2:J:29:LEU:HD23	1.88	0.41
2:H:199:TRP:HB2	2:H:205:ILE:HD11	2.03	0.40
2:J:6:GLU:OE2	2:J:104:GLY:HA3	2.20	0.40
2:H:94:GLN:HG3	2:H:95:GLU:O	2.21	0.40
2:H:205:ILE:H	2:H:205:ILE:HG12	1.70	0.40
1:M:13:VAL:HG21	1:M:78:VAL:HG11	2.03	0.40
2:J:144:VAL:HB	2:J:187:LEU:HB3	2.04	0.40
1:L:34:HIS:CE1	1:L:91:SER:OG	2.74	0.40
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.03	0.40
2:J:58:ARG:NH2	3:Q:312:LYS:O	2.55	0.40
2:H:122:TYR:HA	2:H:123:PRO:HD2	1.94	0.40
2:J:56:ASP:OD2	2:J:58:ARG:NH1	2.54	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	213/218 (98%)	194 (91%)	12 (6%)	7 (3%)	4 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	213/218 (98%)	191 (90%)	14 (7%)	8 (4%)	3 10
2	H	213/222 (96%)	183 (86%)	24 (11%)	6 (3%)	5 17
2	J	213/222 (96%)	188 (88%)	15 (7%)	10 (5%)	2 7
3	P	7/16 (44%)	6 (86%)	1 (14%)	0	100 100
3	Q	7/16 (44%)	6 (86%)	1 (14%)	0	100 100
All	All	866/912 (95%)	768 (89%)	67 (8%)	31 (4%)	3 11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	ASP
1	L	170	ASP
2	H	128	CYS
2	H	215	SER
2	J	64	LYS
2	J	216	SER
1	L	122	SER
1	L	166	GLN
2	H	183	ASP
1	M	51	SER
1	M	167	ASP
2	J	180	SER
1	L	80	ALA
1	L	167	ASP
2	H	180	SER
1	M	68	ARG
1	M	199	LYS
2	J	41	SER
2	J	105	GLN
2	J	134	THR
1	M	200	THR
2	J	82(C)	VAL
2	J	127	VAL
2	J	214	ALA
1	L	200	THR
2	H	40	PRO
2	H	116	THR
1	M	15	LEU
1	M	28	ASP
1	M	60	ASP

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Mol	Chain	Res	Type
2	J	53	TRP

5.3.2 Protein sidechains (i)

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	191/194 (98%)	154 (81%)	37 (19%)	1 4
1	M	191/194 (98%)	168 (88%)	23 (12%)	5 15
2	H	189/195 (97%)	154 (82%)	35 (18%)	1 5
2	J	189/195 (97%)	158 (84%)	31 (16%)	2 7
3	P	7/13 (54%)	4 (57%)	3 (43%)	0 0
3	Q	7/13 (54%)	6 (86%)	1 (14%)	3 10
All	All	774/804 (96%)	644 (83%)	130 (17%)	2 6

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	10	SER
1	L	11	LEU
1	L	18	ARG
1	L	24	ARG
1	L	28	ASP
1	L	30	ASN
1	L	34	HIS
1	L	51	SER
1	L	54	LEU
1	L	58	ILE
1	L	60	ASP
1	L	70	ASP
1	L	72	THR
1	L	77	PRO
1	L	78	VAL
1	L	81	ASP

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Mol	Chain	Res	Type
1	L	92	ASN
1	L	94	ASP
1	L	97	THR
1	L	103	LYS
1	L	114	THR
1	L	134	CYS
1	L	145	ASN
1	L	147	LYS
1	L	151	ASP
1	L	170	ASP
1	L	172	THR
1	L	179	LEU
1	L	181	LEU
1	L	184	ASP
1	L	191	SER
1	L	193	THR
1	L	194	CYS
1	L	201	SER
1	L	202	THR
1	L	208	SER
2	H	3	GLN
2	H	12	LEU
2	H	13	GLN
2	H	28	SER
2	H	29	LEU
2	H	31	THR
2	H	34	MET
2	H	35(B)	SER
2	H	56	ASP
2	H	57	LYS
2	H	58	ARG
2	H	65	SER
2	H	69	ILE
2	H	73	THR
2	H	77	GLN
2	H	82(A)	THR
2	H	94	GLN
2	H	105	GLN
2	H	110	THR
2	H	119	PRO
2	H	128	CYS
2	H	134	THR

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Mol	Chain	Res	Type
2	H	137	SER
2	H	143	LEU
2	H	151	PRO
2	H	153	THR
2	H	163	SER
2	H	166	LEU
2	H	187	LEU
2	H	203	GLN
2	H	205	ILE
2	H	216	SER
2	H	217	THR
2	H	220	ASP
2	H	228	ARG
3	P	311	CYS
3	P	313	ARG
3	P	320	PRO
1	M	1	ASP
1	M	18	ARG
1	M	22	SER
1	M	28	ASP
1	M	33	LEU
1	M	42	GLN
1	M	54	LEU
1	M	58	ILE
1	M	72	THR
1	M	74	THR
1	M	79	GLU
1	M	94	ASP
1	M	105	GLU
1	M	108	ARG
1	M	127	SER
1	M	145	ASN
1	M	162	SER
1	M	164	THR
1	M	165	ASP
1	M	168	SER
1	M	197	THR
1	M	204	PRO
1	M	211	ARG
2	J	4	LEU
2	J	12	LEU
2	J	23	SER

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Mol	Chain	Res	Type
2	J	35(B)	SER
2	J	43	LYS
2	J	58	ARG
2	J	62	SER
2	J	82(A)	THR
2	J	82(C)	VAL
2	J	107	THR
2	J	115	LYS
2	J	116	THR
2	J	123	PRO
2	J	128	CYS
2	J	130	ASP
2	J	137	SER
2	J	143	LEU
2	J	151	PRO
2	J	152	VAL
2	J	154	LEU
2	J	177	VAL
2	J	178	LEU
2	J	183	ASP
2	J	187	LEU
2	J	194	THR
2	J	203	GLN
2	J	216	SER
2	J	217	THR
2	J	220	ASP
2	J	226	GLU
2	J	228	ARG
3	Q	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	HIS
1	L	124	GLN
2	H	94	GLN
2	H	203	GLN
2	H	209	ASN
2	J	16	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.