



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 AM UTC

PDB ID : 1NGQ / pdb_00001ngq
Title : N1G9 (IGG1-LAMBDA) FAB FRAGMENT
Authors : Mizutani, R.; Satow, Y.
Deposited on : 1995-06-23
Resolution : 2.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

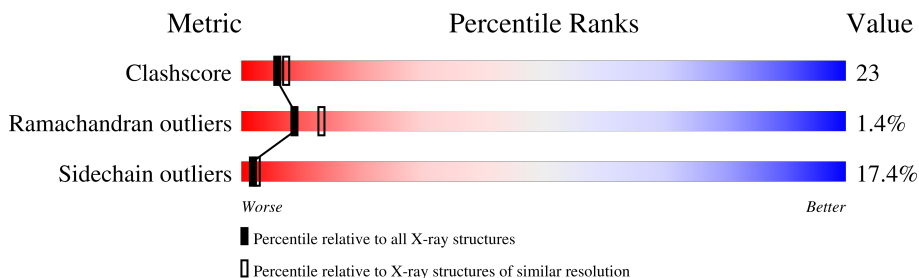
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	
2	H	222	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3369 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 N1G9 (IGG1-LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	2	0
			1595	1000	267	322	6			

- Molecule 2 is a protein called N1G9 (IGG1-LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1629	1041	263	319	6			

There are 32 discrepancies between the modelled and reference sequences:

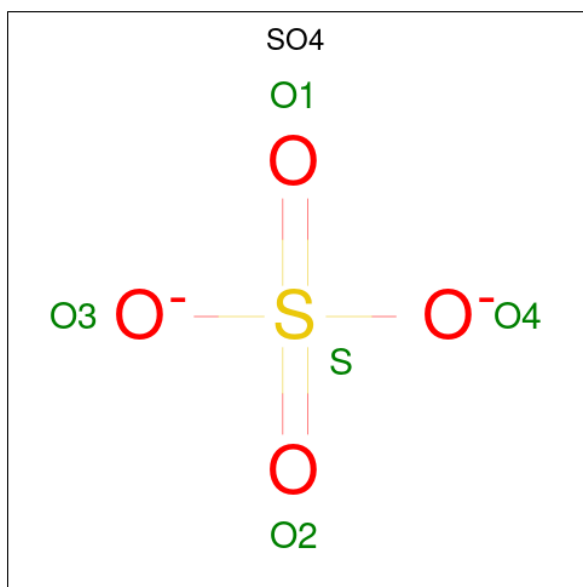
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	GLU	conflict	UNP P01751
H	3	GLN	LYS	conflict	UNP P01751
H	5	GLN	HIS	conflict	UNP P01751
H	6	GLN	GLU	conflict	UNP P01751
H	7	PRO	SER	conflict	UNP P01751
H	9	ALA	PRO	conflict	UNP P01751
H	10	GLU	GLY	conflict	UNP P01751
H	13	LYS	ARG	conflict	UNP P01751
H	16	ALA	THR	conflict	UNP P01751
H	20	LEU	ILE	conflict	UNP P01751
H	31	SER	ASN	conflict	UNP P01751
H	34	MET	LEU	conflict	UNP P01751
H	35	HIS	GLY	conflict	UNP P01751
H	43	ARG	HIS	conflict	UNP P01751
H	50	ARG	ASP	conflict	UNP P01751
H	52	ASP	TYR	conflict	UNP P01751
H	54	ASN	GLY	conflict	UNP P01751
H	55	SER	GLY	conflict	UNP P01751
H	57	GLY	TYR	conflict	UNP P01751
H	59	LYS	ASN	conflict	UNP P01751

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Chain	Residue	Modelled	Actual	Comment	Reference
H	66	SER	GLY	conflict	UNP P01751
H	72	VAL	ALA	conflict	UNP P01751
H	74	LYS	THR	conflict	UNP P01751
H	75	PRO	SER	conflict	UNP P01751
H	95	TYR	PHE	conflict	UNP P01751
H	99	TYR	-	insertion	UNP P01751
H	100	ASP	PHE	conflict	UNP P01751
H	?	-	TYR	deletion	UNP P01751
H	?	-	TRP	deletion	UNP P01751
H	109	TYR	VAL	conflict	UNP P01751
H	116	LEU	VAL	conflict	UNP P01751
H	194	PRO	THR	conflict	UNP P01751

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

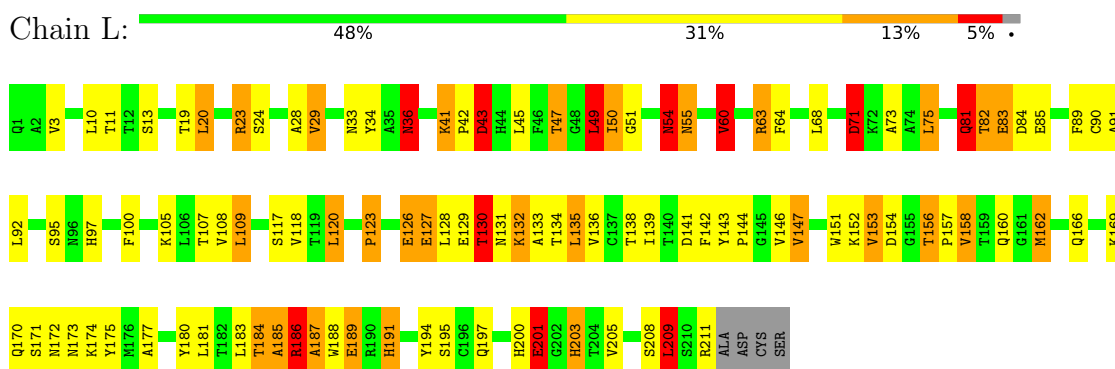
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	75	Total	O	0	0
			75	75		
4	H	65	Total	O	0	0
			65	65		

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: N1G9 (IGG1-LAMBDA)



• Molecule 2: N1G9 (IGG1-LAMBDA)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.89Å 109.89Å 97.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	87.0 (15.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 2.1	Depositor
R, R_{free}	0.194 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3369	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.22	0/1643	2.13	63/2246 (2.8%)
2	H	1.20	1/1677 (0.1%)	2.17	83/2295 (3.6%)
All	All	1.21	1/3320 (0.0%)	2.15	146/4541 (3.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	97	ALA	C-N	-5.06	1.26	1.33

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	201	GLU	CB-CG-CD	12.61	134.04	112.60
2	H	108	ASP	CA-CB-CG	11.13	123.73	112.60
2	H	94	TYR	CA-C-O	-9.30	110.51	120.46
1	L	158	VAL	N-CA-C	-8.97	100.07	110.21
2	H	29	PHE	CA-C-N	8.92	132.24	120.28
2	H	29	PHE	C-N-CA	8.92	132.24	120.28
2	H	20	LEU	CA-C-O	-8.87	110.72	120.92
1	L	203	HIS	CA-CB-CG	-8.60	105.20	113.80
2	H	213	VAL	O-C-N	8.32	132.00	123.10
1	L	75	LEU	CA-C-O	-8.01	111.73	120.30
2	H	107	PHE	CA-CB-CG	7.87	121.67	113.80
2	H	40	ARG	N-CA-C	-7.85	98.33	109.24
2	H	77	SER	CA-C-O	-7.83	112.76	121.84
1	L	158	VAL	CB-CA-C	7.75	120.13	111.45
1	L	174	LYS	CA-C-O	-7.74	111.82	121.88
1	L	33	ASN	CA-CB-CG	7.62	120.22	112.60
2	H	71	THR	CA-CB-CG2	7.59	123.40	110.50
1	L	127	GLU	CB-CG-CD	7.50	125.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	30	THR	N-CA-C	7.32	119.25	111.28
1	L	89	PHE	CA-C-O	-7.26	113.01	120.71
2	H	41	PRO	CB-CA-C	7.15	119.36	111.56
2	H	61	ASN	N-CA-C	-7.12	98.44	109.76
2	H	111	GLY	N-CA-C	-7.10	101.67	112.89
1	L	41	LYS	CA-C-O	-7.08	113.54	120.97
2	H	150	LYS	N-CA-C	7.03	120.91	109.59
2	H	46	GLU	CA-C-O	-7.02	112.52	120.32
2	H	8	GLY	N-CA-C	6.98	121.70	112.77
2	H	96	CYS	N-CA-CB	6.87	121.75	110.69
1	L	201	GLU	N-CA-CB	6.86	122.09	110.49
1	L	187	ALA	N-CA-C	-6.81	103.86	111.28
2	H	96	CYS	CA-C-O	-6.78	113.53	120.71
1	L	134	THR	CA-CB-OG1	-6.70	99.55	109.60
1	L	186	ARG	N-CA-C	6.61	118.28	111.14
2	H	6	GLN	OE1-CD-NE2	6.59	129.19	122.60
2	H	12	VAL	CB-CA-C	6.58	121.42	110.30
1	L	41	LYS	N-CA-C	-6.50	101.88	110.40
2	H	163	SER	CA-C-O	-6.50	112.96	121.08
1	L	63	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	L	82	THR	CA-C-O	6.37	127.30	120.10
1	L	64	PHE	CA-CB-CG	6.35	120.15	113.80
2	H	16	ALA	CA-C-O	-6.33	113.57	121.55
1	L	81	GLN	OE1-CD-NE2	6.32	128.92	122.60
2	H	16	ALA	O-C-N	6.24	130.12	122.14
2	H	5	GLN	OE1-CD-NE2	6.23	128.83	122.60
1	L	60	VAL	N-CA-C	-6.14	101.20	107.89
1	L	135	LEU	CA-CB-CG	6.07	137.56	116.30
1	L	177	ALA	O-C-N	6.04	129.44	123.46
1	L	85	GLU	CB-CG-CD	6.04	122.87	112.60
2	H	104	SER	N-CA-C	6.03	120.34	112.92
1	L	100	PHE	CA-C-O	-5.97	114.23	121.28
1	L	185	ALA	CA-C-N	5.94	128.52	120.44
1	L	185	ALA	C-N-CA	5.94	128.52	120.44
2	H	97	ALA	CA-C-O	-5.94	114.17	121.06
2	H	13	LYS	N-CA-C	-5.93	102.42	110.36
1	L	36	ASN	CA-C-O	-5.92	114.42	121.11
2	H	101	TYR	N-CA-C	5.87	117.76	111.36
2	H	30	THR	CA-CB-OG1	-5.86	100.81	109.60
2	H	160	THR	CA-CB-CG2	5.86	120.46	110.50
2	H	105	SER	N-CA-C	5.84	119.17	111.28
1	L	11	THR	CA-C-O	-5.84	114.05	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	141	ASP	CA-C-O	-5.83	114.78	121.54
2	H	18	VAL	CB-CA-C	-5.82	100.64	110.71
2	H	61	ASN	CA-C-O	-5.81	114.07	120.69
2	H	218	VAL	O-C-N	5.80	127.72	121.10
1	L	177	ALA	CA-C-O	-5.76	114.77	121.10
1	L	54	ASN	CA-C-O	-5.74	113.54	119.51
2	H	18	VAL	N-CA-CB	5.68	120.76	111.45
2	H	30	THR	OG1-CB-CG2	5.62	120.55	109.30
2	H	89	GLU	CA-C-O	-5.61	112.04	119.10
1	L	90	CYS	N-CA-CB	5.60	119.47	110.85
1	L	147	VAL	N-CA-CB	5.54	120.60	112.35
2	H	112	GLN	O-C-N	5.53	130.00	122.37
1	L	134	THR	CA-CB-CG2	5.52	119.89	110.50
2	H	33	TRP	CA-C-O	-5.52	115.20	121.72
2	H	125	PRO	CB-CA-C	5.50	116.34	111.17
2	H	61	ASN	CB-CA-C	5.50	118.80	109.84
2	H	121	ALA	CA-C-N	5.50	132.59	122.92
2	H	121	ALA	C-N-CA	5.50	132.59	122.92
1	L	63	ARG	N-CA-C	-5.49	106.42	113.01
2	H	112	GLN	CA-C-O	-5.48	112.64	119.28
1	L	117	SER	O-C-N	5.48	130.04	123.13
1	L	201	GLU	CA-C-N	5.48	132.14	121.41
1	L	201	GLU	C-N-CA	5.48	132.14	121.41
2	H	7	PRO	CA-C-N	5.47	126.02	120.00
2	H	7	PRO	C-N-CA	5.47	126.02	120.00
2	H	89	GLU	CB-CG-CD	5.46	121.89	112.60
2	H	88	SER	CA-CB-OG	-5.46	100.18	111.10
1	L	47	THR	CB-CA-C	-5.46	97.45	109.56
2	H	118	VAL	CA-C-O	-5.44	114.71	120.53
1	L	156	THR	CA-CB-OG1	-5.43	101.46	109.60
1	L	107	THR	CA-C-O	-5.43	114.35	120.32
2	H	206	HIS	CA-C-N	5.42	126.62	119.84
2	H	206	HIS	C-N-CA	5.42	126.62	119.84
1	L	34	TYR	CA-C-O	-5.36	115.75	122.03
2	H	200	VAL	N-CA-C	-5.36	100.60	108.11
2	H	79	ALA	N-CA-C	-5.36	101.54	110.17
2	H	113	GLY	CA-C-N	5.36	130.39	123.00
2	H	113	GLY	C-N-CA	5.36	130.39	123.00
2	H	186	SER	CA-C-O	-5.35	114.18	120.60
1	L	43	ASP	CA-C-O	-5.35	112.86	120.51
2	H	197	SER	CA-C-N	5.35	130.10	122.72
2	H	197	SER	C-N-CA	5.35	130.10	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	57	GLY	CA-C-O	-5.34	115.96	120.98
2	H	56	GLY	N-CA-C	-5.34	107.90	115.43
2	H	202	CYS	CB-CA-C	5.33	118.44	109.48
1	L	82	THR	N-CA-CB	-5.33	102.02	110.22
2	H	45	LEU	N-CA-C	-5.32	101.61	110.17
1	L	29	VAL	CA-C-O	-5.31	114.79	121.11
2	H	24	ALA	N-CA-CB	-5.31	101.76	110.52
2	H	163	SER	CB-CA-C	-5.31	103.33	111.66
2	H	39	GLN	N-CA-CB	5.30	118.90	110.84
2	H	5	GLN	N-CA-C	5.30	117.37	108.73
2	H	132	ALA	N-CA-C	-5.29	103.51	110.39
1	L	153	VAL	O-C-N	5.29	128.98	122.95
2	H	117	THR	CA-C-O	-5.29	114.64	120.30
2	H	200	VAL	N-CA-CB	5.27	118.69	111.41
1	L	130	THR	CA-CB-CG2	5.25	119.42	110.50
1	L	55	ASN	CA-C-O	-5.25	114.74	120.36
2	H	155	GLU	N-CA-CB	-5.25	102.95	110.04
2	H	71	THR	CA-CB-OG1	-5.25	101.73	109.60
1	L	123	PRO	CA-C-O	-5.24	115.37	121.34
2	H	42	GLY	CA-C-O	5.24	124.78	118.97
2	H	92	ALA	N-CA-CB	-5.24	101.64	110.49
1	L	3	VAL	N-CA-CB	-5.21	105.33	111.90
1	L	146	VAL	CA-C-O	-5.21	114.75	120.43
1	L	175	TYR	O-C-N	5.20	130.06	122.94
1	L	71	ASP	CA-C-N	-5.19	113.81	122.21
1	L	71	ASP	C-N-CA	-5.19	113.81	122.21
2	H	20	LEU	O-C-N	5.17	129.16	123.16
2	H	213	VAL	CA-C-O	-5.15	114.90	120.67
1	L	13	SER	O-C-N	5.12	126.53	121.57
1	L	68	LEU	N-CA-C	-5.11	100.56	108.90
2	H	30	THR	N-CA-CB	-5.11	102.61	110.12
2	H	193	SER	O-C-N	5.10	127.19	121.32
1	L	34	TYR	N-CA-CB	-5.10	104.33	111.62
2	H	5	GLN	CA-C-O	-5.09	114.91	120.36
1	L	49	LEU	CA-C-N	5.09	130.78	122.69
1	L	49	LEU	C-N-CA	5.09	130.78	122.69
1	L	123	PRO	N-CA-C	-5.07	103.23	111.14
2	H	115	THR	CA-C-O	-5.07	115.16	120.58
1	L	147	VAL	CA-CB-CG1	5.06	119.01	110.40
2	H	86	LEU	N-CA-CB	-5.05	102.89	110.17
2	H	190	VAL	N-CA-CB	-5.05	104.14	111.21
1	L	126	GLU	CB-CG-CD	5.02	121.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	209	LEU	CB-CA-C	5.01	118.73	109.71
2	H	159	VAL	CB-CA-C	5.00	118.08	110.62

There are no chirality outliers.

There are no planarity outliers.

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	1595	0	1535	80	0
2	H	1629	0	1564	68	1
3	H	5	0	0	1	0
4	H	65	0	0	4	0
4	L	75	0	0	3	0
All	All	3369	0	3099	145	1

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 23.

All (145) 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:12:VAL:HG21	2:H:18:VAL:HG13	1.47	0.97
1:L:194:TYR:HB2	1:L:209:LEU:HD22	1.50	0.93
1:L:131:ASN:HA	1:L:185:ALA:HB2	1.47	0.93
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.16	0.91
1:L:194:TYR:HB2	1:L:209:LEU:CD2	2.03	0.89
2:H:191:PRO:O	2:H:194:PRO:HD2	1.74	0.87
1:L:153:VAL:HG23	1:L:158:VAL:HG21	1.60	0.83
1:L:183:LEU:HD11	1:L:194:TYR:HE2	1.44	0.82
2:H:63:LYS:NZ	3:H:301:SO4:O4	2.14	0.78
1:L:42:PRO:O	1:L:43:ASP:HB2	1.81	0.78
1:L:195:SER:HB2	1:L:208:SER:OG	1.83	0.77
1:L:54:ASN:HD22	1:L:54:ASN:C	1.93	0.76
2:H:12:VAL:HG21	2:H:18:VAL:CG1	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ALA:O	1:L:188:TRP:HB3	1.85	0.76
2:H:199:THR:HB	2:H:216:LYS:HD2	1.67	0.76
2:H:190:VAL:HG13	2:H:194:PRO:HG2	1.68	0.75
1:L:81:GLN:HG2	1:L:83[A]:GLU:OE2	1.87	0.75
1:L:131:ASN:CA	1:L:185:ALA:HB2	2.16	0.74
2:H:218:VAL:HG23	2:H:219:PRO:HD2	1.70	0.74
1:L:81:GLN:HB3	1:L:83[A]:GLU:HG2	1.68	0.74
2:H:218:VAL:CG2	2:H:219:PRO:HD2	2.19	0.72
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.06	0.72
2:H:193:SER:N	2:H:194:PRO:CD	2.52	0.70
1:L:127:GLU:OE2	2:H:150:LYS:NZ	2.19	0.70
2:H:193:SER:N	2:H:194:PRO:HD2	2.07	0.68
2:H:141:SER:O	2:H:192:SER:N	2.25	0.67
1:L:152:LYS:HG2	1:L:157:PRO:HA	1.79	0.65
1:L:172:ASN:O	1:L:173:ASN:HB2	1.95	0.65
2:H:193:SER:H	2:H:194:PRO:HD2	1.60	0.64
1:L:183:LEU:HD11	1:L:194:TYR:CE2	2.29	0.63
2:H:79:ALA:HB1	4:H:351:HOH:O	1.98	0.63
2:H:160:THR:HG22	2:H:203:ASN:HB2	1.80	0.63
2:H:50:ARG:HD2	2:H:50:ARG:C	2.24	0.63
1:L:147:VAL:HG12	1:L:200:HIS:HB2	1.80	0.62
1:L:131:ASN:C	1:L:185:ALA:HB2	2.25	0.62
1:L:109:LEU:HD12	1:L:143:TYR:CE2	2.36	0.61
1:L:63:ARG:NH2	1:L:84:ASP:OD1	2.24	0.61
1:L:131:ASN:HA	1:L:185:ALA:CB	2.25	0.60
1:L:162:MET:HA	1:L:180:TYR:O	2.01	0.60
1:L:10:LEU:HD12	1:L:20:LEU:HD22	1.82	0.59
1:L:186:ARG:HG3	1:L:186:ARG:HH11	1.67	0.59
2:H:141:SER:O	2:H:192:SER:CB	2.50	0.59
2:H:91:SER:O	2:H:92:ALA:HB2	2.02	0.59
1:L:97:HIS:CD2	1:L:97:HIS:N	2.69	0.58
1:L:189:GLU:HA	1:L:211:ARG:NH2	2.18	0.58
1:L:200:HIS:O	1:L:201:GLU:C	2.46	0.58
2:H:152:TYR:CE1	2:H:157:VAL:HG13	2.37	0.58
2:H:194:PRO:HA	2:H:198:GLU:HG2	1.85	0.58
1:L:188:TRP:CZ2	1:L:211:ARG:HG3	2.39	0.57
2:H:166:LEU:HD13	2:H:188:VAL:HG21	1.86	0.57
1:L:109:LEU:HD12	1:L:143:TYR:HE2	1.70	0.57
2:H:40:ARG:NH2	2:H:89:GLU:O	2.38	0.56
2:H:154:PRO:HD2	2:H:208:ALA:CB	2.34	0.56
1:L:153:VAL:HG23	1:L:158:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:THR:O	1:L:185:ALA:C	2.48	0.56
2:H:193:SER:H	2:H:194:PRO:CD	2.18	0.55
1:L:120:LEU:HD23	1:L:136:VAL:O	2.06	0.55
1:L:120:LEU:HD21	1:L:151:TRP:HH2	1.72	0.55
1:L:189:GLU:HA	1:L:211:ARG:HH21	1.72	0.55
1:L:153:VAL:CG2	1:L:158:VAL:HG21	2.35	0.55
2:H:218:VAL:CG2	2:H:219:PRO:CD	2.86	0.54
1:L:123:PRO:HA	4:L:270:HOH:O	2.08	0.54
2:H:112:GLN:HB2	4:H:366:HOH:O	2.08	0.54
1:L:10:LEU:CD1	1:L:20:LEU:HD22	2.38	0.54
1:L:154:ASP:OD2	1:L:191:HIS:HB3	2.08	0.54
2:H:191:PRO:C	2:H:194:PRO:HD2	2.33	0.54
2:H:74:LYS:HB3	2:H:75:PRO:HD3	1.89	0.54
1:L:189:GLU:HA	1:L:211:ARG:HE	1.72	0.53
1:L:189:GLU:HA	1:L:211:ARG:NE	2.23	0.53
1:L:97:HIS:H	1:L:97:HIS:HD2	1.56	0.53
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.91	0.53
1:L:183:LEU:HD22	1:L:187:ALA:HB1	1.91	0.53
2:H:38:LYS:HG3	2:H:94:TYR:CE1	2.44	0.52
1:L:36:ASN:OD1	2:H:106:TYR:HA	2.09	0.52
1:L:130:THR:HG22	1:L:132:LYS:HB2	1.91	0.52
1:L:81:GLN:C	1:L:108:VAL:HG11	2.35	0.52
2:H:199:THR:HA	4:H:322:HOH:O	2.09	0.52
2:H:207:PRO:O	2:H:208:ALA:C	2.52	0.52
2:H:153:PHE:HB2	2:H:181:LEU:HD12	1.93	0.51
1:L:20:LEU:N	1:L:20:LEU:HD23	2.25	0.51
2:H:184:LEU:C	2:H:184:LEU:HD23	2.36	0.51
1:L:143:TYR:HA	1:L:144:PRO:C	2.36	0.50
2:H:134:GLY:O	2:H:135:SER:CB	2.59	0.50
2:H:50:ARG:C	2:H:50:ARG:CD	2.85	0.50
2:H:128:VAL:CG1	2:H:204:VAL:HG21	2.42	0.50
1:L:51:GLY:HA3	2:H:106:TYR:HB3	1.94	0.50
1:L:28:ALA:HA	1:L:71:ASP:HB2	1.94	0.49
2:H:35:HIS:HD2	2:H:47:TRP:NE1	1.97	0.49
2:H:122:LYS:O	2:H:123:THR:C	2.56	0.49
1:L:49:LEU:HA	1:L:60:VAL:HG21	1.94	0.49
1:L:19:THR:C	1:L:20:LEU:HD23	2.38	0.49
1:L:47:THR:HG21	4:L:263:HOH:O	2.11	0.48
1:L:197:GLN:C	4:L:231:HOH:O	2.55	0.48
2:H:191:PRO:O	2:H:194:PRO:CD	2.54	0.47
1:L:189:GLU:HA	1:L:211:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD12	2:H:58:THR:CG2	2.44	0.47
1:L:41:LYS:HB3	1:L:42:PRO:HD2	1.96	0.47
1:L:23:ARG:HG2	1:L:24:SER:N	2.28	0.47
2:H:190:VAL:HG11	2:H:195:TRP:HB2	1.97	0.47
1:L:203:HIS:N	1:L:203:HIS:ND1	2.63	0.46
1:L:162:MET:HE3	1:L:162:MET:HB2	1.60	0.46
1:L:169:LYS:HB3	1:L:169:LYS:HE2	1.73	0.46
2:H:218:VAL:HA	2:H:219:PRO:HD3	1.80	0.46
2:H:147:CYS:O	2:H:185:SER:HA	2.15	0.46
1:L:153:VAL:H	1:L:158:VAL:HG23	1.81	0.45
2:H:195:TRP:CD1	2:H:196:PRO:HA	2.52	0.45
1:L:54:ASN:C	1:L:54:ASN:ND2	2.62	0.45
2:H:34:MET:HE2	2:H:34:MET:HB2	1.92	0.45
2:H:98:ARG:HH21	2:H:108:ASP:CG	2.25	0.45
2:H:218:VAL:HG23	2:H:219:PRO:CD	2.44	0.44
2:H:194:PRO:O	2:H:198:GLU:N	2.27	0.44
2:H:65:LYS:HB3	2:H:65:LYS:HE3	1.21	0.43
2:H:128:VAL:HG11	2:H:204:VAL:HG21	2.00	0.43
1:L:183:LEU:HD22	1:L:187:ALA:CB	2.48	0.43
1:L:138:THR:C	1:L:139:ILE:HG13	2.43	0.43
1:L:81:GLN:CA	1:L:81:GLN:HE21	2.28	0.43
1:L:109:LEU:HD12	1:L:109:LEU:HA	1.66	0.43
1:L:97:HIS:N	1:L:97:HIS:HD2	2.12	0.43
2:H:162:ASN:O	2:H:163:SER:HB2	2.18	0.43
1:L:63:ARG:HH11	1:L:63:ARG:HD3	1.58	0.43
1:L:123:PRO:CG	1:L:133:ALA:HB1	2.49	0.43
2:H:73:ASP:OD1	2:H:76:SER:OG	2.30	0.42
1:L:139:ILE:HG22	1:L:142:PHE:CD2	2.54	0.42
1:L:189:GLU:O	1:L:189:GLU:HG3	2.17	0.42
2:H:192:SER:O	2:H:193:SER:OG	2.30	0.42
1:L:128:LEU:HD23	1:L:128:LEU:HA	1.89	0.42
2:H:122:LYS:HA	4:H:353:HOH:O	2.19	0.42
2:H:154:PRO:HD2	2:H:208:ALA:HB3	2.01	0.42
2:H:161:TRP:CE3	2:H:188:VAL:HG11	2.54	0.42
2:H:51:ILE:HD12	2:H:58:THR:HG22	2.02	0.42
2:H:194:PRO:HA	2:H:198:GLU:CG	2.50	0.42
1:L:189:GLU:CA	1:L:211:ARG:HH21	2.33	0.41
1:L:183:LEU:CD1	1:L:194:TYR:CE2	3.01	0.41
2:H:64:PHE:O	2:H:65:LYS:C	2.63	0.41
1:L:97:HIS:CD2	1:L:97:HIS:H	2.32	0.41
1:L:156:THR:HA	1:L:157:PRO:HD2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:THR:HG22	2:H:203:ASN:OD1	2.20	0.41
2:H:164:GLY:O	2:H:165:SER:C	2.62	0.41
1:L:50:ILE:HA	1:L:55:ASN:O	2.20	0.41
1:L:91:ALA:O	1:L:92:LEU:HD23	2.21	0.41
2:H:218:VAL:HG22	2:H:219:PRO:HD2	1.97	0.41
1:L:29:VAL:HG11	1:L:73:ALA:HB2	2.03	0.40
1:L:189:GLU:CA	1:L:211:ARG:NH2	2.83	0.40
2:H:130:PRO:HG2	2:H:130:PRO:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:NZ	2:H:19:LYS:NZ[8_665]	1.73	0.47

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	211/215 (98%)	192 (91%)	17 (8%)	2 (1%)	14	22
2	H	211/222 (95%)	193 (92%)	14 (7%)	4 (2%)	6	8
All	All	422/437 (97%)	385 (91%)	31 (7%)	6 (1%)	9	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP
2	H	193	SER
1	L	201	GLU
2	H	92	ALA
2	H	179	SER

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Mol	Chain	Res	Type
2	H	207	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	177/182 (97%)	140 (79%)	37 (21%)	1	1
2	H	181/192 (94%)	154 (85%)	27 (15%)	3	3
All	All	358/374 (96%)	294 (82%)	64 (18%)	2	2

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	LEU
1	L	23	ARG
1	L	36	ASN
1	L	45	LEU
1	L	49	LEU
1	L	50	ILE
1	L	54	ASN
1	L	60	VAL
1	L	71	ASP
1	L	75	LEU
1	L	81	GLN
1	L	82	THR
1	L	83[A]	GLU
1	L	83[B]	GLU
1	L	95	SER
1	L	105[A]	LYS
1	L	105[B]	LYS
1	L	109	LEU
1	L	118	VAL
1	L	120	LEU
1	L	126	GLU
1	L	129	GLU

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Mol	Chain	Res	Type
1	L	130	THR
1	L	132	LYS
1	L	135	LEU
1	L	160	GLN
1	L	162	MET
1	L	166	GLN
1	L	170	GLN
1	L	171	SER
1	L	181	LEU
1	L	184	THR
1	L	186	ARG
1	L	189	GLU
1	L	191	HIS
1	L	205	VAL
1	L	209	LEU
2	H	4	LEU
2	H	11	LEU
2	H	18	VAL
2	H	20	LEU
2	H	23	LYS
2	H	28	THR
2	H	30	THR
2	H	59	LYS
2	H	65	LYS
2	H	71	THR
2	H	72	VAL
2	H	93	VAL
2	H	112	GLN
2	H	128	VAL
2	H	147	CYS
2	H	158	THR
2	H	160	THR
2	H	168	SER
2	H	181	LEU
2	H	184	LEU
2	H	190	VAL
2	H	193	SER
2	H	197	SER
2	H	202	CYS
2	H	211	THR
2	H	213	VAL
2	H	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	54	ASN
1	L	81	GLN
1	L	173	ASN
2	H	1	GLN
2	H	3	GLN
2	H	5	GLN
2	H	35	HIS
2	H	112	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	H	301	-	4,4,4	0.71	0	6,6,6	0.54	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	SO4	1	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.