Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:32 PM GMT

PDB ID	:	1BBJ
Title	:	CRYSTAL STRUCTURE OF A CHIMERIC FAB' FRAGMENT OF AN ANTIBODY BINDING TUMOUR CELLS
Authors	:	Brady, R.L.; Hubbard, R.E.; Todd, R.J.
Deposited on	:	1992-04-30
Resolution	:	3.10 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 (i) symbol.

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

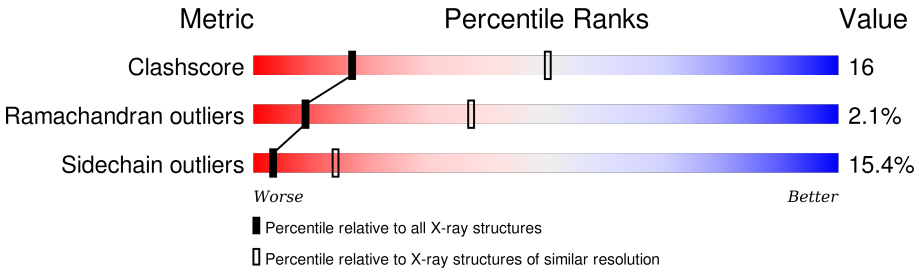
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 <=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	A	211	50% 39% 9%
1	L	211	50% 40% 9%
2	B	212	58% 34% 7%
2	H	212	58% 34% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6466 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 IGG4-KAPPA B72.3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1630	1019	274	332	5			
1	A	211	Total	C	N	O	S	0	0	0
			1630	1019	274	332	5			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLN	GLU	CONFLICT	GB 11692743
L	4	MET	LEU	CONFLICT	GB 11692743
L	11	LEU	GLN	CONFLICT	GB 11692743
L	13	VAL	ALA	CONFLICT	GB 11692743
L	15	VAL	LEU	CONFLICT	GB 11692743
L	18	THR	SER	CONFLICT	GB 11692743
L	24	ARG	LEU	CONFLICT	GB 11692743
L	27	GLU	GLN	CONFLICT	GB 11692743
L	28	ASN	THR	CONFLICT	GB 11692743
L	30	TYR	GLY	CONFLICT	GB 11692743
L	31	SER	THR	CONFLICT	GB 11692743
L	32	ASN	TRP	CONFLICT	GB 11692743
L	40	GLN	PRO	CONFLICT	GB 11692743
L	48	VAL	ILE	CONFLICT	GB 11692743
L	53	ASN	SER	CONFLICT	GB 11692743
L	70	GLN	LYS	CONFLICT	GB 11692743
L	71	TYR	PHE	CONFLICT	GB 11692743
L	73	LEU	PHE	CONFLICT	GB 11692743
L	76	ASN	SER	CONFLICT	GB 11692743
L	80	SER	ALA	CONFLICT	GB 11692743
L	84	GLY	VAL	CONFLICT	GB 11692743
L	90	HIS	GLN	CONFLICT	GB 11692743
L	91	PHE	LEU	CONFLICT	GB 11692743
L	92	TRP	TYR	CONFLICT	GB 11692743
L	93	GLY	SER	CONFLICT	GB 11692743

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Chain	Residue	Modelled	Actual	Comment	Reference
L	103	ARG	LYS	CONFLICT	GB 11692743
L	109	ALA	THR	CONFLICT	GB 11692743
L	110	ASP	VAL	CONFLICT	GB 11692743
L	114	THR	SER	CONFLICT	GB 11692743
A	3	GLN	GLU	CONFLICT	GB 11692743
A	4	MET	LEU	CONFLICT	GB 11692743
A	11	LEU	GLN	CONFLICT	GB 11692743
A	13	VAL	ALA	CONFLICT	GB 11692743
A	15	VAL	LEU	CONFLICT	GB 11692743
A	18	THR	SER	CONFLICT	GB 11692743
A	24	ARG	LEU	CONFLICT	GB 11692743
A	27	GLU	GLN	CONFLICT	GB 11692743
A	28	ASN	THR	CONFLICT	GB 11692743
A	30	TYR	GLY	CONFLICT	GB 11692743
A	31	SER	THR	CONFLICT	GB 11692743
A	32	ASN	TRP	CONFLICT	GB 11692743
A	40	GLN	PRO	CONFLICT	GB 11692743
A	48	VAL	ILE	CONFLICT	GB 11692743
A	53	ASN	SER	CONFLICT	GB 11692743
A	70	GLN	LYS	CONFLICT	GB 11692743
A	71	TYR	PHE	CONFLICT	GB 11692743
A	73	LEU	PHE	CONFLICT	GB 11692743
A	76	ASN	SER	CONFLICT	GB 11692743
A	80	SER	ALA	CONFLICT	GB 11692743
A	84	GLY	VAL	CONFLICT	GB 11692743
A	90	HIS	GLN	CONFLICT	GB 11692743
A	91	PHE	LEU	CONFLICT	GB 11692743
A	92	TRP	TYR	CONFLICT	GB 11692743
A	93	GLY	SER	CONFLICT	GB 11692743
A	103	ARG	LYS	CONFLICT	GB 11692743
A	109	ALA	THR	CONFLICT	GB 11692743
A	110	ASP	VAL	CONFLICT	GB 11692743
A	114	THR	SER	CONFLICT	GB 11692743

- Molecule 2 is a protein called IGG4-KAPPA B72.3 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1603	1009	266	322	6			
2	B	212	Total	C	N	O	S	0	0	0
			1603	1009	266	322	6			

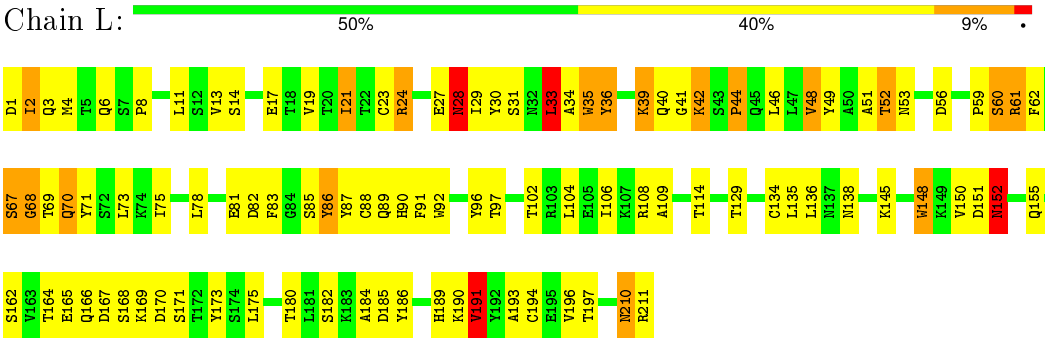
3 Residue-property plots (i)

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.

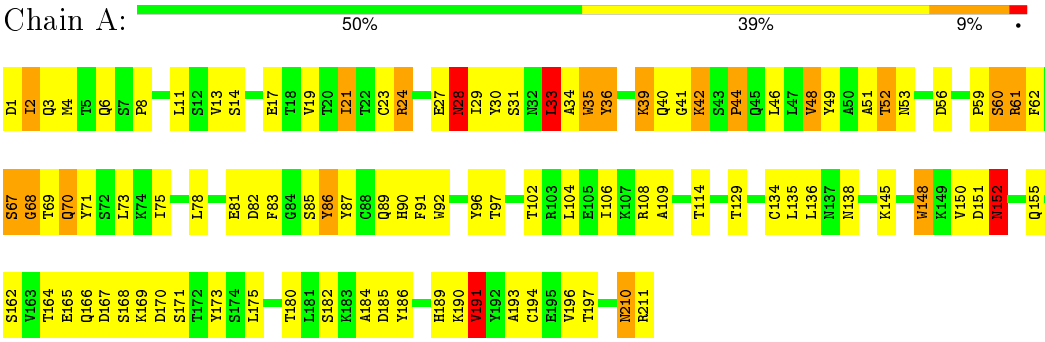
- Molecule 1: IGG4-KAPPA B72.3 FAB (LIGHT CHAIN)

Chain L:



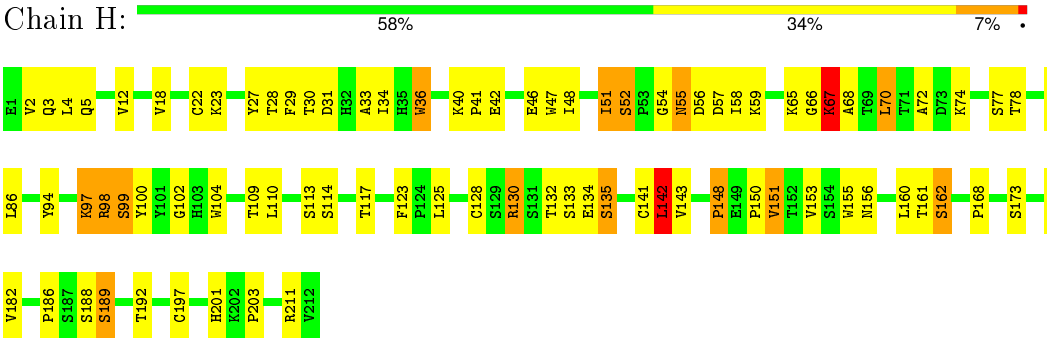
- Molecule 1: IGG4-KAPPA B72.3 FAB (LIGHT CHAIN)

Chain A:



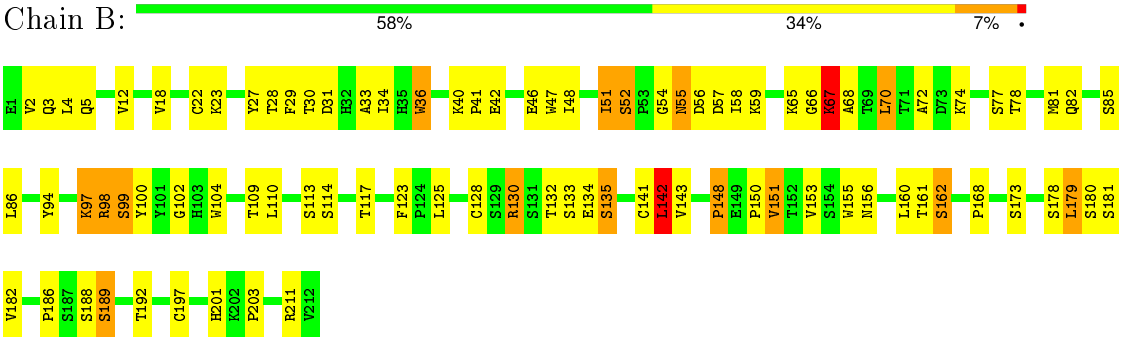
- Molecule 2: IGG4-KAPPA B72.3 FAB (HEAVY CHAIN)

Chain H:



• Molecule 2: IGG4-KAPPA B72.3 FAB (HEAVY CHAIN)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.50Å 93.20Å 208.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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: PCA

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	A	1.13	6/1666 (0.4%)	1.81	44/2261 (1.9%)
1	L	1.13	6/1666 (0.4%)	1.81	44/2261 (1.9%)
2	B	1.12	5/1635 (0.3%)	1.67	29/2225 (1.3%)
2	H	1.12	5/1635 (0.3%)	1.67	29/2225 (1.3%)
All	All	1.13	22/6602 (0.3%)	1.74	146/8972 (1.6%)

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	A	0	4
1	L	0	4
2	B	0	4
2	H	0	4
All	All	0	16

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	LEU	C-N	-12.31	1.05	1.34
2	H	142	LEU	C-N	-12.29	1.05	1.34
2	B	54	GLY	C-N	11.50	1.60	1.34
2	H	54	GLY	C-N	11.48	1.60	1.34
1	A	148	TRP	C-N	-9.16	1.12	1.34
1	L	148	TRP	C-N	-9.14	1.13	1.34
1	L	36	TYR	C-N	-7.43	1.17	1.34
1	A	36	TYR	C-N	-7.43	1.17	1.34
1	A	152	ASN	C-N	7.24	1.50	1.34
1	L	152	ASN	C-N	7.22	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	4	MET	C-N	-7.16	1.17	1.34
1	A	4	MET	C-N	-7.16	1.17	1.34
2	B	28	THR	C-N	-6.89	1.18	1.34
2	H	28	THR	C-N	-6.87	1.18	1.34
1	L	135	LEU	C-N	-6.80	1.18	1.34
1	A	135	LEU	C-N	-6.79	1.18	1.34
1	A	168	SER	C-N	6.25	1.48	1.34
1	L	168	SER	C-N	6.23	1.48	1.34
2	B	47	TRP	CG-CD2	-5.25	1.34	1.43
2	H	47	TRP	CG-CD2	-5.21	1.34	1.43
2	H	66	GLY	C-N	-5.12	1.22	1.34
2	B	66	GLY	C-N	-5.11	1.22	1.34

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	ASN	O-C-N	-14.55	99.42	122.70
1	L	28	ASN	O-C-N	-14.52	99.47	122.70
1	A	168	SER	C-N-CA	-10.79	94.74	121.70
1	L	168	SER	C-N-CA	-10.77	94.77	121.70
1	A	148	TRP	CD1-CG-CD2	10.26	114.51	106.30
1	A	28	ASN	CA-C-N	10.23	139.70	117.20
1	L	28	ASN	CA-C-N	10.21	139.65	117.20
1	L	148	TRP	CD1-CG-CD2	10.21	114.47	106.30
1	A	42	LYS	CA-C-N	-9.77	95.70	117.20
1	L	42	LYS	CA-C-N	-9.77	95.71	117.20
2	H	28	THR	O-C-N	-9.74	107.11	122.70
2	B	28	THR	O-C-N	-9.73	107.13	122.70
2	H	28	THR	C-N-CA	9.73	146.02	121.70
2	B	28	THR	C-N-CA	9.72	146.00	121.70
1	A	42	LYS	O-C-N	9.21	137.44	122.70
1	L	42	LYS	O-C-N	9.20	137.42	122.70
1	A	23	CYS	CA-CB-SG	8.92	130.06	114.00
1	L	23	CYS	CA-CB-SG	8.91	130.04	114.00
1	L	168	SER	O-C-N	8.54	136.36	122.70
1	A	168	SER	O-C-N	8.53	136.35	122.70
2	B	151	VAL	CG1-CB-CG2	-8.40	97.46	110.90
2	H	151	VAL	CG1-CB-CG2	-8.38	97.49	110.90
1	A	35	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	96	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	L	96	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	A	33	LEU	O-C-N	-8.19	109.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	33	LEU	O-C-N	-8.18	109.61	122.70
1	L	35	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	A	148	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	L	148	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	A	152	ASN	CA-C-N	-7.98	99.64	117.20
1	L	152	ASN	CA-C-N	-7.98	99.64	117.20
2	B	36	TRP	CD1-CG-CD2	7.98	112.68	106.30
2	H	36	TRP	CD1-CG-CD2	7.93	112.64	106.30
2	B	102	GLY	O-C-N	7.88	135.31	122.70
2	H	102	GLY	O-C-N	7.87	135.28	122.70
1	L	39	LYS	O-C-N	-7.80	110.22	122.70
1	A	39	LYS	O-C-N	-7.77	110.27	122.70
2	B	47	TRP	CD1-CG-CD2	7.69	112.45	106.30
2	H	47	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	L	24	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	H	28	THR	CA-C-N	7.41	133.50	117.20
2	B	28	THR	CA-C-N	7.41	133.50	117.20
1	A	24	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	B	36	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	H	130	ARG	NE-CZ-NH2	7.27	123.94	120.30
2	H	155	TRP	CD1-CG-CD2	7.25	112.10	106.30
2	B	130	ARG	NE-CZ-NH2	7.24	123.92	120.30
2	B	155	TRP	CD1-CG-CD2	7.24	112.09	106.30
2	H	36	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	35	TRP	CE2-CD2-CG	-7.18	101.55	107.30
2	H	98	ARG	NE-CZ-NH2	7.17	123.89	120.30
2	B	155	TRP	CE2-CD2-CG	-7.17	101.57	107.30
2	H	155	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	L	35	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	B	98	ARG	NE-CZ-NH2	7.13	123.87	120.30
2	B	47	TRP	CE2-CD2-CG	-7.05	101.66	107.30
2	H	47	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	L	96	TYR	CB-CG-CD1	6.96	125.18	121.00
1	A	96	TYR	CB-CG-CD1	6.93	125.16	121.00
1	A	148	TRP	CG-CD1-NE1	-6.89	103.21	110.10
1	L	148	TRP	CG-CD1-NE1	-6.85	103.25	110.10
1	L	168	SER	CA-C-N	-6.76	102.33	117.20
1	A	168	SER	CA-C-N	-6.75	102.34	117.20
2	B	141	CYS	CA-CB-SG	-6.63	102.06	114.00
2	H	141	CYS	CA-CB-SG	-6.61	102.10	114.00
1	A	148	TRP	O-C-N	-6.60	112.14	122.70
1	L	148	TRP	O-C-N	-6.60	112.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	GLU	O-C-N	-6.49	112.32	122.70
1	L	27	GLU	O-C-N	-6.46	112.36	122.70
1	L	194	CYS	CA-CB-SG	-6.39	102.50	114.00
1	A	194	CYS	CA-CB-SG	-6.39	102.50	114.00
2	B	102	GLY	CA-C-N	-6.34	103.25	117.20
2	H	102	GLY	CA-C-N	-6.32	103.29	117.20
2	B	27	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	L	191	VAL	CA-CB-CG2	-6.31	101.44	110.90
2	H	27	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	191	VAL	CA-CB-CG2	-6.30	101.46	110.90
1	L	148	TRP	CA-C-N	6.28	131.03	117.20
1	A	148	TRP	CA-C-N	6.28	131.01	117.20
2	B	179	LEU	CA-CB-CG	6.26	129.70	115.30
2	H	179	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	59	PRO	CA-C-N	-6.01	103.97	117.20
1	L	59	PRO	CA-C-N	-6.00	104.00	117.20
1	A	152	ASN	O-C-N	-5.98	113.13	122.70
1	A	211	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	L	152	ASN	O-C-N	-5.97	113.14	122.70
1	A	92	TRP	CE2-CD2-CE3	5.94	125.83	118.70
1	L	92	TRP	CE2-CD2-CE3	5.93	125.81	118.70
1	L	211	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	L	114	THR	N-CA-CB	-5.76	99.35	110.30
1	A	114	THR	N-CA-CB	-5.76	99.36	110.30
2	H	113	SER	CA-C-N	-5.71	104.65	117.20
2	B	113	SER	CA-C-N	-5.68	104.70	117.20
2	H	156	ASN	CA-CB-CG	-5.61	101.06	113.40
2	B	156	ASN	CA-CB-CG	-5.61	101.06	113.40
2	H	211	ARG	CB-CG-CD	5.57	126.09	111.60
2	B	211	ARG	CB-CG-CD	5.57	126.09	111.60
2	H	197	CYS	CA-CB-SG	5.56	124.00	114.00
2	B	197	CYS	CA-CB-SG	5.55	124.00	114.00
1	L	39	LYS	CA-C-N	5.55	129.41	117.20
1	A	39	LYS	CA-C-N	5.54	129.39	117.20
2	H	65	LYS	CA-CB-CG	5.53	125.57	113.40
2	B	65	LYS	CA-CB-CG	5.52	125.54	113.40
2	B	211	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	B	52	SER	N-CA-C	-5.52	96.11	111.00
2	H	52	SER	N-CA-C	-5.50	96.14	111.00
2	H	54	GLY	C-N-CA	-5.47	108.02	121.70
2	H	211	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	B	54	GLY	C-N-CA	-5.47	108.03	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	A	135	LEU	O-C-N	-5.46	113.96	122.70
1	L	211	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	L	135	LEU	O-C-N	-5.44	114.00	122.70
2	B	98	ARG	CB-CA-C	-5.43	99.54	110.40
1	A	211	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	L	1	ASP	N-CA-C	-5.41	96.40	111.00
2	H	98	ARG	CB-CA-C	-5.40	99.60	110.40
1	A	1	ASP	N-CA-C	-5.40	96.42	111.00
1	L	35	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	L	186	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	186	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	L	86	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	86	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	A	134	CYS	CA-CB-SG	-5.29	104.47	114.00
1	L	134	CYS	CA-CB-SG	-5.29	104.48	114.00
2	B	94	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	L	56	ASP	CA-C-N	5.24	126.69	116.20
2	H	94	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	56	ASP	CA-C-N	5.23	126.66	116.20
1	A	186	TYR	C-N-CA	-5.23	108.63	121.70
1	L	186	TYR	C-N-CA	-5.22	108.65	121.70
1	L	210	ASN	CA-C-O	-5.18	109.22	120.10
1	A	21	ILE	CA-CB-CG2	-5.18	100.54	110.90
1	L	21	ILE	CA-CB-CG2	-5.17	100.56	110.90
1	A	210	ASN	CA-C-O	-5.17	109.25	120.10
1	A	24	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	B	36	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	L	24	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	H	36	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	L	194	CYS	CA-C-N	5.07	128.35	117.20
1	A	194	CYS	CA-C-N	5.06	128.33	117.20
2	H	36	TRP	CB-CG-CD1	-5.03	120.46	127.00
2	B	36	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	L	35	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	A	35	TRP	CB-CG-CD1	-5.00	120.50	127.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	28	ASN	Peptide
1	A	33	LEU	Mainchain
1	A	70	GLN	Mainchain
2	B	135	SER	Mainchain
2	B	142	LEU	Mainchain
2	B	42	GLU	Mainchain
2	B	67	LYS	Mainchain
2	H	135	SER	Mainchain
2	H	142	LEU	Mainchain
2	H	42	GLU	Mainchain
2	H	67	LYS	Mainchain
1	L	152	ASN	Mainchain
1	L	28	ASN	Peptide
1	L	33	LEU	Mainchain
1	L	70	GLN	Mainchain

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	A	1630	0	1561	65	0
1	L	1630	0	1561	65	1
2	B	1603	0	1561	42	0
2	H	1603	0	1561	42	1
All	All	6466	0	6244	208	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 16.

All (208) 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)
1:L:106:ILE:HD11	1:L:171:SER:OG	1.55	1.07
1:A:106:ILE:HD11	1:A:171:SER:OG	1.55	1.07
2:H:98:ARG:O	2:H:98:ARG:HG2	1.50	1.06
2:B:98:ARG:HG2	2:B:98:ARG:O	1.50	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:HG11	2:B:98:ARG:HH21	0.94	1.06
2:H:2:VAL:HG11	2:H:98:ARG:HH21	0.94	1.05
2:B:2:VAL:HG11	2:B:98:ARG:NH2	1.73	1.02
2:H:2:VAL:HG11	2:H:98:ARG:NH2	1.73	1.01
1:A:28:ASN:ND2	1:A:68:GLY:O	2.01	0.93
1:L:28:ASN:ND2	1:L:68:GLY:O	2.01	0.92
1:L:40:GLN:O	1:L:40:GLN:HG3	1.70	0.92
1:A:40:GLN:HG3	1:A:40:GLN:O	1.70	0.92
1:A:28:ASN:HD21	1:A:68:GLY:HA2	1.38	0.87
1:L:28:ASN:HD21	1:L:68:GLY:HA2	1.38	0.87
1:A:28:ASN:OD1	1:A:30:TYR:CE1	2.31	0.84
1:L:28:ASN:OD1	1:L:30:TYR:CE1	2.31	0.83
1:A:28:ASN:OD1	1:A:30:TYR:HE1	1.61	0.83
1:L:28:ASN:OD1	1:L:30:TYR:HE1	1.61	0.82
1:L:29:ILE:HG21	1:L:90:HIS:HB2	1.62	0.81
1:L:40:GLN:O	1:L:40:GLN:CG	2.29	0.81
1:A:29:ILE:HG21	1:A:90:HIS:HB2	1.62	0.81
1:A:40:GLN:O	1:A:40:GLN:CG	2.29	0.80
2:H:12:VAL:HG21	2:H:18:VAL:HB	1.68	0.76
2:B:12:VAL:HG21	2:B:18:VAL:HB	1.68	0.75
2:B:2:VAL:CG1	2:B:98:ARG:HH21	1.89	0.75
2:H:2:VAL:CG1	2:H:98:ARG:HH21	1.89	0.74
2:H:98:ARG:O	2:H:98:ARG:CG	2.35	0.73
2:B:33:ALA:HA	2:B:52:SER:HA	1.75	0.69
1:A:82:ASP:O	1:A:104:LEU:HD23	1.93	0.69
1:L:82:ASP:O	1:L:104:LEU:HD23	1.93	0.68
2:H:33:ALA:HA	2:H:52:SER:HA	1.75	0.68
2:B:18:VAL:HG21	2:B:110:LEU:HD11	1.75	0.68
1:L:28:ASN:ND2	1:L:68:GLY:HA2	2.09	0.67
1:A:28:ASN:ND2	1:A:68:GLY:HA2	2.09	0.67
2:H:18:VAL:HG21	2:H:110:LEU:HD11	1.75	0.67
2:B:98:ARG:CG	2:B:98:ARG:O	2.35	0.66
1:A:35:TRP:HB2	1:A:48:VAL:HG13	1.78	0.66
2:H:51:ILE:HG12	2:H:58:ILE:HG22	1.78	0.66
1:A:150:VAL:O	1:A:191:VAL:O	2.14	0.66
1:L:35:TRP:HB2	1:L:48:VAL:HG13	1.78	0.66
2:B:51:ILE:HG12	2:B:58:ILE:HG22	1.78	0.66
1:L:150:VAL:O	1:L:191:VAL:O	2.14	0.66
2:B:99:SER:OG	2:B:100:TYR:N	2.30	0.65
2:H:99:SER:OG	2:H:100:TYR:N	2.30	0.65
2:H:48:ILE:HD13	2:H:81:MET:SD	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HD13	2:B:81:MET:SD	2.38	0.64
2:H:143:VAL:HG11	2:H:151:VAL:HG11	1.80	0.64
1:A:13:VAL:HG21	1:A:19:VAL:HG22	1.79	0.64
1:L:24:ARG:HA	1:L:69:THR:O	1.99	0.63
1:L:13:VAL:HG21	1:L:19:VAL:HG22	1.79	0.63
2:B:143:VAL:HG11	2:B:151:VAL:HG11	1.80	0.63
1:A:24:ARG:HA	1:A:69:THR:O	1.99	0.63
1:A:42:LYS:HE2	1:A:42:LYS:HA	1.81	0.63
1:L:42:LYS:HE2	1:L:42:LYS:HA	1.81	0.62
1:A:13:VAL:HG23	1:A:78:LEU:HD22	1.80	0.62
1:L:13:VAL:HG23	1:L:78:LEU:HD22	1.80	0.62
1:L:106:ILE:HD11	1:L:171:SER:HG	1.60	0.61
1:A:51:ALA:O	1:A:52:THR:HB	2.01	0.60
1:L:136:LEU:N	1:L:136:LEU:HD12	2.16	0.60
1:A:167:ASP:HB3	1:A:170:ASP:OD1	2.02	0.59
1:L:167:ASP:HB3	1:L:170:ASP:OD1	2.02	0.59
1:L:51:ALA:O	1:L:52:THR:HB	2.01	0.59
1:A:136:LEU:HD12	1:A:136:LEU:N	2.16	0.59
2:B:134:GLU:HG2	2:B:135:SER:H	1.68	0.59
1:A:85:SER:HA	1:A:102:THR:O	2.03	0.58
2:H:134:GLU:HG2	2:H:135:SER:H	1.68	0.58
2:B:51:ILE:HB	2:B:70:LEU:HB3	1.86	0.58
1:L:85:SER:HA	1:L:102:THR:O	2.03	0.58
2:H:51:ILE:HB	2:H:70:LEU:HB3	1.86	0.58
1:A:29:ILE:O	1:A:29:ILE:HG13	2.03	0.57
1:L:40:GLN:O	1:L:40:GLN:NE2	2.38	0.57
1:A:40:GLN:NE2	1:A:40:GLN:O	2.38	0.57
1:A:36:TYR:O	1:A:86:TYR:HA	2.05	0.56
1:L:29:ILE:O	1:L:29:ILE:HG13	2.03	0.56
2:H:18:VAL:HG11	2:H:110:LEU:HD21	1.87	0.56
1:L:36:TYR:O	1:L:86:TYR:HA	2.05	0.56
2:B:18:VAL:HG11	2:B:110:LEU:HD21	1.87	0.56
1:A:166:GLN:HG2	1:A:173:TYR:CZ	2.41	0.56
1:L:166:GLN:HG2	1:L:173:TYR:CZ	2.41	0.56
2:H:34:ILE:HA	2:H:97:LYS:O	2.06	0.55
2:B:34:ILE:HA	2:B:97:LYS:O	2.06	0.55
2:B:68:ALA:HA	2:B:82:GLN:O	2.07	0.55
2:B:123:PHE:HB2	2:B:142:LEU:HB3	1.89	0.54
1:A:106:ILE:HD11	1:A:171:SER:HG	1.67	0.54
2:H:68:ALA:HA	2:H:82:GLN:O	2.07	0.54
2:H:123:PHE:HB2	2:H:142:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG23	1:A:155:GLN:CG	2.38	0.53
1:A:167:ASP:C	1:A:169:LYS:N	2.61	0.53
1:L:150:VAL:HG23	1:L:155:GLN:CG	2.38	0.53
1:L:167:ASP:C	1:L:169:LYS:N	2.61	0.52
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.45	0.52
2:H:55:ASN:O	2:H:57:ASP:N	2.43	0.52
2:B:55:ASN:O	2:B:57:ASP:N	2.43	0.52
1:A:62:PHE:CE1	1:A:75:ILE:HG12	2.45	0.51
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.92	0.51
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.92	0.51
2:B:189:SER:HA	2:B:192:THR:OG1	2.10	0.51
1:A:167:ASP:O	1:A:169:LYS:N	2.44	0.51
1:L:167:ASP:O	1:L:169:LYS:N	2.44	0.51
1:A:29:ILE:HG21	1:A:90:HIS:CB	2.38	0.50
2:H:189:SER:HA	2:H:192:THR:OG1	2.10	0.50
1:L:29:ILE:HG21	1:L:90:HIS:CB	2.38	0.50
2:B:125:LEU:HD11	2:B:142:LEU:HB2	1.94	0.50
1:L:145:LYS:CG	1:L:197:THR:HB	2.41	0.50
2:H:125:LEU:HD11	2:H:142:LEU:HB2	1.94	0.50
1:A:108:ARG:NH1	1:A:109:ALA:O	2.45	0.50
1:L:108:ARG:NH1	1:L:109:ALA:O	2.45	0.50
1:L:162:SER:HB2	2:H:168:PRO:HG2	1.94	0.49
2:H:51:ILE:HG12	2:H:58:ILE:CG2	2.41	0.49
1:A:66:GLY:HA3	1:A:71:TYR:HA	1.94	0.49
1:A:145:LYS:CG	1:A:197:THR:HB	2.41	0.49
2:B:51:ILE:HG12	2:B:58:ILE:CG2	2.41	0.49
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.94	0.49
1:A:162:SER:HB2	2:B:168:PRO:HG2	1.94	0.49
1:A:136:LEU:N	1:A:136:LEU:CD1	2.75	0.49
1:L:136:LEU:CD1	1:L:136:LEU:N	2.75	0.48
1:A:49:TYR:O	1:A:53:ASN:HB2	2.13	0.48
1:L:49:TYR:O	1:L:53:ASN:HB2	2.13	0.48
2:H:67:LYS:HE2	2:H:67:LYS:HB2	1.48	0.48
2:B:67:LYS:HE2	2:B:67:LYS:HB2	1.49	0.47
1:L:28:ASN:ND2	1:L:68:GLY:C	2.65	0.47
1:L:91:PHE:CE2	2:H:100:TYR:O	2.67	0.47
1:A:28:ASN:ND2	1:A:68:GLY:CA	2.75	0.47
1:L:148:TRP:HA	1:L:193:ALA:O	2.14	0.47
1:A:167:ASP:C	1:A:169:LYS:H	2.16	0.47
1:L:167:ASP:C	1:L:169:LYS:H	2.16	0.47
1:A:148:TRP:HA	1:A:193:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:CE2	2:B:100:TYR:O	2.67	0.47
1:L:28:ASN:ND2	1:L:68:GLY:CA	2.75	0.47
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.97	0.47
1:L:33:LEU:HD13	1:L:33:LEU:C	2.35	0.47
1:L:136:LEU:HD21	1:L:196:VAL:HG13	1.97	0.47
1:L:185:ASP:O	1:L:189:HIS:HD2	1.97	0.47
2:B:153:VAL:HG11	2:B:181:SER:CB	2.45	0.46
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.97	0.46
1:A:185:ASP:O	1:A:189:HIS:HD2	1.97	0.46
1:A:28:ASN:ND2	1:A:68:GLY:C	2.65	0.46
2:H:201:HIS:CE1	2:H:203:PRO:HG2	2.51	0.46
2:H:153:VAL:HG11	2:H:181:SER:CB	2.44	0.46
1:A:150:VAL:HG23	1:A:155:GLN:HG3	1.98	0.46
2:B:201:HIS:CE1	2:B:203:PRO:HG2	2.51	0.46
1:A:33:LEU:HD13	1:A:33:LEU:C	2.35	0.46
1:A:136:LEU:HD21	1:A:196:VAL:HG13	1.97	0.46
1:L:150:VAL:HG23	1:L:155:GLN:HG3	1.98	0.46
1:A:33:LEU:HD13	1:A:34:ALA:N	2.30	0.46
1:A:190:LYS:O	1:A:210:ASN:HA	2.15	0.46
1:L:33:LEU:HD13	1:L:34:ALA:N	2.30	0.46
1:L:190:LYS:O	1:L:210:ASN:HA	2.15	0.46
1:A:36:TYR:HE2	1:A:89:GLN:HE21	1.64	0.46
1:L:29:ILE:CG2	1:L:90:HIS:HB2	2.42	0.45
2:B:186:PRO:HG2	2:B:189:SER:OG	2.15	0.45
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.64	0.45
1:L:61:ARG:HE	1:L:61:ARG:HB3	1.58	0.45
2:B:81:MET:HE2	2:B:81:MET:HB3	1.84	0.45
2:H:186:PRO:HG2	2:H:189:SER:OG	2.15	0.45
2:H:81:MET:HE2	2:H:81:MET:HB3	1.84	0.45
1:L:39:LYS:HE3	1:L:83:PHE:O	2.17	0.45
2:H:29:PHE:CD2	2:H:77:SER:HA	2.52	0.44
1:A:39:LYS:HE3	1:A:83:PHE:O	2.17	0.44
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.53	0.44
1:L:11:LEU:HB3	1:L:104:LEU:HD12	2.00	0.44
2:B:22:CYS:HB2	2:B:36:TRP:CH2	2.53	0.44
1:A:29:ILE:CG2	1:A:90:HIS:HB2	2.42	0.44
1:A:11:LEU:HB3	1:A:104:LEU:HD12	2.00	0.44
1:A:31:SER:HB3	1:A:51:ALA:HB3	2.00	0.44
2:B:29:PHE:CD2	2:B:77:SER:HA	2.53	0.44
1:L:52:THR:HA	1:L:64:GLY:HA3	1.99	0.43
1:L:138:ASN:HA	1:L:173:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HA	1:A:64:GLY:HA3	1.99	0.43
1:L:31:SER:HB3	1:L:51:ALA:HB3	2.00	0.43
1:A:138:ASN:HA	1:A:173:TYR:O	2.18	0.43
1:A:155:GLN:HB3	1:A:158:ASN:OD1	2.18	0.43
2:B:135:SER:O	2:B:186:PRO:HA	2.19	0.43
2:H:97:LYS:HD2	2:H:104:TRP:CE2	2.53	0.43
1:L:155:GLN:HB3	1:L:158:ASN:OD1	2.18	0.43
2:B:97:LYS:HD2	2:B:104:TRP:CE2	2.53	0.43
1:A:61:ARG:HB3	1:A:61:ARG:HE	1.58	0.43
2:H:135:SER:O	2:H:186:PRO:HA	2.19	0.43
1:A:145:LYS:HG2	1:A:197:THR:HB	2.01	0.42
1:L:44:PRO:HD2	2:H:104:TRP:CE3	2.54	0.42
1:A:6:GLN:OE1	1:A:87:TYR:HA	2.19	0.42
2:B:22:CYS:O	2:B:78:THR:HA	2.19	0.42
2:H:18:VAL:HG11	2:H:110:LEU:CD2	2.48	0.42
1:L:145:LYS:HG2	1:L:197:THR:HB	2.01	0.42
1:L:6:GLN:OE1	1:L:87:TYR:HA	2.19	0.42
2:H:3:GLN:HG3	2:H:5:GLN:OE1	2.19	0.42
2:H:22:CYS:O	2:H:78:THR:HA	2.19	0.42
2:B:3:GLN:HG3	2:B:5:GLN:OE1	2.19	0.42
2:H:4:LEU:HD13	2:H:22:CYS:SG	2.59	0.42
2:B:4:LEU:HD13	2:B:22:CYS:SG	2.59	0.42
2:B:18:VAL:HG11	2:B:110:LEU:CD2	2.49	0.42
1:L:145:LYS:HG3	1:L:197:THR:HB	2.02	0.42
1:A:44:PRO:HD2	2:B:104:TRP:CE3	2.54	0.41
1:A:67:SER:O	1:A:69:THR:N	2.53	0.41
1:L:67:SER:O	1:L:69:THR:N	2.53	0.41
1:A:2:ILE:HD11	1:A:29:ILE:HG23	2.03	0.41
2:H:51:ILE:HD12	2:H:72:ALA:HB2	2.03	0.41
1:A:145:LYS:HG3	1:A:197:THR:HB	2.02	0.41
2:B:18:VAL:CG1	2:B:86:LEU:HD11	2.50	0.41
2:B:51:ILE:HD12	2:B:72:ALA:HB2	2.03	0.41
1:L:33:LEU:HD21	1:L:88:CYS:HB2	2.04	0.40
1:L:8:PRO:HD2	1:L:21:ILE:HG23	2.04	0.40
1:L:2:ILE:HD11	1:L:29:ILE:HG23	2.03	0.40
1:A:8:PRO:HD2	1:A:21:ILE:HG23	2.04	0.40
1:A:40:GLN:O	1:A:40:GLN:CD	2.60	0.40
2:H:18:VAL:CG1	2:H:86:LEU:HD11	2.50	0.40
2:H:117:THR:HG23	2:H:148:PRO:HD3	2.04	0.40
2:B:117:THR:HG23	2:B:148:PRO:HD3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:CG1	2:H:192:THR:CG2[4_466]	1.87	0.33

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	A	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	7 33
1	L	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	7 33
2	B	210/212 (99%)	186 (89%)	20 (10%)	4 (2%)	10 40
2	H	210/212 (99%)	186 (89%)	20 (10%)	4 (2%)	10 40
All	All	838/846 (99%)	746 (89%)	74 (9%)	18 (2%)	9 37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	THR
2	H	56	ASP
1	A	52	THR
2	B	56	ASP
1	L	60	SER
1	L	68	GLY
2	H	162	SER
1	A	60	SER
1	A	68	GLY
2	B	162	SER
2	H	99	SER
2	B	99	SER
1	L	41	GLY
2	H	41	PRO
1	A	41	GLY
2	B	41	PRO

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Mol	Chain	Res	Type
1	A	184	ALA
1	L	184	ALA

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	A	183/183 (100%)	158 (86%)	25 (14%)	4	19
1	L	183/183 (100%)	158 (86%)	25 (14%)	4	19
2	B	181/181 (100%)	150 (83%)	31 (17%)	2	11
2	H	181/181 (100%)	150 (83%)	31 (17%)	2	11
All	All	728/728 (100%)	616 (85%)	112 (15%)	3	14

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	3	GLN
1	L	14	SER
1	L	17	GLU
1	L	28	ASN
1	L	44	PRO
1	L	46	LEU
1	L	48	VAL
1	L	60	SER
1	L	61	ARG
1	L	67	SER
1	L	70	GLN
1	L	73	LEU
1	L	81	GLU
1	L	97	THR
1	L	129	THR
1	L	151	ASP
1	L	152	ASN
1	L	161	GLU

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Mol	Chain	Res	Type
1	L	164	THR
1	L	165	GLU
1	L	175	LEU
1	L	180	THR
1	L	182	SER
1	L	191	VAL
2	H	23	LYS
2	H	30	THR
2	H	31	ASP
2	H	40	LYS
2	H	46	GLU
2	H	51	ILE
2	H	55	ASN
2	H	59	LYS
2	H	67	LYS
2	H	70	LEU
2	H	74	LYS
2	H	85	SER
2	H	97	LYS
2	H	109	THR
2	H	114	SER
2	H	128	CYS
2	H	130	ARG
2	H	132	THR
2	H	133	SER
2	H	148	PRO
2	H	150	PRO
2	H	160	LEU
2	H	161	THR
2	H	162	SER
2	H	173	SER
2	H	178	SER
2	H	179	LEU
2	H	180	SER
2	H	182	VAL
2	H	188	SER
2	H	189	SER
1	A	2	ILE
1	A	3	GLN
1	A	14	SER
1	A	17	GLU
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	44	PRO
1	A	46	LEU
1	A	48	VAL
1	A	60	SER
1	A	61	ARG
1	A	67	SER
1	A	70	GLN
1	A	73	LEU
1	A	81	GLU
1	A	97	THR
1	A	129	THR
1	A	151	ASP
1	A	152	ASN
1	A	161	GLU
1	A	164	THR
1	A	165	GLU
1	A	175	LEU
1	A	180	THR
1	A	182	SER
1	A	191	VAL
2	B	23	LYS
2	B	30	THR
2	B	31	ASP
2	B	40	LYS
2	B	46	GLU
2	B	51	ILE
2	B	55	ASN
2	B	59	LYS
2	B	67	LYS
2	B	70	LEU
2	B	74	LYS
2	B	85	SER
2	B	97	LYS
2	B	109	THR
2	B	114	SER
2	B	128	CYS
2	B	130	ARG
2	B	132	THR
2	B	133	SER
2	B	148	PRO
2	B	150	PRO
2	B	160	LEU

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Mol	Chain	Res	Type
2	B	161	THR
2	B	162	SER
2	B	173	SER
2	B	178	SER
2	B	179	LEU
2	B	180	SER
2	B	182	VAL
2	B	188	SER
2	B	189	SER

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

Mol	Chain	Res	Type
1	L	32	ASN
1	L	89	GLN
2	H	156	ASN
1	A	32	ASN
1	A	89	GLN
2	B	156	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
2	PCA	B	1	2	7,8,9	1.49	1 (14%)	9,10,12	1.68	3 (33%)
2	PCA	H	1	2	7,8,9	1.47	1 (14%)	9,10,12	1.68	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	3.51	1.45	1.33
2	B	1	PCA	CD-N	3.55	1.45	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	PCA	O-C-CA	-2.66	118.42	125.44
2	B	1	PCA	O-C-CA	-2.65	118.43	125.44
2	H	1	PCA	OE-CD-CG	-2.51	121.20	126.81
2	B	1	PCA	OE-CD-CG	-2.51	121.20	126.81
2	H	1	PCA	OE-CD-N	-2.03	118.70	124.85
2	B	1	PCA	OE-CD-N	-2.03	118.71	124.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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