



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:26 am BST

PDB ID : 1BM3
Title : IMMUNOGLOBULIN OPG2 FAB-PEPTIDE COMPLEX
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Deposited on : 1999-04-15
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

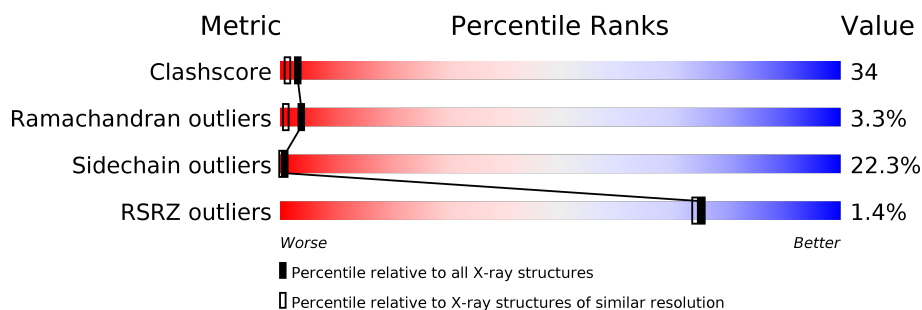
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	L	214	<div> <div>2%</div> <div>39% 36% 20% 5%</div> </div>
2	H	227	<div> <div>2%</div> <div>35% 31% 20% 9% 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3589 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 IMMUNOGLOBULIN OPG2 FAB, CONSTANT DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1654	1023	280	344	7			

- Molecule 2 is a protein called IMMUNOGLOBULIN OPG2 FAB, VARIABLE DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1622	1016	280	317	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	153	Total	O	0	0
			153	153		
3	H	160	Total	O	0	0
			160	160		

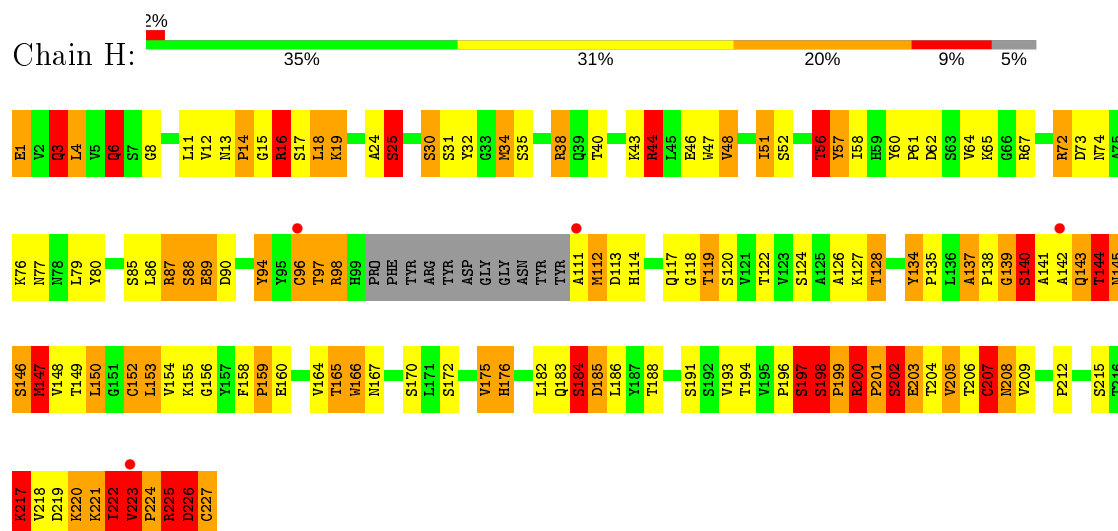
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

• Molecule 1: IMMUNOGLOBULIN OPG2 FAB, CONSTANT DOMAIN



• Molecule 2: IMMUNOGLOBULIN OPG2 FAB, VARIABLE DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	A 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 90.05Å 79.11Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 18.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	78.0 (8.00-2.00) 83.2 (18.63-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.152 , (Not available) 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.00	0/1691	2.60	109/2293 (4.8%)
2	H	0.99	1/1662 (0.1%)	2.60	110/2266 (4.9%)
All	All	1.00	1/3353 (0.0%)	2.60	219/4559 (4.8%)

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
2	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	67	ARG	NE-CZ	-6.10	1.25	1.33

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	188	ARG	CD-NE-CZ	24.31	157.63	123.60
2	H	90	ASP	CB-CG-OD1	22.93	138.94	118.30
1	L	1	ASP	CB-CG-OD1	19.29	135.66	118.30
2	H	225	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	L	11	LEU	CA-CB-CG	17.46	155.45	115.30
1	L	192	TYR	CB-CG-CD2	-17.38	110.57	121.00
2	H	67	ARG	NE-CZ-NH2	17.04	128.82	120.30
2	H	87	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	L	192	TYR	CB-CG-CD1	16.69	131.02	121.00
2	H	72	ARG	NE-CZ-NH1	-15.80	112.40	120.30
2	H	67	ARG	CD-NE-CZ	13.96	143.15	123.60
1	L	136	LEU	CA-CB-CG	13.06	145.33	115.30
2	H	119	THR	N-CA-CB	11.99	133.08	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2	GLU	OE1-CD-OE2	11.99	137.68	123.30
1	L	211	ARG	NE-CZ-NH1	11.97	126.28	120.30
2	H	73	ASP	CB-CG-OD1	11.62	128.76	118.30
2	H	200	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	L	211	ARG	CD-NE-CZ	11.21	139.30	123.60
1	L	45	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	L	188	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	L	211	ARG	CB-CA-C	10.73	131.86	110.40
1	L	184	ASP	CB-CG-OD2	-10.40	108.94	118.30
2	H	90	ASP	CB-CG-OD2	-10.30	109.03	118.30
2	H	64	VAL	N-CA-CB	-10.24	88.98	111.50
2	H	226	ASP	CB-CG-OD1	9.89	127.20	118.30
1	L	13	VAL	CA-CB-CG1	9.70	125.45	110.90
1	L	1	ASP	N-CA-CB	9.56	127.81	110.60
2	H	57	TYR	CA-CB-CG	9.54	131.52	113.40
2	H	225	ARG	NE-CZ-NH2	-9.47	115.56	120.30
2	H	38	ARG	NE-CZ-NH1	9.29	124.95	120.30
2	H	200	ARG	N-CA-C	-9.26	86.01	111.00
2	H	199	PRO	CA-C-O	9.23	142.37	120.20
1	L	184	ASP	CB-CG-OD1	9.21	126.59	118.30
2	H	18	LEU	CA-CB-CG	9.18	136.41	115.30
1	L	195	GLU	OE1-CD-OE2	9.11	134.24	123.30
1	L	212	ASN	N-CA-C	9.09	135.54	111.00
2	H	199	PRO	C-N-CA	9.05	144.32	121.70
2	H	226	ASP	N-CA-C	9.03	135.38	111.00
2	H	77	ASN	CA-CB-CG	8.98	133.15	113.40
1	L	1	ASP	OD1-CG-OD2	-8.97	106.26	123.30
2	H	40	THR	CA-CB-CG2	8.85	124.78	112.40
2	H	87	ARG	NH1-CZ-NH2	-8.80	109.72	119.40
1	L	108	ARG	NE-CZ-NH2	-8.69	115.95	120.30
2	H	16	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	H	197	SER	N-CA-CB	-8.39	97.91	110.50
1	L	181	LEU	N-CA-CB	-8.27	93.86	110.40
2	H	205	VAL	N-CA-CB	8.24	129.63	111.50
1	L	107	LYS	CA-CB-CG	8.23	131.51	113.40
1	L	1	ASP	CA-CB-CG	8.13	131.30	113.40
1	L	162	SER	CA-CB-OG	-8.13	89.24	111.20
1	L	54	SER	N-CA-CB	8.09	122.64	110.50
1	L	70	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	L	45	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	L	4	LEU	CA-CB-CG	8.04	133.80	115.30
1	L	74	SER	N-CA-CB	-7.95	98.57	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	87	ARG	CD-NE-CZ	-7.94	112.48	123.60
2	H	155	LYS	CA-CB-CG	7.91	130.81	113.40
1	L	17	ASP	CB-CG-OD1	7.83	125.35	118.30
2	H	175	VAL	CA-CB-CG1	7.81	122.62	110.90
2	H	217	LYS	N-CA-CB	7.81	124.65	110.60
2	H	46	GLU	N-CA-CB	7.68	124.42	110.60
1	L	2	GLU	CG-CD-OE2	-7.64	103.01	118.30
2	H	67	ARG	NH1-CZ-NH2	-7.63	111.00	119.40
2	H	199	PRO	O-C-N	-7.60	110.55	122.70
1	L	211	ARG	NH1-CZ-NH2	-7.59	111.05	119.40
1	L	82	ASP	CB-CG-OD1	7.58	125.12	118.30
1	L	155	ARG	CD-NE-CZ	7.52	134.13	123.60
1	L	70	ASP	CB-CG-OD1	7.52	125.07	118.30
2	H	67	ARG	CB-CG-CD	7.48	131.05	111.60
1	L	90	GLN	CA-CB-CG	7.45	129.78	113.40
2	H	98	ARG	NE-CZ-NH2	7.31	123.96	120.30
2	H	139	GLY	N-CA-C	-7.30	94.86	113.10
2	H	72	ARG	NH1-CZ-NH2	7.24	127.37	119.40
1	L	127	SER	CB-CA-C	7.23	123.83	110.10
1	L	33	LEU	CB-CG-CD2	-7.22	98.73	111.00
2	H	205	VAL	CA-CB-CG2	7.19	121.69	110.90
1	L	212	ASN	N-CA-CB	-7.14	97.75	110.60
1	L	94	TRP	CB-CG-CD1	7.14	136.28	127.00
1	L	49	LYS	C-N-CA	7.14	139.54	121.70
2	H	225	ARG	CB-CG-CD	7.04	129.90	111.60
2	H	184	SER	C-N-CA	7.03	139.27	121.70
2	H	8	GLY	CA-C-O	-7.02	107.96	120.60
1	L	2	GLU	CB-CG-CD	-6.97	95.39	114.20
1	L	165	ASP	CB-CG-OD1	-6.96	112.04	118.30
2	H	137	ALA	N-CA-CB	6.88	119.73	110.10
1	L	155	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	L	167	ASP	CB-CG-OD1	6.84	124.46	118.30
2	H	57	TYR	CB-CG-CD1	6.83	125.10	121.00
2	H	94	TYR	CB-CG-CD1	6.83	125.10	121.00
1	L	153	SER	CB-CA-C	-6.82	97.14	110.10
1	L	4	LEU	CB-CG-CD2	-6.81	99.43	111.00
2	H	153	LEU	CA-CB-CG	6.79	130.92	115.30
1	L	94	TRP	CB-CG-CD2	-6.79	117.77	126.60
1	L	212	ASN	CB-CA-C	-6.79	96.82	110.40
1	L	153	SER	CA-CB-OG	6.75	129.42	111.20
1	L	153	SER	N-CA-CB	6.71	120.57	110.50
1	L	187	GLU	OE1-CD-OE2	6.71	131.35	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	179	LEU	CB-CG-CD2	-6.68	99.64	111.00
2	H	19	LYS	CA-CB-CG	-6.66	98.74	113.40
2	H	25	SER	CB-CA-C	-6.64	97.48	110.10
2	H	166	TRP	CB-CA-C	6.63	123.67	110.40
1	L	181	LEU	CA-CB-CG	6.63	130.54	115.30
2	H	154	VAL	CA-CB-CG2	6.62	120.84	110.90
1	L	82	ASP	CB-CG-OD2	-6.62	112.34	118.30
2	H	183	GLN	CB-CG-CD	6.55	128.63	111.60
2	H	15	GLY	CA-C-O	-6.51	108.88	120.60
2	H	18	LEU	N-CA-CB	6.44	123.29	110.40
1	L	204	PRO	N-CD-CG	-6.44	93.54	103.20
1	L	103	LYS	CA-CB-CG	6.44	127.56	113.40
2	H	46	GLU	CG-CD-OE2	-6.41	105.49	118.30
2	H	146	SER	N-CA-C	-6.38	93.78	111.00
1	L	61	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	L	123	GLU	CG-CD-OE1	6.37	131.03	118.30
1	L	105	GLU	CA-CB-CG	6.34	127.34	113.40
2	H	34	MET	CG-SD-CE	6.32	110.32	100.20
1	L	123	GLU	N-CA-CB	6.32	121.98	110.60
2	H	184	SER	CA-C-O	6.31	133.35	120.10
1	L	59	PRO	CB-CA-C	6.30	127.76	112.00
1	L	205	ILE	N-CA-CB	6.30	125.28	110.80
1	L	117	ILE	CG1-CB-CG2	-6.29	97.56	111.40
1	L	132	VAL	CA-CB-CG1	-6.27	101.50	110.90
2	H	16	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	H	46	GLU	OE1-CD-OE2	6.21	130.75	123.30
2	H	207	CYS	N-CA-CB	6.17	121.70	110.60
1	L	73	LEU	CA-CB-CG	6.16	129.47	115.30
2	H	226	ASP	CA-C-O	6.15	133.02	120.10
2	H	112	MET	CG-SD-CE	6.15	110.04	100.20
2	H	220	LYS	N-CA-CB	6.10	121.59	110.60
2	H	24	ALA	CB-CA-C	6.07	119.21	110.10
2	H	48	VAL	N-CA-CB	-6.04	98.21	111.50
1	L	47	LEU	CA-CB-CG	6.00	129.10	115.30
2	H	85	SER	N-CA-CB	5.96	119.44	110.50
1	L	188	ARG	CB-CA-C	5.95	122.29	110.40
2	H	90	ASP	OD1-CG-OD2	-5.93	112.02	123.30
2	H	191	SER	N-CA-CB	5.93	119.39	110.50
1	L	3	LEU	O-C-N	5.92	132.18	122.70
2	H	38	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
2	H	184	SER	N-CA-CB	-5.90	101.64	110.50
1	L	72	THR	C-N-CA	5.90	136.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	90	GLN	CB-CG-CD	5.90	126.94	111.60
2	H	226	ASP	CA-CB-CG	5.87	126.31	113.40
2	H	165	THR	N-CA-CB	5.84	121.40	110.30
2	H	185	ASP	CB-CA-C	5.83	122.06	110.40
1	L	167	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	L	73	LEU	N-CA-CB	5.82	122.04	110.40
2	H	222	ILE	CA-C-O	5.80	132.29	120.10
2	H	48	VAL	CA-CB-CG1	5.77	119.56	110.90
1	L	140	TYR	CA-CB-CG	-5.76	102.45	113.40
1	L	22	SER	N-CA-CB	5.75	119.13	110.50
2	H	223	VAL	CB-CA-C	5.75	122.31	111.40
2	H	18	LEU	CB-CA-C	-5.74	99.29	110.20
2	H	140	SER	C-N-CA	5.72	136.01	121.70
1	L	138	ASN	CA-CB-CG	5.71	125.96	113.40
2	H	64	VAL	CB-CA-C	5.69	122.22	111.40
2	H	217	LYS	N-CA-C	-5.68	95.67	111.00
2	H	4	LEU	O-C-N	5.67	131.77	122.70
1	L	85	MET	N-CA-CB	-5.66	100.41	110.60
1	L	21	LEU	CA-C-O	-5.64	108.26	120.10
1	L	94	TRP	N-CA-CB	5.63	120.74	110.60
1	L	142	LYS	CA-CB-CG	5.63	125.78	113.40
2	H	143	GLN	CB-CG-CD	5.62	126.21	111.60
1	L	153	SER	O-C-N	5.61	131.68	122.70
1	L	187	GLU	CG-CD-OE1	-5.60	107.11	118.30
2	H	128	THR	CA-CB-CG2	5.58	120.22	112.40
1	L	188	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
1	L	174	SER	N-CA-CB	5.56	118.84	110.50
1	L	145	ASN	O-C-N	5.56	131.59	122.70
2	H	198	SER	N-CA-CB	5.56	118.84	110.50
2	H	200	ARG	CB-CA-C	5.55	121.50	110.40
1	L	168	SER	CB-CA-C	-5.54	99.58	110.10
2	H	164	VAL	O-C-N	5.52	131.54	122.70
2	H	80	TYR	O-C-N	5.52	131.53	122.70
1	L	22	SER	CB-CA-C	-5.52	99.62	110.10
2	H	88	SER	CB-CA-C	5.51	120.57	110.10
1	L	152	GLY	CA-C-O	-5.47	110.75	120.60
1	L	59	PRO	N-CA-CB	-5.46	96.59	102.60
1	L	138	ASN	OD1-CG-ND2	-5.46	109.35	121.90
2	H	44	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	L	211	ARG	CA-C-O	5.41	131.46	120.10
2	H	86	LEU	CB-CG-CD2	5.40	120.18	111.00
1	L	213	GLU	N-CA-C	5.40	125.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	196	ALA	N-CA-CB	-5.39	102.55	110.10
2	H	3	GLN	N-CA-CB	5.39	120.31	110.60
2	H	191	SER	O-C-N	5.37	131.30	122.70
1	L	55	ILE	CB-CA-C	5.37	122.34	111.60
2	H	16	ARG	CD-NE-CZ	5.37	131.12	123.60
2	H	140	SER	CA-C-O	5.37	131.37	120.10
2	H	134	TYR	CB-CG-CD1	5.37	124.22	121.00
2	H	124	SER	N-CA-CB	-5.35	102.47	110.50
2	H	176	HIS	CB-CA-C	-5.33	99.75	110.40
2	H	188	THR	N-CA-CB	5.32	120.42	110.30
2	H	6	GLN	O-C-N	5.32	131.21	122.70
2	H	225	ARG	CD-NE-CZ	5.31	131.04	123.60
1	L	75	ILE	CA-CB-CG1	5.31	121.09	111.00
1	L	90	GLN	N-CA-CB	-5.29	101.07	110.60
1	L	4	LEU	N-CA-C	-5.26	96.79	111.00
1	L	96	LEU	O-C-N	5.26	131.12	122.70
2	H	160	GLU	CA-CB-CG	5.26	124.96	113.40
1	L	12	SER	N-CA-CB	-5.24	102.64	110.50
2	H	56	THR	CA-C-O	-5.21	109.16	120.10
1	L	123	GLU	CA-C-O	-5.20	109.19	120.10
1	L	15	PRO	N-CA-CB	5.19	109.53	103.30
2	H	1	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	L	206	VAL	CA-CB-CG1	5.17	118.66	110.90
1	L	208	SER	O-C-N	5.16	130.95	122.70
2	H	224	PRO	N-CD-CG	-5.15	95.47	103.20
2	H	60	TYR	O-C-N	5.13	130.85	121.10
1	L	137	ASN	CA-C-O	5.10	130.81	120.10
2	H	30	SER	O-C-N	5.10	130.86	122.70
1	L	184	ASP	CB-CA-C	5.10	120.59	110.40
2	H	199	PRO	CA-N-CD	-5.10	104.36	111.50
1	L	205	ILE	CB-CA-C	-5.09	101.43	111.60
2	H	205	VAL	N-CA-C	-5.07	97.32	111.00
1	L	71	PHE	O-C-N	5.06	130.80	122.70
1	L	13	VAL	N-CA-CB	-5.06	100.37	111.50
1	L	87	PHE	CB-CG-CD1	-5.05	117.26	120.80
2	H	31	SER	O-C-N	5.02	130.73	122.70
2	H	72	ARG	N-CA-CB	5.01	119.62	110.60
2	H	18	LEU	CA-C-N	-5.00	106.19	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	225	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	1654	0	1569	81	6
2	H	1622	0	1588	142	1
3	H	160	0	0	19	6
3	L	153	0	0	17	3
All	All	3589	0	3157	216	9

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 34.

All (216) 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:16:ARG:HG3	2:H:17:SER:H	1.08	1.08
1:L:36:TYR:OH	2:H:111:ALA:HB1	1.67	0.94
1:L:8:PRO:HG2	1:L:11:LEU:HD22	1.50	0.92
1:L:11:LEU:HD21	1:L:21:LEU:CD1	1.99	0.92
1:L:1:ASP:HB2	1:L:95:PRO:HD2	1.53	0.91
1:L:11:LEU:HD21	1:L:21:LEU:HD11	1.51	0.90
1:L:90:GLN:HE21	1:L:92:ASN:H	1.20	0.89
2:H:137:ALA:HB2	2:H:225:ARG:HD3	1.54	0.89
2:H:97:THR:HA	2:H:114:HIS:O	1.72	0.89
2:H:182:LEU:HD11	2:H:185:ASP:HA	1.54	0.88
1:L:34:HIS:CD2	2:H:111:ALA:HB2	2.13	0.82
1:L:198:HIS:HB3	3:L:901:HOH:O	1.81	0.80
2:H:16:ARG:HG3	2:H:17:SER:N	1.92	0.80
2:H:97:THR:CG2	2:H:112:MET:HB3	2.11	0.80
2:H:98:ARG:O	2:H:113:ASP:OD1	2.00	0.79
1:L:40:SER:HA	3:L:697:HOH:O	1.82	0.79
1:L:137:ASN:ND2	3:L:706:HOH:O	2.13	0.78
2:H:4:LEU:HD11	3:H:637:HOH:O	1.82	0.77
1:L:205:ILE:N	1:L:205:ILE:HD12	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:CYS:O	2:H:97:THR:HG23	1.85	0.76
2:H:44:ARG:HG3	3:H:930:HOH:O	1.87	0.74
2:H:16:ARG:HG2	3:H:767:HOH:O	1.85	0.74
2:H:185:ASP:HA	3:H:858:HOH:O	1.86	0.74
2:H:143:GLN:HB2	3:H:689:HOH:O	1.89	0.72
2:H:199:PRO:HB3	2:H:203:GLU:N	2.05	0.71
1:L:12:SER:HA	1:L:105:GLU:O	1.91	0.71
2:H:199:PRO:HB3	2:H:203:GLU:H	1.56	0.71
2:H:98:ARG:NH2	2:H:113:ASP:OD2	2.23	0.71
2:H:203:GLU:O	2:H:223:VAL:HG13	1.90	0.70
1:L:50:TYR:HB2	3:L:840:HOH:O	1.93	0.69
2:H:51:ILE:HG13	2:H:58:ILE:HG12	1.76	0.68
1:L:77:SER:HB2	3:L:748:HOH:O	1.93	0.68
2:H:97:THR:HB	2:H:112:MET:HB3	1.76	0.67
1:L:125:LEU:O	1:L:128:GLY:N	2.27	0.67
1:L:90:GLN:HE21	1:L:92:ASN:N	1.92	0.66
2:H:225:ARG:HG2	2:H:226:ASP:HB3	1.77	0.66
1:L:113:PRO:HD2	3:L:901:HOH:O	1.95	0.66
2:H:139:GLY:O	2:H:142:ALA:N	2.29	0.65
2:H:225:ARG:HG3	3:H:908:HOH:O	1.96	0.65
2:H:32:TYR:CG	2:H:98:ARG:HD2	2.31	0.64
2:H:143:GLN:HG2	2:H:200:ARG:NH2	2.12	0.64
1:L:205:ILE:H	1:L:205:ILE:HD12	1.62	0.64
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.28	0.63
2:H:200:ARG:O	2:H:202:SER:N	2.32	0.62
2:H:97:THR:CB	2:H:112:MET:HB3	2.30	0.62
2:H:6:GLN:HE21	2:H:6:GLN:H	1.47	0.62
2:H:199:PRO:HG3	2:H:203:GLU:HB2	1.82	0.62
2:H:145:ASN:HD22	2:H:146:SER:H	1.48	0.62
1:L:205:ILE:HD11	3:L:773:HOH:O	2.00	0.61
1:L:205:ILE:HD11	3:L:901:HOH:O	1.99	0.61
2:H:139:GLY:O	2:H:141:ALA:N	2.28	0.61
2:H:97:THR:CB	2:H:112:MET:HG2	2.30	0.61
2:H:223:VAL:O	2:H:225:ARG:HD2	2.01	0.61
2:H:217:LYS:HB2	3:H:846:HOH:O	2.00	0.60
2:H:97:THR:HG21	2:H:112:MET:CB	2.31	0.60
2:H:135:PRO:HG2	2:H:225:ARG:NH2	2.17	0.60
2:H:199:PRO:CG	2:H:203:GLU:HB2	2.31	0.60
1:L:147:LYS:HB2	3:L:828:HOH:O	2.01	0.60
1:L:214:CYS:HA	2:H:227:CYS:HB2	1.83	0.60
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:SER:HB2	3:H:659:HOH:O	2.02	0.59
2:H:97:THR:CG2	2:H:112:MET:CB	2.78	0.59
1:L:211:ARG:HA	3:L:822:HOH:O	2.01	0.59
2:H:200:ARG:C	2:H:202:SER:H	2.05	0.59
2:H:223:VAL:O	2:H:225:ARG:N	2.34	0.59
2:H:196:PRO:C	2:H:198:SER:H	2.04	0.59
1:L:19:VAL:HG22	1:L:75:ILE:HD12	1.85	0.59
1:L:90:GLN:NE2	1:L:92:ASN:H	1.94	0.59
2:H:143:GLN:HG2	2:H:200:ARG:HH21	1.68	0.58
1:L:90:GLN:NE2	1:L:92:ASN:N	2.50	0.58
2:H:11:LEU:HD22	2:H:159:PRO:HG3	1.85	0.58
2:H:205:VAL:H	2:H:223:VAL:HG22	1.68	0.58
2:H:16:ARG:CG	2:H:17:SER:H	1.91	0.57
2:H:225:ARG:HG2	2:H:226:ASP:N	2.18	0.57
1:L:127:SER:HB3	3:L:864:HOH:O	2.04	0.57
2:H:128:THR:HA	2:H:158:PHE:O	2.05	0.57
2:H:200:ARG:C	2:H:202:SER:N	2.57	0.57
2:H:97:THR:HG21	2:H:112:MET:HG2	1.87	0.56
2:H:144:THR:HG23	3:H:920:HOH:O	2.05	0.56
2:H:52:SER:OG	2:H:56:THR:O	2.23	0.56
2:H:223:VAL:HG21	3:H:843:HOH:O	2.04	0.56
2:H:76:LYS:HD3	3:H:870:HOH:O	2.05	0.56
2:H:150:LEU:HG	2:H:222:ILE:HG21	1.87	0.56
2:H:96:CYS:O	2:H:97:THR:CG2	2.53	0.55
1:L:19:VAL:CG2	1:L:75:ILE:HD12	2.35	0.55
1:L:11:LEU:HG	1:L:104:LEU:HD12	1.88	0.55
3:L:707:HOH:O	2:H:43:LYS:HD2	2.05	0.55
1:L:29:ILE:CD1	1:L:33:LEU:HD23	2.37	0.55
2:H:12:VAL:HG23	2:H:16:ARG:HB3	1.88	0.55
1:L:108:ARG:NE	1:L:109:ALA:O	2.40	0.55
2:H:12:VAL:HG11	2:H:18:LEU:HG	1.89	0.55
2:H:201:PRO:HD3	2:H:224:PRO:O	2.07	0.54
2:H:87:ARG:HB3	2:H:89:GLU:HG3	1.90	0.54
2:H:145:ASN:ND2	3:H:680:HOH:O	2.40	0.54
2:H:200:ARG:HH11	2:H:224:PRO:CB	2.21	0.54
2:H:32:TYR:O	2:H:72:ARG:NH2	2.36	0.54
2:H:201:PRO:HA	2:H:223:VAL:HG12	1.90	0.54
2:H:96:CYS:O	2:H:97:THR:OG1	2.26	0.53
1:L:108:ARG:HG2	1:L:171:SER:HB3	1.91	0.53
2:H:167:ASN:HA	2:H:206:THR:HG23	1.89	0.53
2:H:207:CYS:N	2:H:220:LYS:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:SER:HA	2:H:200:ARG:NH2	2.24	0.53
2:H:38:ARG:HG2	2:H:48:VAL:HG21	1.91	0.53
2:H:47:TRP:CZ3	2:H:61:PRO:HD3	2.43	0.53
1:L:1:ASP:HB2	1:L:95:PRO:CD	2.34	0.53
1:L:195:GLU:HB2	1:L:206:VAL:CG2	2.40	0.52
1:L:1:ASP:CB	1:L:95:PRO:HD2	2.34	0.52
2:H:145:ASN:ND2	2:H:146:SER:H	2.08	0.52
2:H:196:PRO:O	2:H:198:SER:N	2.35	0.51
2:H:182:LEU:HD11	2:H:185:ASP:CA	2.35	0.51
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.93	0.50
2:H:167:ASN:OD1	2:H:206:THR:HG22	2.11	0.50
2:H:200:ARG:HB3	2:H:201:PRO:HD2	1.92	0.50
2:H:96:CYS:O	2:H:97:THR:CB	2.59	0.50
1:L:138:ASN:OD1	2:H:176:HIS:HE1	1.95	0.50
1:L:18:SER:HA	1:L:76:ASN:O	2.11	0.50
2:H:156:GLY:HA2	2:H:186:LEU:HB3	1.93	0.50
2:H:6:GLN:NE2	2:H:118:GLY:H	2.10	0.50
2:H:97:THR:HB	2:H:112:MET:CB	2.41	0.50
1:L:127:SER:OG	3:L:723:HOH:O	2.14	0.49
1:L:175:MET:HG2	1:L:176:SER:N	2.26	0.49
2:H:200:ARG:CA	2:H:224:PRO:HG2	2.42	0.49
2:H:97:THR:OG1	2:H:112:MET:HG2	2.12	0.49
2:H:200:ARG:NH1	2:H:224:PRO:HB3	2.27	0.49
2:H:145:ASN:O	2:H:197:SER:HB3	2.13	0.49
2:H:126:ALA:HB2	2:H:185:ASP:HB3	1.95	0.49
2:H:220:LYS:NZ	3:H:783:HOH:O	2.46	0.49
2:H:16:ARG:HB2	2:H:16:ARG:CZ	2.43	0.49
2:H:32:TYR:CD1	2:H:98:ARG:HD2	2.47	0.48
1:L:136:LEU:CD1	1:L:196:ALA:HB2	2.43	0.48
1:L:136:LEU:HD21	1:L:146:VAL:HG21	1.94	0.48
2:H:146:SER:HA	2:H:197:SER:OG	2.13	0.48
1:L:195:GLU:HG3	1:L:204:PRO:HB2	1.94	0.48
2:H:6:GLN:HE22	2:H:117:GLN:N	2.12	0.48
2:H:97:THR:HG21	2:H:112:MET:CG	2.43	0.48
2:H:4:LEU:HD13	2:H:96:CYS:HB3	1.93	0.48
2:H:97:THR:CB	2:H:112:MET:CG	2.91	0.48
1:L:142:LYS:HE3	3:L:814:HOH:O	2.14	0.48
1:L:210:ASN:HB2	1:L:212:ASN:HB2	1.96	0.48
1:L:55:ILE:O	1:L:58:ILE:HG12	2.13	0.48
1:L:33:LEU:HG	1:L:71:PHE:CG	2.49	0.47
1:L:30:SER:HB3	1:L:31:ASN:H	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:NH2	1:L:109:ALA:O	2.45	0.47
1:L:142:LYS:HG2	3:L:928:HOH:O	2.15	0.47
1:L:213:GLU:HG2	2:H:141:ALA:HB2	1.96	0.47
2:H:87:ARG:HG2	3:H:951:HOH:O	2.15	0.46
1:L:213:GLU:HG2	2:H:141:ALA:CB	2.46	0.46
2:H:97:THR:HG22	2:H:112:MET:HB3	1.95	0.46
2:H:200:ARG:HH11	2:H:224:PRO:HB3	1.78	0.46
2:H:138:PRO:HD3	2:H:150:LEU:HD12	1.97	0.46
1:L:90:GLN:HE22	1:L:93:SER:H	1.61	0.46
2:H:200:ARG:HA	2:H:224:PRO:HG2	1.98	0.46
2:H:6:GLN:NE2	2:H:6:GLN:H	2.13	0.46
2:H:147:MET:CE	2:H:194:THR:HG22	2.46	0.46
2:H:221:LYS:HD2	2:H:221:LYS:H	1.80	0.46
2:H:97:THR:CG2	2:H:112:MET:HG2	2.45	0.46
2:H:147:MET:CB	3:H:609:HOH:O	2.63	0.46
2:H:200:ARG:HD3	2:H:201:PRO:HD2	1.98	0.46
2:H:137:ALA:CB	2:H:225:ARG:HD3	2.35	0.45
2:H:199:PRO:O	2:H:224:PRO:HG2	2.17	0.45
2:H:98:ARG:HB2	3:H:637:HOH:O	2.16	0.45
2:H:204:THR:HA	2:H:223:VAL:HG22	1.99	0.45
2:H:217:LYS:HD2	2:H:218:VAL:N	2.32	0.45
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.98	0.45
2:H:199:PRO:HA	2:H:202:SER:HB2	1.99	0.45
1:L:163:TRP:N	1:L:163:TRP:CD1	2.84	0.45
1:L:167:ASP:OD1	1:L:169:LYS:N	2.47	0.45
1:L:205:ILE:CD1	3:L:901:HOH:O	2.59	0.45
1:L:85:MET:HG2	1:L:87:PHE:CZ	2.51	0.45
2:H:134:TYR:HA	2:H:135:PRO:HD3	1.80	0.45
2:H:208:ASN:HB3	2:H:219:ASP:OD1	2.17	0.44
2:H:221:LYS:HD3	2:H:221:LYS:O	2.17	0.44
2:H:97:THR:HB	2:H:112:MET:CG	2.47	0.44
2:H:200:ARG:O	2:H:201:PRO:C	2.56	0.44
1:L:116:SER:O	1:L:134:CYS:HA	2.18	0.44
1:L:55:ILE:HD11	1:L:58:ILE:HD11	1.99	0.43
1:L:113:PRO:HG3	1:L:144:ILE:CD1	2.48	0.43
1:L:183:LYS:O	1:L:187:GLU:HG2	2.19	0.43
2:H:13:ASN:HA	2:H:14:PRO:HD3	1.87	0.43
1:L:29:ILE:HG22	1:L:92:ASN:HB3	2.01	0.43
1:L:8:PRO:CG	1:L:11:LEU:HD22	2.36	0.43
2:H:147:MET:HB3	3:H:609:HOH:O	2.19	0.43
2:H:117:GLN:HG3	3:H:635:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASP:OD1	2:H:65:LYS:HE3	2.19	0.43
1:L:112:ALA:HB2	1:L:200:THR:OG1	2.18	0.43
1:L:80:THR:HA	1:L:83:PHE:CE2	2.54	0.42
2:H:11:LEU:HA	2:H:122:THR:O	2.19	0.42
1:L:13:VAL:HG11	1:L:19:VAL:HG11	2.02	0.42
1:L:49:LYS:HG3	1:L:53:GLN:HB2	2.01	0.42
1:L:24:ARG:HG3	1:L:70:ASP:OD1	2.19	0.42
1:L:204:PRO:O	3:L:733:HOH:O	2.21	0.42
2:H:222:ILE:O	2:H:225:ARG:HD2	2.19	0.42
1:L:34:HIS:CG	2:H:111:ALA:HB2	2.54	0.42
1:L:113:PRO:HG3	1:L:144:ILE:HD11	2.01	0.42
2:H:152:CYS:HB2	2:H:166:TRP:CZ2	2.55	0.42
1:L:106:ILE:HG21	1:L:106:ILE:HD13	1.93	0.42
2:H:147:MET:HG2	3:H:625:HOH:O	2.19	0.42
1:L:191:SER:HB3	1:L:210:ASN:OD1	2.19	0.42
2:H:94:TYR:O	2:H:118:GLY:HA2	2.20	0.41
1:L:170:ASP:O	1:L:171:SER:HB2	2.20	0.41
2:H:200:ARG:HD3	2:H:201:PRO:CD	2.51	0.41
2:H:200:ARG:HH11	2:H:224:PRO:HB2	1.83	0.41
1:L:14:THR:O	1:L:17:ASP:HB2	2.21	0.41
1:L:90:GLN:NE2	1:L:93:SER:H	2.19	0.41
2:H:3:GLN:HB2	2:H:25:SER:HB3	2.02	0.41
2:H:220:LYS:HD2	2:H:220:LYS:HA	1.77	0.41
2:H:150:LEU:HD11	2:H:224:PRO:HG3	2.02	0.41
1:L:19:VAL:O	1:L:74:SER:HA	2.20	0.41
2:H:149:THR:HA	2:H:193:VAL:O	2.21	0.41
2:H:196:PRO:C	2:H:198:SER:N	2.69	0.41
2:H:221:LYS:CD	2:H:221:LYS:H	2.32	0.41
1:L:12:SER:O	1:L:13:VAL:HG23	2.20	0.41
2:H:135:PRO:HG2	2:H:225:ARG:HH22	1.86	0.41
1:L:142:LYS:HB2	1:L:173:TYR:CE2	2.55	0.41
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.69	0.40
1:L:205:ILE:N	1:L:205:ILE:CD1	2.79	0.40

All (9) 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)
3:L:834:HOH:O	3:H:829:HOH:O[2_657]	1.26	0.94
3:L:763:HOH:O	3:L:763:HOH:O[2_556]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:LEU:CA	3:H:952:HOH:O[2_657]	1.53	0.67
1:L:181:LEU:CB	3:H:952:HOH:O[2_657]	1.69	0.51
2:H:57:TYR:OH	2:H:140:SER:CB[1_455]	1.84	0.36
1:L:156:GLN:OE1	3:L:712:HOH:O[2_657]	1.84	0.36
1:L:181:LEU:C	3:H:952:HOH:O[2_657]	1.93	0.27
1:L:182:THR:N	3:H:952:HOH:O[2_657]	2.06	0.14
1:L:181:LEU:CG	3:H:952:HOH:O[2_657]	2.18	0.02

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	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	23
2	H	212/227 (93%)	180 (85%)	19 (9%)	13 (6%)	1	0
All	All	424/441 (96%)	383 (90%)	27 (6%)	14 (3%)	4	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	THR
2	H	140	SER
2	H	147	MET
2	H	226	ASP
1	L	76	ASN
2	H	144	THR
2	H	184	SER
2	H	197	SER
2	H	202	SER
2	H	200	ARG
2	H	222	ILE
2	H	223	VAL
2	H	201	PRO

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Mol	Chain	Res	Type
2	H	159	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	193/193 (100%)	153 (79%)	40 (21%)	1	0
2	H	184/193 (95%)	140 (76%)	44 (24%)	0	0
All	All	377/386 (98%)	293 (78%)	84 (22%)	1	0

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	13	VAL
1	L	21	LEU
1	L	24	ARG
1	L	29	ILE
1	L	30	SER
1	L	41	HIS
1	L	45	ARG
1	L	46	LEU
1	L	67	SER
1	L	69	THR
1	L	70	ASP
1	L	72	THR
1	L	73	LEU
1	L	90	GLN
1	L	93	SER
1	L	94	TRP
1	L	105	GLU
1	L	116	SER
1	L	121	SER
1	L	122	SER
1	L	123	GLU

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Mol	Chain	Res	Type
1	L	136	LEU
1	L	138	ASN
1	L	142	LYS
1	L	160	LEU
1	L	163	TRP
1	L	168	SER
1	L	175	MET
1	L	180	THR
1	L	187	GLU
1	L	188	ARG
1	L	191	SER
1	L	197	THR
1	L	199	LYS
1	L	201	SER
1	L	202	THR
1	L	205	ILE
1	L	207	LYS
1	L	214	CYS
2	H	1	GLU
2	H	3	GLN
2	H	6	GLN
2	H	14	PRO
2	H	16	ARG
2	H	19	LYS
2	H	25	SER
2	H	30	SER
2	H	35	SER
2	H	44	ARG
2	H	51	ILE
2	H	56	THR
2	H	88	SER
2	H	89	GLU
2	H	96	CYS
2	H	119	THR
2	H	120	SER
2	H	127	LYS
2	H	144	THR
2	H	145	ASN
2	H	147	MET
2	H	148	VAL
2	H	150	LEU
2	H	152	CYS

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Mol	Chain	Res	Type
2	H	153	LEU
2	H	165	THR
2	H	170	SER
2	H	172	SER
2	H	175	VAL
2	H	184	SER
2	H	198	SER
2	H	200	ARG
2	H	202	SER
2	H	203	GLU
2	H	207	CYS
2	H	208	ASN
2	H	209	VAL
2	H	212	PRO
2	H	215	SER
2	H	217	LYS
2	H	221	LYS
2	H	225	ARG
2	H	226	ASP
2	H	227	CYS

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

Mol	Chain	Res	Type
1	L	6	GLN
1	L	90	GLN
1	L	157	ASN
1	L	161	ASN
2	H	6	GLN
2	H	74	ASN
2	H	145	ASN
2	H	176	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	214/214 (100%)	-0.42	2 (0%) 84 83	4, 17, 36, 126	0
2	H	216/227 (95%)	-0.25	4 (1%) 66 65	4, 21, 56, 112	0
All	All	430/441 (97%)	-0.33	6 (1%) 75 74	4, 18, 46, 126	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	223	VAL	4.7
2	H	142	ALA	3.9
2	H	96	CYS	3.6
2	H	111	ALA	3.6
1	L	212	ASN	2.7
1	L	214	CYS	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.