Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:32 pm BST

PDB ID	:	1FVD
Title	:	X-RAY STRUCTURES OF THE ANTIGEN-BINDING DOMAINS FROM THREE VARIANTS OF HUMANIZED ANTI-P185-HER2 ANTIBODY 4D5 AND COMPARISON WITH MOLECULAR MODELING
Authors	:	Eigenbrot, C.; Presta, L.; Randal, M.; Kossiakoff, A.A.
Deposited on	:	1992-10-20
Resolution	:	2.50 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 ①) were used in the production of this report:

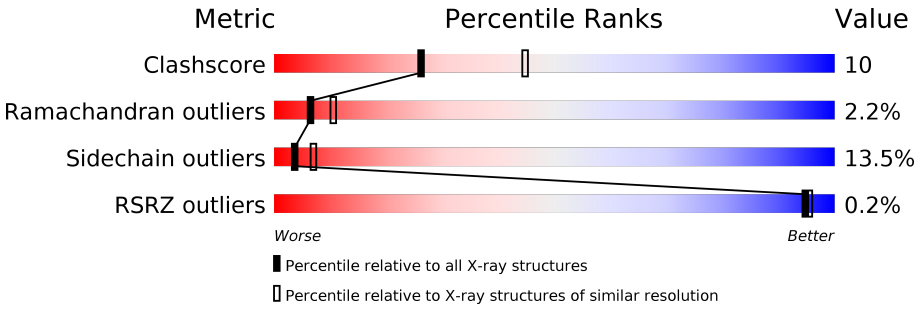
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	A	214	63% 28% 8%
1	C	214	60% 30% 10%
2	B	223	60% 29% 11%
2	D	223	% 69% 24% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGG1-KAPPA 4D5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	19	0	0
			1647	1028	277	336	6			
1	C	214	Total	C	N	O	S	20	0	0
			1647	1028	277	336	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	PHE	CONFLICT	EMBL X95750
A	28	ASP	SER	CONFLICT	EMBL X95750
A	29	VAL	ILE	CONFLICT	EMBL X95750
A	30	ASN	SER	CONFLICT	EMBL X95750
A	31	THR	SER	CONFLICT	EMBL X95750
A	32	ALA	TYR	CONFLICT	EMBL X95750
A	33	VAL	LEU	CONFLICT	EMBL X95750
A	34	ALA	ASN	CONFLICT	EMBL X95750
A	50	SER	ALA	CONFLICT	EMBL X95750
A	53	PHE	SER	CONFLICT	EMBL X95750
A	55	GLU	GLN	CONFLICT	EMBL X95750
A	66	ARG	GLY	CONFLICT	EMBL X95750
A	91	HIS	SER	CONFLICT	EMBL X95750
A	92	TYR	HIS	CONFLICT	EMBL X95750
A	93	THR	SER	CONFLICT	EMBL X95750
A	96	PRO	TYR	CONFLICT	EMBL X95750
A	103	LYS	ASN	CONFLICT	EMBL X95750
A	104	VAL	LEU	CONFLICT	EMBL X95750
C	14	SER	PHE	CONFLICT	EMBL X95750
C	28	ASP	SER	CONFLICT	EMBL X95750
C	29	VAL	ILE	CONFLICT	EMBL X95750
C	30	ASN	SER	CONFLICT	EMBL X95750
C	31	THR	SER	CONFLICT	EMBL X95750
C	32	ALA	TYR	CONFLICT	EMBL X95750
C	33	VAL	LEU	CONFLICT	EMBL X95750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	ALA	ASN	CONFLICT	EMBL X95750
C	50	SER	ALA	CONFLICT	EMBL X95750
C	53	PHE	SER	CONFLICT	EMBL X95750
C	55	GLU	GLN	CONFLICT	EMBL X95750
C	66	ARG	GLY	CONFLICT	EMBL X95750
C	91	HIS	SER	CONFLICT	EMBL X95750
C	92	TYR	HIS	CONFLICT	EMBL X95750
C	93	THR	SER	CONFLICT	EMBL X95750
C	96	PRO	TYR	CONFLICT	EMBL X95750
C	103	LYS	ASN	CONFLICT	EMBL X95750
C	104	VAL	LEU	CONFLICT	EMBL X95750

- Molecule 2 is a protein called IGG1-KAPPA 4D5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	44	0	0
			1669	1053	282	327	7			
2	D	223	Total	C	N	O	S	44	0	0
			1669	1053	282	327	7			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASN	ALA	CONFLICT	EMBL Y14735
B	29	ILE	TYR	CONFLICT	EMBL Y14735
B	30	LYS	SER	CONFLICT	EMBL Y14735
B	31	ASP	SER	CONFLICT	EMBL Y14735
B	32	THR	PHE	CONFLICT	EMBL Y14735
B	33	TYR	TRP	CONFLICT	EMBL Y14735
B	34	ILE	MET	CONFLICT	EMBL Y14735
B	43	LYS	ARG	CONFLICT	EMBL Y14735
B	46	GLU	VAL	CONFLICT	EMBL Y14735
B	49	ALA	SER	CONFLICT	EMBL Y14735
B	52	TYR	ASN	CONFLICT	EMBL Y14735
B	54	THR	ASP	CONFLICT	EMBL Y14735
B	55	ASN	GLY	CONFLICT	EMBL Y14735
B	56	GLY	ARG	CONFLICT	EMBL Y14735
B	57	TYR	ILE	CONFLICT	EMBL Y14735
B	59	ARG	VAL	CONFLICT	EMBL Y14735
B	63	SER	ALA	CONFLICT	EMBL Y14735
B	72	ALA	ARG	CONFLICT	EMBL Y14735
B	74	THR	ASN	CONFLICT	EMBL Y14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	SER	ALA	CONFLICT	EMBL Y14735
B	85	SER	ASN	CONFLICT	EMBL Y14735
B	97	SER	ALA	CONFLICT	EMBL Y14735
B	99	TRP	-	INSERTION	EMBL Y14735
B	100	GLY	-	INSERTION	EMBL Y14735
B	102	ASP	THR	CONFLICT	EMBL Y14735
B	103	GLY	ARG	CONFLICT	EMBL Y14735
B	?	-	LEU	DELETION	EMBL Y14735
B	?	-	GLU	DELETION	EMBL Y14735
B	?	-	LEU	DELETION	EMBL Y14735
B	?	-	THR	DELETION	EMBL Y14735
B	?	-	SER	DELETION	EMBL Y14735
B	?	-	ARG	DELETION	EMBL Y14735
B	105	TYR	GLY	CONFLICT	EMBL Y14735
B	106	ALA	GLN	CONFLICT	EMBL Y14735
B	109	VAL	GLN	CONFLICT	EMBL Y14735
D	28	ASN	ALA	CONFLICT	EMBL Y14735
D	29	ILE	TYR	CONFLICT	EMBL Y14735
D	30	LYS	SER	CONFLICT	EMBL Y14735
D	31	ASP	SER	CONFLICT	EMBL Y14735
D	32	THR	PHE	CONFLICT	EMBL Y14735
D	33	TYR	TRP	CONFLICT	EMBL Y14735
D	34	ILE	MET	CONFLICT	EMBL Y14735
D	43	LYS	ARG	CONFLICT	EMBL Y14735
D	46	GLU	VAL	CONFLICT	EMBL Y14735
D	49	ALA	SER	CONFLICT	EMBL Y14735
D	52	TYR	ASN	CONFLICT	EMBL Y14735
D	54	THR	ASP	CONFLICT	EMBL Y14735
D	55	ASN	GLY	CONFLICT	EMBL Y14735
D	56	GLY	ARG	CONFLICT	EMBL Y14735
D	57	TYR	ILE	CONFLICT	EMBL Y14735
D	59	ARG	VAL	CONFLICT	EMBL Y14735
D	63	SER	ALA	CONFLICT	EMBL Y14735
D	72	ALA	ARG	CONFLICT	EMBL Y14735
D	74	THR	ASN	CONFLICT	EMBL Y14735
D	75	SER	ALA	CONFLICT	EMBL Y14735
D	85	SER	ASN	CONFLICT	EMBL Y14735
D	97	SER	ALA	CONFLICT	EMBL Y14735
D	99	TRP	-	INSERTION	EMBL Y14735
D	100	GLY	-	INSERTION	EMBL Y14735
D	102	ASP	THR	CONFLICT	EMBL Y14735
D	103	GLY	ARG	CONFLICT	EMBL Y14735

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	EMBL Y14735
D	?	-	GLU	DELETION	EMBL Y14735
D	?	-	LEU	DELETION	EMBL Y14735
D	?	-	THR	DELETION	EMBL Y14735
D	?	-	SER	DELETION	EMBL Y14735
D	?	-	ARG	DELETION	EMBL Y14735
D	105	TYR	GLY	CONFLICT	EMBL Y14735
D	106	ALA	GLN	CONFLICT	EMBL Y14735
D	109	VAL	GLN	CONFLICT	EMBL Y14735

- Molecule 3 is water.

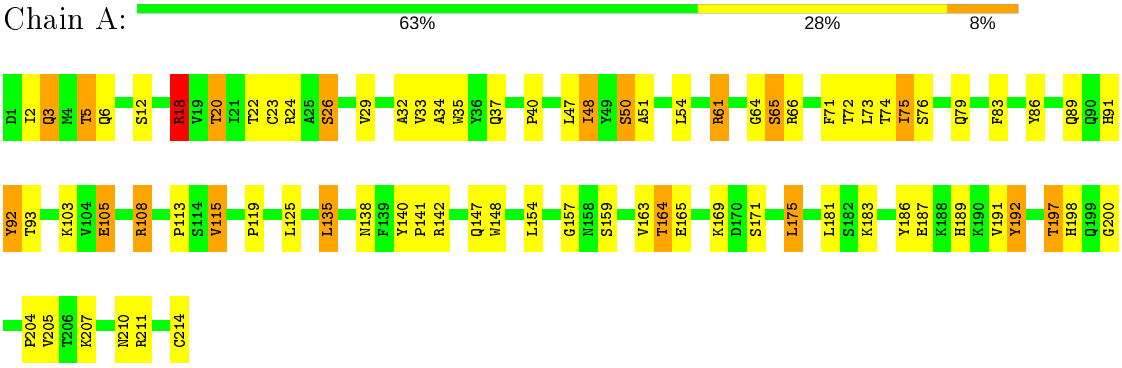
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	50	Total O 50 50	0	0
3	C	39	Total O 39 39	0	0
3	D	64	Total O 64 64	0	0

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 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.

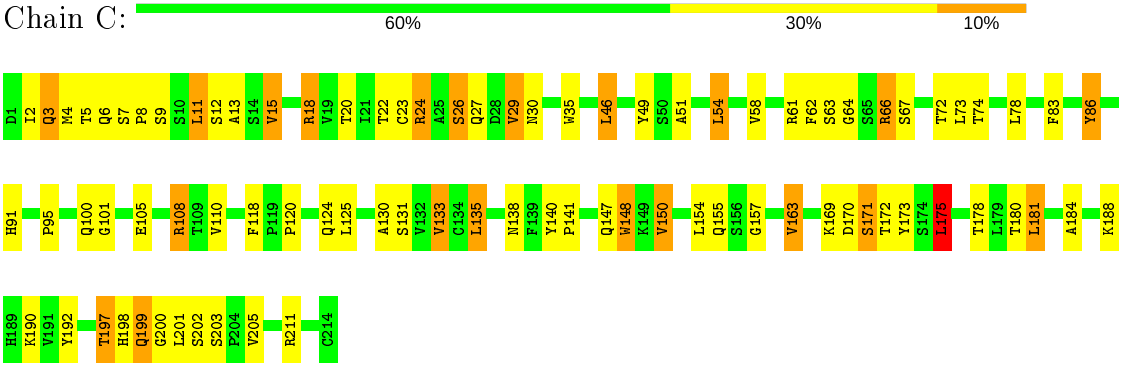
- Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)

Chain A:



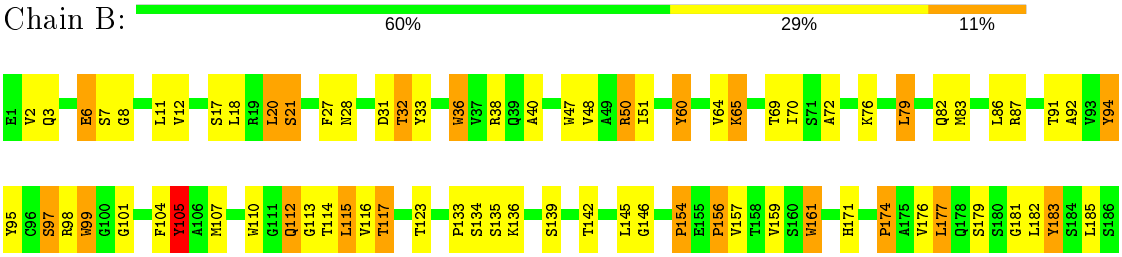
- Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)

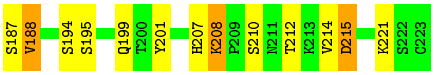
Chain C:



- Molecule 2: IGG1-KAPPA 4D5 FAB (HEAVY CHAIN)

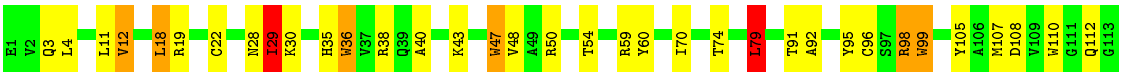
Chain B:





- Molecule 2: IGG1-KAPPA 4D5 FAB (HEAVY CHAIN)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.20Å 80.20Å 86.10Å 113.10° 92.70° 102.60°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 82.6 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 72.2	EDS
L-test for twinning[1]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6831	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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	A	0.94	0/1683	1.80	32/2286 (1.4%)
1	C	0.95	2/1683 (0.1%)	1.78	33/2286 (1.4%)
2	B	1.06	0/1710	1.88	38/2329 (1.6%)
2	D	1.05	2/1710 (0.1%)	1.89	49/2329 (2.1%)
All	All	1.00	4/6786 (0.1%)	1.84	152/9230 (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	2
2	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	VAL	CA-CB	5.79	1.67	1.54
2	D	183	TYR	CA-CB	-5.32	1.42	1.53
1	C	26	SER	CA-CB	-5.29	1.45	1.52
2	D	187	SER	CA-CB	-5.00	1.45	1.52

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	A	61	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	C	18	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	C	163	VAL	CG1-CB-CG2	-10.88	93.49	110.90
2	B	95	TYR	CB-CG-CD2	-10.51	114.69	121.00
1	C	86	TYR	CB-CG-CD2	-10.41	114.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	18	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	D	183	TYR	CB-CG-CD1	-10.27	114.84	121.00
1	A	192	TYR	CB-CG-CD2	-9.86	115.09	121.00
1	C	108	ARG	NE-CZ-NH1	9.85	125.22	120.30
2	D	110	TRP	CD1-CG-CD2	9.62	114.00	106.30
1	A	175	LEU	CA-CB-CG	9.40	136.92	115.30
1	C	175	LEU	CA-CB-CG	9.28	136.65	115.30
1	C	66	ARG	NE-CZ-NH2	-9.26	115.67	120.30
2	B	185	LEU	CA-CB-CG	9.15	136.35	115.30
2	B	50	ARG	NE-CZ-NH1	9.14	124.87	120.30
2	B	161	TRP	CD1-CG-CD2	8.94	113.45	106.30
2	D	47	TRP	CD1-CG-CD2	8.89	113.42	106.30
1	C	108	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	D	19	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	D	98	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	86	TYR	CB-CG-CD2	-8.61	115.84	121.00
2	B	183	TYR	CB-CG-CD2	-8.60	115.84	121.00
2	D	99	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	A	148	TRP	CD1-CG-CD2	8.53	113.13	106.30
2	B	99	TRP	CD1-CG-CD2	8.49	113.09	106.30
2	D	161	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	61	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	B	50	ARG	NE-CZ-NH2	-8.26	116.17	120.30
2	D	47	TRP	CE2-CD2-CG	-8.17	100.77	107.30
2	B	110	TRP	CD1-CG-CD2	8.10	112.78	106.30
2	D	185	LEU	CA-CB-CG	8.04	133.79	115.30
2	D	59	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	61	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	B	47	TRP	CD1-CG-CD2	7.82	112.56	106.30
2	D	4	LEU	CB-CG-CD2	-7.58	98.11	111.00
1	A	35	TRP	CD1-CG-CD2	7.54	112.33	106.30
2	D	98	ARG	CB-CG-CD	-7.25	92.74	111.60
2	D	110	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	C	173	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	A	148	TRP	CE2-CD2-CG	-7.21	101.53	107.30
2	B	161	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	C	11	LEU	CA-CB-CG	7.08	131.59	115.30
2	D	48	VAL	CG1-CB-CG2	-7.06	99.61	110.90
2	B	115	LEU	CA-CB-CG	7.05	131.52	115.30
2	D	47	TRP	CG-CD2-CE3	7.01	140.21	133.90
1	A	91	HIS	CA-CB-CG	6.89	125.31	113.60
2	D	183	TYR	CG-CD2-CE2	-6.87	115.80	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	TRP	CE2-CD2-CG	-6.87	101.80	107.30
2	B	47	TRP	CE2-CD2-CG	-6.86	101.81	107.30
2	D	50	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	B	33	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	B	60	TYR	CB-CG-CD2	-6.72	116.97	121.00
2	D	47	TRP	NE1-CE2-CZ2	-6.71	123.02	130.40
1	A	33	VAL	CG1-CB-CG2	-6.70	100.18	110.90
1	C	24	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	135	LEU	CA-CB-CG	6.68	130.67	115.30
2	D	47	TRP	CG-CD1-NE1	-6.63	103.47	110.10
1	A	18	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	35	TRP	CE2-CD2-CG	-6.56	102.05	107.30
2	B	145	LEU	CA-CB-CG	6.53	130.31	115.30
2	B	99	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	C	46	LEU	CA-CB-CG	6.48	130.21	115.30
1	C	148	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	A	135	LEU	CA-CB-CG	6.45	130.14	115.30
1	C	30	ASN	N-CA-CB	-6.44	99.00	110.60
1	C	35	TRP	CD1-CG-CD2	6.43	111.45	106.30
2	D	176	VAL	CA-CB-CG2	-6.42	101.28	110.90
2	D	99	TRP	CE2-CD2-CG	-6.36	102.22	107.30
1	A	163	VAL	CG1-CB-CG2	-6.33	100.77	110.90
2	D	110	TRP	CG-CD1-NE1	-6.32	103.78	110.10
2	D	161	TRP	CE2-CD2-CG	-6.32	102.24	107.30
1	C	197	THR	CA-CB-CG2	6.28	121.20	112.40
1	A	148	TRP	CG-CD1-NE1	-6.27	103.83	110.10
1	C	192	TYR	CB-CG-CD2	-6.24	117.25	121.00
2	D	59	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	192	TYR	CB-CG-CD1	6.18	124.71	121.00
2	D	95	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	A	24	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	B	36	TRP	CE2-CD2-CG	-6.03	102.48	107.30
1	C	35	TRP	CE2-CD2-CG	-6.02	102.48	107.30
1	C	91	HIS	CA-CB-CG	6.02	123.83	113.60
2	B	50	ARG	CB-CG-CD	-6.00	95.99	111.60
1	C	197	THR	CA-CB-OG1	-5.98	96.45	109.00
1	C	148	TRP	CE2-CD2-CG	-5.97	102.52	107.30
2	D	4	LEU	CA-CB-CG	5.97	129.03	115.30
2	B	87	ARG	CB-CG-CD	-5.97	96.09	111.60
2	D	47	TRP	CB-CG-CD1	-5.95	119.26	127.00
2	B	201	TYR	CB-CG-CD1	-5.94	117.44	121.00
2	D	36	TRP	CD1-CG-CD2	5.90	111.02	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	VAL	CG1-CB-CG2	-5.88	101.49	110.90
2	D	60	TYR	CG-CD2-CE2	-5.86	116.62	121.30
1	C	49	TYR	CB-CG-CD1	-5.85	117.49	121.00
2	B	215	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	142	ARG	CB-CG-CD	-5.79	96.53	111.60
2	D	12	VAL	CA-CB-CG1	-5.79	102.21	110.90
1	A	113	PRO	CA-C-N	5.79	129.93	117.20
2	D	38	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	D	176	VAL	CA-CB-CG1	5.78	119.56	110.90
2	D	95	TYR	CB-CG-CD2	5.77	124.46	121.00
2	D	220	PRO	N-CA-C	5.77	127.10	112.10
2	B	112	GLN	CA-CB-CG	5.75	126.04	113.40
2	D	161	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	A	175	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	A	197	THR	CA-CB-CG2	5.69	120.36	112.40
1	A	18	ARG	CB-CG-CD	-5.68	96.83	111.60
1	A	50	SER	CA-C-N	-5.68	104.70	117.20
2	D	183	TYR	CD1-CG-CD2	5.66	124.12	117.90
2	B	99	TRP	CA-C-N	5.65	127.49	116.20
1	C	124	GLN	CA-CB-CG	-5.64	100.99	113.40
2	B	36	TRP	CD1-CG-CD2	5.63	110.81	106.30
2	D	99	TRP	CB-CG-CD2	-5.63	119.28	126.60
2	D	201	TYR	CB-CG-CD1	-5.62	117.63	121.00
2	B	21	SER	N-CA-CB	-5.61	102.08	110.50
1	A	115	VAL	CA-CB-CG2	-5.61	102.49	110.90
2	B	47	TRP	CG-CD1-NE1	-5.56	104.54	110.10
2	D	148	LEU	CA-CB-CG	5.55	128.06	115.30
2	D	36	TRP	CE2-CD2-CG	-5.53	102.87	107.30
2	D	213	LYS	N-CA-C	-5.51	96.11	111.00
2	B	176	VAL	CG1-CB-CG2	-5.50	102.11	110.90
1	A	35	TRP	CG-CD1-NE1	-5.49	104.61	110.10
2	B	50	ARG	CA-CB-CG	5.46	125.42	113.40
1	A	164	THR	CA-CB-CG2	5.44	120.01	112.40
1	A	92	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	D	29	ILE	N-CA-CB	-5.39	98.39	110.80
1	A	75	ILE	N-CA-C	-5.38	96.47	111.00
2	D	158	THR	CA-CB-OG1	-5.38	97.71	109.00
2	B	94	TYR	CB-CG-CD1	-5.38	117.77	121.00
2	D	29	ILE	CA-CB-CG1	-5.35	100.84	111.00
1	C	24	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	99	TRP	CG-CD1-NE1	-5.32	104.78	110.10
2	B	60	TYR	CG-CD2-CE2	-5.32	117.05	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	161	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	197	THR	CA-CB-OG1	-5.25	97.97	109.00
1	C	140	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	C	54	LEU	CA-CB-CG	5.22	127.31	115.30
2	D	112	GLN	CB-CG-CD	5.21	125.16	111.60
2	B	97	SER	CB-CA-C	-5.21	100.20	110.10
2	D	4	LEU	CB-CG-CD1	5.17	119.78	111.00
2	B	110	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	C	66	ARG	CG-CD-NE	-5.15	100.98	111.80
1	C	181	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	86	TYR	O-C-N	5.13	130.91	122.70
2	D	18	LEU	CA-CB-CG	5.09	127.00	115.30
2	B	99	TRP	CB-CG-CD2	-5.08	120.00	126.60
2	B	95	TYR	CB-CG-CD1	5.05	124.03	121.00
1	C	29	VAL	N-CA-CB	-5.05	100.39	111.50
1	C	171	SER	N-CA-C	5.03	124.59	111.00
1	A	175	LEU	CB-CG-CD1	5.02	119.54	111.00
2	D	99	TRP	CG-CD1-NE1	-5.02	105.08	110.10
2	D	79	LEU	CA-CB-CG	5.01	126.83	115.30
2	B	8	GLY	CA-C-N	5.01	126.21	116.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	A	192	TYR	Sidechain
2	D	105	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	A	1647	0	1596	34	0
1	C	1647	0	1596	36	0
2	B	1669	0	1634	38	0
2	D	1669	0	1634	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	46	0	0	0	0
3	B	50	0	0	0	0
3	C	39	0	0	0	0
3	D	64	0	0	0	0
All	All	6831	0	6460	133	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 10.

All (133) 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:D:35:HIS:HD2	2:D:47:TRP:HE1	1.25	0.84
2:B:91:THR:HG23	2:B:117:THR:HA	1.62	0.81
1:A:187:GLU:HA	1:A:211:ARG:HD2	1.69	0.75
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.72	0.71
1:A:83:PHE:HZ	1:A:165:GLU:HG3	1.57	0.68
1:A:20:THR:HG22	1:A:74:THR:HG22	1.78	0.65
1:C:170:ASP:O	1:C:172:THR:HG23	1.98	0.64
1:C:110:VAL:HG21	1:C:199:GLN:HE22	1.64	0.62
2:D:35:HIS:CD2	2:D:47:TRP:HE1	2.14	0.61
2:B:177:LEU:HD11	2:B:181:GLY:HA2	1.83	0.61
2:D:91:THR:HG23	2:D:117:THR:HA	1.81	0.60
2:D:35:HIS:HD2	2:D:47:TRP:NE1	2.00	0.59
1:A:189:HIS:O	1:A:211:ARG:HD3	2.03	0.59
1:A:48:ILE:HG13	1:A:54:LEU:HD23	1.83	0.59
1:A:64:GLY:HA2	1:A:72:THR:O	2.03	0.58
2:B:20:LEU:CD1	2:B:83:MET:SD	2.92	0.58
2:B:20:LEU:HD12	2:B:83:MET:SD	2.44	0.58
1:C:54:LEU:HD21	1:C:62:PHE:O	2.04	0.57
2:D:28:ASN:HD22	2:D:30:LYS:HG2	1.69	0.57
1:A:191:VAL:HG22	1:A:210:ASN:HD22	1.70	0.57
1:A:66:ARG:HG3	1:A:71:PHE:CE2	2.41	0.55
1:C:184:ALA:O	1:C:188:LYS:HG3	2.06	0.55
2:B:208:LYS:HZ2	2:B:208:LYS:H	1.55	0.55
1:A:2:ILE:HG21	1:A:29:VAL:HG21	1.89	0.55
2:D:169:GLY:O	2:D:189:VAL:HA	2.07	0.55
1:A:191:VAL:HG22	1:A:210:ASN:ND2	2.22	0.54
1:C:3:GLN:HB2	1:C:26:SER:OG	2.07	0.54
2:D:204:ASN:HB3	2:D:213:LYS:NZ	2.22	0.54
1:C:13:ALA:HB3	1:C:78:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLY:HA2	2:B:161:TRP:CH2	2.43	0.54
1:C:110:VAL:HG21	1:C:199:GLN:NE2	2.23	0.54
1:A:12:SER:HA	1:A:105:GLU:O	2.07	0.53
1:C:15:VAL:HA	1:C:78:LEU:O	2.08	0.53
2:B:171:HIS:HB2	2:B:188:VAL:HG12	1.90	0.53
2:D:203:CYS:SG	2:D:203:CYS:O	2.66	0.52
1:A:2:ILE:HD12	1:A:93:THR:OG1	2.08	0.52
2:B:156:PRO:HG2	2:B:208:LYS:NZ	2.25	0.52
1:A:2:ILE:HG21	1:A:29:VAL:CG2	2.41	0.51
2:D:154:PRO:O	2:D:207:HIS:HE1	1.94	0.51
1:A:198:HIS:CD2	1:A:200:GLY:H	2.29	0.51
2:D:202:ILE:HD13	2:D:217:LYS:HA	1.93	0.51
2:B:156:PRO:HG2	2:B:208:LYS:HZ3	1.76	0.51
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.41	0.51
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.75	0.51
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.92	0.50
1:C:163:VAL:HG23	1:C:175:LEU:HD23	1.93	0.50
1:C:150:VAL:HG13	1:C:155:GLN:NE2	2.26	0.50
1:C:198:HIS:CD2	1:C:200:GLY:H	2.29	0.50
1:C:148:TRP:O	1:C:154:LEU:HD22	2.12	0.49
1:A:32:ALA:HB3	1:A:92:TYR:HB2	1.95	0.49
2:B:60:TYR:HB2	2:B:65:LYS:HB3	1.93	0.49
2:B:159:VAL:HG11	2:B:187:SER:HB2	1.95	0.49
1:A:3:GLN:H	1:A:26:SER:HB3	1.78	0.49
2:B:159:VAL:HG11	2:B:187:SER:CB	2.43	0.49
1:C:5:THR:O	1:C:23:CYS:HA	2.13	0.48
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.49	0.48
2:B:27:PHE:CE2	2:B:98:ARG:HD3	2.48	0.48
2:B:32:THR:HG21	2:B:98:ARG:HG3	1.94	0.48
1:C:63:SER:O	1:C:73:LEU:HD12	2.13	0.48
2:B:212:THR:HG22	2:B:214:VAL:HG23	1.96	0.48
1:C:169:LYS:HD2	1:C:169:LYS:HA	1.58	0.48
1:C:13:ALA:HB3	1:C:78:LEU:CD2	2.44	0.48
1:C:170:ASP:O	1:C:172:THR:N	2.47	0.47
1:A:34:ALA:HA	1:A:48:ILE:O	2.14	0.47
2:B:154:PRO:O	2:B:207:HIS:HE1	1.97	0.47
2:B:146:GLY:HA2	2:B:161:TRP:HH2	1.79	0.47
1:C:5:THR:HA	1:C:100:GLN:HE22	1.79	0.47
2:B:72:ALA:HB2	2:B:79:LEU:HD12	1.96	0.47
2:B:51:ILE:HG21	2:B:79:LEU:HD11	1.96	0.47
1:C:64:GLY:HA2	1:C:72:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLN:HA	1:C:22:THR:O	2.15	0.47
1:A:83:PHE:CZ	1:A:165:GLU:HG3	2.44	0.46
2:B:83:MET:HE1	2:B:86:LEU:HD21	1.96	0.46
2:B:195:SER:HB2	2:B:199:GLN:HG3	1.96	0.46
1:A:79:GLN:OE1	1:A:79:GLN:HA	2.14	0.46
2:D:35:HIS:O	2:D:96:CYS:HA	2.14	0.46
2:B:98:ARG:O	2:B:107:MET:HA	2.15	0.46
2:D:133:PRO:HB3	2:D:144:ALA:O	2.16	0.46
2:D:30:LYS:HE3	2:D:74:THR:HB	1.98	0.46
1:C:201:LEU:HB3	1:C:203:SER:O	2.16	0.46
1:C:95:PRO:HB3	2:D:47:TRP:CE3	2.51	0.46
1:C:147:GLN:HB3	1:C:154:LEU:HD21	1.97	0.45
2:B:177:LEU:HD23	2:B:183:TYR:CE1	2.51	0.45
1:A:141:PRO:O	1:A:198:HIS:HE1	2.00	0.45
2:B:40:ALA:HA	2:B:92:ALA:HA	1.99	0.45
2:D:28:ASN:HB2	2:D:30:LYS:NZ	2.31	0.45
2:D:204:ASN:HB3	2:D:213:LYS:HZ1	1.81	0.45
2:B:36:TRP:HD1	2:B:70:ILE:HD12	1.82	0.45
1:A:119:PRO:HG2	2:B:221:LYS:NZ	2.32	0.44
1:A:125:LEU:O	1:A:183:LYS:HD3	2.17	0.44
1:A:119:PRO:HD3	2:B:135:SER:HB2	1.98	0.44
1:C:2:ILE:HG12	1:C:27:GLN:OE1	2.17	0.44
2:D:36:TRP:HE1	2:D:79:LEU:HD12	1.81	0.44
1:A:147:GLN:HB3	1:A:154:LEU:HD21	2.00	0.44
1:A:61:ARG:O	1:A:75:ILE:HA	2.17	0.44
1:C:163:VAL:HG23	1:C:175:LEU:CD2	2.48	0.44
2:B:6:GLU:HA	2:B:21:SER:O	2.19	0.43
1:C:66:ARG:HG2	1:C:67:SER:N	2.34	0.43
2:D:40:ALA:HB3	2:D:43:LYS:HB2	2.00	0.43
1:C:12:SER:HA	1:C:105:GLU:O	2.18	0.43
1:C:141:PRO:O	1:C:198:HIS:HE1	2.01	0.43
1:C:201:LEU:HD13	1:C:205:VAL:HG23	1.99	0.43
1:C:8:PRO:HG3	1:C:11:LEU:HD12	2.00	0.43
1:C:118:PHE:HD2	1:C:133:VAL:HG22	1.84	0.43
2:B:7:SER:HA	2:B:114:THR:HG21	2.00	0.42
1:C:4:MET:O	1:C:100:GLN:NE2	2.51	0.42
2:B:123:THR:HG22	2:B:210:SER:HB3	2.01	0.42
1:A:65:SER:O	1:A:71:PHE:HA	2.19	0.42
2:B:101:GLY:HA2	2:B:105:TYR:CE1	2.55	0.42
1:C:2:ILE:HG21	1:C:29:VAL:CG2	2.49	0.42
2:B:94:TYR:O	2:B:113:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HG2	1:A:171:SER:HB2	2.01	0.42
2:D:162:ASN:OD1	2:D:201:TYR:HA	2.19	0.42
1:A:186:TYR:CE2	1:A:211:ARG:HG3	2.55	0.42
1:C:86:TYR:O	1:C:101:GLY:HA2	2.20	0.42
1:C:54:LEU:CD1	1:C:58:VAL:HG12	2.50	0.42
2:D:98:ARG:O	2:D:107:MET:HA	2.20	0.42
2:D:125:GLY:HA2	2:D:207:HIS:HD2	1.85	0.41
1:A:6:GLN:HA	1:A:22:THR:O	2.20	0.41
2:B:69:THR:HB	2:B:82:GLN:HB3	2.03	0.41
2:D:22:CYS:HB2	2:D:36:TRP:CZ2	2.55	0.41
1:A:115:VAL:HG12	1:A:207:LYS:HB2	2.03	0.41
1:A:5:THR:O	1:A:23:CYS:HA	2.21	0.41
2:D:125:GLY:HA2	2:D:207:HIS:CD2	2.56	0.41
2:D:133:PRO:HG3	2:D:145:LEU:HD22	2.02	0.41
2:B:214:VAL:HG12	2:B:215:ASP:N	2.36	0.40
2:D:98:ARG:HD3	2:D:108:ASP:OD1	2.22	0.40
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.83	0.40
2:B:17:SER:HA	2:B:83:MET:O	2.21	0.40
2:D:91:THR:O	2:D:92:ALA:HB2	2.21	0.40
1:C:120:PRO:HG3	1:C:130:ALA:HB1	2.03	0.40
1:A:18:ARG:HA	1:A:76:SER:O	2.21	0.40
2:B:94:TYR:HE1	2:B:116:VAL:HB	1.87	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	A	212/214 (99%)	194 (92%)	13 (6%)	5 (2%)	6 9
1	C	212/214 (99%)	197 (93%)	11 (5%)	4 (2%)	8 13
2	B	221/223 (99%)	197 (89%)	18 (8%)	6 (3%)	5 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	221/223 (99%)	199 (90%)	18 (8%)	4 (2%)	8 14
All	All	866/874 (99%)	787 (91%)	60 (7%)	19 (2%)	6 10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	PRO
2	B	134	SER
2	B	139	SER
1	C	171	SER
2	D	220	PRO
1	A	51	ALA
2	B	105	TYR
2	D	29	ILE
2	D	196	LEU
1	A	138	ASN
1	C	51	ALA
1	C	138	ASN
1	C	157	GLY
2	B	136	LYS
2	B	174	PRO
2	D	54	THR
1	A	50	SER
1	A	157	GLY
1	A	204	PRO

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	189/189 (100%)	168 (89%)	21 (11%)	6 11
1	C	189/189 (100%)	165 (87%)	24 (13%)	4 8
2	B	185/185 (100%)	153 (83%)	32 (17%)	2 3
2	D	185/185 (100%)	161 (87%)	24 (13%)	4 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	748/748 (100%)	647 (86%)	101 (14%)	4 7

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	THR
1	A	18	ARG
1	A	20	THR
1	A	26	SER
1	A	40	PRO
1	A	48	ILE
1	A	65	SER
1	A	73	LEU
1	A	89	GLN
1	A	103	LYS
1	A	105	GLU
1	A	108	ARG
1	A	135	LEU
1	A	159	SER
1	A	164	THR
1	A	169	LYS
1	A	175	LEU
1	A	181	LEU
1	A	197	THR
1	A	214	CYS
2	B	3	GLN
2	B	6	GLU
2	B	11	LEU
2	B	12	VAL
2	B	18	LEU
2	B	20	LEU
2	B	28	ASN
2	B	31	ASP
2	B	32	THR
2	B	50	ARG
2	B	64	VAL
2	B	65	LYS
2	B	76	LYS
2	B	79	LEU
2	B	97	SER
2	B	99	TRP

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Mol	Chain	Res	Type
2	B	104	PHE
2	B	105	TYR
2	B	112	GLN
2	B	115	LEU
2	B	117	THR
2	B	142	THR
2	B	154	PRO
2	B	156	PRO
2	B	157	VAL
2	B	174	PRO
2	B	177	LEU
2	B	179	SER
2	B	182	LEU
2	B	188	VAL
2	B	194	SER
2	B	208	LYS
1	C	3	GLN
1	C	7	SER
1	C	9	SER
1	C	18	ARG
1	C	20	THR
1	C	24	ARG
1	C	46	LEU
1	C	74	THR
1	C	83	PHE
1	C	108	ARG
1	C	125	LEU
1	C	131	SER
1	C	133	VAL
1	C	135	LEU
1	C	150	VAL
1	C	175	LEU
1	C	178	THR
1	C	180	THR
1	C	181	LEU
1	C	190	LYS
1	C	197	THR
1	C	199	GLN
1	C	202	SER
1	C	211	ARG
2	D	3	GLN
2	D	11	LEU

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Mol	Chain	Res	Type
2	D	12	VAL
2	D	18	LEU
2	D	29	ILE
2	D	79	LEU
2	D	99	TRP
2	D	114	THR
2	D	117	THR
2	D	127	SER
2	D	145	LEU
2	D	148	LEU
2	D	149	VAL
2	D	160	SER
2	D	166	LEU
2	D	168	SER
2	D	176	VAL
2	D	177	LEU
2	D	182	LEU
2	D	185	LEU
2	D	208	LYS
2	D	213	LYS
2	D	216	LYS
2	D	220	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	89	GLN
1	A	147	GLN
1	A	198	HIS
1	A	199	GLN
1	A	210	ASN
2	B	178	GLN
2	B	207	HIS
1	C	89	GLN
1	C	100	GLN
1	C	198	HIS
1	C	199	GLN
2	D	3	GLN
2	D	28	ASN
2	D	35	HIS
2	D	207	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

There are no carbohydrates 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

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, 95^{th} 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	A	212/214 (99%)	-0.97	0	100	100	4, 20, 43, 55	1 (0%)
1	C	211/214 (98%)	-1.01	0	100	100	4, 20, 41, 49	0
2	B	216/223 (96%)	-1.02	0	100	100	2, 13, 44, 64	0
2	D	217/223 (97%)	-1.04	2 (0%)	84	86	2, 11, 38, 59	0
All	All	856/874 (97%)	-1.01	2 (0%)	95	95	2, 17, 42, 64	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	135	SER	3.3
2	D	140	GLY	3.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.