



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:08 PM EDT

PDB ID : 1FVD / pdb_00001fvd
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

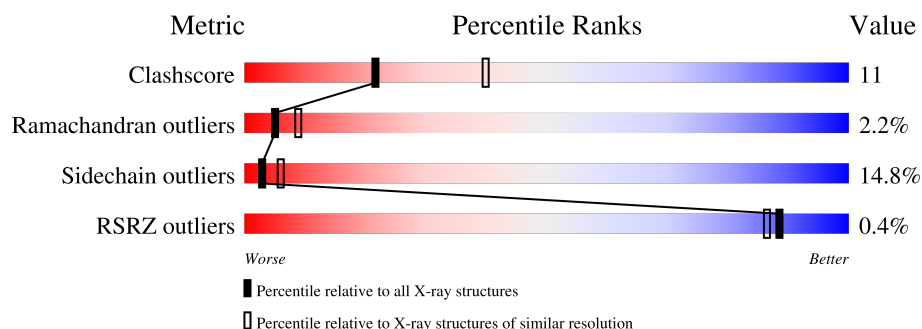
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	C	214	
2	B	223	
2	D	223	

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

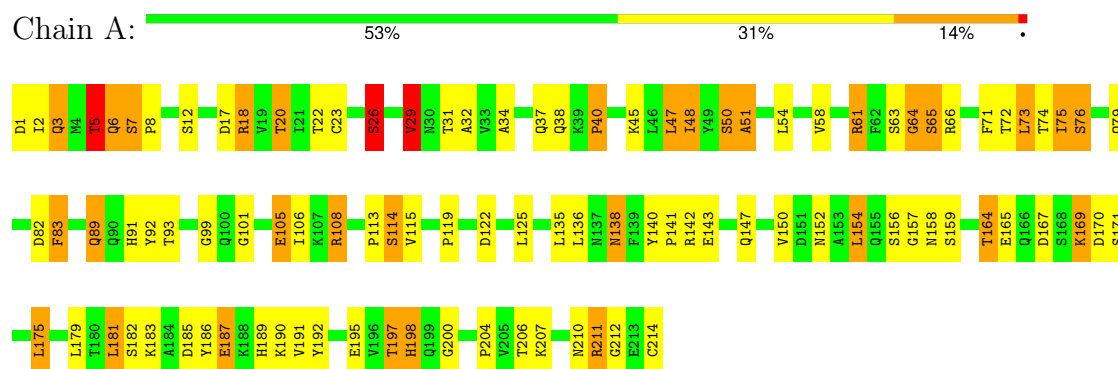
- Molecule 3 is water.

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

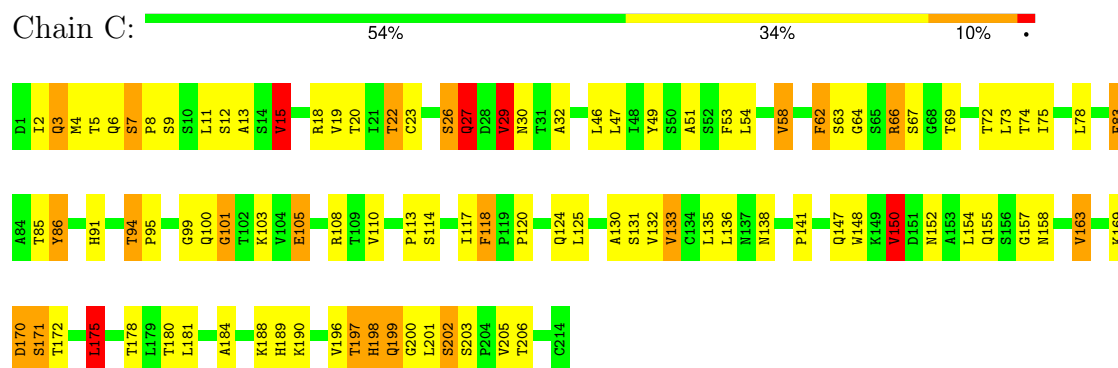
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

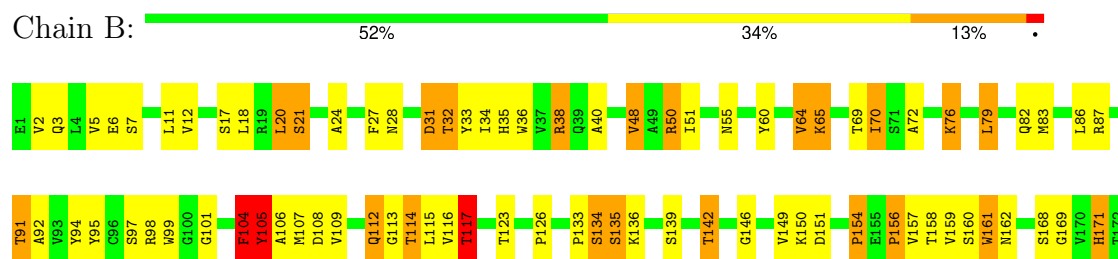
• Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)

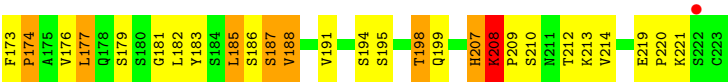


• Molecule 1: IGG1-KAPPA 4D5 FAB (LIGHT CHAIN)

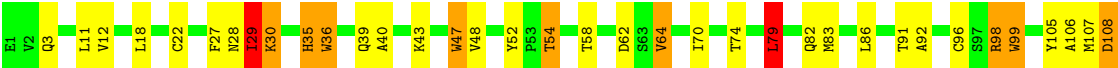


• Molecule 2: IGG1-KAPPA 4D5 FAB (HEAVY CHAIN)





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



4 Data and refinement statistics

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) 81.3 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	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 , 71.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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.*

¹Theoretical 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	A	1.19	3/1683 (0.2%)	2.08	70/2286 (3.1%)
1	C	1.24	7/1683 (0.4%)	2.03	52/2286 (2.3%)
2	B	1.37	10/1710 (0.6%)	2.13	59/2329 (2.5%)
2	D	1.34	9/1710 (0.5%)	2.13	66/2329 (2.8%)
All	All	1.29	29/6786 (0.4%)	2.09	247/9230 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	D	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	VAL	CA-CB	11.17	1.67	1.54
2	B	117	THR	CA-CB	9.21	1.66	1.53
2	D	117	THR	CA-CB	9.11	1.65	1.53
2	B	35	HIS	CD2-NE2	-7.76	1.29	1.37
2	D	35	HIS	CD2-NE2	-7.50	1.29	1.37
2	D	99	TRP	CA-CB	-7.23	1.43	1.52
2	D	183	TYR	CA-CB	-7.20	1.42	1.53
1	C	198	HIS	CD2-NE2	-7.08	1.30	1.37
2	B	198	THR	CA-CB	6.88	1.64	1.53
1	A	198	HIS	CD2-NE2	-6.84	1.30	1.37
2	B	171	HIS	CD2-NE2	-6.75	1.30	1.37
2	B	207	HIS	CD2-NE2	-6.54	1.30	1.37
2	B	24	ALA	CA-C	-6.48	1.44	1.52
1	C	189	HIS	CD2-NE2	-6.44	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	29	VAL	CA-CB	-6.09	1.46	1.54
2	D	171	HIS	CD2-NE2	-5.95	1.31	1.37
2	D	35	HIS	CG-ND1	-5.84	1.31	1.38
1	A	198	HIS	CG-ND1	-5.72	1.31	1.38
2	B	35	HIS	CG-ND1	-5.56	1.32	1.38
1	C	150	VAL	CA-CB	5.53	1.61	1.54
2	D	149	VAL	CA-CB	5.53	1.60	1.53
1	C	117	ILE	CA-CB	5.50	1.63	1.55
2	D	207	HIS	CD2-NE2	-5.34	1.31	1.37
2	B	213	LYS	CA-CB	-5.23	1.45	1.52
2	B	207	HIS	CG-ND1	-5.21	1.32	1.38
2	D	47	TRP	NE1-CE2	-5.14	1.31	1.37
1	A	195	GLU	CA-CB	5.14	1.60	1.53
1	C	26	SER	CA-CB	-5.06	1.45	1.53
2	B	191	VAL	CA-CB	5.03	1.60	1.55

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	HIS	CA-CB-CG	11.51	125.31	113.80
1	C	91	HIS	CA-CB-CG	10.03	123.83	113.80
2	B	31	ASP	CA-CB-CG	9.66	122.26	112.60
2	B	108	ASP	CA-CB-CG	9.42	122.02	112.60
1	C	197	THR	CA-CB-OG1	-8.77	96.45	109.60
1	A	17	ASP	CA-CB-CG	8.74	121.34	112.60
2	D	64	VAL	CB-CA-C	8.66	118.77	110.63
2	B	150	LYS	N-CA-C	8.48	124.20	109.96
1	A	211	ARG	N-CA-C	8.43	121.20	110.24
2	D	176	VAL	N-CA-CB	-8.32	100.98	111.46
1	A	158	ASN	CA-CB-CG	8.13	120.73	112.60
2	D	98	ARG	CB-CG-CD	-8.07	92.74	111.30
2	B	198	THR	N-CA-C	-8.04	102.37	112.90
2	D	158	THR	CA-CB-OG1	-7.93	97.71	109.60
1	A	83	PHE	CA-CB-CG	7.91	121.71	113.80
1	C	163	VAL	CG1-CB-CG2	-7.87	93.49	110.80
2	D	219	GLU	CA-C-N	7.87	129.68	119.84
2	D	219	GLU	C-N-CA	7.87	129.68	119.84
2	D	29	ILE	N-CA-CB	-7.78	98.39	111.23
1	A	167	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	197	THR	CA-CB-OG1	-7.75	97.97	109.60
2	B	104	PHE	CA-CB-CG	7.66	121.46	113.80
1	A	29	VAL	N-CA-C	-7.44	105.10	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	112	GLN	CB-CG-CD	7.39	125.16	112.60
1	C	7	SER	O-C-N	-7.38	116.64	121.88
1	A	75	ILE	N-CA-C	-7.36	96.47	107.37
1	C	83	PHE	CA-CB-CG	7.27	121.07	113.80
2	D	191	VAL	N-CA-C	7.24	115.87	107.84
2	B	28	ASN	CB-CG-ND2	7.20	127.20	116.40
1	A	113	PRO	O-C-N	-7.17	115.07	123.10
2	B	55	ASN	OD1-CG-ND2	-7.13	115.47	122.60
2	D	129	PHE	CA-C-N	7.10	126.86	119.76
2	D	129	PHE	C-N-CA	7.10	126.86	119.76
2	D	220	PRO	N-CA-C	7.10	127.10	112.47
1	A	29	VAL	N-CA-CB	-7.09	102.85	112.28
2	B	168	SER	N-CA-C	7.01	120.11	108.96
2	B	112	GLN	CG-CD-NE2	7.00	126.90	116.40
1	A	206	THR	CA-CB-OG1	-6.99	99.12	109.60
1	C	99	GLY	N-CA-C	-6.98	101.61	112.85
2	B	162	ASN	CA-CB-CG	-6.97	105.63	112.60
1	C	30	ASN	CA-CB-CG	6.93	119.53	112.60
1	C	101	GLY	O-C-N	6.92	130.52	122.56
1	A	1	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	122	ASP	CA-CB-CG	-6.88	105.72	112.60
2	D	62	ASP	CA-CB-CG	6.88	119.48	112.60
2	D	64	VAL	N-CA-C	-6.83	107.22	113.71
2	D	213	LYS	N-CA-C	-6.76	96.11	107.80
2	D	27	PHE	CA-CB-CG	6.75	120.55	113.80
1	A	99	GLY	N-CA-C	-6.70	102.26	112.51
2	B	112	GLN	CB-CG-CD	6.70	123.98	112.60
2	D	52	TYR	CA-C-O	-6.70	114.17	119.99
2	B	50	ARG	CB-CG-CD	-6.66	95.99	111.30
2	D	153	PHE	O-C-N	-6.65	115.28	122.06
2	B	208	LYS	CA-C-N	6.63	126.88	119.32
2	B	208	LYS	C-N-CA	6.63	126.88	119.32
2	B	87	ARG	CB-CG-CD	-6.61	96.09	111.30
1	C	198	HIS	CB-CG-CD2	-6.61	122.61	131.20
2	D	64	VAL	N-CA-CB	-6.59	101.42	111.57
1	C	124	GLN	OE1-CD-NE2	6.56	129.16	122.60
1	C	124	GLN	CA-CB-CG	-6.55	100.99	114.10
1	A	187	GLU	N-CA-C	6.54	121.12	113.20
1	A	101	GLY	N-CA-C	6.49	120.33	112.48
2	D	187	SER	N-CA-C	-6.48	98.34	108.90
1	C	171	SER	N-CA-C	6.47	124.59	110.80
1	C	118	PHE	CA-C-O	6.46	124.63	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	VAL	CA-C-N	6.44	126.47	119.90
1	C	58	VAL	C-N-CA	6.44	126.47	119.90
1	C	22	THR	N-CA-C	6.42	120.00	109.72
1	A	142	ARG	CB-CG-CD	-6.42	96.53	111.30
2	D	30	LYS	CA-C-O	6.41	127.30	120.70
2	D	35	HIS	CA-CB-CG	6.38	120.19	113.80
1	A	58	VAL	CA-C-N	6.33	126.35	119.89
1	A	58	VAL	C-N-CA	6.33	126.35	119.89
2	D	35	HIS	CB-CG-ND1	6.31	132.17	122.70
2	D	47	TRP	CG-CD2-CE3	6.31	140.21	133.90
2	B	64	VAL	N-CA-CB	-6.29	101.88	111.57
1	A	18	ARG	CB-CG-CD	-6.29	96.83	111.30
1	C	197	THR	CA-CB-CG2	6.29	121.20	110.50
1	A	182	SER	CA-C-O	-6.29	114.88	121.55
2	B	33	TYR	N-CA-C	-6.27	98.97	109.07
1	C	86	TYR	O-C-N	6.26	130.91	123.27
2	D	206	ASN	O-C-N	-6.24	116.03	123.27
2	B	126	PRO	N-CA-C	6.24	121.30	111.38
2	D	39	GLN	OE1-CD-NE2	6.23	128.83	122.60
2	B	38	ARG	N-CA-C	6.20	120.03	110.42
2	D	82	GLN	OE1-CD-NE2	-6.20	116.40	122.60
2	B	220	PRO	N-CA-C	6.19	120.69	111.41
1	A	138	ASN	N-CA-C	6.18	123.96	110.80
1	A	164	THR	N-CA-CB	-6.14	101.01	110.04
1	C	22	THR	CA-CB-OG1	-6.14	100.38	109.60
2	B	135	SER	N-CA-C	6.13	120.31	112.34
2	B	208	LYS	CA-C-O	-6.13	112.69	118.33
2	B	64	VAL	CB-CA-C	6.12	116.39	110.63
1	A	164	THR	CA-CB-OG1	-6.12	100.43	109.60
1	C	158	ASN	N-CA-C	-6.08	104.07	112.03
2	B	151	ASP	N-CA-C	6.07	118.60	111.02
1	A	170	ASP	N-CA-C	6.05	121.47	112.94
1	A	179	LEU	N-CA-C	-6.05	99.38	109.24
1	A	91	HIS	CB-CG-CD2	-6.04	123.35	131.20
2	B	70	ILE	N-CA-C	-6.03	99.78	108.53
2	B	162	ASN	N-CA-C	6.03	119.74	111.54
1	A	40	PRO	N-CA-C	6.03	124.89	112.47
1	C	124	GLN	CG-CD-NE2	-6.01	107.38	116.40
1	C	49	TYR	CA-C-O	-6.01	114.19	121.28
2	B	112	GLN	CA-CB-CG	5.97	126.04	114.10
1	A	76	SER	N-CA-C	5.96	117.44	111.07
2	D	27	PHE	O-C-N	-5.93	116.49	123.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	PHE	CA-CB-CG	5.92	119.72	113.80
2	D	27	PHE	CA-C-N	-5.91	114.36	122.93
2	D	27	PHE	C-N-CA	-5.91	114.36	122.93
1	C	32	ALA	N-CA-C	5.90	118.83	108.56
1	A	175	LEU	CA-CB-CG	5.89	136.92	116.30
1	C	163	VAL	CA-C-O	-5.88	114.21	120.39
2	D	153	PHE	CA-CB-CG	-5.85	107.95	113.80
2	D	110	TRP	O-C-N	-5.83	115.65	123.23
1	A	190	LYS	CA-C-N	-5.83	115.59	122.93
1	A	190	LYS	C-N-CA	-5.83	115.59	122.93
2	D	129	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	175	LEU	CA-CB-CG	5.82	136.65	116.30
1	A	61	ARG	N-CA-C	5.81	120.10	113.19
2	B	76	LYS	N-CA-C	-5.80	105.96	113.16
1	A	197	THR	CA-CB-CG2	5.80	120.36	110.50
2	D	99	TRP	CE2-CD2-CE3	5.79	124.59	118.80
1	A	181	LEU	CA-C-N	5.79	129.49	120.75
1	A	181	LEU	C-N-CA	5.79	129.49	120.75
1	C	47	LEU	N-CA-C	-5.76	106.90	114.04
2	D	165	ALA	N-CA-C	5.75	118.41	111.40
2	B	185	LEU	CA-CB-CG	5.73	136.35	116.30
2	D	79	LEU	N-CA-CB	-5.69	100.95	111.13
2	B	50	ARG	CA-CB-CG	5.66	125.42	114.10
2	B	219	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	61	ARG	NE-CZ-NH2	-5.64	114.12	119.20
2	B	209	PRO	N-CA-C	5.64	122.16	113.75
2	D	106	ALA	CB-CA-C	-5.64	108.44	115.89
2	D	54	THR	CA-CB-OG1	-5.64	101.14	109.60
1	C	18	ARG	N-CA-C	-5.63	100.80	109.76
2	B	21	SER	N-CA-CB	-5.63	102.08	111.20
2	B	187	SER	N-CA-C	-5.63	99.73	108.90
2	B	160	SER	N-CA-C	-5.62	100.80	109.52
2	D	207	HIS	CB-CG-CD2	-5.62	123.89	131.20
2	D	29	ILE	CA-CB-CG1	-5.62	100.84	110.40
2	D	175	ALA	O-C-N	5.62	129.35	123.06
1	A	156	SER	CA-CB-OG	5.61	122.33	111.10
1	A	31	THR	N-CA-CB	-5.60	102.19	111.49
2	B	76	LYS	N-CA-CB	-5.60	101.88	110.44
1	A	164	THR	CA-CB-CG2	5.60	120.01	110.50
1	C	85	THR	N-CA-C	-5.58	99.91	109.24
1	C	69	THR	CA-C-O	-5.58	112.82	119.35
2	D	99	TRP	CD2-CE2-CZ2	-5.58	116.83	122.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	171	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	114	SER	O-C-N	-5.56	116.45	123.01
1	A	89	GLN	CG-CD-NE2	5.54	124.71	116.40
2	B	142	THR	N-CA-C	-5.54	100.66	109.96
1	A	106	ILE	N-CA-C	5.52	116.13	108.84
2	B	169	GLY	O-C-N	5.51	127.59	122.57
1	A	26	SER	CA-CB-OG	5.50	122.10	111.10
2	B	35	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	D	35	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	C	114	SER	N-CA-C	-5.49	101.73	109.96
1	A	38	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	73	LEU	N-CA-C	-5.47	100.78	109.59
2	B	79	LEU	N-CA-CB	-5.44	102.23	111.69
1	C	196	VAL	N-CA-C	5.43	116.81	108.71
2	B	104	PHE	N-CA-C	5.43	119.13	107.67
1	C	53	PHE	O-C-N	-5.43	116.89	123.13
2	B	134	SER	N-CA-C	5.42	122.35	110.80
2	D	126	PRO	N-CA-C	5.42	119.70	111.19
1	C	103	LYS	CB-CG-CD	5.41	123.74	111.30
2	B	171	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	D	206	ASN	N-CA-CB	-5.40	102.22	110.65
1	A	212	GLY	N-CA-C	5.40	117.53	112.08
1	C	113	PRO	N-CA-C	5.39	118.95	110.80
1	A	63	SER	CA-CB-OG	-5.39	100.32	111.10
2	D	176	VAL	CA-CB-CG1	5.39	119.56	110.40
1	C	136	LEU	N-CA-C	-5.39	100.40	109.07
2	B	5	VAL	O-C-N	-5.38	117.39	123.20
2	D	99	TRP	CB-CG-CD2	-5.37	119.28	126.80
2	D	176	VAL	CA-CB-CG2	-5.37	101.28	110.40
2	B	158	THR	OG1-CB-CG2	-5.37	98.57	109.30
2	D	47	TRP	CE2-CD2-CG	-5.36	100.77	107.20
2	B	173	PHE	CA-C-N	5.35	126.53	119.84
2	B	173	PHE	C-N-CA	5.35	126.53	119.84
1	C	198	HIS	CA-C-N	5.35	127.76	120.54
1	C	198	HIS	C-N-CA	5.35	127.76	120.54
1	A	113	PRO	CA-C-O	-5.34	114.94	121.03
2	B	91	THR	N-CA-C	-5.31	101.79	109.59
2	D	29	ILE	N-CA-C	5.30	120.37	109.34
2	D	198	THR	CA-CB-OG1	-5.30	101.64	109.60
2	D	36	TRP	CD2-CE2-CZ2	-5.30	117.10	122.40
1	C	170	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	7	SER	O-C-N	-5.29	118.13	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ASN	CA-CB-CG	-5.29	107.31	112.60
2	B	117	THR	OG1-CB-CG2	5.28	119.86	109.30
2	B	48	VAL	N-CA-CB	-5.27	107.32	111.64
1	C	29	VAL	N-CA-C	-5.27	106.74	112.80
1	A	154	LEU	CA-C-N	5.26	128.95	121.42
1	A	154	LEU	C-N-CA	5.26	128.95	121.42
1	A	152	ASN	CA-CB-CG	-5.26	107.34	112.60
2	D	116	VAL	CA-C-O	-5.25	114.51	120.66
1	A	5	THR	CA-C-O	5.25	126.03	120.36
1	A	198	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	C	53	PHE	CA-CB-CG	5.24	119.04	113.80
2	D	58	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	6	GLN	N-CA-CB	-5.23	102.35	110.57
2	D	52	TYR	CA-C-N	5.23	125.28	119.32
2	D	52	TYR	C-N-CA	5.23	125.28	119.32
1	C	202	SER	O-C-N	5.22	127.66	122.12
1	A	18	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	C	75	ILE	N-CA-C	-5.20	100.39	107.99
1	A	106	ILE	O-C-N	-5.20	116.68	122.66
2	D	176	VAL	O-C-N	-5.19	117.03	123.10
2	B	112	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	47	LEU	N-CA-C	-5.18	106.04	112.93
2	D	158	THR	CA-CB-CG2	5.18	119.30	110.50
2	B	95	TYR	CA-C-O	-5.17	115.11	120.70
2	D	47	TRP	CG-CD1-NE1	-5.17	103.47	110.20
1	A	169	LYS	N-CA-C	-5.17	104.57	111.24
1	A	185	ASP	CA-CB-CG	5.17	117.77	112.60
2	D	111	GLY	O-C-N	-5.16	118.37	122.81
2	B	213	LYS	N-CA-C	-5.16	98.62	107.23
1	C	91	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	150	VAL	N-CA-CB	-5.14	105.19	111.67
2	B	108	ASP	N-CA-C	5.13	118.00	111.69
1	A	158	ASN	CA-C-N	5.12	130.28	122.65
1	A	158	ASN	C-N-CA	5.12	130.28	122.65
2	D	108	ASP	N-CA-C	5.11	119.57	113.23
2	B	34	ILE	CA-C-O	-5.11	114.90	120.72
1	A	64	GLY	O-C-N	-5.10	118.78	123.42
1	C	113	PRO	O-C-N	-5.10	117.39	123.10
1	C	27	GLN	CA-CB-CG	5.10	124.30	114.10
1	C	29	VAL	N-CA-CB	-5.10	100.39	111.81
2	B	161	TRP	CE2-CD2-CE3	5.10	123.90	118.80
2	D	47	TRP	CB-CG-CD1	-5.09	119.26	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	VAL	N-CA-CB	-5.09	106.60	111.89
2	D	48	VAL	CG1-CB-CG2	-5.09	99.61	110.80
1	C	62	PHE	CA-C-O	5.08	125.85	120.36
2	D	151	ASP	N-CA-C	5.07	116.84	110.91
1	A	51	ALA	N-CA-C	5.07	121.59	110.80
2	B	28	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	136	LEU	N-CA-C	-5.02	99.24	108.02
1	C	19	VAL	N-CA-C	-5.02	100.98	108.46
2	D	158	THR	N-CA-CB	-5.01	102.26	110.68
1	C	66	ARG	CG-CD-NE	-5.01	100.98	112.00
2	B	186	SER	N-CA-C	-5.01	101.47	109.23
1	A	82	ASP	N-CA-C	-5.00	106.76	112.92
1	C	94	THR	N-CA-C	-5.00	102.76	110.32
1	A	114	SER	N-CA-C	-5.00	102.29	110.20

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	35	0
1	C	1647	0	1596	37	0
2	B	1669	0	1634	39	0
2	D	1669	0	1634	31	0
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	139	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 11.

All (139) 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:B:83:MET:HE2	2:B:86:LEU:HD21	1.56	0.87
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:D:83:MET:HE2	2:D:86:LEU:HD21	1.83	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ARG:HG2	2:B:48:VAL:CG2	2.41	0.51
2:B:156:PRO:HG2	2:B:208:LYS:HZ3	1.76	0.51
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.75	0.51
2:D:208:LYS:H	2:D:208:LYS:HZ2	1.59	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:13:ALA:HB3	1:C:78:LEU:CD2	2.44	0.48
1:C:169:LYS:HD2	1:C:169:LYS:HA	1.58	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
2:B:72:ALA:HB2	2:B:79:LEU:HD12	1.96	0.47
1:C:5:THR:HA	1:C:100:GLN:HE22	1.79	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
1:C:6:GLN:HA	1:C:22:THR:O	2.15	0.47
2:B:83:MET:HE2	2:B:86:LEU:CD2	2.36	0.46
1:A:83:PHE:CZ	1:A:165:GLU:HG3	2.44	0.46
2:B:195:SER:HB2	2:B:199:GLN:HG3	1.96	0.46
1:A:79:GLN:HA	1:A:79:GLN:OE1	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:LYS:HE3	2:D:74:THR:HB	1.98	0.46
2:D:133:PRO:HB3	2:D:144:ALA:O	2.16	0.46
2:D:204:ASN:HB3	2:D:213:LYS:HZ1	1.80	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: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
2:D:83:MET:HE2	2:D:86:LEU:CD2	2.47	0.44
1:A:61:ARG:O	1:A:75:ILE:HA	2.17	0.44
1:A:147:GLN:HB3	1:A:154:LEU:HD21	2.00	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:104:PHE:C	2:B:106:ALA:H	2.29	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: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
1:C:3:GLN:HB2	1:C:26:SER:HG	1.86	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:7:SER:HA	1:A:8:PRO:C	2.46	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%)	4	8
1	C	212/214 (99%)	197 (93%)	11 (5%)	4 (2%)	6	11
2	B	221/223 (99%)	197 (89%)	18 (8%)	6 (3%)	4	6
2	D	221/223 (99%)	199 (90%)	18 (8%)	4 (2%)	6	12
All	All	866/874 (99%)	787 (91%)	60 (7%)	19 (2%)	5	9

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 ⓘ

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%)	165 (87%)	24 (13%)	4	9
1	C	189/189 (100%)	161 (85%)	28 (15%)	3	6
2	B	185/185 (100%)	151 (82%)	34 (18%)	1	3
2	D	185/185 (100%)	160 (86%)	25 (14%)	4	8
All	All	748/748 (100%)	637 (85%)	111 (15%)	3	6

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	5	THR
1	A	20	THR
1	A	26	SER
1	A	29	VAL
1	A	40	PRO
1	A	45	LYS
1	A	48	ILE
1	A	50	SER
1	A	65	SER
1	A	73	LEU
1	A	89	GLN
1	A	105	GLU
1	A	108	ARG
1	A	114	SER
1	A	135	LEU
1	A	143	GLU
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	11	LEU
2	B	12	VAL
2	B	18	LEU
2	B	20	LEU
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	97	SER
2	B	99	TRP
2	B	104	PHE
2	B	105	TYR
2	B	109	VAL
2	B	112	GLN
2	B	114	THR
2	B	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	176	VAL
2	B	177	LEU
2	B	179	SER
2	B	182	LEU
2	B	185	LEU
2	B	188	VAL
2	B	194	SER
2	B	198	THR
2	B	208	LYS
1	C	3	GLN
1	C	7	SER
1	C	9	SER
1	C	15	VAL
1	C	20	THR
1	C	27	GLN
1	C	29	VAL
1	C	46	LEU
1	C	74	THR
1	C	83	PHE
1	C	94	THR
1	C	105	GLU
1	C	108	ARG
1	C	125	LEU
1	C	131	SER
1	C	132	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	206	THR
2	D	3	GLN
2	D	11	LEU
2	D	12	VAL
2	D	18	LEU
2	D	29	ILE
2	D	64	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	91	HIS
1	A	199	GLN
1	A	210	ASN
2	B	3	GLN
2	B	178	GLN
2	B	207	HIS
1	C	100	GLN
1	C	198	HIS
1	C	199	GLN
2	D	3	GLN
2	D	28	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	35	HIS
2	D	207	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	212/214 (99%)	-0.73	0 100 100	4, 20, 43, 55	1 (0%)
1	C	211/214 (98%)	-0.78	0 100 100	4, 20, 41, 49	0
2	B	216/223 (96%)	-0.79	1 (0%) 87 85	2, 13, 44, 64	0
2	D	217/223 (97%)	-0.81	2 (0%) 81 78	2, 11, 38, 59	0
All	All	856/874 (97%)	-0.78	3 (0%) 88 86	2, 17, 42, 64	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	135	SER	2.6
2	B	222	SER	2.3
2	D	140	GLY	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.