



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:02 AM UTC

PDB ID : 3EYQ / pdb_00003eyq
Title : Crystal structure of MJ5 Fab, a germline antibody variant of anti-human cytomegalovirus antibody 8f9
Authors : Thomson, C.A.; Bryson, S.; McLean, G.R.; Creagh, A.L.; Pai, E.F.; Schrader, J.W.
Deposited on : 2008-10-21
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

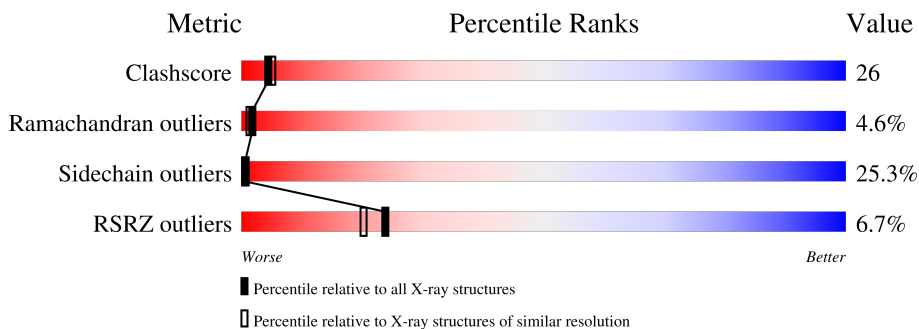
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	C	216	
2	D	242	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3294 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 M2J5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	212	Total	C	N	O	S	0	0	0
			1638	1026	280	328	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	expression tag	PDB 3EYQ

- Molecule 2 is a protein called 8f9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total	C	N	O	S	0	0	0
			1568	994	264	304	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	235	LEU	-	expression tag	PDB 3EYQ
D	236	GLU	-	expression tag	PDB 3EYQ
D	237	HIS	-	expression tag	PDB 3EYQ
D	238	HIS	-	expression tag	PDB 3EYQ
D	239	HIS	-	expression tag	PDB 3EYQ
D	240	HIS	-	expression tag	PDB 3EYQ
D	241	HIS	-	expression tag	PDB 3EYQ
D	242	HIS	-	expression tag	PDB 3EYQ

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	55	Total	O	0	0
			55	55		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	33	Total	O	0	0
			33	33		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.38Å 76.05Å 111.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 85.9 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.270 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3294	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 6.50% 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	C	3.03	170/1675 (10.1%)	2.13	78/2279 (3.4%)
2	D	2.83	119/1603 (7.4%)	1.97	58/2177 (2.7%)
All	All	2.93	289/3278 (8.8%)	2.05	136/4456 (3.1%)

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	C	4	8
2	D	4	14
All	All	8	22

All (289) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	ALA	CA-CB	-10.74	1.38	1.53
1	C	84	ALA	CA-CB	-10.60	1.41	1.54
1	C	33	LEU	C-O	-9.94	1.12	1.24
2	D	61	ALA	CA-CB	-9.94	1.36	1.53
1	C	118	ILE	C-O	-9.56	1.13	1.24
1	C	37	GLN	C-O	-9.54	1.12	1.24
2	D	170	ALA	CA-CB	-9.47	1.38	1.53
2	D	40	ALA	CA-CB	-9.43	1.38	1.53
1	C	196	GLU	C-O	-8.89	1.13	1.24
2	D	217	THR	C-O	-8.71	1.14	1.24
2	D	50	VAL	C-O	-8.64	1.15	1.24
2	D	37	VAL	C-O	-8.62	1.15	1.24
2	D	162	VAL	C-O	-8.59	1.15	1.24
2	D	114	TYR	C-O	-8.58	1.13	1.23
1	C	164	VAL	C-O	-8.48	1.15	1.24
2	D	121	VAL	C-O	-8.30	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	93	VAL	CA-C	-8.29	1.43	1.52
1	C	9	ALA	CA-CB	-8.13	1.40	1.53
2	D	154	VAL	C-O	-8.12	1.14	1.24
1	C	107	ILE	C-O	-8.10	1.15	1.24
1	C	173	THR	C-O	-8.09	1.13	1.23
1	C	34	ALA	CA-C	-8.08	1.43	1.52
1	C	110	THR	N-CA	-8.08	1.36	1.46
2	D	185	SER	C-O	-8.01	1.13	1.24
1	C	30	SER	C-O	-7.99	1.17	1.24
1	C	32	TYR	C-O	-7.98	1.15	1.23
1	C	133	VAL	C-O	-7.88	1.15	1.24
1	C	112	ALA	C-O	-7.84	1.15	1.24
2	D	175	VAL	C-O	-7.83	1.16	1.24
2	D	7	SER	C-O	-7.78	1.14	1.23
2	D	64	VAL	C-O	-7.78	1.15	1.24
1	C	9	ALA	CA-C	-7.75	1.43	1.52
2	D	155	LYS	CE-NZ	-7.74	1.26	1.49
2	D	70	ILE	C-O	-7.73	1.14	1.24
1	C	201	GLY	C-O	-7.72	1.15	1.23
1	C	58	ILE	CA-C	-7.70	1.47	1.53
1	C	150	LYS	C-O	-7.66	1.14	1.23
1	C	6	GLN	C-O	-7.62	1.14	1.24
1	C	156	GLN	C-O	-7.61	1.15	1.24
1	C	155	LEU	N-CA	-7.57	1.35	1.45
1	C	149	TRP	C-O	-7.50	1.15	1.23
1	C	86	TYR	C-O	-7.42	1.15	1.24
2	D	189	SER	C-O	-7.42	1.14	1.23
1	C	180	LEU	C-O	-7.41	1.14	1.24
1	C	162	GLU	C-O	-7.31	1.14	1.23
2	D	169	GLY	C-O	-7.30	1.16	1.24
1	C	151	VAL	CA-C	-7.23	1.43	1.52
1	C	44	PRO	C-O	-7.22	1.14	1.24
1	C	137	LEU	C-O	-7.22	1.15	1.23
2	D	158	PHE	C-O	-7.21	1.15	1.24
1	C	77	SER	C-O	-7.21	1.15	1.24
1	C	14	SER	C-O	-7.20	1.16	1.24
1	C	48	ILE	C-O	-7.20	1.16	1.24
1	C	141	TYR	C-O	-7.17	1.16	1.24
2	D	5	VAL	C-O	-7.15	1.16	1.24
1	C	186	ASP	C-O	-7.08	1.16	1.24
1	C	105	LEU	C-O	-7.04	1.15	1.24
2	D	48	VAL	C-O	-7.04	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	ALA	C-O	-7.01	1.15	1.24
1	C	177	SER	C-O	-7.01	1.15	1.24
1	C	151	VAL	C-O	-6.96	1.16	1.24
1	C	202	LEU	C-O	-6.96	1.15	1.24
1	C	144	GLU	CA-C	-6.95	1.42	1.52
2	D	153	LEU	C-O	-6.95	1.15	1.24
2	D	150	LEU	C-O	-6.94	1.15	1.23
1	C	179	THR	C-O	-6.90	1.15	1.24
1	C	9	ALA	C-O	-6.89	1.16	1.24
2	D	37	VAL	CA-CB	6.86	1.66	1.55
1	C	29	VAL	CA-CB	-6.85	1.45	1.54
2	D	121	VAL	N-CA	-6.79	1.38	1.46
1	C	182	LEU	C-O	-6.77	1.15	1.24
1	C	14	SER	CA-C	-6.73	1.43	1.52
1	C	171	ASP	CB-CG	-6.72	1.35	1.52
2	D	130	GLY	C-O	-6.72	1.14	1.24
1	C	198	THR	CB-CG2	-6.71	1.30	1.52
2	D	156	ASP	C-O	-6.70	1.15	1.24
1	C	183	SER	C-O	-6.70	1.15	1.23
2	D	218	LYS	C-O	-6.69	1.16	1.24
1	C	83	PHE	N-CA	-6.68	1.38	1.46
1	C	189	LYS	C-O	-6.68	1.16	1.24
1	C	114	PRO	C-O	-6.67	1.14	1.23
1	C	198	THR	C-O	-6.64	1.16	1.24
1	C	82	ASP	CA-C	-6.64	1.44	1.52
2	D	188	TYR	C-O	-6.60	1.15	1.23
1	C	160	SER	C-O	-6.57	1.16	1.23
2	D	129	LYS	C-O	-6.55	1.15	1.23
1	C	185	ALA	CA-CB	-6.53	1.43	1.53
1	C	39	LYS	C-O	-6.52	1.15	1.23
1	C	108	LYS	C-O	-6.51	1.16	1.24
1	C	11	LEU	C-O	-6.51	1.16	1.24
1	C	104	ARG	N-CA	-6.51	1.38	1.46
2	D	147	THR	CB-CG2	-6.50	1.31	1.52
2	D	186	GLY	C-O	-6.49	1.15	1.24
1	C	127	LYS	CB-CG	-6.47	1.33	1.52
2	D	192	SER	C-O	-6.47	1.16	1.24
2	D	23	ALA	CA-CB	-6.45	1.44	1.52
2	D	170	ALA	N-CA	-6.45	1.38	1.46
1	C	184	LYS	C-O	-6.44	1.16	1.24
2	D	33	GLY	C-O	-6.44	1.16	1.24
2	D	166	TRP	C-O	-6.43	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	ASN	C-O	-6.42	1.15	1.24
1	C	190	HIS	C-O	-6.42	1.16	1.23
2	D	38	ARG	N-CA	-6.41	1.37	1.45
1	C	133	VAL	CA-C	-6.41	1.45	1.52
1	C	66	GLY	C-O	-6.39	1.17	1.23
1	C	134	VAL	CB-CG2	-6.39	1.31	1.52
2	D	157	TYR	C-O	-6.39	1.15	1.23
1	C	36	TYR	C-O	-6.38	1.16	1.24
1	C	99	PHE	C-O	-6.38	1.16	1.24
2	D	129	LYS	CG-CD	-6.35	1.33	1.52
1	C	157	SER	C-O	-6.35	1.16	1.23
2	D	61	ALA	C-O	-6.33	1.15	1.23
1	C	85	VAL	C-O	-6.31	1.17	1.24
2	D	93	VAL	C-O	-6.30	1.16	1.24
1	C	178	SER	C-O	-6.28	1.16	1.24
1	C	12	SER	C-O	-6.28	1.16	1.24
2	D	204	GLN	N-CA	-6.28	1.38	1.46
1	C	206	VAL	CB-CG1	-6.25	1.31	1.52
1	C	111	VAL	C-O	-6.24	1.18	1.24
2	D	164	VAL	C-O	-6.23	1.17	1.24
2	D	28	THR	C-O	-6.21	1.16	1.24
1	C	68	GLY	C-O	-6.20	1.15	1.23
2	D	11	VAL	CB-CG2	-6.20	1.32	1.52
1	C	192	VAL	C-O	-6.19	1.17	1.24
1	C	49	TYR	C-O	-6.19	1.16	1.24
1	C	151	VAL	CA-CB	-6.19	1.46	1.54
2	D	131	PRO	C-O	-6.18	1.16	1.23
1	C	211	ASN	C-O	-6.18	1.16	1.23
1	C	122	SER	C-O	-6.17	1.16	1.24
1	C	44	PRO	CA-C	-6.15	1.43	1.52
1	C	147	VAL	C-O	-6.14	1.16	1.24
2	D	114	TYR	CA-C	-6.14	1.45	1.52
2	D	11	VAL	C-O	-6.13	1.17	1.24
1	C	175	SER	C-O	-6.11	1.16	1.23
2	D	133	VAL	C-O	-6.11	1.17	1.24
2	D	148	ALA	CA-CB	-6.10	1.38	1.53
1	C	193	TYR	C-O	-6.08	1.17	1.24
1	C	193	TYR	N-CA	-6.08	1.39	1.46
2	D	177	THR	N-CA	-6.08	1.38	1.46
2	D	116	GLY	C-O	-6.07	1.18	1.23
2	D	172	THR	C-O	-6.07	1.16	1.24
2	D	155	LYS	C-O	-6.07	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	PHE	C-O	-6.05	1.17	1.24
1	C	165	THR	C-O	-6.04	1.16	1.23
1	C	150	LYS	N-CA	-6.03	1.38	1.46
1	C	103	THR	N-CA	-6.02	1.38	1.46
1	C	131	ALA	C-O	-6.00	1.16	1.23
2	D	34	MET	C-O	-6.00	1.16	1.23
1	C	10	THR	C-O	-5.99	1.17	1.24
2	D	24	ALA	CA-CB	-5.98	1.44	1.53
1	C	110	THR	CA-CB	-5.98	1.43	1.53
2	D	196	VAL	C-O	-5.94	1.17	1.24
1	C	169	SER	C-O	-5.94	1.16	1.24
2	D	47	TRP	CA-C	-5.93	1.45	1.52
1	C	13	LEU	C-O	-5.92	1.16	1.23
1	C	143	ARG	C-O	-5.90	1.17	1.24
2	D	44	GLY	C-O	-5.88	1.18	1.23
1	C	64	GLY	C-O	-5.86	1.16	1.23
2	D	161	PRO	CG-CD	-5.86	1.35	1.51
2	D	4	LEU	N-CA	-5.86	1.38	1.46
1	C	46	LEU	C-O	-5.85	1.17	1.24
1	C	174	TYR	CE1-CZ	-5.85	1.24	1.38
1	C	10	THR	CB-CG2	-5.83	1.33	1.52
2	D	48	VAL	CA-CB	-5.81	1.49	1.55
1	C	79	GLU	C-O	-5.78	1.16	1.23
1	C	119	PHE	C-O	-5.78	1.18	1.24
1	C	82	ASP	C-O	-5.76	1.16	1.24
1	C	70	ASP	CB-CG	-5.75	1.37	1.52
1	C	61	ARG	C-O	-5.75	1.16	1.24
1	C	164	VAL	CB-CG2	-5.75	1.33	1.52
2	D	68	PHE	C-O	-5.75	1.17	1.23
1	C	145	ALA	C-O	-5.74	1.16	1.24
1	C	124	GLU	CA-C	-5.74	1.44	1.52
2	D	15	GLY	C-O	-5.74	1.15	1.24
1	C	205	PRO	CA-C	5.74	1.58	1.52
2	D	36	TRP	C-O	-5.72	1.17	1.24
2	D	81	LEU	C-O	-5.72	1.17	1.24
2	D	174	GLY	C-O	-5.72	1.16	1.23
1	C	134	VAL	CB-CG1	-5.71	1.33	1.52
1	C	154	ALA	CA-C	-5.71	1.45	1.52
2	D	51	ILE	C-O	-5.71	1.18	1.24
1	C	113	ALA	C-O	-5.69	1.17	1.24
1	C	127	LYS	CA-CB	-5.69	1.44	1.53
2	D	16	ARG	CA-C	-5.68	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	THR	CB-CG2	-5.67	1.33	1.52
2	D	166	TRP	N-CA	-5.67	1.39	1.46
2	D	194	VAL	C-O	-5.66	1.17	1.23
1	C	2	ILE	CG1-CD1	-5.66	1.29	1.51
2	D	190	LEU	CG-CD2	-5.66	1.33	1.52
1	C	120	PRO	CB-CG	-5.66	1.21	1.49
1	C	84	ALA	C-O	-5.65	1.20	1.24
1	C	174	TYR	C-O	-5.65	1.17	1.23
2	D	205	THR	C-O	-5.65	1.17	1.23
2	D	180	ALA	CA-CB	-5.64	1.44	1.53
2	D	158	PHE	CD1-CE1	-5.63	1.21	1.38
1	C	182	LEU	CG-CD2	-5.62	1.34	1.52
2	D	196	VAL	CA-CB	5.62	1.61	1.54
1	C	100	GLY	C-O	-5.61	1.16	1.23
1	C	78	LEU	C-O	-5.61	1.17	1.24
2	D	136	LEU	C-O	-5.61	1.17	1.23
1	C	21	LEU	C-O	-5.61	1.16	1.24
1	C	207	THR	N-CA	-5.60	1.40	1.46
1	C	63	SER	C-O	-5.59	1.17	1.23
2	D	34	MET	SD-CE	-5.57	1.65	1.79
1	C	132	SER	C-O	-5.57	1.17	1.24
1	C	185	ALA	N-CA	-5.56	1.39	1.46
2	D	206	TYR	C-O	-5.56	1.17	1.24
2	D	118	GLY	C-O	-5.56	1.16	1.23
1	C	52	SER	N-CA	-5.56	1.39	1.46
2	D	119	THR	C-O	-5.56	1.17	1.23
1	C	70	ASP	C-O	-5.54	1.17	1.24
2	D	197	PRO	CG-CD	-5.53	1.31	1.50
1	C	69	THR	C-O	-5.53	1.16	1.24
1	C	109	ARG	N-CA	-5.51	1.39	1.45
2	D	210	VAL	CA-CB	5.50	1.60	1.53
2	D	182	LEU	C-O	-5.49	1.17	1.24
1	C	73	LEU	C-O	-5.48	1.17	1.24
2	D	57	ASN	C-O	-5.48	1.17	1.24
1	C	2	ILE	C-O	-5.47	1.18	1.24
1	C	113	ALA	CA-CB	-5.47	1.44	1.53
1	C	181	THR	CA-CB	-5.46	1.44	1.53
1	C	140	PHE	C-O	-5.45	1.17	1.23
2	D	17	SER	C-O	-5.44	1.17	1.23
2	D	12	VAL	C-O	-5.43	1.17	1.23
1	C	120	PRO	C-O	-5.42	1.18	1.24
2	D	77	ASN	C-O	-5.40	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	100	GLY	C-O	-5.40	1.18	1.23
2	D	5	VAL	CA-C	-5.39	1.46	1.52
1	C	134	VAL	C-O	-5.38	1.18	1.24
2	D	47	TRP	C-O	-5.37	1.17	1.23
1	C	6	GLN	CA-C	-5.37	1.46	1.52
1	C	15	PRO	C-O	-5.35	1.17	1.23
1	C	20	THR	C-O	-5.35	1.18	1.24
1	C	208	LYS	C-O	-5.34	1.17	1.24
1	C	58	ILE	N-CA	-5.34	1.42	1.46
1	C	163	SER	C-O	-5.33	1.17	1.23
2	D	17	SER	CA-C	-5.32	1.46	1.52
1	C	150	LYS	CG-CD	-5.32	1.36	1.52
2	D	40	ALA	C-N	-5.30	1.29	1.33
1	C	133	VAL	CA-CB	-5.29	1.48	1.54
1	C	143	ARG	CB-CG	-5.29	1.36	1.52
1	C	200	GLN	C-O	-5.29	1.17	1.24
2	D	198	SER	C-O	-5.29	1.18	1.24
1	C	32	TYR	CD1-CE1	-5.28	1.22	1.38
1	C	70	ASP	N-CA	-5.28	1.40	1.46
2	D	176	HIS	C-O	-5.28	1.18	1.24
1	C	154	ALA	C-O	-5.26	1.17	1.24
2	D	158	PHE	CA-C	-5.26	1.46	1.52
2	D	2	VAL	CA-CB	-5.26	1.48	1.54
2	D	123	VAL	CB-CG1	-5.25	1.35	1.52
1	C	8	PRO	CB-CG	-5.25	1.30	1.51
1	C	123	ASP	C-O	-5.24	1.17	1.24
1	C	144	GLU	C-O	-5.23	1.17	1.24
2	D	19	ARG	C-O	-5.22	1.17	1.24
2	D	83	MET	SD-CE	-5.22	1.66	1.79
1	C	32	TYR	CD2-CE2	-5.20	1.23	1.38
1	C	26	SER	C-O	-5.19	1.17	1.24
2	D	83	MET	C-O	-5.19	1.17	1.23
2	D	6	GLU	N-CA	-5.19	1.39	1.45
2	D	58	LYS	C-O	-5.19	1.17	1.23
2	D	161	PRO	CA-CB	-5.18	1.44	1.53
1	C	83	PHE	C-O	-5.17	1.17	1.23
1	C	74	THR	C-O	-5.17	1.17	1.24
2	D	120	LEU	C-O	-5.15	1.17	1.24
1	C	22	SER	C-O	-5.15	1.17	1.24
1	C	206	VAL	C-O	-5.14	1.17	1.24
1	C	149	TRP	CA-C	-5.14	1.46	1.52
1	C	205	PRO	C-O	-5.14	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	SER	C-O	-5.14	1.17	1.24
1	C	191	LYS	CG-CD	-5.13	1.37	1.52
1	C	34	ALA	N-CA	-5.13	1.39	1.45
2	D	86	LEU	C-O	-5.12	1.17	1.23
2	D	159	PRO	CB-CG	-5.12	1.31	1.51
1	C	60	ALA	C-O	-5.11	1.17	1.24
2	D	167	ASN	C-O	-5.11	1.17	1.23
2	D	115	TRP	CA-C	-5.09	1.46	1.52
2	D	71	SER	C-O	-5.09	1.17	1.23
2	D	123	VAL	CA-CB	5.08	1.59	1.53
2	D	98	LYS	C-O	-5.07	1.18	1.24
2	D	9	GLY	C-O	-5.07	1.17	1.23
2	D	93	VAL	CA-CB	5.06	1.60	1.54
1	C	150	LYS	CB-CG	-5.05	1.37	1.52
1	C	139	ASN	CG-OD1	-5.04	1.14	1.23
2	D	215	SER	C-O	-5.04	1.17	1.24
1	C	118	ILE	CB-CG2	-5.02	1.35	1.52
2	D	97	ALA	C-O	-5.02	1.17	1.23
1	C	125	GLN	C-O	-5.01	1.18	1.24
2	D	71	SER	CA-C	-5.01	1.46	1.52
1	C	160	SER	CA-C	-5.01	1.46	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	113	ASP	N-CA-C	13.62	126.12	111.28
1	C	130	THR	N-CA-C	12.42	127.76	110.24
2	D	54	ASP	N-CA-C	-12.22	99.35	114.75
1	C	10	THR	N-CA-C	10.20	125.03	108.41
1	C	65	SER	N-CA-C	9.07	122.94	109.24
1	C	143	ARG	N-CA-C	8.89	121.05	111.36
1	C	149	TRP	N-CA-C	8.80	123.17	109.96
1	C	101	GLN	N-CA-C	8.78	123.54	113.01
1	C	118	ILE	N-CA-C	8.76	120.88	108.36
1	C	64	GLY	N-CA-C	8.72	124.24	110.90
2	D	181	VAL	N-CA-C	8.72	120.40	108.89
2	D	24	ALA	N-CA-C	8.69	123.57	109.76
1	C	164	VAL	N-CA-C	8.62	120.53	108.12
2	D	188	TYR	N-CA-C	8.49	122.85	110.28
1	C	3	VAL	N-CA-C	8.38	120.63	107.98
2	D	164	VAL	N-CA-C	8.35	120.50	108.48
1	C	51	ALA	N-CA-C	8.32	128.52	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	28	THR	N-CA-C	8.31	128.51	110.80
2	D	184	SER	N-CA-C	8.29	125.04	111.37
2	D	175	VAL	N-CA-C	8.23	120.72	108.54
2	D	190	LEU	N-CA-C	8.17	120.52	108.60
1	C	116	VAL	N-CA-C	8.14	119.64	107.75
2	D	97	ALA	N-CA-C	8.14	122.36	109.50
2	D	19	ARG	N-CA-C	7.97	121.72	108.73
1	C	134	VAL	N-CA-C	7.92	119.26	108.17
1	C	188	GLU	N-CA-C	7.86	124.33	111.37
1	C	32	TYR	N-CA-C	7.84	121.86	109.39
1	C	192	VAL	N-CA-C	7.79	119.51	108.36
1	C	25	ALA	N-CA-C	7.71	120.96	110.55
2	D	90	ASP	N-CA-C	-7.68	103.00	113.30
2	D	210	VAL	N-CA-C	7.68	118.73	107.37
1	C	35	TRP	N-CA-C	7.68	121.95	109.59
1	C	179	THR	N-CA-C	7.60	121.20	108.20
1	C	37	GLN	N-CA-C	7.54	120.95	108.96
2	D	30	SER	N-CA-C	-7.46	104.02	113.72
2	D	129	LYS	N-CA-C	7.44	121.47	108.75
1	C	144	GLU	N-CA-C	7.42	121.02	109.96
2	D	53	TYR	CA-CB-CG	7.37	127.17	113.90
2	D	50	VAL	N-CA-C	7.34	119.40	108.46
1	C	183	SER	N-CA-C	7.28	120.94	110.24
1	C	202	LEU	N-CA-C	7.27	121.09	109.24
1	C	115	SER	N-CA-C	7.20	126.14	110.80
1	C	201	GLY	N-CA-C	7.12	127.26	115.66
1	C	134	VAL	CB-CA-C	7.04	121.32	110.83
2	D	148	ALA	N-CA-C	7.03	120.99	109.24
1	C	119	PHE	N-CA-C	6.99	121.98	108.85
1	C	113	ALA	N-CA-C	6.97	119.52	109.48
1	C	194	ALA	N-CA-C	6.93	120.04	108.13
2	D	206	TYR	N-CA-C	6.90	120.10	108.02
2	D	149	ALA	N-CA-C	6.90	120.92	109.95
1	C	148	GLN	N-CA-C	6.88	119.62	108.41
2	D	65	LYS	N-CA-C	6.87	121.05	110.20
2	D	16	ARG	N-CA-C	6.87	121.47	109.80
1	C	138	ASN	N-CA-C	6.86	119.86	108.96
1	C	105	LEU	N-CA-C	6.74	119.26	108.41
2	D	115	TRP	N-CA-C	-6.74	99.07	109.52
1	C	112	ALA	N-CA-C	6.68	119.30	108.41
2	D	29	PHE	N-CA-C	-6.68	103.66	112.34
1	C	159	ASN	N-CA-C	6.67	125.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	N-CA-C	6.64	120.06	109.24
1	C	56	THR	N-CA-C	6.63	120.45	110.64
1	C	200	GLN	N-CA-C	6.61	124.87	110.80
1	C	204	SER	N-CA-C	6.60	117.72	110.13
2	D	62	ASP	N-CA-C	6.58	118.11	111.07
1	C	190	HIS	N-CA-C	6.56	120.73	110.17
1	C	72	THR	OG1-CB-CG2	-6.50	96.30	109.30
1	C	185	ALA	N-CA-C	6.49	118.90	111.11
1	C	4	LEU	N-CA-C	6.47	119.25	108.96
2	D	123	VAL	N-CA-C	6.43	115.98	106.85
1	C	60	ALA	N-CA-C	6.41	120.35	112.54
1	C	98	THR	N-CA-C	6.35	119.88	109.72
2	D	132	SER	N-CA-C	6.33	119.85	110.48
2	D	64	VAL	N-CA-C	6.28	120.94	113.22
1	C	3	VAL	CB-CA-C	6.18	117.91	111.23
2	D	78	THR	N-CA-C	6.17	119.62	108.69
2	D	160	GLU	N-CA-C	6.16	117.66	109.83
1	C	74	THR	N-CA-C	6.13	118.50	108.52
2	D	80	TYR	N-CA-C	6.12	119.38	109.40
1	C	184	LYS	N-CA-C	6.12	121.47	111.37
1	C	147	VAL	N-CA-C	6.11	117.38	108.58
2	D	198	SER	N-CA-C	6.06	117.89	111.28
2	D	182	LEU	N-CA-C	6.03	123.65	110.80
1	C	21	LEU	N-CA-C	6.02	119.21	109.40
1	C	66	GLY	N-CA-C	6.01	118.54	111.63
1	C	71	PHE	N-CA-C	6.01	119.27	109.24
1	C	209	SER	N-CA-C	5.99	118.17	109.07
2	D	205	THR	N-CA-C	5.98	118.94	109.96
1	C	81	GLU	N-CA-C	5.97	123.51	110.80
1	C	162	GLU	N-CA-C	5.97	118.93	109.50
1	C	117	PHE	N-CA-C	5.95	118.81	108.76
1	C	178	SER	N-CA-C	5.94	118.21	108.52
2	D	199	SER	N-CA-C	5.91	123.39	110.80
1	C	70	ASP	N-CA-C	5.89	118.50	108.02
1	C	26	SER	N-CA-C	-5.84	106.29	113.41
2	D	76	LYS	N-CA-C	5.80	119.33	112.72
1	C	160	SER	N-CA-C	5.76	118.85	109.06
1	C	5	THR	OG1-CB-CG2	-5.75	97.81	109.30
2	D	88	ALA	N-CA-C	5.67	122.89	110.80
1	C	78	LEU	N-CA-C	5.65	118.38	109.96
2	D	155	LYS	N-CA-C	5.62	119.41	109.96
2	D	134	PHE	N-CA-C	5.60	118.04	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	THR	N-CA-C	5.59	118.22	108.76
1	C	165	THR	N-CA-C	5.57	118.31	110.23
2	D	133	VAL	CB-CA-C	5.55	117.25	111.09
2	D	185	SER	N-CA-C	5.54	122.60	110.80
2	D	215	SER	N-CA-C	5.54	120.03	113.16
1	C	191	LYS	N-CA-C	5.52	119.74	111.96
1	C	46	LEU	N-CA-C	5.51	117.70	109.59
2	D	153	LEU	N-CA-C	5.49	117.60	108.20
1	C	63	SER	N-CA-C	5.46	117.57	108.99
1	C	176	LEU	N-CA-C	5.44	117.96	108.76
2	D	118	GLY	N-CA-C	5.44	118.38	112.29
1	C	76	SER	N-CA-C	5.43	118.24	111.24
1	C	84	ALA	N-CA-C	5.42	115.70	108.23
2	D	221	LYS	N-CA-C	5.39	117.20	108.41
2	D	32	TYR	N-CA-C	5.38	122.25	110.80
1	C	180	LEU	N-CA-C	5.36	117.04	108.41
2	D	20	LEU	N-CA-C	5.32	118.73	110.17
2	D	176	HIS	N-CA-C	5.30	117.30	108.02
2	D	21	SER	N-CA-C	5.29	118.19	109.72
1	C	120	PRO	N-CD-CG	-5.29	95.27	103.20
1	C	153	ASN	N-CA-C	5.25	120.86	113.56
1	C	125	GLN	N-CA-C	-5.24	105.65	111.36
2	D	49	ALA	N-CA-C	5.21	116.76	108.79
2	D	213	LYS	N-CA-C	5.19	120.52	113.16
1	C	31	SER	N-CA-C	5.17	119.69	113.17
2	D	78	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	C	7	SER	N-CA-C	5.15	117.97	109.58
2	D	3	GLN	N-CA-C	5.11	117.78	109.24
1	C	127	LYS	CB-CA-C	-5.11	101.14	109.56
1	C	211	ASN	N-CA-C	5.08	116.92	107.99
2	D	196	VAL	N-CA-CB	5.07	118.30	111.21
1	C	30	SER	N-CA-C	5.05	117.11	108.67
2	D	171	LEU	N-CA-C	5.05	116.97	109.25
2	D	183	GLN	N-CA-C	5.03	121.51	110.80
2	D	81	LEU	N-CA-C	5.02	116.81	108.02

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	51	ALA	CA
1	C	115	SER	CA
1	C	123	ASP	CA

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Mol	Chain	Res	Type	Atom
1	C	130	THR	CA
2	D	28	THR	CA
2	D	113	ASP	CA
2	D	147	THR	CA
2	D	183	GLN	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	114	PRO	Peptide
1	C	122	SER	Peptide
1	C	129	GLY	Peptide
1	C	181	THR	Peptide
1	C	51	ALA	Peptide
1	C	54	ARG	Peptide
1	C	80	PRO	Peptide
1	C	99	PHE	Peptide
2	D	10	GLY	Peptide
2	D	131	PRO	Peptide
2	D	155	LYS	Peptide
2	D	181	VAL	Peptide
2	D	182	LEU	Peptide
2	D	184	SER	Peptide
2	D	198	SER	Peptide
2	D	199	SER	Peptide
2	D	202	GLY	Peptide
2	D	29	PHE	Peptide
2	D	52	SER	Peptide
2	D	53	TYR	Peptide
2	D	75	SER	Peptide
2	D	9	GLY	Peptide

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	C	1638	0	1597	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1568	0	1539	73	5
3	C	55	0	0	5	0
3	D	33	0	0	2	0
All	All	3294	0	3136	168	5

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 26.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:HB3	1:C:173:THR:OG1	1.50	1.11
1:C:130:THR:HG22	1:C:131:ALA:H	0.94	1.05
1:C:127:LYS:N	1:C:127:LYS:HD2	1.73	1.03
1:C:130:THR:HG22	1:C:131:ALA:N	1.74	0.97
2:D:67:ARG:NH2	2:D:90:ASP:OD2	1.96	0.96
1:C:130:THR:CG2	1:C:131:ALA:H	1.81	0.94
1:C:126:LEU:O	1:C:184:LYS:HD2	1.72	0.89
1:C:12:SER:OG	1:C:106:GLU:OE2	1.91	0.87
2:D:53:TYR:HB3	2:D:54:ASP:CB	2.05	0.87
2:D:36:TRP:NE1	2:D:79:LEU:HD11	1.91	0.86
1:C:127:LYS:C	1:C:129:GLY:H	1.81	0.85
2:D:36:TRP:CE2	2:D:79:LEU:HD11	2.11	0.85
1:C:29:VAL:O	1:C:29:VAL:HG22	1.79	0.80
2:D:87:ARG:CD	2:D:89:GLU:OE2	2.30	0.80
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.64	0.79
2:D:177:THR:OG1	2:D:192:SER:OG	1.94	0.79
2:D:36:TRP:CE2	2:D:79:LEU:CD1	2.64	0.79
1:C:127:LYS:N	1:C:127:LYS:CD	2.30	0.79
1:C:126:LEU:O	1:C:184:LYS:CD	2.31	0.78
2:D:200:SER:O	2:D:201:LEU:HB2	1.83	0.78
1:C:29:VAL:HG23	1:C:92:SER:HB2	1.64	0.78
1:C:171:ASP:CB	1:C:173:THR:OG1	2.30	0.77
2:D:87:ARG:HD3	2:D:89:GLU:OE2	1.85	0.77
2:D:28:THR:C	2:D:30:SER:H	1.89	0.77
2:D:67:ARG:HH22	2:D:90:ASP:CG	1.93	0.76
2:D:36:TRP:CZ2	2:D:79:LEU:HD13	2.22	0.75
2:D:12:VAL:HG11	2:D:86:LEU:HD13	1.68	0.75
2:D:199:SER:C	2:D:200:SER:O	2.28	0.75
2:D:53:TYR:HB3	2:D:54:ASP:HB2	1.68	0.75
2:D:200:SER:O	2:D:201:LEU:CB	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ARG:NH2	3:C:252:HOH:O	2.20	0.73
1:C:29:VAL:O	1:C:29:VAL:CG2	2.36	0.73
2:D:12:VAL:HG12	2:D:123:VAL:HG22	1.70	0.73
1:C:156:GLN:HB3	1:C:159:ASN:HD21	1.52	0.72
1:C:107:ILE:H	1:C:167:GLN:HE22	1.38	0.72
2:D:54:ASP:OD2	2:D:56:SER:HB2	1.90	0.72
2:D:67:ARG:HB3	2:D:84:ASN:O	1.91	0.71
2:D:36:TRP:CZ2	2:D:79:LEU:CD1	2.74	0.70
1:C:15:PRO:HD3	1:C:83:PHE:CZ	2.26	0.70
2:D:36:TRP:NE1	2:D:79:LEU:CD1	2.56	0.67
1:C:202:LEU:O	1:C:203:SER:C	2.35	0.67
2:D:87:ARG:HD2	2:D:89:GLU:OE2	1.93	0.67
2:D:29:PHE:O	2:D:72:ARG:NH2	2.27	0.66
2:D:13:GLN:OE1	2:D:16:ARG:NH2	2.29	0.66
2:D:129:LYS:HG3	2:D:130:GLY:N	2.11	0.65
1:C:125:GLN:O	1:C:127:LYS:N	2.30	0.65
2:D:28:THR:O	2:D:30:SER:N	2.30	0.65
2:D:53:TYR:HB3	2:D:54:ASP:HB3	1.79	0.64
1:C:127:LYS:C	1:C:129:GLY:N	2.44	0.64
1:C:21:LEU:HB2	1:C:73:LEU:HB3	1.81	0.63
1:C:29:VAL:HG23	1:C:92:SER:CB	2.29	0.63
1:C:123:ASP:O	1:C:127:LYS:HD3	2.00	0.62
2:D:196:VAL:HB	2:D:197:PRO:HD2	1.81	0.62
2:D:196:VAL:HB	2:D:197:PRO:CD	2.29	0.62
2:D:54:ASP:OD2	2:D:56:SER:CB	2.47	0.62
1:C:126:LEU:C	1:C:127:LYS:HD2	2.26	0.61
1:C:38:GLN:NE2	1:C:44:PRO:HD3	2.16	0.60
1:C:38:GLN:HE21	1:C:44:PRO:HD3	1.66	0.60
1:C:83:PHE:CE1	1:C:107:ILE:HG13	2.35	0.60
1:C:130:THR:CG2	1:C:131:ALA:N	2.49	0.60
1:C:144:GLU:H	1:C:144:GLU:CD	2.10	0.59
1:C:104:ARG:NH1	3:C:263:HOH:O	2.35	0.59
1:C:116:VAL:HG12	1:C:208:LYS:HG2	1.83	0.59
1:C:116:VAL:HG12	1:C:208:LYS:CG	2.32	0.59
1:C:90:GLN:OE1	1:C:98:THR:OG1	2.21	0.58
2:D:52:SER:O	2:D:53:TYR:C	2.45	0.58
2:D:52:SER:O	2:D:54:ASP:N	2.37	0.58
1:C:117:PHE:HB2	1:C:136:LEU:HB3	1.84	0.58
1:C:85:VAL:HG22	1:C:104:ARG:HB2	1.85	0.57
1:C:150:LYS:HG2	1:C:153:ASN:HA	1.85	0.57
2:D:53:TYR:CG	2:D:54:ASP:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:TYR:CE1	2:D:70:ILE:HG22	2.39	0.57
2:D:52:SER:C	2:D:54:ASP:N	2.63	0.56
1:C:15:PRO:HD3	1:C:83:PHE:HZ	1.68	0.56
2:D:199:SER:OG	2:D:200:SER:N	2.28	0.55
2:D:62:ASP:HA	2:D:65:LYS:HD2	1.89	0.55
1:C:30:SER:OG	1:C:31:SER:N	2.30	0.55
1:C:83:PHE:CD1	1:C:107:ILE:HG13	2.43	0.54
1:C:35:TRP:CE3	1:C:73:LEU:HD22	2.42	0.54
1:C:124:GLU:O	1:C:124:GLU:HG3	2.06	0.54
2:D:47:TRP:HZ2	2:D:50:VAL:HG12	1.73	0.53
1:C:197:VAL:HB	1:C:206:VAL:HG23	1.91	0.53
2:D:53:TYR:CB	2:D:54:ASP:HB2	2.36	0.53
1:C:37:GLN:HG3	1:C:86:TYR:CE1	2.44	0.52
1:C:125:GLN:C	1:C:127:LYS:H	2.16	0.52
1:C:168:ASP:CG	1:C:171:ASP:HB2	2.35	0.52
1:C:11:LEU:HB3	1:C:105:LEU:HG	1.92	0.52
1:C:197:VAL:HB	1:C:206:VAL:CG2	2.40	0.52
1:C:168:ASP:HB3	1:C:173:THR:H	1.74	0.52
1:C:61:ARG:O	1:C:75:ILE:HA	2.10	0.51
1:C:125:GLN:NE2	1:C:132:SER:H	2.08	0.51
1:C:125:GLN:HE22	1:C:132:SER:H	1.57	0.51
2:D:22:CYS:HB3	2:D:79:LEU:HD12	1.93	0.51
2:D:52:SER:C	2:D:54:ASP:H	2.19	0.51
2:D:22:CYS:N	2:D:79:LEU:O	2.43	0.51
2:D:36:TRP:CE2	2:D:79:LEU:HD13	2.43	0.51
2:D:199:SER:O	2:D:200:SER:C	2.53	0.51
2:D:29:PHE:HB3	2:D:77:ASN:OD1	2.11	0.50
1:C:182:LEU:HD13	1:C:187:TYR:HB2	1.94	0.50
1:C:124:GLU:O	1:C:127:LYS:HG2	2.11	0.50
1:C:141:TYR:CG	1:C:142:PRO:HA	2.46	0.50
2:D:129:LYS:O	2:D:212:HIS:CE1	2.64	0.50
1:C:144:GLU:O	3:C:251:HOH:O	2.20	0.49
1:C:55:ALA:HB3	1:C:58:ILE:HG13	1.95	0.49
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.48	0.49
2:D:129:LYS:O	2:D:212:HIS:HE1	1.96	0.48
2:D:51:ILE:HB	2:D:70:ILE:HG12	1.93	0.48
2:D:135:PRO:HD3	2:D:221:LYS:HE2	1.96	0.48
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.95	0.48
2:D:54:ASP:OD2	2:D:56:SER:OG	2.30	0.48
2:D:165:SER:HB3	2:D:209:ASN:OD1	2.14	0.48
1:C:94:TRP:HB2	1:C:95:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:NE2	1:C:93:ASN:O	2.47	0.47
2:D:151:GLY:HA2	2:D:166:TRP:CH2	2.48	0.47
1:C:62:PHE:CE1	1:C:75:ILE:HD13	2.49	0.47
1:C:168:ASP:O	1:C:172:SER:HA	2.14	0.47
1:C:90:GLN:HE21	1:C:93:ASN:H	1.63	0.47
1:C:116:VAL:HA	1:C:136:LEU:O	2.15	0.47
1:C:165:THR:HG23	2:D:178:PHE:CE2	2.50	0.47
1:C:54:ARG:HG2	1:C:58:ILE:HB	1.97	0.46
1:C:164:VAL:HG22	1:C:176:LEU:HB2	1.96	0.46
1:C:124:GLU:O	1:C:124:GLU:CG	2.62	0.46
1:C:21:LEU:O	1:C:72:THR:HA	2.17	0.45
2:D:79:LEU:HD22	2:D:80:TYR:N	2.32	0.45
1:C:34:ALA:O	1:C:88:CYS:HA	2.16	0.45
1:C:124:GLU:O	1:C:127:LYS:CG	2.65	0.45
1:C:8:PRO:O	1:C:103:THR:HG23	2.17	0.45
1:C:202:LEU:HB2	1:C:204:SER:O	2.17	0.45
1:C:114:PRO:HD3	1:C:140:PHE:HB2	1.99	0.44
2:D:151:GLY:HA2	2:D:166:TRP:CZ2	2.52	0.44
1:C:116:VAL:CG1	1:C:208:LYS:HG2	2.47	0.44
1:C:90:GLN:HG2	1:C:92:SER:H	1.83	0.44
2:D:6:GLU:CD	2:D:118:GLY:H	2.22	0.44
1:C:139:ASN:HB3	1:C:173:THR:HG21	1.99	0.43
2:D:158:PHE:HA	2:D:159:PRO:HA	1.66	0.43
1:C:116:VAL:HG12	1:C:208:LYS:HG3	1.99	0.43
2:D:32:TYR:CE2	2:D:101:LYS:HD2	2.54	0.43
1:C:127:LYS:HE2	1:C:127:LYS:HB3	1.64	0.43
1:C:137:LEU:HD22	1:C:176:LEU:HG	1.99	0.43
2:D:29:PHE:CB	2:D:77:ASN:OD1	2.65	0.43
2:D:22:CYS:CB	2:D:79:LEU:HD12	2.49	0.43
2:D:149:ALA:HB2	2:D:195:THR:HG22	2.01	0.43
2:D:60:TYR:CZ	2:D:70:ILE:HG22	2.54	0.43
2:D:156:ASP:HB3	2:D:187:LEU:HD13	2.01	0.42
1:C:80:PRO:HA	1:C:83:PHE:HD2	1.84	0.42
1:C:127:LYS:H	1:C:127:LYS:HG2	1.36	0.42
2:D:22:CYS:HB3	2:D:79:LEU:HB3	2.02	0.42
2:D:28:THR:O	2:D:29:PHE:C	2.61	0.42
2:D:207:ILE:HG12	2:D:222:LYS:HA	2.02	0.42
1:C:155:LEU:HD12	1:C:156:GLN:N	2.35	0.41
1:C:165:THR:HG1	1:C:175:SER:H	1.68	0.41
2:D:30:SER:HB2	3:D:273:HOH:O	2.20	0.41
2:D:160:GLU:HA	2:D:161:PRO:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:NE	1:C:79:GLU:HG2	2.35	0.41
1:C:200:GLN:NE2	3:C:226:HOH:O	2.35	0.41
1:C:196:GLU:HG3	1:C:207:THR:OG1	2.19	0.41
1:C:91:ARG:NH1	2:D:109:SER:HB2	2.36	0.41
1:C:181:THR:HG22	1:C:182:LEU:N	2.36	0.41
2:D:183:GLN:H	2:D:183:GLN:HG3	1.40	0.41
1:C:58:ILE:HA	1:C:59:PRO:HD3	1.90	0.41
1:C:162:GLU:HB3	3:C:243:HOH:O	2.21	0.41
2:D:113:ASP:C	2:D:114:TYR:CD2	2.99	0.41
1:C:116:VAL:HG21	1:C:206:VAL:HG21	2.02	0.40
1:C:164:VAL:HG22	1:C:176:LEU:CB	2.52	0.40
2:D:124:SER:OG	3:D:255:HOH:O	2.17	0.40
1:C:126:LEU:O	1:C:184:LYS:HD3	2.17	0.40
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.85	0.40
1:C:182:LEU:HD22	1:C:183:SER:N	2.37	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:TYR:OH	2:D:216:ASN:ND2[4_546]	0.45	1.75
2:D:53:TYR:OH	2:D:216:ASN:CG[4_546]	1.12	1.08
2:D:53:TYR:CZ	2:D:216:ASN:ND2[4_546]	1.27	0.93
2:D:53:TYR:OH	2:D:216:ASN:OD1[4_546]	1.82	0.38
2:D:53:TYR:CE1	2:D:216:ASN:ND2[4_546]	2.00	0.20

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	C	210/216 (97%)	180 (86%)	22 (10%)	8 (4%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	202/242 (84%)	180 (89%)	11 (5%)	11 (5%)	1	1
All	All	412/458 (90%)	360 (87%)	33 (8%)	19 (5%)	2	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	GLU
1	C	123	ASP
2	D	28	THR
2	D	53	TYR
2	D	88	ALA
2	D	183	GLN
2	D	199	SER
2	D	200	SER
1	C	115	SER
1	C	200	GLN
2	D	185	SER
2	D	201	LEU
2	D	203	THR
1	C	126	LEU
1	C	203	SER
1	C	139	ASN
2	D	156	ASP
1	C	44	PRO
2	D	161	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	C	185/188 (98%)	135 (73%)	50 (27%)	0	0
2	D	174/202 (86%)	133 (76%)	41 (24%)	1	1
All	All	359/390 (92%)	268 (75%)	91 (25%)	0	1

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	LEU
1	C	7	SER
1	C	10	THR
1	C	13	LEU
1	C	18	ARG
1	C	20	THR
1	C	22	SER
1	C	29	VAL
1	C	31	SER
1	C	33	LEU
1	C	54	ARG
1	C	67	SER
1	C	70	ASP
1	C	74	THR
1	C	75	ILE
1	C	77	SER
1	C	81	GLU
1	C	93	ASN
1	C	97	ILE
1	C	101	GLN
1	C	104	ARG
1	C	105	LEU
1	C	110	THR
1	C	127	LYS
1	C	128	SER
1	C	130	THR
1	C	133	VAL
1	C	134	VAL
1	C	138	ASN
1	C	143	ARG
1	C	144	GLU
1	C	146	LYS
1	C	148	GLN
1	C	150	LYS
1	C	155	LEU
1	C	157	SER
1	C	159	ASN
1	C	163	SER
1	C	167	GLN
1	C	170	LYS
1	C	171	ASP
1	C	173	THR
1	C	176	LEU

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Mol	Chain	Res	Type
1	C	182	LEU
1	C	183	SER
1	C	189	LYS
1	C	191	LYS
1	C	200	GLN
1	C	202	LEU
1	C	207	THR
2	D	1	GLN
2	D	12	VAL
2	D	16	ARG
2	D	18	LEU
2	D	20	LEU
2	D	25	SER
2	D	28	THR
2	D	31	SER
2	D	35	HIS
2	D	43	LYS
2	D	51	ILE
2	D	64	VAL
2	D	65	LYS
2	D	72	ARG
2	D	75	SER
2	D	76	LYS
2	D	78	THR
2	D	79	LEU
2	D	85	SER
2	D	87	ARG
2	D	109	SER
2	D	124	SER
2	D	127	SER
2	D	129	LYS
2	D	132	SER
2	D	150	LEU
2	D	154	VAL
2	D	162	VAL
2	D	164	VAL
2	D	165	SER
2	D	172	THR
2	D	182	LEU
2	D	183	GLN
2	D	184	SER
2	D	188	TYR

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Mol	Chain	Res	Type
2	D	190	LEU
2	D	192	SER
2	D	200	SER
2	D	205	THR
2	D	209	ASN
2	D	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN
1	C	38	GLN
1	C	125	GLN
1	C	148	GLN
1	C	153	ASN
1	C	156	GLN
1	C	159	ASN
1	C	167	GLN
1	C	190	HIS
1	C	211	ASN
2	D	39	GLN
2	D	82	GLN
2	D	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	C	212/216 (98%)	0.31	6 (2%) 55 51	8, 20, 31, 39	0
2	D	208/242 (85%)	0.65	22 (10%) 11 8	11, 24, 41, 48	0
All	All	420/458 (91%)	0.47	28 (6%) 24 20	8, 22, 39, 48	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	TYR	4.6
2	D	199	SER	3.8
2	D	201	LEU	3.5
1	C	129	GLY	3.3
2	D	87	ARG	2.9
2	D	28	THR	2.7
2	D	2	VAL	2.7
1	C	127	LYS	2.7
2	D	216	ASN	2.7
2	D	76	LYS	2.6
1	C	32	TYR	2.6
2	D	25	SER	2.5
2	D	200	SER	2.5
2	D	203	THR	2.4
2	D	22	CYS	2.4
2	D	78	THR	2.2
2	D	101	LYS	2.2
2	D	30	SER	2.2
1	C	124	GLU	2.1
2	D	117	GLN	2.1
2	D	42	GLY	2.1
2	D	66	GLY	2.1
2	D	202	GLY	2.1
2	D	114	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	75	SER	2.1
1	C	5	THR	2.1
2	D	214	PRO	2.0
1	C	128	SER	2.0

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.