



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2026 – 04:37 am BST

PDB ID : 9TVR / pdb_00009tvr
Title : FgFR4-D2 domain in complex with Fab 4012
Authors : Mathieu, M.; Pouzieux, S.
Deposited on : 2026-01-13
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.2
Xtriage (Phenix) : 2.2
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

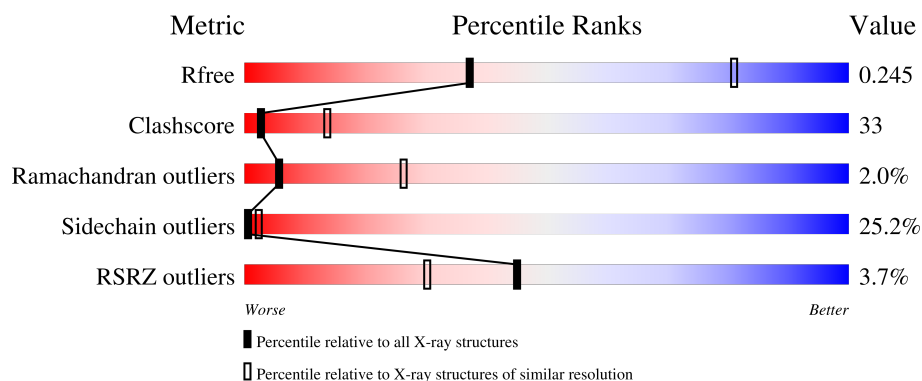
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	213	8% 40% 45% 15%
1	D	213	9% 37% 49% 14%
1	G	213	3% 39% 44% 15% .
1	J	213	2% 37% 47% 15% .
2	B	221	3% 36% 45% 16% .

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Mol	Chain	Length	Quality of chain
2	E	221	7%38%43%15% . .
2	H	221	%39%46%13% .
2	K	221	%39%45%13% . .
3	C	114	33%32%17%18%
3	F	114	32%36%13%18%
3	I	114	33%36%12%18%
3	L	114	2%32%34%13% . 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16147 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 Fab 4012 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1665	1037	282	340	6			
1	D	213	Total	C	N	O	S	0	0	0
			1665	1037	282	340	6			
1	G	213	Total	C	N	O	S	0	0	0
			1665	1037	282	340	6			
1	J	211	Total	C	N	O	S	0	0	0
			1648	1028	279	335	6			

- Molecule 2 is a protein called Fab 4012 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1627	1033	264	324	6			
2	E	213	Total	C	N	O	S	0	0	0
			1623	1031	263	323	6			
2	H	216	Total	C	N	O	S	0	0	0
			1638	1039	266	327	6			
2	K	216	Total	C	N	O	S	0	0	0
			1638	1039	266	327	6			

- Molecule 3 is a protein called Fibroblast growth factor receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	94	Total	C	N	O	S	0	0	0
			753	480	136	133	4			
3	F	93	Total	C	N	O	S	0	0	0
			745	474	135	132	4			
3	I	93	Total	C	N	O	S	0	0	0
			745	474	135	132	4			
3	L	92	Total	C	N	O	S	0	0	0
			735	468	132	131	4			

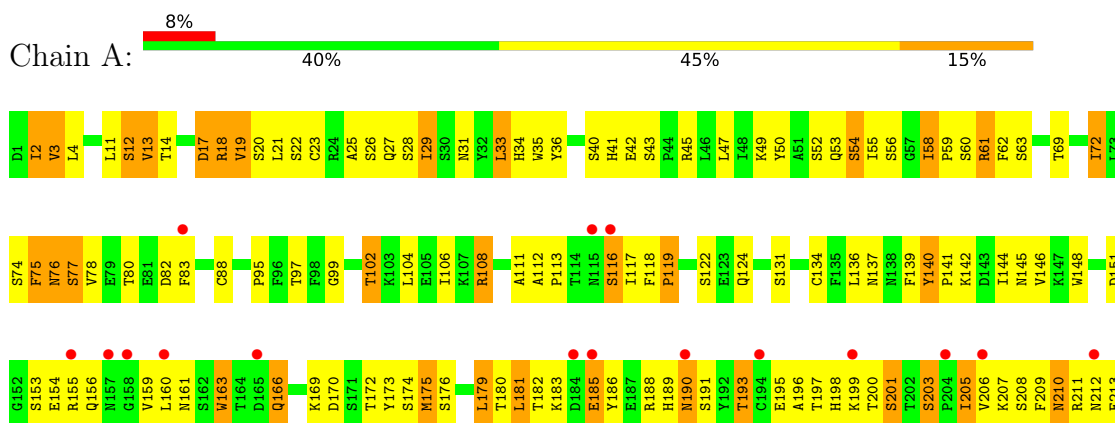
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P22455
C	107	LEU	-	expression tag	UNP P22455
C	108	GLU	-	expression tag	UNP P22455
C	109	HIS	-	expression tag	UNP P22455
C	110	HIS	-	expression tag	UNP P22455
C	111	HIS	-	expression tag	UNP P22455
C	112	HIS	-	expression tag	UNP P22455
C	113	HIS	-	expression tag	UNP P22455
C	114	HIS	-	expression tag	UNP P22455
F	1	MET	-	initiating methionine	UNP P22455
F	107	LEU	-	expression tag	UNP P22455
F	108	GLU	-	expression tag	UNP P22455
F	109	HIS	-	expression tag	UNP P22455
F	110	HIS	-	expression tag	UNP P22455
F	111	HIS	-	expression tag	UNP P22455
F	112	HIS	-	expression tag	UNP P22455
F	113	HIS	-	expression tag	UNP P22455
F	114	HIS	-	expression tag	UNP P22455
I	1	MET	-	initiating methionine	UNP P22455
I	107	LEU	-	expression tag	UNP P22455
I	108	GLU	-	expression tag	UNP P22455
I	109	HIS	-	expression tag	UNP P22455
I	110	HIS	-	expression tag	UNP P22455
I	111	HIS	-	expression tag	UNP P22455
I	112	HIS	-	expression tag	UNP P22455
I	113	HIS	-	expression tag	UNP P22455
I	114	HIS	-	expression tag	UNP P22455
L	1	MET	-	initiating methionine	UNP P22455
L	107	LEU	-	expression tag	UNP P22455
L	108	GLU	-	expression tag	UNP P22455
L	109	HIS	-	expression tag	UNP P22455
L	110	HIS	-	expression tag	UNP P22455
L	111	HIS	-	expression tag	UNP P22455
L	112	HIS	-	expression tag	UNP P22455
L	113	HIS	-	expression tag	UNP P22455
L	114	HIS	-	expression tag	UNP P22455

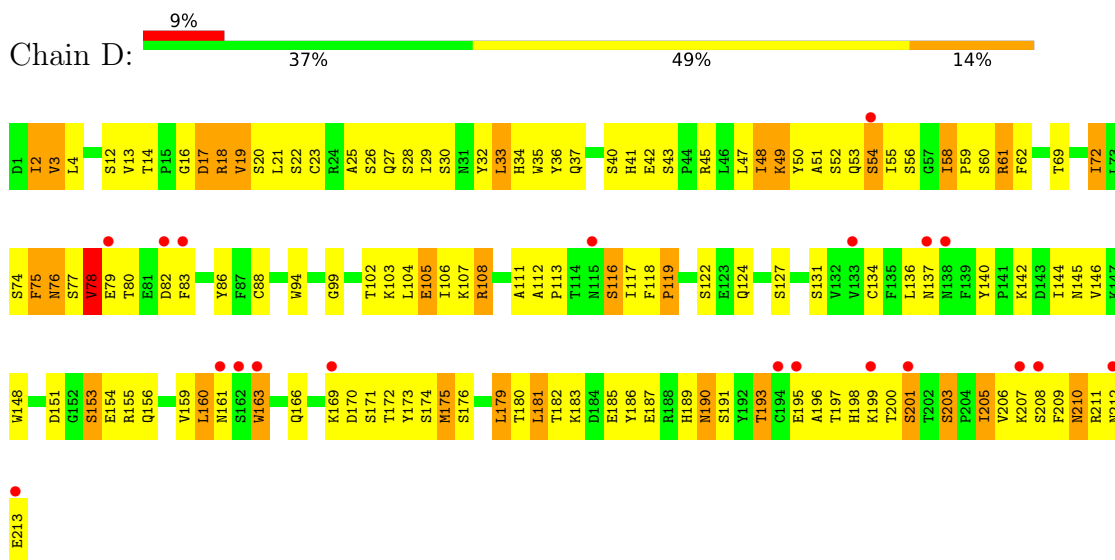
3 Residue-property plots

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.

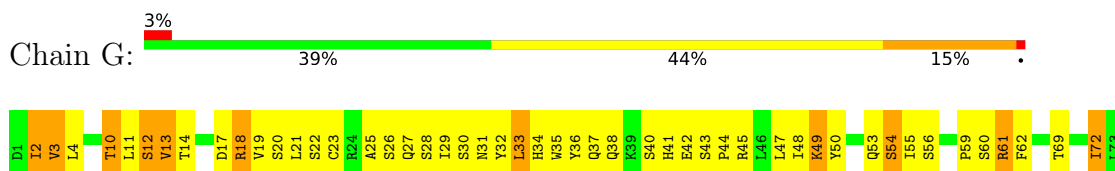
• Molecule 1: Fab 4012 Light chain

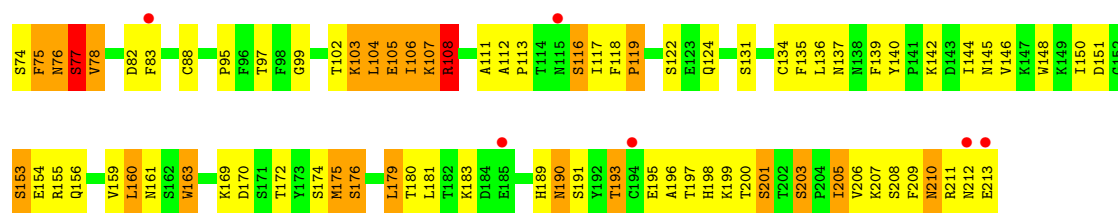


• Molecule 1: Fab 4012 Light chain

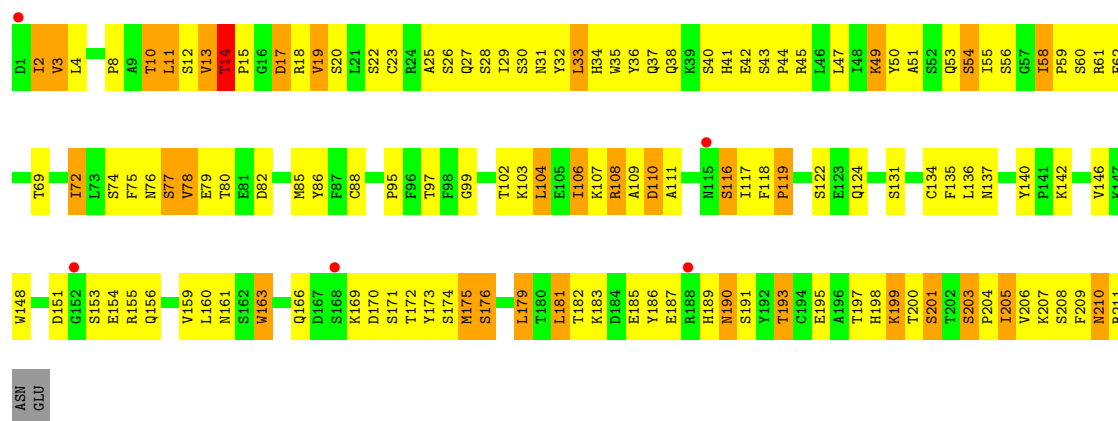


• Molecule 1: Fab 4012 Light chain

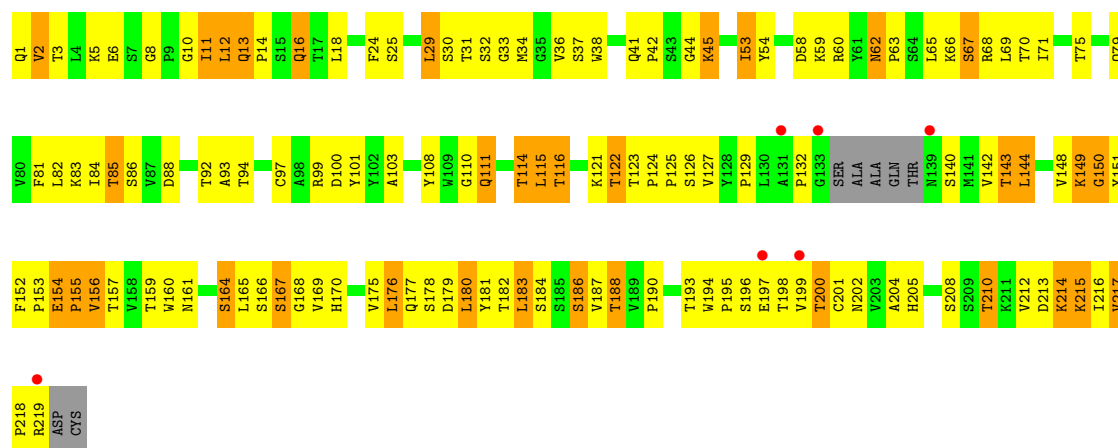




• Molecule 1: Fab 4012 Light chain

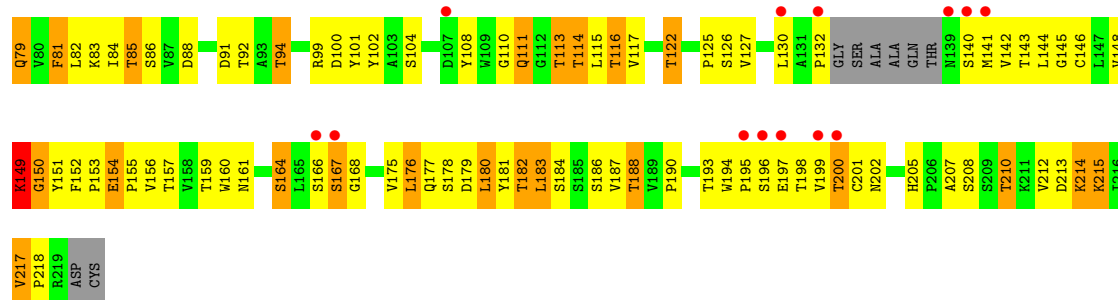


• Molecule 2: Fab 4012 Heavy Chain

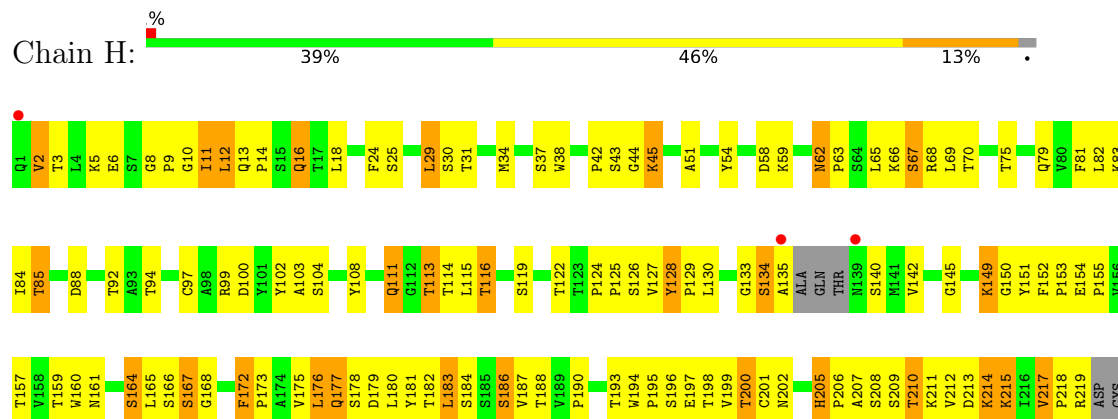


• Molecule 2: Fab 4012 Heavy Chain

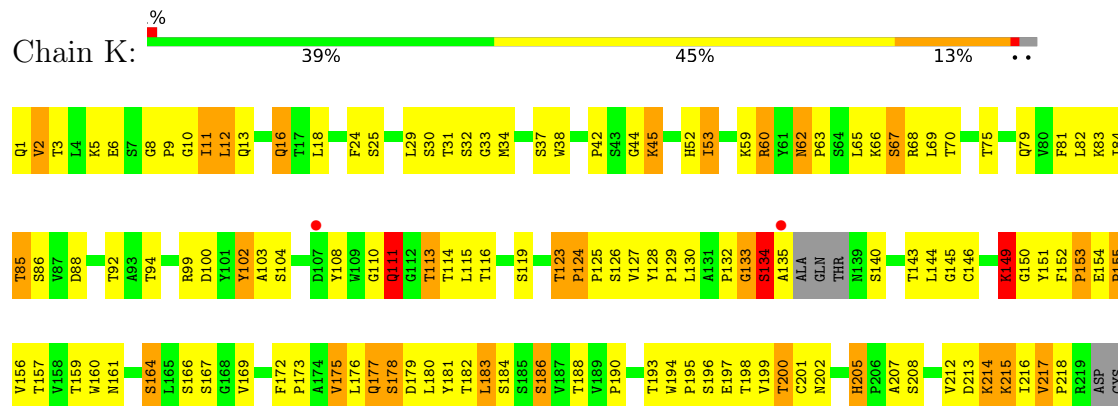




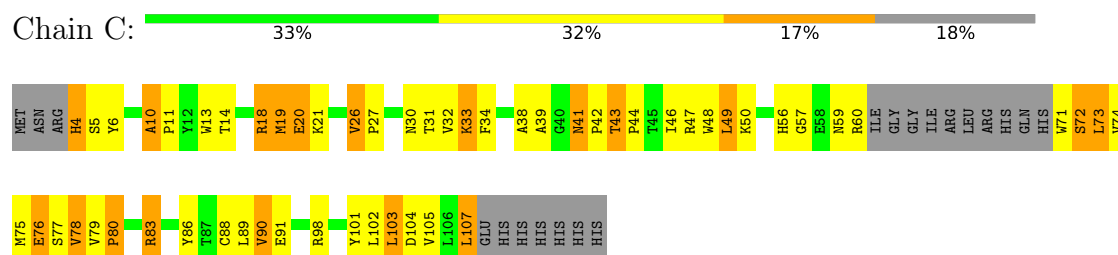
• Molecule 2: Fab 4012 Heavy Chain

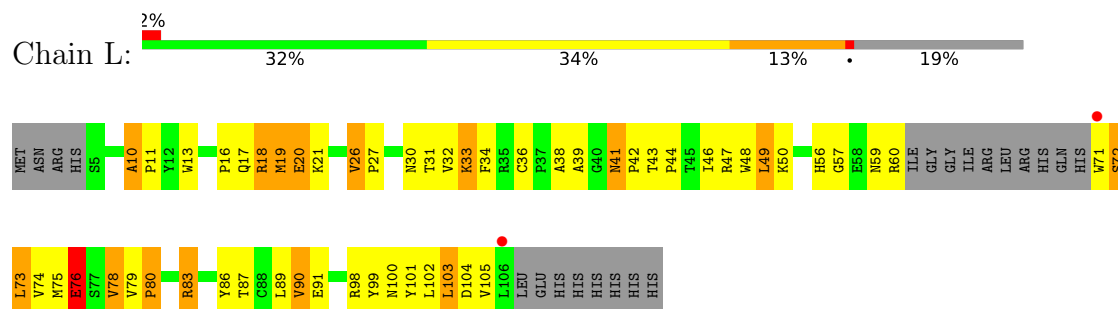


• Molecule 2: Fab 4012 Heavy Chain



• Molecule 3: Fibroblast growth factor receptor 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.54Å 121.64Å 319.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.66 – 3.25 113.66 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.6 (113.66-3.25) 97.8 (113.66-3.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.5.1	Depositor
R, R_{free}	(Not available) , 0.233 0.208 , 0.245	Depositor DCC
R_{free} test set	3392 reflections (7.72%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16147	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1705	0.94	7/2313 (0.3%)
1	D	0.39	0/1705	0.89	4/2313 (0.2%)
1	G	0.45	0/1705	0.96	7/2313 (0.3%)
1	J	0.47	0/1688	0.99	9/2290 (0.4%)
2	B	0.48	0/1671	1.06	12/2287 (0.5%)
2	E	0.43	0/1667	1.01	11/2282 (0.5%)
2	H	0.48	0/1682	1.10	19/2302 (0.8%)
2	K	0.50	0/1682	1.17	20/2302 (0.9%)
3	C	0.62	0/776	1.03	4/1058 (0.4%)
3	F	0.56	0/768	1.03	5/1047 (0.5%)
3	I	0.57	0/768	1.03	2/1047 (0.2%)
3	L	0.56	0/757	1.01	5/1032 (0.5%)
All	All	0.48	0/16574	1.02	105/22586 (0.5%)

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	8	GLY	CA-C-N	11.86	133.22	119.47
2	K	8	GLY	C-N-CA	11.86	133.22	119.47
2	E	8	GLY	CA-C-N	11.11	132.35	119.47
2	E	8	GLY	C-N-CA	11.11	132.35	119.47
2	K	123	THR	CA-C-N	-10.81	111.88	119.66

There are no chirality outliers.

There are no planarity outliers.

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	1665	0	1580	96	0
1	D	1665	0	1580	131	0
1	G	1665	0	1580	110	0
1	J	1648	0	1568	131	0
2	B	1627	0	1591	100	0
2	E	1623	0	1588	128	0
2	H	1638	0	1601	89	0
2	K	1638	0	1601	102	0
3	C	753	0	731	58	0
3	F	745	0	720	56	0
3	I	745	0	720	49	0
3	L	735	0	713	49	0
All	All	16147	0	15573	1060	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 33.

The worst 5 of 1060 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:THR:HG23	2:H:116:THR:HA	1.20	1.18
1:J:11:LEU:HD11	1:J:13:VAL:HG12	1.21	1.17
2:K:92:THR:HG23	2:K:116:THR:HA	1.19	1.16
1:D:47:LEU:HD23	1:D:58:ILE:HD12	1.25	1.15
1:J:49:LYS:HG2	1:J:55:ILE:HD11	1.16	1.13

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	211/213 (99%)	197 (93%)	12 (6%)	2 (1%)	14	42
1	D	211/213 (99%)	195 (92%)	13 (6%)	3 (1%)	9	33
1	G	211/213 (99%)	196 (93%)	14 (7%)	1 (0%)	24	55
1	J	209/213 (98%)	193 (92%)	14 (7%)	2 (1%)	12	40
2	B	210/221 (95%)	188 (90%)	13 (6%)	9 (4%)	2	13
2	E	209/221 (95%)	185 (88%)	17 (8%)	7 (3%)	3	18
2	H	212/221 (96%)	187 (88%)	19 (9%)	6 (3%)	4	20
2	K	212/221 (96%)	191 (90%)	14 (7%)	7 (3%)	3	18
3	C	90/114 (79%)	86 (96%)	3 (3%)	1 (1%)	11	38
3	F	89/114 (78%)	83 (93%)	5 (6%)	1 (1%)	11	38
3	I	89/114 (78%)	85 (96%)	3 (3%)	1 (1%)	11	38
3	L	88/114 (77%)	85 (97%)	2 (2%)	1 (1%)	11	38
All	All	2041/2192 (93%)	1871 (92%)	129 (6%)	41 (2%)	6	26

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	122	THR
1	D	17	ASP
1	D	78	VAL
2	H	134	SER
2	B	150	GLY

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	193/193 (100%)	145 (75%)	48 (25%)	0	2
1	D	193/193 (100%)	145 (75%)	48 (25%)	0	2
1	G	193/193 (100%)	143 (74%)	50 (26%)	0	2
1	J	191/193 (99%)	146 (76%)	45 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	190/195 (97%)	133 (70%)	57 (30%)	0	1
2	E	190/195 (97%)	139 (73%)	51 (27%)	0	2
2	H	191/195 (98%)	147 (77%)	44 (23%)	1	3
2	K	191/195 (98%)	145 (76%)	46 (24%)	1	3
3	C	81/99 (82%)	62 (76%)	19 (24%)	1	3
3	F	80/99 (81%)	60 (75%)	20 (25%)	0	2
3	I	80/99 (81%)	62 (78%)	18 (22%)	1	4
3	L	79/99 (80%)	59 (75%)	20 (25%)	0	2
All	All	1852/1948 (95%)	1386 (75%)	466 (25%)	0	2

5 of 466 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	43	THR
2	K	202	ASN
1	G	193	THR
2	K	188	THR
1	J	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	4	HIS
1	J	156	GLN
3	I	30	ASN
1	J	38	GLN
1	J	189	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	213/213 (100%)	0.54	16 (7%) 20 15	6, 40, 72, 84	0
1	D	213/213 (100%)	1.02	20 (9%) 14 11	22, 53, 73, 82	0
1	G	213/213 (100%)	0.25	6 (2%) 55 36	5, 33, 53, 71	0
1	J	211/213 (99%)	0.29	5 (2%) 59 40	4, 28, 51, 58	0
2	B	214/221 (96%)	0.15	6 (2%) 55 36	5, 28, 49, 67	0
2	E	213/221 (96%)	0.68	16 (7%) 20 15	12, 50, 72, 83	0
2	H	216/221 (97%)	-0.09	3 (1%) 73 54	3, 24, 44, 57	0
2	K	216/221 (97%)	0.03	2 (0%) 81 65	4, 24, 39, 66	0
3	C	94/114 (82%)	-0.20	0 100 100	3, 12, 27, 40	0
3	F	93/114 (81%)	0.02	0 100 100	9, 23, 34, 43	0
3	I	93/114 (81%)	-0.20	0 100 100	6, 16, 27, 33	0
3	L	92/114 (80%)	0.06	2 (2%) 62 43	12, 26, 40, 50	0
All	All	2081/2192 (94%)	0.28	76 (3%) 45 30	3, 29, 65, 84	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	132	PRO	3.9
1	G	115	ASN	3.6
1	D	212	ASN	3.5
1	A	184	ASP	3.1
1	A	158	GLY	3.0

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.