



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 AM UTC

PDB ID : 8K4V / pdb_00008k4v
Title : Crystal structure of HLA-A*11:01 in complex with KRAS G12R peptide (VVVGARGVGK)
Authors : Xu, Y.
Deposited on : 2023-07-20
Resolution : 3.10 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

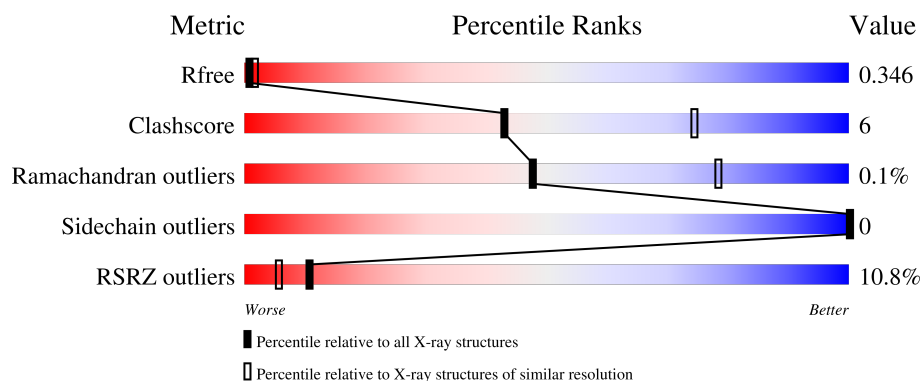
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	276	10% 82% 18%
1	D	276	11% 84% 16%
1	G	276	12% 85% 15%
1	J	276	12% 86% 14%
2	B	122	12% 65% 17% 18%

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Mol	Chain	Length	Quality of chain
2	E	122	7% 64% 18% 18%
2	H	122	5% 71% 11% 18%
2	K	122	7% 64% 18% 18%
3	C	10	70% 20% 10%
3	F	10	20% 80% 20%
3	I	10	10% 70% 10% 20%
3	L	10	10% 50% 30% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12560 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 HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	D	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	G	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			
1	J	275	Total	C	N	O	S	0	1	0
			2250	1398	409	434	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P04439
A	33	TYR	PHE	variant	UNP P04439
A	114	ASP	ALA	variant	UNP P04439
A	129	PRO	SER	variant	UNP P04439
D	24	MET	-	initiating methionine	UNP P04439
D	33	TYR	PHE	variant	UNP P04439
D	114	ASP	ALA	variant	UNP P04439
D	129	PRO	SER	variant	UNP P04439
G	24	MET	-	initiating methionine	UNP P04439
G	33	TYR	PHE	variant	UNP P04439
G	114	ASP	ALA	variant	UNP P04439
G	129	PRO	SER	variant	UNP P04439
J	24	MET	-	initiating methionine	UNP P04439
J	33	TYR	PHE	variant	UNP P04439
J	114	ASP	ALA	variant	UNP P04439
J	129	PRO	SER	variant	UNP P04439

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	E	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	H	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	K	100	Total 836	C 533	N 141	O 158	S 4	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
B	100	GLY	-	expression tag	UNP P61769
B	101	SER	-	expression tag	UNP P61769
B	102	GLY	-	expression tag	UNP P61769
B	103	GLY	-	expression tag	UNP P61769
B	104	SER	-	expression tag	UNP P61769
B	105	GLY	-	expression tag	UNP P61769
B	106	ALA	-	expression tag	UNP P61769
B	107	GLY	-	expression tag	UNP P61769
B	108	LEU	-	expression tag	UNP P61769
B	109	ASN	-	expression tag	UNP P61769
B	110	ASP	-	expression tag	UNP P61769
B	111	ILE	-	expression tag	UNP P61769
B	112	PHE	-	expression tag	UNP P61769
B	113	GLU	-	expression tag	UNP P61769
B	114	ALA	-	expression tag	UNP P61769
B	115	GLN	-	expression tag	UNP P61769
B	116	LYS	-	expression tag	UNP P61769
B	117	ILE	-	expression tag	UNP P61769
B	118	GLU	-	expression tag	UNP P61769
B	119	TRP	-	expression tag	UNP P61769
B	120	HIS	-	expression tag	UNP P61769
B	121	GLU	-	expression tag	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
E	100	GLY	-	expression tag	UNP P61769
E	101	SER	-	expression tag	UNP P61769
E	102	GLY	-	expression tag	UNP P61769
E	103	GLY	-	expression tag	UNP P61769
E	104	SER	-	expression tag	UNP P61769
E	105	GLY	-	expression tag	UNP P61769
E	106	ALA	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	GLY	-	expression tag	UNP P61769
E	108	LEU	-	expression tag	UNP P61769
E	109	ASN	-	expression tag	UNP P61769
E	110	ASP	-	expression tag	UNP P61769
E	111	ILE	-	expression tag	UNP P61769
E	112	PHE	-	expression tag	UNP P61769
E	113	GLU	-	expression tag	UNP P61769
E	114	ALA	-	expression tag	UNP P61769
E	115	GLN	-	expression tag	UNP P61769
E	116	LYS	-	expression tag	UNP P61769
E	117	ILE	-	expression tag	UNP P61769
E	118	GLU	-	expression tag	UNP P61769
E	119	TRP	-	expression tag	UNP P61769
E	120	HIS	-	expression tag	UNP P61769
E	121	GLU	-	expression tag	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
H	100	GLY	-	expression tag	UNP P61769
H	101	SER	-	expression tag	UNP P61769
H	102	GLY	-	expression tag	UNP P61769
H	103	GLY	-	expression tag	UNP P61769
H	104	SER	-	expression tag	UNP P61769
H	105	GLY	-	expression tag	UNP P61769
H	106	ALA	-	expression tag	UNP P61769
H	107	GLY	-	expression tag	UNP P61769
H	108	LEU	-	expression tag	UNP P61769
H	109	ASN	-	expression tag	UNP P61769
H	110	ASP	-	expression tag	UNP P61769
H	111	ILE	-	expression tag	UNP P61769
H	112	PHE	-	expression tag	UNP P61769
H	113	GLU	-	expression tag	UNP P61769
H	114	ALA	-	expression tag	UNP P61769
H	115	GLN	-	expression tag	UNP P61769
H	116	LYS	-	expression tag	UNP P61769
H	117	ILE	-	expression tag	UNP P61769
H	118	GLU	-	expression tag	UNP P61769
H	119	TRP	-	expression tag	UNP P61769
H	120	HIS	-	expression tag	UNP P61769
H	121	GLU	-	expression tag	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
K	100	GLY	-	expression tag	UNP P61769
K	101	SER	-	expression tag	UNP P61769
K	102	GLY	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
K	103	GLY	-	expression tag	UNP P61769
K	104	SER	-	expression tag	UNP P61769
K	105	GLY	-	expression tag	UNP P61769
K	106	ALA	-	expression tag	UNP P61769
K	107	GLY	-	expression tag	UNP P61769
K	108	LEU	-	expression tag	UNP P61769
K	109	ASN	-	expression tag	UNP P61769
K	110	ASP	-	expression tag	UNP P61769
K	111	ILE	-	expression tag	UNP P61769
K	112	PHE	-	expression tag	UNP P61769
K	113	GLU	-	expression tag	UNP P61769
K	114	ALA	-	expression tag	UNP P61769
K	115	GLN	-	expression tag	UNP P61769
K	116	LYS	-	expression tag	UNP P61769
K	117	ILE	-	expression tag	UNP P61769
K	118	GLU	-	expression tag	UNP P61769
K	119	TRP	-	expression tag	UNP P61769
K	120	HIS	-	expression tag	UNP P61769
K	121	GLU	-	expression tag	UNP P61769

- Molecule 3 is a protein called KRAS G12R peptide (VVVGARGVVGK).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			66	41	14	11			
3	F	8	Total	C	N	O	0	0	0
			50	32	9	9			
3	I	8	Total	C	N	O	0	0	0
			50	32	9	9			
3	L	8	Total	C	N	O	0	0	0
			50	32	9	9			

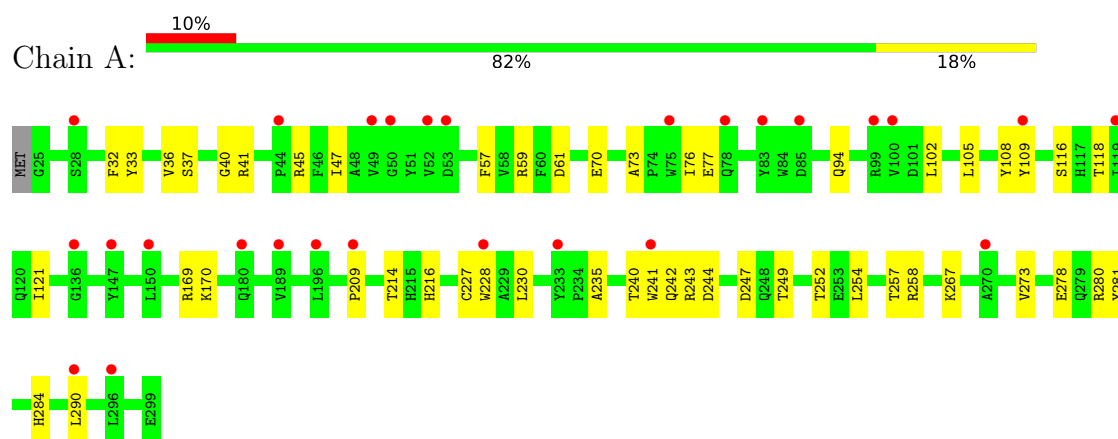
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ARG	GLY	engineered mutation	UNP P01116
F	6	ARG	GLY	engineered mutation	UNP P01116
I	6	ARG	GLY	engineered mutation	UNP P01116
L	6	ARG	GLY	engineered mutation	UNP P01116

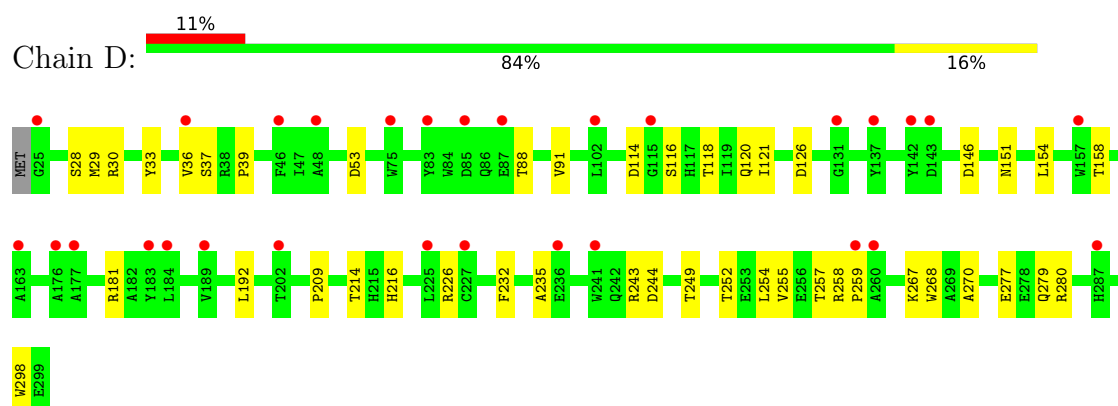
3 Residue-property plots [i](#)

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.

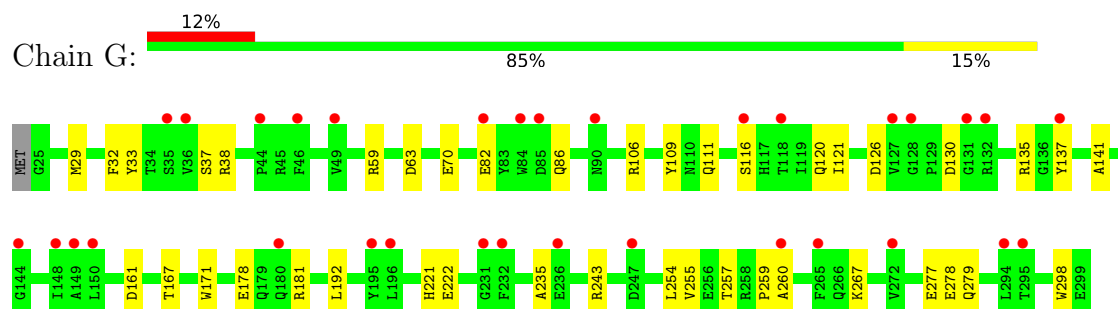
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



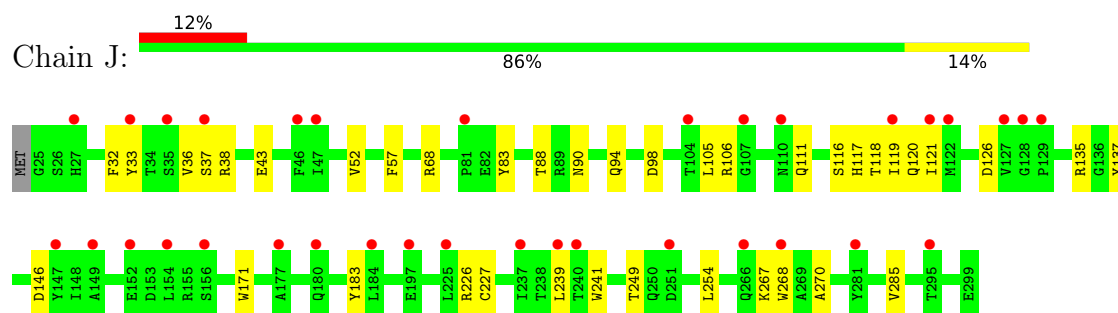
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



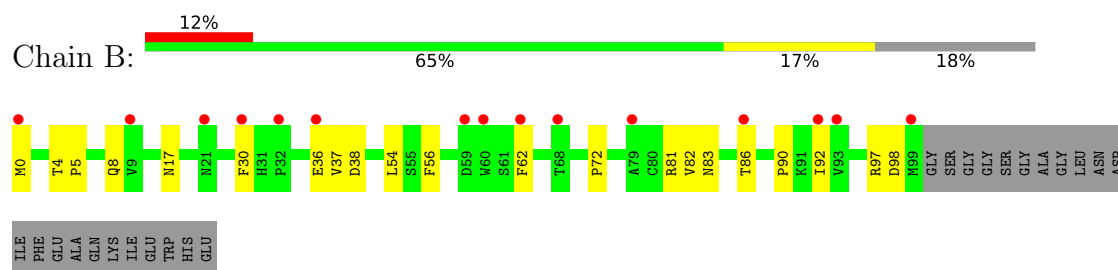
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



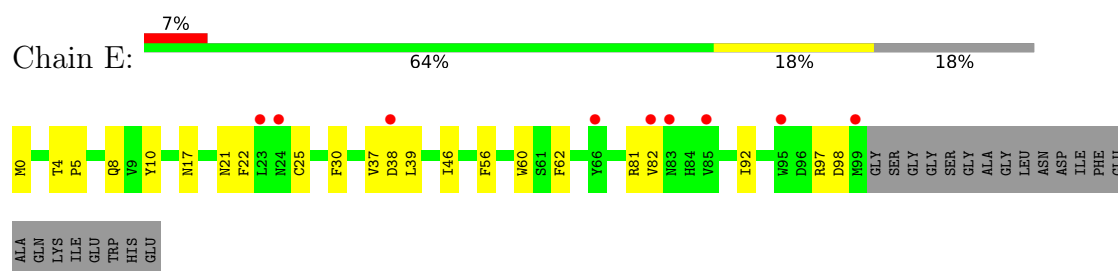
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



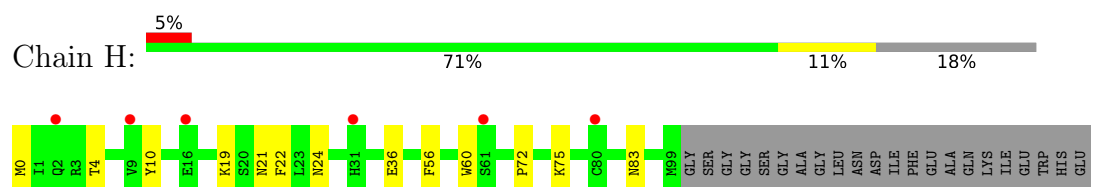
- Molecule 2: Beta-2-microglobulin



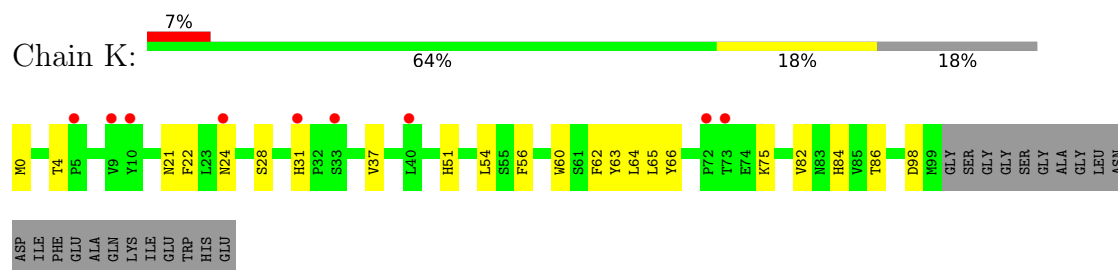
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

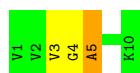


- Molecule 2: Beta-2-microglobulin



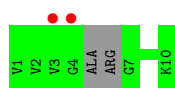
- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain C:  70% 20% 10%



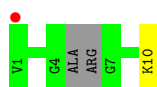
- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain F:  20% 80% 20%



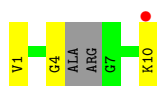
- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain I:  10% 70% 10% 20%



- Molecule 3: KRAS G12R peptide (VVVGARGVGK)

Chain L:  10% 50% 30% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.65Å 121.60Å 155.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.39 – 3.10 25.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.39-3.10) 79.6 (25.39-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.21 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.296 , 0.347 0.297 , 0.346	Depositor DCC
R_{free} test set	1998 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	1.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	12560	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6469e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.12	0/2314	0.37	0/3141
1	D	0.14	0/2314	0.37	0/3141
1	G	0.13	0/2314	0.36	0/3141
1	J	0.12	0/2314	0.35	0/3141
2	B	0.13	0/859	0.35	0/1162
2	E	0.13	0/859	0.34	0/1162
2	H	0.12	0/859	0.35	0/1162
2	K	0.12	0/859	0.38	0/1162
3	C	0.16	0/65	0.44	0/84
3	F	0.10	0/48	0.21	0/60
3	I	0.12	0/48	0.27	0/60
3	L	0.11	0/48	0.25	0/60
All	All	0.13	0/12901	0.36	0/17476

There are no bond length outliers.

There are no bond angle outliers.

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	2250	0	2096	32	0
1	D	2250	0	2096	28	0
1	G	2250	0	2096	27	0
1	J	2250	0	2096	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	836	0	803	22	0
2	E	836	0	803	18	0
2	H	836	0	803	16	0
2	K	836	0	803	16	0
3	C	66	0	78	1	0
3	F	50	0	59	0	0
3	I	50	0	59	2	0
3	L	50	0	59	4	0
All	All	12560	0	11851	151	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 6.

All (151) 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:92:ILE:HG12	2:H:75:LYS:HD2	1.62	0.82
1:G:279:GLN:NE2	1:G:298:TRP:O	2.18	0.76
1:A:169:ARG:NH1	1:J:249:THR:OG1	2.19	0.75
1:G:120:GLN:NE2	2:H:60:TRP:O	2.21	0.74
1:A:216:HIS:NE2	2:B:98:ASP:OD2	2.21	0.73
2:E:92:ILE:HD12	2:K:75:LYS:HG2	1.71	0.71
1:D:244:ASP:OD2	1:D:280:ARG:NH2	2.23	0.68
2:B:0:MET:N	2:K:4:THR:OG1	2.27	0.67
2:B:56:PHE:HA	2:B:62:PHE:HA	1.78	0.66
1:D:216:HIS:NE2	2:E:98:ASP:OD2	2.18	0.66
2:E:4:THR:OG1	2:H:0:MET:N	2.27	0.66
1:G:126:ASP:OD2	1:G:135:ARG:NH2	2.30	0.65
1:J:94[A]:GLN:NE2	1:J:98:ASP:OD1	2.29	0.65
1:A:244:ASP:OD2	1:A:280:ARG:NH2	2.26	0.64
1:G:243:ARG:NH1	1:G:277:GLU:OE1	2.26	0.64
1:G:29:MET:HB2	1:G:192:LEU:HD13	1.78	0.64
1:A:254:LEU:HD11	1:A:267:LYS:HE3	1.79	0.63
1:J:33:TYR:HB2	1:J:121:ILE:HB	1.81	0.63
2:E:0:MET:N	2:H:4:THR:OG1	2.31	0.63
1:G:106:ARG:HG3	1:G:111:GLN:HB2	1.79	0.63
2:E:17:ASN:OD1	2:E:97:ARG:NH2	2.28	0.63
1:G:33:TYR:HB2	1:G:121:ILE:HB	1.81	0.62
1:D:279:GLN:NE2	1:D:298:TRP:O	2.28	0.62
2:B:90:PRO:HG2	2:H:75:LYS:O	2.02	0.60
1:D:36:VAL:HG22	1:D:118:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:SER:O	1:J:116:SER:OG	2.17	0.59
1:G:135:ARG:NE	1:G:137:TYR:OH	2.32	0.58
1:A:227:CYS:HB2	1:A:241:TRP:CZ2	2.38	0.58
1:A:258:ARG:NH1	2:B:8:GLN:OE1	2.34	0.58
1:A:273:VAL:HG21	1:A:278:GLU:HG3	1.85	0.58
1:J:32:PHE:HB3	2:K:56:PHE:CE2	2.40	0.57
1:J:268:TRP:HZ3	1:J:270:ALA:HB2	1.70	0.57
1:J:36:VAL:HG22	1:J:118:THR:HG23	1.89	0.55
1:J:254:LEU:HD11	1:J:267:LYS:HE3	1.89	0.55
1:D:214:THR:HG21	2:E:98:ASP:OD1	2.07	0.55
1:G:178:GLU:HG3	1:G:181:ARG:HH22	1.71	0.55
1:A:243:ARG:NH1	1:A:281:TYR:OH	2.35	0.55
1:G:59:ARG:NE	1:G:70:GLU:OE1	2.31	0.54
1:J:135:ARG:NE	1:J:137:TYR:OH	2.33	0.53
1:A:235:ALA:HB1	1:A:257:THR:HG21	1.89	0.53
1:G:259:PRO:O	2:H:10:TYR:OH	2.17	0.53
1:A:37:SER:HB3	1:A:102:LEU:HD13	1.90	0.53
1:D:151:ASN:OD1	1:D:158:THR:OG1	2.21	0.53
1:A:228:TRP:HE3	1:A:230:LEU:HD21	1.74	0.53
2:B:92:ILE:HG12	2:H:75:LYS:CD	2.37	0.53
3:C:3:VAL:O	3:C:5:ALA:N	2.42	0.53
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.90	0.52
1:D:258:ARG:NH1	2:E:8:GLN:OE1	2.38	0.52
1:J:106:ARG:HG3	1:J:111:GLN:HB2	1.92	0.52
1:D:243:ARG:NH1	1:D:277:GLU:OE1	2.36	0.52
1:J:68:ARG:HD2	1:J:88:THR:HG21	1.92	0.52
1:G:235:ALA:HB1	1:G:257:THR:HG21	1.90	0.51
2:E:21:ASN:OD1	2:E:22:PHE:N	2.38	0.51
1:D:28:SER:N	1:D:53:ASP:OD1	2.38	0.51
2:H:21:ASN:OD1	2:H:22:PHE:N	2.38	0.51
1:G:254:LEU:HD11	1:G:267:LYS:HE3	1.92	0.51
2:E:38:ASP:OD2	2:E:81:ARG:NH2	2.35	0.50
2:B:72:PRO:HB2	2:B:97:ARG:NH2	2.26	0.50
1:A:228:TRP:CE3	1:A:230:LEU:HD21	2.46	0.50
2:B:90:PRO:HB2	2:H:75:LYS:HB3	1.92	0.50
1:J:105:LEU:HD22	1:J:119:ILE:HD11	1.93	0.50
1:A:108:TYR:HH	1:A:170:LYS:HZ2	1.56	0.50
1:D:255:VAL:O	1:D:267:LYS:NZ	2.37	0.50
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.43	0.50
2:K:37:VAL:HG22	2:K:82:VAL:HG22	1.94	0.49
1:D:30:ARG:NH2	1:D:126:ASP:OD1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLY:C	1:D:39:PRO:HB2	2.36	0.49
2:E:56:PHE:HA	2:E:62:PHE:HA	1.95	0.49
1:A:47:ILE:HG21	2:B:54:LEU:HB3	1.94	0.49
1:A:36:VAL:HG22	1:A:118:THR:HG23	1.94	0.49
1:J:126:ASP:OD2	1:J:135:ARG:NH2	2.45	0.49
1:J:183:TYR:OH	3:L:1:VAL:O	2.24	0.49
2:K:28:SER:HA	2:K:63:TYR:HA	1.95	0.48
1:D:259:PRO:O	2:E:10:TYR:OH	2.24	0.48
1:A:32:PHE:HB3	2:B:56:PHE:CE2	2.49	0.48
1:D:268:TRP:HZ3	1:D:270:ALA:HB2	1.79	0.48
2:B:83:ASN:OD1	2:B:90:PRO:HG3	2.14	0.48
1:J:227:CYS:HB2	1:J:241:TRP:CZ2	2.49	0.48
1:G:255:VAL:O	1:G:267:LYS:NZ	2.35	0.47
2:B:81:ARG:HG3	2:H:75:LYS:HG2	1.97	0.47
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.96	0.47
1:J:120:GLN:CD	2:K:31:HIS:HE2	2.22	0.47
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.96	0.47
2:K:56:PHE:HA	2:K:62:PHE:HA	1.96	0.47
2:H:19:LYS:O	2:H:72:PRO:HD2	2.15	0.47
1:G:37:SER:O	1:G:116:SER:OG	2.18	0.46
1:J:90:ASN:O	1:J:94[B]:GLN:NE2	2.48	0.46
1:D:37:SER:O	1:D:116:SER:OG	2.25	0.46
1:D:146:ASP:OD1	2:E:60:TRP:NE1	2.35	0.46
1:A:73:ALA:O	1:A:76:ILE:HG22	2.15	0.46
1:J:146:ASP:OD1	2:K:60:TRP:NE1	2.39	0.46
2:H:36:GLU:HB3	2:H:83:ASN:HB2	1.98	0.46
1:J:37:SER:HG	1:J:117:HIS:H	1.63	0.46
2:K:21:ASN:OD1	2:K:22:PHE:N	2.44	0.46
1:D:249:THR:O	1:D:252:THR:OG1	2.28	0.46
1:A:249:THR:O	1:A:252:THR:OG1	2.28	0.45
2:K:54:LEU:HA	2:K:64:LEU:HD21	1.99	0.45
1:J:226:ARG:NH1	2:K:98:ASP:OD2	2.48	0.45
2:B:38:ASP:CG	2:B:81:ARG:HH21	2.25	0.45
1:G:221:HIS:ND1	1:G:222:GLU:HG3	2.32	0.45
2:K:24:ASN:HB3	2:K:65:LEU:HD11	1.99	0.44
1:A:59:ARG:NH2	1:A:70:GLU:OE1	2.47	0.44
1:J:38:ARG:NE	1:J:43:GLU:O	2.27	0.44
2:B:92:ILE:HA	2:H:75:LYS:HZ3	1.81	0.44
1:D:209:PRO:HB3	1:D:232:PHE:HB3	2.00	0.44
1:D:235:ALA:HB1	1:D:257:THR:HG21	1.98	0.43
1:A:105:LEU:O	1:A:109:TYR:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:GLN:NE2	2:K:60:TRP:O	2.46	0.43
1:J:171:TRP:CZ2	3:L:10:LYS:HG2	2.54	0.43
1:D:154:LEU:O	1:D:181:ARG:NH1	2.48	0.43
1:D:120:GLN:HB3	2:E:56:PHE:CZ	2.53	0.43
1:J:83:TYR:HE2	3:L:1:VAL:HG12	1.82	0.43
1:D:88:THR:HA	1:D:91:VAL:HG12	2.01	0.43
2:E:37:VAL:HG22	2:E:82:VAL:HG22	1.99	0.43
1:J:90:ASN:ND2	3:L:4:GLY:HA2	2.33	0.43
2:B:4:THR:OG1	2:K:0:MET:N	2.52	0.43
1:G:130:ASP:OD1	1:G:130:ASP:N	2.49	0.43
2:K:51:HIS:HB3	2:K:66:TYR:CD2	2.53	0.43
1:A:57:PHE:O	1:A:76:ILE:HG21	2.19	0.43
1:J:239:LEU:HD22	1:J:285:VAL:HG22	2.00	0.43
1:G:109:TYR:OH	1:G:161:ASP:OD2	2.29	0.42
1:D:254:LEU:HD11	1:D:267:LYS:HE3	2.00	0.42
1:A:242:GLN:NE2	1:A:247:ASP:OD1	2.53	0.42
1:A:33:TYR:HB2	1:A:121:ILE:HB	2.01	0.42
2:B:36:GLU:O	2:B:82:VAL:HA	2.20	0.42
1:A:209:PRO:HD2	1:A:290:LEU:HG	2.01	0.42
2:B:4:THR:HG22	2:B:86:THR:HB	2.01	0.42
1:G:278:GLU:OE1	1:G:278:GLU:N	2.44	0.42
1:A:37:SER:O	1:A:116:SER:OG	2.35	0.42
1:J:52:VAL:HG23	1:J:57:PHE:CE1	2.55	0.41
1:A:33:TYR:CE2	1:A:94[A]:GLN:HG2	2.56	0.41
1:A:73:ALA:O	1:A:77:GLU:HG3	2.20	0.41
1:D:33:TYR:HB2	1:D:121:ILE:HB	2.01	0.41
1:A:214:THR:HG21	2:B:98:ASP:OD1	2.21	0.41
1:G:167:THR:HG23	3:I:10:LYS:HA	2.03	0.41
1:D:226:ARG:NH1	2:E:98:ASP:O	2.53	0.41
1:D:30:ARG:HH22	1:D:126:ASP:CG	2.25	0.41
2:E:39:LEU:HB3	2:E:46:ILE:HD12	2.02	0.41
1:D:29:MET:HB2	1:D:192:LEU:HD13	2.03	0.41
1:G:32:PHE:HB3	2:H:56:PHE:CE2	2.56	0.41
1:G:82:GLU:OE2	1:G:86:GLN:HB2	2.21	0.41
1:G:171:TRP:CZ2	3:I:10:LYS:HG2	2.56	0.41
1:G:260:ALA:O	2:H:24:ASN:ND2	2.53	0.41
2:K:84:HIS:CE1	2:K:86:THR:HG23	2.56	0.41
2:E:5:PRO:HB3	2:E:30:PHE:HB3	2.02	0.40
1:G:135:ARG:HE	1:G:137:TYR:HH	1.66	0.40
1:G:141:ALA:HB2	2:H:60:TRP:CE2	2.56	0.40
1:A:240:THR:O	1:A:284:HIS:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HG2	1:D:114:ASP:OD1	2.21	0.40
1:A:45:ARG:NH2	1:A:61:ASP:OD2	2.40	0.40
1:G:38:ARG:NH2	1:G:63:ASP:OD1	2.50	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	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	D	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	G	274/276 (99%)	269 (98%)	5 (2%)	0	100	100
1	J	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
2	B	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	E	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	H	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
2	K	98/122 (80%)	95 (97%)	3 (3%)	0	100	100
3	C	8/10 (80%)	5 (62%)	1 (12%)	2 (25%)	0	0
3	F	4/10 (40%)	4 (100%)	0	0	100	100
3	I	4/10 (40%)	4 (100%)	0	0	100	100
3	L	4/10 (40%)	4 (100%)	0	0	100	100
All	All	1508/1632 (92%)	1471 (98%)	35 (2%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	4	GLY

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Mol	Chain	Res	Type
3	C	5	ALA

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	233/233 (100%)	233 (100%)	0	100	100
1	D	233/233 (100%)	233 (100%)	0	100	100
1	G	233/233 (100%)	233 (100%)	0	100	100
1	J	233/233 (100%)	233 (100%)	0	100	100
2	B	95/110 (86%)	95 (100%)	0	100	100
2	E	95/110 (86%)	95 (100%)	0	100	100
2	H	95/110 (86%)	95 (100%)	0	100	100
2	K	95/110 (86%)	95 (100%)	0	100	100
3	C	6/6 (100%)	6 (100%)	0	100	100
3	F	5/6 (83%)	5 (100%)	0	100	100
3	I	5/6 (83%)	5 (100%)	0	100	100
3	L	5/6 (83%)	5 (100%)	0	100	100
All	All	1333/1396 (96%)	1333 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	D	27	HIS
1	D	78	GLN
1	D	215	HIS
1	G	198	ASN
1	G	286	GLN
2	H	13	HIS

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Mol	Chain	Res	Type
1	J	90	ASN
1	J	198	ASN

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 ⓘ

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, 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	275/276 (99%)	1.05	27 (9%) 13 7	27, 54, 73, 86	1 (0%)
1	D	275/276 (99%)	0.93	29 (10%) 11 6	19, 47, 72, 85	1 (0%)
1	G	275/276 (99%)	0.97	32 (11%) 9 5	23, 50, 74, 96	1 (0%)
1	J	275/276 (99%)	1.14	34 (12%) 8 5	30, 70, 95, 107	1 (0%)
2	B	100/122 (81%)	1.14	15 (15%) 5 3	26, 48, 66, 87	0
2	E	100/122 (81%)	0.96	9 (9%) 15 8	25, 43, 62, 75	0
2	H	100/122 (81%)	0.96	6 (6%) 27 15	26, 44, 63, 71	0
2	K	100/122 (81%)	1.18	9 (9%) 15 8	40, 63, 85, 111	0
3	C	10/10 (100%)	0.80	0 100 100	48, 62, 80, 82	0
3	F	8/10 (80%)	0.96	2 (25%) 2 1	34, 49, 57, 58	0
3	I	8/10 (80%)	0.67	1 (12%) 8 5	31, 40, 48, 50	0
3	L	8/10 (80%)	1.63	1 (12%) 8 5	75, 83, 95, 104	0
All	All	1534/1632 (93%)	1.03	165 (10%) 11 6	19, 52, 84, 111	4 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	THR	6.3
2	B	32	PRO	5.0
2	K	31	HIS	4.7
1	G	247	ASP	4.7
2	E	23	LEU	4.6
1	J	149	ALA	4.4
2	H	31	HIS	4.0
1	G	144	GLY	3.9
1	J	46	PHE	3.8
1	D	142	TYR	3.8
1	J	281	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	92	ILE	3.7
1	G	36	VAL	3.5
1	D	48	ALA	3.4
1	J	147	TYR	3.3
1	J	81	PRO	3.3
1	G	46	PHE	3.3
1	D	143	ASP	3.2
1	A	119	ILE	3.2
1	G	265	PHE	3.2
2	H	9	VAL	3.2
1	D	85	ASP	3.2
2	E	38	ASP	3.2
1	A	28	SER	3.2
2	E	99	MET	3.1
1	G	90	ASN	3.0
2	B	99	MET	3.0
2	K	40	LEU	3.0
1	G	118	THR	3.0
1	G	131	GLY	3.0
1	G	231	GLY	3.0
1	J	180	GLN	3.0
1	D	102	LEU	2.9
1	D	163	ALA	2.9
2	K	9	VAL	2.9
2	B	60	TRP	2.9
1	A	52	VAL	2.9
1	D	83	TYR	2.9
1	G	148	ILE	2.9
1	J	47	ILE	2.9
2	E	95	TRP	2.9
1	J	104	THR	2.8
1	G	232	PHE	2.8
1	A	83	TYR	2.8
1	D	137	TYR	2.8
2	E	82	VAL	2.8
1	A	53	ASP	2.8
1	G	150	LEU	2.7
1	A	99	ARG	2.7
2	E	85	VAL	2.7
1	D	46	PHE	2.7
1	A	228	TRP	2.7
1	G	44	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	119	ILE	2.7
1	G	82	GLU	2.7
1	A	75	TRP	2.7
1	A	49	VAL	2.7
2	B	79	ALA	2.7
1	D	87	GLU	2.6
1	D	189	VAL	2.6
2	H	61	SER	2.6
1	G	195	TYR	2.6
2	E	24	ASN	2.6
1	G	260	ALA	2.6
1	A	100	VAL	2.6
1	D	287	HIS	2.6
1	J	156	SER	2.5
1	D	225	LEU	2.5
1	J	152	GLU	2.5
2	B	30	PHE	2.5
1	D	184	LEU	2.5
1	A	44	PRO	2.5
1	D	36	VAL	2.5
1	D	227	CYS	2.5
2	K	72	PRO	2.5
1	D	183	TYR	2.5
1	J	37	SER	2.4
1	D	241	TRP	2.4
1	J	268	TRP	2.4
1	A	150	LEU	2.4
1	G	35	SER	2.4
1	J	33	TYR	2.4
2	B	62	PHE	2.4
2	B	21	ASN	2.4
1	G	272	VAL	2.4
1	A	270	ALA	2.4
2	B	0	MET	2.4
1	J	197	GLU	2.4
1	J	239	LEU	2.4
1	J	266	GLN	2.4
1	A	189	VAL	2.4
1	G	149	ALA	2.3
1	J	177	ALA	2.3
1	A	50	GLY	2.3
1	J	295	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	73	THR	2.3
1	G	294	LEU	2.3
1	J	127	VAL	2.3
2	K	5	PRO	2.3
2	H	2	GLN	2.3
2	H	16	GLU	2.3
1	A	136	GLY	2.3
1	J	237	ILE	2.3
1	D	75	TRP	2.3
3	F	4	GLY	2.3
1	J	240	THR	2.3
1	J	110	ASN	2.3
3	F	3	VAL	2.3
2	K	10	TYR	2.3
1	A	78	GLN	2.3
3	L	10	LYS	2.3
1	J	129	PRO	2.2
1	A	290	LEU	2.2
1	D	157	TRP	2.2
1	J	35	SER	2.2
2	B	36	GLU	2.2
1	A	241	TRP	2.2
1	G	84	TRP	2.2
1	G	132	ARG	2.2
1	J	27	HIS	2.2
1	J	121	ILE	2.2
1	J	184	LEU	2.2
1	D	176	ALA	2.2
1	G	128	GLY	2.2
1	J	251	ASP	2.2
1	A	180	GLN	2.1
1	A	209	PRO	2.1
1	D	25	GLY	2.1
1	G	295	THR	2.1
1	A	233	TYR	2.1
1	J	128	GLY	2.1
2	E	83	ASN	2.1
2	B	93	VAL	2.1
1	D	202	THR	2.1
1	A	147	TYR	2.1
1	D	260	ALA	2.1
1	D	115	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	49	VAL	2.1
1	G	196	LEU	2.1
2	B	86	THR	2.1
1	J	122	MET	2.1
1	D	177	ALA	2.1
1	D	236	GLU	2.1
1	G	236	GLU	2.1
2	K	24	ASN	2.1
1	A	296	LEU	2.1
1	J	154	LEU	2.1
1	G	85	ASP	2.1
1	A	109	TYR	2.1
2	K	33	SER	2.0
1	J	225	LEU	2.0
1	A	85	ASP	2.0
2	E	66	TYR	2.0
1	D	131	GLY	2.0
1	G	180	GLN	2.0
1	J	107	GLY	2.0
2	B	9	VAL	2.0
1	G	116	SER	2.0
1	G	137	TYR	2.0
2	B	59	ASP	2.0
2	H	80	CYS	2.0
1	D	259	PRO	2.0
1	G	127	VAL	2.0
3	I	1	VAL	2.0
1	A	196	LEU	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.