



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:16 AM UTC

PDB ID : 9EE0 / pdb_00009ee0
Title : HIV CA - GLFG peptide (9 mM)
Authors : Melcak, I.; Sarafianos, S.G.
Deposited on : 2024-11-18
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

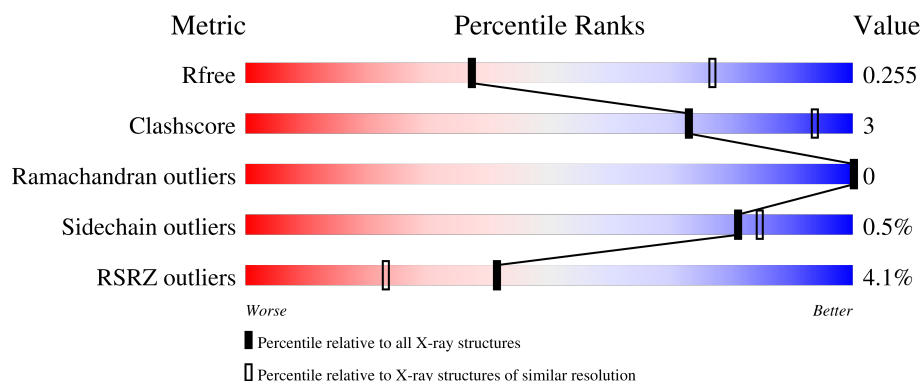
1 Overall quality at a glance

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.













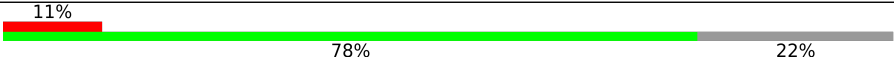

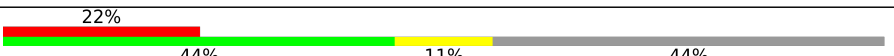
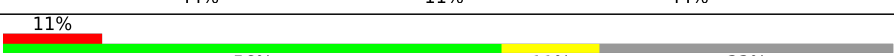

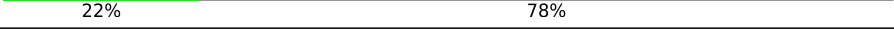


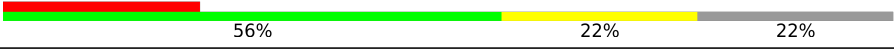
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	231	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	231	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	231	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	D	231	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>12%</div> </div> </div>
1	E	231	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	
2	M	9	
2	N	9	
2	O	9	
2	P	9	
2	Q	9	
2	R	9	
2	S	9	
2	T	9	
2	U	9	
2	V	9	
2	W	9	
2	X	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19394 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1600	1011	278	297	14			
1	B	208	Total	C	N	O	S	0	0	0
			1587	999	276	298	14			
1	C	212	Total	C	N	O	S	0	0	0
			1622	1018	284	306	14			
1	D	204	Total	C	N	O	S	0	0	0
			1534	964	266	290	14			
1	E	205	Total	C	N	O	S	0	0	0
			1561	985	272	291	13			
1	F	215	Total	C	N	O	S	0	0	0
			1629	1025	283	307	14			
1	G	218	Total	C	N	O	S	0	0	0
			1650	1036	290	310	14			
1	H	208	Total	C	N	O	S	0	0	0
			1583	996	277	296	14			
1	I	214	Total	C	N	O	S	0	0	0
			1603	1014	277	298	14			
1	J	216	Total	C	N	O	S	0	0	0
			1645	1032	290	309	14			
1	K	203	Total	C	N	O	S	0	0	0
			1529	963	264	288	14			
1	L	202	Total	C	N	O	S	0	0	0
			1515	955	260	287	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12493
A	45	CYS	GLU	engineered mutation	UNP P12493
A	184	ALA	TRP	engineered mutation	UNP P12493
A	185	ALA	MET	engineered mutation	UNP P12493
B	14	CYS	ALA	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12493
B	184	ALA	TRP	engineered mutation	UNP P12493
B	185	ALA	MET	engineered mutation	UNP P12493
C	14	CYS	ALA	engineered mutation	UNP P12493
C	45	CYS	GLU	engineered mutation	UNP P12493
C	184	ALA	TRP	engineered mutation	UNP P12493
C	185	ALA	MET	engineered mutation	UNP P12493
D	14	CYS	ALA	engineered mutation	UNP P12493
D	45	CYS	GLU	engineered mutation	UNP P12493
D	184	ALA	TRP	engineered mutation	UNP P12493
D	185	ALA	MET	engineered mutation	UNP P12493
E	14	CYS	ALA	engineered mutation	UNP P12493
E	45	CYS	GLU	engineered mutation	UNP P12493
E	184	ALA	TRP	engineered mutation	UNP P12493
E	185	ALA	MET	engineered mutation	UNP P12493
F	14	CYS	ALA	engineered mutation	UNP P12493
F	45	CYS	GLU	engineered mutation	UNP P12493
F	184	ALA	TRP	engineered mutation	UNP P12493
F	185	ALA	MET	engineered mutation	UNP P12493
G	14	CYS	ALA	engineered mutation	UNP P12493
G	45	CYS	GLU	engineered mutation	UNP P12493
G	184	ALA	TRP	engineered mutation	UNP P12493
G	185	ALA	MET	engineered mutation	UNP P12493
H	14	CYS	ALA	engineered mutation	UNP P12493
H	45	CYS	GLU	engineered mutation	UNP P12493
H	184	ALA	TRP	engineered mutation	UNP P12493
H	185	ALA	MET	engineered mutation	UNP P12493
I	14	CYS	ALA	engineered mutation	UNP P12493
I	45	CYS	GLU	engineered mutation	UNP P12493
I	184	ALA	TRP	engineered mutation	UNP P12493
I	185	ALA	MET	engineered mutation	UNP P12493
J	14	CYS	ALA	engineered mutation	UNP P12493
J	45	CYS	GLU	engineered mutation	UNP P12493
J	184	ALA	TRP	engineered mutation	UNP P12493
J	185	ALA	MET	engineered mutation	UNP P12493
K	14	CYS	ALA	engineered mutation	UNP P12493
K	45	CYS	GLU	engineered mutation	UNP P12493
K	184	ALA	TRP	engineered mutation	UNP P12493
K	185	ALA	MET	engineered mutation	UNP P12493
L	14	CYS	ALA	engineered mutation	UNP P12493
L	45	CYS	GLU	engineered mutation	UNP P12493
L	184	ALA	TRP	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12493

- Molecule 2 is a protein called GLFG peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	2	Total	C	N	O	0	0	0
			19	15	2	2			
2	O	6	Total	C	N	O	0	0	0
			37	24	6	7			
2	P	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	Q	3	Total	C	N	O	0	0	0
			23	17	3	3			
2	R	5	Total	C	N	O	0	0	0
			32	22	5	5			
2	S	6	Total	C	N	O	0	0	0
			37	25	6	6			
2	T	2	Total	C	N	O	0	0	0
			15	11	2	2			
2	U	3	Total	C	N	O	0	0	0
			23	17	3	3			
2	V	6	Total	C	N	O	0	0	0
			36	24	6	6			
2	W	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	X	2	Total	C	N	O	0	0	0
			19	15	2	2			
2	N	1	Total	C	N	O	0	0	0
			11	9	1	1			

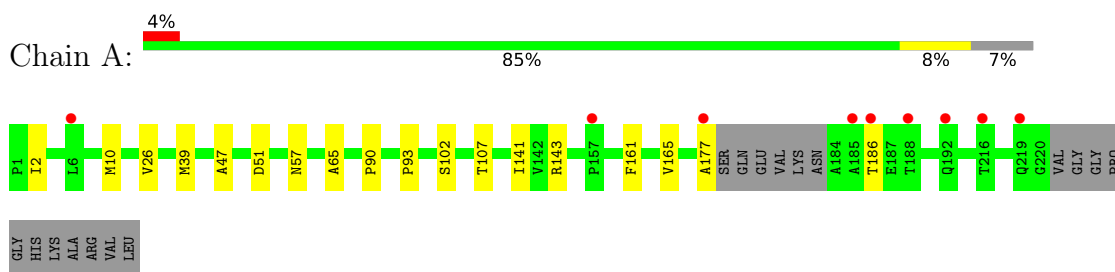
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

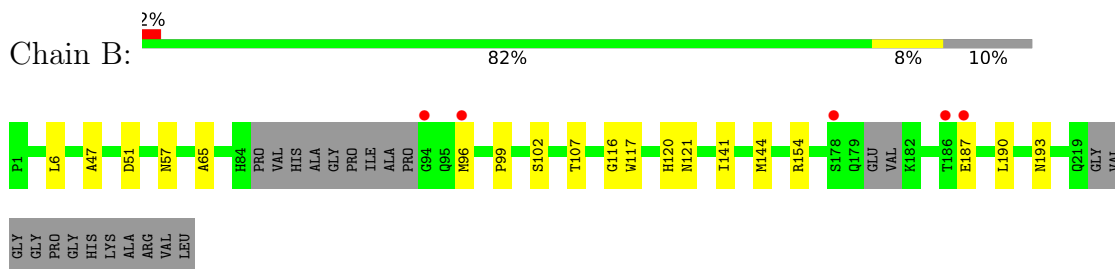
3 Residue-property plots [i](#)

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.

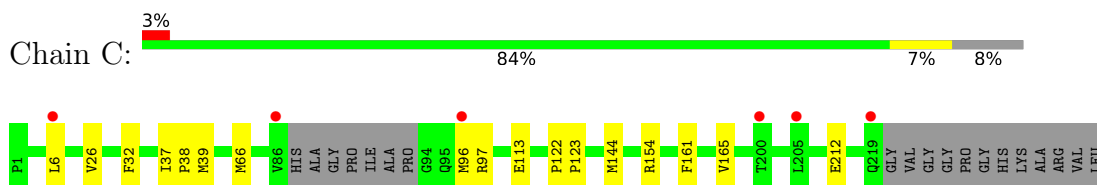
- Molecule 1: Capsid protein p24



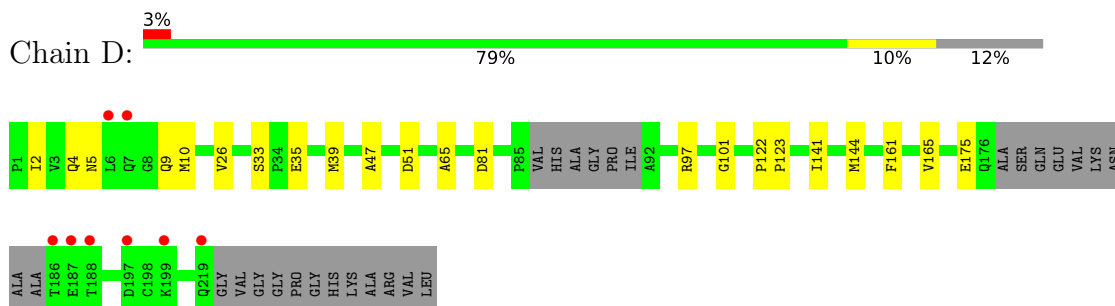
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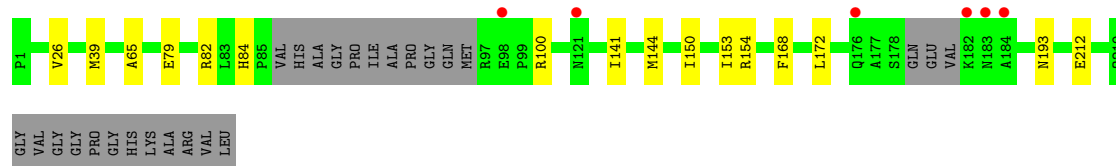
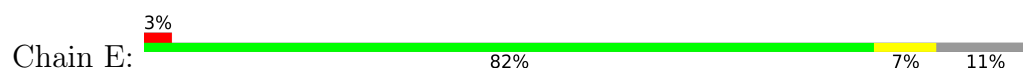
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



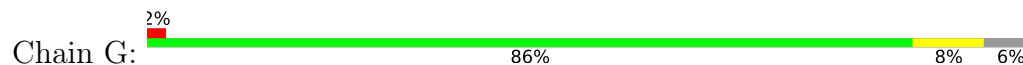
● Molecule 1: Capsid protein p24



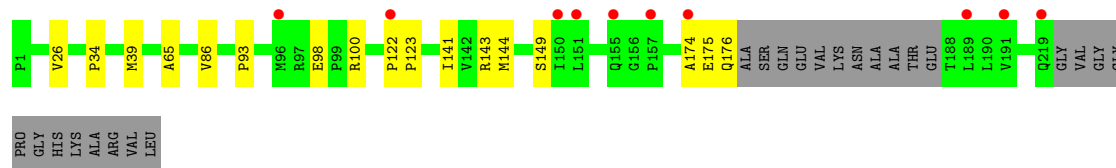
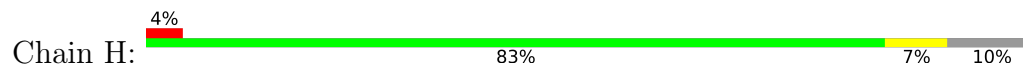
● Molecule 1: Capsid protein p24



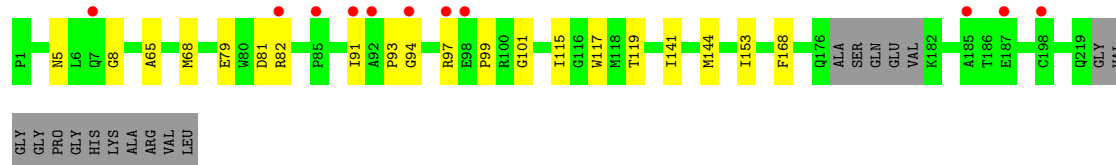
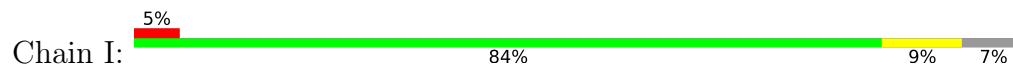
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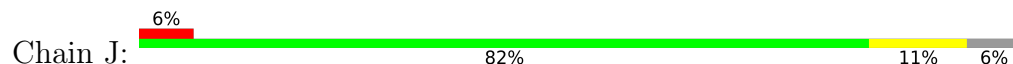
● Molecule 1: Capsid protein p24

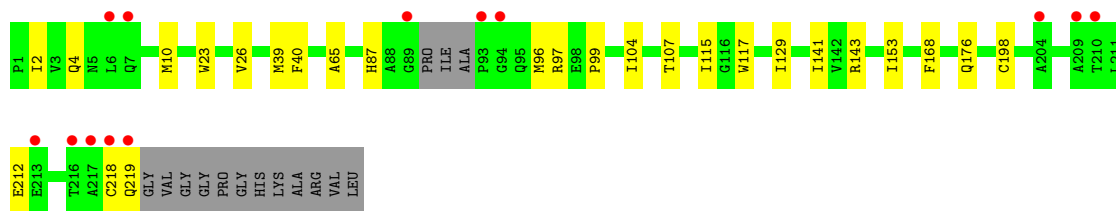


● Molecule 1: Capsid protein p24

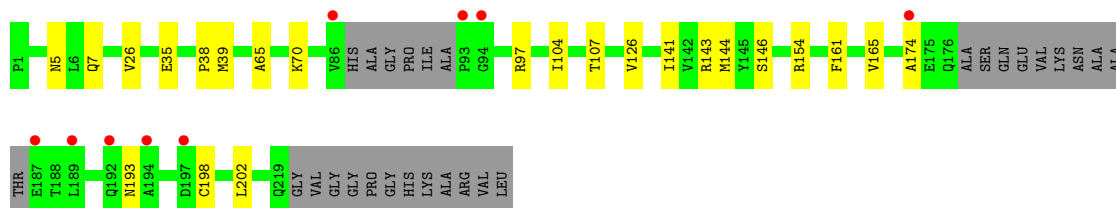
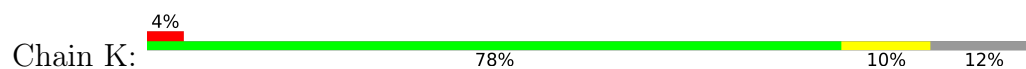


● Molecule 1: Capsid protein p24

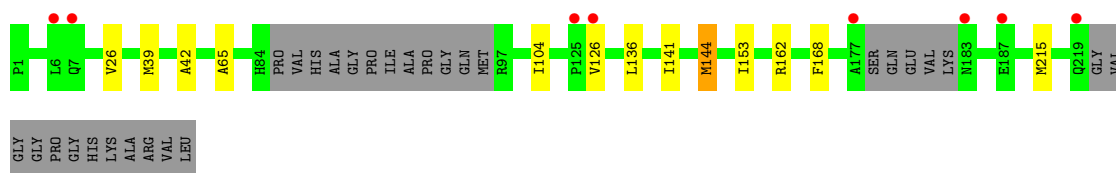
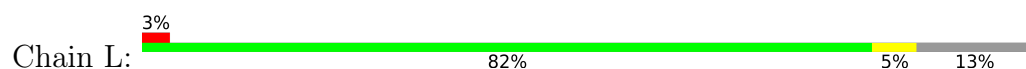




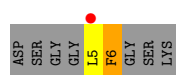
- Molecule 1: Capsid protein p24



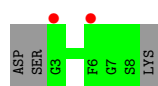
- Molecule 1: Capsid protein p24



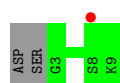
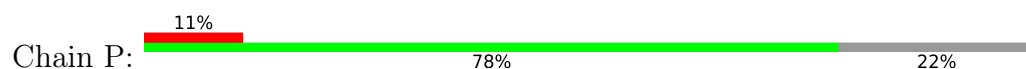
- Molecule 2: GLFG peptide



- Molecule 2: GLFG peptide

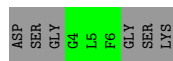


- Molecule 2: GLFG peptide




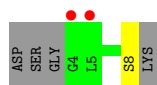
● Molecule 2: GLFG peptide

Chain Q:  33% 67%



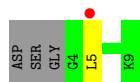
● Molecule 2: GLFG peptide

Chain R:  22% 44% 11% 44%



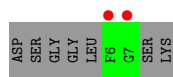
● Molecule 2: GLFG peptide

Chain S:  11% 56% 11% 33%



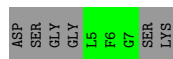
● Molecule 2: GLFG peptide

Chain T:  22% 22% 78%




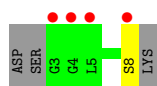
● Molecule 2: GLFG peptide

Chain U:  33% 67%



● Molecule 2: GLFG peptide

Chain V:  44% 56% 11% 33%



● Molecule 2: GLFG peptide

Chain W:  22% 56% 22% 22%



- Molecule 2: GLFG peptide

Chain X:  22% 78%

ASP	SER	GLY	GLY	L5	F6	GLY	SER	LYS
-----	-----	-----	-----	----	----	-----	-----	-----

- Molecule 2: GLFG peptide

Chain N:  11% 89%

ASP	SER	GLY	GLY	LEU	F6	GLY	SER	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.06Å 135.22Å 205.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.90 – 3.10 33.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (33.90-3.10) 95.6 (33.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.229 , 0.255 0.229 , 0.255	Depositor DCC
R_{free} test set	3346 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19394	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.09	0/1636	0.24	0/2230
1	B	0.08	0/1618	0.21	0/2197
1	C	0.09	0/1655	0.22	0/2250
1	D	0.08	0/1567	0.21	0/2133
1	E	0.08	0/1593	0.21	0/2166
1	F	0.08	0/1664	0.21	0/2265
1	G	0.08	0/1685	0.20	0/2294
1	H	0.09	0/1619	0.21	0/2206
1	I	0.09	0/1639	0.21	0/2234
1	J	0.09	0/1680	0.23	0/2283
1	K	0.09	0/1562	0.22	0/2126
1	L	0.08	0/1546	0.21	0/2108
2	M	0.23	0/19	0.78	0/24
2	N	0.05	0/11	0.03	0/13
2	O	0.07	0/37	0.12	0/47
2	P	0.09	0/41	0.24	0/53
2	Q	0.12	0/23	0.15	0/29
2	R	0.05	0/32	0.15	0/41
2	S	0.05	0/37	0.09	0/48
2	T	0.05	0/15	0.13	0/18
2	U	0.03	0/23	0.08	0/29
2	V	0.05	0/36	0.12	0/46
2	W	0.05	0/41	0.12	0/53
2	X	0.07	0/19	0.15	0/24
All	All	0.09	0/19798	0.22	0/26917

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 ⓘ

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	1600	0	1550	10	0
1	B	1587	0	1553	13	0
1	C	1622	0	1584	10	0
1	D	1534	0	1454	11	0
1	E	1561	0	1529	9	0
1	F	1629	0	1577	9	0
1	G	1650	0	1605	12	0
1	H	1583	0	1535	10	0
1	I	1603	0	1552	13	0
1	J	1645	0	1603	16	0
1	K	1529	0	1458	14	0
1	L	1515	0	1447	8	0
2	M	19	0	19	2	0
2	N	11	0	8	1	0
2	O	37	0	33	0	0
2	P	41	0	32	0	0
2	Q	23	0	22	0	0
2	R	32	0	27	1	0
2	S	37	0	29	1	0
2	T	15	0	11	0	0
2	U	23	0	22	0	0
2	V	36	0	30	1	0
2	W	41	0	32	2	0
2	X	19	0	19	0	0
3	A	1	0	0	0	0
3	H	1	0	0	0	0
All	All	19394	0	18731	122	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 3.

All (122) 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:K:70:LYS:HZ1	2:W:9:LYS:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.80	0.63
1:D:5:ASN:HB3	1:D:9:GLN:H	1.64	0.62
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.81	0.62
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.82	0.61
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.82	0.61
1:J:219:GLN:NE2	1:K:146:SER:O	2.34	0.60
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.85	0.58
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.85	0.58
1:L:104:ILE:HG12	1:L:126:VAL:HG12	1.84	0.58
1:K:104:ILE:HG12	1:K:126:VAL:HG12	1.86	0.57
1:B:6:LEU:HB3	1:C:6:LEU:HG	1.87	0.56
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.88	0.56
1:B:96:MET:HE2	1:I:94:GLY:H	1.71	0.55
1:J:143:ARG:NH1	1:J:176:GLN:OE1	2.37	0.55
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.88	0.55
1:G:81:ASP:OD1	1:G:101:GLY:N	2.38	0.54
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.89	0.54
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.90	0.53
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.89	0.53
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.89	0.53
1:H:143:ARG:NH1	1:H:176:GLN:O	2.42	0.53
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.89	0.53
1:B:99:PRO:HG3	1:B:117:TRP:CE2	2.45	0.52
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.90	0.52
1:I:81:ASP:OD1	1:I:101:GLY:N	2.42	0.52
1:E:84:HIS:O	1:E:100:ARG:NH1	2.33	0.52
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.91	0.51
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.91	0.51
1:E:153:ILE:HG21	1:E:168:PHE:HA	1.93	0.51
1:E:79:GLU:OE2	1:E:82:ARG:NH2	2.34	0.50
1:J:212:GLU:HG3	1:K:144:MET:SD	2.51	0.50
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.93	0.50
1:I:79:GLU:CD	1:I:82:ARG:HH21	2.20	0.49
1:G:86:VAL:HG21	1:G:100:ARG:HG2	1.94	0.49
1:K:154:ARG:HA	1:K:193:ASN:HB3	1.94	0.49
1:D:81:ASP:OD1	1:D:101:GLY:N	2.43	0.49
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.93	0.49
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.94	0.49
1:H:86:VAL:HG21	1:H:100:ARG:HG2	1.95	0.49
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.95	0.49
1:B:154:ARG:HG2	1:B:193:ASN:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ALA:HB1	1:F:51:ASP:HB2	1.94	0.49
1:G:144:MET:HE1	1:L:215:MET:HE2	1.95	0.48
1:H:144:MET:HB3	1:H:144:MET:HE2	1.80	0.48
1:F:99:PRO:HG3	1:F:117:TRP:CE2	2.49	0.48
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.96	0.48
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.95	0.48
1:G:70:LYS:NZ	2:S:5:LEU:O	2.46	0.47
1:I:5:ASN:OD1	1:I:8:GLY:N	2.42	0.47
1:B:57:ASN:HD21	2:N:6:PHE:N	2.11	0.47
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.96	0.47
1:H:86:VAL:HG13	1:H:98:GLU:HB2	1.96	0.47
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.96	0.47
1:K:107:THR:HG23	2:W:8:SER:HA	1.96	0.47
1:A:143:ARG:HG3	1:A:177:ALA:HB2	1.96	0.47
1:I:79:GLU:OE2	1:I:82:ARG:NH2	2.47	0.46
1:J:198:CYS:SG	1:J:218:CYS:HB3	2.56	0.46
1:A:57:ASN:ND2	2:M:5:LEU:O	2.48	0.46
1:I:153:ILE:HG21	1:I:168:PHE:HA	1.97	0.46
1:B:117:TRP:CZ2	1:I:93:PRO:HG2	2.51	0.46
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.98	0.46
1:B:47:ALA:HB1	1:B:51:ASP:HB2	1.97	0.45
1:B:144:MET:HE2	1:B:144:MET:HB3	1.84	0.45
1:J:107:THR:HG23	2:V:8:SER:HA	1.99	0.45
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.98	0.45
1:E:154:ARG:HA	1:E:193:ASN:HB3	1.98	0.45
1:A:102:SER:HB2	1:A:107:THR:HB	1.99	0.45
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.52	0.45
1:H:34:PRO:HG3	1:H:174:ALA:HA	1.99	0.45
1:L:144:MET:HE2	1:L:144:MET:HB3	1.93	0.45
1:C:96:MET:HE2	1:H:93:PRO:HA	1.99	0.44
1:E:144:MET:HE2	1:E:144:MET:HB3	1.81	0.44
1:B:116:GLY:O	1:B:120:HIS:HB2	2.18	0.44
1:C:97:ARG:NH2	1:C:113:GLU:OE2	2.50	0.44
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.98	0.44
1:J:4:GLN:HB2	1:J:10:MET:SD	2.58	0.43
1:C:212:GLU:HA	1:D:144:MET:HE1	1.99	0.43
1:C:32:PHE:HZ	1:C:66:MET:HE3	1.83	0.43
1:D:33:SER:OG	1:D:35:GLU:OE1	2.32	0.43
1:C:37:ILE:HB	1:C:38:PRO:HD3	2.00	0.43
1:E:212:GLU:HG3	1:F:144:MET:HE1	2.01	0.43
1:L:153:ILE:HG21	1:L:168:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:ARG:HA	1:L:215:MET:HE3	1.99	0.43
1:G:86:VAL:HG13	1:G:98:GLU:HB2	2.01	0.43
1:D:47:ALA:HB1	1:D:51:ASP:HB2	2.01	0.42
1:J:2:ILE:HD11	1:J:115:ILE:HG12	2.00	0.42
1:C:122:PRO:HA	1:C:123:PRO:HD3	1.88	0.42
1:B:187:GLU:HA	1:B:190:LEU:HB3	2.00	0.42
1:I:144:MET:HE2	1:I:144:MET:HB3	1.83	0.42
1:J:153:ILE:HG21	1:J:168:PHE:HA	2.01	0.42
1:A:90:PRO:HB2	1:J:97:ARG:HB2	2.00	0.42
1:J:104:ILE:HD13	1:J:129:ILE:HG21	2.01	0.42
1:F:90:PRO:HB2	1:K:97:ARG:HB2	2.02	0.42
1:K:5:ASN:HD21	1:K:7:GLN:HB2	1.84	0.42
1:G:68:MET:HE2	1:G:68:MET:HB3	1.96	0.42
1:K:143:ARG:HA	1:K:174:ALA:O	2.19	0.42
1:D:161:PHE:O	1:D:165:VAL:HG23	2.20	0.42
1:H:122:PRO:HA	1:H:123:PRO:HD3	1.89	0.42
1:I:99:PRO:HG3	1:I:117:TRP:CE2	2.55	0.42
1:C:144:MET:HE2	1:C:144:MET:HB3	1.97	0.41
1:F:81:ASP:OD1	1:F:101:GLY:N	2.52	0.41
1:G:4:GLN:HE21	1:G:8:GLY:HA2	1.85	0.41
1:G:161:PHE:O	1:G:165:VAL:HG23	2.20	0.41
2:M:5:LEU:HB3	2:M:6:PHE:CD2	2.55	0.41
1:D:122:PRO:HA	1:D:123:PRO:HD3	1.88	0.41
1:F:124:ILE:O	1:F:126:VAL:N	2.52	0.41
1:I:68:MET:HE2	1:I:68:MET:HB3	1.89	0.41
1:B:120:HIS:CG	1:B:121:ASN:H	2.39	0.41
1:K:198:CYS:O	1:K:202:LEU:N	2.52	0.41
1:B:102:SER:HB2	1:B:107:THR:HB	2.02	0.41
1:I:91:ILE:HG12	1:I:97:ARG:HB3	2.03	0.41
1:C:161:PHE:O	1:C:165:VAL:HG23	2.21	0.41
1:F:107:THR:HG23	2:R:8:SER:HA	2.03	0.41
1:G:54:THR:HG21	1:L:42:ALA:HB2	2.03	0.41
1:J:23:TRP:CZ3	1:J:40:PHE:HB2	2.56	0.41
1:A:161:PHE:O	1:A:165:VAL:HG23	2.21	0.40
1:K:35:GLU:C	1:K:38:PRO:HD2	2.45	0.40
1:E:150:ILE:HG12	1:E:172:LEU:HD13	2.03	0.40
1:H:149:SER:HA	1:H:175:GLU:OE2	2.21	0.40
1:K:161:PHE:O	1:K:165:VAL:HG23	2.22	0.40
1:I:115:ILE:O	1:I:119:THR:OG1	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	210/231 (91%)	208 (99%)	2 (1%)	0	100	100
1	B	202/231 (87%)	200 (99%)	2 (1%)	0	100	100
1	C	208/231 (90%)	203 (98%)	5 (2%)	0	100	100
1	D	198/231 (86%)	196 (99%)	2 (1%)	0	100	100
1	E	199/231 (86%)	194 (98%)	5 (2%)	0	100	100
1	F	211/231 (91%)	205 (97%)	6 (3%)	0	100	100
1	G	214/231 (93%)	206 (96%)	8 (4%)	0	100	100
1	H	204/231 (88%)	201 (98%)	3 (2%)	0	100	100
1	I	210/231 (91%)	206 (98%)	4 (2%)	0	100	100
1	J	212/231 (92%)	204 (96%)	8 (4%)	0	100	100
1	K	197/231 (85%)	192 (98%)	5 (2%)	0	100	100
1	L	196/231 (85%)	192 (98%)	4 (2%)	0	100	100
2	O	4/9 (44%)	4 (100%)	0	0	100	100
2	P	5/9 (56%)	5 (100%)	0	0	100	100
2	Q	1/9 (11%)	1 (100%)	0	0	100	100
2	R	3/9 (33%)	3 (100%)	0	0	100	100
2	S	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	U	1/9 (11%)	1 (100%)	0	0	100	100
2	V	4/9 (44%)	4 (100%)	0	0	100	100
2	W	5/9 (56%)	5 (100%)	0	0	100	100
All	All	2488/2844 (88%)	2433 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	164/193 (85%)	163 (99%)	1 (1%)	78	83
1	B	167/193 (86%)	167 (100%)	0	100	100
1	C	172/193 (89%)	171 (99%)	1 (1%)	78	83
1	D	157/193 (81%)	155 (99%)	2 (1%)	61	77
1	E	164/193 (85%)	164 (100%)	0	100	100
1	F	169/193 (88%)	169 (100%)	0	100	100
1	G	172/193 (89%)	170 (99%)	2 (1%)	63	78
1	H	167/193 (86%)	167 (100%)	0	100	100
1	I	165/193 (86%)	165 (100%)	0	100	100
1	J	173/193 (90%)	172 (99%)	1 (1%)	78	83
1	K	158/193 (82%)	158 (100%)	0	100	100
1	L	156/193 (81%)	154 (99%)	2 (1%)	61	77
2	M	2/6 (33%)	1 (50%)	1 (50%)	0	0
2	N	1/6 (17%)	1 (100%)	0	100	100
2	O	3/6 (50%)	3 (100%)	0	100	100
2	P	2/6 (33%)	2 (100%)	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	100	100
2	R	2/6 (33%)	2 (100%)	0	100	100
2	S	2/6 (33%)	2 (100%)	0	100	100
2	T	1/6 (17%)	1 (100%)	0	100	100
2	U	2/6 (33%)	2 (100%)	0	100	100
2	V	2/6 (33%)	2 (100%)	0	100	100
2	W	2/6 (33%)	2 (100%)	0	100	100
2	X	2/6 (33%)	2 (100%)	0	100	100
All	All	2007/2388 (84%)	1997 (100%)	10 (0%)	81	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	THR
1	C	154	ARG
1	D	4	GLN
1	D	175	GLU
1	G	70	LYS
1	G	136	LEU
1	J	87	HIS
1	L	136	LEU
1	L	144	MET
2	M	6	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
1	B	121	ASN
1	C	7	GLN
1	C	12	HIS
1	C	95	GLN
1	D	193	ASN
1	E	12	HIS
1	F	7	GLN
1	F	67	GLN
1	G	84	HIS
1	H	84	HIS
1	I	95	GLN
1	I	193	ASN
1	J	4	GLN
1	K	12	HIS
1	K	62	HIS
1	K	121	ASN
1	L	67	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	214/231 (92%)	0.03	9 (4%) 40 22	34, 55, 102, 130	0
1	B	208/231 (90%)	0.03	5 (2%) 59 38	36, 57, 93, 135	0
1	C	212/231 (91%)	0.03	6 (2%) 55 34	32, 55, 103, 132	0
1	D	204/231 (88%)	0.17	8 (3%) 43 24	34, 56, 128, 157	0
1	E	205/231 (88%)	0.03	6 (2%) 53 32	34, 55, 97, 127	0
1	F	215/231 (93%)	0.05	1 (0%) 87 73	34, 59, 115, 123	0
1	G	218/231 (94%)	0.05	4 (1%) 67 47	42, 63, 112, 144	0
1	H	208/231 (90%)	0.29	10 (4%) 35 19	41, 69, 127, 198	0
1	I	214/231 (92%)	0.30	11 (5%) 33 18	38, 64, 108, 158	0
1	J	216/231 (93%)	0.14	13 (6%) 27 15	35, 53, 119, 153	0
1	K	203/231 (87%)	0.17	9 (4%) 39 21	37, 59, 131, 170	0
1	L	202/231 (87%)	0.16	8 (3%) 42 23	41, 67, 103, 164	0
2	M	2/9 (22%)	2.72	1 (50%) 0 0	83, 83, 83, 125	0
2	N	1/9 (11%)	1.40	0 100 100	54, 54, 54, 54	1 (100%)
2	O	6/9 (66%)	1.63	2 (33%) 1 0	66, 71, 86, 98	0
2	P	7/9 (77%)	1.54	1 (14%) 6 3	45, 65, 72, 83	7 (100%)
2	Q	3/9 (33%)	1.39	0 100 100	59, 59, 73, 75	0
2	R	5/9 (55%)	1.56	2 (40%) 1 0	60, 60, 75, 84	0
2	S	6/9 (66%)	1.39	1 (16%) 4 2	55, 65, 68, 73	0
2	T	2/9 (22%)	2.45	2 (100%) 0 0	64, 64, 64, 79	2 (100%)
2	U	3/9 (33%)	0.72	0 100 100	66, 66, 68, 72	0
2	V	6/9 (66%)	2.48	4 (66%) 0 0	53, 67, 86, 92	0
2	W	7/9 (77%)	1.60	2 (28%) 1 1	59, 76, 95, 106	0
2	X	2/9 (22%)	0.81	0 100 100	49, 49, 49, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2569/2880 (89%)	0.15	105 (4%)	41	23	32, 61, 114, 198	10 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	217	ALA	5.3
1	E	183	ASN	5.0
1	C	219	GLN	4.8
1	I	82	ARG	4.5
2	P	8	SER	4.4
1	L	6	LEU	4.4
1	D	197	ASP	4.2
1	J	216	THR	4.0
2	M	5	LEU	3.9
1	D	186	THR	3.7
1	D	188	THR	3.6
1	D	6	LEU	3.6
1	L	183	ASN	3.6
2	W	8	SER	3.4
1	H	157	PRO	3.4
1	G	180	GLU	3.4
2	V	3	GLY	3.3
1	I	92	ALA	3.2
1	H	96	MET	3.2
2	V	4	GLY	3.1
1	K	174	ALA	3.1
1	J	89	GLY	3.1
1	K	197	ASP	3.0
1	J	93	PRO	2.9
1	B	186	THR	2.9
2	V	8	SER	2.9
1	J	6	LEU	2.9
1	K	192	GLN	2.9
1	J	209	ALA	2.9
1	K	187	GLU	2.8
1	H	150	ILE	2.8
2	R	4	GLY	2.7
1	L	126	VAL	2.7
1	I	7	GLN	2.7
1	J	219	GLN	2.7
1	F	194	ALA	2.7
1	C	96	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	219	GLN	2.6
1	G	220	GLY	2.6
1	D	7	GLN	2.6
1	A	157	PRO	2.6
1	L	7	GLN	2.6
1	I	94	GLY	2.6
2	V	5	LEU	2.6
1	K	86	VAL	2.6
1	B	187	GLU	2.5
1	H	191	VAL	2.5
1	I	91	ILE	2.5
1	A	188	THR	2.5
2	W	7	GLY	2.5
1	J	204	ALA	2.5
1	E	176	GLN	2.5
1	A	6	LEU	2.5
2	O	3	GLY	2.5
2	T	7	GLY	2.5
1	D	219	GLN	2.5
2	T	6	PHE	2.4
1	J	210	THR	2.4
1	B	96	MET	2.4
1	I	187	GLU	2.4
2	S	5	LEU	2.4
1	E	98	GLU	2.4
1	J	213	GLU	2.4
1	J	218	CYS	2.4
2	O	6	PHE	2.3
1	A	186	THR	2.3
1	E	184	ALA	2.3
1	L	177	ALA	2.3
1	E	121	ASN	2.3
1	K	93	PRO	2.3
1	A	177	ALA	2.3
1	E	182	LYS	2.3
1	L	187	GLU	2.3
1	H	122	PRO	2.3
1	C	205	LEU	2.3
1	H	189	LEU	2.3
2	R	5	LEU	2.3
1	D	199	LYS	2.3
1	H	155	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	125	PRO	2.2
1	G	87	HIS	2.2
1	I	97	ARG	2.2
1	J	94	GLY	2.2
1	K	189	LEU	2.2
1	H	219	GLN	2.2
1	D	187	GLU	2.2
1	A	192	GLN	2.2
1	K	94	GLY	2.2
1	A	216	THR	2.2
1	B	178	SER	2.2
1	C	86	VAL	2.1
1	H	174	ALA	2.1
1	H	151	LEU	2.1
1	A	219	GLN	2.1
1	I	185	ALA	2.1
1	G	202	LEU	2.1
1	A	185	ALA	2.1
1	J	7	GLN	2.1
1	I	85	PRO	2.1
1	I	98	GLU	2.1
1	C	200	THR	2.1
1	B	94	GLY	2.0
1	C	6	LEU	2.0
1	K	194	ALA	2.0
1	I	198	CYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	301	1/1	0.87	0.15	71,71,71,71	0
3	CL	H	301	1/1	0.89	0.09	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.