



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:34 PM UTC

PDB ID : 9EE4 / pdb\_00009ee4  
Title : HIV CA - FG peptide (34 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](mailto: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>.

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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

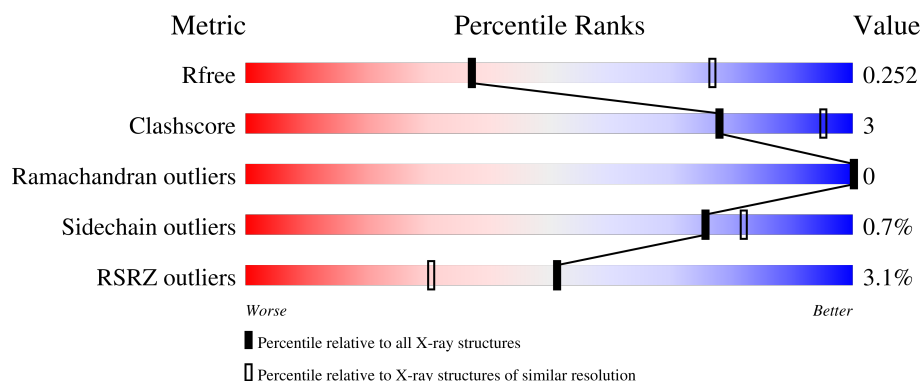
# 1 Overall quality at a glance

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.



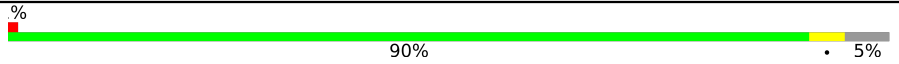
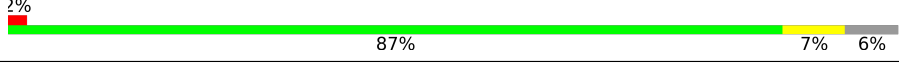



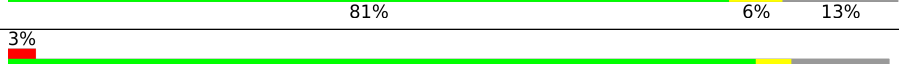

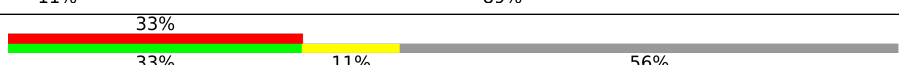


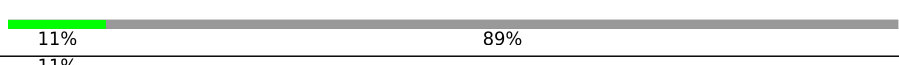





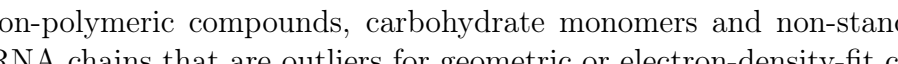
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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  $\geq 3$ , 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>5%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	231	<div> <div>84%</div> <div>5%</div> <div>10%</div> </div>
1	C	231	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	231	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	E	231	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</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	O	9	
2	P	9	
2	Q	9	
2	R	9	
2	S	9	
2	U	9	
2	V	9	
2	W	9	
2	X	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19347 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	218	Total	C	N	O	S	0	0	0
			1628	1026	284	304	14			
1	B	207	Total	C	N	O	S	0	0	0
			1586	998	275	299	14			
1	C	212	Total	C	N	O	S	0	0	0
			1622	1018	284	306	14			
1	D	202	Total	C	N	O	S	0	0	0
			1534	962	268	290	14			
1	E	213	Total	C	N	O	S	0	0	0
			1612	1015	282	301	14			
1	F	219	Total	C	N	O	S	0	0	0
			1661	1044	292	311	14			
1	G	218	Total	C	N	O	S	0	0	0
			1663	1043	293	313	14			
1	H	210	Total	C	N	O	S	0	0	0
			1593	1003	279	297	14			
1	I	212	Total	C	N	O	S	0	0	0
			1595	1010	274	297	14			
1	J	214	Total	C	N	O	S	0	0	0
			1634	1025	287	308	14			
1	K	201	Total	C	N	O	S	0	0	0
			1525	960	265	286	14			
1	L	205	Total	C	N	O	S	0	0	0
			1540	971	265	291	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 FG peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	4	Total	C	N	O	0	0	0
			25	17	4	4			
2	P	2	Total	C	N	O	0	0	0
			16	12	2	2			
2	S	2	Total	C	N	O	0	0	0
			16	12	2	2			
2	W	4	Total	C	N	O	0	0	0
			25	17	4	4			
2	X	2	Total	C	N	O	0	0	0
			15	11	2	2			
2	M	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	Q	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	R	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	U	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	V	1	Total	C	N	O	0	0	0
			11	9	1	1			

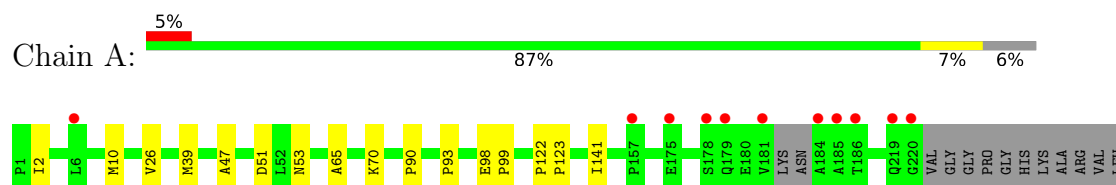
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		

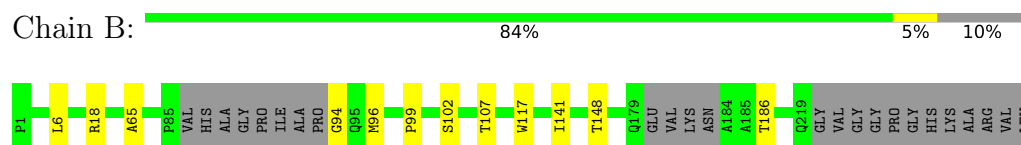
### 3 Residue-property plots [i](#)

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.

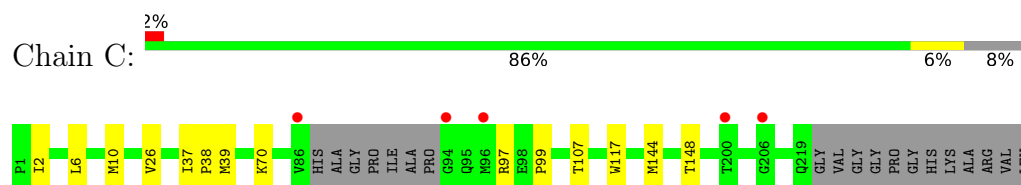
- Molecule 1: Capsid protein p24



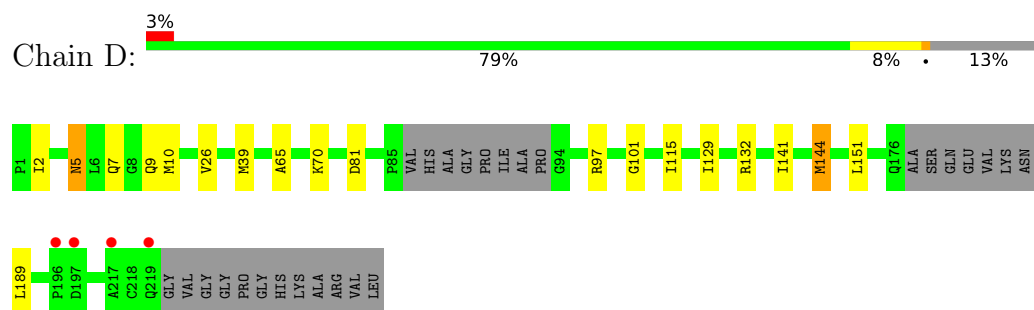
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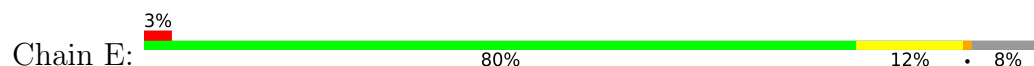
- Molecule 1: Capsid protein p24

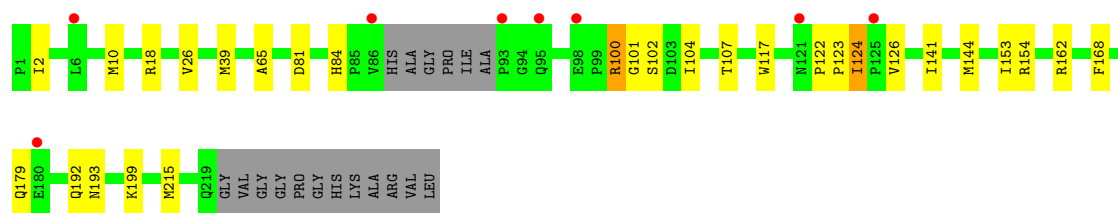


- Molecule 1: Capsid protein p24

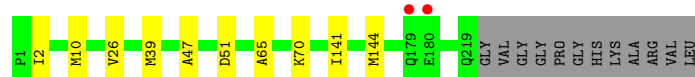
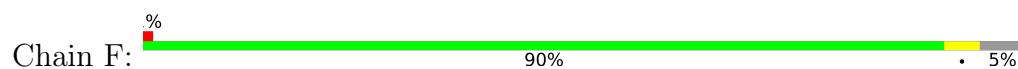


- Molecule 1: Capsid protein p24

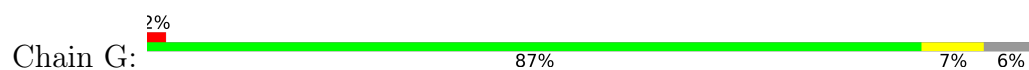




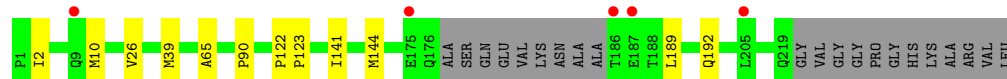
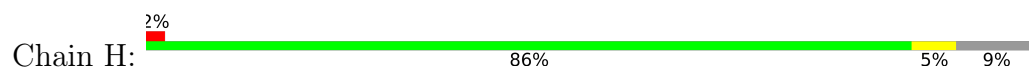
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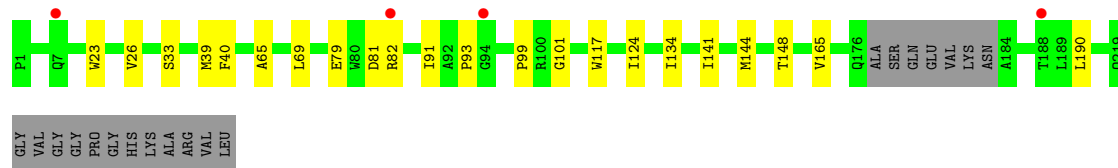
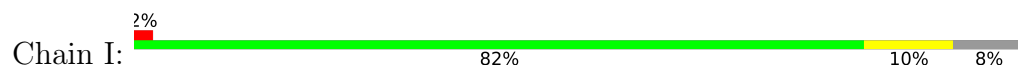
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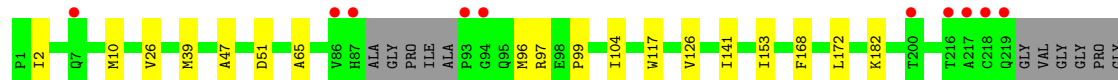
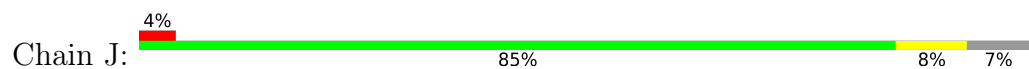
- Molecule 1: Capsid protein p24



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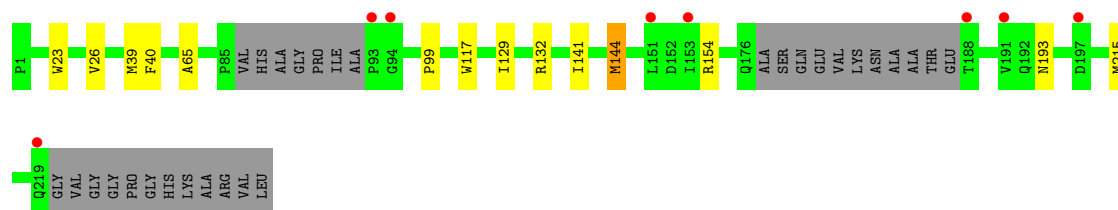
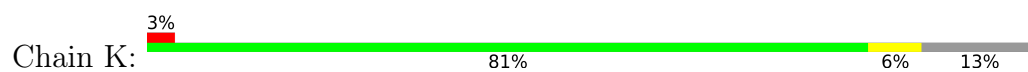


- Molecule 1: Capsid protein p24

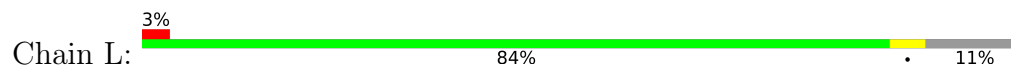


- Molecule 1: Capsid protein p24

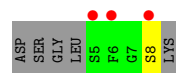
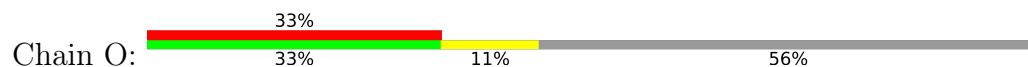




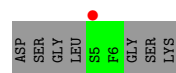
- Molecule 1: Capsid protein p24



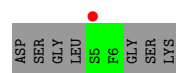
- Molecule 2: FG peptide



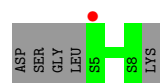
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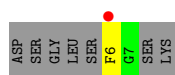


- Molecule 2: FG peptide

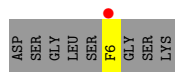


- Molecule 2: FG peptide

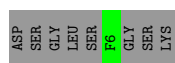




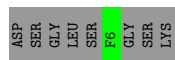
- Molecule 2: FG peptide



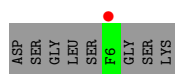
- Molecule 2: FG peptide



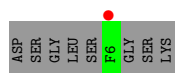
- Molecule 2: FG peptide



- Molecule 2: FG peptide



- Molecule 2: FG peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.91Å 136.40Å 207.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.07 – 3.10 33.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (33.07-3.10) 95.9 (33.07-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.219 , 0.252 0.219 , 0.252	Depositor DCC
$R_{free}$ test set	3441 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0/1664	0.21	0/2268
1	B	0.08	0/1618	0.20	0/2198
1	C	0.09	0/1655	0.21	0/2250
1	D	0.08	0/1566	0.21	0/2129
1	E	0.08	0/1646	0.21	0/2239
1	F	0.08	0/1698	0.20	0/2312
1	G	0.09	0/1699	0.20	0/2312
1	H	0.08	0/1629	0.20	0/2219
1	I	0.08	0/1631	0.20	0/2223
1	J	0.09	0/1668	0.22	0/2267
1	K	0.08	0/1558	0.19	0/2119
1	L	0.08	0/1572	0.20	0/2143
2	M	0.05	0/11	0.06	0/13
2	O	0.07	0/25	0.26	0/32
2	P	0.05	0/16	0.06	0/20
2	Q	0.05	0/11	0.05	0/13
2	R	0.07	0/11	0.09	0/13
2	S	0.06	0/16	0.09	0/20
2	U	0.08	0/11	0.10	0/13
2	V	0.05	0/11	0.08	0/13
2	W	0.04	0/25	0.15	0/32
2	X	0.05	0/15	0.09	0/18
All	All	0.08	0/19756	0.20	0/26866

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	1628	0	1571	10	0
1	B	1586	0	1556	7	0
1	C	1622	0	1584	9	0
1	D	1534	0	1464	13	0
1	E	1612	0	1570	16	0
1	F	1661	0	1611	5	0
1	G	1663	0	1620	10	0
1	H	1593	0	1545	8	0
1	I	1595	0	1554	12	0
1	J	1634	0	1594	11	0
1	K	1525	0	1465	8	0
1	L	1540	0	1475	7	0
2	M	11	0	8	2	0
2	O	25	0	15	1	0
2	P	16	0	10	0	0
2	Q	11	0	8	0	0
2	R	11	0	8	0	0
2	S	16	0	10	0	0
2	U	11	0	8	0	0
2	V	11	0	8	0	0
2	W	25	0	15	0	0
2	X	15	0	11	1	0
3	B	1	0	0	2	0
3	G	1	0	0	1	0
All	All	19347	0	18710	105	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 (105) 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)
3:G:301:CL:CL	1:L:18:ARG:NH2	2.52	0.80
1:B:18:ARG:NH2	3:B:301:CL:CL	2.65	0.67
1:E:104:ILE:HG12	1:E:126:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HG3	2:M:6:PHE:HB3	1.81	0.62
1:E:84:HIS:O	1:E:100:ARG:NH2	2.33	0.61
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.83	0.61
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.84	0.60
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.82	0.60
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.84	0.60
3:B:301:CL:CL	1:E:18:ARG:NH2	2.72	0.59
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.87	0.57
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.85	0.57
1:G:192:GLN:HA	1:G:199:LYS:HE2	1.87	0.56
1:J:104:ILE:HG12	1:J:126:VAL:HG12	1.87	0.56
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.86	0.56
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.87	0.56
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.87	0.56
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.87	0.56
1:A:53:ASN:OD1	2:M:6:PHE:N	2.39	0.55
1:B:96:MET:HE2	1:I:93:PRO:HA	1.88	0.55
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.88	0.55
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.88	0.55
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.89	0.55
1:G:2:ILE:HG22	1:G:10:MET:HE3	1.89	0.55
1:C:2:ILE:HG22	1:C:10:MET:HE3	1.88	0.54
1:D:129:ILE:HG12	1:D:132:ARG:HH12	1.72	0.54
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.90	0.54
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.88	0.53
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.89	0.53
1:I:81:ASP:OD1	1:I:101:GLY:N	2.42	0.53
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.89	0.53
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.91	0.52
1:D:5:ASN:HD21	1:D:7:GLN:HB2	1.76	0.51
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.91	0.51
1:K:129:ILE:HG12	1:K:132:ARG:HH12	1.75	0.51
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.92	0.51
1:E:117:TRP:HB3	1:E:124:ILE:O	2.11	0.51
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.93	0.51
1:D:5:ASN:OD1	1:D:9:GLN:N	2.45	0.50
1:A:90:PRO:HB2	1:J:97:ARG:HB2	1.94	0.50
1:E:179:GLN:HB3	1:F:70:LYS:HE3	1.93	0.50
1:J:153:ILE:HG21	1:J:168:PHE:HA	1.94	0.50
1:I:79:GLU:OE2	1:I:82:ARG:NH2	2.31	0.49
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:LEU:HD21	1:I:134:ILE:HG23	1.95	0.48
1:D:151:LEU:HA	1:D:189:LEU:HD21	1.95	0.48
1:H:189:LEU:HA	1:H:192:GLN:HB3	1.96	0.48
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.96	0.48
1:E:153:ILE:HG21	1:E:168:PHE:HA	1.95	0.48
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.49	0.47
1:B:99:PRO:HG3	1:B:117:TRP:CE2	2.49	0.47
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.96	0.47
1:G:81:ASP:OD1	1:G:101:GLY:N	2.47	0.47
1:I:117:TRP:HB3	1:I:124:ILE:HB	1.97	0.47
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.98	0.46
1:K:99:PRO:HG3	1:K:117:TRP:CE2	2.50	0.46
1:I:99:PRO:HG3	1:I:117:TRP:CE2	2.50	0.46
1:G:215:MET:HB2	1:H:144:MET:HE1	1.98	0.46
1:K:154:ARG:HA	1:K:193:ASN:HB3	1.97	0.46
1:D:81:ASP:OD1	1:D:101:GLY:N	2.49	0.46
1:E:117:TRP:HD1	1:E:124:ILE:HD12	1.80	0.45
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.98	0.45
1:H:2:ILE:HG22	1:H:10:MET:HE3	1.98	0.45
1:E:192:GLN:HA	1:E:199:LYS:HE3	1.99	0.45
1:J:172:LEU:HD21	1:J:182:LYS:HA	1.98	0.45
1:D:5:ASN:CG	1:D:7:GLN:H	2.24	0.45
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.52	0.44
1:G:158:LYS:HD3	1:G:158:LYS:H	1.82	0.44
1:K:215:MET:HE2	1:L:144:MET:HE1	1.98	0.44
1:L:57:ASN:HD21	2:X:6:PHE:N	2.15	0.44
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.99	0.44
1:E:102:SER:HB2	1:E:107:THR:HB	2.00	0.43
1:C:107:THR:HG23	2:O:8:SER:HA	2.00	0.43
1:I:144:MET:HE2	1:I:144:MET:HB3	1.90	0.43
1:B:6:LEU:HB3	1:C:6:LEU:HG	2.00	0.43
1:E:81:ASP:OD1	1:E:101:GLY:N	2.50	0.43
1:F:47:ALA:HB1	1:F:51:ASP:HB2	1.99	0.43
1:D:144:MET:HE2	1:D:144:MET:HB3	1.85	0.43
1:E:122:PRO:HA	1:E:123:PRO:HD3	1.91	0.43
1:C:97:ARG:HB2	1:H:90:PRO:HB2	2.01	0.43
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.92	0.42
1:D:2:ILE:HD11	1:D:115:ILE:HG12	2.00	0.42
1:H:122:PRO:HA	1:H:123:PRO:HD3	1.92	0.42
1:I:165:VAL:HG22	1:I:190:LEU:HD11	2.01	0.42
1:I:26:VAL:HG21	1:I:39:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:MET:HE2	1:C:144:MET:HB3	1.97	0.42
1:D:2:ILE:HG22	1:D:10:MET:HE3	2.00	0.42
1:A:2:ILE:HG22	1:A:10:MET:HE3	2.01	0.42
1:E:154:ARG:HA	1:E:193:ASN:HB3	2.02	0.42
1:A:122:PRO:HA	1:A:123:PRO:HD3	1.92	0.41
1:J:99:PRO:HG3	1:J:117:TRP:CD2	2.55	0.41
1:H:144:MET:HE2	1:H:144:MET:HB3	1.85	0.41
1:B:102:SER:HB2	1:B:107:THR:HB	2.01	0.41
1:G:54:THR:HG21	1:L:42:ALA:HB2	2.02	0.41
1:G:122:PRO:HA	1:G:123:PRO:HD3	1.93	0.41
1:J:47:ALA:HB1	1:J:51:ASP:HB2	2.02	0.41
1:C:37:ILE:HB	1:C:38:PRO:HD3	2.02	0.41
1:D:70:LYS:HB2	1:D:70:LYS:HE2	1.85	0.41
1:E:162:ARG:HA	1:E:215:MET:HE3	2.03	0.41
1:C:70:LYS:HE3	1:C:70:LYS:HB2	1.81	0.41
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.56	0.41
1:L:122:PRO:HA	1:L:123:PRO:HD3	1.89	0.41
1:B:94:GLY:HA2	1:I:91:ILE:HD13	2.02	0.41
1:I:23:TRP:CZ3	1:I:40:PHE:HB2	2.56	0.41
1:K:144:MET:HE2	1:K:144:MET:HB3	1.91	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	214/231 (93%)	210 (98%)	4 (2%)	0	100	100
1	B	201/231 (87%)	196 (98%)	5 (2%)	0	100	100
1	C	208/231 (90%)	200 (96%)	8 (4%)	0	100	100
1	D	196/231 (85%)	190 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	209/231 (90%)	202 (97%)	7 (3%)	0	100	100
1	F	217/231 (94%)	212 (98%)	5 (2%)	0	100	100
1	G	214/231 (93%)	205 (96%)	9 (4%)	0	100	100
1	H	206/231 (89%)	202 (98%)	4 (2%)	0	100	100
1	I	208/231 (90%)	203 (98%)	5 (2%)	0	100	100
1	J	210/231 (91%)	199 (95%)	11 (5%)	0	100	100
1	K	195/231 (84%)	189 (97%)	6 (3%)	0	100	100
1	L	199/231 (86%)	192 (96%)	7 (4%)	0	100	100
2	O	2/9 (22%)	2 (100%)	0	0	100	100
2	W	2/9 (22%)	2 (100%)	0	0	100	100
All	All	2481/2790 (89%)	2404 (97%)	77 (3%)	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	167/193 (86%)	167 (100%)	0	100	100
1	B	169/193 (88%)	167 (99%)	2 (1%)	63	78
1	C	172/193 (89%)	171 (99%)	1 (1%)	78	83
1	D	159/193 (82%)	156 (98%)	3 (2%)	50	73
1	E	168/193 (87%)	165 (98%)	3 (2%)	51	73
1	F	172/193 (89%)	171 (99%)	1 (1%)	78	83
1	G	175/193 (91%)	174 (99%)	1 (1%)	78	83
1	H	167/193 (86%)	167 (100%)	0	100	100
1	I	166/193 (86%)	164 (99%)	2 (1%)	63	78
1	J	173/193 (90%)	173 (100%)	0	100	100
1	K	159/193 (82%)	158 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	159/193 (82%)	158 (99%)	1 (1%)	78	83
2	M	1/7 (14%)	1 (100%)	0	100	100
2	O	1/7 (14%)	1 (100%)	0	100	100
2	P	1/7 (14%)	1 (100%)	0	100	100
2	Q	1/7 (14%)	1 (100%)	0	100	100
2	R	1/7 (14%)	1 (100%)	0	100	100
2	S	1/7 (14%)	1 (100%)	0	100	100
2	U	1/7 (14%)	1 (100%)	0	100	100
2	V	1/7 (14%)	1 (100%)	0	100	100
2	W	1/7 (14%)	1 (100%)	0	100	100
2	X	1/7 (14%)	1 (100%)	0	100	100
All	All	2016/2386 (84%)	2001 (99%)	15 (1%)	76	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	148	THR
1	B	186	THR
1	C	148	THR
1	D	5	ASN
1	D	144	MET
1	D	186	THR
1	E	100	ARG
1	E	124	ILE
1	E	144	MET
1	F	144	MET
1	G	100	ARG
1	I	33	SER
1	I	148	THR
1	K	144	MET
1	L	144	MET

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

Mol	Chain	Res	Type
1	B	7	GLN
1	B	9	GLN

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Mol	Chain	Res	Type
1	C	4	GLN
1	C	62	HIS
1	D	193	ASN
1	F	155	GLN
1	G	62	HIS
1	H	95	GLN
1	I	67	GLN
1	J	21	ASN
1	J	95	GLN
1	K	155	GLN
1	L	57	ASN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	218/231 (94%)	0.06	11 (5%) 34 18	38, 58, 106, 127	0
1	B	207/231 (89%)	-0.03	0 100 100	40, 62, 91, 111	0
1	C	212/231 (91%)	-0.01	5 (2%) 59 38	37, 59, 102, 138	0
1	D	202/231 (87%)	0.16	6 (2%) 52 31	36, 61, 125, 148	0
1	E	213/231 (92%)	0.12	8 (3%) 44 25	36, 62, 104, 140	0
1	F	219/231 (94%)	-0.01	2 (0%) 81 63	38, 62, 101, 117	0
1	G	218/231 (94%)	0.07	4 (1%) 67 47	44, 67, 109, 130	0
1	H	210/231 (90%)	0.20	5 (2%) 59 38	43, 69, 115, 152	0
1	I	212/231 (91%)	0.11	4 (1%) 66 45	42, 68, 101, 128	0
1	J	214/231 (92%)	0.08	10 (4%) 36 19	39, 59, 112, 146	0
1	K	201/231 (87%)	0.21	8 (3%) 42 23	40, 65, 128, 159	0
1	L	205/231 (88%)	0.20	7 (3%) 48 28	43, 70, 114, 146	0
2	M	1/9 (11%)	2.40	1 (100%) 0 0	73, 73, 73, 73	1 (100%)
2	O	4/9 (44%)	2.46	3 (75%) 0 0	73, 78, 81, 104	0
2	P	2/9 (22%)	2.49	1 (50%) 0 0	48, 48, 48, 57	2 (100%)
2	Q	1/9 (11%)	0.84	0 100 100	70, 70, 70, 70	0
2	R	1/9 (11%)	1.52	0 100 100	63, 63, 63, 63	1 (100%)
2	S	2/9 (22%)	2.69	1 (50%) 0 0	61, 61, 61, 82	0
2	U	1/9 (11%)	2.16	1 (100%) 0 0	94, 94, 94, 94	0
2	V	1/9 (11%)	3.43	1 (100%) 0 0	72, 72, 72, 72	0
2	W	4/9 (44%)	1.39	1 (25%) 2 1	56, 59, 62, 66	4 (100%)
2	X	2/9 (22%)	1.98	1 (50%) 0 0	75, 75, 75, 84	0
All	All	2550/2862 (89%)	0.11	80 (3%) 51 30	36, 64, 111, 159	8 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	GLN	6.0
1	J	217	ALA	5.0
2	S	5	SER	4.3
1	E	95	GLN	4.2
1	A	181	VAL	4.1
1	E	180	GLU	3.7
2	V	6	PHE	3.4
2	P	5	SER	3.4
1	L	180	GLU	3.4
1	J	86	VAL	3.2
1	D	196	PRO	3.2
1	A	178	SER	3.2
2	O	8	SER	3.1
1	A	184	ALA	3.1
1	D	188	THR	3.1
1	L	186	THR	3.1
2	O	5	SER	3.0
2	W	5	SER	2.9
1	G	160	PRO	2.8
1	G	220	GLY	2.8
1	E	121	ASN	2.7
1	J	219	GLN	2.7
1	I	94	GLY	2.7
1	J	218	CYS	2.7
1	L	183	ASN	2.7
1	A	157	PRO	2.6
1	H	205	LEU	2.6
1	D	197	ASP	2.6
1	E	86	VAL	2.5
1	E	6	LEU	2.5
1	C	94	GLY	2.5
1	K	94	GLY	2.5
1	D	187	GLU	2.5
1	L	219	GLN	2.5
1	C	200	THR	2.4
1	A	179	GLN	2.4
1	K	151	LEU	2.4
1	A	186	THR	2.4
1	E	93	PRO	2.4
2	M	6	PHE	2.4
1	C	96	MET	2.4
1	F	179	GLN	2.4
1	A	175	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	187	GLU	2.4
1	C	86	VAL	2.4
1	J	216	THR	2.3
1	K	197	ASP	2.3
1	L	85	PRO	2.3
1	I	188	THR	2.3
1	G	188	THR	2.3
1	J	200	THR	2.3
1	I	82	ARG	2.3
1	I	7	GLN	2.3
1	K	153	ILE	2.2
1	J	93	PRO	2.2
1	L	178	SER	2.2
1	A	219	GLN	2.2
1	E	125	PRO	2.2
1	J	87	HIS	2.2
1	K	219	GLN	2.2
1	D	217	ALA	2.2
2	U	6	PHE	2.2
1	A	6	LEU	2.1
1	E	98	GLU	2.1
2	X	6	PHE	2.1
1	K	93	PRO	2.1
1	H	9	GLN	2.1
1	H	187	GLU	2.1
1	K	191	VAL	2.1
1	A	220	GLY	2.1
2	O	6	PHE	2.1
1	G	218	CYS	2.1
1	A	185	ALA	2.1
1	C	206	GLY	2.1
1	H	186	THR	2.0
1	J	7	GLN	2.0
1	J	94	GLY	2.0
1	H	175	GLU	2.0
1	K	188	THR	2.0
1	F	180	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CL	G	301	1/1	0.90	0.05	68,68,68,68	0
3	CL	B	301	1/1	0.95	0.05	77,77,77,77	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.