



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 07:02 AM EDT

PDB ID : 3JTL  
Title : Crystal structure of archaeal 20S proteasome in complex with mutated P26 activator  
Authors : Stadtmueller, B.M.; Whitby, F.G.; Hill, C.P.  
Deposited on : 2009-09-12  
Resolution : 3.20 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>.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

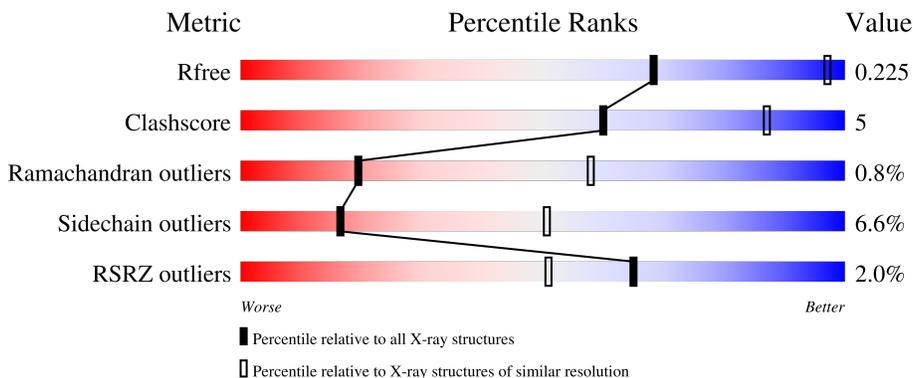
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	227	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">3%      82%      17%      .</p>
1	B	227	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">4%      86%      12%      .</p>
1	C	227	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      85%      13%      .</p>
1	D	227	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">4%      83%      15%      .</p>
1	E	227	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">3%      82%      17%      .</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	 4% 82% 17% .
1	G	227	 3% 78% 20% .
2	H	203	 % 82% 15% .
2	I	203	 % 85% 14% .
2	J	203	 2% 83% 14% .
2	K	203	 % 84% 14% .
2	L	203	 % 84% 14% .
2	M	203	 % 84% 14% .
2	N	203	 % 84% 14% .
3	O	228	 % 84% 11% .
3	P	228	 2% 82% 12% .
3	Q	228	 2% 83% 12% .
3	R	228	 % 84% 11% .
3	S	228	 % 84% 11% .
3	T	228	 2% 85% 10% .
3	U	228	 % 83% 11% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35140 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	B	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	C	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	D	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	E	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	F	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	G	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	I	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	J	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	K	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	L	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	M	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	N	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0

- Molecule 3 is a protein called Proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	P	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	Q	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	R	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	S	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	T	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	U	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	variant	UNP Q9U8G2
O	225	HIS	GLY	engineered mutation	UNP Q9U8G2
O	226	LEU	SER	engineered mutation	UNP Q9U8G2
O	228	VAL	HIS	engineered mutation	UNP Q9U8G2
O	229	LEU	MET	engineered mutation	UNP Q9U8G2
O	230	TYR	VAL	engineered mutation	UNP Q9U8G2
O	231	ARG	SER	engineered mutation	UNP Q9U8G2
P	49	VAL	THR	variant	UNP Q9U8G2
P	225	HIS	GLY	engineered mutation	UNP Q9U8G2
P	226	LEU	SER	engineered mutation	UNP Q9U8G2
P	228	VAL	HIS	engineered mutation	UNP Q9U8G2
P	229	LEU	MET	engineered mutation	UNP Q9U8G2
P	230	TYR	VAL	engineered mutation	UNP Q9U8G2
P	231	ARG	SER	engineered mutation	UNP Q9U8G2
Q	49	VAL	THR	variant	UNP Q9U8G2
Q	225	HIS	GLY	engineered mutation	UNP Q9U8G2
Q	226	LEU	SER	engineered mutation	UNP Q9U8G2
Q	228	VAL	HIS	engineered mutation	UNP Q9U8G2
Q	229	LEU	MET	engineered mutation	UNP Q9U8G2
Q	230	TYR	VAL	engineered mutation	UNP Q9U8G2
Q	231	ARG	SER	engineered mutation	UNP Q9U8G2
R	49	VAL	THR	variant	UNP Q9U8G2
R	225	HIS	GLY	engineered mutation	UNP Q9U8G2
R	226	LEU	SER	engineered mutation	UNP Q9U8G2

*Continued on next page...*

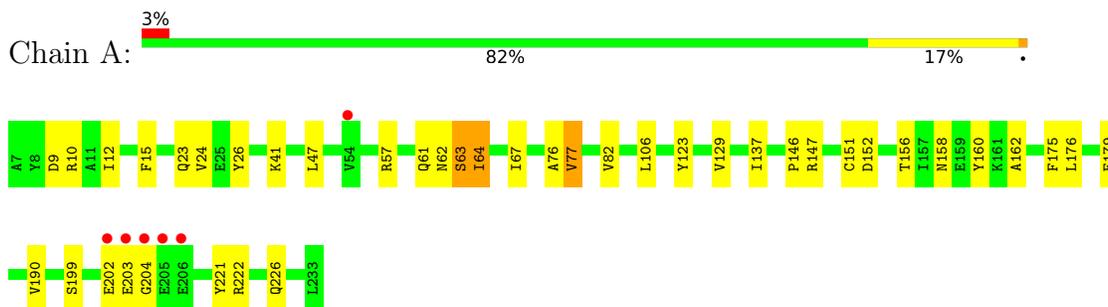
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
R	228	VAL	HIS	engineered mutation	UNP Q9U8G2
R	229	LEU	MET	engineered mutation	UNP Q9U8G2
R	230	TYR	VAL	engineered mutation	UNP Q9U8G2
R	231	ARG	SER	engineered mutation	UNP Q9U8G2
S	49	VAL	THR	variant	UNP Q9U8G2
S	225	HIS	GLY	engineered mutation	UNP Q9U8G2
S	226	LEU	SER	engineered mutation	UNP Q9U8G2
S	228	VAL	HIS	engineered mutation	UNP Q9U8G2
S	229	LEU	MET	engineered mutation	UNP Q9U8G2
S	230	TYR	VAL	engineered mutation	UNP Q9U8G2
S	231	ARG	SER	engineered mutation	UNP Q9U8G2
T	49	VAL	THR	variant	UNP Q9U8G2
T	225	HIS	GLY	engineered mutation	UNP Q9U8G2
T	226	LEU	SER	engineered mutation	UNP Q9U8G2
T	228	VAL	HIS	engineered mutation	UNP Q9U8G2
T	229	LEU	MET	engineered mutation	UNP Q9U8G2
T	230	TYR	VAL	engineered mutation	UNP Q9U8G2
T	231	ARG	SER	engineered mutation	UNP Q9U8G2
U	49	VAL	THR	variant	UNP Q9U8G2
U	225	HIS	GLY	engineered mutation	UNP Q9U8G2
U	226	LEU	SER	engineered mutation	UNP Q9U8G2
U	228	VAL	HIS	engineered mutation	UNP Q9U8G2
U	229	LEU	MET	engineered mutation	UNP Q9U8G2
U	230	TYR	VAL	engineered mutation	UNP Q9U8G2
U	231	ARG	SER	engineered mutation	UNP Q9U8G2

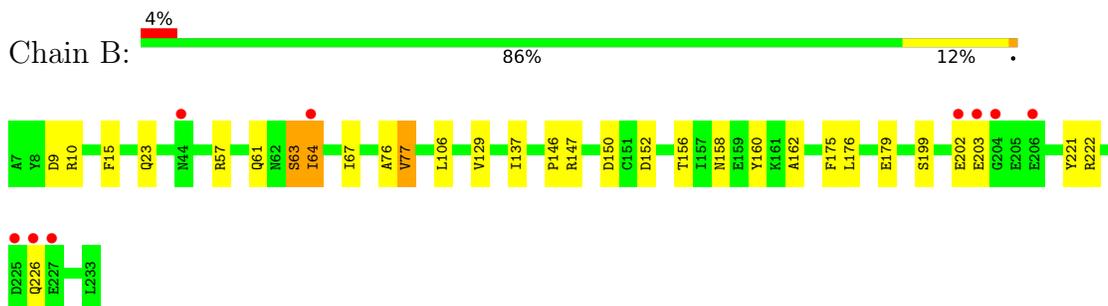
### 3 Residue-property plots [i](#)

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.

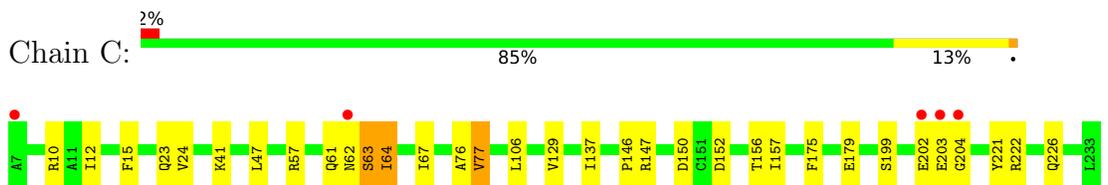
- Molecule 1: Proteasome subunit alpha



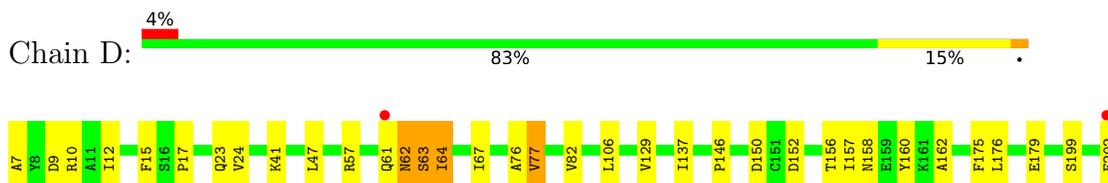
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

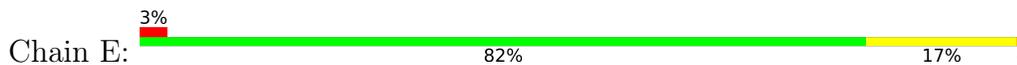


- Molecule 1: Proteasome subunit alpha

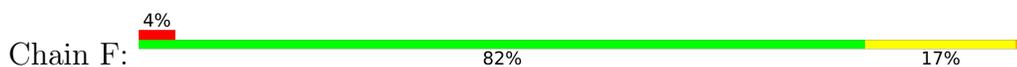




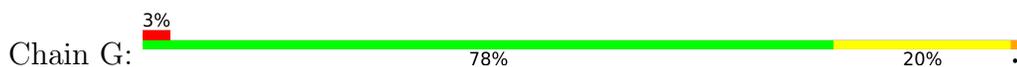
- Molecule 1: Proteasome subunit alpha



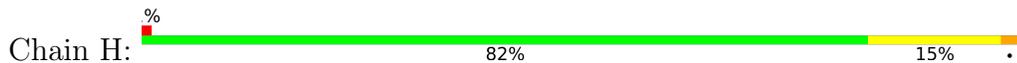
- Molecule 1: Proteasome subunit alpha



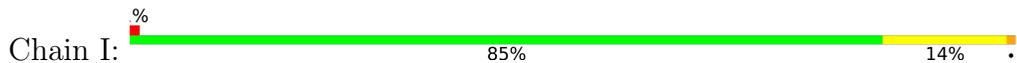
- Molecule 1: Proteasome subunit alpha



- Molecule 2: Proteasome subunit beta

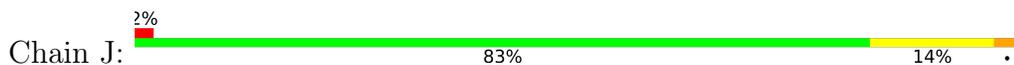


- Molecule 2: Proteasome subunit beta

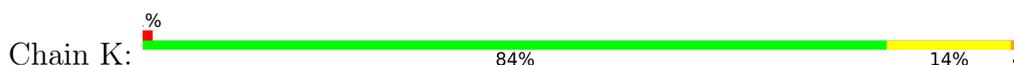




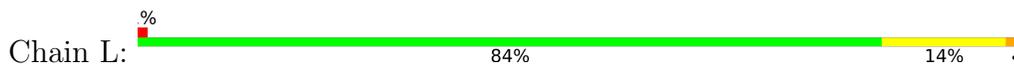
• Molecule 2: Proteasome subunit beta



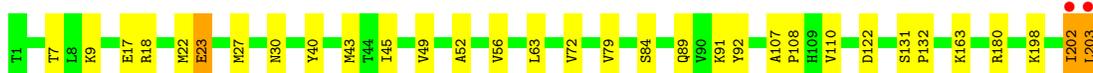
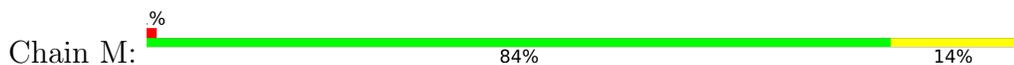
• Molecule 2: Proteasome subunit beta



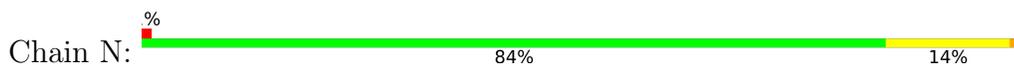
• Molecule 2: Proteasome subunit beta



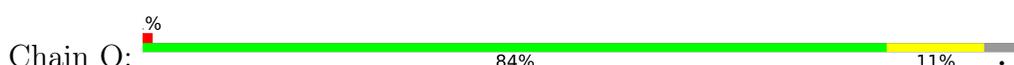
• Molecule 2: Proteasome subunit beta

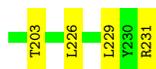


• Molecule 2: Proteasome subunit beta

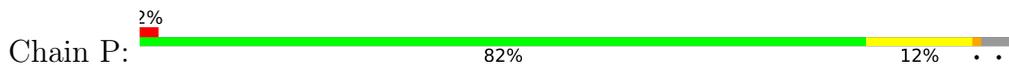


• Molecule 3: Proteasome activator protein PA26

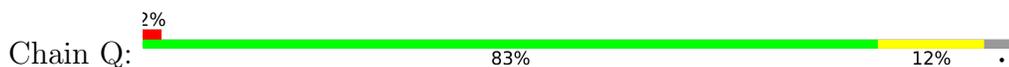




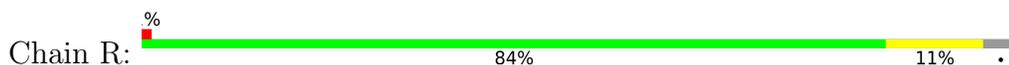
- Molecule 3: Proteasome activator protein PA26



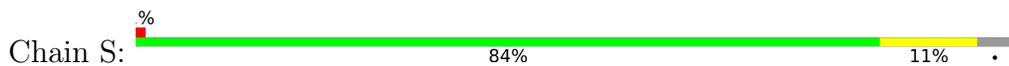
- Molecule 3: Proteasome activator protein PA26



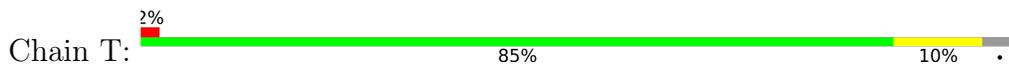
- Molecule 3: Proteasome activator protein PA26



- Molecule 3: Proteasome activator protein PA26

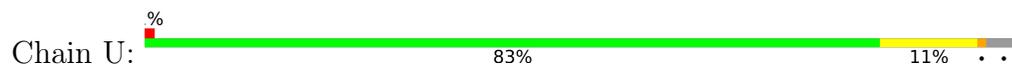


- Molecule 3: Proteasome activator protein PA26





● Molecule 3: Proteasome activator protein PA26



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.83Å 126.58Å 182.17Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	29.85 – 3.20 29.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.85-3.20) 99.0 (29.85-3.20)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.18Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.226 0.199 , 0.225	Depositor DCC
$R_{free}$ test set	1905 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	35140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 [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	0.78	1/1793 (0.1%)	0.75	0/2416
1	B	0.77	0/1793	0.74	0/2416
1	C	0.77	0/1793	0.75	0/2416
1	D	0.81	1/1793 (0.1%)	0.75	0/2416
1	E	0.81	1/1793 (0.1%)	0.78	0/2416
1	F	0.77	1/1793 (0.1%)	0.77	0/2416
1	G	0.77	1/1793 (0.1%)	0.74	0/2416
2	H	0.83	1/1576 (0.1%)	0.80	0/2129
2	I	0.83	3/1576 (0.2%)	0.80	1/2129 (0.0%)
2	J	0.81	1/1576 (0.1%)	0.80	2/2129 (0.1%)
2	K	0.84	3/1576 (0.2%)	0.80	1/2129 (0.0%)
2	L	0.83	1/1576 (0.1%)	0.78	1/2129 (0.0%)
2	M	0.86	2/1576 (0.1%)	0.81	2/2129 (0.1%)
2	N	0.85	3/1576 (0.2%)	0.81	2/2129 (0.1%)
3	O	0.74	0/1718	0.72	0/2322
3	P	0.71	0/1718	0.73	2/2322 (0.1%)
3	Q	0.72	0/1718	0.72	0/2322
3	R	0.75	0/1718	0.72	1/2322 (0.0%)
3	S	0.74	0/1718	0.71	0/2322
3	T	0.73	0/1718	0.72	0/2322
3	U	0.77	1/1718 (0.1%)	0.72	1/2322 (0.0%)
All	All	0.78	20/35609 (0.1%)	0.76	13/48069 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	T	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	22	MET	CG-SD	6.40	1.97	1.81
3	U	35	GLU	CG-CD	6.27	1.61	1.51
1	E	7	ALA	CA-CB	6.17	1.65	1.52
1	A	151	CYS	CB-SG	-6.11	1.71	1.82
2	M	22	MET	CB-CG	5.91	1.70	1.51
2	N	22	MET	CB-CG	5.89	1.70	1.51
2	K	22	MET	CB-CG	5.78	1.69	1.51
2	N	22	MET	CG-SD	5.68	1.96	1.81
1	G	151	CYS	CB-SG	-5.60	1.72	1.81
2	H	22	MET	CB-CG	5.59	1.69	1.51
2	I	22	MET	CG-SD	5.54	1.95	1.81
2	I	22	MET	CB-CG	5.51	1.69	1.51
2	J	22	MET	CB-CG	5.32	1.68	1.51
2	K	22	MET	CG-SD	5.31	1.95	1.81
1	F	151	CYS	CB-SG	-5.28	1.73	1.81
2	L	22	MET	CB-CG	5.24	1.68	1.51
2	N	122	ASP	CB-CG	5.13	1.62	1.51
1	D	7	ALA	CA-CB	5.08	1.63	1.52
2	K	202	ILE	CA-CB	5.03	1.66	1.54
2	I	62	GLU	CG-CD	5.00	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	184	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	J	22	MET	CG-SD-CE	5.59	109.15	100.20
2	M	22	MET	CB-CG-SD	5.54	129.01	112.40
2	N	22	MET	CG-SD-CE	5.52	109.03	100.20
2	N	22	MET	CB-CG-SD	5.50	128.89	112.40
2	I	22	MET	CB-CG-SD	5.30	128.31	112.40
2	J	22	MET	CB-CG-SD	5.16	127.87	112.40
2	M	22	MET	CG-SD-CE	5.11	108.38	100.20
3	U	226	LEU	CA-CB-CG	5.09	127.01	115.30
3	R	226	LEU	CA-CB-CG	5.06	126.94	115.30
3	P	226	LEU	CA-CB-CG	5.02	126.85	115.30
2	K	22	MET	CB-CG-SD	5.01	127.44	112.40
2	L	22	MET	CB-CG-SD	5.01	127.44	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	223	ARG	Peptide

## 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	1769	0	1800	19	0
1	B	1769	0	1800	12	0
1	C	1769	0	1800	13	0
1	D	1769	0	1800	24	0
1	E	1769	0	1800	25	2
1	F	1769	0	1800	28	0
1	G	1769	0	1800	25	0
2	H	1557	0	1609	18	0
2	I	1557	0	1609	17	0
2	J	1557	0	1609	16	0
2	K	1557	0	1609	16	0
2	L	1557	0	1609	16	0
2	M	1557	0	1609	15	2
2	N	1557	0	1609	15	0
3	O	1694	0	1722	19	0
3	P	1694	0	1722	18	0
3	Q	1694	0	1722	16	0
3	R	1694	0	1722	15	1
3	S	1694	0	1722	13	0
3	T	1694	0	1722	15	0
3	U	1694	0	1722	20	1
All	All	35140	0	35917	325	3

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 5.

All (325) 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:N:43:MET:CE	2:N:56:VAL:HG22	2.02	0.90
2:I:43:MET:CE	2:I:56:VAL:HG22	2.03	0.89
3:T:89:ARG:HD3	3:U:203:THR:HG21	1.54	0.86
2:J:43:MET:CE	2:J:56:VAL:HG22	2.06	0.85
3:S:89:ARG:HD3	3:T:203:THR:HG21	1.59	0.84
2:K:43:MET:CE	2:K:56:VAL:HG22	2.11	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:ARG:HD3	3:Q:203:THR:HG21	1.61	0.81
2:L:43:MET:CE	2:L:56:VAL:HG22	2.12	0.80
2:M:202:ILE:HG22	2:M:203:LEU:H	1.48	0.79
2:I:202:ILE:HG22	2:I:203:LEU:H	1.47	0.79
2:K:202:ILE:HG22	2:K:203:LEU:H	1.47	0.78
2:N:202:ILE:HG22	2:N:203:LEU:H	1.49	0.78
2:L:202:ILE:HG22	2:L:203:LEU:H	1.48	0.77
2:H:43:MET:CE	2:H:56:VAL:HG22	2.15	0.77
3:O:203:THR:HG21	3:U:89:ARG:HD3	1.68	0.76
2:H:202:ILE:HG22	2:H:203:LEU:H	1.49	0.76
3:O:89:ARG:HD3	3:P:203:THR:HG21	1.68	0.76
2:J:202:ILE:HG22	2:J:203:LEU:H	1.51	0.75
3:R:89:ARG:HD3	3:S:203:THR:HG21	1.71	0.73
3:Q:89:ARG:HD3	3:R:203:THR:HG21	1.71	0.71
1:E:17:PRO:HA	1:F:26:TYR:CG	2.29	0.68
2:I:202:ILE:HG22	2:I:203:LEU:N	2.10	0.67
2:K:202:ILE:HG22	2:K:203:LEU:N	2.11	0.65
2:M:202:ILE:HG22	2:M:203:LEU:N	2.10	0.65
2:M:43:MET:CE	2:M:56:VAL:HG22	2.27	0.65
2:L:202:ILE:HG22	2:L:203:LEU:N	2.11	0.65
2:J:202:ILE:HG22	2:J:203:LEU:N	2.14	0.63
2:N:202:ILE:HG22	2:N:203:LEU:N	2.13	0.62
1:D:82:VAL:CG1	3:T:231:ARG:HB2	2.29	0.62
2:H:202:ILE:HG22	2:H:203:LEU:N	2.13	0.61
1:C:77:VAL:HG23	1:C:137:ILE:HB	1.83	0.60
2:L:163:LYS:NZ	2:L:203:LEU:HB3	2.16	0.60
1:F:77:VAL:HG23	1:F:137:ILE:HB	1.84	0.60
1:B:77:VAL:HG23	1:B:137:ILE:HB	1.83	0.60
1:D:77:VAL:HG23	1:D:137:ILE:HB	1.84	0.60
2:I:163:LYS:NZ	2:I:203:LEU:HB3	2.17	0.59
1:G:77:VAL:HG23	1:G:137:ILE:HB	1.85	0.57
2:I:107:ALA:HB1	2:I:108:PRO:CD	2.35	0.56
1:A:77:VAL:HG23	1:A:137:ILE:HB	1.87	0.56
2:I:63:LEU:HD21	2:I:79:VAL:HG22	1.86	0.56
2:M:107:ALA:HB1	2:M:108:PRO:CD	2.35	0.56
2:H:107:ALA:HB1	2:H:108:PRO:CD	2.37	0.55
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.21	0.55
2:I:43:MET:HE3	2:I:56:VAL:HG22	1.87	0.55
2:J:107:ALA:HB1	2:J:108:PRO:CD	2.36	0.55
3:O:67:LEU:HD11	3:O:187:ASP:HB3	1.89	0.55
2:L:107:ALA:HB1	2:L:108:PRO:CD	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.88	0.54
2:K:63:LEU:HD21	2:K:79:VAL:HG22	1.89	0.54
1:E:82:VAL:HG22	3:U:229:LEU:O	2.07	0.54
1:G:9:ASP:O	1:G:23:GLN:NE2	2.41	0.54
1:E:82:VAL:CG1	3:U:231:ARG:HB2	2.37	0.54
2:J:63:LEU:HD21	2:J:79:VAL:HG22	1.90	0.54
2:N:43:MET:HE1	2:N:56:VAL:HG22	1.87	0.54
1:B:15:PHE:N	1:C:23:GLN:OE1	2.41	0.54
1:A:152:ASP:OD1	1:A:156:THR:HB	2.08	0.53
1:E:77:VAL:HG23	1:E:137:ILE:HB	1.89	0.53
2:K:107:ALA:HB1	2:K:108:PRO:CD	2.38	0.53
3:O:178:SER:HG	3:U:63:SER:HG	1.57	0.53
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.90	0.53
3:R:50:ILE:HD11	3:R:67:LEU:HD21	1.89	0.53
1:F:67:ILE:HG12	1:F:77:VAL:HG13	1.90	0.53
3:Q:50:ILE:HD11	3:Q:67:LEU:HD21	1.91	0.53
2:L:63:LEU:HD21	2:L:79:VAL:HG22	1.90	0.53
1:D:152:ASP:OD1	1:D:156:THR:HB	2.09	0.52
2:N:107:ALA:HB1	2:N:108:PRO:CD	2.39	0.52
3:R:36:ILE:HG12	3:R:77:LEU:HD21	1.91	0.52
2:H:7:THR:HG22	2:H:110:VAL:HG23	1.90	0.52
3:O:36:ILE:CG1	3:O:77:LEU:HD21	2.39	0.52
3:Q:36:ILE:CG1	3:Q:77:LEU:HD21	2.38	0.52
3:P:50:ILE:HD11	3:P:67:LEU:HD21	1.92	0.52
3:R:36:ILE:CG1	3:R:77:LEU:HD21	2.40	0.52
3:T:36:ILE:CG1	3:T:77:LEU:HD21	2.39	0.52
3:U:24:VAL:HG13	3:U:84:GLN:HB3	1.91	0.52
3:P:36:ILE:CG1	3:P:77:LEU:HD21	2.39	0.52
3:P:36:ILE:HG12	3:P:77:LEU:HD21	1.91	0.51
1:F:9:ASP:O	1:F:23:GLN:NE2	2.44	0.51
3:T:36:ILE:HG12	3:T:77:LEU:HD21	1.91	0.51
2:M:163:LYS:NZ	2:M:203:LEU:HB3	2.26	0.51
2:K:7:THR:HG22	2:K:110:VAL:HG23	1.91	0.51
3:R:67:LEU:HD11	3:R:187:ASP:HB3	1.93	0.51
1:F:63:SER:OG	1:F:64:ILE:N	2.44	0.51
2:I:7:THR:HG22	2:I:110:VAL:HG23	1.93	0.51
2:J:163:LYS:NZ	2:J:203:LEU:HB3	2.26	0.51
2:L:45:ILE:HB	2:L:52:ALA:HB1	1.92	0.51
3:T:24:VAL:HG13	3:T:84:GLN:HB3	1.93	0.51
1:F:152:ASP:OD1	1:F:156:THR:HB	2.10	0.51
1:D:12:ILE:HD11	1:D:24:VAL:HG23	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:THR:HG22	2:L:110:VAL:HG23	1.93	0.50
1:E:17:PRO:HB3	3:P:105:LEU:HD11	1.92	0.50
2:M:63:LEU:HD21	2:M:79:VAL:HG22	1.93	0.50
1:E:175:PHE:CE1	1:E:179:GLU:HG3	2.46	0.50
1:G:67:ILE:HG12	1:G:77:VAL:HG13	1.92	0.50
3:Q:24:VAL:HG13	3:Q:84:GLN:HB3	1.93	0.50
3:Q:67:LEU:HD11	3:Q:187:ASP:HB3	1.92	0.50
3:U:36:ILE:HG12	3:U:77:LEU:HD21	1.93	0.50
3:P:67:LEU:HD11	3:P:187:ASP:HB3	1.93	0.50
3:Q:36:ILE:HG12	3:Q:77:LEU:HD21	1.92	0.50
2:N:7:THR:HG22	2:N:110:VAL:HG23	1.93	0.50
1:E:63:SER:OG	1:E:64:ILE:N	2.44	0.49
1:F:82:VAL:CG1	3:O:231:ARG:HB2	2.41	0.49
1:E:67:ILE:HG12	1:E:77:VAL:HG13	1.94	0.49
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.94	0.49
2:H:3:THR:HB	2:H:16:THR:HG22	1.95	0.49
3:S:67:LEU:HD11	3:S:187:ASP:HB3	1.94	0.49
2:J:45:ILE:HB	2:J:52:ALA:HB1	1.95	0.49
1:E:17:PRO:HA	1:F:26:TYR:CD2	2.48	0.49
3:O:36:ILE:HG12	3:O:77:LEU:HD21	1.93	0.49
3:R:99:HIS:HB3	3:S:109:VAL:HG22	1.95	0.48
3:U:36:ILE:CG1	3:U:77:LEU:HD21	2.42	0.48
1:A:67:ILE:HG12	1:A:77:VAL:HG13	1.95	0.48
2:K:163:LYS:NZ	2:K:203:LEU:HB3	2.28	0.48
3:U:50:ILE:HD11	3:U:67:LEU:HD21	1.95	0.48
3:T:50:ILE:HD11	3:T:67:LEU:HD21	1.95	0.48
2:K:3:THR:HB	2:K:16:THR:HG22	1.96	0.48
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.95	0.48
3:U:50:ILE:HD11	3:U:67:LEU:HD11	1.95	0.48
3:O:99:HIS:HB3	3:P:109:VAL:HG22	1.95	0.48
1:A:175:PHE:CE1	1:A:179:GLU:HG3	2.49	0.48
2:N:7:THR:CG2	2:N:110:VAL:HG23	2.44	0.48
1:A:82:VAL:HG21	1:G:156:THR:HG23	1.96	0.48
1:D:12:ILE:HD11	1:D:24:VAL:CG2	2.44	0.48
2:J:43:MET:HE3	2:J:56:VAL:HG22	1.90	0.48
3:S:113:VAL:HA	3:S:116:ILE:HG22	1.96	0.48
3:U:89:ARG:NH2	3:U:118:ASP:OD1	2.46	0.47
3:U:67:LEU:HD11	3:U:187:ASP:HB3	1.96	0.47
2:H:63:LEU:HD21	2:H:79:VAL:HG22	1.95	0.47
2:J:131:SER:N	2:J:132:PRO:CD	2.78	0.47
2:K:45:ILE:HB	2:K:52:ALA:HB1	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:43:MET:HE3	2:N:56:VAL:HG22	1.92	0.47
3:R:140:ILE:CD1	3:R:144:ALA:HB1	2.45	0.47
1:C:15:PHE:N	1:D:23:GLN:OE1	2.47	0.47
1:F:17:PRO:HB3	3:Q:105:LEU:HD11	1.97	0.47
1:F:175:PHE:CE1	1:F:179:GLU:HG3	2.49	0.47
1:B:158:ASN:HB2	1:B:160:TYR:CE1	2.49	0.47
3:S:24:VAL:HG13	3:S:84:GLN:HB3	1.95	0.47
1:D:9:ASP:O	1:D:23:GLN:NE2	2.47	0.47
1:D:63:SER:OG	1:D:64:ILE:N	2.46	0.47
2:I:43:MET:HE1	2:I:56:VAL:HG22	1.90	0.47
1:F:17:PRO:HA	1:G:26:TYR:CG	2.49	0.47
1:A:23:GLN:OE1	1:G:15:PHE:N	2.48	0.47
1:E:15:PHE:N	1:F:23:GLN:OE1	2.48	0.47
2:J:7:THR:HG22	2:J:110:VAL:HG23	1.95	0.47
1:B:67:ILE:HG12	1:B:77:VAL:HG13	1.97	0.47
1:C:63:SER:OG	1:C:64:ILE:N	2.47	0.47
1:C:152:ASP:OD1	1:C:156:THR:HB	2.15	0.47
1:D:82:VAL:CG1	3:T:231:ARG:CB	2.93	0.47
3:T:67:LEU:HD11	3:T:187:ASP:HB3	1.96	0.47
2:K:43:MET:HE3	2:K:56:VAL:HG22	1.95	0.46
2:M:131:SER:N	2:M:132:PRO:CD	2.78	0.46
1:B:146:PRO:O	1:B:147:ARG:HD2	2.16	0.46
1:C:67:ILE:HG12	1:C:77:VAL:HG13	1.96	0.46
2:I:45:ILE:HB	2:I:52:ALA:HB1	1.98	0.46
3:T:113:VAL:HA	3:T:116:ILE:HG22	1.97	0.46
2:I:43:MET:CE	2:I:56:VAL:CG2	2.86	0.46
1:E:12:ILE:HD11	1:E:24:VAL:HG23	1.97	0.46
2:H:7:THR:CG2	2:H:110:VAL:HG23	2.46	0.46
1:D:175:PHE:CE1	1:D:179:GLU:HG3	2.50	0.46
2:N:63:LEU:HD21	2:N:79:VAL:HG22	1.98	0.46
2:N:163:LYS:NZ	2:N:203:LEU:HB3	2.31	0.46
3:S:99:HIS:HB3	3:T:109:VAL:HG22	1.97	0.46
3:T:99:HIS:HB3	3:U:109:VAL:HG22	1.97	0.46
2:I:163:LYS:HZ3	2:I:203:LEU:HB3	1.80	0.46
2:K:202:ILE:CG2	2:K:203:LEU:N	2.79	0.46
1:G:63:SER:OG	1:G:64:ILE:N	2.50	0.45
1:E:126:TYR:HH	1:F:123:TYR:HH	1.65	0.45
2:H:91:LYS:HE2	2:H:92:TYR:CE1	2.52	0.45
2:K:7:THR:CG2	2:K:110:VAL:HG23	2.46	0.45
3:S:36:ILE:HG12	3:S:77:LEU:HD21	1.97	0.45
1:B:76:ALA:HA	1:B:137:ILE:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ALA:HA	1:D:137:ILE:O	2.17	0.45
3:O:82:TYR:CD2	3:P:196:LEU:HD22	2.51	0.45
1:A:123:TYR:HH	1:G:126:TYR:HH	1.62	0.45
3:U:113:VAL:HA	3:U:116:ILE:HG22	1.98	0.45
2:H:131:SER:N	2:H:132:PRO:CD	2.80	0.45
1:F:15:PHE:N	1:G:23:GLN:OE1	2.49	0.45
2:I:43:MET:HE1	2:I:56:VAL:CG2	2.47	0.45
2:L:202:ILE:CG2	2:L:203:LEU:N	2.80	0.45
1:C:76:ALA:HA	1:C:137:ILE:O	2.16	0.45
2:K:131:SER:N	2:K:132:PRO:CD	2.80	0.45
1:A:63:SER:OG	1:A:64:ILE:N	2.50	0.45
3:O:109:VAL:HG22	3:U:99:HIS:HB3	1.99	0.45
3:O:178:SER:OG	3:U:63:SER:OG	2.26	0.45
1:C:157:ILE:HG21	1:C:157:ILE:HD13	1.73	0.44
3:P:50:ILE:HD13	3:P:187:ASP:HB3	1.99	0.44
3:R:50:ILE:HD13	3:R:187:ASP:HB3	1.99	0.44
1:G:76:ALA:HA	1:G:137:ILE:O	2.17	0.44
3:Q:113:VAL:HA	3:Q:116:ILE:HG22	1.99	0.44
1:D:67:ILE:HG12	1:D:77:VAL:HG13	1.98	0.44
2:I:131:SER:N	2:I:132:PRO:CD	2.80	0.44
2:N:91:LYS:HE2	2:N:92:TYR:CE1	2.51	0.44
1:D:47:LEU:C	1:D:47:LEU:HD12	2.37	0.44
2:K:43:MET:HE1	2:K:56:VAL:HG22	1.97	0.44
2:H:45:ILE:HB	2:H:52:ALA:HB1	1.98	0.44
1:C:12:ILE:HD11	1:C:24:VAL:HG23	1.99	0.44
1:E:9:ASP:O	1:E:23:GLN:NE2	2.50	0.44
1:F:38:LEU:HD12	1:F:38:LEU:C	2.38	0.44
2:I:7:THR:CG2	2:I:110:VAL:HG23	2.48	0.44
1:E:41:LYS:HE3	1:E:146:PRO:O	2.18	0.44
1:E:156:THR:HG23	1:F:82:VAL:HG21	2.00	0.44
1:F:41:LYS:HE3	1:F:146:PRO:O	2.18	0.44
3:R:89:ARG:NH2	3:R:118:ASP:OD1	2.50	0.44
3:R:113:VAL:HA	3:R:116:ILE:HG22	1.99	0.44
1:B:9:ASP:O	1:B:23:GLN:NE2	2.49	0.44
1:E:76:ALA:HA	1:E:137:ILE:O	2.18	0.44
1:G:152:ASP:HB2	1:G:153:PRO:HD2	2.00	0.44
2:H:43:MET:HE3	2:H:56:VAL:HG22	1.98	0.44
3:Q:201:LEU:O	3:Q:205:VAL:HG23	2.18	0.44
3:T:140:ILE:CD1	3:T:144:ALA:HB1	2.48	0.44
1:B:162:ALA:HB1	1:B:176:LEU:HD13	2.00	0.43
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:ASN:O	2:H:89:GLN:C	2.55	0.43
1:D:41:LYS:HE3	1:D:146:PRO:O	2.18	0.43
1:F:17:PRO:HA	1:G:26:TYR:CD2	2.53	0.43
1:F:12:ILE:HD11	1:F:24:VAL:CG2	2.48	0.43
2:M:45:ILE:HB	2:M:52:ALA:HB1	1.99	0.43
3:P:67:LEU:HD23	3:P:67:LEU:N	2.33	0.43
1:F:156:THR:HG23	1:G:82:VAL:HG21	2.00	0.43
2:N:202:ILE:CG2	2:N:203:LEU:N	2.81	0.43
3:O:113:VAL:HA	3:O:116:ILE:HG22	1.99	0.43
3:P:82:TYR:CD2	3:Q:196:LEU:HD22	2.54	0.43
3:P:113:VAL:HA	3:P:116:ILE:HG22	2.00	0.43
1:F:12:ILE:HD11	1:F:24:VAL:HG23	2.00	0.43
1:F:158:ASN:HB2	1:F:160:TYR:CE1	2.53	0.43
2:J:7:THR:CG2	2:J:110:VAL:HG23	2.49	0.43
3:U:50:ILE:HD13	3:U:187:ASP:HB3	2.00	0.43
1:C:175:PHE:CE1	1:C:179:GLU:HG3	2.54	0.43
2:I:202:ILE:CG2	2:I:203:LEU:N	2.79	0.43
1:C:41:LYS:HE3	1:C:146:PRO:O	2.19	0.43
3:S:36:ILE:CG1	3:S:77:LEU:HD21	2.48	0.43
1:D:15:PHE:N	1:E:23:GLN:OE1	2.51	0.43
2:H:202:ILE:CG2	2:H:203:LEU:N	2.82	0.43
3:Q:140:ILE:CD1	3:Q:144:ALA:HB1	2.47	0.43
1:D:17:PRO:HB3	3:O:105:LEU:HD11	2.01	0.43
1:E:64:ILE:HG22	3:U:231:ARG:HE	1.84	0.43
2:L:18:ARG:CD	2:L:31:GLY:O	2.67	0.43
3:Q:82:TYR:CD2	3:R:196:LEU:HD22	2.53	0.43
1:E:17:PRO:HA	1:F:26:TYR:CD1	2.53	0.43
1:E:111:ASN:HD21	2:L:69:GLN:HB3	1.84	0.43
2:H:87:LEU:HD23	2:H:114:ASP:O	2.19	0.42
2:J:18:ARG:CD	2:J:31:GLY:O	2.67	0.42
2:L:131:SER:N	2:L:132:PRO:CD	2.82	0.42
3:O:36:ILE:HG12	3:O:77:LEU:CD2	2.49	0.42
1:D:157:ILE:HG22	1:D:158:ASN:N	2.34	0.42
1:G:41:LYS:HE3	1:G:146:PRO:O	2.19	0.42
2:K:18:ARG:CD	2:K:31:GLY:O	2.66	0.42
1:B:175:PHE:CE1	1:B:179:GLU:HG3	2.54	0.42
1:F:157:ILE:HG22	1:F:158:ASN:N	2.34	0.42
2:M:202:ILE:CG2	2:M:203:LEU:N	2.80	0.42
2:N:88:ASN:O	2:N:89:GLN:C	2.55	0.42
2:J:3:THR:HB	2:J:16:THR:HG22	2.00	0.42
2:K:91:LYS:HE2	2:K:92:TYR:CE1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:67:LEU:N	3:O:67:LEU:HD23	2.34	0.42
3:P:39:ILE:HD13	3:P:74:TYR:HA	2.01	0.42
1:G:146:PRO:O	1:G:147:ARG:HD2	2.19	0.42
2:L:43:MET:HE3	2:L:56:VAL:HG22	1.97	0.42
1:D:17:PRO:HA	1:E:26:TYR:CG	2.55	0.42
2:L:104:ILE:HD13	2:L:108:PRO:HA	2.01	0.42
3:P:63:SER:HA	3:P:64:PRO:HD3	1.88	0.42
3:S:140:ILE:CD1	3:S:144:ALA:HB1	2.50	0.42
1:C:47:LEU:C	1:C:47:LEU:HD12	2.40	0.42
3:U:67:LEU:HD23	3:U:67:LEU:N	2.35	0.42
1:D:82:VAL:HG13	3:T:231:ARG:HB2	2.00	0.42
1:G:158:ASN:HB2	1:G:160:TYR:CE1	2.55	0.42
1:G:175:PHE:CE1	1:G:179:GLU:HG3	2.55	0.42
2:J:91:LYS:HE2	2:J:92:TYR:CE1	2.54	0.42
2:L:7:THR:CG2	2:L:110:VAL:HG23	2.49	0.42
2:M:91:LYS:HE2	2:M:92:TYR:CE1	2.55	0.42
2:N:45:ILE:HB	2:N:52:ALA:HB1	2.01	0.42
1:D:175:PHE:CD1	1:D:175:PHE:C	2.94	0.42
1:E:152:ASP:OD1	1:E:156:THR:HB	2.19	0.42
2:M:43:MET:HE3	2:M:56:VAL:HG22	2.02	0.42
3:S:63:SER:HA	3:S:64:PRO:HD3	1.93	0.42
3:P:36:ILE:HG12	3:P:77:LEU:CD2	2.50	0.42
1:A:76:ALA:HA	1:A:137:ILE:O	2.20	0.41
1:D:162:ALA:HB1	1:D:176:LEU:HD13	2.02	0.41
2:L:107:ALA:HB1	2:L:108:PRO:HD2	2.02	0.41
3:R:140:ILE:HD11	3:R:144:ALA:HB1	2.02	0.41
3:T:140:ILE:HD11	3:T:144:ALA:HB1	2.02	0.41
1:B:63:SER:OG	1:B:64:ILE:N	2.52	0.41
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.50	0.41
2:J:43:MET:HE1	2:J:56:VAL:HG22	1.96	0.41
3:Q:140:ILE:HD11	3:Q:144:ALA:HB1	2.02	0.41
1:G:162:ALA:HB1	1:G:176:LEU:HD13	2.01	0.41
2:J:88:ASN:O	2:J:89:GLN:C	2.57	0.41
2:M:40:TYR:CE2	2:M:180:ARG:NH2	2.89	0.41
1:A:26:TYR:CG	1:G:17:PRO:HA	2.55	0.41
1:A:41:LYS:HE3	1:A:146:PRO:O	2.20	0.41
1:B:152:ASP:OD1	1:B:156:THR:HB	2.20	0.41
2:I:91:LYS:HE2	2:I:92:TYR:CE1	2.55	0.41
3:R:24:VAL:HG13	3:R:84:GLN:HB3	2.01	0.41
3:U:140:ILE:CD1	3:U:144:ALA:HB1	2.51	0.41
3:S:89:ARG:NH2	3:S:118:ASP:OD1	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ASN:OD1	1:D:62:ASN:N	2.51	0.41
1:F:82:VAL:HG22	3:O:229:LEU:O	2.20	0.41
3:Q:50:ILE:HD13	3:Q:187:ASP:HB3	2.02	0.41
1:A:15:PHE:N	1:B:23:GLN:OE1	2.53	0.41
1:E:16:SER:O	1:F:26:TYR:HB3	2.20	0.41
1:F:175:PHE:CD1	1:F:175:PHE:C	2.94	0.41
1:G:47:LEU:HD22	1:G:190:VAL:HG22	2.02	0.41
1:E:47:LEU:HD12	1:E:47:LEU:C	2.41	0.41
2:H:18:ARG:CD	2:H:31:GLY:O	2.69	0.41
2:N:131:SER:N	2:N:132:PRO:CD	2.84	0.41
3:P:50:ILE:HD11	3:P:67:LEU:HD11	2.02	0.41
1:C:146:PRO:O	1:C:147:ARG:HD2	2.21	0.41
1:D:158:ASN:HB2	1:D:160:TYR:CE1	2.56	0.41
2:M:7:THR:HG22	2:M:110:VAL:HG23	2.02	0.41
3:Q:99:HIS:HB3	3:R:109:VAL:HG22	2.02	0.41
1:A:158:ASN:HB2	1:A:160:TYR:CE1	2.55	0.41
1:D:47:LEU:HD12	1:D:47:LEU:O	2.21	0.41
1:F:162:ALA:HB1	1:F:176:LEU:HD13	2.02	0.41
1:G:36:THR:HG22	1:G:37:ALA:N	2.36	0.41
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.03	0.40
1:G:198:LYS:HG3	1:G:207:LEU:HD22	2.02	0.40
2:M:7:THR:CG2	2:M:110:VAL:HG23	2.51	0.40
1:A:12:ILE:HD11	1:A:24:VAL:HG23	2.03	0.40
1:A:47:LEU:HD22	1:A:190:VAL:HG22	2.04	0.40
1:A:47:LEU:C	1:A:47:LEU:HD12	2.42	0.40
1:A:146:PRO:O	1:A:147:ARG:HD2	2.22	0.40
1:A:9:ASP:O	1:A:23:GLN:NE2	2.54	0.40
1:G:12:ILE:HD11	1:G:24:VAL:CG2	2.51	0.40
2:H:163:LYS:HZ3	2:H:203:LEU:HB3	1.86	0.40
1:A:162:ALA:HB1	1:A:176:LEU:HD13	2.03	0.40
3:O:89:ARG:NH2	3:O:118:ASP:OD1	2.53	0.40
2:M:107:ALA:HB1	2:M:108:PRO:HD2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:14:ASP:OD1	3:U:45:GLU:OE1[4_555]	1.98	0.22
1:E:181:LYS:NZ	2:M:180:ARG:O[4_546]	2.03	0.17
1:E:181:LYS:CE	2:M:180:ARG:O[4_546]	2.14	0.06

## 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	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	12	47
1	B	225/227 (99%)	214 (95%)	9 (4%)	2 (1%)	17	56
1	C	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
1	D	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	17	56
1	E	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
1	F	225/227 (99%)	214 (95%)	8 (4%)	3 (1%)	12	47
1	G	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
2	H	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	I	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	J	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	15	54
2	K	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	L	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	M	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	15	54
2	N	201/203 (99%)	186 (92%)	13 (6%)	2 (1%)	15	54
3	O	214/228 (94%)	208 (97%)	5 (2%)	1 (0%)	29	67
3	P	214/228 (94%)	206 (96%)	7 (3%)	1 (0%)	29	67
3	Q	214/228 (94%)	209 (98%)	4 (2%)	1 (0%)	29	67
3	R	214/228 (94%)	207 (97%)	6 (3%)	1 (0%)	29	67
3	S	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
3	T	214/228 (94%)	208 (97%)	5 (2%)	1 (0%)	29	67
3	U	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
All	All	4480/4606 (97%)	4260 (95%)	182 (4%)	38 (1%)	19	58

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	B	64	ILE
1	C	64	ILE
1	D	64	ILE
1	E	64	ILE
1	F	64	ILE
1	G	64	ILE
2	I	23	GLU
2	J	23	GLU
2	K	23	GLU
2	L	23	GLU
1	A	203	GLU
1	B	203	GLU
1	C	203	GLU
1	D	203	GLU
1	E	203	GLU
1	F	203	GLU
1	G	203	GLU
2	H	23	GLU
2	M	23	GLU
2	N	23	GLU
2	L	202	ILE
1	F	56	SER
2	H	202	ILE
2	I	202	ILE
2	J	202	ILE
2	K	202	ILE
2	M	202	ILE
2	N	202	ILE
1	E	56	SER
3	O	173	GLY
3	P	173	GLY
1	G	204	GLY
3	Q	173	GLY
3	R	173	GLY
3	T	173	GLY
1	A	204	GLY
1	C	204	GLY

### 5.3.2 Protein sidechains [i](#)

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	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	B	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	C	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	D	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	E	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	F	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	G	188/188 (100%)	175 (93%)	13 (7%)	15	49
2	H	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	I	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	J	170/170 (100%)	156 (92%)	14 (8%)	11	41
2	K	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	L	170/170 (100%)	156 (92%)	14 (8%)	11	41
2	M	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	N	170/170 (100%)	155 (91%)	15 (9%)	10	36
3	O	180/188 (96%)	172 (96%)	8 (4%)	28	64
3	P	180/188 (96%)	170 (94%)	10 (6%)	21	57
3	Q	180/188 (96%)	170 (94%)	10 (6%)	21	57
3	R	180/188 (96%)	173 (96%)	7 (4%)	32	67
3	S	180/188 (96%)	171 (95%)	9 (5%)	24	60
3	T	180/188 (96%)	173 (96%)	7 (4%)	32	67
3	U	180/188 (96%)	172 (96%)	8 (4%)	28	64
All	All	3766/3822 (98%)	3518 (93%)	248 (7%)	16	51

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	57	ARG
1	A	61	GLN
1	A	62	ASN
1	A	63	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	77	VAL
1	A	106	LEU
1	A	129	VAL
1	A	199	SER
1	A	202	GLU
1	A	221	TYR
1	A	222	ARG
1	A	226	GLN
1	B	10	ARG
1	B	57	ARG
1	B	61	GLN
1	B	63	SER
1	B	77	VAL
1	B	106	LEU
1	B	129	VAL
1	B	150	ASP
1	B	199	SER
1	B	202	GLU
1	B	221	TYR
1	B	222	ARG
1	B	226	GLN
1	C	10	ARG
1	C	57	ARG
1	C	61	GLN
1	C	62	ASN
1	C	63	SER
1	C	77	VAL
1	C	106	LEU
1	C	129	VAL
1	C	150	ASP
1	C	199	SER
1	C	202	GLU
1	C	221	TYR
1	C	222	ARG
1	C	226	GLN
1	D	10	ARG
1	D	57	ARG
1	D	61	GLN
1	D	62	ASN
1	D	63	SER
1	D	77	VAL
1	D	106	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	129	VAL
1	D	150	ASP
1	D	199	SER
1	D	202	GLU
1	D	221	TYR
1	D	222	ARG
1	D	226	GLN
1	E	10	ARG
1	E	57	ARG
1	E	61	GLN
1	E	62	ASN
1	E	63	SER
1	E	77	VAL
1	E	106	LEU
1	E	129	VAL
1	E	199	SER
1	E	202	GLU
1	E	221	TYR
1	E	222	ARG
1	E	226	GLN
1	F	10	ARG
1	F	57	ARG
1	F	61	GLN
1	F	62	ASN
1	F	63	SER
1	F	77	VAL
1	F	106	LEU
1	F	129	VAL
1	F	150	ASP
1	F	199	SER
1	F	202	GLU
1	F	221	TYR
1	F	222	ARG
1	F	226	GLN
1	G	10	ARG
1	G	57	ARG
1	G	61	GLN
1	G	62	ASN
1	G	63	SER
1	G	77	VAL
1	G	106	LEU
1	G	129	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	199	SER
1	G	202	GLU
1	G	221	TYR
1	G	222	ARG
1	G	226	GLN
2	H	9	LYS
2	H	17	GLU
2	H	18	ARG
2	H	23	GLU
2	H	27	MET
2	H	30	ASN
2	H	49	VAL
2	H	72	VAL
2	H	84	SER
2	H	89	GLN
2	H	122	ASP
2	H	198	LYS
2	H	203	LEU
2	I	9	LYS
2	I	17	GLU
2	I	18	ARG
2	I	23	GLU
2	I	27	MET
2	I	30	ASN
2	I	49	VAL
2	I	72	VAL
2	I	84	SER
2	I	89	GLN
2	I	122	ASP
2	I	198	LYS
2	I	203	LEU
2	J	3	THR
2	J	9	LYS
2	J	17	GLU
2	J	18	ARG
2	J	23	GLU
2	J	27	MET
2	J	30	ASN
2	J	49	VAL
2	J	72	VAL
2	J	84	SER
2	J	89	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	122	ASP
2	J	198	LYS
2	J	203	LEU
2	K	9	LYS
2	K	17	GLU
2	K	18	ARG
2	K	23	GLU
2	K	27	MET
2	K	30	ASN
2	K	49	VAL
2	K	72	VAL
2	K	84	SER
2	K	89	GLN
2	K	122	ASP
2	K	198	LYS
2	K	203	LEU
2	L	3	THR
2	L	9	LYS
2	L	17	GLU
2	L	18	ARG
2	L	23	GLU
2	L	27	MET
2	L	30	ASN
2	L	49	VAL
2	L	72	VAL
2	L	84	SER
2	L	89	GLN
2	L	122	ASP
2	L	198	LYS
2	L	203	LEU
2	M	9	LYS
2	M	17	GLU
2	M	18	ARG
2	M	23	GLU
2	M	27	MET
2	M	30	ASN
2	M	49	VAL
2	M	72	VAL
2	M	84	SER
2	M	89	GLN
2	M	122	ASP
2	M	198	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	203	LEU
2	N	3	THR
2	N	9	LYS
2	N	17	GLU
2	N	18	ARG
2	N	23	GLU
2	N	27	MET
2	N	30	ASN
2	N	49	VAL
2	N	72	VAL
2	N	84	SER
2	N	89	GLN
2	N	122	ASP
2	N	157	ARG
2	N	198	LYS
2	N	203	LEU
3	O	19	THR
3	O	45	GLU
3	O	65	GLU
3	O	68	LEU
3	O	89	ARG
3	O	119	GLU
3	O	130	LYS
3	O	226	LEU
3	P	19	THR
3	P	45	GLU
3	P	65	GLU
3	P	68	LEU
3	P	89	ARG
3	P	115	LYS
3	P	119	GLU
3	P	130	LYS
3	P	154	THR
3	P	226	LEU
3	Q	19	THR
3	Q	45	GLU
3	Q	65	GLU
3	Q	68	LEU
3	Q	89	ARG
3	Q	115	LYS
3	Q	119	GLU
3	Q	130	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Q	154	THR
3	Q	226	LEU
3	R	19	THR
3	R	45	GLU
3	R	65	GLU
3	R	68	LEU
3	R	119	GLU
3	R	130	LYS
3	R	226	LEU
3	S	19	THR
3	S	45	GLU
3	S	65	GLU
3	S	68	LEU
3	S	89	ARG
3	S	115	LYS
3	S	119	GLU
3	S	130	LYS
3	S	226	LEU
3	T	19	THR
3	T	45	GLU
3	T	65	GLU
3	T	68	LEU
3	T	89	ARG
3	T	119	GLU
3	T	226	LEU
3	U	19	THR
3	U	45	GLU
3	U	65	GLU
3	U	68	LEU
3	U	115	LYS
3	U	119	GLU
3	U	130	LYS
3	U	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	B	226	GLN
1	C	226	GLN
1	D	226	GLN
1	E	111	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	226	GLN
1	F	226	GLN
1	G	226	GLN
2	H	191	GLN
2	I	191	GLN
2	J	191	GLN
2	K	191	GLN
2	L	98	GLN
2	L	191	GLN
2	M	191	GLN
2	N	98	GLN
2	N	191	GLN
3	O	79	HIS
3	U	79	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	227/227 (100%)	-0.27	6 (2%) 56 40	23, 40, 69, 79	0
1	B	227/227 (100%)	-0.21	9 (3%) 38 25	23, 40, 69, 79	0
1	C	227/227 (100%)	-0.26	5 (2%) 62 48	23, 40, 69, 79	0
1	D	227/227 (100%)	-0.22	9 (3%) 38 25	23, 40, 69, 79	0
1	E	227/227 (100%)	-0.20	6 (2%) 56 40	23, 40, 69, 79	0
1	F	227/227 (100%)	-0.23	8 (3%) 44 28	23, 40, 69, 79	0
1	G	227/227 (100%)	-0.17	7 (3%) 49 32	23, 40, 69, 79	0
2	H	203/203 (100%)	-0.33	2 (0%) 82 72	24, 34, 54, 71	0
2	I	203/203 (100%)	-0.42	2 (0%) 82 72	24, 34, 54, 71	0
2	J	203/203 (100%)	-0.37	4 (1%) 65 51	24, 34, 54, 71	0
2	K	203/203 (100%)	-0.38	2 (0%) 82 72	24, 34, 54, 71	0
2	L	203/203 (100%)	-0.37	2 (0%) 82 72	24, 34, 54, 71	0
2	M	203/203 (100%)	-0.37	2 (0%) 82 72	24, 34, 54, 71	0
2	N	203/203 (100%)	-0.39	2 (0%) 82 72	24, 35, 54, 71	0
3	O	218/228 (95%)	-0.28	3 (1%) 75 63	25, 40, 55, 64	0
3	P	218/228 (95%)	-0.32	5 (2%) 60 47	26, 40, 55, 64	0
3	Q	218/228 (95%)	-0.35	5 (2%) 60 47	26, 40, 55, 64	0
3	R	218/228 (95%)	-0.30	3 (1%) 75 63	25, 40, 55, 64	0
3	S	218/228 (95%)	-0.40	3 (1%) 75 63	25, 40, 55, 64	0
3	T	218/228 (95%)	-0.31	4 (1%) 68 55	25, 40, 55, 64	0
3	U	218/228 (95%)	-0.34	3 (1%) 75 63	25, 40, 55, 64	0
All	All	4536/4606 (98%)	-0.31	92 (2%) 65 51	23, 38, 63, 79	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	202	ILE	7.4
2	K	202	ILE	6.1
2	H	202	ILE	5.4
2	J	202	ILE	5.3
2	N	202	ILE	5.1
2	I	202	ILE	4.6
2	L	202	ILE	4.6
3	P	172	GLY	4.4
1	G	202	GLU	4.3
2	I	203	LEU	4.2
3	O	133	SER	4.1
1	G	204	GLY	4.1
2	H	203	LEU	3.8
1	A	203	GLU	3.8
1	G	203	GLU	3.6
1	E	204	GLY	3.6
3	Q	133	SER	3.5
3	R	172	GLY	3.5
1	G	206	GLU	3.5
1	A	202	GLU	3.5
2	M	203	LEU	3.4
1	C	203	GLU	3.3
1	C	202	GLU	3.3
2	N	203	LEU	3.2
1	B	203	GLU	3.2
3	R	133	SER	3.1
1	F	206	GLU	3.1
3	U	172	GLY	3.1
3	R	227	ASP	3.0
1	F	203	GLU	3.0
1	A	204	GLY	2.9
3	P	133	SER	2.9
3	O	172	GLY	2.9
1	E	203	GLU	2.9
1	B	204	GLY	2.8
1	D	202	GLU	2.8
1	D	204	GLY	2.8
1	B	226	GLN	2.8
3	O	132	GLY	2.7
1	C	204	GLY	2.7
3	P	173	GLY	2.7
1	A	205	GLU	2.6
1	F	204	GLY	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	T	133	SER	2.6
1	A	206	GLU	2.6
1	F	54	VAL	2.6
1	B	206	GLU	2.6
1	F	202	GLU	2.5
2	K	203	LEU	2.5
1	B	44	ASN	2.5
1	B	202	GLU	2.5
2	L	203	LEU	2.5
3	S	133	SER	2.5
1	D	203	GLU	2.5
1	D	226	GLN	2.4
1	G	54	VAL	2.4
1	D	208	LYS	2.4
1	D	233	LEU	2.4
3	Q	227	ASP	2.4
1	B	64	ILE	2.4
3	P	132	GLY	2.4
3	Q	132	GLY	2.4
1	B	225	ASP	2.4
3	T	225	HIS	2.3
3	Q	172	GLY	2.3
3	S	172	GLY	2.3
1	C	7	ALA	2.3
3	S	227	ASP	2.3
1	D	206	GLU	2.3
1	F	55	ARG	2.3
2	J	190	ASP	2.3
1	A	54	VAL	2.3
3	Q	225	HIS	2.3
3	T	131	SER	2.2
3	U	133	SER	2.2
1	E	202	GLU	2.2
1	D	61	GLN	2.2
1	G	205	GLU	2.2
1	F	233	LEU	2.1
1	D	205	GLU	2.1
1	E	7	ALA	2.1
1	C	62	ASN	2.1
1	G	227	GLU	2.1
3	P	135	GLY	2.1
3	U	52	ASN	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	55	ARG	2.0
1	B	227	GLU	2.0
1	F	205	GLU	2.0
3	T	132	GLY	2.0
1	E	61	GLN	2.0
2	J	145	LYS	2.0
2	J	197	ARG	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 monosaccharides 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.