



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:30 am GMT

PDB ID : 5E17  
Title : T. thermophilus transcription initiation complex having a RRR discriminator sequence and a nontemplate-strand length corresponding to TSS selection at position 7 (RPo-GGG-7)  
Authors : Zhang, Y.; Ebright, R.H.  
Deposited on : 2015-09-29  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

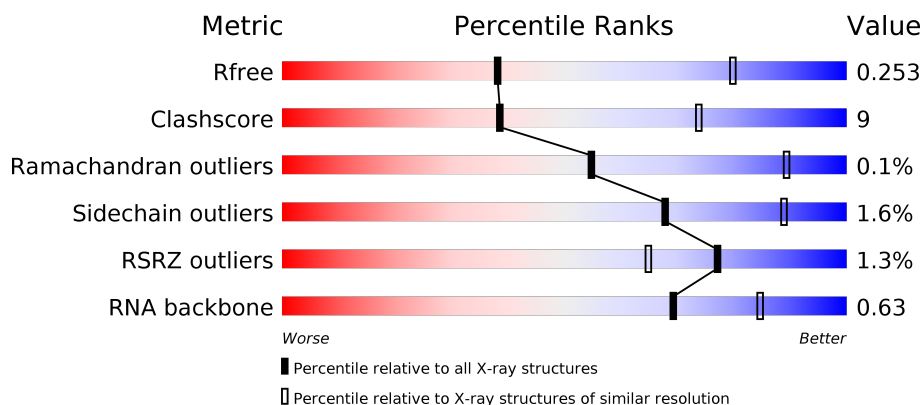
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	315	<div> <div></div> <div>57% 16% 27%</div> </div>
1	B	315	<div> <div></div> <div>51% 19% 30%</div> </div>
2	C	1119	<div> <div></div> <div>76% 22% ..</div> </div>
3	D	1524	<div> <div></div> <div>76% 20% ..</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>83%12%5%</div></div>
5	F	443	<div><div>3%</div><div></div><div>63%13%24%</div></div>
6	G	21	<div><div></div><div>48%38%14%</div></div>
7	H	27	<div><div></div><div>41%48%11%</div></div>
8	I	7	<div><div>14%</div><div></div><div>71%14%14%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28784 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1814	1158	316	338	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1120	303	325	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	3	0
			8792	5562	1570	1636	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	3	0
			11759	7458	2070	2195	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	337	Total	C	N	O	S	0	0	0
			2737	1726	499	508	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*CP\*T\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*T  
P\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			372	176	73	106	17			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-R(\*CP\*CP\*CP\*UP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

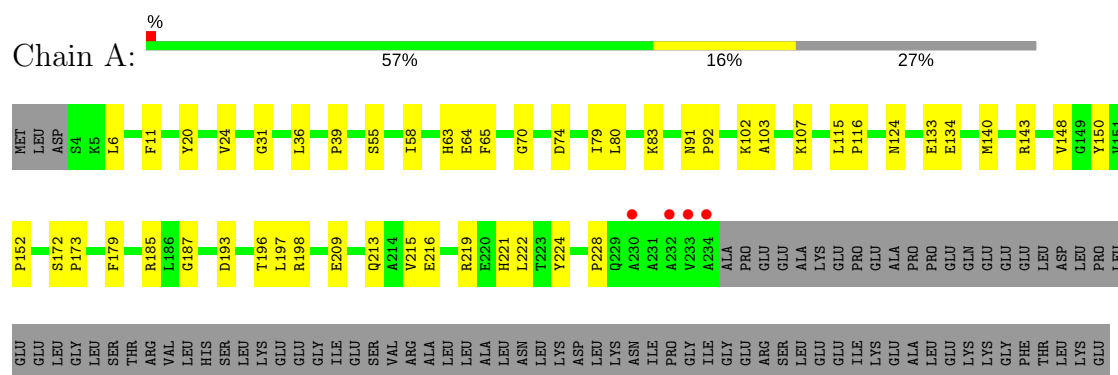
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	12	Total O 12 12	0	0
11	B	12	Total O 12 12	0	0
11	C	49	Total O 49 49	0	0
11	D	62	Total O 62 62	0	0
11	E	5	Total O 5 5	0	0
11	F	8	Total O 8 8	0	0
11	G	5	Total O 5 5	0	0
11	H	4	Total O 4 4	0	0
11	I	2	Total O 2 2	0	0

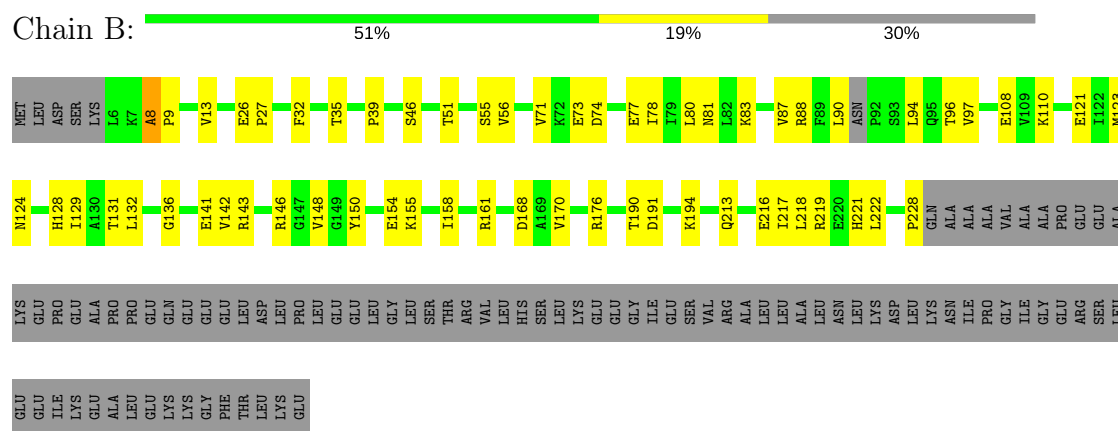
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

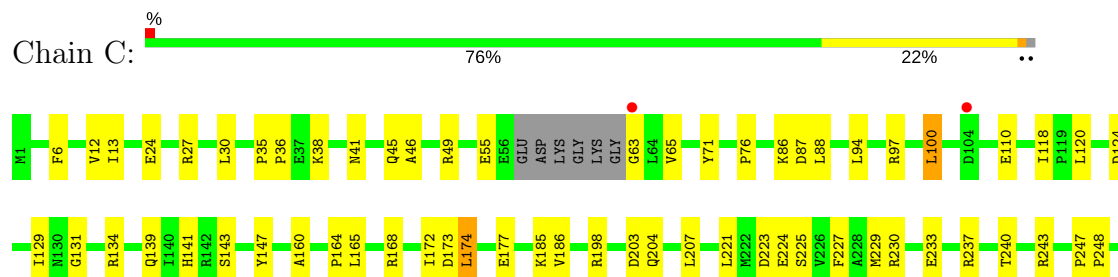
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

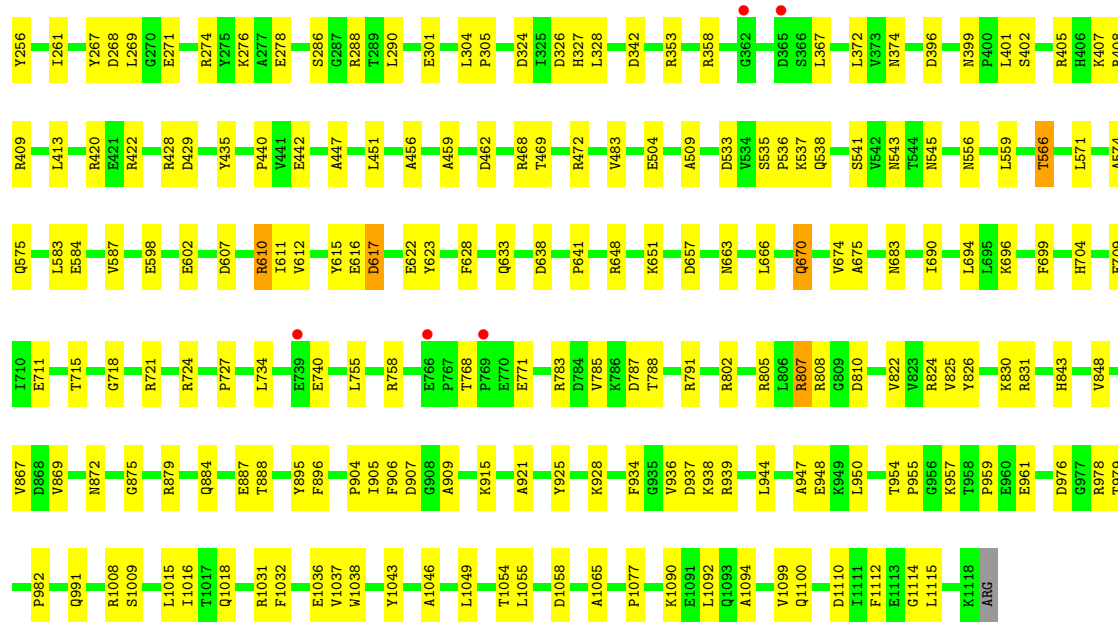


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

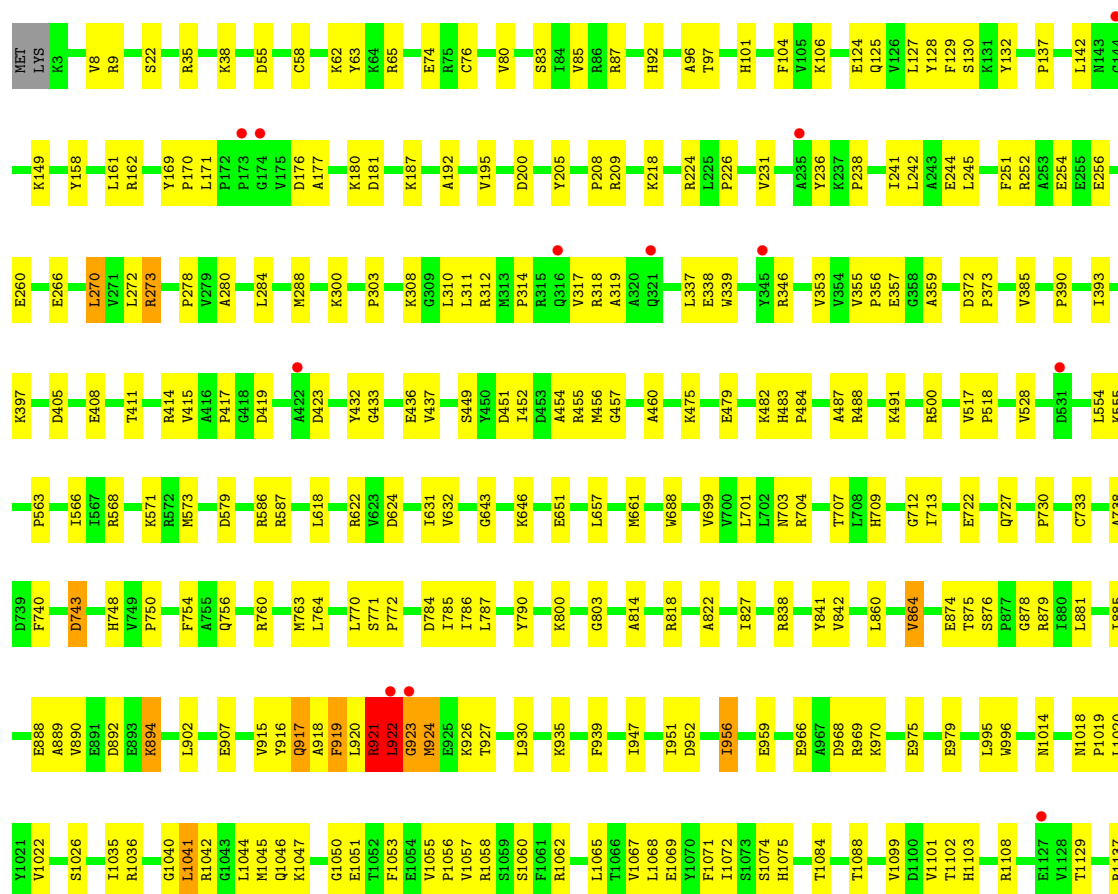
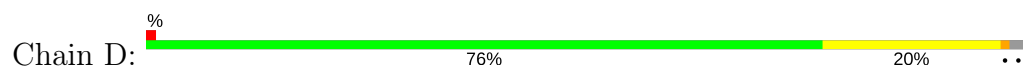


#### • Molecule 2: DNA-directed RNA polymerase subunit beta

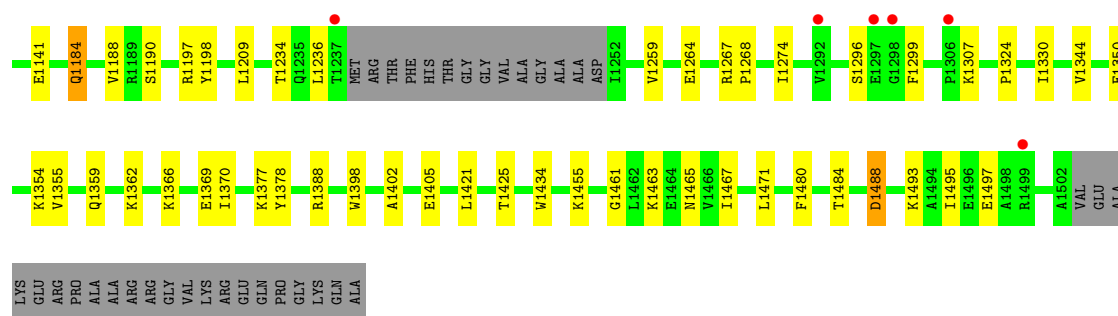




• Molecule 3: DNA-directed RNA polymerase subunit beta'







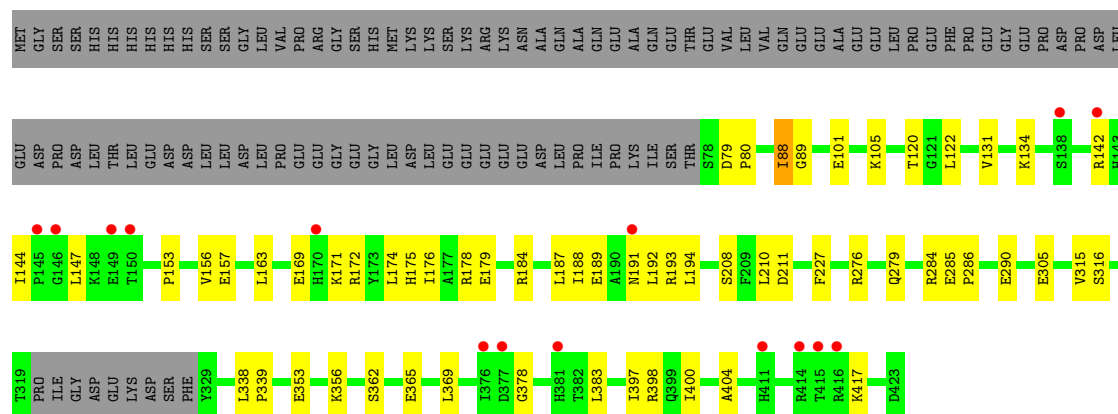
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 83% 12% 5%



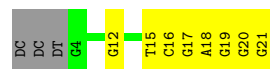
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 3% 63% 13% 24%



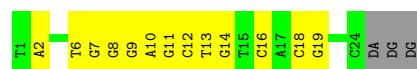
- Molecule 6: DNA (5'-D(\*CP\*CP\*T\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*GP\*G)-3')

Chain G: 48% 38% 14%

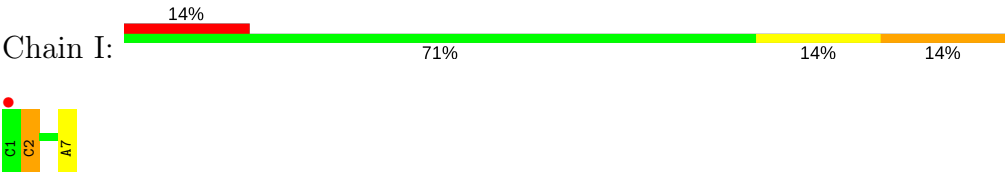


- Molecule 7: DNA (27-MER)

Chain H: 41% 48% 11%



- Molecule 8: RNA (5'-R(\*CP\*CP\*CP\*UP\*CP\*GP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.01Å 103.57Å 294.94Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	39.82 – 3.20 39.82 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (39.82-3.20) 93.2 (39.82-3.18)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.260 0.210 , 0.253	Depositor DCC
$R_{free}$ test set	4211 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.023 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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](#)

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

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	0.25	0/1849	0.46	0/2515
1	B	0.23	0/1781	0.45	0/2420
2	C	0.25	0/8969	0.45	0/12129
3	D	0.31	4/11975 (0.0%)	0.49	7/16189 (0.0%)
4	E	0.24	0/772	0.42	0/1040
5	F	0.30	0/2779	0.44	0/3737
6	G	0.49	0/418	0.83	0/645
7	H	0.53	0/556	0.90	0/858
8	I	0.30	0/157	0.96	0/242
All	All	0.29	4/29256 (0.0%)	0.49	7/39775 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	921	ARG	C-O	9.12	1.40	1.23
3	D	923	GLY	CA-C	-7.58	1.39	1.51
3	D	917	GLN	C-O	6.03	1.34	1.23
3	D	923	GLY	N-CA	-5.26	1.38	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	924	MET	C-N-CA	-7.41	103.17	121.70
3	D	923	GLY	C-N-CA	-6.01	106.67	121.70
3	D	922	LEU	N-CA-C	-5.57	95.97	111.00
3	D	919	PHE	N-CA-CB	5.19	119.95	110.60
3	D	1041	LEU	CA-CB-CG	5.14	127.12	115.30
3	D	921	ARG	CA-C-N	-5.10	105.98	117.20
3	D	922	LEU	C-N-CA	-5.09	111.61	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	922	LEU	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	1814	0	1869	38	0
1	B	1750	0	1802	44	0
2	C	8792	0	8902	160	0
3	D	11759	0	12002	231	0
4	E	758	0	770	10	0
5	F	2737	0	2819	41	0
6	G	372	0	203	10	0
7	H	495	0	272	13	0
8	I	142	0	78	2	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	12	0	0	1	0
11	B	12	0	0	6	0
11	C	49	0	0	0	0
11	D	62	0	0	5	0
11	E	5	0	0	1	0
11	F	8	0	0	0	0
11	G	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	4	0	0	2	0
11	I	2	0	0	0	0
All	All	28784	0	28717	488	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 9.

All (488) 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:D:918:ALA:O	3:D:923:GLY:N	1.80	1.12
3:D:919:PHE:O	3:D:923:GLY:HA2	1.51	1.09
3:D:919:PHE:C	3:D:923:GLY:HA2	1.98	0.84
3:D:921:ARG:O	3:D:923:GLY:HA3	1.80	0.82
6:G:20:DG:H1	8:I:2:C:H42	1.32	0.77
1:B:74:ASP:O	11:B:2101:HOH:O	2.02	0.76
3:D:921:ARG:C	3:D:923:GLY:HA3	2.07	0.75
2:C:628:PHE:H	2:C:638:ASP:HB3	1.54	0.73
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.71
3:D:65:ARG:NH1	5:F:378:GLY:O	2.24	0.70
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.24	0.70
3:D:919:PHE:O	3:D:923:GLY:CA	2.37	0.70
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.75	0.68
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.75	0.68
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.74	0.68
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.75	0.68
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.27	0.68
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.25	0.67
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.27	0.67
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.24	0.67
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.76	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.76	0.67
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.76	0.66
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.77	0.66
2:C:428:ARG:NH2	2:C:447:ALA:O	2.29	0.66
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.78	0.66
3:D:1046:GLN:NE2	3:D:1050:GLY:O	2.28	0.65
3:D:918:ALA:C	3:D:923:GLY:H	1.90	0.65
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.30	0.65
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.16	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.30	0.64
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.14	0.63
1:A:185:ARG:NH2	1:A:187:GLY:O	2.30	0.63
2:C:758:ARG:HH21	2:C:788:THR:HB	1.63	0.63
2:C:884:GLN:O	2:C:888:THR:OG1	2.15	0.63
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.81	0.62
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.81	0.62
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.80	0.62
2:C:223:ASP:OD1	2:C:225:SER:OG	2.16	0.61
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.81	0.61
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.82	0.61
3:D:224:ARG:H	3:D:251:PHE:HE1	1.48	0.61
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.33	0.61
1:A:133:GLU:OE1	2:C:610:ARG:NH1	2.34	0.61
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.83	0.60
2:C:409:ARG:NH2	2:C:442:GLU:OE2	2.33	0.60
3:D:432:TYR:O	11:D:2101:HOH:O	2.16	0.60
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.82	0.60
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.34	0.60
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.35	0.59
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.85	0.59
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.83	0.59
2:C:598:GLU:O	2:C:651:LYS:NZ	2.33	0.59
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.84	0.59
5:F:227:PHE:HA	11:H:101:HOH:O	2.01	0.59
3:D:433:GLY:HA2	11:D:2101:HOH:O	2.02	0.59
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.85	0.59
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.67	0.58
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.33	0.58
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.58
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.85	0.58
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.69	0.58
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.86	0.57
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.86	0.57
7:H:10:DA:H2'	7:H:11:DG:O4'	2.04	0.57
7:H:2:DA:N1	11:H:101:HOH:O	2.33	0.57
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.85	0.57
3:D:922:LEU:O	3:D:927:THR:N	2.37	0.57
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.85	0.57
2:C:420:ARG:O	2:C:422:ARG:NH2	2.35	0.57
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:OG1	1:B:87:VAL:O	2.19	0.57
3:D:449:SER:N	11:D:2101:HOH:O	2.13	0.57
1:A:31:GLY:N	1:A:193:ASP:OD2	2.35	0.57
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.86	0.57
3:D:308:LYS:NZ	11:D:2113:HOH:O	2.36	0.56
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.87	0.56
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.87	0.56
3:D:1184:GLN:O	11:D:2102:HOH:O	2.17	0.56
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.38	0.56
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.87	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.87	0.56
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.56
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.37	0.56
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.86	0.56
5:F:79:ASP:OD2	7:H:8:DG:N1	2.30	0.56
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.87	0.56
2:C:12:VAL:HG12	2:C:13:ILE:HG23	1.88	0.56
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.88	0.56
2:C:94:LEU:HD22	2:C:118:ILE:HD11	1.87	0.55
5:F:171:LYS:O	5:F:175:HIS:ND1	2.37	0.55
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.70	0.55
3:D:231:VAL:O	3:D:236:TYR:OH	2.23	0.55
3:D:1071:PHE:O	3:D:1074:SER:OG	2.13	0.55
1:B:78:ILE:HG23	1:B:129:ILE:HG23	1.88	0.55
3:D:162:ARG:NH1	3:D:451:ASP:OD1	2.40	0.55
3:D:921:ARG:C	3:D:923:GLY:CA	2.74	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
1:B:191:ASP:N	1:B:191:ASP:OD1	2.37	0.54
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.88	0.54
6:G:16:DC:H2'	6:G:17:DG:H8	1.70	0.54
1:B:8:ALA:HB1	1:B:27:PRO:HD2	1.89	0.54
1:B:8:ALA:HB1	1:B:9:PRO:HA	1.89	0.54
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.19	0.54
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.39	0.54
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.72	0.54
6:G:15:DT:H2'	6:G:16:DC:C6	2.43	0.54
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.88	0.54
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.89	0.54
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.90	0.54
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.89	0.54
1:A:209:GLU:O	1:A:213:GLN:HG2	2.08	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:ARG:NH1	2:C:456:ALA:O	2.41	0.53
2:C:413:LEU:HD11	2:C:451:LEU:HD13	1.90	0.53
4:E:2:ALA:N	11:E:102:HOH:O	2.41	0.53
7:H:9:DG:H2"	7:H:10:DA:C8	2.44	0.53
2:C:617:ASP:N	2:C:617:ASP:OD1	2.42	0.53
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.89	0.53
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.09	0.53
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.34	0.53
5:F:169:GLU:O	5:F:172:ARG:HB3	2.08	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.74	0.53
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.09	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.53
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.91	0.53
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.91	0.53
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.90	0.53
2:C:168:ARG:O	2:C:267:TYR:HA	2.09	0.53
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.44	0.52
2:C:543:ASN:ND2	2:C:566:THR:HG22	2.25	0.52
2:C:715:THR:OG1	2:C:718:GLY:O	2.23	0.52
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.91	0.52
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.90	0.52
2:C:616:GLU:OE1	2:C:648:ARG:NH1	2.42	0.52
5:F:276:ARG:O	5:F:279:GLN:HG3	2.10	0.52
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.92	0.52
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.41	0.52
6:G:12:DG:N2	7:H:16:DC:O2	2.19	0.52
2:C:1008:ARG:NH2	3:D:624:ASP:OD1	2.35	0.52
5:F:105:LYS:HD3	5:F:179:GLU:HG2	1.92	0.52
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.92	0.52
3:D:919:PHE:HA	3:D:927:THR:OG1	2.10	0.52
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.92	0.52
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.36	0.51
2:C:848:VAL:HG22	3:D:740:PHE:O	2.10	0.51
3:D:701:LEU:HB2	3:D:748:HIS:HB2	1.92	0.51
3:D:921:ARG:C	3:D:923:GLY:N	2.59	0.51
5:F:194:LEU:HB2	7:H:6:DT:C2	2.45	0.51
2:C:872:ASN:ND2	3:D:784:ASP:OD2	2.41	0.51
3:D:187:LYS:N	3:D:200:ASP:OD2	2.36	0.51
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.92	0.51
1:B:32:PHE:HA	1:B:35:THR:HB	1.92	0.51
5:F:189:GLU:HA	5:F:192:LEU:HG	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HG2	11:B:2103:HOH:O	2.09	0.51
1:B:136:GLY:N	11:B:2107:HOH:O	2.44	0.51
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.43	0.51
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.93	0.51
5:F:187:LEU:O	5:F:191:ASN:ND2	2.42	0.51
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.50
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.94	0.50
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.44	0.50
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.94	0.50
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.28	0.50
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.92	0.50
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.93	0.50
2:C:584:GLU:HB3	2:C:666:LEU:H	1.76	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.50
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.93	0.50
3:D:106:LYS:O	3:D:586:ARG:NH1	2.45	0.50
2:C:657:ASP:OD2	2:C:663:ASN:N	2.42	0.49
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.12	0.49
2:C:286:SER:OG	2:C:301:GLU:OE2	2.25	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.93	0.49
2:C:274:ARG:NH2	2:C:278:GLU:OE2	2.46	0.49
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.47	0.49
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.95	0.49
6:G:16:DC:H2'	6:G:17:DG:C8	2.47	0.49
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	1.94	0.49
5:F:172:ARG:O	5:F:176:ILE:HG12	2.12	0.49
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.94	0.49
2:C:326:ASP:OD1	7:H:14:DG:N2	2.41	0.49
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.42	0.49
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.94	0.49
2:C:41:ASN:O	2:C:46:ALA:HB2	2.12	0.49
3:D:920:LEU:C	3:D:923:GLY:HA2	2.32	0.49
3:D:555:LYS:HA	5:F:142:ARG:HH12	1.77	0.49
2:C:1015:LEU:HD11	3:D:528:VAL:HG11	1.93	0.48
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.94	0.48
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.45	0.48
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.48	0.48
3:D:1047:LYS:HG2	3:D:1053[A]:PHE:CE2	2.48	0.48
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.12	0.48
5:F:315:VAL:HG22	5:F:316:SER:H	1.78	0.48
7:H:18:DC:H2''	7:H:19:DG:C8	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.94	0.48
2:C:143:SER:O	2:C:147:TYR:OH	2.29	0.48
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.46	0.48
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.94	0.48
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.48
3:D:487:ALA:O	3:D:491:LYS:HG2	2.13	0.48
2:C:198:ARG:HE	2:C:227:PHE:HA	1.78	0.48
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.94	0.48
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.49	0.48
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.13	0.48
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.96	0.48
3:D:1084:THR:O	3:D:1088:THR:HG23	2.14	0.48
3:D:411:THR:HG23	3:D:436:GLU:HA	1.96	0.48
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.79	0.48
3:D:1103:HIS:CE1	3:D:1463:LYS:H	2.32	0.48
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.30	0.48
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.95	0.47
2:C:615:TYR:OH	2:C:623:TYR:OH	2.17	0.47
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	1.95	0.47
3:D:966:GLU:O	3:D:969:ARG:HG2	2.15	0.47
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.96	0.47
5:F:189:GLU:O	5:F:192:LEU:HB2	2.15	0.47
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.96	0.47
1:B:46:SER:O	1:B:148:VAL:HB	2.14	0.47
3:D:1047:LYS:N	3:D:1051:GLU:O	2.38	0.47
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.47	0.47
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.47
3:D:176:ASP:OD1	3:D:177:ALA:N	2.47	0.47
1:B:190:THR:O	11:B:2102:HOH:O	2.20	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.47
3:D:1053[B]:PHE:CE2	3:D:1055:VAL:HB	2.50	0.47
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.96	0.47
3:D:923:GLY:O	3:D:927:THR:HB	2.15	0.47
3:D:923:GLY:O	3:D:927:THR:CB	2.62	0.47
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.48	0.47
3:D:923:GLY:O	3:D:924:MET:C	2.49	0.47
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.50	0.47
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.96	0.47
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.96	0.47
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.50	0.47
1:B:83:LYS:NZ	3:D:842:VAL:O	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:924:MET:HB3	4:E:7:ASP:OD1	2.15	0.47
3:D:1484:THR:O	4:E:25:LYS:NZ	2.27	0.47
3:D:770:LEU:HD11	3:D:919:PHE:CD1	2.50	0.47
3:D:890:VAL:HG21	3:D:922:LEU:HD13	1.97	0.47
2:C:1009:SER:O	3:D:624:ASP:HB3	2.14	0.46
3:D:417:PRO:HD3	3:D:432:TYR:HA	1.98	0.46
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.97	0.46
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.96	0.46
3:D:915:VAL:O	3:D:919:PHE:HB2	2.15	0.46
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.72	0.46
2:C:224:GLU:CD	2:C:224:GLU:H	2.18	0.46
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.98	0.46
3:D:55:ASP:OD1	3:D:83:SER:OG	2.31	0.46
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.97	0.46
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.98	0.46
2:C:541:SER:O	2:C:545:ASN:ND2	2.41	0.46
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.97	0.46
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.50	0.46
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.98	0.46
3:D:319:ALA:HA	3:D:337:LEU:HD23	1.98	0.46
3:D:975:GLU:O	3:D:979:GLU:HG2	2.16	0.46
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.98	0.46
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.97	0.46
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.46
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.98	0.46
3:D:411:THR:O	5:F:178:ARG:NH1	2.44	0.46
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.51	0.46
5:F:353:GLU:HA	5:F:356:LYS:HD2	1.98	0.46
1:A:124:ASN:N	1:A:124:ASN:OD1	2.49	0.46
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.51	0.46
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.98	0.46
1:B:190:THR:HG21	3:D:722:GLU:OE2	2.15	0.46
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.48	0.46
7:H:12:DC:H1'	7:H:13:DT:C4	2.51	0.46
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.98	0.45
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.41	0.45
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.31	0.45
3:D:353:VAL:HG12	3:D:355:VAL:H	1.81	0.45
3:D:875:THR:OG1	3:D:876:SER:N	2.48	0.45
1:A:221:HIS:O	1:A:224:TYR:N	2.50	0.45
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:N	11:B:2101:HOH:O	2.15	0.45
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.51	0.45
2:C:243:ARG:NH1	7:H:9:DG:O6	2.49	0.45
2:C:602:GLU:HB2	2:C:648:ARG:HH21	1.82	0.45
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.45
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	1.99	0.45
3:D:252:ARG:HA	3:D:303:PRO:HA	1.99	0.45
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.57	0.45
3:D:58:CYS:SG	3:D:62:LYS:N	2.90	0.45
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.99	0.45
5:F:89:GLY:HA3	7:H:7:DG:C6	2.51	0.45
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.98	0.45
2:C:556:ASN:O	2:C:559:LEU:HB3	2.16	0.45
3:D:743:ASP:OD1	3:D:743:ASP:N	2.50	0.45
3:D:951:ILE:HG13	3:D:1062:ARG:HD2	1.98	0.45
3:D:1455:LYS:HE3	3:D:1455:LYS:HB2	1.84	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.45
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	1.98	0.45
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.98	0.45
3:D:63:TYR:HB2	3:D:80:VAL:HG21	1.98	0.45
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.31	0.45
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.97	0.45
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.17	0.45
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.40	0.45
3:D:38:LYS:HD3	3:D:38:LYS:HA	1.84	0.45
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.99	0.45
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.99	0.44
3:D:760:ARG:O	3:D:764:LEU:HB2	2.17	0.44
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.99	0.44
3:D:921:ARG:HG2	3:D:921:ARG:H	1.60	0.44
2:C:440:PRO:HB2	3:D:1074:SER:HB2	2.00	0.44
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.00	0.44
3:D:890:VAL:O	3:D:926:LYS:HD3	2.17	0.44
1:A:179:PHE:HB3	1:A:197:LEU:HD23	2.00	0.44
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.32	0.44
3:D:879:ARG:HD3	3:D:902:LEU:O	2.17	0.44
1:A:222:LEU:HD11	1:B:218:LEU:HG	1.98	0.44
2:C:88:LEU:O	2:C:131:GLY:N	2.50	0.44
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.43	0.44
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.98	0.44
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.87	0.44
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.00	0.44
2:C:256:TYR:HE1	7:H:11:DG:H22	1.65	0.44
1:B:94:LEU:HD11	1:B:97:VAL:HG22	1.98	0.44
2:C:237:ARG:O	2:C:240:THR:OG1	2.29	0.44
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.98	0.44
6:G:17:DG:H2'	6:G:18:DA:C8	2.53	0.44
1:B:155:LYS:HA	1:B:155:LYS:HD3	1.74	0.44
2:C:670:GLN:HG2	2:C:699:PHE:CG	2.52	0.44
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.49	0.43
2:C:587:VAL:HG11	2:C:666:LEU:HD22	2.00	0.43
3:D:1362:LYS:HB2	3:D:1362:LYS:HE2	1.75	0.43
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.46	0.43
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.00	0.43
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.82	0.43
3:D:926:LYS:H	3:D:926:LYS:HG3	1.50	0.43
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.53	0.43
2:C:1094:ALA:HA	3:D:518:PRO:HB2	2.01	0.43
3:D:959:GLU:N	3:D:959:GLU:OE1	2.36	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.85	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.84	0.43
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.52	0.43
2:C:947:ALA:HA	2:C:950:LEU:HB2	1.99	0.43
3:D:704:ARG:HD2	3:D:738:ALA:HB2	2.01	0.43
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.52	0.43
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.18	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.43
2:C:63:GLY:N	2:C:367:LEU:HD12	2.34	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.99	0.43
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.33	0.43
3:D:730:PRO:O	3:D:733:CYS:HB2	2.19	0.43
3:D:860:LEU:O	3:D:876:SER:HB2	2.19	0.43
2:C:928:LYS:HB2	2:C:928:LYS:HE3	1.82	0.43
3:D:236:TYR:CE2	3:D:242:LEU:HD12	2.53	0.43
3:D:137:PRO:HA	3:D:452:ILE:HG23	2.00	0.43
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.19	0.43
6:G:19:DG:H2'	6:G:20:DG:C8	2.53	0.43
1:B:124:ASN:OD1	1:B:124:ASN:N	2.50	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	2.01	0.43
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.01	0.43
3:D:699:VAL:O	3:D:756:GLN:NE2	2.48	0.43
5:F:134:LYS:NZ	5:F:157:GLU:OE1	2.37	0.43
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.83	0.43
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.43
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.23	0.43
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.01	0.43
3:D:1045[B]:MET:HE3	3:D:1072:ILE:HG21	2.01	0.43
3:D:142:LEU:HB2	3:D:161:LEU:HD21	2.00	0.43
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.18	0.43
3:D:921:ARG:O	3:D:922:LEU:C	2.57	0.43
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.53	0.42
2:C:895:TYR:HB2	2:C:991:GLN:HG3	1.99	0.42
3:D:310:LEU:HD12	3:D:310:LEU:H	1.84	0.42
3:D:771:SER:HA	3:D:772:PRO:HD3	1.85	0.42
2:C:399:ASN:OD1	2:C:401:LEU:HB3	2.19	0.42
2:C:139:GLN:NE2	2:C:413:LEU:O	2.49	0.42
2:C:875:GLY:O	2:C:879:ARG:HD3	2.19	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.19	0.42
1:B:110:LYS:HD3	1:B:128:HIS:HA	2.02	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:535:SER:O	2:C:538:GLN:HG2	2.18	0.42
3:D:125:GLN:O	3:D:130:SER:N	2.52	0.42
3:D:657:LEU:HG	3:D:661:MET:HE2	2.00	0.42
3:D:860:LEU:HD22	3:D:878:GLY:HA2	2.01	0.42
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	2.01	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.42
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.42
3:D:1072:ILE:HA	3:D:1075:HIS:HD2	1.83	0.42
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.18	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.42
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.20	0.42
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.01	0.42
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.89	0.42
1:A:103:ALA:HB1	1:A:107:LYS:HD3	2.02	0.42
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.20	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.90	0.42
3:D:917:GLN:O	3:D:918:ALA:C	2.58	0.42
3:D:1053[A]:PHE:CE2	3:D:1072:ILE:HG23	2.55	0.42
3:D:200:ASP:O	3:D:397:LYS:HG2	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:N	11:B:2103:HOH:O	2.52	0.42
2:C:420:ARG:HB2	2:C:420:ARG:HE	1.61	0.42
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.02	0.42
4:E:44:GLU:OE1	4:E:72:ARG:NH2	2.49	0.42
1:B:213:GLN:O	1:B:217:ILE:HG13	2.19	0.42
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.36	0.42
2:C:721:ARG:HH12	2:C:785:VAL:HG11	1.85	0.42
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	2.01	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.90	0.42
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.55	0.41
2:C:203:ASP:OD1	2:C:204:GLN:N	2.53	0.41
2:C:896:PHE:HB2	2:C:921:ALA:HB1	2.01	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.01	0.41
6:G:20:DG:H2'	6:G:21:DG:O4'	2.20	0.41
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.55	0.41
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.02	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.93	0.41
3:D:803:GLY:HA2	3:D:827:ILE:HA	2.02	0.41
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.56	0.41
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.01	0.41
2:C:740:GLU:OE1	2:C:807[B]:ARG:NH2	2.53	0.41
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.90	0.41
3:D:209:ARG:O	3:D:346:ARG:HD3	2.21	0.41
3:D:414:ARG:HD3	3:D:451:ASP:HB2	2.01	0.41
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.55	0.41
3:D:790:TYR:CE1	3:D:1022:VAL:HG13	2.55	0.41
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.49	0.41
1:A:148:VAL:O	11:A:402:HOH:O	2.21	0.41
1:A:172:SER:HA	1:A:173:PRO:HD2	1.87	0.41
1:A:80:LEU:O	1:A:83:LYS:HB2	2.21	0.41
2:C:164:PRO:HA	2:C:269:LEU:HD23	2.03	0.41
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.56	0.41
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.55	0.41
3:D:814:ALA:O	3:D:818:ARG:HG3	2.21	0.41
1:B:150:TYR:HE1	1:B:170:VAL:HG22	1.86	0.41
2:C:607:ASP:HB3	2:C:610:ARG:H	1.85	0.41
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.56	0.41
3:D:890:VAL:HA	3:D:926:LYS:HB3	2.02	0.41
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.03	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.88	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	2.03	0.41
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.53	0.41
3:D:408:GLU:HA	5:F:171:LYS:NZ	2.36	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.21	0.41
2:C:276:LYS:HE3	2:C:276:LYS:HB3	1.89	0.41
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.89	0.41
2:C:45:GLN:O	2:C:49:ARG:HG2	2.20	0.41
2:C:611:ILE:HD11	2:C:641:PRO:HB3	2.03	0.41
2:C:690:ILE:HB	2:C:694:LEU:HD12	2.01	0.41
2:C:944:LEU:O	2:C:948:GLU:HB2	2.21	0.41
3:D:923:GLY:O	3:D:927:THR:OG1	2.39	0.41
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.84	0.41
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.56	0.41
3:D:1072:ILE:HA	3:D:1075:HIS:CD2	2.55	0.41
3:D:618:LEU:HA	3:D:618:LEU:HD13	1.85	0.41
3:D:743:ASP:HA	8:I:7:A:H4'	2.02	0.41
3:D:784:ASP:HB2	3:D:939:PHE:HE1	1.86	0.41
3:D:920:LEU:O	3:D:923:GLY:HA2	2.20	0.41
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	2.03	0.41
5:F:397:ILE:HD12	5:F:400:ILE:HD12	2.02	0.41
6:G:15:DT:C4	6:G:16:DC:N4	2.89	0.41
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.48	0.41
2:C:30:LEU:O	2:C:71:TYR:OH	2.28	0.40
2:C:55:GLU:HG2	2:C:65:VAL:HG22	2.01	0.40
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.03	0.40
3:D:226:PRO:HG2	3:D:245:LEU:HD11	2.02	0.40
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.94	0.40
2:C:1018:GLN:O	2:C:1058:ASP:HA	2.21	0.40
2:C:807[A]:ARG:NH1	2:C:810:ASP:OD2	2.45	0.40
2:C:976:ASP:HB3	2:C:979:THR:OG1	2.21	0.40
3:D:956:ILE:H	3:D:956:ILE:HG12	1.61	0.40
3:D:573:MET:SD	5:F:210:LEU:HB3	2.61	0.40
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.03	0.40
7:H:12:DC:H1'	7:H:13:DT:C5	2.56	0.40
1:B:94:LEU:O	1:B:146:ARG:NH2	2.54	0.40
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.03	0.40
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	2.03	0.40
3:D:786:ILE:HG22	3:D:1026:SER:HB2	2.03	0.40
3:D:622:ARG:NH1	6:G:17:DG:OP1	2.35	0.40
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.57	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:683:ASN:HB2	2:C:872:ASN:HB2	2.04	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.83	0.40
5:F:362:SER:OG	5:F:365:GLU:HG2	2.21	0.40
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.22	0.40
3:D:916:TYR:O	3:D:919:PHE:HB3	2.22	0.40
5:F:184:ARG:O	5:F:188:ILE:HG13	2.21	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	230/315 (73%)	228 (99%)	2 (1%)	0	100	100
1	B	218/315 (69%)	210 (96%)	7 (3%)	1 (0%)	32	74
2	C	1111/1119 (99%)	1081 (97%)	29 (3%)	1 (0%)	55	89
3	D	1485/1524 (97%)	1445 (97%)	40 (3%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	333/443 (75%)	329 (99%)	4 (1%)	0	100	100
All	All	3469/3815 (91%)	3383 (98%)	84 (2%)	2 (0%)	55	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	925	TYR
1	B	8	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/273 (74%)	199 (99%)	2 (1%)	80	93
1	B	195/273 (71%)	192 (98%)	3 (2%)	70	90
2	C	939/941 (100%)	922 (98%)	17 (2%)	64	87
3	D	1256/1279 (98%)	1234 (98%)	22 (2%)	64	87
4	E	82/88 (93%)	81 (99%)	1 (1%)	75	91
5	F	293/388 (76%)	290 (99%)	3 (1%)	80	93
All	All	2966/3242 (92%)	2918 (98%)	48 (2%)	68	89

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	74	ASP
1	B	55	SER
1	B	96	THR
1	B	154	GLU
2	C	100	LEU
2	C	141	HIS
2	C	174	LEU
2	C	177	GLU
2	C	230	ARG
2	C	342	ASP
2	C	353	ARG
2	C	358	ARG
2	C	402	SER
2	C	429	ASP
2	C	566	THR
2	C	575	GLN
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	807[A]	ARG
2	C	807[B]	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	35	ARG
3	D	149	LYS
3	D	270	LEU
3	D	273	ARG
3	D	288	MET
3	D	632	VAL
3	D	709	HIS
3	D	743	ASP
3	D	754	PHE
3	D	864	VAL
3	D	894	LYS
3	D	907	GLU
3	D	921	ARG
3	D	956	ILE
3	D	1014	ASN
3	D	1041	LEU
3	D	1129	THR
3	D	1184	GLN
3	D	1188	VAL
3	D	1234	THR
3	D	1307	LYS
3	D	1488	ASP
4	E	50	THR
5	F	88	ILE
5	F	369	LEU
5	F	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
2	C	99	GLN
2	C	117	HIS
2	C	506	ASN
2	C	538	GLN
2	C	962	GLN
3	D	66	GLN
3	D	143	ASN
3	D	669	ASN
3	D	1124	GLN
5	F	83	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	2	C

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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	231/315 (73%)	-0.36	4 (1%) 70 57	40, 54, 82, 135	0
1	B	222/315 (70%)	-0.29	0 100 100	38, 61, 96, 118	0
2	C	1112/1119 (99%)	-0.34	7 (0%) 89 83	20, 49, 113, 153	0
3	D	1486/1524 (97%)	-0.18	18 (1%) 79 67	18, 53, 118, 151	1 (0%)
4	E	94/99 (94%)	-0.41	0 100 100	24, 49, 86, 107	0
5	F	337/443 (76%)	-0.03	15 (4%) 34 21	42, 73, 124, 149	0
6	G	18/21 (85%)	-0.17	0 100 100	36, 64, 143, 151	0
7	H	24/27 (88%)	-0.01	0 100 100	59, 83, 139, 168	0
8	I	7/7 (100%)	-0.07	1 (14%) 3 2	33, 35, 85, 108	0
All	All	3531/3870 (91%)	-0.24	45 (1%) 77 65	18, 55, 116, 168	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	5.0
5	F	146	GLY	4.9
5	F	149	GLU	4.6
1	A	232	ALA	4.5
3	D	422	ALA	3.7
5	F	377	ASP	3.7
3	D	173	PRO	3.7
3	D	144	GLY	3.6
3	D	922	LEU	3.5
5	F	414	ARG	3.1
2	C	365	ASP	3.1
3	D	1237	THR	3.1
3	D	531	ASP	3.0
5	F	138	SER	3.0
2	C	766	GLU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	362	GLY	2.8
3	D	316	GLN	2.8
3	D	1499	ARG	2.8
5	F	415	THR	2.6
5	F	170	HIS	2.6
3	D	1297	GLU	2.6
3	D	174	GLY	2.4
3	D	1306	PRO	2.4
3	D	321	GLN	2.4
8	I	1	C	2.4
1	A	230	ALA	2.4
5	F	150	THR	2.3
5	F	381	HIS	2.3
2	C	739	GLU	2.3
5	F	191	ASN	2.3
1	A	234	ALA	2.3
5	F	145	PRO	2.3
2	C	104	ASP	2.3
3	D	235	ALA	2.3
5	F	416	ARG	2.3
3	D	345	TYR	2.3
3	D	923	GLY	2.3
5	F	411	HIS	2.3
3	D	1292	VAL	2.2
5	F	376	ILE	2.2
1	A	233	VAL	2.2
3	D	1298	GLY	2.2
5	F	142	ARG	2.1
2	C	769	PRO	2.0
3	D	1127	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	MG	D	1601	1/1	0.97	0.18	-0.34	37,37,37,37	0
10	ZN	D	1603	1/1	0.90	0.07	-1.45	45,45,45,45	0
9	MG	F	2001	1/1	0.95	0.14	-1.60	62,62,62,62	0
10	ZN	D	1602	1/1	0.98	0.03	-3.80	6,6,6,6	0
9	MG	D	1604	1/1	0.98	0.12	-	19,19,19,19	0
9	MG	B	2001	1/1	0.69	0.27	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.