



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2017 – 05:42 AM EST

PDB ID : 5UH9  
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex containing 2nt RNA  
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.  
Deposited on : unknown  
Resolution : 4.40 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.

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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	:	rb-20030345
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)	:	rb-20030345

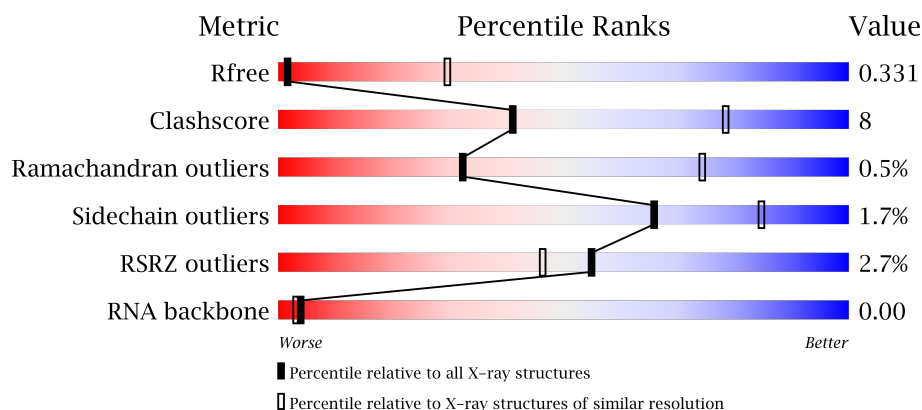
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.40 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	1024 (5.08-3.62)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1007 (5.08-3.64)
RNA backbone	2435	1036 (5.90-2.90)

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	347	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>12%</div> <div>35%</div> </div> </div>
1	B	347	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>12%</div> <div>35%</div> </div> </div>
2	C	1178	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>.</div> </div> </div>
3	D	1316	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	110	 2% 65% 8% 26%
5	F	528	 3% 49% 11% 39%
6	H	23	 48% 43% 9%
7	G	16	 63% 25% 6% 6%
8	I	2	 100%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 26030 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	224	Total	C	N	O	S	0	0	0
			1704	1072	295	335	2			
1	B	226	Total	C	N	O	S	0	0	0
			1709	1077	290	340	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8714	5454	1528	1693	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9887	6188	1793	1866	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O	0	0	0
			637	408	106	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	322	Total	C	N	O	S	0	0	0
			2555	1589	461	496	9			

- Molecule 6 is a DNA chain called DNA (5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*CP\*GP\*GP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

- Molecule 7 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*CP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

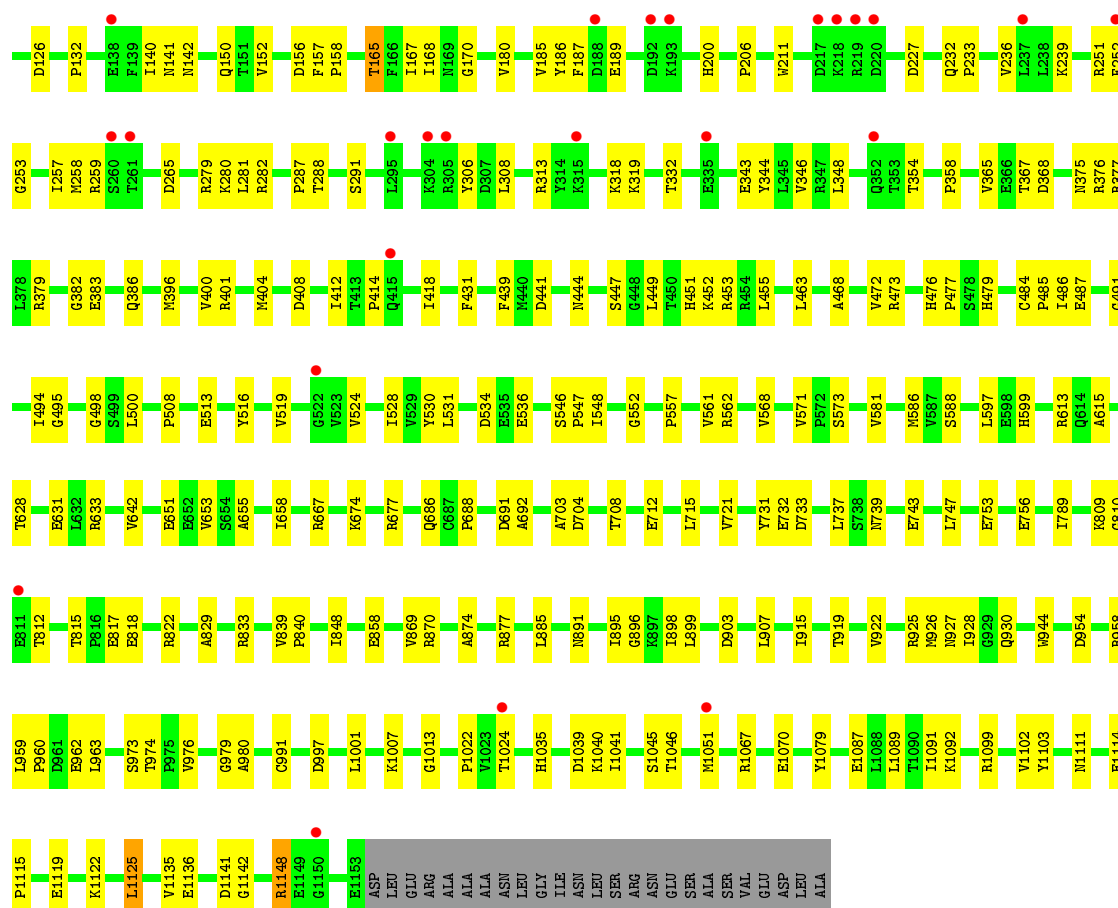
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

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 ( $\text{RSRZ} > 2$ ). 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.

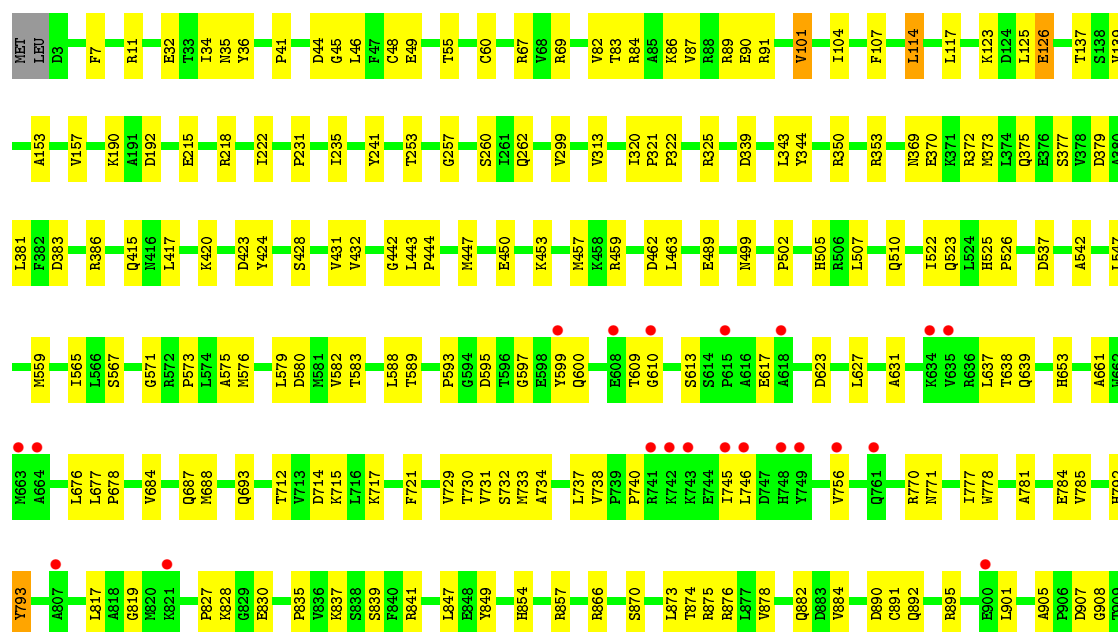
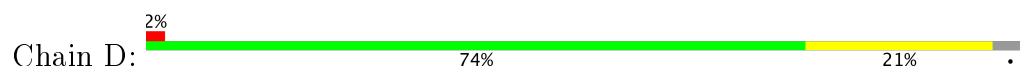
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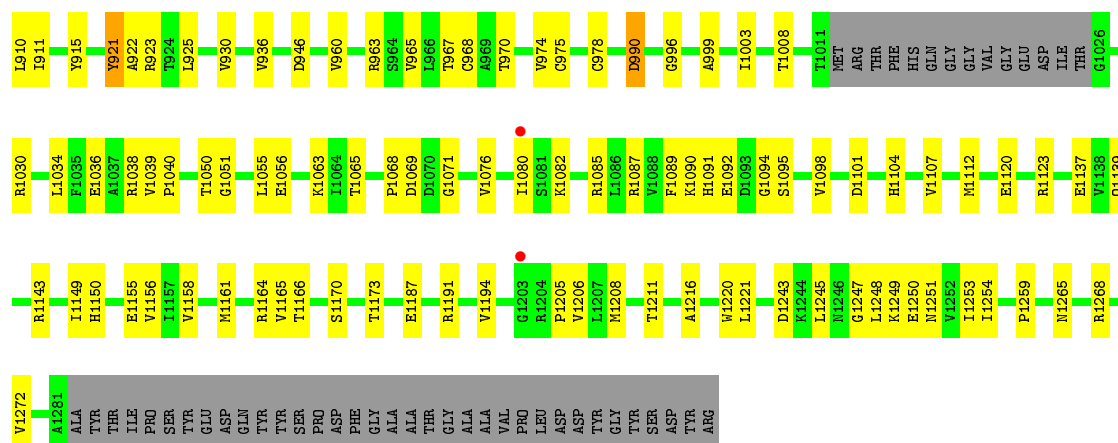
- Chain B:
- 
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1        | MET        | 0.00                       |
| 2        | LEU        | 0.00                       |
| 3        | ILE        | 0.00                       |
| 4        | SER        | 0.00                       |
| 5        | GLN        | 0.00                       |
| 6        | R6         | 0.00                       |
| 7        | E11        | 0.00                       |
| 8        | V22        | 0.00                       |
| 9        | I23        | 0.00                       |
| 10       | E27        | 0.00                       |
| 11       | P28        | 0.00                       |
| 12       | G35        | 0.00                       |
| 13       | R39        | 0.00                       |
| 14       | L42        | 0.00                       |
| 15       | S45        | 0.00                       |
| 16       | V51        | 0.00                       |
| 17       | I56        | 0.00                       |
| 18       | W59        | 0.00                       |
| 19       | L60        | 0.00                       |
| 20       | H61        | 0.00                       |
| 21       | E62        | 0.00                       |
| 22       | D72        | 0.00                       |
| 23       | V73        | 0.00                       |
| 24       | T74        | 0.00                       |
| 25       | E75        | 0.00                       |
| 26       | I76        | 0.00                       |
| 27       | I77        | 0.00                       |
| 28       | L78        | 0.00                       |
| 29       | N79        | 0.00                       |
| 30       | L80        | 0.00                       |
| 31       | K81        | 0.00                       |
| 32       | V84        | 0.00                       |
| 33       | H85        | 0.00                       |
| 34       | S86        | 0.00                       |
| 35       | S87        | 0.00                       |
| 36       | D90        | 0.00                       |
| 37       | E91        | 0.00                       |
| 38       | P92        | 0.00                       |
| 39       | W93        | 0.00                       |
| 40       | T94        | 0.00                       |
| 41       | K95        | 0.00                       |
| 42       | I96        | 0.00                       |
| 43       | L97        | 0.00                       |
| 44       | K98        | 0.00                       |
| 45       | K99        | 0.00                       |
| 46       | V100       | 0.00                       |

- Chain C:
- 
- | Amino Acid | Conservation (%) |
|------------|------------------|
| MET        | 2%               |
| LEU        | 74%              |
| LEU        | 74%              |
| GLU        | 74%              |
| GLY        | 74%              |
| CYS        | 74%              |
| ILE        | 74%              |
| LEU        | 74%              |
| ALA        | 74%              |
| ASP        | 74%              |
| SER        | 74%              |
| ARG        | 74%              |
| GLN        | 74%              |
| LYS        | 74%              |
| THR        | 74%              |
| ALA        | 74%              |
| SER        | 74%              |
| PRO        | 74%              |
| SER        | 74%              |
| PRO        | 74%              |
| ARG        | 74%              |
| PRO        | 74%              |
| GLN        | 74%              |
| SER        | 74%              |
| SER        | 74%              |
| S28        | 74%              |
| Y29        | 74%              |
| N30        | 74%              |
| V39        | 21%              |
| S40        | 21%              |
| F41        | 21%              |
| E46        | 21%              |
| P47        | 21%              |
| L48        | 21%              |
| E49        | 21%              |
| V50        | 21%              |
| L53        | 21%              |
| T58        | 21%              |
| D59        | 21%              |
| S60        | 21%              |
| F61        | 21%              |
| E62        | 21%              |
| S94        | 21%              |
| P95        | 21%              |
| I96        | 21%              |
| G101       | 21%              |
| S102       | 21%              |
| M103       | 21%              |
| S104       | 21%              |
| L105       | 21%              |
| V110       | 21%              |

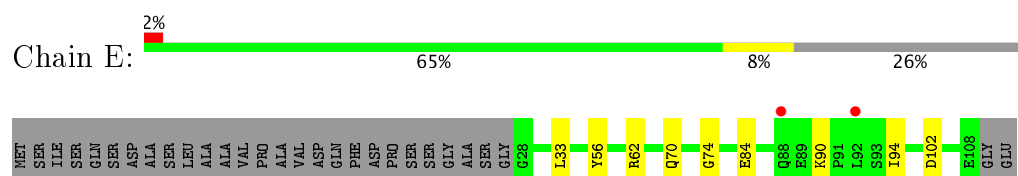


• Molecule 3: DNA-directed RNA polymerase subunit beta'

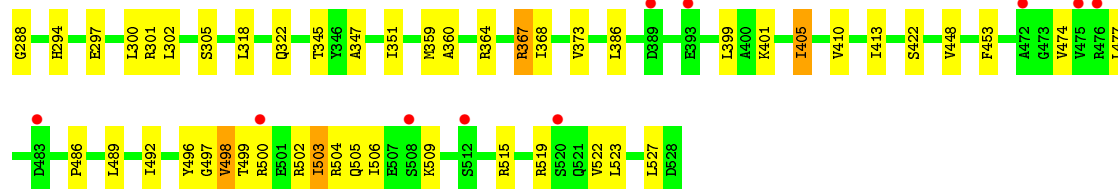
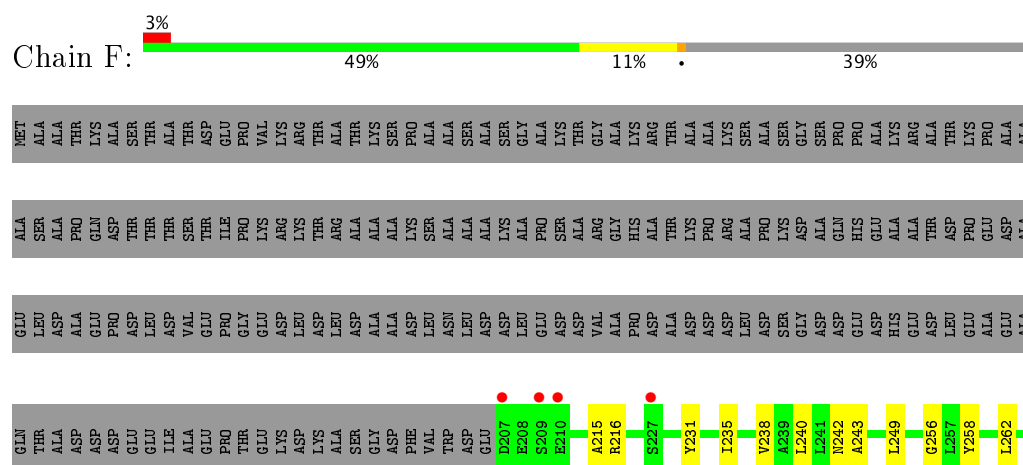




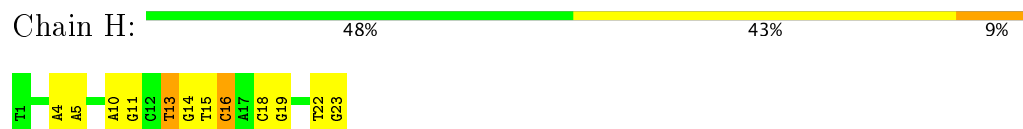
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*CP\*GP\*GP\*AP\*TP\*G)-3')





- Molecule 7: DNA (5'-D(\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*CP\*AP\*GP\*G)-3')

Chain G:  63% 25% 6% 6%



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

Chain I:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.46Å 164.63Å 201.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 4.40 49.89 – 4.40	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.89-4.40) 71.6 (49.89-4.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 4.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.281 , 0.332 0.285 , 0.331	Depositor DCC
$R_{free}$ test set	1991 reflections (6.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.65	EDS
Total number of atoms	26030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.23	0/1730	0.45	0/2354
1	B	0.24	0/1734	0.44	0/2360
2	C	0.24	0/8873	0.42	1/12031 (0.0%)
3	D	0.24	0/10052	0.41	0/13591
4	E	0.23	0/650	0.42	0/886
5	F	0.24	0/2585	0.41	0/3485
6	H	0.68	2/535 (0.4%)	1.07	4/826 (0.5%)
7	G	0.82	1/339 (0.3%)	0.95	2/521 (0.4%)
8	I	0.30	0/47	0.60	0/72
All	All	0.27	3/26545 (0.0%)	0.46	7/36126 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	12	DG	O3'-P	10.61	1.73	1.61
6	H	13	DT	O3'-P	6.39	1.68	1.61
6	H	16	DC	O3'-P	5.84	1.68	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	16	DC	P-O3'-C3'	8.31	129.67	119.70
6	H	19	DG	C5'-C4'-O4'	7.34	123.24	109.30
6	H	19	DG	O4'-C4'-C3'	-6.85	101.76	104.50
7	G	12	DG	P-O3'-C3'	-6.21	112.25	119.70
6	H	16	DC	OP1-P-O3'	5.77	117.89	105.20
2	C	48	LEU	CA-CB-CG	5.14	127.13	115.30
7	G	9	DC	P-O3'-C3'	5.13	125.85	119.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1704	0	1741	25	0
1	B	1709	0	1733	25	0
2	C	8714	0	8636	164	0
3	D	9887	0	9943	186	0
4	E	637	0	635	6	0
5	F	2555	0	2579	42	0
6	H	476	0	261	15	0
7	G	303	0	170	4	0
8	I	42	0	22	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	26030	0	25720	414	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 8.

All (414) 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)
6:H:16:DC:O2	7:G:12:DG:N2	1.92	1.03
3:D:891:CYS:SG	3:D:970:THR:OG1	2.23	0.96
2:C:211:TRP:NE1	6:H:13:DT:O2	2.00	0.94
6:H:16:DC:N3	7:G:12:DG:N1	2.23	0.83
6:H:15:DT:H2''	6:H:16:DC:H5'	1.68	0.73
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.73	0.71
2:C:104:SER:HB3	2:C:140:ILE:HB	1.73	0.70
2:C:1024:THR:H	3:D:730:THR:HG21	1.56	0.69
1:B:11:GLU:HB2	1:B:22:VAL:HB	1.74	0.69
2:C:401:ARG:HA	2:C:404:MET:HE2	1.76	0.68
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.76	0.68
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.27	0.68
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.75	0.68
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.76	0.67
2:C:1067:ARG:NH2	3:D:415:GLN:O	2.27	0.67
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.76	0.67
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.76	0.66
2:C:101:GLY:O	2:C:142:ASN:ND2	2.29	0.66
3:D:891:CYS:O	3:D:892:GLN:HB2	1.96	0.65
2:C:815:THR:HG22	2:C:817:GLU:H	1.61	0.65
1:B:75:GLU:O	1:B:79:ASN:ND2	2.30	0.64
2:C:1035:HIS:HB3	2:C:1040:LYS:HE2	1.77	0.64
1:A:11:GLU:HB2	1:A:22:VAL:HB	1.80	0.64
3:D:676:LEU:HG	3:D:715:LYS:HB3	1.80	0.64
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.80	0.64
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.80	0.63
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.79	0.63
3:D:589:THR:HG21	3:D:688:MET:HG2	1.78	0.63
3:D:350:ARG:HG2	3:D:353:ARG:HH12	1.62	0.63
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.81	0.63
2:C:485:PRO:O	3:D:857:ARG:NH2	2.31	0.63
3:D:369:ASN:OD1	3:D:372:ARG:NH2	2.33	0.62
3:D:45:GLY:H	3:D:48:CYS:HB2	1.65	0.62
5:F:360:ALA:HB1	5:F:373:VAL:HG21	1.82	0.62
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.82	0.61
2:C:944:TRP:HB2	2:C:991:CYS:HB2	1.82	0.61
5:F:401:LYS:HA	5:F:405:ILE:HA	1.82	0.61
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	1.82	0.61
5:F:515:ARG:O	5:F:519:ARG:N	2.33	0.61
2:C:453:ARG:NH1	2:C:500:LEU:O	2.35	0.60
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.83	0.60
2:C:704:ASP:HB2	2:C:708:THR:HB	1.82	0.60
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.84	0.59
2:C:102:SER:O	2:C:141:ASN:ND2	2.35	0.59
1:A:87:SER:O	1:A:142:ARG:NH1	2.31	0.59
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.85	0.59
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.84	0.59
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.83	0.59
2:C:1136:GLU:OE1	3:D:11:ARG:NH1	2.36	0.59
5:F:499:THR:OG1	5:F:500:ARG:N	2.36	0.58
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.86	0.58
3:D:107:PHE:HE1	3:D:125:LEU:HB3	1.68	0.58
3:D:215:GLU:OE1	3:D:218:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.85	0.58
3:D:712:THR:HA	3:D:715:LYS:HD2	1.84	0.58
3:D:882:GLN:HE22	3:D:1249:LYS:HG3	1.67	0.58
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.85	0.58
3:D:443:LEU:HD12	3:D:444:PRO:HD2	1.86	0.58
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.85	0.57
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.86	0.57
3:D:32:GLU:HG3	5:F:367:ARG:HB2	1.86	0.57
7:G:15:DT:H2'	7:G:16:DC:C6	2.39	0.57
2:C:50:VAL:O	2:C:633:ARG:NH1	2.37	0.57
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.68	0.57
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.86	0.57
3:D:600:GLN:HB2	3:D:609:THR:HB	1.86	0.57
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.86	0.57
3:D:262:GLN:HB2	3:D:313:VAL:HG11	1.86	0.57
4:E:70:GLN:O	4:E:74:GLY:N	2.20	0.57
3:D:873:LEU:HA	3:D:876:ARG:HE	1.70	0.56
1:A:18:ARG:NH2	1:A:195:ASP:OD1	2.37	0.56
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.85	0.56
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.87	0.56
2:C:96:ILE:N	2:C:105:LEU:O	2.24	0.56
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.87	0.56
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.88	0.56
6:H:22:DT:H1'	6:H:23:DG:H5'	1.88	0.56
2:C:677:ARG:HE	2:C:753:GLU:HA	1.71	0.56
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.88	0.56
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.20	0.56
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.87	0.55
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.87	0.55
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.89	0.55
2:C:739:ASN:ND2	2:C:743:GLU:OE2	2.39	0.55
3:D:257:GLY:O	3:D:260:SER:OG	2.25	0.55
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.88	0.55
5:F:496:TYR:O	5:F:498:VAL:N	2.40	0.55
5:F:238:VAL:HG21	5:F:297:GLU:HB3	1.89	0.55
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.87	0.54
2:C:733:ASP:OD2	2:C:925:ARG:NH2	2.40	0.54
2:C:96:ILE:HB	2:C:105:LEU:HB3	1.89	0.54
3:D:502:PRO:HG3	7:G:14:DG:H21	1.72	0.54
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.88	0.54
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.39	0.54
2:C:1041:ILE:HD11	3:D:447:MET:HG3	1.89	0.53
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.72	0.53
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.89	0.53
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.88	0.53
3:D:1080:ILE:HG22	3:D:1082:LYS:H	1.73	0.53
2:C:919:THR:HG21	3:D:729:VAL:HG12	1.89	0.53
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.91	0.53
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.90	0.53
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.91	0.53
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.23	0.53
2:C:318:LYS:NZ	2:C:534:ASP:OD2	2.38	0.53
2:C:651:GLU:OE2	2:C:667:ARG:NH1	2.41	0.53
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.90	0.53
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.42	0.52
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.90	0.52
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.91	0.52
2:C:974:THR:HG23	2:C:980:ALA:H	1.75	0.52
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.90	0.52
3:D:67:ARG:HG2	3:D:69:ARG:H	1.75	0.52
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.92	0.52
2:C:119:VAL:HG13	2:C:167:ILE:HD11	1.91	0.52
2:C:344:TYR:OH	2:C:365:VAL:HA	2.09	0.52
3:D:737:LEU:N	3:D:793:TYR:OH	2.33	0.52
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.92	0.52
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.74	0.51
2:C:186:TYR:HE1	2:C:375:ASN:HB3	1.74	0.51
3:D:1069:ASP:OD2	3:D:1104:HIS:NE2	2.43	0.51
2:C:1045:SER:OG	2:C:1046:THR:N	2.44	0.51
3:D:746:LEU:HD13	3:D:837:LYS:HB3	1.93	0.51
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.91	0.51
5:F:345:THR:HB	6:H:4:DA:H8	1.75	0.51
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.92	0.51
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.74	0.51
3:D:613:SER:N	3:D:617:GLU:OE1	2.34	0.51
3:D:35:ASN:OD1	3:D:36:TYR:N	2.44	0.51
5:F:477:LEU:HB3	5:F:492:ILE:HD13	1.93	0.51
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.93	0.50
3:D:49:GLU:OE2	3:D:55:THR:N	2.35	0.50
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.94	0.50
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:206:PRO:HB3	2:C:306:TYR:CZ	2.47	0.50
3:D:589:THR:HB	3:D:687:GLN:HA	1.94	0.50
3:D:320:ILE:HG22	3:D:344:TYR:HE2	1.77	0.50
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.94	0.50
2:C:817:GLU:OE1	2:C:817:GLU:N	2.45	0.49
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.93	0.49
3:D:383:ASP:OD2	3:D:386:ARG:NE	2.43	0.49
2:C:1089:LEU:HB3	3:D:420:LYS:NZ	2.26	0.49
2:C:150:GLN:HG2	2:C:414:PRO:HG2	1.94	0.49
3:D:827:PRO:HD3	3:D:854:HIS:NE2	2.28	0.49
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.47	0.49
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.37	0.49
3:D:417:LEU:HD22	3:D:1253:ILE:HG23	1.95	0.49
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.28	0.49
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.95	0.49
2:C:747:LEU:HD13	2:C:885:LEU:HD11	1.95	0.49
3:D:580:ASP:HB2	3:D:721:PHE:HE1	1.78	0.49
5:F:410:VAL:HA	5:F:413:ILE:HD12	1.94	0.49
5:F:499:THR:O	5:F:502:ARG:HG2	2.12	0.49
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.95	0.49
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.94	0.49
2:C:288:THR:N	2:C:291:SER:OG	2.44	0.49
2:C:891:ASN:OD1	2:C:891:ASN:N	2.39	0.49
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.33	0.49
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.45	0.49
5:F:492:ILE:HG22	5:F:503:ILE:HG21	1.94	0.49
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.94	0.48
2:C:485:PRO:HG3	2:C:586:MET:HE3	1.94	0.48
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.95	0.48
2:C:28:SER:N	2:C:962:GLU:OE1	2.46	0.48
2:C:944:TRP:NE1	2:C:963:LEU:O	2.42	0.48
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.94	0.48
5:F:262:LEU:O	5:F:266:LEU:HG	2.13	0.48
1:A:64:THR:OG1	1:A:65:THR:N	2.46	0.48
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.95	0.48
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.46	0.48
5:F:489:LEU:HD23	5:F:489:LEU:H	1.78	0.48
2:C:494:ILE:HD11	3:D:857:ARG:HG3	1.95	0.48
2:C:400:VAL:O	2:C:404:MET:HG3	2.14	0.48
2:C:885:LEU:HD12	2:C:895:ILE:HD11	1.96	0.48
3:D:428:SER:HB3	3:D:522:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.95	0.48
2:C:557:PRO:O	2:C:573:SER:N	2.46	0.48
3:D:1056:GLU:HB3	3:D:1063:LYS:HE3	1.96	0.48
2:C:180:VAL:HG21	2:C:379:ARG:HE	1.79	0.47
2:C:165:THR:HG22	2:C:452:LYS:HE2	1.96	0.47
2:C:46:GLU:N	2:C:47:PRO:HD3	2.29	0.47
3:D:907:ASP:OD1	3:D:907:ASP:N	2.48	0.47
2:C:252:PHE:HB3	2:C:258:MET:HG3	1.96	0.47
3:D:83:THR:HG22	3:D:84:ARG:H	1.79	0.47
2:C:200:HIS:CE1	2:C:348:LEU:HG	2.50	0.47
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.96	0.47
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.95	0.47
2:C:1070:GLU:OE1	3:D:875:ARG:NH2	2.33	0.47
2:C:877:ARG:HH12	2:C:1039:ASP:CG	2.17	0.47
3:D:339:ASP:OD1	5:F:422:SER:OG	2.21	0.47
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.97	0.47
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.15	0.47
3:D:373:MET:HE1	5:F:322:GLN:HG3	1.96	0.47
1:A:213:LYS:HA	1:B:223:ARG:HG3	1.96	0.47
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.74	0.47
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.80	0.46
4:E:33:LEU:H	4:E:33:LEU:HD23	1.79	0.46
2:C:211:TRP:HH2	6:H:14:DG:OP1	1.97	0.46
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.79	0.46
3:D:44:ASP:N	3:D:48:CYS:SG	2.86	0.46
1:B:39:ARG:NH2	3:D:623:ASP:OD2	2.46	0.46
3:D:884:VAL:HG11	3:D:1156:VAL:HG13	1.98	0.46
3:D:996:GLY:HA2	3:D:1156:VAL:HG11	1.98	0.46
6:H:10:DA:C2	6:H:11:DG:C4	3.03	0.46
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.30	0.46
5:F:489:LEU:HD12	5:F:504:ARG:HD3	1.97	0.46
2:C:1089:LEU:HD13	3:D:420:LYS:HZ2	1.80	0.46
2:C:487:GLU:OE1	2:C:588:SER:OG	2.24	0.46
3:D:778:TRP:CE2	3:D:835:PRO:HG3	2.51	0.46
1:A:120:ASN:OD1	1:A:120:ASN:N	2.48	0.46
3:D:373:MET:SD	5:F:318:LEU:HB3	2.56	0.46
2:C:281:LEU:HD22	2:C:282:ARG:HG3	1.98	0.46
3:D:1120:GLU:HA	3:D:1123:ARG:HG2	1.98	0.46
2:C:472:VAL:HG22	6:H:14:DG:N2	2.30	0.46
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.98	0.46
2:C:287:PRO:HD2	5:F:216:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:ALA:HB2	3:D:911:ILE:HG13	1.97	0.46
2:C:1007:LYS:HA	2:C:1024:THR:HA	1.98	0.45
2:C:463:LEU:HD13	2:C:468:ALA:HB2	1.99	0.45
3:D:1036:GLU:OE2	3:D:1211:THR:OG1	2.29	0.45
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.45
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.97	0.45
3:D:137:THR:OG1	3:D:253:THR:O	2.33	0.45
3:D:373:MET:O	3:D:377:SER:OG	2.29	0.45
2:C:731:TYR:CE1	3:D:579:LEU:HB2	2.49	0.45
6:H:15:DT:H2"	6:H:16:DC:H6	1.80	0.45
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.99	0.45
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.98	0.45
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.50	0.45
1:A:18:ARG:NH1	2:C:997:ASP:OD1	2.49	0.45
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.48	0.45
1:A:56:ILE:HB	1:A:59:VAL:HB	1.98	0.45
3:D:537:ASP:N	3:D:537:ASP:OD1	2.43	0.45
3:D:588:LEU:HD12	3:D:589:THR:HG23	1.98	0.45
2:C:1111:ASN:HB3	4:E:62:ARG:NH1	2.31	0.45
2:C:396:MET:HE1	2:C:418:ILE:HG12	1.98	0.45
3:D:1068:PRO:HB2	3:D:1071:GLY:O	2.17	0.45
3:D:457:MET:HE2	3:D:457:MET:HB2	1.81	0.45
2:C:41:PHE:O	2:C:979:GLY:HA2	2.17	0.45
2:C:447:SER:HB2	2:C:613:ARG:O	2.17	0.45
5:F:235:ILE:HG23	5:F:300:LEU:HB3	1.97	0.45
3:D:1248:LEU:HD23	3:D:1259:PRO:HD2	1.98	0.45
3:D:580:ASP:HB2	3:D:721:PHE:CE1	2.52	0.45
1:B:87:SER:O	1:B:142:ARG:NH1	2.49	0.45
2:C:455:LEU:N	2:C:498:GLY:O	2.44	0.45
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.36	0.45
5:F:347:ALA:O	5:F:351:ILE:HG13	2.17	0.45
2:C:1092:LYS:O	3:D:423:ASP:N	2.48	0.44
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.50	0.44
3:D:525:HIS:HA	3:D:526:PRO:HD3	1.86	0.44
3:D:1272:VAL:HG11	4:E:56:TYR:O	2.17	0.44
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.82	0.44
3:D:320:ILE:HG13	3:D:321:PRO:HD2	1.98	0.44
3:D:499:ASN:HB3	3:D:542:ALA:HB3	1.98	0.44
3:D:819:GLY:O	3:D:839:SER:HB3	2.18	0.44
1:B:182:ARG:HA	1:B:187:THR:HA	1.99	0.44
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:907:LEU:HD13	2:C:1001:LEU:HD13	2.00	0.44
2:C:444:ASN:H	2:C:447:SER:HB3	1.82	0.44
3:D:999:ALA:O	3:D:1003:ILE:HG13	2.17	0.44
3:D:905:ALA:HB3	3:D:908:GLY:O	2.16	0.44
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.53	0.44
4:E:90:LYS:O	4:E:94:ILE:HG13	2.17	0.44
5:F:249:LEU:HD11	5:F:294:HIS:ND1	2.32	0.44
2:C:568:VAL:HG21	3:D:847:LEU:HD23	2.00	0.44
3:D:453:LYS:O	3:D:457:MET:HG3	2.17	0.44
3:D:990:ASP:N	3:D:990:ASP:OD1	2.50	0.44
3:D:1250:GLU:OE2	3:D:1250:GLU:N	2.46	0.44
2:C:928:ILE:H	2:C:928:ILE:HG13	1.53	0.44
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.99	0.44
2:C:954:ASP:O	2:C:958:ARG:NH1	2.51	0.44
3:D:895:ARG:NH1	3:D:967:THR:O	2.51	0.44
3:D:925:LEU:HD11	3:D:960:VAL:HG11	2.00	0.44
3:D:117:LEU:HD12	3:D:299:VAL:HG22	1.99	0.43
2:C:615:ALA:HB3	2:C:715:LEU:HD22	2.00	0.43
3:D:1065:THR:HG23	3:D:1076:VAL:HB	2.00	0.43
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.24	0.43
3:D:125:LEU:HA	3:D:125:LEU:HD12	1.79	0.43
3:D:965:VAL:HG13	3:D:974:VAL:HG11	2.00	0.43
2:C:674:LYS:NZ	2:C:686:GLN:O	2.46	0.43
3:D:372:ARG:HH22	5:F:231:TYR:HB2	1.83	0.43
3:D:637:LEU:O	3:D:661:ALA:HA	2.19	0.43
1:A:149:ALA:HB2	1:A:165:ASP:N	2.34	0.43
2:C:383:GLU:HA	2:C:386:GLN:HB3	2.00	0.43
3:D:1170:SER:O	3:D:1173:THR:OG1	2.36	0.43
3:D:350:ARG:HD2	3:D:377:SER:OG	2.18	0.43
2:C:628:THR:N	2:C:631:GLU:OE2	2.50	0.43
3:D:87:VAL:O	3:D:90:GLU:HG2	2.18	0.43
6:H:15:DT:C2	6:H:16:DC:C5	3.07	0.43
2:C:899:LEU:HB3	2:C:903:ASP:HB2	2.01	0.43
2:C:319:LYS:HE3	2:C:344:TYR:CZ	2.54	0.43
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.54	0.43
2:C:132:PRO:HA	2:C:156:ASP:HA	2.01	0.43
2:C:1045:SER:HB3	3:D:450:GLU:O	2.19	0.43
1:B:77:ILE:O	1:B:81:LYS:HG3	2.19	0.43
2:C:441:ASP:H	2:C:451:HIS:CD2	2.37	0.43
2:C:731:TYR:HB3	3:D:432:VAL:HG21	2.01	0.43
2:C:896:GLY:HA2	3:D:431:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1003:ILE:HA	3:D:1149:ILE:HD13	2.01	0.43
3:D:123:LYS:HD2	3:D:123:LYS:HA	1.68	0.43
3:D:153:ALA:O	3:D:157:VAL:HG23	2.18	0.43
3:D:424:TYR:CD2	3:D:547:LEU:HD11	2.54	0.43
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.53	0.43
2:C:1007:LYS:HD2	2:C:1022:PRO:HB2	2.01	0.42
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.52	0.42
3:D:350:ARG:NH1	3:D:373:MET:HB3	2.34	0.42
3:D:459:ARG:NH1	3:D:463:LEU:HD11	2.34	0.42
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.88	0.42
3:D:1050:THR:HB	3:D:1107:VAL:N	2.34	0.42
3:D:732:SER:OG	3:D:733:MET:N	2.51	0.42
2:C:313:ARG:NH1	2:C:332:THR:O	2.52	0.42
3:D:218:ARG:O	3:D:222:ILE:HG13	2.19	0.42
5:F:345:THR:HA	6:H:5:DA:N7	2.34	0.42
1:A:100:GLN:HG3	1:A:133:LYS:HB2	2.01	0.42
2:C:839:VAL:HA	2:C:840:PRO:HD3	1.92	0.42
3:D:1158:VAL:HA	3:D:1161:MET:SD	2.59	0.42
5:F:474:VAL:HA	5:F:477:LEU:HD12	2.01	0.42
1:A:69:VAL:O	2:C:655:ALA:N	2.48	0.42
1:B:95:MET:HB3	1:B:113:PRO:HD3	2.02	0.42
1:B:212:GLY:O	1:B:216:VAL:HG23	2.19	0.42
2:C:233:PRO:HB2	2:C:236:VAL:HG23	2.02	0.42
2:C:441:ASP:H	2:C:451:HIS:HD2	1.68	0.42
3:D:1030:ARG:NH2	3:D:1034:LEU:HD21	2.35	0.42
3:D:459:ARG:NH1	3:D:489:GLU:OE1	2.53	0.42
3:D:567:SER:O	3:D:571:GLY:N	2.50	0.42
5:F:300:LEU:HD12	5:F:300:LEU:HA	1.84	0.42
1:B:173:LYS:HA	1:B:173:LYS:HD2	1.92	0.42
2:C:408:ASP:O	2:C:412:ILE:HG13	2.19	0.42
3:D:734:ALA:O	3:D:737:LEU:HG	2.20	0.42
1:B:208:LEU:O	1:B:212:GLY:N	2.49	0.42
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.20	0.42
2:C:60:SER:HG	2:C:382:GLY:H	1.62	0.42
2:C:737:LEU:HG	2:C:895:ILE:HD12	2.02	0.42
2:C:809:LYS:HD2	2:C:833:ARG:HD3	2.02	0.42
3:D:1085:ARG:HA	3:D:1112:MET:HA	2.01	0.42
3:D:1164:ARG:HH11	3:D:1208:MET:HE1	1.85	0.42
3:D:46:LEU:O	3:D:325:ARG:NH2	2.35	0.42
3:D:828:LYS:HE3	3:D:830:GLU:HB2	2.01	0.42
2:C:815:THR:HG21	5:F:453:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:TYR:CZ	5:F:448:VAL:HB	2.54	0.42
2:C:444:ASN:O	2:C:447:SER:HB3	2.19	0.42
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.16	0.42
3:D:369:ASN:O	3:D:373:MET:HG3	2.20	0.42
3:D:874:THR:O	3:D:878:VAL:HG23	2.20	0.42
2:C:251:ARG:NH2	2:C:343:GLU:OE1	2.44	0.42
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.55	0.42
2:C:94:SER:HA	2:C:95:PRO:HA	1.79	0.42
1:B:191:LYS:HE2	1:B:193:ILE:HD11	2.02	0.41
3:D:866:ARG:NH1	3:D:1008:THR:O	2.48	0.41
3:D:353:ARG:NH1	3:D:370:GLU:OE1	2.44	0.41
3:D:87:VAL:O	3:D:91:ARG:HG3	2.19	0.41
1:A:40:ARG:HD2	2:C:1013:GLY:O	2.20	0.41
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	2.02	0.41
2:C:472:VAL:HG22	6:H:14:DG:C2	2.55	0.41
2:C:926:MET:HE1	3:D:817:LEU:HA	2.01	0.41
5:F:302:LEU:O	5:F:305:SER:OG	2.22	0.41
1:B:45:SER:OG	1:B:214:THR:HG21	2.20	0.41
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.19	0.41
2:C:519:VAL:HG22	2:C:524:VAL:HA	2.02	0.41
2:C:53:LEU:HD13	2:C:449:LEU:HD21	2.00	0.41
3:D:573:PRO:O	3:D:576:MET:HE3	2.20	0.41
1:A:100:GLN:HG2	1:A:101:GLY:H	1.85	0.41
1:A:21:PHE:HZ	1:A:205:ARG:HA	1.84	0.41
1:B:23:ILE:HD12	1:B:192:LEU:HD23	2.03	0.41
2:C:1089:LEU:HD22	3:D:420:LYS:HG3	2.02	0.41
2:C:344:TYR:CE2	2:C:365:VAL:HG13	2.54	0.41
1:A:98:ARG:HG2	1:A:135:GLU:HG3	2.02	0.41
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.54	0.41
2:C:927:ASN:OD1	2:C:930:GLN:NE2	2.54	0.41
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.85	0.41
5:F:242:ASN:OD1	5:F:243:ALA:N	2.53	0.41
1:A:185:GLN:HG2	1:A:186:ARG:H	1.85	0.41
2:C:187:PHE:O	2:C:368:ASP:N	2.49	0.41
2:C:810:GLY:O	2:C:812:THR:N	2.53	0.41
5:F:519:ARG:HD3	5:F:519:ARG:HA	1.85	0.41
2:C:58:THR:O	2:C:62:GLU:HG3	2.21	0.41
3:D:459:ARG:HH11	3:D:463:LEU:HD11	1.86	0.41
3:D:600:GLN:N	3:D:609:THR:O	2.28	0.41
1:A:66:VAL:HA	1:A:67:PRO:HD3	1.95	0.41
2:C:444:ASN:OD1	2:C:447:SER:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:15:DT:C2'	6:H:16:DC:H5'	2.43	0.41
1:B:72:ASP:OD1	1:B:73:VAL:N	2.53	0.41
2:C:47:PRO:HG2	2:C:581:VAL:O	2.20	0.41
2:C:732:GLU:HG2	3:D:579:LEU:HD12	2.02	0.41
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.86	0.41
3:D:320:ILE:HG23	3:D:325:ARG:HD3	2.03	0.41
3:D:597:GLY:HA3	3:D:627:LEU:HA	2.03	0.41
4:E:84:GLU:H	4:E:84:GLU:CD	2.25	0.41
1:A:181:THR:O	1:A:188:ASP:HA	2.21	0.41
2:C:253:GLY:HA2	2:C:259:ARG:HE	1.86	0.41
2:C:40:SER:HB2	2:C:973:SER:HB2	2.03	0.41
1:A:225:LEU:HD13	1:A:225:LEU:H	1.85	0.40
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.86	0.40
2:C:708:THR:HA	2:C:712:GLU:O	2.21	0.40
2:C:958:ARG:HD2	2:C:958:ARG:N	2.35	0.40
3:D:1221:LEU:HD12	3:D:1221:LEU:HA	1.91	0.40
3:D:756:VAL:HG21	3:D:777:ILE:HD11	2.03	0.40
3:D:781:ALA:O	3:D:785:VAL:HG23	2.20	0.40
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.04	0.40
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.81	0.40
2:C:546:SER:HA	2:C:547:PRO:HD3	1.86	0.40
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.87	0.40
2:C:928:ILE:HG12	3:D:817:LEU:HD11	2.03	0.40
1:A:61:HIS:HE1	1:A:63:PHE:O	2.04	0.40
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.96	0.40
2:C:789:ILE:HD12	2:C:869:VAL:HG11	2.03	0.40
1:A:162:ILE:HA	1:A:163:PRO:HD2	1.88	0.40
1:A:55:ARG:HG3	1:A:161:ARG:HA	2.04	0.40
2:C:157:PHE:HA	2:C:158:PRO:HD3	1.96	0.40
2:C:152:VAL:HG21	2:C:418:ILE:HD12	2.03	0.40
3:D:507:LEU:HB3	3:D:510:GLN:HE21	1.87	0.40
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.74	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	222/347 (64%)	209 (94%)	11 (5%)	2 (1%)	20	63
1	B	222/347 (64%)	202 (91%)	18 (8%)	2 (1%)	20	63
2	C	1124/1178 (95%)	1055 (94%)	62 (6%)	7 (1%)	28	71
3	D	1261/1316 (96%)	1192 (94%)	67 (5%)	2 (0%)	51	85
4	E	79/110 (72%)	77 (98%)	2 (2%)	0	100	100
5	F	320/528 (61%)	304 (95%)	13 (4%)	3 (1%)	20	63
All	All	3228/3826 (84%)	3039 (94%)	173 (5%)	16 (0%)	32	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
5	F	497	GLY
1	A	184	GLU
2	C	1148	ARG
3	D	593	PRO
2	C	508	PRO
2	C	47	PRO
2	C	922	VAL
5	F	405	ILE
1	B	227	VAL
1	B	35	GLY
1	A	156	GLY
2	C	491	GLY
2	C	358	PRO
2	C	552	GLY
5	F	486	PRO

### 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	192/297 (65%)	188 (98%)	4 (2%)	59	80
1	B	191/297 (64%)	190 (100%)	1 (0%)	91	95
2	C	948/998 (95%)	935 (99%)	13 (1%)	71	86
3	D	1048/1095 (96%)	1026 (98%)	22 (2%)	59	80
4	E	68/90 (76%)	67 (98%)	1 (2%)	70	86
5	F	271/427 (64%)	265 (98%)	6 (2%)	57	79
All	All	2718/3204 (85%)	2671 (98%)	47 (2%)	66	85

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	VAL
1	A	159	ILE
1	A	182	ARG
1	A	225	LEU
1	B	42	LEU
2	C	39	VAL
2	C	48	LEU
2	C	165	THR
2	C	185	VAL
2	C	354	THR
2	C	376	ARG
2	C	439	PHE
2	C	479	HIS
2	C	691	ASP
2	C	858	GLU
2	C	1051	MET
2	C	1099	ARG
2	C	1125	LEU
3	D	7	PHE
3	D	60	CYS
3	D	82	VAL
3	D	101	VAL
3	D	114	LEU
3	D	126	GLU
3	D	582	VAL
3	D	583	THR
3	D	653	HIS
3	D	677	LEU
3	D	684	VAL
3	D	714	ASP

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Mol	Chain	Res	Type
3	D	793	TYR
3	D	870	SER
3	D	901	LEU
3	D	910	LEU
3	D	921	TYR
3	D	968	CYS
3	D	975	CYS
3	D	978	CYS
3	D	990	ASP
3	D	1194	VAL
4	E	102	ASP
5	F	258	TYR
5	F	359	MET
5	F	367	ARG
5	F	498	VAL
5	F	503	ILE
5	F	527	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	ASN
2	C	930	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

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 3 ligands modelled in this entry, 3 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	224/347 (64%)	0.12	7 (3%) 49 41	61, 73, 133, 185	0
1	B	226/347 (65%)	0.43	15 (6%) 19 16	66, 116, 184, 220	0
2	C	1126/1178 (95%)	0.08	25 (2%) 62 55	59, 72, 145, 193	0
3	D	1265/1316 (96%)	-0.07	23 (1%) 69 61	59, 73, 131, 183	0
4	E	81/110 (73%)	0.09	2 (2%) 58 49	63, 79, 125, 199	0
5	F	322/528 (60%)	0.11	16 (4%) 30 25	62, 84, 204, 218	0
6	H	23/23 (100%)	0.06	0 100 100	69, 90, 119, 133	0
7	G	15/16 (93%)	0.32	0 100 100	65, 91, 114, 121	0
8	I	2/2 (100%)	0.09	0 100 100	89, 89, 89, 91	0
All	All	3284/3867 (84%)	0.05	88 (2%) 55 46	59, 75, 157, 220	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	219	ARG	5.2
2	C	218	LYS	5.0
5	F	500	ARG	5.0
2	C	192	ASP	4.3
5	F	475	VAL	4.2
5	F	520	SER	4.1
5	F	207	ASP	4.1
2	C	193	LYS	3.9
3	D	745	ILE	3.8
1	A	12	ASP	3.7
1	B	60	LEU	3.7
2	C	138	GLU	3.7
3	D	746	LEU	3.6
1	B	138	LEU	3.5
3	D	749	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
3	D	635	VAL	3.3
3	D	610	GLY	3.2
1	B	151	GLN	3.2
2	C	352	GLN	3.2
2	C	220	ASP	3.2
1	B	62	GLU	3.2
3	D	743	LYS	3.2
1	A	226	ASN	3.1
1	B	59	VAL	3.1
2	C	237	LEU	3.1
2	C	295	LEU	3.0
3	D	615	PRO	3.0
1	A	224	GLU	3.0
1	B	140	VAL	2.9
5	F	483	ASP	2.9
3	D	742	LYS	2.9
2	C	304	LYS	2.8
3	D	618	ALA	2.8
3	D	900	GLU	2.8
3	D	664	ALA	2.7
1	B	115	GLY	2.7
2	C	811	GLU	2.7
5	F	272	LYS	2.7
3	D	741	ARG	2.6
5	F	508	SER	2.6
1	A	8	THR	2.6
3	D	807	ALA	2.6
2	C	261	THR	2.6
3	D	821	LYS	2.6
1	A	57	ASP	2.6
1	A	3	ILE	2.5
2	C	1024	THR	2.5
2	C	30	ASN	2.5
2	C	217	ASP	2.5
5	F	210	GLU	2.5
3	D	748	HIS	2.4
3	D	1203	GLY	2.4
1	B	110	ILE	2.4
5	F	227	SER	2.4
2	C	260	SER	2.4
2	C	305	ARG	2.4
2	C	1051	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	522	GLY	2.4
2	C	415	GLN	2.3
5	F	476	ARG	2.3
1	B	56	ILE	2.3
3	D	1080	ILE	2.2
3	D	634	LYS	2.2
3	D	608	GLU	2.2
5	F	273	LEU	2.2
3	D	756	VAL	2.2
1	B	128	LEU	2.2
3	D	599	TYR	2.2
2	C	188	ASP	2.2
5	F	472	ALA	2.2
2	C	315	LYS	2.1
5	F	209	SER	2.1
5	F	393	GLU	2.1
1	B	51	VAL	2.1
2	C	1150	GLY	2.1
3	D	663	MET	2.1
5	F	512	SER	2.1
1	A	225	LEU	2.1
1	B	134	LEU	2.1
2	C	335	GLU	2.1
3	D	761	GLN	2.1
2	C	252	PHE	2.1
1	B	219	PHE	2.0
5	F	389	ASP	2.0
1	B	86	SER	2.0
1	B	93	VAL	2.0
4	E	92	LEU	2.0
4	E	88	GLN	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( $\text{\AA}^2$ )	Q<0.9
9	ZN	D	1401	1/1	0.92	0.08	-1.80	116,116,116,116	0
9	ZN	D	1402	1/1	0.97	0.09	-2.17	116,116,116,116	0
10	MG	D	1403	1/1	0.92	0.12	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.