



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID : 2ID0  
Title : Escherichia coli RNase II  
Authors : Zuo, Y.; Zhang, J.; Wang, Y.; Malhotra, A.  
Deposited on : 2006-09-13  
Resolution : 2.35 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

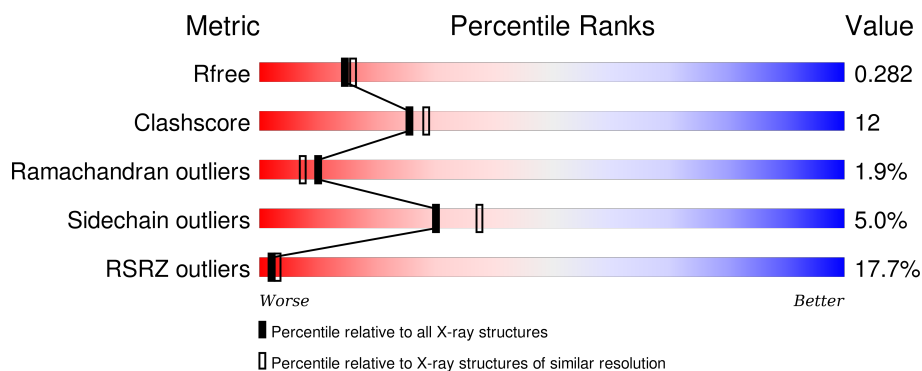
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	644	<div> <div>27%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	B	644	<div> <div>13%</div> <div>74%</div> <div>24%</div> <div>..</div> </div>
1	C	644	<div> <div>11%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	D	644	<div> <div>18%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19820 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 Exoribonuclease 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	Se	0	0	0
			4838	3078	860	879	7	14			
1	B	636	Total	C	N	O	S	Se	0	0	0
			4937	3128	879	909	7	14			
1	C	636	Total	C	N	O	S	Se	0	0	0
			4930	3129	876	904	7	14			
1	D	636	Total	C	N	O	S	Se	0	0	0
			4824	3072	853	878	7	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	208	MSE	MET	MODIFIED RESIDUE	UNP P30850

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	633	MSE	MET	MODIFIED RESIDUE	UNP P30850

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

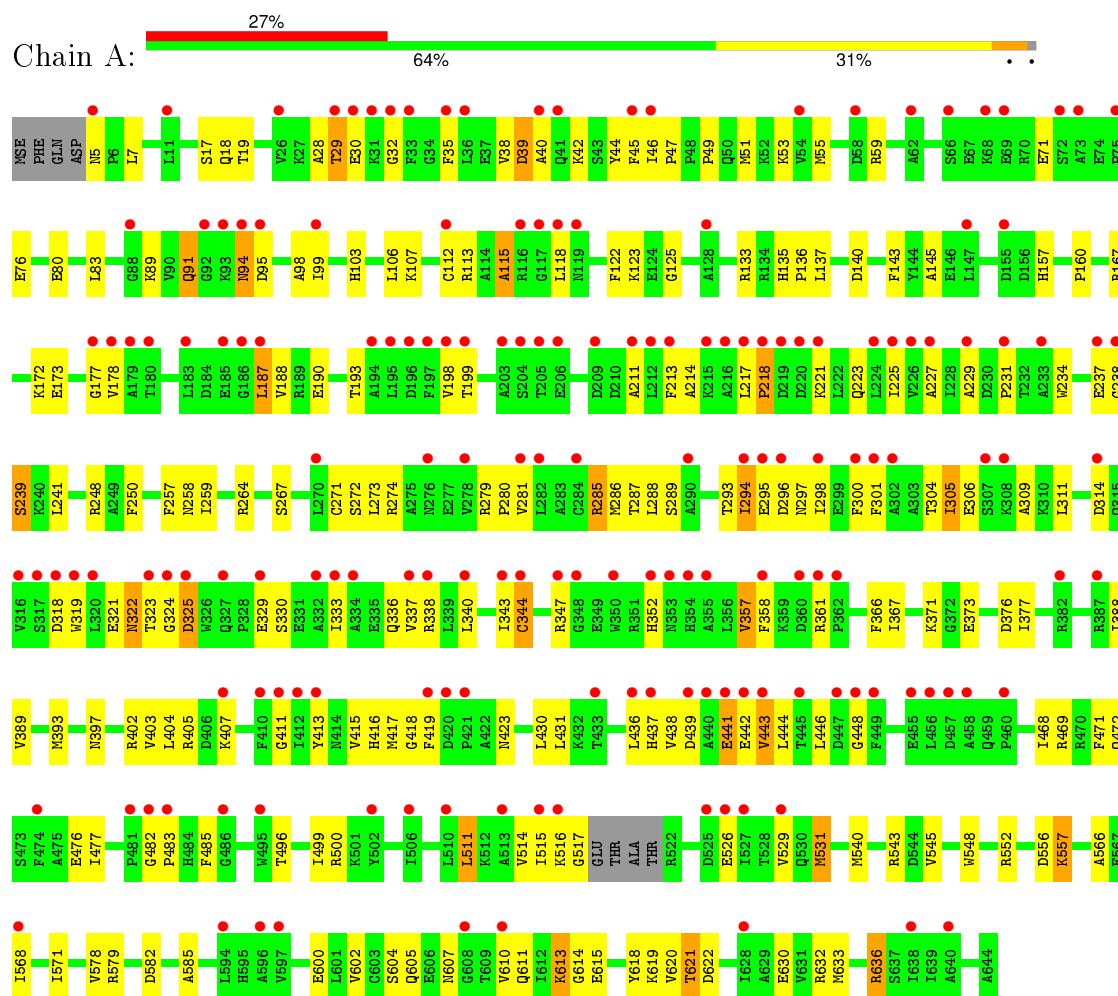
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	96	Total 96	O 96	0	0
3	C	82	Total 82	O 82	0	0
3	D	59	Total 59	O 59	0	0

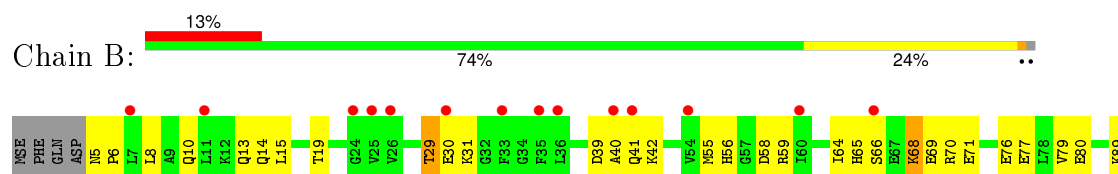
### 3 Residue-property plots

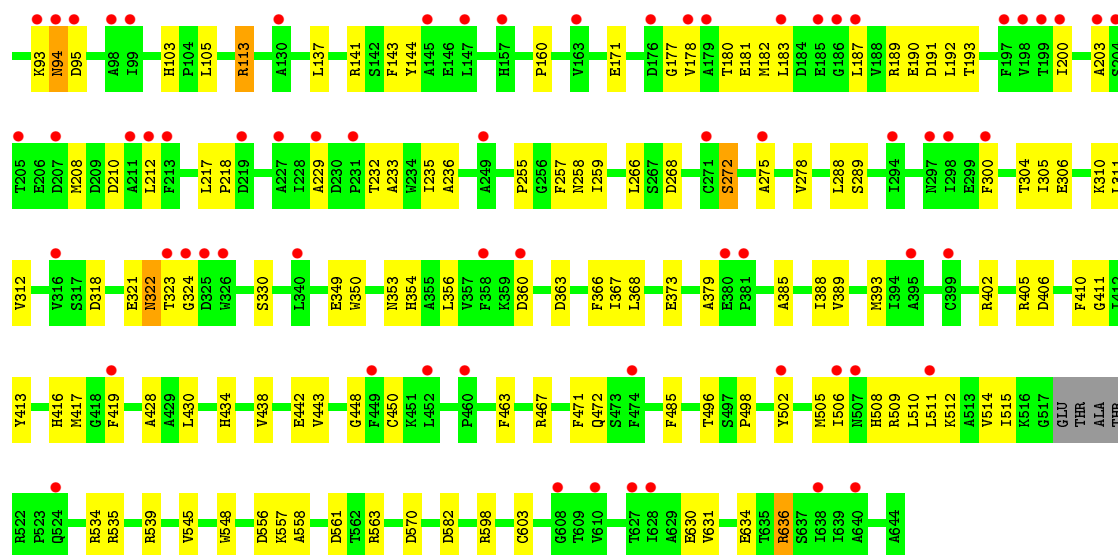
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Exoribonuclease 2

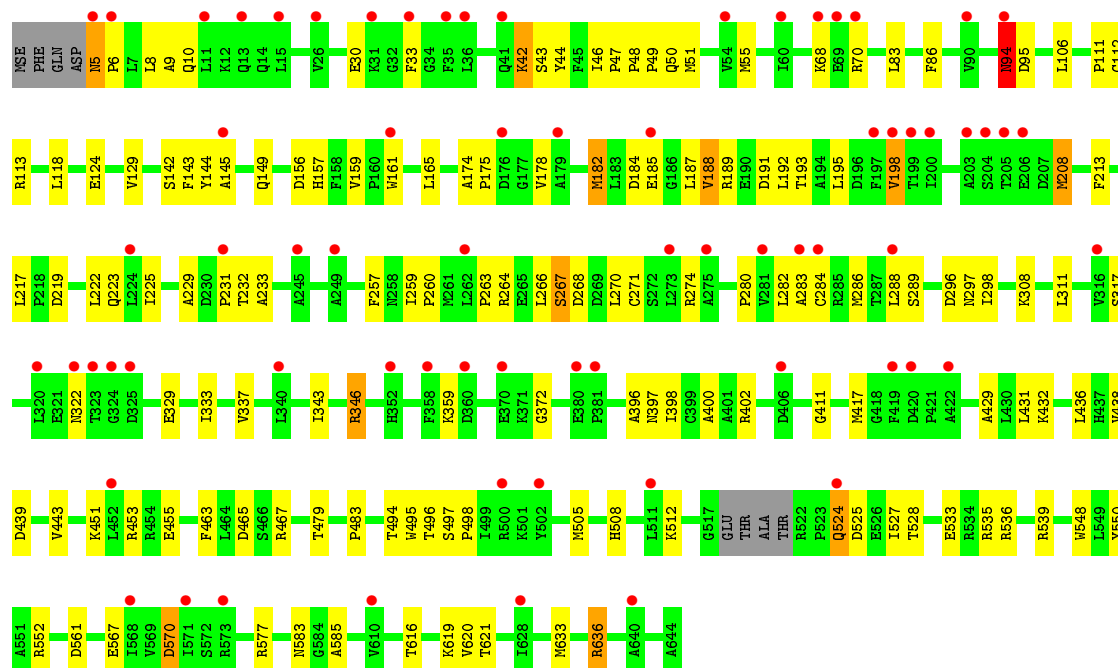
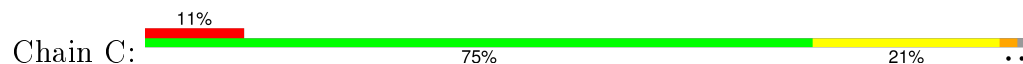


#### • Molecule 1: Exoribonuclease 2

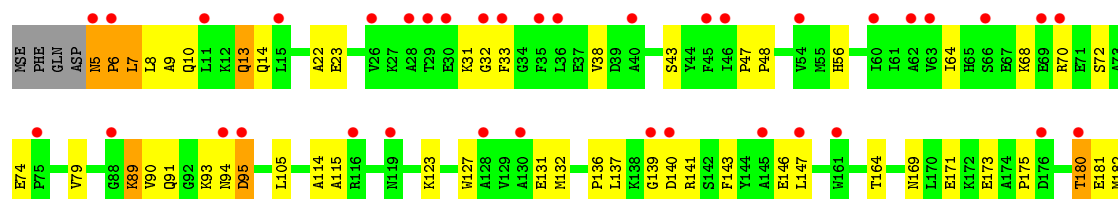


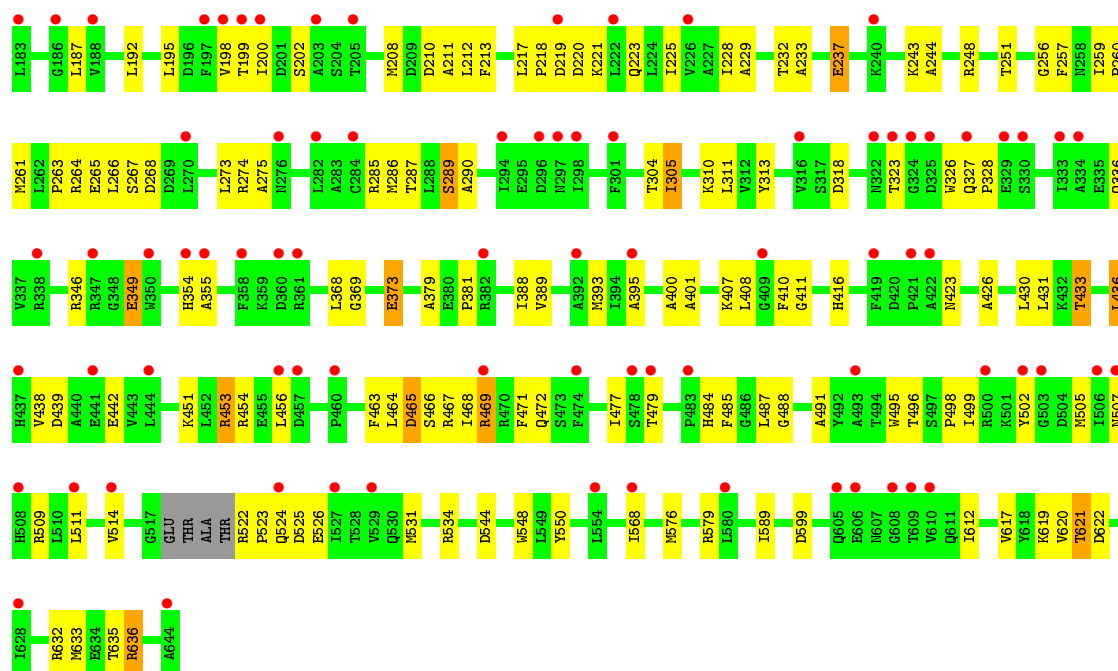


• Molecule 1: Exoribonuclease 2



• Molecule 1: Exoribonuclease 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.76Å 118.43Å 122.38Å 107.80° 98.36° 91.40°	Depositor
Resolution (Å)	17.95 – 2.35 17.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.3 (17.95-2.35) 77.9 (17.95-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.80 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.286 0.221 , 0.282	Depositor DCC
$R_{free}$ test set	5045 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 100807 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN

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	0.81	9/4925 (0.2%)	0.78	2/6674 (0.0%)
1	B	0.83	3/5025 (0.1%)	0.80	3/6800 (0.0%)
1	C	0.80	0/5018	0.80	2/6788 (0.0%)
1	D	0.86	8/4911 (0.2%)	0.83	3/6659 (0.0%)
All	All	0.82	20/19879 (0.1%)	0.80	10/26921 (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
1	A	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CZ-NH1	16.16	1.54	1.33
1	B	190	GLU	CD-OE1	15.89	1.43	1.25
1	B	190	GLU	CD-OE2	15.08	1.42	1.25
1	D	5	ASN	CG-ND2	14.79	1.69	1.32
1	D	285	ARG	NE-CZ	13.06	1.50	1.33
1	D	14	GLN	C-O	12.78	1.47	1.23
1	A	301	PHE	CE2-CZ	8.16	1.52	1.37
1	A	285	ARG	CZ-NH2	6.98	1.42	1.33
1	A	301	PHE	CG-CD2	6.90	1.49	1.38
1	D	13	GLN	CD-OE1	6.37	1.38	1.24
1	D	5	ASN	N-CA	6.21	1.58	1.46
1	A	188	VAL	C-O	6.12	1.34	1.23
1	D	14	GLN	C-N	6.08	1.48	1.34
1	A	517	GLY	CA-C	5.73	1.61	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	LYS	C-O	5.19	1.33	1.23
1	B	603	CYS	CB-SG	-5.18	1.73	1.81
1	A	298	ILE	C-N	5.16	1.46	1.34
1	D	550	TYR	CD1-CE1	5.07	1.47	1.39
1	D	13	GLN	CG-CD	5.06	1.62	1.51
1	A	285	ARG	CD-NE	5.01	1.54	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	285	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	D	285	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	C	535	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	58	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	8	LEU	CB-CG-CD2	-6.81	99.42	111.00
1	B	8	LEU	CA-CB-CG	6.36	129.92	115.30
1	C	535	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	301	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	D	599	ASP	CB-CG-OD1	5.47	123.22	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ASN	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	4838	0	4707	142	0
1	B	4937	0	4850	98	0
1	C	4930	0	4860	99	0
1	D	4824	0	4698	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	50	0	0	5	0
3	B	96	0	0	3	0
3	C	82	0	0	2	0
3	D	59	0	0	3	0
All	All	19820	0	19115	481	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 12.

All (481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:ND2	1:D:5:ASN:CG	1.69	1.44
1:A:431:LEU:HD13	1:A:438:VAL:HG21	1.30	1.12
1:D:217:LEU:HB3	1:D:218:PRO:HD2	1.30	1.07
1:D:5:ASN:HB2	1:D:6:PRO:HD3	1.44	0.99
1:D:393:MSE:SE	1:D:496:THR:HG21	2.16	0.95
1:A:439:ASP:O	1:A:443:VAL:HG23	1.69	0.93
1:D:275:ALA:H	1:D:310:LYS:HE3	1.34	0.90
1:B:103:HIS:HE1	1:B:105:LEU:HD12	1.38	0.88
1:A:59:ARG:HH21	1:A:80:GLU:HG2	1.38	0.88
1:D:5:ASN:HB2	1:D:6:PRO:CD	2.06	0.86
1:D:217:LEU:HB3	1:D:218:PRO:CD	2.05	0.84
1:C:68:LYS:HB3	1:C:70:ARG:O	1.76	0.84
1:B:582:ASP:OD2	3:B:1044:HOH:O	1.96	0.83
1:D:407:LYS:HG3	1:D:514:VAL:HG13	1.61	0.82
1:B:217:LEU:HB3	1:B:218:PRO:HD2	1.61	0.81
1:B:416:HIS:HB3	1:B:485:PHE:H	1.45	0.81
1:A:115:ALA:O	3:A:1051:HOH:O	1.99	0.80
1:A:318:ASP:HB3	1:A:323:THR:HG21	1.64	0.79
1:D:182:MSE:HE2	1:D:233:ALA:HB1	1.64	0.78
1:A:264:ARG:HA	1:A:267:SER:OG	1.84	0.77
1:C:182:MSE:HE3	1:C:233:ALA:HB1	1.68	0.76
1:C:451:LYS:O	1:C:455:GLU:HG3	1.85	0.76
1:A:430:LEU:HD22	1:A:471:PHE:HE1	1.51	0.76
1:A:403:VAL:HG13	1:A:407:LYS:HE3	1.68	0.75
1:D:208:MSE:HE3	1:D:310:LYS:HE2	1.69	0.75
1:B:180:THR:HG22	1:B:181:GLU:H	1.52	0.74
1:D:318:ASP:HB3	1:D:323:THR:HB	1.67	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ALA:H	1:D:310:LYS:CE	2.00	0.74
1:D:416:HIS:HB3	1:D:485:PHE:H	1.51	0.74
1:D:379:ALA:O	1:D:381:PRO:HD3	1.88	0.74
1:B:498:PRO:HG3	1:B:508:HIS:NE2	2.01	0.74
1:D:393:MSE:SE	1:D:496:THR:CG2	2.85	0.74
1:B:182:MSE:HE3	1:B:233:ALA:HB1	1.70	0.74
1:C:182:MSE:CE	1:C:233:ALA:HB1	2.18	0.73
1:D:469:ARG:HA	1:D:472:GLN:HE21	1.51	0.73
1:A:620:VAL:O	1:A:621:THR:HB	1.88	0.73
1:B:39:ASP:HB3	1:B:42:LYS:HB3	1.70	0.72
1:B:39:ASP:OD1	1:B:40:ALA:N	2.23	0.71
1:A:630:GLU:CD	1:A:632:ARG:HE	1.93	0.71
1:A:55:MSE:SE	1:A:83:LEU:HD12	2.40	0.71
1:B:217:LEU:HB3	1:B:218:PRO:CD	2.21	0.70
1:D:198:VAL:HG22	1:D:199:THR:N	2.06	0.70
1:C:182:MSE:HE3	1:C:233:ALA:CB	2.22	0.70
1:D:93:LYS:HG2	1:D:94:ASN:H	1.55	0.70
1:A:468:ILE:O	1:A:471:PHE:HB2	1.92	0.70
1:D:439:ASP:HB3	1:D:442:GLU:HB2	1.72	0.70
1:B:305:ILE:HG22	1:B:306:GLU:N	2.07	0.69
1:B:76:GLU:HG2	1:B:77:GLU:HG3	1.74	0.68
1:B:318:ASP:HB3	1:B:323:THR:HB	1.75	0.68
1:A:29:THR:HG22	1:A:30:GLU:H	1.57	0.68
1:A:214:ALA:HA	1:A:223:GLN:O	1.94	0.68
1:A:611:GLN:HA	1:A:615:GLU:O	1.93	0.68
1:B:417:MSE:HA	1:B:417:MSE:HE2	1.76	0.68
1:D:484:HIS:CE1	1:D:487:LEU:HG	2.28	0.68
1:D:132:MSE:CE	1:D:143:PHE:HD2	2.08	0.67
1:C:525:ASP:O	1:C:528:THR:HG22	1.94	0.67
1:B:598:ARG:NH1	3:B:1073:HOH:O	2.27	0.67
1:D:463:PHE:CE2	1:D:467:ARG:HD2	2.29	0.67
1:A:411:GLY:HA3	1:A:413:TYR:HE1	1.58	0.67
1:D:453:ARG:HD3	1:D:456:LEU:HD12	1.76	0.67
1:D:198:VAL:HG21	1:D:311:LEU:CD1	2.25	0.66
1:A:397:ASN:HD21	1:A:496:THR:HB	1.60	0.66
1:B:511:LEU:O	1:B:514:VAL:HG12	1.96	0.66
1:A:39:ASP:OD1	1:A:42:LYS:HB2	1.96	0.66
1:B:13:GLN:HG3	1:B:14:GLN:HG2	1.77	0.66
1:C:55:MSE:HE3	1:C:143:PHE:CE2	2.31	0.65
1:D:290:ALA:O	1:D:346:ARG:HD2	1.96	0.65
1:D:431:LEU:HD22	1:D:436:LEU:HD22	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ALA:HA	1:D:488:GLY:O	1.96	0.65
1:A:411:GLY:HA3	1:A:413:TYR:CE1	2.32	0.64
1:A:319:TRP:HH2	1:A:338:ARG:HG3	1.62	0.64
1:A:53:LYS:HG2	1:A:137:LEU:HD23	1.80	0.64
1:D:423:ASN:HB3	1:D:471:PHE:HD2	1.64	0.63
1:D:132:MSE:HE1	1:D:143:PHE:HD2	1.63	0.63
1:A:38:VAL:HB	1:A:42:LYS:HB3	1.79	0.63
1:B:416:HIS:HB3	1:B:485:PHE:N	2.14	0.63
1:C:161:TRP:O	1:C:165:LEU:HD12	1.99	0.63
1:A:604:SER:OG	1:A:607:ASN:HB2	1.99	0.63
1:D:430:LEU:O	1:D:433:THR:HB	1.99	0.62
1:D:182:MSE:HE2	1:D:233:ALA:CB	2.29	0.61
1:A:571:ILE:HD13	1:A:610:VAL:HG23	1.82	0.61
1:A:499:ILE:HG23	1:A:500:ARG:NE	2.16	0.61
1:D:5:ASN:CB	1:D:6:PRO:CD	2.78	0.61
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.61
1:B:512:LYS:HA	1:B:515:ILE:HD12	1.80	0.61
1:C:498:PRO:HG3	1:C:508:HIS:CE1	2.36	0.61
1:A:431:LEU:HD22	1:A:436:LEU:HD23	1.83	0.61
1:A:199:THR:O	1:A:311:LEU:HB2	2.01	0.61
1:C:175:PRO:HG2	1:C:263:PRO:HD3	1.84	0.60
1:C:561:ASP:OD1	3:C:1048:HOH:O	2.15	0.60
1:D:620:VAL:O	1:D:621:THR:HB	2.01	0.60
1:A:371:LYS:HE2	1:A:373:GLU:HB2	1.82	0.60
1:B:356:LEU:HD21	1:B:450:CYS:HA	1.84	0.60
1:C:5:ASN:HB2	1:C:6:PRO:CD	2.32	0.60
1:C:174:ALA:HB2	1:C:260:PRO:HG2	1.83	0.59
1:B:208:MSE:HE3	1:B:310:LYS:HG2	1.84	0.59
1:D:198:VAL:CG2	1:D:199:THR:N	2.65	0.59
1:A:294:ILE:HD12	1:A:294:ILE:H	1.67	0.59
1:A:630:GLU:OE2	1:A:632:ARG:NE	2.32	0.59
1:A:213:PHE:HD2	1:A:225:ILE:HD12	1.66	0.59
1:B:305:ILE:CG2	1:B:306:GLU:N	2.65	0.59
1:C:229:ALA:HB1	1:C:271:CYS:HB3	1.85	0.59
1:B:535:ARG:O	1:B:539:ARG:HG3	2.03	0.59
1:A:568:ILE:HD12	1:A:622:ASP:HB2	1.85	0.59
1:C:439:ASP:O	1:C:443:VAL:HG23	2.03	0.58
1:D:633:MSE:HG2	3:D:1015:HOH:O	2.03	0.58
1:B:389:VAL:O	1:B:393:MSE:HG2	2.03	0.58
1:A:619:LYS:HE2	1:A:622:ASP:OD1	2.03	0.58
1:C:189:ARG:HH21	1:C:280:PRO:HB2	1.69	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:O	1:A:272:SER:HB2	2.04	0.58
1:D:257:PHE:CE2	1:D:259:ILE:HD11	2.39	0.58
1:D:507:ASN:O	1:D:511:LEU:HB2	2.04	0.57
1:D:213:PHE:CD2	1:D:225:ILE:HD12	2.40	0.57
1:C:195:LEU:HD22	1:C:213:PHE:CZ	2.38	0.57
1:A:177:GLY:HA2	1:A:241:LEU:HD21	1.85	0.57
1:D:5:ASN:ND2	1:D:5:ASN:CB	2.65	0.57
1:A:198:VAL:HG12	1:A:309:ALA:HB3	1.87	0.57
1:C:329:GLU:O	1:C:329:GLU:HG3	2.03	0.57
1:C:616:THR:HG21	1:C:619:LYS:HE3	1.86	0.57
1:A:367:ILE:HD12	1:A:376:ASP:HB3	1.87	0.56
1:C:47:PRO:C	1:C:49:PRO:HD2	2.25	0.56
1:A:403:VAL:O	1:A:407:LYS:HG2	2.05	0.56
1:C:229:ALA:O	1:C:231:PRO:HD3	2.06	0.56
1:C:189:ARG:NH2	1:C:280:PRO:HB2	2.21	0.56
1:B:556:ASP:OD1	1:B:557:LYS:NZ	2.37	0.56
1:A:415:VAL:HG12	1:A:482:GLY:HA3	1.88	0.56
1:B:305:ILE:CG2	1:B:306:GLU:H	2.19	0.56
1:B:113:ARG:CZ	1:B:113:ARG:HB2	2.35	0.55
1:A:439:ASP:OD1	1:A:441:GLU:HB3	2.06	0.55
1:D:524:GLN:C	1:D:526:GLU:H	2.08	0.55
1:C:296:ASP:O	1:C:298:ILE:N	2.35	0.55
1:C:5:ASN:HB2	1:C:6:PRO:HD3	1.88	0.55
1:D:568:ILE:HD12	1:D:622:ASP:HB2	1.88	0.55
1:B:278:VAL:HG13	1:B:304:THR:HG22	1.89	0.55
1:A:419:PHE:HA	1:A:472:GLN:HA	1.87	0.54
1:D:416:HIS:HB3	1:D:485:PHE:N	2.19	0.54
1:D:400:ALA:HB2	1:D:495:TRP:CD1	2.41	0.54
1:D:408:LEU:HB2	1:D:410:PHE:H	1.72	0.54
1:C:68:LYS:HG3	1:C:70:ARG:H	1.71	0.54
1:D:93:LYS:HG2	1:D:94:ASN:N	2.21	0.54
1:C:174:ALA:CB	1:C:260:PRO:HG2	2.38	0.54
1:A:103:HIS:HB3	1:A:106:LEU:HD12	1.90	0.54
1:D:23:GLU:O	1:D:38:VAL:HG13	2.07	0.54
1:B:442:GLU:O	1:B:448:GLY:HA3	2.07	0.54
1:C:431:LEU:HD13	1:C:438:VAL:HG21	1.89	0.54
1:B:141:ARG:O	1:B:141:ARG:HG2	2.07	0.54
1:A:294:ILE:HD11	1:A:347:ARG:HH12	1.72	0.53
1:D:208:MSE:HB3	1:D:273:LEU:HB2	1.91	0.53
1:D:198:VAL:HG21	1:D:311:LEU:HD12	1.89	0.53
1:D:423:ASN:HB3	1:D:471:PHE:CD2	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:VAL:O	1:D:621:THR:CB	2.57	0.53
1:A:477:ILE:HD13	1:A:531:MSE:HE2	1.90	0.53
1:D:173:GLU:O	1:D:248:ARG:NH2	2.36	0.53
1:D:89:LYS:HD3	1:D:127:TRP:CZ2	2.43	0.53
1:B:463:PHE:CZ	1:B:467:ARG:HD3	2.44	0.53
1:D:175:PRO:O	1:D:263:PRO:HG3	2.09	0.53
1:A:272:SER:O	1:A:279:ARG:HD2	2.09	0.53
1:A:257:PHE:CE2	1:A:259:ILE:HD11	2.43	0.53
1:C:431:LEU:HD22	1:C:436:LEU:HD23	1.91	0.53
1:A:47:PRO:HB2	1:A:49:PRO:HD2	1.91	0.53
1:A:211:ALA:HB3	1:A:227:ALA:HB3	1.90	0.53
1:C:400:ALA:HB2	1:C:495:TRP:CD1	2.44	0.53
1:A:279:ARG:HH11	1:A:280:PRO:HD2	1.74	0.53
1:C:217:LEU:HD11	1:C:223:GLN:HB2	1.91	0.53
1:B:208:MSE:CE	1:B:310:LYS:HG2	2.39	0.53
1:C:533:GLU:OE1	1:C:536:ARG:NH2	2.42	0.53
1:D:463:PHE:CZ	1:D:467:ARG:HD2	2.43	0.52
1:B:6:PRO:O	1:B:10:GLN:HG3	2.09	0.52
1:D:136:PRO:HA	1:D:141:ARG:O	2.09	0.52
1:A:446:LEU:HG	1:A:485:PHE:CZ	2.45	0.52
1:C:620:VAL:O	1:C:621:THR:HB	2.09	0.52
1:C:548:TRP:HA	1:C:636:ARG:HG2	1.90	0.52
1:A:118:LEU:HD21	1:A:122:PHE:CE1	2.45	0.52
1:B:366:PHE:HB3	1:B:368:LEU:HD21	1.92	0.52
1:A:611:GLN:NE2	1:A:614:GLY:O	2.42	0.52
1:A:352:HIS:HA	1:A:357:VAL:HG22	1.90	0.52
1:A:29:THR:HG22	1:A:30:GLU:HG3	1.92	0.52
1:C:5:ASN:HD21	1:C:8:LEU:H	1.57	0.52
1:A:431:LEU:HB3	1:A:436:LEU:HB3	1.92	0.52
1:D:612:ILE:HD12	1:D:617:VAL:HG21	1.92	0.52
1:B:321:GLU:O	1:B:322:ASN:CB	2.58	0.52
1:C:208:MSE:HE1	1:C:274:ARG:HA	1.91	0.52
1:C:5:ASN:ND2	1:C:8:LEU:H	2.08	0.51
1:D:401:ALA:HB1	1:D:491:ALA:HB1	1.92	0.51
1:D:251:THR:HG23	1:D:260:PRO:HA	1.91	0.51
1:A:579:ARG:HA	1:A:585:ALA:O	2.11	0.51
1:B:203:ALA:HB2	1:B:312:VAL:HG22	1.91	0.51
1:C:286:MSE:HE1	1:C:396:ALA:HA	1.92	0.51
1:D:438:VAL:HG22	1:D:439:ASP:N	2.26	0.51
1:D:465:ASP:O	1:D:468:ILE:HG12	2.09	0.51
1:A:227:ALA:HB1	1:A:281:VAL:HG11	1.93	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PHE:CE2	1:A:377:ILE:HD13	2.45	0.51
1:D:115:ALA:HA	1:D:146:GLU:OE2	2.11	0.51
1:D:389:VAL:O	1:D:393:MSE:HG2	2.11	0.51
1:C:174:ALA:HB2	1:C:260:PRO:CG	2.41	0.51
1:D:208:MSE:HB2	1:D:273:LEU:H	1.76	0.51
1:B:305:ILE:HG22	1:B:306:GLU:H	1.76	0.51
1:C:188:VAL:O	1:C:188:VAL:HG12	2.11	0.51
1:B:59:ARG:HG2	1:B:79:VAL:HB	1.92	0.50
1:D:579:ARG:NH2	3:D:1041:HOH:O	2.32	0.50
1:C:438:VAL:CG1	1:C:443:VAL:CG2	2.89	0.50
1:D:632:ARG:HB2	1:D:635:THR:CG2	2.41	0.50
1:D:304:THR:C	1:D:305:ILE:HG12	2.32	0.50
1:A:393:MSE:SE	1:A:496:THR:OG1	2.79	0.50
1:D:408:LEU:HB3	1:D:410:PHE:CD1	2.47	0.50
1:C:417:MSE:HE1	1:C:483:PRO:HD2	1.94	0.50
1:B:275:ALA:HB2	1:B:310:LYS:HG3	1.93	0.50
1:A:39:ASP:CG	1:A:40:ALA:N	2.64	0.50
1:B:428:ALA:HA	1:B:438:VAL:HG12	1.94	0.50
1:A:330:SER:HB2	1:A:333:ILE:HG12	1.94	0.50
1:D:217:LEU:CD1	1:D:287:THR:HG23	2.42	0.50
1:D:286:MSE:SE	1:D:395:ALA:HB1	2.62	0.49
1:A:571:ILE:O	1:A:605:GLN:HA	2.12	0.49
1:D:180:THR:HG22	1:D:181:GLU:H	1.77	0.49
1:A:407:LYS:HG3	1:A:514:VAL:HG22	1.94	0.49
1:C:112:CYS:HA	1:C:145:ALA:O	2.12	0.49
1:D:477:ILE:HD13	1:D:531:MSE:HE2	1.95	0.49
1:D:451:LYS:HA	1:D:454:ARG:HE	1.78	0.49
1:A:213:PHE:CD2	1:A:225:ILE:HD12	2.46	0.49
1:B:235:ILE:HD11	1:B:266:LEU:CD2	2.43	0.49
1:C:46:ILE:HG22	1:C:50:GLN:HB2	1.94	0.49
1:C:397:ASN:OD1	1:C:494:THR:HA	2.12	0.49
1:D:275:ALA:N	1:D:310:LYS:HE3	2.16	0.49
1:D:198:VAL:CG2	1:D:199:THR:H	2.26	0.49
1:B:419:PHE:HD2	1:B:471:PHE:O	1.94	0.49
1:B:561:ASP:HB2	1:B:563:ARG:NH2	2.27	0.49
1:D:171:GLU:CD	1:D:171:GLU:H	2.16	0.49
1:C:570:ASP:OD2	1:C:577:ARG:HD3	2.13	0.49
1:D:200:ILE:HG22	1:D:313:TYR:CE2	2.47	0.49
1:A:431:LEU:HD13	1:A:438:VAL:CG2	2.21	0.49
1:B:55:MSE:HE3	1:B:143:PHE:CE2	2.48	0.49
1:A:112:CYS:HA	1:A:145:ALA:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:O	1:B:13:GLN:HG2	2.13	0.48
1:D:213:PHE:HA	1:D:336:GLN:OE1	2.13	0.48
1:A:89:LYS:HZ2	1:A:89:LYS:HB3	1.78	0.48
1:D:274:ARG:HA	1:D:310:LYS:HE2	1.96	0.48
1:A:229:ALA:O	1:A:231:PRO:HD3	2.13	0.48
1:B:300:PHE:CD2	1:B:511:LEU:HD22	2.48	0.48
1:B:323:THR:OG1	1:B:324:GLY:N	2.47	0.48
1:A:300:PHE:O	1:A:515:ILE:HG12	2.13	0.48
1:C:55:MSE:HG3	1:C:106:LEU:HD22	1.94	0.48
1:D:22:ALA:HB3	1:D:64:ILE:HD11	1.95	0.48
1:D:182:MSE:CE	1:D:233:ALA:CB	2.92	0.48
1:A:59:ARG:NH2	1:A:80:GLU:HG2	2.17	0.48
1:D:632:ARG:HB2	1:D:635:THR:HG22	1.96	0.48
1:C:142:SER:HB3	3:C:1055:HOH:O	2.13	0.48
1:C:33:PHE:HB3	1:C:48:PRO:HD3	1.95	0.48
1:A:91:GLN:NE2	1:A:98:ALA:HB3	2.29	0.48
1:D:139:GLY:O	1:D:140:ASP:HB2	2.14	0.48
1:B:191:ASP:O	1:B:193:THR:N	2.43	0.48
1:C:453:ARG:HH22	1:C:465:ASP:CG	2.17	0.48
1:A:468:ILE:HG13	1:A:469:ARG:N	2.29	0.47
1:A:389:VAL:O	1:A:393:MSE:HG2	2.14	0.47
1:A:135:HIS:CE1	1:A:137:LEU:HB2	2.49	0.47
1:C:156:ASP:HB3	1:C:159:VAL:HG23	1.96	0.47
1:B:278:VAL:HA	1:B:305:ILE:O	2.14	0.47
1:A:333:ILE:O	1:A:337:VAL:HG23	2.14	0.47
1:C:129:VAL:HB	1:C:149:GLN:HB3	1.96	0.47
1:A:526:GLU:O	1:A:529:VAL:HB	2.14	0.47
1:D:7:LEU:O	1:D:10:GLN:HB2	2.14	0.47
1:A:113:ARG:HD2	3:A:1037:HOH:O	2.14	0.47
1:D:576:MSE:HE2	1:D:589:ILE:HD12	1.96	0.47
1:A:442:GLU:HG2	1:A:448:GLY:HA3	1.96	0.47
1:A:402:ARG:O	1:A:405:ARG:HB3	2.14	0.47
1:C:463:PHE:CZ	1:C:467:ARG:HD3	2.50	0.47
1:B:548:TRP:HA	1:B:636:ARG:HG2	1.96	0.47
1:C:266:LEU:HD23	1:C:270:LEU:HD12	1.96	0.47
1:A:600:GLU:HG2	1:A:613:LYS:HG3	1.96	0.47
1:A:32:GLY:O	1:A:51:MSE:HG3	2.14	0.47
1:B:257:PHE:CE2	1:B:259:ILE:HD11	2.48	0.47
1:A:234:TRP:HH2	1:A:280:PRO:CG	2.27	0.47
1:A:118:LEU:HD21	1:A:122:PHE:HE1	1.79	0.47
1:B:438:VAL:HG22	1:B:443:VAL:HG13	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ALA:HB2	1:A:51:MSE:CE	2.45	0.47
1:B:182:MSE:HE2	1:B:182:MSE:HB3	1.84	0.47
1:A:250:PHE:HE1	1:A:531:MSE:O	1.97	0.47
1:D:327:GLN:HG2	1:D:328:PRO:HD2	1.95	0.47
1:B:65:HIS:O	1:B:71:GLU:HA	2.15	0.47
1:D:318:ASP:HB3	1:D:323:THR:CB	2.40	0.47
1:A:39:ASP:CG	1:A:40:ALA:H	2.17	0.47
1:A:566:ALA:HB1	1:A:578:VAL:HB	1.96	0.47
1:A:404:LEU:HD21	1:A:511:LEU:HD13	1.97	0.47
1:A:416:HIS:CE1	1:A:418:GLY:HA2	2.49	0.47
1:A:620:VAL:O	1:A:621:THR:CB	2.60	0.46
1:D:263:PRO:HB2	1:D:266:LEU:HG	1.96	0.46
1:A:499:ILE:HG23	1:A:500:ARG:HE	1.79	0.46
1:A:556:ASP:OD1	1:A:557:LYS:HE2	2.15	0.46
1:B:66:SER:HB3	1:B:71:GLU:HG2	1.96	0.46
1:A:540:MSE:HE3	1:A:543:ARG:HH22	1.80	0.46
1:D:164:THR:HG21	1:D:544:ASP:HB2	1.98	0.46
1:C:157:HIS:HE1	1:C:372:GLY:HA3	1.80	0.46
1:D:132:MSE:HE2	1:D:143:PHE:HD2	1.79	0.46
1:A:416:HIS:O	1:A:485:PHE:HB2	2.16	0.46
1:D:164:THR:CG2	1:D:544:ASP:HB2	2.45	0.46
1:A:107:LYS:HE3	3:A:1030:HOH:O	2.14	0.46
1:C:550:TYR:OH	1:C:583:ASN:O	2.24	0.46
1:C:232:THR:OG1	1:C:512:LYS:NZ	2.34	0.46
1:D:264:ARG:O	1:D:268:ASP:N	2.40	0.46
1:A:404:LEU:HB2	1:A:413:TYR:OH	2.16	0.46
1:C:257:PHE:CE2	1:C:259:ILE:HD11	2.51	0.46
1:B:19:THR:HG22	1:B:64:ILE:O	2.16	0.46
1:D:217:LEU:HD11	1:D:223:GLN:HB2	1.98	0.46
1:D:484:HIS:HE1	1:D:487:LEU:HG	1.80	0.46
1:D:132:MSE:HE1	1:D:143:PHE:CD2	2.48	0.46
1:D:524:GLN:O	1:D:526:GLU:N	2.49	0.46
1:D:23:GLU:OE2	1:D:79:VAL:HG21	2.15	0.46
1:D:349:GLU:HA	1:D:349:GLU:OE1	2.16	0.46
1:B:558:ALA:HB2	1:B:631:VAL:HG23	1.97	0.46
1:D:548:TRP:HA	1:D:636:ARG:HG2	1.97	0.46
1:D:323:THR:HG21	1:D:326:TRP:O	2.16	0.46
1:A:286:MSE:HE3	1:A:294:ILE:HG12	1.98	0.46
1:A:28:ALA:HB2	1:A:51:MSE:HE1	1.98	0.46
1:C:184:ASP:HA	1:C:187:LEU:HD11	1.97	0.46
1:A:55:MSE:SE	1:A:83:LEU:CD1	3.14	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:ARG:HD3	1:D:636:ARG:N	2.31	0.45
1:C:94:ASN:HB2	1:C:95:ASP:H	1.60	0.45
1:A:430:LEU:HD22	1:A:471:PHE:CE1	2.42	0.45
1:C:5:ASN:ND2	1:C:8:LEU:HB3	2.30	0.45
1:A:376:ASP:OD1	1:A:377:ILE:N	2.48	0.45
1:A:446:LEU:HD21	1:A:483:PRO:HB2	1.97	0.45
1:C:225:ILE:HA	1:C:284:CYS:O	2.16	0.45
1:C:333:ILE:O	1:C:337:VAL:HG23	2.15	0.45
1:B:416:HIS:ND1	1:B:485:PHE:HB2	2.31	0.45
1:C:5:ASN:HD22	1:C:8:LEU:HB3	1.81	0.45
1:A:231:PRO:HA	1:A:271:CYS:SG	2.56	0.45
1:B:68:LYS:HB2	1:B:69:GLU:H	1.50	0.45
1:B:506:ILE:O	1:B:510:LEU:HG	2.17	0.45
1:A:305:ILE:HG22	1:A:306:GLU:H	1.81	0.45
1:C:198:VAL:HG21	1:C:311:LEU:HD11	1.99	0.45
1:C:438:VAL:CG1	1:C:443:VAL:HG21	2.47	0.45
1:C:533:GLU:OE1	1:C:533:GLU:HA	2.17	0.45
1:C:185:GLU:H	1:C:187:LEU:HG	1.80	0.45
1:C:398:ILE:O	1:C:402:ARG:HG3	2.17	0.45
1:C:222:LEU:HD12	1:C:346:ARG:HD2	1.99	0.45
1:A:319:TRP:CH2	1:A:338:ARG:HG3	2.47	0.45
1:B:430:LEU:O	1:B:434:HIS:HD2	2.00	0.45
1:D:289:SER:HB3	1:D:290:ALA:H	1.56	0.44
1:C:5:ASN:O	1:C:9:ALA:HB2	2.17	0.44
1:B:235:ILE:O	1:B:509:ARG:NH2	2.47	0.44
1:B:558:ALA:HB1	1:B:630:GLU:HA	1.99	0.44
1:D:237:GLU:HB2	1:D:509:ARG:CZ	2.46	0.44
1:A:633:MSE:HG2	3:A:1012:HOH:O	2.16	0.44
1:A:548:TRP:HA	1:A:636:ARG:HG2	2.00	0.44
1:D:137:LEU:HA	1:D:137:LEU:HD23	1.70	0.44
1:C:30:GLU:OE1	1:C:30:GLU:HA	2.17	0.44
1:C:192:LEU:HB3	1:C:195:LEU:HD12	2.00	0.44
1:D:524:GLN:C	1:D:526:GLU:N	2.70	0.44
1:C:552:ARG:HA	1:C:633:MSE:HE1	2.00	0.44
1:A:238:GLY:O	1:A:239:SER:C	2.55	0.44
1:A:135:HIS:ND1	1:A:137:LEU:HB2	2.31	0.44
1:A:344:CYS:HB2	1:A:388:ILE:HA	1.98	0.44
1:D:263:PRO:HB3	1:D:265:GLU:OE1	2.16	0.44
1:A:221:LYS:HD3	1:A:289:SER:HB3	1.99	0.44
1:D:369:GLY:HA3	1:D:373:GLU:OE1	2.18	0.44
1:D:33:PHE:HB3	1:D:48:PRO:HG3	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:ARG:HA	1:D:523:PRO:HD3	1.90	0.44
1:A:321:GLU:O	1:A:322:ASN:CB	2.65	0.44
1:B:29:THR:C	1:B:31:LYS:H	2.21	0.44
1:D:208:MSE:HB2	1:D:273:LEU:N	2.33	0.44
1:C:182:MSE:HE3	1:C:233:ALA:HB3	2.00	0.44
1:D:579:ARG:NE	3:D:1041:HOH:O	2.48	0.44
1:A:295:GLU:C	1:A:297:ASN:H	2.21	0.44
1:A:423:ASN:HB3	1:A:471:PHE:CD2	2.53	0.43
1:D:32:GLY:O	1:D:48:PRO:HA	2.18	0.43
1:C:42:LYS:HE2	1:C:44:TYR:CE1	2.52	0.43
1:B:373:GLU:HG3	3:B:1055:HOH:O	2.18	0.43
1:D:426:ALA:HB3	1:D:471:PHE:HE2	1.83	0.43
1:A:157:HIS:CE1	1:A:552:ARG:NH1	2.87	0.43
1:C:308:LYS:HD3	1:C:308:LYS:HA	1.86	0.43
1:B:570:ASP:OD1	1:B:570:ASP:N	2.50	0.43
1:A:279:ARG:O	1:A:281:VAL:HG23	2.18	0.43
1:B:113:ARG:CB	1:B:113:ARG:NH1	2.81	0.43
1:C:550:TYR:CD2	1:C:585:ALA:HB2	2.54	0.43
1:D:47:PRO:HA	1:D:48:PRO:HD3	1.87	0.43
1:D:114:ALA:HA	1:D:147:LEU:HB2	2.01	0.43
1:B:10:GLN:HA	1:B:13:GLN:HG2	2.01	0.43
1:B:502:TYR:O	1:B:505:MSE:HB2	2.19	0.43
1:C:411:GLY:O	1:C:479:THR:HA	2.18	0.43
1:D:229:ALA:HB3	1:D:499:ILE:HD11	2.00	0.43
1:B:385:ALA:HA	1:B:388:ILE:HD12	2.01	0.43
1:D:95:ASP:OD1	1:D:95:ASP:N	2.52	0.43
1:D:453:ARG:HA	1:D:453:ARG:HD3	1.72	0.43
1:C:111:PRO:HD2	1:C:143:PHE:O	2.19	0.43
1:B:275:ALA:H	1:B:310:LYS:HE3	1.83	0.43
1:C:191:ASP:OD1	1:C:193:THR:HB	2.19	0.43
1:B:349:GLU:O	1:B:353:ASN:ND2	2.51	0.43
1:C:467:ARG:HA	1:C:467:ARG:NE	2.34	0.43
1:A:35:PHE:HA	1:A:44:TYR:O	2.18	0.43
1:A:99:ILE:HG23	1:A:99:ILE:O	2.18	0.43
1:B:171:GLU:H	1:B:171:GLU:CD	2.22	0.43
1:B:56:HIS:NE2	1:B:105:LEU:HD13	2.34	0.43
1:B:182:MSE:HE1	1:B:189:ARG:HH12	1.84	0.43
1:A:157:HIS:HD2	1:A:371:LYS:O	2.02	0.43
1:B:177:GLY:O	1:B:178:VAL:C	2.57	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.81	0.43
1:D:619:LYS:N	1:D:622:ASP:OD2	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:TYR:CE2	1:B:506:ILE:HD11	2.54	0.42
1:C:524:GLN:OE1	1:C:527:ILE:HG13	2.19	0.42
1:D:9:ALA:O	1:D:13:GLN:HB2	2.19	0.42
1:B:363:ASP:O	1:B:379:ALA:HA	2.20	0.42
1:C:429:ALA:HA	1:C:432:LYS:HG2	2.02	0.42
1:A:217:LEU:HB3	1:A:218:PRO:CD	2.49	0.42
1:C:359:LYS:HE2	1:C:359:LYS:HB3	1.73	0.42
1:D:411:GLY:O	1:D:479:THR:HA	2.19	0.42
1:B:103:HIS:CE1	1:B:105:LEU:HD12	2.30	0.42
1:A:160:PRO:O	1:A:545:VAL:HG22	2.20	0.42
1:B:402:ARG:O	1:B:406:ASP:OD2	2.37	0.42
1:C:48:PRO:O	1:C:51:MSE:HB2	2.19	0.42
1:B:93:LYS:O	1:B:94:ASN:C	2.57	0.42
1:C:5:ASN:CB	1:C:6:PRO:CD	2.97	0.42
1:A:324:GLY:O	1:A:325:ASP:HB2	2.19	0.42
1:D:466:SER:OG	1:D:620:VAL:HG21	2.20	0.42
1:D:275:ALA:HB2	1:D:310:LYS:HG3	2.02	0.42
1:B:561:ASP:HB2	1:B:563:ARG:HH21	1.85	0.42
1:B:5:ASN:HB2	1:B:6:PRO:HD2	2.01	0.41
1:C:55:MSE:CE	1:C:143:PHE:CE2	3.01	0.41
1:D:192:LEU:HB3	1:D:195:LEU:HD12	2.02	0.41
1:A:280:PRO:HA	1:A:304:THR:HG22	2.01	0.41
1:A:55:MSE:HE3	1:A:143:PHE:CE2	2.54	0.41
1:A:136:PRO:HA	1:A:140:ASP:O	2.20	0.41
1:D:408:LEU:HB3	1:D:410:PHE:HD1	1.85	0.41
1:B:59:ARG:HB3	1:B:80:GLU:HB2	2.01	0.41
1:A:173:GLU:O	1:A:248:ARG:NH2	2.49	0.41
1:B:212:LEU:HD21	1:B:393:MSE:CE	2.51	0.41
1:A:257:PHE:HE2	1:A:259:ILE:HD11	1.83	0.41
1:D:243:LYS:HG3	1:D:244:ALA:N	2.35	0.41
1:D:416:HIS:ND1	1:D:485:PHE:HB2	2.35	0.41
1:A:336:GLN:HA	1:A:336:GLN:NE2	2.34	0.41
1:D:228:ILE:HG13	1:D:496:THR:HA	2.01	0.41
1:D:453:ARG:HH11	1:D:453:ARG:HG2	1.85	0.41
1:C:111:PRO:HB2	1:C:144:TYR:CD1	2.55	0.41
1:A:221:LYS:NZ	1:A:289:SER:HB3	2.35	0.41
1:B:94:ASN:O	1:B:95:ASP:C	2.58	0.41
1:C:288:LEU:HD11	1:C:343:ILE:HG23	2.02	0.41
1:A:288:LEU:HD23	1:A:294:ILE:HG13	2.03	0.41
1:B:350:TRP:CD1	1:B:354:HIS:HD2	2.38	0.41
1:A:59:ARG:HB3	1:A:80:GLU:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LYS:HG3	1:D:514:VAL:CG1	2.39	0.41
1:D:171:GLU:CD	1:D:534:ARG:HH12	2.23	0.41
1:B:29:THR:C	1:B:31:LYS:N	2.71	0.41
1:D:169:ASN:HD22	1:D:169:ASN:HA	1.68	0.41
1:B:200:ILE:HG12	1:B:311:LEU:HD12	2.03	0.41
1:A:287:THR:H	1:A:294:ILE:HG23	1.85	0.41
1:C:83:LEU:HD13	1:C:86:PHE:CD2	2.56	0.41
1:A:89:LYS:NZ	1:A:125:GLY:O	2.54	0.41
1:D:211:ALA:O	1:D:212:LEU:HD23	2.21	0.41
1:D:90:VAL:CG1	1:D:91:GLN:N	2.84	0.41
1:B:268:ASP:O	1:B:272:SER:HB3	2.21	0.41
1:D:464:LEU:HD23	1:D:464:LEU:N	2.35	0.41
1:B:41:GLN:OE1	1:B:41:GLN:HA	2.19	0.41
1:D:256:GLY:HA3	1:D:368:LEU:HD12	2.03	0.41
1:C:5:ASN:N	1:C:5:ASN:HD22	2.19	0.41
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.97	0.41
1:D:56:HIS:CE1	1:D:105:LEU:HD13	2.56	0.41
1:D:198:VAL:HG22	1:D:199:THR:H	1.84	0.40
1:A:157:HIS:CD2	1:A:371:LYS:O	2.74	0.40
1:D:633:MSE:C	1:D:635:THR:H	2.24	0.40
1:A:602:VAL:O	1:A:610:VAL:HA	2.21	0.40
1:A:288:LEU:CD2	1:A:294:ILE:HG13	2.52	0.40
1:C:229:ALA:C	1:C:231:PRO:HD3	2.41	0.40
1:A:46:ILE:HA	1:A:47:PRO:HD3	1.78	0.40
1:D:502:TYR:CD1	1:D:505:MSE:HE2	2.55	0.40
1:C:264:ARG:HA	1:C:267:SER:OG	2.21	0.40
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.88	0.40
1:A:95:ASP:HB2	3:A:1039:HOH:O	2.21	0.40
1:B:498:PRO:HG3	1:B:508:HIS:CE1	2.55	0.40
1:D:199:THR:HG22	1:D:210:ASP:O	2.21	0.40
1:A:135:HIS:HA	1:A:136:PRO:HD2	1.91	0.40
1:D:498:PRO:HB2	1:D:505:MSE:HG2	2.03	0.40
1:C:282:LEU:HD12	1:C:283:ALA:H	1.87	0.40
1:D:304:THR:O	1:D:305:ILE:HG12	2.22	0.40
1:B:160:PRO:O	1:B:545:VAL:HG22	2.21	0.40
1:A:273:LEU:HD22	1:A:281:VAL:HG22	2.02	0.40
1:B:187:LEU:HD22	1:B:189:ARG:HH21	1.87	0.40
1:C:55:MSE:CG	1:C:106:LEU:HD22	2.52	0.40
1:C:55:MSE:HB2	1:C:55:MSE:HE3	1.92	0.40
1:A:568:ILE:HD13	1:A:618:TYR:HB3	2.03	0.40
1:C:400:ALA:CB	1:C:495:TRP:CD1	3.05	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLY:O	1:B:413:TYR:HD1	2.04	0.40
1:B:183:LEU:HD11	1:B:236:ALA:HB2	2.02	0.40
1:C:539:ARG:HH11	1:C:539:ARG:HG3	1.86	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	632/644 (98%)	546 (86%)	68 (11%)	18 (3%)	6	3
1	B	632/644 (98%)	577 (91%)	47 (7%)	8 (1%)	15	13
1	C	632/644 (98%)	580 (92%)	45 (7%)	7 (1%)	17	17
1	D	632/644 (98%)	557 (88%)	61 (10%)	14 (2%)	8	5
All	All	2528/2576 (98%)	2260 (89%)	221 (9%)	47 (2%)	10	7

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	218	PRO
1	A	274	ARG
1	A	322	ASN
1	A	325	ASP
1	A	437	HIS
1	A	443	VAL
1	B	322	ASN
1	C	297	ASN
1	D	31	LYS
1	D	221	LYS
1	D	289	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	433	THR
1	A	115	ALA
1	A	123	LYS
1	A	187	LEU
1	A	621	THR
1	C	42	LYS
1	C	289	SER
1	C	322	ASN
1	D	68	LYS
1	D	219	ASP
1	D	469	ARG
1	D	525	ASP
1	D	621	THR
1	A	190	GLU
1	A	239	SER
1	A	441	GLU
1	B	15	LEU
1	B	192	LEU
1	B	272	SER
1	C	94	ASN
1	C	182	MSE
1	D	237	GLU
1	D	465	ASP
1	A	39	ASP
1	A	193	THR
1	A	296	ASP
1	B	30	GLU
1	D	220	ASP
1	B	94	ASN
1	B	229	ALA
1	C	188	VAL
1	D	6	PRO
1	A	361	ARG
1	B	255	PRO
1	D	388	ILE

### 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	480/522 (92%)	445 (93%)	35 (7%)	17	19
1	B	505/522 (97%)	485 (96%)	20 (4%)	38	49
1	C	504/522 (97%)	483 (96%)	21 (4%)	36	46
1	D	479/522 (92%)	456 (95%)	23 (5%)	31	40
All	All	1968/2088 (94%)	1869 (95%)	99 (5%)	30	37

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	SER
1	A	18	GLN
1	A	19	THR
1	A	29	THR
1	A	45	PHE
1	A	71	GLU
1	A	76	GLU
1	A	91	GLN
1	A	94	ASN
1	A	133	ARG
1	A	167	ARG
1	A	172	LYS
1	A	178	VAL
1	A	187	LEU
1	A	237	GLU
1	A	258	ASN
1	A	285	ARG
1	A	293	THR
1	A	294	ILE
1	A	305	ILE
1	A	314	ASP
1	A	329	GLU
1	A	344	CYS
1	A	357	VAL
1	A	358	PHE
1	A	417	MSE
1	A	444	LEU
1	A	476	GLU
1	A	511	LEU
1	A	531	MSE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	557	LYS
1	A	582	ASP
1	A	613	LYS
1	A	636	ARG
1	B	29	THR
1	B	68	LYS
1	B	70	ARG
1	B	89	LYS
1	B	113	ARG
1	B	144	TYR
1	B	210	ASP
1	B	232	THR
1	B	258	ASN
1	B	288	LEU
1	B	289	SER
1	B	330	SER
1	B	360	ASP
1	B	367	ILE
1	B	405	ARG
1	B	410	PHE
1	B	472	GLN
1	B	496	THR
1	B	634	GLU
1	B	636	ARG
1	C	5	ASN
1	C	10	GLN
1	C	43	SER
1	C	94	ASN
1	C	113	ARG
1	C	124	GLU
1	C	178	VAL
1	C	198	VAL
1	C	208	MSE
1	C	219	ASP
1	C	267	SER
1	C	268	ASP
1	C	317	SER
1	C	346	ARG
1	C	496	THR
1	C	497	SER
1	C	505	MSE
1	C	524	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	567	GLU
1	C	570	ASP
1	C	636	ARG
1	D	7	LEU
1	D	8	LEU
1	D	43	SER
1	D	70	ARG
1	D	72	SER
1	D	74	GLU
1	D	89	LYS
1	D	95	ASP
1	D	123	LYS
1	D	131	GLU
1	D	180	THR
1	D	187	LEU
1	D	202	SER
1	D	232	THR
1	D	261	MSE
1	D	267	SER
1	D	305	ILE
1	D	349	GLU
1	D	354	HIS
1	D	373	GLU
1	D	436	LEU
1	D	453	ARG
1	D	636	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	91	GLN
1	A	94	ASN
1	A	157	HIS
1	A	605	GLN
1	B	354	HIS
1	B	434	HIS
1	B	507	ASN
1	C	5	ASN
1	C	157	HIS
1	C	315	GLN
1	C	353	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	472	GLN
1	C	611	GLN
1	D	169	ASN
1	D	297	ASN
1	D	342	GLN
1	D	437	HIS
1	D	472	GLN
1	D	607	ASN
1	D	611	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	622/644 (96%)	1.35	173 (27%) 1 1	31, 57, 80, 89	0
1	B	622/644 (96%)	0.77	81 (13%) 5 9	33, 54, 74, 84	0
1	C	622/644 (96%)	0.66	70 (11%) 7 12	41, 53, 72, 84	0
1	D	622/644 (96%)	1.04	117 (18%) 2 3	31, 53, 74, 85	0
All	All	2488/2576 (96%)	0.95	441 (17%) 2 3	31, 54, 76, 89	0

All (441) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	GLY	9.4
1	A	324	GLY	7.8
1	A	290	ALA	7.7
1	D	33	PHE	6.4
1	A	68	LYS	6.2
1	C	324	GLY	6.1
1	A	212	LEU	6.0
1	A	318	ASP	6.0
1	D	219	ASP	6.0
1	A	294	ILE	5.9
1	A	474	PHE	5.9
1	A	296	ASP	5.8
1	A	354	HIS	5.8
1	B	323	THR	5.8
1	D	324	GLY	5.7
1	C	36	LEU	5.7
1	A	220	ASP	5.7
1	C	5	ASN	5.6
1	D	36	LEU	5.3
1	B	275	ALA	5.3
1	C	203	ALA	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	41	GLN	5.2
1	A	410	PHE	5.2
1	D	421	PRO	5.2
1	D	322	ASN	5.2
1	A	327	GLN	5.1
1	A	195	LEU	5.1
1	A	117	GLY	5.0
1	A	278	VAL	5.0
1	D	183	LEU	5.0
1	A	319	TRP	5.0
1	D	35	PHE	5.0
1	A	358	PHE	4.9
1	D	358	PHE	4.8
1	A	340	LEU	4.8
1	A	316	VAL	4.7
1	A	199	THR	4.7
1	A	344	CYS	4.7
1	A	211	ALA	4.7
1	A	35	PHE	4.7
1	C	6	PRO	4.6
1	D	32	GLY	4.6
1	A	66	SER	4.6
1	A	217	LEU	4.6
1	A	196	ASP	4.6
1	A	216	ALA	4.5
1	B	36	LEU	4.5
1	A	353	ASN	4.5
1	A	282	LEU	4.5
1	D	474	PHE	4.5
1	A	502	TYR	4.4
1	A	116	ARG	4.4
1	A	180	THR	4.4
1	D	419	PHE	4.3
1	A	94	ASN	4.3
1	A	276	ASN	4.3
1	A	350	TRP	4.3
1	A	218	PRO	4.3
1	A	421	PRO	4.2
1	D	382	ARG	4.2
1	A	178	VAL	4.2
1	A	407	LYS	4.2
1	A	36	LEU	4.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	26	VAL	4.1
1	C	206	GLU	4.1
1	A	186	GLY	4.1
1	C	610	VAL	4.1
1	A	11	LEU	4.1
1	D	323	THR	4.1
1	A	183	LEU	4.1
1	A	198	VAL	4.0
1	D	11	LEU	4.0
1	C	94	ASN	4.0
1	A	118	LEU	4.0
1	C	54	VAL	3.9
1	D	30	GLU	4.0
1	D	60	ILE	3.9
1	C	26	VAL	3.9
1	A	203	ALA	3.9
1	A	445	THR	3.9
1	D	29	THR	3.9
1	D	94	ASN	3.9
1	C	200	ILE	3.8
1	D	527	ILE	3.8
1	C	197	PHE	3.8
1	D	128	ALA	3.8
1	D	483	PRO	3.8
1	D	316	VAL	3.8
1	A	329	GLU	3.8
1	A	437	HIS	3.8
1	A	325	ASP	3.8
1	A	458	ALA	3.7
1	B	179	ALA	3.7
1	A	568	ILE	3.7
1	C	198	VAL	3.7
1	A	5	ASN	3.7
1	B	54	VAL	3.7
1	A	206	GLU	3.7
1	A	338	ARG	3.7
1	B	205	THR	3.7
1	A	112	CYS	3.7
1	D	296	ASP	3.6
1	B	93	LYS	3.6
1	A	73	ALA	3.6
1	A	227	ALA	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	644	ALA	3.6
1	D	69	GLU	3.6
1	A	284	CYS	3.6
1	B	60	ILE	3.6
1	C	176	ASP	3.6
1	D	506	ILE	3.5
1	B	197	PHE	3.5
1	A	26	VAL	3.5
1	A	32	GLY	3.5
1	A	360	ASP	3.5
1	A	420	ASP	3.5
1	D	176	ASP	3.5
1	B	99	ILE	3.5
1	A	194	ALA	3.5
1	A	516	LYS	3.5
1	D	199	THR	3.5
1	B	41	GLN	3.5
1	C	380	GLU	3.5
1	B	33	PHE	3.4
1	D	198	VAL	3.4
1	D	329	GLU	3.4
1	C	69	GLU	3.4
1	A	221	LYS	3.4
1	B	325	ASP	3.4
1	D	140	ASP	3.4
1	D	46	ILE	3.4
1	D	628	ILE	3.4
1	A	33	PHE	3.3
1	A	69	GLU	3.3
1	A	382	ARG	3.3
1	A	529	VAL	3.3
1	D	524	GLN	3.3
1	A	361	ARG	3.3
1	C	381	PRO	3.3
1	D	28	ALA	3.3
1	D	70	ARG	3.3
1	C	33	PHE	3.3
1	D	284	CYS	3.3
1	A	323	THR	3.3
1	A	334	ALA	3.3
1	B	176	ASP	3.3
1	B	35	PHE	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	474	PHE	3.2
1	A	355	ALA	3.2
1	D	54	VAL	3.2
1	A	205	THR	3.2
1	B	271	CYS	3.2
1	B	231	PRO	3.2
1	D	437	HIS	3.2
1	A	177	GLY	3.2
1	B	449	PHE	3.1
1	A	41	GLN	3.1
1	A	525	ASP	3.1
1	A	610	VAL	3.1
1	D	297	ASN	3.1
1	B	7	LEU	3.1
1	A	439	ASP	3.1
1	D	355	ALA	3.1
1	A	119	ASN	3.1
1	C	204	SER	3.1
1	D	5	ASN	3.1
1	D	327	GLN	3.1
1	A	308	LYS	3.1
1	A	307	SER	3.1
1	B	249	ALA	3.0
1	D	493	ALA	3.0
1	D	240	LYS	3.0
1	B	399	CYS	3.0
1	B	460	PRO	3.0
1	B	419	PHE	3.0
1	B	94	ASN	3.0
1	D	350	TRP	3.0
1	C	35	PHE	3.0
1	A	147	LEU	3.0
1	A	31	LYS	3.0
1	A	187	LEU	3.0
1	A	231	PRO	3.0
1	D	460	PRO	3.0
1	B	26	VAL	3.0
1	D	130	ALA	3.0
1	B	358	PHE	3.0
1	C	199	THR	3.0
1	D	75	PRO	2.9
1	B	219	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	608	GLY	2.9
1	A	455	GLU	2.9
1	D	197	PHE	2.9
1	C	323	THR	2.9
1	A	92	GLY	2.9
1	A	238	GLY	2.9
1	D	456	LEU	2.9
1	D	502	TYR	2.9
1	A	412	ILE	2.9
1	B	204	SER	2.9
1	A	295	GLU	2.8
1	A	515	ILE	2.8
1	C	13	GLN	2.8
1	C	502	TYR	2.8
1	A	75	PRO	2.8
1	D	605	GLN	2.8
1	A	527	ILE	2.8
1	C	185	GLU	2.8
1	A	88	GLY	2.8
1	A	229	ALA	2.8
1	A	481	PRO	2.8
1	D	6	PRO	2.8
1	A	40	ALA	2.8
1	A	348	GLY	2.8
1	B	211	ALA	2.8
1	A	219	ASP	2.8
1	D	119	ASN	2.8
1	A	93	LYS	2.8
1	A	213	PHE	2.8
1	D	298	ILE	2.8
1	C	422	ALA	2.8
1	D	514	VAL	2.8
1	A	300	PHE	2.8
1	D	15	LEU	2.8
1	D	580	LEU	2.8
1	C	70	ARG	2.8
1	A	413	TYR	2.8
1	B	297	ASN	2.8
1	D	325	ASP	2.7
1	D	347	ARG	2.7
1	A	225	ILE	2.7
1	A	270	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	231	PRO	2.7
1	D	222	LEU	2.7
1	B	627	THR	2.7
1	A	54	VAL	2.7
1	D	63	VAL	2.7
1	C	511	LEU	2.7
1	B	229	ALA	2.7
1	C	322	ASN	2.7
1	D	503	GLY	2.7
1	D	188	VAL	2.7
1	A	460	PRO	2.7
1	B	298	ILE	2.7
1	D	444	LEU	2.7
1	D	360	ASP	2.7
1	A	436	LEU	2.7
1	A	333	ILE	2.7
1	B	628	ILE	2.7
1	A	72	SER	2.7
1	C	275	ALA	2.7
1	D	145	ALA	2.7
1	A	29	THR	2.7
1	C	420	ASP	2.7
1	D	276	ASN	2.6
1	B	294	ILE	2.6
1	A	197	PHE	2.6
1	A	204	SER	2.6
1	B	185	GLU	2.6
1	D	186	GLY	2.6
1	C	224	LEU	2.6
1	C	571	ILE	2.6
1	D	200	ILE	2.6
1	C	284	CYS	2.6
1	D	529	VAL	2.6
1	A	314	ASP	2.6
1	A	513	ALA	2.6
1	B	183	LEU	2.6
1	B	395	ALA	2.6
1	B	452	LEU	2.6
1	B	640	ALA	2.6
1	C	452	LEU	2.6
1	D	62	ALA	2.6
1	A	46	ILE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	628	ILE	2.6
1	A	320	LEU	2.6
1	D	610	VAL	2.6
1	B	608	GLY	2.5
1	B	502	TYR	2.5
1	C	205	THR	2.5
1	C	406	ASP	2.5
1	B	147	LEU	2.5
1	D	88	GLY	2.5
1	A	30	GLU	2.5
1	A	441	GLU	2.5
1	C	249	ALA	2.5
1	A	347	ARG	2.5
1	D	554	LEU	2.5
1	A	99	ILE	2.5
1	C	60	ILE	2.5
1	D	294	ILE	2.5
1	A	419	PHE	2.5
1	D	270	LEU	2.5
1	D	354	HIS	2.5
1	A	440	ALA	2.4
1	B	203	ALA	2.4
1	D	40	ALA	2.4
1	A	483	PRO	2.4
1	B	95	ASP	2.4
1	B	610	VAL	2.4
1	A	449	PHE	2.4
1	A	433	THR	2.4
1	B	524	GLN	2.4
1	A	362	PRO	2.4
1	A	456	LEU	2.4
1	C	68	LYS	2.4
1	B	316	VAL	2.4
1	D	330	SER	2.4
1	A	179	ALA	2.4
1	A	332	ALA	2.4
1	B	187	LEU	2.4
1	D	147	LEU	2.4
1	B	25	VAL	2.4
1	C	90	VAL	2.4
1	C	179	ALA	2.4
1	C	640	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	2.4
1	B	198	VAL	2.4
1	D	95	ASP	2.4
1	A	237	GLU	2.4
1	C	262	LEU	2.4
1	A	317	SER	2.4
1	A	337	VAL	2.4
1	D	203	ALA	2.4
1	A	387	ARG	2.4
1	A	510	LEU	2.3
1	B	11	LEU	2.3
1	B	178	VAL	2.3
1	D	338	ARG	2.3
1	A	62	ALA	2.3
1	B	186	GLY	2.3
1	C	573	ARG	2.3
1	A	443	VAL	2.3
1	D	226	VAL	2.3
1	D	334	ALA	2.3
1	C	15	LEU	2.3
1	D	508	HIS	2.3
1	A	482	GLY	2.3
1	B	380	GLU	2.3
1	D	282	LEU	2.3
1	A	155	ASP	2.3
1	C	281	VAL	2.3
1	C	568	ILE	2.3
1	A	209	ASP	2.3
1	B	340	LEU	2.3
1	C	340	LEU	2.3
1	A	226	VAL	2.3
1	A	638	ILE	2.3
1	D	422	ALA	2.3
1	A	352	HIS	2.3
1	A	447	ASP	2.3
1	A	596	ALA	2.2
1	B	360	ASP	2.2
1	D	66	SER	2.2
1	B	213	PHE	2.2
1	C	358	PHE	2.2
1	D	511	LEU	2.2
1	A	215	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	448	GLY	2.2
1	A	58	ASP	2.2
1	C	316	VAL	2.2
1	C	419	PHE	2.2
1	D	45	PHE	2.2
1	B	30	GLU	2.2
1	C	360	ASP	2.2
1	D	205	THR	2.2
1	B	40	ALA	2.2
1	A	298	ILE	2.2
1	B	200	ILE	2.2
1	A	281	VAL	2.2
1	A	411	GLY	2.2
1	C	273	LEU	2.2
1	B	638	ILE	2.2
1	A	185	GLU	2.2
1	C	325	ASP	2.2
1	D	478	SER	2.2
1	D	606	GLU	2.2
1	D	333	ILE	2.2
1	A	597	VAL	2.2
1	A	594	LEU	2.2
1	A	640	ALA	2.2
1	D	392	ALA	2.2
1	D	161	TRP	2.1
1	B	300	PHE	2.1
1	B	507	ASN	2.1
1	D	301	PHE	2.1
1	D	507	ASN	2.1
1	B	212	LEU	2.1
1	B	227	ALA	2.1
1	D	500	ARG	2.1
1	B	381	PRO	2.1
1	A	45	PHE	2.1
1	D	479	THR	2.1
1	A	442	GLU	2.1
1	B	98	ALA	2.1
1	B	145	ALA	2.1
1	D	395	ALA	2.1
1	C	628	ILE	2.1
1	C	500	ARG	2.1
1	D	116	ARG	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	326	TRP	2.1
1	B	511	LEU	2.1
1	A	486	GLY	2.1
1	A	608	GLY	2.1
1	A	343	ILE	2.1
1	A	506	ILE	2.1
1	B	506	ILE	2.1
1	C	352	HIS	2.1
1	C	370	GLU	2.1
1	D	469	ARG	2.1
1	B	199	THR	2.1
1	C	31	LYS	2.1
1	C	161	TRP	2.1
1	C	288	LEU	2.1
1	D	609	THR	2.1
1	A	128	ALA	2.1
1	A	233	ALA	2.1
1	B	207	ASP	2.1
1	D	457	ASP	2.1
1	C	320	LEU	2.1
1	D	441	GLU	2.1
1	B	130	ALA	2.1
1	A	495	TRP	2.1
1	D	568	ILE	2.1
1	B	24	GLY	2.0
1	D	180	THR	2.0
1	C	145	ALA	2.0
1	C	245	ALA	2.0
1	C	524	GLN	2.0
1	B	66	SER	2.0
1	A	526	GLU	2.0
1	D	139	GLY	2.0
1	D	361	ARG	2.0
1	B	163	VAL	2.0
1	A	224	LEU	2.0
1	A	301	PHE	2.0
1	C	283	ALA	2.0
1	D	409	GLY	2.0
1	A	95	ASP	2.0
1	A	457	ASP	2.0
1	A	302	ALA	2.0
1	B	157	HIS	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 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
2	MN	B	1002	1/1	0.98	0.04	-	83,83,83,83	0
2	MN	A	1001	1/1	0.93	0.14	-	100,100,100,100	0
2	MN	D	1004	1/1	0.96	0.08	-	94,94,94,94	0
2	MN	C	1003	1/1	0.95	0.03	-	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.