



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID : 4IMP  
Title : The missing linker: a dimerization motif located within polyketide synthase modules  
Authors : Zheng, J.; Keatinge-Clay, A.T.  
Deposited on : 2013-01-03  
Resolution : 2.57 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  
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

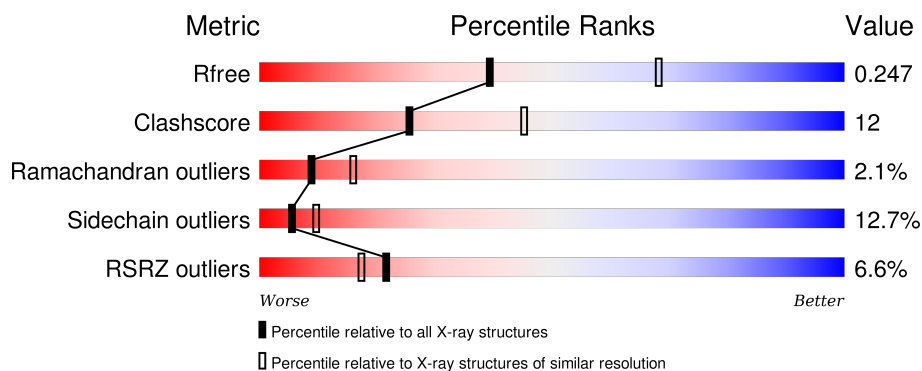
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	580	<div> <div>8%</div> <div>68% 18% • 10%</div> </div>
1	B	580	<div> <div>8%</div> <div>63% 21% 5% • 11%</div> </div>
1	C	580	<div> <div>5%</div> <div>64% 21% 5% 11%</div> </div>
1	D	580	<div> <div>9%</div> <div>62% 22% 5% 11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15710 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 Polyketide synthase extender modules 3-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			3885	2429	719	727	10			
1	B	518	Total	C	N	O	S	0	0	0
			3871	2422	717	722	10			
1	C	519	Total	C	N	O	S	0	0	0
			3875	2422	718	725	10			
1	D	515	Total	C	N	O	S	0	0	0
			3850	2407	714	719	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q9ALM4
A	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM4
A	-18	SER	-	EXPRESSION TAG	UNP Q9ALM4
A	-17	SER	-	EXPRESSION TAG	UNP Q9ALM4
A	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	-10	SER	-	EXPRESSION TAG	UNP Q9ALM4
A	-9	SER	-	EXPRESSION TAG	UNP Q9ALM4
A	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM4
A	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM4
A	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM4
A	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM4
A	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM4
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM4
A	-2	SER	-	EXPRESSION TAG	UNP Q9ALM4
A	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM4
A	0	MET	-	EXPRESSION TAG	UNP Q9ALM4

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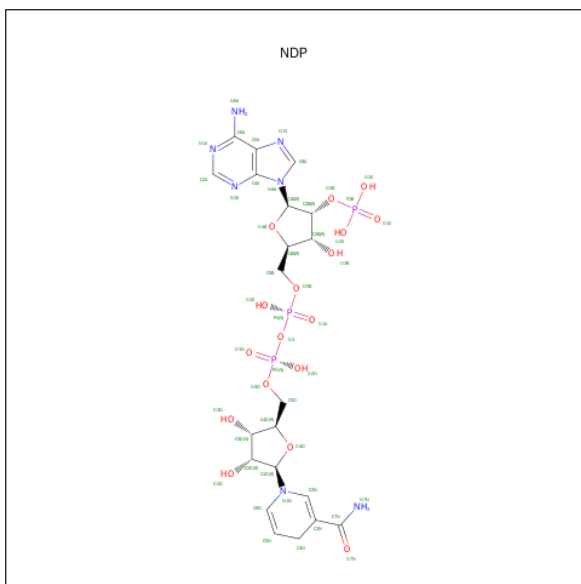
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q9ALM4
B	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM4
B	-18	SER	-	EXPRESSION TAG	UNP Q9ALM4
B	-17	SER	-	EXPRESSION TAG	UNP Q9ALM4
B	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	-10	SER	-	EXPRESSION TAG	UNP Q9ALM4
B	-9	SER	-	EXPRESSION TAG	UNP Q9ALM4
B	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM4
B	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM4
B	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM4
B	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM4
B	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM4
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM4
B	-2	SER	-	EXPRESSION TAG	UNP Q9ALM4
B	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM4
B	0	MET	-	EXPRESSION TAG	UNP Q9ALM4
C	-20	MET	-	EXPRESSION TAG	UNP Q9ALM4
C	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM4
C	-18	SER	-	EXPRESSION TAG	UNP Q9ALM4
C	-17	SER	-	EXPRESSION TAG	UNP Q9ALM4
C	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	-10	SER	-	EXPRESSION TAG	UNP Q9ALM4
C	-9	SER	-	EXPRESSION TAG	UNP Q9ALM4
C	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM4
C	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM4
C	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM4
C	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM4
C	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM4
C	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM4
C	-2	SER	-	EXPRESSION TAG	UNP Q9ALM4
C	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM4
C	0	MET	-	EXPRESSION TAG	UNP Q9ALM4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q9ALM4
D	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM4
D	-18	SER	-	EXPRESSION TAG	UNP Q9ALM4
D	-17	SER	-	EXPRESSION TAG	UNP Q9ALM4
D	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	-10	SER	-	EXPRESSION TAG	UNP Q9ALM4
D	-9	SER	-	EXPRESSION TAG	UNP Q9ALM4
D	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM4
D	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM4
D	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM4
D	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM4
D	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM4
D	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM4
D	-2	SER	-	EXPRESSION TAG	UNP Q9ALM4
D	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM4
D	0	MET	-	EXPRESSION TAG	UNP Q9ALM4

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

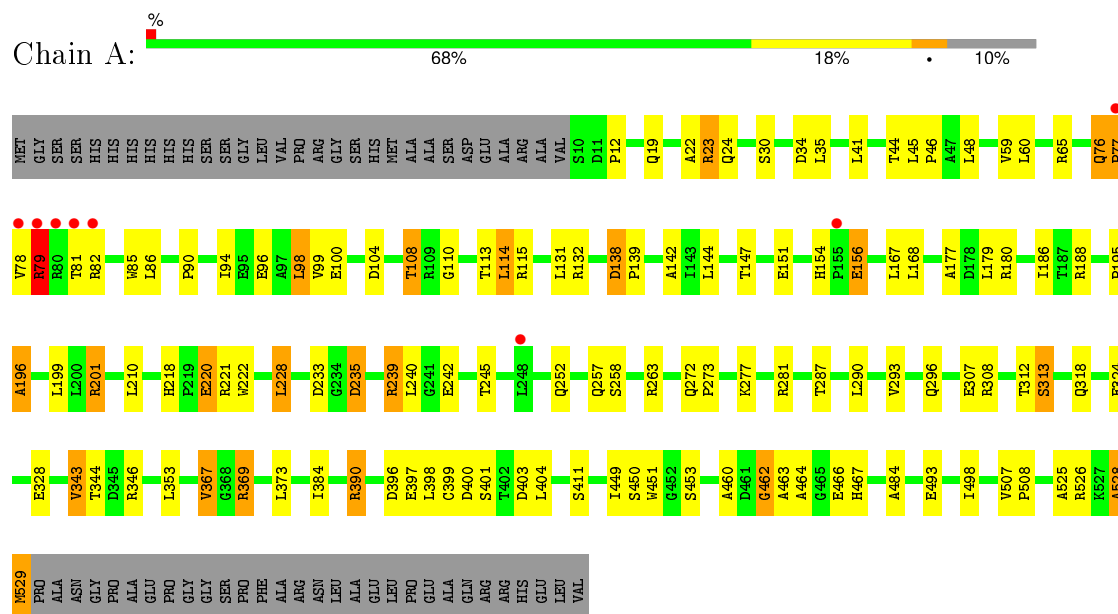
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	7	Total 7	O 7	0	0
3	C	1	Total 1	O 1	0	0
3	D	3	Total 3	O 3	0	0

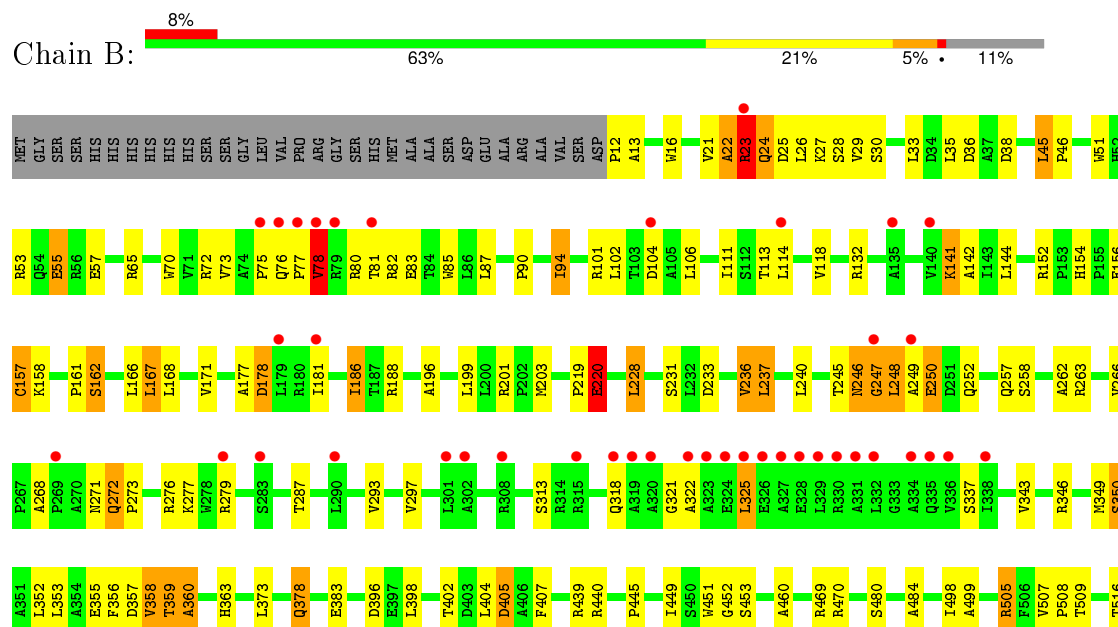
### 3 Residue-property plots [i](#)

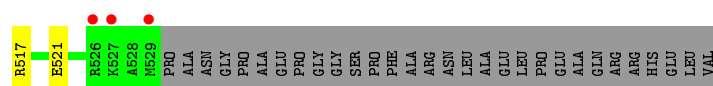
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Polyketide synthase extender modules 3-4

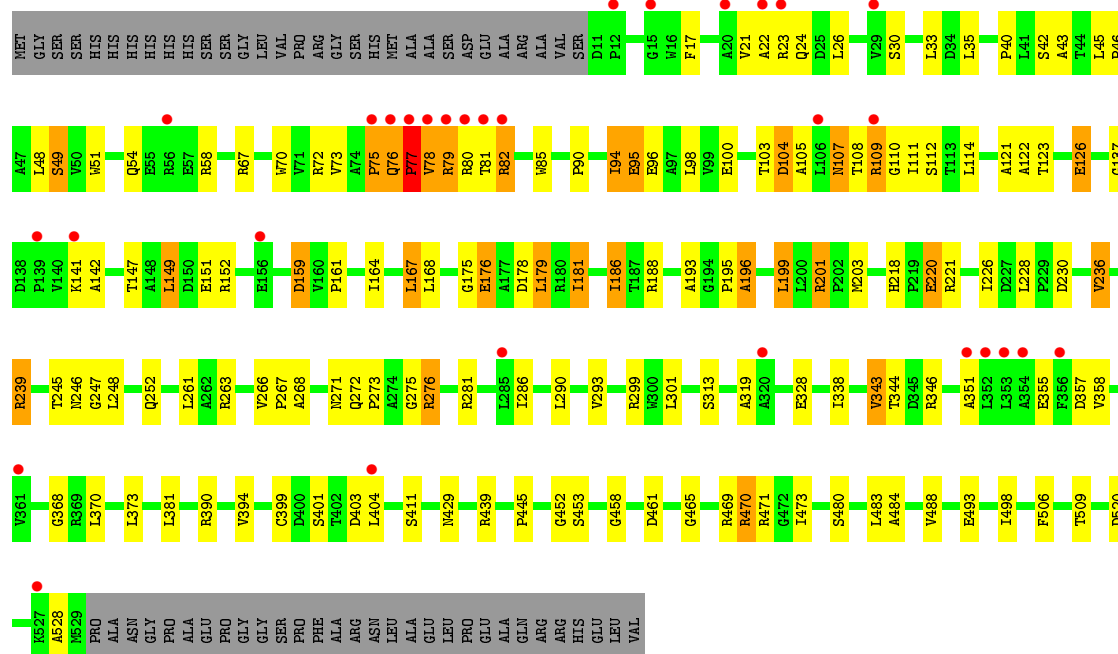


- Molecule 1: Polyketide synthase extender modules 3-4

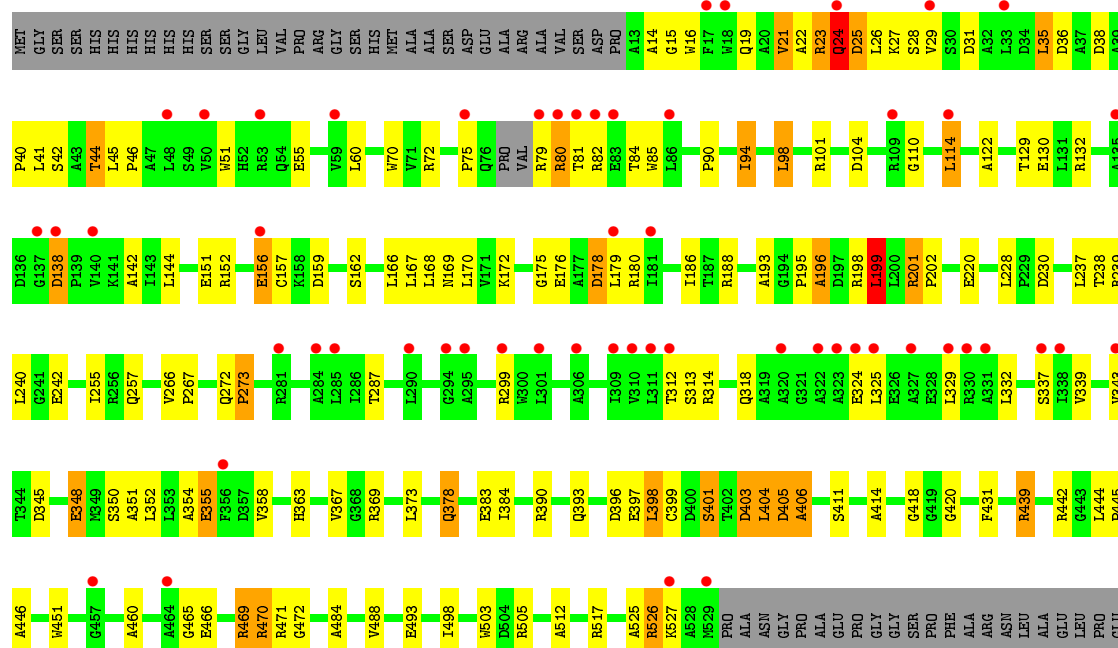




- Molecule 1: Polyketide synthase extender modules 3-4



- Molecule 1: Polyketide synthase extender modules 3-4





ALA
GLN
ARG
ARG
HIS
GLU
LEU
VAL

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.81Å 211.69Å 101.74Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 47.57 – 2.57	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.57) 96.4 (47.57-2.57)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.245 0.204 , 0.247	Depositor DCC
$R_{free}$ test set	3812 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 72966 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: NDP

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	0.69	2/3958 (0.1%)	0.61	1/5395 (0.0%)
1	B	0.62	0/3944	0.56	1/5375 (0.0%)
1	C	0.60	0/3947	0.56	2/5379 (0.0%)
1	D	0.60	0/3920	0.55	2/5339 (0.0%)
All	All	0.63	2/15769 (0.0%)	0.57	6/21488 (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	4
1	B	0	5
1	C	0	2
1	D	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	TRP	CD2-CE2	5.14	1.47	1.41
1	A	296	GLN	CD-OE1	5.00	1.34	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	PRO	N-CA-CB	7.01	111.72	103.30
1	D	199	LEU	CA-CB-CG	5.30	127.48	115.30
1	B	104	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	104	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	104	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	104	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	ASP	Peptide
1	A	462	GLY	Peptide
1	A	528	ALA	Peptide
1	A	79	ARG	Peptide
1	B	196	ALA	Peptide
1	B	23	ARG	Peptide
1	B	24	GLN	Peptide
1	B	248	LEU	Peptide
1	B	78	VAL	Peptide
1	C	368	GLY	Peptide
1	C	77	PRO	Peptide
1	D	451	TRP	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	3885	0	3892	86	0
1	B	3871	0	3884	113	0
1	C	3875	0	3874	104	0
1	D	3850	0	3859	95	0
2	A	48	0	26	3	0
2	B	48	0	26	2	0
2	C	48	0	26	7	0
2	D	48	0	26	3	0
3	A	26	0	0	0	0
3	B	7	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15710	0	15613	390	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 (390) 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:469:ARG:HG2	1:D:469:ARG:HH21	1.10	1.15
1:B:90:PRO:HG2	1:B:94:ILE:HD11	1.29	1.10
1:C:80:ARG:HG3	1:C:81:THR:H	1.08	1.09
1:C:470:ARG:HG2	1:C:470:ARG:HH21	1.10	1.07
1:A:239:ARG:HH21	1:A:239:ARG:HG3	1.14	1.03
1:A:22:ALA:O	1:A:23:ARG:HB2	1.63	0.97
1:C:82:ARG:HE	1:C:110:GLY:HA2	1.29	0.97
1:D:144:LEU:HD11	1:D:186:ILE:CD1	1.97	0.95
1:B:90:PRO:CG	1:B:94:ILE:HD11	1.98	0.93
1:D:144:LEU:HD11	1:D:186:ILE:HD13	1.50	0.93
1:C:78:VAL:CB	1:C:79:ARG:HA	1.99	0.92
1:C:49:SER:HB3	1:D:21:VAL:HG13	1.55	0.89
1:A:76:GLN:H	1:A:77:PRO:HD2	1.38	0.89
1:B:161:PRO:HG3	1:B:203:MET:CE	2.03	0.88
1:C:80:ARG:HG3	1:C:81:THR:N	1.89	0.88
1:C:470:ARG:HG2	1:C:470:ARG:NH2	1.87	0.88
1:B:161:PRO:HG3	1:B:203:MET:HE1	1.58	0.86
1:D:22:ALA:O	1:D:23:ARG:HB2	1.76	0.85
1:A:77:PRO:HB3	1:A:78:VAL:HA	1.59	0.85
1:C:299:ARG:NH2	1:C:328:GLU:OE1	2.10	0.83
1:C:484:ALA:HB1	1:C:498:ILE:HD13	1.57	0.83
1:B:349:MET:O	1:B:353:LEU:HD12	1.80	0.81
1:A:239:ARG:NH2	1:A:239:ARG:HG3	1.89	0.80
1:B:81:THR:HG23	1:B:82:ARG:H	1.46	0.80
1:B:154:HIS:HB3	1:B:157:CYS:HB3	1.64	0.80
1:C:161:PRO:HG2	1:C:164:ILE:HG12	1.64	0.79
1:A:343:VAL:HG22	2:A:1501:NDP:N1A	1.96	0.79
1:D:80:ARG:HG3	1:D:81:THR:N	1.97	0.79
1:C:275:GLY:O	1:C:276:ARG:HB3	1.81	0.78
1:D:195:PRO:O	1:D:196:ALA:CB	2.31	0.78
1:D:45:LEU:HB3	1:D:46:PRO:HD3	1.66	0.77
1:A:195:PRO:O	1:A:196:ALA:HB3	1.83	0.77
1:A:19:GLN:O	1:A:22:ALA:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ARG:CG	1:B:81:THR:H	1.98	0.76
1:D:24:GLN:O	1:D:26:LEU:N	2.18	0.76
1:D:345:ASP:OD1	1:D:348:GLU:HG2	1.86	0.76
1:D:199:LEU:HD13	1:D:199:LEU:O	1.85	0.76
1:C:76:GLN:NE2	1:C:248:LEU:HD12	2.01	0.75
1:B:73:VAL:O	1:B:73:VAL:HG23	1.87	0.75
1:A:41:LEU:HD13	1:A:41:LEU:O	1.87	0.75
1:A:41:LEU:HD12	1:B:26:LEU:CD2	2.17	0.75
1:D:484:ALA:HB1	1:D:498:ILE:HD13	1.69	0.75
1:C:77:PRO:CB	1:C:78:VAL:CB	2.65	0.74
1:B:252:GLN:OE1	1:B:263:ARG:HD3	1.88	0.73
1:A:77:PRO:HG2	1:A:242:GLU:HB2	1.70	0.73
1:C:108:THR:O	1:C:108:THR:HG22	1.88	0.73
1:D:40:PRO:O	1:D:44:THR:HG23	1.88	0.73
1:D:469:ARG:NH2	1:D:469:ARG:HG2	1.90	0.72
1:A:151:GLU:OE2	1:A:201:ARG:HD3	1.89	0.72
1:D:339:VAL:HG21	1:D:352:LEU:HD11	1.70	0.72
1:C:313:SER:OG	2:C:1501:NDP:O1X	2.07	0.72
1:A:154:HIS:CE1	1:A:156:GLU:HB3	2.25	0.72
1:C:343:VAL:HG22	2:C:1501:NDP:N1A	2.05	0.72
1:B:439:ARG:NH2	1:B:445:PRO:O	2.22	0.72
1:D:159:ASP:OD1	1:D:390:ARG:HD3	1.90	0.71
1:A:77:PRO:CB	1:A:78:VAL:HA	2.21	0.71
1:B:353:LEU:HA	1:B:358:VAL:HG13	1.71	0.71
1:A:195:PRO:O	1:A:196:ALA:CB	2.37	0.71
1:A:79:ARG:HH22	1:A:245:THR:HB	1.55	0.71
1:B:83:GLU:HB2	1:B:141:LYS:NZ	2.06	0.70
1:C:78:VAL:CB	1:C:79:ARG:CA	2.70	0.70
1:B:80:ARG:HG2	1:B:81:THR:H	1.56	0.70
1:B:65:ARG:NH2	1:B:268:ALA:O	2.24	0.69
1:C:195:PRO:O	1:C:196:ALA:HB3	1.92	0.69
1:D:144:LEU:HD11	1:D:186:ILE:HD11	1.75	0.69
1:D:151:GLU:OE2	1:D:201:ARG:HD3	1.92	0.69
1:D:469:ARG:CG	1:D:469:ARG:HH21	1.96	0.68
1:A:463:ALA:O	1:A:466:GLU:HB2	1.93	0.68
1:A:41:LEU:HD12	1:B:26:LEU:HD23	1.76	0.68
1:A:22:ALA:O	1:A:23:ARG:CB	2.41	0.67
1:A:344:THR:O	1:A:390:ARG:NH2	2.27	0.67
1:D:314:ARG:N	2:D:1501:NDP:O1X	2.27	0.67
1:C:470:ARG:HH21	1:C:470:ARG:CG	1.94	0.67
1:C:218:HIS:HB3	1:C:221:ARG:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:CD1	1:D:186:ILE:HD13	2.21	0.67
1:A:108:THR:O	1:A:108:THR:CG2	2.42	0.67
1:C:45:LEU:HB3	1:C:46:PRO:HD3	1.76	0.66
1:C:252:GLN:OE1	1:C:263:ARG:HD3	1.96	0.66
1:B:23:ARG:HA	1:B:24:GLN:HB2	1.78	0.65
1:A:94:ILE:HD11	1:A:98:LEU:HB3	1.79	0.65
1:C:480:SER:HA	1:C:483:LEU:HD12	1.79	0.65
1:C:161:PRO:HG2	1:C:164:ILE:CG1	2.28	0.64
1:B:76:GLN:N	1:B:77:PRO:CD	2.61	0.64
1:B:161:PRO:HG3	1:B:203:MET:HE3	1.78	0.64
1:D:470:ARG:HH21	1:D:470:ARG:HB3	1.62	0.64
1:B:359:THR:OG1	1:B:359:THR:O	2.07	0.64
1:B:353:LEU:HA	1:B:358:VAL:CG1	2.27	0.64
1:A:19:GLN:HB3	1:A:23:ARG:HH21	1.61	0.64
1:B:76:GLN:N	1:B:77:PRO:HD3	2.13	0.64
1:C:142:ALA:HA	1:C:181:ILE:HG23	1.79	0.64
1:D:195:PRO:O	1:D:196:ALA:HB3	1.97	0.64
1:C:94:ILE:HD13	1:C:94:ILE:H	1.63	0.64
1:A:528:ALA:O	1:A:529:MET:HG3	1.98	0.64
1:A:154:HIS:ND1	1:A:156:GLU:HB3	2.13	0.63
1:B:233:ASP:O	1:B:236:VAL:HG13	1.99	0.63
1:C:159:ASP:OD1	1:C:159:ASP:N	2.32	0.63
1:B:440:ARG:HH21	1:B:445:PRO:HA	1.64	0.62
1:C:411:SER:OG	1:C:429:ASN:HB3	1.98	0.62
1:C:453:SER:OG	1:C:473:ILE:HG22	2.00	0.62
1:B:76:GLN:H	1:B:77:PRO:HD3	1.62	0.61
1:D:90:PRO:HG2	1:D:94:ILE:HD11	1.82	0.61
1:D:503:TRP:CE3	1:D:525:ALA:HB2	2.35	0.61
1:B:90:PRO:HG2	1:B:94:ILE:CD1	2.20	0.61
1:D:80:ARG:HG3	1:D:81:THR:H	1.65	0.61
1:B:45:LEU:CB	1:B:46:PRO:HD3	2.31	0.61
1:D:35:LEU:HD13	1:D:44:THR:HB	1.82	0.60
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.65	0.60
1:B:440:ARG:NH2	1:B:445:PRO:HA	2.16	0.60
1:B:152:ARG:O	1:B:162:SER:HB2	2.01	0.60
1:D:240:LEU:HA	1:D:255:ILE:CD1	2.32	0.60
1:B:90:PRO:CD	1:B:94:ILE:HD11	2.32	0.60
1:D:23:ARG:C	1:D:25:ASP:H	2.05	0.60
1:B:80:ARG:CG	1:B:81:THR:N	2.63	0.60
1:D:287:THR:OG1	1:D:363:HIS:HA	2.01	0.60
1:C:151:GLU:OE2	1:C:201:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ARG:NH2	1:C:445:PRO:O	2.35	0.60
1:D:122:ALA:O	1:D:169:ASN:ND2	2.34	0.59
1:B:80:ARG:HG2	1:B:81:THR:N	2.18	0.59
1:D:411:SER:O	2:D:1501:NDP:H6N	2.03	0.59
1:B:12:PRO:HG2	1:B:13:ALA:H	1.66	0.59
1:B:13:ALA:HB2	1:B:55:GLU:HG3	1.84	0.59
1:B:83:GLU:HB2	1:B:141:LYS:HZ2	1.66	0.58
1:C:195:PRO:O	1:C:196:ALA:CB	2.52	0.58
1:C:67:ARG:HG2	1:C:268:ALA:HB2	1.86	0.58
1:D:82:ARG:HA	1:D:110:GLY:O	2.04	0.58
1:A:401:SER:HB2	1:A:403:ASP:OD1	2.04	0.57
1:C:111:ILE:HG22	1:C:112:SER:O	2.04	0.57
1:A:453:SER:HB2	1:A:460:ALA:CB	2.34	0.57
1:A:144:LEU:HD11	1:A:186:ILE:HD13	1.86	0.57
1:B:118:VAL:HG11	1:B:166:LEU:HD22	1.87	0.57
1:B:186:ILE:HG23	1:B:228:LEU:HD22	1.87	0.57
1:A:131:LEU:HB3	1:A:179:LEU:HD12	1.87	0.57
1:A:239:ARG:HH21	1:A:239:ARG:CG	2.02	0.57
1:C:40:PRO:HD2	1:C:43:ALA:HB3	1.86	0.57
1:A:90:PRO:HG3	1:A:147:THR:HA	1.87	0.57
1:D:354:ALA:O	1:D:355:GLU:HB2	2.04	0.56
1:A:76:GLN:H	1:A:77:PRO:CD	2.15	0.56
1:C:82:ARG:HE	1:C:110:GLY:CA	2.11	0.56
1:C:76:GLN:HE21	1:C:248:LEU:HD12	1.68	0.56
1:A:525:ALA:O	1:A:529:MET:CE	2.53	0.56
1:C:401:SER:OG	1:C:403:ASP:OD1	2.17	0.56
1:C:17:PHE:O	1:C:21:VAL:HG23	2.05	0.56
1:C:175:GLY:O	1:C:178:ASP:N	2.33	0.56
1:C:351:ALA:O	1:C:355:GLU:HB2	2.05	0.56
1:A:252:GLN:OE1	1:A:263:ARG:HD3	2.05	0.56
1:B:80:ARG:CZ	1:B:245:THR:HG22	2.36	0.56
1:C:161:PRO:HG3	1:C:203:MET:CE	2.35	0.56
1:C:390:ARG:O	1:C:394:VAL:HG23	2.06	0.55
1:B:77:PRO:HG2	1:B:246:ASN:HA	1.87	0.55
1:D:405:ASP:O	1:D:406:ALA:HB2	2.07	0.55
1:A:293:VAL:HB	2:A:1501:NDP:H51N	1.88	0.55
1:B:250:GLU:OE2	1:B:517:ARG:NH2	2.38	0.55
1:A:367:VAL:CG2	1:A:384:ILE:HD12	2.37	0.55
1:D:472:GLY:HA2	1:D:505:ARG:HD2	1.89	0.55
1:C:399:CYS:O	1:C:439:ARG:NH1	2.40	0.55
1:B:90:PRO:HD2	1:B:94:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TRP:CD2	1:B:142:ALA:HB3	2.41	0.54
1:A:41:LEU:HD12	1:B:26:LEU:HD21	1.88	0.54
1:C:22:ALA:O	1:C:23:ARG:HB2	2.08	0.54
1:A:41:LEU:HA	1:A:44:THR:HB	1.90	0.54
1:A:65:ARG:NH1	1:A:493:GLU:OE1	2.39	0.53
1:A:343:VAL:HG22	2:A:1501:NDP:C2A	2.38	0.53
1:D:24:GLN:O	1:D:24:GLN:HG2	2.09	0.53
1:B:13:ALA:O	1:B:16:TRP:HB3	2.08	0.53
1:C:470:ARG:CG	1:C:470:ARG:NH2	2.58	0.53
1:C:82:ARG:HG3	1:C:110:GLY:HA2	1.90	0.53
1:B:177:ALA:O	1:B:178:ASP:C	2.47	0.53
1:D:439:ARG:NH2	1:D:445:PRO:O	2.42	0.53
1:D:240:LEU:HA	1:D:255:ILE:HD11	1.90	0.53
1:B:507:VAL:HB	1:B:508:PRO:HD3	1.89	0.53
1:C:82:ARG:NE	1:C:110:GLY:HA2	2.12	0.53
1:C:26:LEU:HD21	1:D:42:SER:HA	1.89	0.53
1:D:144:LEU:CD1	1:D:186:ILE:CD1	2.81	0.52
1:D:314:ARG:HB2	2:D:1501:NDP:O1X	2.09	0.52
1:A:108:THR:HG22	1:A:108:THR:O	2.09	0.52
1:B:87:LEU:HD12	1:B:144:LEU:O	2.09	0.52
1:B:161:PRO:HB3	1:B:203:MET:HE3	1.90	0.52
1:C:465:GLY:O	1:C:469:ARG:HG3	2.10	0.52
1:D:420:GLY:H	1:D:471:ARG:NH1	2.07	0.52
1:C:54:GLN:O	1:C:58:ARG:HG3	2.10	0.52
1:D:22:ALA:O	1:D:23:ARG:CB	2.56	0.52
1:B:271:ASN:O	1:B:272:GLN:O	2.28	0.52
1:C:488:VAL:HG13	1:C:493:GLU:HB2	1.91	0.52
1:A:82:ARG:HH11	1:A:110:GLY:HA2	1.75	0.51
1:B:73:VAL:O	1:B:73:VAL:CG2	2.58	0.51
1:D:470:ARG:NH2	1:D:470:ARG:HB3	2.25	0.51
1:A:462:GLY:HA3	1:A:464:ALA:H	1.75	0.51
1:A:324:GLU:OE1	1:A:328:GLU:OE2	2.28	0.51
1:C:49:SER:CB	1:D:21:VAL:HG13	2.35	0.51
1:D:299:ARG:HA	1:D:329:LEU:HD21	1.92	0.51
1:B:23:ARG:HA	1:B:24:GLN:CB	2.38	0.51
1:A:45:LEU:HB3	1:A:46:PRO:CD	2.41	0.51
1:C:161:PRO:HG3	1:C:203:MET:HE2	1.93	0.50
1:A:94:ILE:CD1	1:A:98:LEU:HD12	2.41	0.50
1:A:19:GLN:HB3	1:A:23:ARG:NH2	2.26	0.50
1:B:90:PRO:HD2	1:B:94:ILE:HD11	1.93	0.50
1:C:246:ASN:C	1:C:248:LEU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:CYS:O	1:D:439:ARG:NH1	2.44	0.50
1:C:70:TRP:CD1	1:C:193:ALA:HA	2.47	0.50
1:C:123:THR:N	1:C:126:GLU:OE1	2.37	0.50
1:B:470:ARG:HA	1:B:505:ARG:HH11	1.77	0.49
1:C:96:GLU:O	1:C:100:GLU:HG3	2.11	0.49
1:B:453:SER:HB2	1:B:460:ALA:CB	2.42	0.49
1:D:384:ILE:HD13	1:D:384:ILE:N	2.25	0.49
1:C:108:THR:CG2	1:C:108:THR:O	2.60	0.49
1:C:90:PRO:HG3	1:C:147:THR:HA	1.94	0.49
1:A:86:LEU:HD12	1:A:114:LEU:O	2.12	0.49
1:C:82:ARG:HG3	1:C:110:GLY:O	2.12	0.49
1:C:104:ASP:O	1:C:105:ALA:C	2.51	0.49
1:D:45:LEU:HB3	1:D:46:PRO:CD	2.38	0.49
1:D:460:ALA:O	1:D:465:GLY:CA	2.60	0.49
1:B:101:ARG:NH1	1:B:101:ARG:HG3	2.28	0.49
1:B:346:ARG:O	1:B:350:SER:OG	2.31	0.49
1:B:45:LEU:HB2	1:B:46:PRO:HD3	1.95	0.49
1:B:81:THR:HG23	1:B:82:ARG:N	2.22	0.48
1:A:45:LEU:HB3	1:A:46:PRO:HD3	1.95	0.48
1:C:30:SER:HB2	1:C:35:LEU:O	2.12	0.48
1:B:90:PRO:CG	1:B:94:ILE:CD1	2.84	0.48
1:A:30:SER:HB2	1:A:35:LEU:O	2.13	0.48
1:B:167:LEU:O	1:B:171:VAL:HG23	2.14	0.48
1:C:103:THR:O	1:C:107:ASN:HB2	2.14	0.48
1:A:397:GLU:C	1:A:398:LEU:O	2.48	0.48
1:B:355:GLU:HG2	1:B:356:PHE:CE2	2.48	0.48
1:D:460:ALA:O	1:D:465:GLY:HA2	2.14	0.48
1:C:236:VAL:O	1:C:239:ARG:HD2	2.13	0.48
1:A:218:HIS:HB3	1:A:221:ARG:HD3	1.96	0.48
1:B:272:GLN:HB3	1:B:273:PRO:HA	1.95	0.48
1:B:21:VAL:O	1:B:22:ALA:C	2.51	0.48
1:D:101:ARG:HH11	1:D:101:ARG:HG3	1.79	0.48
1:D:242:GLU:HG2	1:D:242:GLU:O	2.14	0.48
1:D:488:VAL:HG22	1:D:493:GLU:OE1	2.13	0.48
1:D:72:ARG:HH12	1:D:75:PRO:HD3	1.79	0.48
1:D:152:ARG:O	1:D:162:SER:HB3	2.14	0.48
1:B:85:TRP:HE1	1:B:141:LYS:CD	2.26	0.48
1:C:85:TRP:CD1	1:C:111:ILE:HG23	2.49	0.47
1:A:180:ARG:NH1	1:A:221:ARG:HD2	2.29	0.47
1:D:90:PRO:HG2	1:D:94:ILE:CD1	2.44	0.47
1:D:195:PRO:O	1:D:196:ALA:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TRP:HE1	1:B:141:LYS:HD2	1.79	0.47
1:B:72:ARG:HH21	1:B:258:SER:HB2	1.79	0.47
1:D:202:PRO:HB2	1:D:431:PHE:CE1	2.48	0.47
1:B:287:THR:OG1	1:B:363:HIS:HA	2.14	0.47
1:D:287:THR:HB	1:D:343:VAL:HG11	1.97	0.47
1:D:14:ALA:O	1:D:16:TRP:N	2.48	0.47
1:D:166:LEU:O	1:D:170:LEU:HB2	2.14	0.47
1:C:22:ALA:C	1:C:24:GLN:H	2.18	0.47
1:D:23:ARG:HB3	1:D:25:ASP:HB2	1.96	0.47
1:D:396:ASP:O	1:D:398:LEU:O	2.33	0.47
1:C:49:SER:HB3	1:D:21:VAL:CG1	2.37	0.46
1:A:528:ALA:C	1:A:529:MET:HG3	2.34	0.46
1:B:186:ILE:CG2	1:B:228:LEU:HD22	2.45	0.46
1:D:152:ARG:HH21	1:D:152:ARG:HB2	1.79	0.46
1:B:237:LEU:HA	1:B:237:LEU:HD22	1.78	0.46
1:B:73:VAL:O	1:B:75:PRO:HD3	2.16	0.46
1:A:396:ASP:O	1:A:398:LEU:O	2.33	0.46
1:D:156:GLU:O	1:D:156:GLU:HG3	2.14	0.46
1:A:239:ARG:O	1:A:242:GLU:HG2	2.16	0.46
1:C:293:VAL:HB	2:C:1501:NDP:H51N	1.98	0.46
1:B:484:ALA:HB1	1:B:498:ILE:CD1	2.45	0.46
1:B:85:TRP:CD1	1:B:111:ILE:HG23	2.50	0.46
1:B:36:ASP:C	1:B:38:ASP:H	2.19	0.46
1:C:75:PRO:O	1:C:76:GLN:CB	2.64	0.46
1:D:439:ARG:HD3	1:D:446:ALA:HB2	1.98	0.46
1:B:13:ALA:HB1	1:B:55:GLU:HG2	1.97	0.46
1:B:45:LEU:CB	1:B:46:PRO:CD	2.94	0.46
1:D:527:LYS:HA	1:D:527:LYS:HD3	1.76	0.46
1:A:76:GLN:N	1:A:77:PRO:HD2	2.18	0.46
1:A:462:GLY:C	1:A:464:ALA:N	2.69	0.46
1:B:161:PRO:CG	1:B:203:MET:HE3	2.46	0.45
1:A:41:LEU:HD13	1:A:41:LEU:C	2.35	0.45
1:D:272:GLN:HA	1:D:273:PRO:HA	1.60	0.45
1:C:290:LEU:HD22	1:C:319:ALA:HB3	1.98	0.45
1:C:272:GLN:CB	1:C:273:PRO:HA	2.45	0.45
1:A:507:VAL:HB	1:A:508:PRO:HD3	1.98	0.45
1:D:442:ARG:NH1	1:D:444:LEU:HD12	2.32	0.45
1:C:186:ILE:HD12	1:C:226:ILE:HB	1.99	0.45
1:B:247:GLY:O	1:B:249:ALA:N	2.50	0.45
1:D:414:ALA:O	1:D:418:GLY:HA2	2.17	0.45
1:D:25:ASP:O	1:D:29:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ILE:HG22	1:C:149:LEU:HD12	1.98	0.45
1:A:272:GLN:HB3	1:A:273:PRO:HA	1.97	0.45
1:C:411:SER:O	2:C:1501:NDP:H6N	2.17	0.45
1:B:102:LEU:HD22	1:B:240:LEU:CD2	2.47	0.45
1:A:85:TRP:CD2	1:A:142:ALA:HB3	2.51	0.45
1:D:172:LYS:O	1:D:175:GLY:N	2.50	0.45
1:A:453:SER:HB2	1:A:460:ALA:HB1	1.98	0.45
1:A:228:LEU:HD11	1:A:240:LEU:HD22	1.99	0.45
1:A:108:THR:HG23	1:A:108:THR:O	2.16	0.45
1:A:65:ARG:HH12	1:A:493:GLU:CD	2.20	0.44
1:A:398:LEU:O	1:A:399:CYS:HB2	2.18	0.44
1:C:75:PRO:O	1:C:76:GLN:HB2	2.17	0.44
1:B:85:TRP:CE2	1:B:142:ALA:HB3	2.52	0.44
1:C:266:VAL:HG12	1:C:267:PRO:O	2.18	0.44
1:D:70:TRP:CD1	1:D:193:ALA:HA	2.52	0.44
1:A:369:ARG:CZ	1:A:384:ILE:HD11	2.48	0.44
1:C:357:ASP:CG	1:C:357:ASP:O	2.55	0.44
1:A:96:GLU:O	1:A:100:GLU:HG3	2.17	0.44
1:B:94:ILE:HG12	1:B:94:ILE:H	1.61	0.44
1:A:525:ALA:O	1:A:529:MET:HE2	2.17	0.44
1:B:453:SER:HB2	1:B:460:ALA:HB2	2.00	0.44
1:C:72:ARG:HA	1:C:261:LEU:HD23	2.00	0.44
1:B:186:ILE:HD13	1:B:186:ILE:N	2.33	0.44
1:C:22:ALA:O	1:C:23:ARG:CB	2.66	0.44
1:B:378:GLN:H	1:B:378:GLN:HG3	1.35	0.44
1:B:321:GLY:O	1:B:325:LEU:HB2	2.17	0.44
1:D:94:ILE:HD13	1:D:94:ILE:N	2.33	0.44
1:C:471:ARG:O	1:C:506:PHE:HA	2.18	0.44
1:A:290:LEU:HD12	1:A:313:SER:HB2	2.00	0.44
1:A:526:ARG:O	1:A:529:MET:HE3	2.17	0.44
1:B:13:ALA:HB2	1:B:55:GLU:CG	2.47	0.44
1:C:85:TRP:CD1	1:C:111:ILE:CG2	3.01	0.44
1:C:17:PHE:HB2	1:C:51:TRP:CH2	2.52	0.44
1:C:95:GLU:H	1:C:95:GLU:HG2	1.40	0.43
1:C:77:PRO:CB	1:C:78:VAL:CA	2.95	0.43
1:C:290:LEU:HD11	1:C:338:ILE:HG23	2.00	0.43
1:A:449:ILE:HG21	1:A:451:TRP:CZ2	2.53	0.43
1:B:78:VAL:O	1:B:80:ARG:N	2.49	0.43
1:C:453:SER:OG	1:C:473:ILE:CG2	2.65	0.43
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.62	0.43
1:C:313:SER:OG	2:C:1501:NDP:P2B	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ARG:CG	1:D:469:ARG:NH2	2.65	0.43
1:C:80:ARG:CG	1:C:81:THR:H	1.94	0.43
1:A:138:ASP:HB3	1:A:139:PRO:CD	2.49	0.43
1:A:411:SER:C	1:A:450:SER:HA	2.38	0.43
1:B:219:PRO:O	1:B:220:GLU:C	2.55	0.43
1:C:104:ASP:O	1:C:107:ASN:N	2.50	0.43
1:B:398:LEU:H	1:B:398:LEU:HG	1.62	0.43
1:A:12:PRO:HG2	1:A:59:VAL:HG11	2.01	0.43
1:C:179:LEU:O	1:C:181:ILE:HD13	2.19	0.43
1:C:252:GLN:OE1	1:C:263:ARG:NH1	2.51	0.43
1:D:350:SER:O	1:D:351:ALA:C	2.57	0.43
1:C:458:GLY:O	1:C:461:ASP:HB3	2.18	0.43
1:B:30:SER:O	1:B:33:LEU:O	2.36	0.43
1:B:85:TRP:CD1	1:B:111:ILE:CG2	3.02	0.43
1:A:484:ALA:HB1	1:A:498:ILE:HD13	2.01	0.43
1:A:235:ASP:OD1	1:A:235:ASP:N	2.52	0.43
1:B:13:ALA:CB	1:B:55:GLU:CG	2.97	0.42
1:A:177:ALA:HB1	1:A:179:LEU:HG	2.00	0.42
1:D:16:TRP:HZ2	1:D:28:SER:HG	1.67	0.42
1:D:526:ARG:HG2	1:D:527:LYS:HE2	2.00	0.42
1:B:396:ASP:O	1:B:398:LEU:O	2.37	0.42
1:B:359:THR:O	1:B:360:ALA:HB2	2.19	0.42
1:C:344:THR:HG22	1:C:390:ARG:HB3	2.02	0.42
1:D:114:LEU:HD21	1:D:138:ASP:OD2	2.19	0.42
1:C:199:LEU:HB2	1:C:230:ASP:HB2	2.00	0.42
1:A:220:GLU:HG3	1:A:220:GLU:H	1.28	0.42
1:C:343:VAL:HG22	2:C:1501:NDP:C6A	2.49	0.42
1:D:403:ASP:O	1:D:404:LEU:C	2.58	0.42
1:D:237:LEU:O	1:D:240:LEU:HB3	2.19	0.42
1:B:90:PRO:HD2	1:B:94:ILE:HD12	2.02	0.42
1:C:75:PRO:HB2	1:C:76:GLN:H	1.68	0.42
1:B:16:TRP:CZ3	1:B:51:TRP:CZ2	3.07	0.41
1:A:99:VAL:HG11	1:A:115:ARG:NH2	2.34	0.41
1:D:266:VAL:HA	1:D:267:PRO:HD3	1.97	0.41
1:B:45:LEU:HD22	1:B:45:LEU:HA	1.89	0.41
1:D:401:SER:OG	1:D:403:ASP:HB2	2.19	0.41
1:A:45:LEU:HD11	1:B:29:VAL:HG21	2.01	0.41
1:B:313:SER:OG	2:B:1501:NDP:O2B	2.39	0.41
1:B:154:HIS:HB3	1:B:157:CYS:CB	2.42	0.41
1:C:275:GLY:O	1:C:276:ARG:CB	2.57	0.41
1:D:85:TRP:CD2	1:D:142:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HA	1:A:312:THR:OG1	2.21	0.41
1:D:98:LEU:HD23	1:D:98:LEU:HA	1.88	0.41
1:B:449:ILE:HG21	1:B:451:TRP:CE2	2.55	0.41
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.81	0.41
1:C:121:ALA:O	1:C:122:ALA:C	2.59	0.41
1:D:345:ASP:OD1	1:D:348:GLU:CG	2.64	0.41
1:C:381:LEU:HD12	1:C:381:LEU:HA	1.88	0.41
1:D:51:TRP:O	1:D:55:GLU:HG2	2.21	0.41
1:B:80:ARG:HG3	1:B:81:THR:H	1.81	0.41
1:B:154:HIS:CE1	1:B:156:GLU:HG2	2.56	0.41
1:B:12:PRO:CG	1:B:13:ALA:H	2.30	0.41
1:D:350:SER:HB3	1:D:398:LEU:HD22	2.03	0.41
1:C:301:LEU:HA	1:C:301:LEU:HD23	1.90	0.41
1:A:76:GLN:N	1:A:77:PRO:CD	2.81	0.41
1:B:293:VAL:O	1:B:297:VAL:HG23	2.21	0.41
1:D:369:ARG:NH1	1:D:383:GLU:OE2	2.54	0.41
1:C:452:GLY:O	2:C:1501:NDP:H42N	2.21	0.40
1:B:313:SER:OG	2:B:1501:NDP:P2B	2.79	0.40
1:B:405:ASP:OD2	1:B:405:ASP:N	2.39	0.40
1:C:286:ILE:HD11	1:C:301:LEU:HD12	2.02	0.40
1:B:70:TRP:HA	1:B:262:ALA:O	2.21	0.40
1:B:452:GLY:H	1:B:499:ALA:HB2	1.87	0.40
1:D:199:LEU:O	1:D:199:LEU:CD1	2.64	0.40
1:A:144:LEU:HD11	1:A:186:ILE:CD1	2.50	0.40
1:D:178:ASP:O	1:D:179:LEU:HD23	2.22	0.40
1:D:393:GLN:O	1:D:397:GLU:HG3	2.21	0.40
1:B:26:LEU:O	1:B:30:SER:HB2	2.22	0.40
1:B:23:ARG:CA	1:B:24:GLN:HB2	2.48	0.40
1:B:266:VAL:HG22	1:B:521:GLU:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/580 (89%)	484 (93%)	29 (6%)	5 (1%)	19	38
1	B	516/580 (89%)	470 (91%)	35 (7%)	11 (2%)	9	16
1	C	517/580 (89%)	459 (89%)	43 (8%)	15 (3%)	6	9
1	D	511/580 (88%)	469 (92%)	29 (6%)	13 (2%)	7	12
All	All	2062/2320 (89%)	1882 (91%)	136 (7%)	44 (2%)	9	16

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	GLU
1	B	272	GLN
1	B	322	ALA
1	B	360	ALA
1	C	42	SER
1	C	75	PRO
1	C	76	GLN
1	C	77	PRO
1	C	78	VAL
1	C	276	ARG
1	D	15	GLY
1	D	25	ASP
1	D	157	CYS
1	D	273	PRO
1	D	355	GLU
1	A	23	ARG
1	A	77	PRO
1	A	281	ARG
1	B	78	VAL
1	C	109	ARG
1	C	220	GLU
1	C	528	ALA
1	D	24	GLN
1	D	196	ALA
1	D	230	ASP
1	A	76	GLN
1	A	196	ALA
1	B	22	ALA
1	B	407	PHE
1	C	176	GLU
1	D	23	ARG
1	D	178	ASP
1	D	378	GLN

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	250	GLU
1	C	520	ASP
1	D	406	ALA
1	B	178	ASP
1	C	196	ALA
1	C	281	ARG
1	D	512	ALA
1	C	247	GLY
1	B	247	GLY
1	C	137	GLY

### 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	383/429 (89%)	342 (89%)	41 (11%)	8	14
1	B	381/429 (89%)	326 (86%)	55 (14%)	4	6
1	C	380/429 (89%)	340 (90%)	40 (10%)	8	15
1	D	378/429 (88%)	320 (85%)	58 (15%)	3	5
All	All	1522/1716 (89%)	1328 (87%)	194 (13%)	5	10

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	34	ASP
1	A	48	LEU
1	A	60	LEU
1	A	79	ARG
1	A	81	THR
1	A	98	LEU
1	A	108	THR
1	A	113	THR
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	132	ARG
1	A	138	ASP
1	A	156	GLU
1	A	167	LEU
1	A	168	LEU
1	A	188	ARG
1	A	199	LEU
1	A	201	ARG
1	A	210	LEU
1	A	220	GLU
1	A	228	LEU
1	A	233	ASP
1	A	235	ASP
1	A	239	ARG
1	A	257	GLN
1	A	258	SER
1	A	277	LYS
1	A	307	GLU
1	A	308	ARG
1	A	313	SER
1	A	318	GLN
1	A	343	VAL
1	A	346	ARG
1	A	353	LEU
1	A	367	VAL
1	A	369	ARG
1	A	373	LEU
1	A	390	ARG
1	A	404	LEU
1	A	467	HIS
1	A	529	MET
1	B	23	ARG
1	B	25	ASP
1	B	27	LYS
1	B	28	SER
1	B	35	LEU
1	B	45	LEU
1	B	53	ARG
1	B	55	GLU
1	B	57	GLU
1	B	94	ILE
1	B	106	LEU

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Mol	Chain	Res	Type
1	B	113	THR
1	B	114	LEU
1	B	132	ARG
1	B	141	LYS
1	B	157	CYS
1	B	158	LYS
1	B	162	SER
1	B	167	LEU
1	B	168	LEU
1	B	181	ILE
1	B	186	ILE
1	B	188	ARG
1	B	199	LEU
1	B	201	ARG
1	B	220	GLU
1	B	228	LEU
1	B	231	SER
1	B	236	VAL
1	B	237	LEU
1	B	246	ASN
1	B	257	GLN
1	B	276	ARG
1	B	277	LYS
1	B	279	ARG
1	B	318	GLN
1	B	325	LEU
1	B	337	SER
1	B	343	VAL
1	B	350	SER
1	B	352	LEU
1	B	357	ASP
1	B	358	VAL
1	B	359	THR
1	B	373	LEU
1	B	378	GLN
1	B	383	GLU
1	B	402	THR
1	B	404	LEU
1	B	405	ASP
1	B	469	ARG
1	B	480	SER
1	B	505	ARG

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Mol	Chain	Res	Type
1	B	509	THR
1	B	516	THR
1	C	33	LEU
1	C	48	LEU
1	C	49	SER
1	C	73	VAL
1	C	79	ARG
1	C	82	ARG
1	C	94	ILE
1	C	95	GLU
1	C	98	LEU
1	C	107	ASN
1	C	109	ARG
1	C	114	LEU
1	C	126	GLU
1	C	141	LYS
1	C	149	LEU
1	C	152	ARG
1	C	159	ASP
1	C	167	LEU
1	C	168	LEU
1	C	176	GLU
1	C	179	LEU
1	C	181	ILE
1	C	186	ILE
1	C	188	ARG
1	C	199	LEU
1	C	201	ARG
1	C	220	GLU
1	C	228	LEU
1	C	236	VAL
1	C	239	ARG
1	C	245	THR
1	C	271	ASN
1	C	343	VAL
1	C	346	ARG
1	C	358	VAL
1	C	370	LEU
1	C	373	LEU
1	C	404	LEU
1	C	470	ARG
1	C	509	THR

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Mol	Chain	Res	Type
1	D	19	GLN
1	D	21	VAL
1	D	24	GLN
1	D	27	LYS
1	D	31	ASP
1	D	35	LEU
1	D	36	ASP
1	D	38	ASP
1	D	41	LEU
1	D	44	THR
1	D	60	LEU
1	D	79	ARG
1	D	80	ARG
1	D	84	THR
1	D	94	ILE
1	D	98	LEU
1	D	114	LEU
1	D	129	THR
1	D	130	GLU
1	D	132	ARG
1	D	138	ASP
1	D	156	GLU
1	D	167	LEU
1	D	168	LEU
1	D	176	GLU
1	D	180	ARG
1	D	188	ARG
1	D	198	ARG
1	D	199	LEU
1	D	201	ARG
1	D	220	GLU
1	D	228	LEU
1	D	238	THR
1	D	239	ARG
1	D	257	GLN
1	D	312	THR
1	D	313	SER
1	D	318	GLN
1	D	324	GLU
1	D	325	LEU
1	D	332	LEU
1	D	337	SER

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Mol	Chain	Res	Type
1	D	348	GLU
1	D	358	VAL
1	D	367	VAL
1	D	373	LEU
1	D	378	GLN
1	D	398	LEU
1	D	401	SER
1	D	403	ASP
1	D	404	LEU
1	D	405	ASP
1	D	439	ARG
1	D	466	GLU
1	D	469	ARG
1	D	470	ARG
1	D	517	ARG
1	D	526	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NDP	A	1501	-	42,52,52	1.68	11 (26%)	55,80,80	1.74	11 (20%)
2	NDP	B	1501	-	42,52,52	1.43	8 (19%)	55,80,80	1.75	10 (18%)
2	NDP	C	1501	-	42,52,52	1.39	8 (19%)	55,80,80	1.60	9 (16%)
2	NDP	D	1501	-	42,52,52	1.34	4 (9%)	55,80,80	1.74	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	1501	-	-	0/30/77/77	0/5/5/5
2	NDP	B	1501	-	-	0/30/77/77	0/5/5/5
2	NDP	C	1501	-	-	0/30/77/77	0/5/5/5
2	NDP	D	1501	-	-	0/30/77/77	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	NDP	C4N-C5N	-3.26	1.42	1.49
2	A	1501	NDP	P2B-O2X	-3.22	1.43	1.54
2	B	1501	NDP	C4N-C5N	-3.11	1.42	1.49
2	A	1501	NDP	PN-O2N	-3.07	1.41	1.54
2	A	1501	NDP	P2B-O3X	-2.77	1.44	1.54
2	A	1501	NDP	PA-O2A	-2.69	1.43	1.54
2	A	1501	NDP	C5A-N7A	-2.60	1.30	1.39
2	B	1501	NDP	P2B-O3X	-2.54	1.45	1.54
2	D	1501	NDP	C4N-C5N	-2.53	1.43	1.49
2	C	1501	NDP	P2B-O2X	-2.46	1.45	1.54
2	C	1501	NDP	C4N-C5N	-2.40	1.43	1.49
2	C	1501	NDP	O7N-C7N	-2.35	1.18	1.24
2	A	1501	NDP	C6N-N1N	-2.33	1.30	1.37
2	B	1501	NDP	PN-O2N	-2.32	1.45	1.54
2	A	1501	NDP	O4D-C4D	-2.30	1.39	1.45
2	D	1501	NDP	P2B-O3X	-2.30	1.46	1.54
2	B	1501	NDP	PA-O2A	-2.30	1.45	1.54
2	C	1501	NDP	P2B-O3X	-2.23	1.46	1.54
2	B	1501	NDP	C6N-N1N	-2.21	1.31	1.37
2	A	1501	NDP	O7N-C7N	-2.19	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	NDP	C2D-C3D	-2.17	1.47	1.53
2	A	1501	NDP	O4B-C4B	-2.16	1.40	1.45
2	B	1501	NDP	P2B-O2X	-2.11	1.47	1.54
2	C	1501	NDP	PA-O2A	-2.11	1.45	1.54
2	C	1501	NDP	C5A-N7A	-2.10	1.32	1.39
2	A	1501	NDP	P2B-O1X	-2.05	1.44	1.51
2	B	1501	NDP	O7N-C7N	-2.03	1.19	1.24
2	D	1501	NDP	C2D-C3D	-2.01	1.47	1.53
2	C	1501	NDP	C6N-N1N	-2.00	1.31	1.37
2	C	1501	NDP	C6N-C5N	2.20	1.37	1.33
2	D	1501	NDP	C6N-C5N	2.27	1.37	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1501	NDP	N3A-C2A-N1A	-8.58	122.32	128.89
2	B	1501	NDP	N3A-C2A-N1A	-7.41	123.22	128.89
2	A	1501	NDP	N3A-C2A-N1A	-7.39	123.23	128.89
2	C	1501	NDP	N3A-C2A-N1A	-6.34	124.04	128.89
2	C	1501	NDP	C4A-C5A-N7A	-3.47	106.28	109.48
2	B	1501	NDP	O3B-C3B-C4B	-3.37	100.96	111.05
2	C	1501	NDP	O4B-C1B-C2B	-3.23	100.75	106.60
2	B	1501	NDP	C4A-C5A-N7A	-3.20	106.54	109.48
2	B	1501	NDP	PN-O3-PA	-3.05	124.17	132.73
2	A	1501	NDP	O3-PN-O5D	-2.95	95.11	102.94
2	D	1501	NDP	C4A-C5A-N7A	-2.84	106.87	109.48
2	B	1501	NDP	O3D-C3D-C2D	-2.63	103.29	111.83
2	C	1501	NDP	O2B-P2B-O1X	-2.61	100.58	107.11
2	A	1501	NDP	O5D-PN-O1N	-2.53	99.78	109.62
2	D	1501	NDP	C1B-N9A-C4A	-2.51	123.15	126.94
2	D	1501	NDP	PN-O3-PA	-2.51	125.67	132.73
2	A	1501	NDP	C4B-O4B-C1B	-2.48	107.00	109.72
2	B	1501	NDP	C1B-N9A-C4A	-2.46	123.23	126.94
2	B	1501	NDP	O2B-P2B-O1X	-2.40	101.11	107.11
2	A	1501	NDP	C4A-C5A-N7A	-2.24	107.42	109.48
2	C	1501	NDP	O3D-C3D-C2D	-2.21	104.64	111.83
2	B	1501	NDP	O5D-PN-O1N	-2.20	101.08	109.62
2	C	1501	NDP	O3B-C3B-C4B	-2.18	104.51	111.05
2	A	1501	NDP	O3D-C3D-C2D	-2.14	104.86	111.83
2	B	1501	NDP	C2B-C3B-C4B	2.01	106.62	101.85
2	A	1501	NDP	C2B-C3B-C4B	2.06	106.73	101.85
2	A	1501	NDP	N6A-C6A-N1A	2.10	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1501	NDP	O3-PA-O5B	2.13	108.58	102.94
2	A	1501	NDP	C2A-N1A-C6A	2.31	122.89	118.77
2	D	1501	NDP	O2N-PN-O1N	2.32	125.08	112.53
2	C	1501	NDP	O2N-PN-O1N	2.32	125.12	112.53
2	C	1501	NDP	O3X-P2B-O2X	2.53	117.03	107.38
2	C	1501	NDP	O4B-C1B-N9A	2.60	113.54	108.10
2	A	1501	NDP	O4B-C1B-N9A	2.92	114.21	108.10
2	A	1501	NDP	P2B-O2B-C2B	3.15	129.12	121.56
2	B	1501	NDP	O4B-C1B-N9A	3.19	114.77	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	NDP	3	0
2	B	1501	NDP	2	0
2	C	1501	NDP	7	0
2	D	1501	NDP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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	520/580 (89%)	0.03	8 (1%) 76 73	26, 46, 78, 137	0
1	B	518/580 (89%)	0.51	44 (8%) 13 10	34, 63, 98, 155	0
1	C	519/580 (89%)	0.36	30 (5%) 26 22	40, 67, 103, 139	0
1	D	515/580 (88%)	0.62	55 (10%) 8 5	40, 68, 103, 135	0
All	All	2072/2320 (89%)	0.38	137 (6%) 22 17	26, 61, 100, 155	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	MET	6.8
1	D	325	LEU	5.9
1	D	309	ILE	5.3
1	C	78	VAL	5.0
1	D	320	ALA	4.7
1	C	22	ALA	4.4
1	C	76	GLN	4.1
1	B	302	ALA	4.1
1	C	82	ARG	4.1
1	D	81	THR	4.1
1	D	529	MET	4.1
1	D	327	ALA	4.0
1	C	77	PRO	3.9
1	D	79	ARG	3.8
1	C	29	VAL	3.8
1	B	78	VAL	3.8
1	D	338	ILE	3.7
1	D	80	ARG	3.7
1	C	139	PRO	3.7
1	B	527	LYS	3.7
1	C	75	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	283	SER	3.6
1	B	325	LEU	3.6
1	A	80	ARG	3.6
1	B	76	GLN	3.5
1	D	527	LYS	3.5
1	B	319	ALA	3.5
1	D	457	GLY	3.5
1	B	322	ALA	3.4
1	D	82	ARG	3.4
1	B	323	ALA	3.4
1	D	311	LEU	3.4
1	D	301	LEU	3.4
1	A	155	PRO	3.4
1	D	33	LEU	3.3
1	B	329	LEU	3.3
1	D	179	LEU	3.3
1	A	82	ARG	3.3
1	C	141	LYS	3.3
1	C	285	LEU	3.3
1	A	81	THR	3.2
1	D	331	ALA	3.2
1	D	290	LEU	3.2
1	A	248	LEU	3.2
1	D	284	ALA	3.2
1	B	334	ALA	3.1
1	B	335	GLN	3.1
1	C	356	PHE	3.1
1	D	109	ARG	3.1
1	B	79	ARG	3.1
1	C	79	ARG	3.0
1	D	323	ALA	3.0
1	B	327	ALA	3.0
1	B	331	ALA	3.0
1	B	318	GLN	2.9
1	D	337	SER	2.9
1	D	135	ALA	2.9
1	D	285	LEU	2.9
1	B	320	ALA	2.9
1	C	353	LEU	2.9
1	B	75	PRO	2.8
1	B	77	PRO	2.8
1	C	351	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.8
1	C	23	ARG	2.8
1	D	312	THR	2.7
1	C	12	PRO	2.7
1	C	80	ARG	2.7
1	C	156	GLU	2.7
1	C	20	ALA	2.7
1	C	106	LEU	2.7
1	D	329	LEU	2.7
1	B	290	LEU	2.7
1	B	23	ARG	2.7
1	B	336	VAL	2.7
1	D	310	VAL	2.6
1	B	330	ARG	2.6
1	D	356	PHE	2.6
1	D	464	ALA	2.6
1	D	299	ARG	2.6
1	D	294	GLY	2.6
1	D	137	GLY	2.5
1	B	179	LEU	2.5
1	B	81	THR	2.5
1	B	308	ARG	2.5
1	C	81	THR	2.5
1	B	324	GLU	2.5
1	B	181	ILE	2.5
1	D	17	PHE	2.5
1	B	140	VAL	2.5
1	D	138	ASP	2.5
1	B	326	GLU	2.5
1	B	114	LEU	2.4
1	D	48	LEU	2.4
1	D	324	GLU	2.4
1	A	79	ARG	2.4
1	D	24	GLN	2.4
1	B	301	LEU	2.4
1	D	140	VAL	2.4
1	D	306	ALA	2.4
1	D	75	PRO	2.4
1	D	156	GLU	2.4
1	C	404	LEU	2.4
1	D	53	ARG	2.3
1	D	322	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	2.3
1	C	361	VAL	2.3
1	C	354	ALA	2.3
1	B	104	ASP	2.2
1	D	343	VAL	2.2
1	C	56	ARG	2.2
1	B	249	ALA	2.2
1	D	50	VAL	2.2
1	D	181	ILE	2.2
1	C	352	LEU	2.2
1	B	269	PRO	2.2
1	D	281	ARG	2.2
1	C	527	LYS	2.2
1	B	338	ILE	2.2
1	B	332	LEU	2.2
1	B	526	ARG	2.2
1	A	77	PRO	2.2
1	D	59	VAL	2.1
1	C	15	GLY	2.1
1	D	83	GLU	2.1
1	C	109	ARG	2.1
1	D	86	LEU	2.1
1	B	247	GLY	2.1
1	D	29	VAL	2.1
1	B	135	ALA	2.0
1	B	315	ARG	2.0
1	D	295	ALA	2.0
1	B	279	ARG	2.0
1	B	328	GLU	2.0
1	D	330	ARG	2.0
1	D	114	LEU	2.0
1	D	18	TRP	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	A	1501	48/48	0.98	0.13	-0.41	22,34,39,46	0
2	NDP	B	1501	48/48	0.95	0.12	-0.74	40,53,69,73	0
2	NDP	C	1501	48/48	0.96	0.11	-0.88	42,54,64,74	0
2	NDP	D	1501	48/48	0.95	0.12	-0.91	39,61,85,97	0

## 6.5 Other polymers

There are no such residues in this entry.