



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 PM GMT

PDB ID : 4OHF  
Title : Crystal structure of cytosolic nucleotidase II (LPG0095) in complex with GMP from Legionella pneumophila, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET LGR1  
Authors : Srinivisan, B.; Forouhar, F.; Shukla, A.; Sampangi, C.; Kulkarni, S.; Abashidze, M.; Seetharaman, J.; Lew, S.; Mao, L.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.M.; Tong, L.; Balaram, H.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2014-01-17  
Resolution : 2.53 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

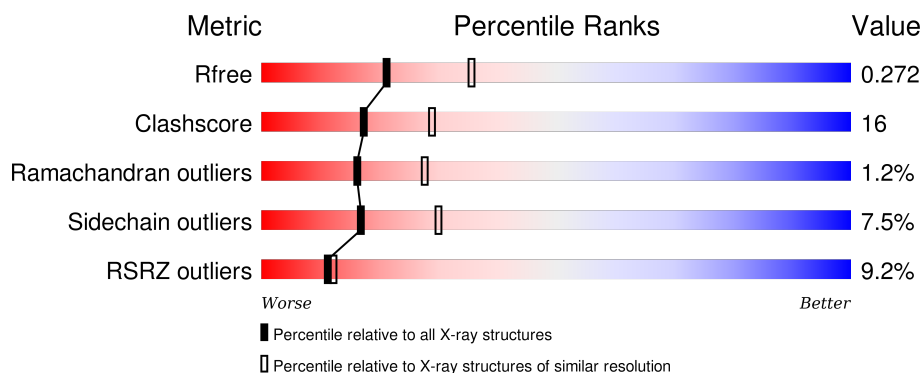
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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	470	<div> <div>10%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
1	B	470	<div> <div>6%</div> <div>65%</div> <div>29%</div> <div>• •</div> </div>
1	C	470	<div> <div>10%</div> <div>57%</div> <div>33%</div> <div>• 7%</div> </div>
1	D	470	<div> <div>9%</div> <div>67%</div> <div>26%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15143 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 Cytosolic IMP-GMP specific 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3736	2405	628	690	13			
1	B	458	Total	C	N	O	S	0	0	0
			3752	2412	630	697	13			
1	C	438	Total	C	N	O	S	0	0	0
			3594	2319	605	658	12			
1	D	456	Total	C	N	O	S	0	0	0
			3742	2405	631	693	13			

There are 44 discrepancies between the modelled and reference sequences:

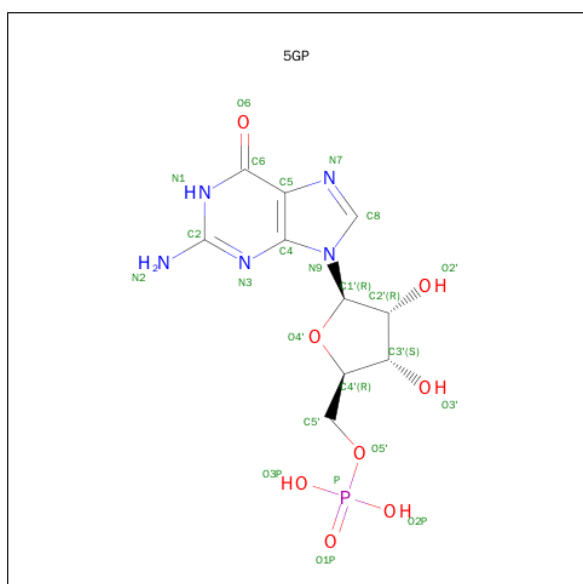
Chain	Residue	Modelled	Actual	Comment	Reference
A	459A	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
A	459B	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
A	459C	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
A	460	LEU	-	EXPRESSION TAG	UNP Q5ZZB6
A	461	GLU	-	EXPRESSION TAG	UNP Q5ZZB6
A	462	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
A	463	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
A	464	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
A	465	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
A	466	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
A	467	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
B	460	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
B	461	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
B	462	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
B	463	LEU	-	EXPRESSION TAG	UNP Q5ZZB6
B	464	GLU	-	EXPRESSION TAG	UNP Q5ZZB6
B	465	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
B	466	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
B	467	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
B	468	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
B	469	HIS	-	EXPRESSION TAG	UNP Q5ZZB6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	460	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
C	461	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
C	462	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
C	463	LEU	-	EXPRESSION TAG	UNP Q5ZZB6
C	464	GLU	-	EXPRESSION TAG	UNP Q5ZZB6
C	465	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	466	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	467	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	468	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	469	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
C	470	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	460	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
D	461	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
D	462	ALA	-	EXPRESSION TAG	UNP Q5ZZB6
D	463	LEU	-	EXPRESSION TAG	UNP Q5ZZB6
D	464	GLU	-	EXPRESSION TAG	UNP Q5ZZB6
D	465	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	466	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	467	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	468	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	469	HIS	-	EXPRESSION TAG	UNP Q5ZZB6
D	470	HIS	-	EXPRESSION TAG	UNP Q5ZZB6

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

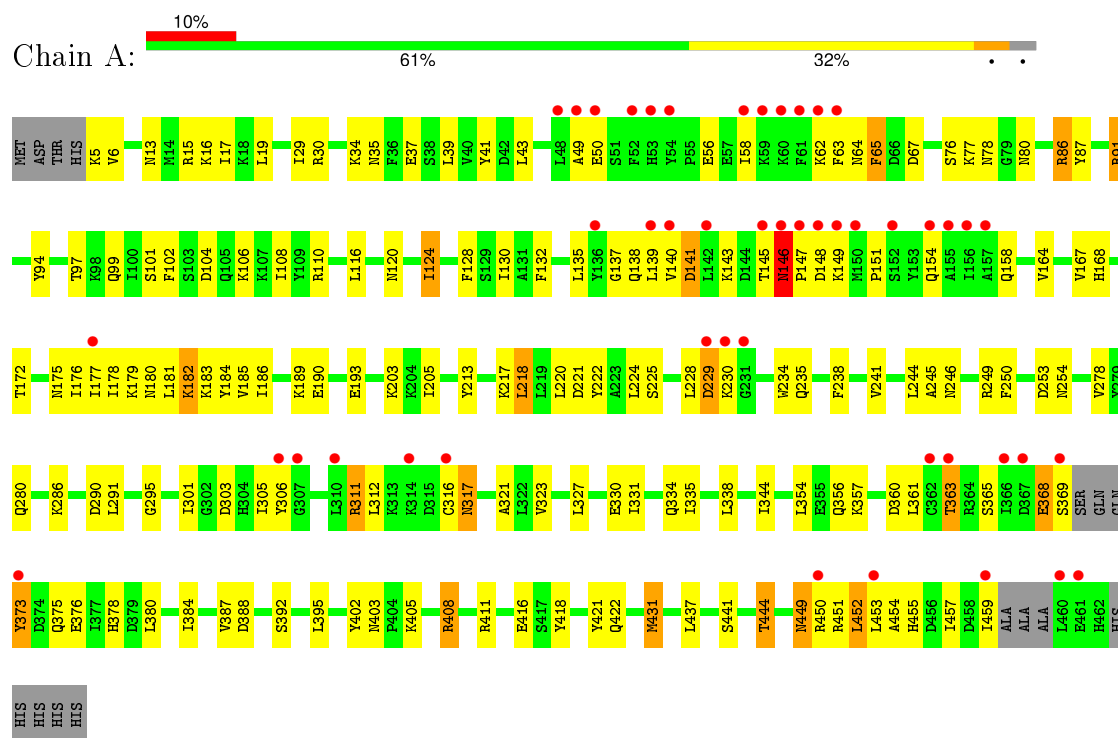
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	67	Total O 67 67	0	0
5	C	48	Total O 48 48	0	0
5	D	58	Total O 58 58	0	0

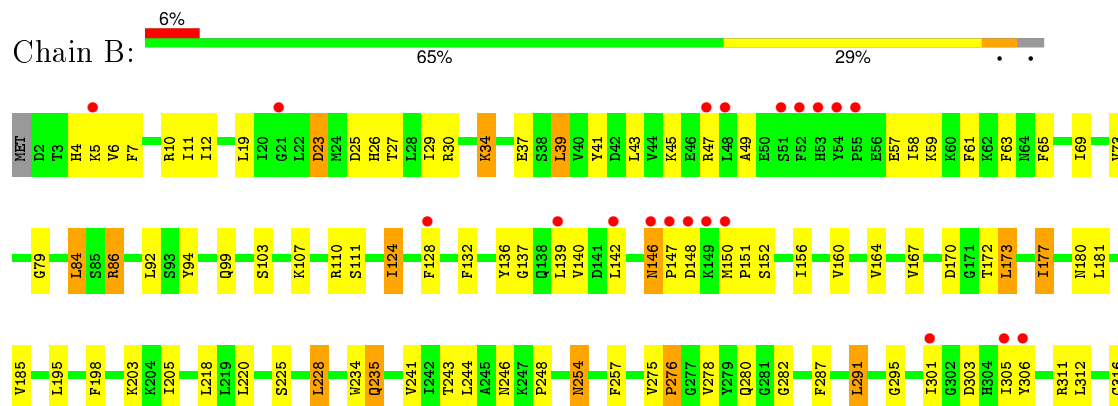
### 3 Residue-property plots [i](#)

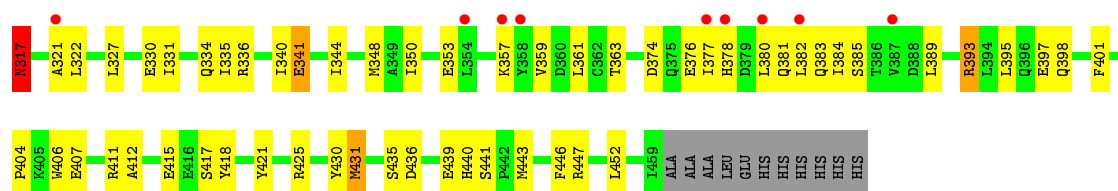
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cytosolic IMP-GMP specific 5'-nucleotidase

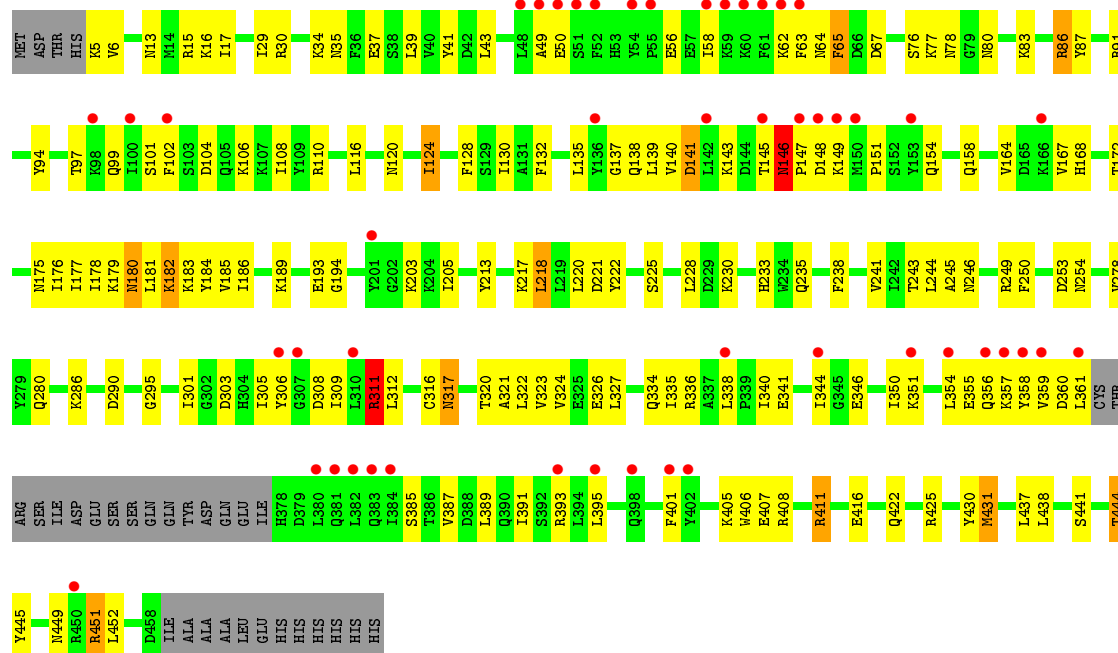


- Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase

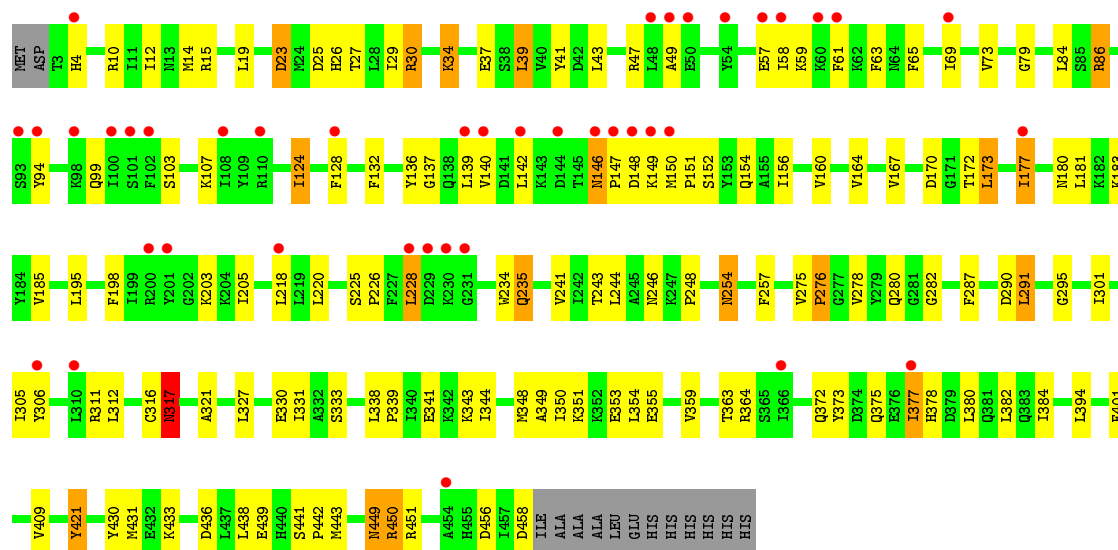




• Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase



• Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.33Å 92.72Å 161.89Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	44.70 – 2.53 44.70 – 2.53	Depositor EDS
% Data completeness (in resolution range)	92.8 (44.70-2.53) 92.9 (44.70-2.53)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.54Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.231 , 0.272 0.231 , 0.272	Depositor DCC
$R_{free}$ test set	6753 reflections (9.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 76184 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: PO4, 5GP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/3814	0.80	11/5139 (0.2%)
1	B	0.41	0/3831	0.61	0/5165
1	C	0.39	0/3670	0.81	11/4944 (0.2%)
1	D	0.40	0/3821	0.62	0/5150
All	All	0.40	0/15136	0.71	22/20398 (0.1%)

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	D	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	ARG	NE-CZ-NH2	-14.53	113.04	120.30
1	A	91	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	411	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	C	411	ARG	NE-CZ-NH1	13.61	127.11	120.30
1	C	311	ARG	NE-CZ-NH1	-13.48	113.56	120.30
1	A	91	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	311	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	C	91	ARG	NE-CZ-NH1	-12.91	113.85	120.30
1	C	311	ARG	NE-CZ-NH2	12.87	126.74	120.30
1	A	311	ARG	NE-CZ-NH1	12.63	126.62	120.30
1	A	411	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	C	91	ARG	NE-CZ-NH2	11.97	126.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	249	ARG	NE-CZ-NH1	-11.11	114.75	120.30
1	A	249	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	C	249	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	C	411	ARG	CD-NE-CZ	7.12	133.57	123.60
1	A	91	ARG	CD-NE-CZ	6.58	132.82	123.60
1	C	311	ARG	CD-NE-CZ	6.46	132.64	123.60
1	A	311	ARG	CD-NE-CZ	6.44	132.61	123.60
1	C	91	ARG	CD-NE-CZ	6.21	132.30	123.60
1	A	411	ARG	CD-NE-CZ	6.06	132.09	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	421	TYR	Sidechain

## 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	3736	0	3739	135	0
1	B	3752	0	3744	114	0
1	C	3594	0	3610	131	0
1	D	3742	0	3740	112	0
2	A	24	0	12	0	0
2	C	24	0	12	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	55	0	0	2	0
5	B	67	0	0	3	0
5	C	48	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	58	0	0	3	0
All	All	15143	0	14857	480	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 16.

All (480) 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:A:441:SER:O	1:A:444:THR:HG22	1.58	1.02
1:C:441:SER:O	1:C:444:THR:HG22	1.59	1.01
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.29	0.96
1:B:311:ARG:HG3	1:B:311:ARG:HH11	1.29	0.95
1:B:235:GLN:HE21	1:B:235:GLN:H	0.98	0.94
1:D:235:GLN:H	1:D:235:GLN:HE21	1.00	0.93
1:D:235:GLN:H	1:D:235:GLN:NE2	1.69	0.89
1:B:235:GLN:NE2	1:B:235:GLN:H	1.70	0.89
1:C:334:GLN:HE22	1:D:456:ASP:HA	1.39	0.87
1:C:305:ILE:HD13	1:C:422:GLN:HB3	1.56	0.85
1:A:13:ASN:HD22	1:A:16:LYS:HD3	1.44	0.83
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.44	0.81
1:C:83:LYS:HZ2	1:C:407:GLU:HG3	1.43	0.81
1:C:13:ASN:HD22	1:C:16:LYS:HD3	1.44	0.80
1:A:189:LYS:HE2	1:A:193:GLU:OE1	1.82	0.79
1:C:189:LYS:HE2	1:C:193:GLU:OE1	1.81	0.79
1:A:230:LYS:HD2	1:A:230:LYS:H	1.48	0.78
1:C:83:LYS:NZ	1:C:407:GLU:HG3	1.98	0.77
1:D:235:GLN:HE21	1:D:235:GLN:N	1.81	0.76
1:B:235:GLN:HE21	1:B:235:GLN:N	1.80	0.76
1:A:241:VAL:CG1	1:A:278:VAL:HG22	2.17	0.74
1:B:49:ALA:HB2	1:B:58:ILE:HD11	1.70	0.74
1:C:241:VAL:CG1	1:C:278:VAL:HG22	2.18	0.73
1:B:359:VAL:O	1:B:363:THR:HG23	1.89	0.73
1:C:387:VAL:O	1:C:391:ILE:HG12	1.88	0.73
1:C:64:ASN:HB3	1:C:67:ASP:OD2	1.89	0.73
1:A:357:LYS:O	1:A:361:LEU:HD13	1.90	0.72
1:A:230:LYS:HD2	1:A:230:LYS:N	2.05	0.72
1:C:360:ASP:O	1:C:361:LEU:HD23	1.88	0.71
1:D:49:ALA:HB2	1:D:58:ILE:HD11	1.71	0.71
1:A:64:ASN:HB3	1:A:67:ASP:OD2	1.90	0.70
1:A:441:SER:OG	1:B:363:THR:HG21	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HD11	1:A:220:LEU:HD23	1.74	0.70
1:C:29:ILE:HD11	1:C:220:LEU:HD23	1.72	0.70
1:A:327:LEU:O	1:A:331:ILE:HG12	1.92	0.70
1:A:305:ILE:HD13	1:A:422:GLN:HB3	1.73	0.69
1:A:334:GLN:HG2	1:A:402:TYR:OH	1.91	0.69
1:C:451:ARG:H	1:C:451:ARG:NE	1.89	0.69
1:D:449:ASN:HD22	1:D:449:ASN:N	1.90	0.69
1:B:124:ILE:H	1:B:124:ILE:HD12	1.58	0.68
1:D:248:PRO:HB3	1:D:306:TYR:HB3	1.75	0.68
1:A:124:ILE:H	1:A:124:ILE:HD12	1.59	0.68
1:C:30:ARG:HH11	1:C:30:ARG:HG2	1.58	0.68
1:C:124:ILE:HD12	1:C:124:ILE:H	1.58	0.68
1:D:311:ARG:NH1	1:D:311:ARG:HG3	2.05	0.67
1:D:449:ASN:H	1:D:449:ASN:ND2	1.93	0.67
1:A:30:ARG:CZ	1:A:186:ILE:HD11	2.25	0.67
1:B:248:PRO:HB3	1:B:306:TYR:HB3	1.76	0.67
1:A:360:ASP:O	1:A:363:THR:HG22	1.94	0.67
1:D:124:ILE:H	1:D:124:ILE:HD12	1.59	0.66
1:A:13:ASN:ND2	1:A:16:LYS:HD3	2.10	0.66
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.60	0.66
1:C:13:ASN:ND2	1:C:16:LYS:HD3	2.11	0.66
1:A:49:ALA:HB2	1:A:58:ILE:HD11	1.78	0.65
1:D:241:VAL:CG1	1:D:278:VAL:HG22	2.26	0.65
1:C:86:ARG:HD2	1:C:87:TYR:CZ	2.31	0.65
1:C:451:ARG:HD2	1:C:451:ARG:O	1.96	0.65
1:C:449:ASN:O	1:C:451:ARG:NH1	2.30	0.65
1:C:30:ARG:CZ	1:C:186:ILE:HD11	2.27	0.65
1:C:336:ARG:HB3	1:C:401:PHE:HD2	1.61	0.65
1:C:49:ALA:HB2	1:C:58:ILE:HD11	1.77	0.65
1:D:128:PHE:CD1	1:D:164:VAL:HG11	2.32	0.65
1:D:339:PRO:O	1:D:343:LYS:HG2	1.97	0.64
1:C:295:GLY:HA3	1:C:317:ASN:HD21	1.62	0.64
1:A:330:GLU:O	1:A:334:GLN:HG3	1.96	0.64
1:D:61:PHE:HE1	1:D:139:LEU:HD23	1.63	0.64
1:C:182:LYS:HB3	1:C:182:LYS:NZ	2.12	0.64
1:A:228:LEU:HD21	1:A:234:TRP:HA	1.80	0.64
1:B:311:ARG:HG3	1:B:311:ARG:NH1	2.06	0.64
1:D:330:GLU:HG2	5:D:627:HOH:O	1.97	0.64
1:B:61:PHE:HE1	1:B:139:LEU:HD23	1.62	0.64
1:A:77:LYS:HB2	1:A:120:ASN:OD1	1.98	0.64
1:A:30:ARG:NH2	1:A:186:ILE:HD11	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLY:HA3	1:A:317:ASN:HD21	1.63	0.63
1:A:86:ARG:HD2	1:A:87:TYR:CZ	2.33	0.63
1:B:241:VAL:CG1	1:B:278:VAL:HG22	2.29	0.63
1:B:128:PHE:CD1	1:B:164:VAL:HG11	2.34	0.63
1:A:6:VAL:HG13	1:A:431:MET:HE3	1.81	0.63
1:D:142:LEU:HD12	1:D:150:MET:SD	2.39	0.63
1:D:350:ILE:O	1:D:354:LEU:HD23	1.98	0.63
1:D:449:ASN:HD22	1:D:449:ASN:H	1.44	0.62
1:A:17:ILE:O	1:A:203:LYS:HE3	1.99	0.62
1:A:182:LYS:HB3	1:A:182:LYS:NZ	2.14	0.62
1:D:442:PRO:O	1:D:443:MET:HE2	1.99	0.62
1:B:377:ILE:HD12	1:B:378:HIS:N	2.14	0.62
1:D:225:SER:HA	1:D:228:LEU:HD22	1.82	0.62
1:D:344:ILE:O	1:D:348:MET:HG3	1.99	0.62
1:A:178:ILE:HD11	1:A:218:LEU:HB3	1.82	0.62
1:D:244:LEU:HB2	1:D:280:GLN:HG3	1.82	0.61
1:B:225:SER:HA	1:B:228:LEU:HD22	1.81	0.61
1:B:142:LEU:HD12	1:B:150:MET:SD	2.41	0.61
1:B:311:ARG:HH11	1:B:311:ARG:CG	2.09	0.61
1:C:77:LYS:HB2	1:C:120:ASN:OD1	1.99	0.61
1:A:380:LEU:O	1:A:384:ILE:HG12	2.00	0.61
1:C:6:VAL:HG13	1:C:431:MET:HE3	1.82	0.60
1:C:41:TYR:CE1	1:C:63:PHE:HB2	2.36	0.60
1:A:295:GLY:HA3	1:A:317:ASN:ND2	2.17	0.60
1:C:17:ILE:O	1:C:203:LYS:HE3	2.00	0.60
1:C:178:ILE:HD11	1:C:218:LEU:HB3	1.83	0.60
1:B:327:LEU:O	1:B:331:ILE:HG12	2.01	0.60
1:C:30:ARG:NH2	1:C:186:ILE:HD11	2.16	0.60
1:C:6:VAL:HG22	1:C:431:MET:HE2	1.84	0.60
1:B:317:ASN:HD22	1:B:317:ASN:C	2.05	0.59
1:A:41:TYR:CE1	1:A:63:PHE:HB2	2.37	0.59
1:C:225:SER:HA	1:C:228:LEU:HD22	1.83	0.59
1:B:295:GLY:HA3	1:B:317:ASN:HD21	1.67	0.59
1:D:195:LEU:HD22	1:D:205:ILE:HD13	1.84	0.59
1:C:305:ILE:HD13	1:C:422:GLN:CB	2.31	0.59
1:A:286:LYS:NZ	1:A:290:ASP:OD2	2.36	0.59
1:C:140:VAL:HA	1:C:143:LYS:HB3	1.85	0.59
1:C:295:GLY:HA3	1:C:317:ASN:ND2	2.17	0.59
1:C:336:ARG:HB3	1:C:401:PHE:CD2	2.38	0.59
1:C:301:ILE:HG12	1:C:321:ALA:HB3	1.85	0.59
1:D:359:VAL:O	1:D:363:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLY:HA3	1:D:317:ASN:HD21	1.68	0.58
1:D:327:LEU:O	1:D:331:ILE:HG12	2.02	0.58
1:C:451:ARG:H	1:C:451:ARG:CZ	2.16	0.58
1:A:241:VAL:HG13	1:A:278:VAL:HG22	1.85	0.58
1:A:454:ALA:O	1:A:457:ILE:HG23	2.03	0.58
1:C:241:VAL:HG13	1:C:278:VAL:HG22	1.86	0.58
1:A:205:ILE:HG22	1:A:238:PHE:HD1	1.68	0.57
1:A:175:ASN:O	1:A:178:ILE:HG22	2.05	0.57
1:B:374:ASP:O	1:B:377:ILE:HG13	2.04	0.57
1:B:336:ARG:O	1:B:401:PHE:CE2	2.57	0.57
1:B:195:LEU:HD22	1:B:205:ILE:HD13	1.86	0.57
1:A:451:ARG:CG	1:A:451:ARG:HH11	2.17	0.57
1:B:317:ASN:ND2	1:B:317:ASN:C	2.58	0.57
1:D:317:ASN:HD22	1:D:317:ASN:C	2.08	0.57
1:B:244:LEU:HB2	1:B:280:GLN:HG3	1.87	0.57
1:C:309:ILE:HG21	1:C:425:ARG:CG	2.34	0.57
1:C:221:ASP:O	1:C:225:SER:HB2	2.05	0.56
1:A:143:LYS:O	1:A:143:LYS:HD2	2.04	0.56
1:D:29:ILE:HD11	1:D:220:LEU:HD23	1.87	0.56
1:A:35:ASN:HD22	1:A:183:LYS:HG2	1.70	0.56
1:C:35:ASN:HD22	1:C:183:LYS:HG2	1.70	0.56
1:A:451:ARG:NH1	1:A:451:ARG:HG3	2.18	0.56
1:A:140:VAL:HA	1:A:143:LYS:HB3	1.87	0.56
1:B:254:ASN:H	1:B:254:ASN:HD22	1.53	0.56
1:D:449:ASN:N	1:D:449:ASN:ND2	2.52	0.56
1:C:175:ASN:O	1:C:178:ILE:HG22	2.06	0.56
1:D:4:HIS:HB3	1:D:436:ASP:HA	1.88	0.56
1:D:39:LEU:HD22	1:D:43:LEU:HG	1.88	0.55
1:B:344:ILE:HD13	1:B:395:LEU:HD23	1.87	0.55
1:B:406:TRP:O	1:B:407:GLU:HB2	2.05	0.55
1:D:311:ARG:CG	1:D:311:ARG:HH11	2.08	0.55
1:D:354:LEU:HB3	1:D:384:ILE:CG1	2.37	0.55
1:C:177:ILE:HG22	1:C:184:TYR:CD2	2.42	0.55
1:D:317:ASN:ND2	1:D:317:ASN:C	2.60	0.55
1:D:235:GLN:NE2	1:D:235:GLN:N	2.49	0.55
1:D:73:VAL:HG21	1:D:84:LEU:HD22	1.88	0.55
1:C:94:TYR:CE2	1:C:405:LYS:HE3	2.41	0.55
1:C:143:LYS:O	1:C:143:LYS:HD2	2.07	0.55
1:C:180:ASN:HB2	5:C:621:HOH:O	2.05	0.54
1:B:73:VAL:HG21	1:B:84:LEU:HD22	1.89	0.54
1:D:373:TYR:O	1:D:377:ILE:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLU:HG3	1:D:65:PHE:HE2	1.72	0.54
1:B:39:LEU:HD22	1:B:43:LEU:HG	1.89	0.54
1:B:34:LYS:NZ	1:B:34:LYS:HB3	2.22	0.54
1:D:441:SER:C	1:D:443:MET:H	2.09	0.54
1:A:408:ARG:HH21	1:A:408:ARG:HG2	1.73	0.54
1:C:451:ARG:C	1:C:452:LEU:HD12	2.27	0.54
1:D:128:PHE:CE1	1:D:164:VAL:HG11	2.42	0.54
1:A:441:SER:CB	1:B:363:THR:HG21	2.38	0.54
1:C:335:ILE:O	1:C:338:LEU:HB2	2.07	0.54
1:B:37:GLU:HG3	1:B:65:PHE:HE2	1.71	0.54
1:A:102:PHE:HB3	5:A:641:HOH:O	2.07	0.54
1:C:286:LYS:NZ	1:C:290:ASP:OD2	2.40	0.54
1:D:301:ILE:HG12	1:D:321:ALA:HB3	1.89	0.53
1:A:221:ASP:O	1:A:225:SER:HB2	2.08	0.53
1:C:351:LYS:O	1:C:355:GLU:HB2	2.08	0.53
1:D:341:GLU:O	1:D:344:ILE:HG13	2.09	0.53
1:A:177:ILE:HG22	1:A:184:TYR:CD2	2.44	0.53
1:D:137:GLY:O	1:D:140:VAL:HG22	2.09	0.53
1:C:205:ILE:HD12	1:C:205:ILE:N	2.23	0.53
1:B:146:ASN:O	1:B:148:ASP:N	2.38	0.53
1:D:254:ASN:HD22	1:D:254:ASN:H	1.55	0.53
1:A:138:GLN:HA	1:A:141:ASP:HB2	1.92	0.52
1:A:301:ILE:HG12	1:A:321:ALA:HB3	1.90	0.52
1:A:354:LEU:HB3	1:A:384:ILE:HD11	1.90	0.52
1:B:94:TYR:CE2	1:B:99:GLN:HB2	2.44	0.52
1:B:128:PHE:CE1	1:B:164:VAL:HG11	2.43	0.52
1:D:344:ILE:HG22	1:D:394:LEU:HB3	1.90	0.52
1:B:4:HIS:HD1	1:B:436:ASP:HA	1.75	0.52
1:C:205:ILE:HG22	1:C:238:PHE:HD1	1.75	0.52
1:A:452:LEU:HA	1:A:455:HIS:HB3	1.92	0.52
1:C:244:LEU:HB2	1:C:280:GLN:HG3	1.91	0.52
1:C:316:CYS:O	1:C:317:ASN:HB3	2.08	0.52
1:D:34:LYS:HB3	1:D:34:LYS:NZ	2.25	0.52
1:D:86:ARG:HB2	1:D:421:TYR:HB2	1.92	0.51
1:B:124:ILE:N	1:B:124:ILE:HD12	2.24	0.51
1:B:146:ASN:HD22	1:B:146:ASN:C	2.13	0.51
1:B:322:LEU:O	1:B:430:TYR:HA	2.11	0.51
1:C:182:LYS:HZ2	1:C:182:LYS:HB3	1.76	0.51
1:C:309:ILE:HG21	1:C:425:ARG:HG2	1.93	0.51
1:A:94:TYR:CE2	1:A:405:LYS:HE3	2.46	0.51
1:D:164:VAL:O	1:D:167:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLN:NE2	1:B:235:GLN:N	2.50	0.51
1:D:124:ILE:HD12	1:D:124:ILE:N	2.25	0.51
1:B:331:ILE:O	1:B:335:ILE:HG13	2.10	0.50
1:C:146:ASN:HD21	1:C:148:ASP:HB2	1.76	0.50
1:A:354:LEU:HB3	1:A:384:ILE:CD1	2.41	0.50
1:D:295:GLY:HA3	1:D:317:ASN:ND2	2.26	0.50
1:C:138:GLN:HA	1:C:141:ASP:HB2	1.93	0.50
1:A:146:ASN:HD21	1:A:148:ASP:HB2	1.77	0.50
1:B:137:GLY:O	1:B:140:VAL:HG22	2.11	0.50
1:A:172:THR:O	1:A:176:ILE:HG12	2.11	0.50
1:C:172:THR:O	1:C:176:ILE:HG12	2.11	0.50
1:D:275:VAL:O	1:D:276:PRO:C	2.50	0.50
1:A:408:ARG:NH2	1:A:408:ARG:HG2	2.26	0.50
1:A:178:ILE:HG12	1:A:218:LEU:HD23	1.93	0.50
1:C:177:ILE:O	1:C:181:LEU:HD23	2.12	0.50
1:B:295:GLY:HA3	1:B:317:ASN:ND2	2.25	0.50
1:A:365:SER:O	1:A:369:SER:HA	2.12	0.50
1:B:441:SER:C	1:B:443:MET:H	2.16	0.50
1:B:301:ILE:HG12	1:B:321:ALA:HB3	1.93	0.50
1:A:86:ARG:HA	1:A:418:TYR:HA	1.94	0.49
1:C:244:LEU:HD12	1:C:280:GLN:CD	2.33	0.49
1:B:29:ILE:HD11	1:B:220:LEU:HD23	1.93	0.49
1:B:198:PHE:O	1:B:203:LYS:HB2	2.12	0.49
1:A:244:LEU:HB2	1:A:280:GLN:HG3	1.93	0.49
1:B:311:ARG:NH1	1:B:311:ARG:CG	2.71	0.49
1:D:241:VAL:HG11	1:D:278:VAL:HG22	1.93	0.49
1:A:6:VAL:HG22	1:A:431:MET:HE2	1.93	0.49
1:D:146:ASN:C	1:D:146:ASN:HD22	2.16	0.49
1:A:177:ILE:O	1:A:181:LEU:HD23	2.12	0.49
1:C:309:ILE:HG21	1:C:425:ARG:HG3	1.94	0.49
1:A:450:ARG:O	1:A:453:LEU:HB3	2.12	0.49
1:A:331:ILE:HG22	1:A:335:ILE:HD13	1.93	0.49
1:B:164:VAL:O	1:B:167:VAL:HG12	2.12	0.49
1:D:4:HIS:CD2	1:D:439:GLU:HG3	2.48	0.49
1:A:37:GLU:OE1	1:A:130:ILE:HB	2.12	0.49
1:C:37:GLU:OE1	1:C:130:ILE:HB	2.12	0.49
1:C:178:ILE:HG12	1:C:218:LEU:HD23	1.95	0.49
1:B:92:LEU:HD11	1:B:406:TRP:CE3	2.47	0.49
1:B:23:ASP:O	1:B:27:THR:HB	2.13	0.49
1:B:412:ALA:HB2	1:B:417:SER:HA	1.94	0.49
1:B:160:VAL:O	1:B:164:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:O	1:B:393:ARG:HG3	2.11	0.49
1:D:94:TYR:CE2	1:D:99:GLN:HB2	2.47	0.49
1:C:94:TYR:OH	1:C:405:LYS:HG3	2.13	0.48
1:A:244:LEU:HD12	1:A:280:GLN:CD	2.33	0.48
1:A:316:CYS:O	1:A:317:ASN:HB3	2.13	0.48
1:B:275:VAL:O	1:B:276:PRO:C	2.52	0.48
1:A:41:TYR:CD1	1:A:63:PHE:HB2	2.49	0.48
1:B:11:ILE:HA	1:B:446:PHE:O	2.12	0.48
1:D:160:VAL:O	1:D:164:VAL:HG23	2.13	0.48
1:A:137:GLY:O	1:A:140:VAL:HG22	2.14	0.48
1:A:402:TYR:O	1:A:403:ASN:C	2.52	0.48
1:D:195:LEU:CD2	1:D:205:ILE:HD13	2.43	0.48
1:C:441:SER:OG	1:D:363:THR:HG21	2.14	0.48
1:C:177:ILE:HG22	1:C:184:TYR:CG	2.48	0.48
1:B:407:GLU:HB3	5:B:652:HOH:O	2.14	0.48
1:C:441:SER:O	1:C:444:THR:CG2	2.47	0.48
1:C:146:ASN:HD22	1:C:146:ASN:C	2.17	0.48
1:B:350:ILE:O	1:B:353:GLU:HB2	2.13	0.48
1:C:101:SER:HB3	1:C:104:ASP:OD1	2.14	0.48
1:B:330:GLU:HG2	5:B:603:HOH:O	2.13	0.48
1:A:452:LEU:HD11	1:B:411:ARG:CZ	2.44	0.47
1:A:224:LEU:O	1:A:228:LEU:HD13	2.14	0.47
1:B:7:PHE:HE2	1:B:327:LEU:HD13	1.79	0.47
1:B:124:ILE:H	1:B:124:ILE:CD1	2.19	0.47
1:C:316:CYS:O	1:C:317:ASN:CB	2.61	0.47
1:C:41:TYR:CD1	1:C:63:PHE:HB2	2.49	0.47
1:B:19:LEU:HD11	1:B:291:LEU:HD22	1.97	0.47
1:D:25:ASP:O	1:D:26:HIS:HB2	2.14	0.47
1:A:205:ILE:N	1:A:205:ILE:HD12	2.30	0.47
1:C:338:LEU:O	1:C:341:GLU:HB3	2.14	0.47
1:B:4:HIS:O	1:B:440:HIS:HE1	1.97	0.47
1:B:287:PHE:CE1	1:B:291:LEU:HD13	2.50	0.47
1:B:431:MET:HB3	1:B:431:MET:HE3	1.63	0.47
1:C:324:VAL:O	1:C:327:LEU:HB2	2.15	0.47
1:D:173:LEU:O	1:D:177:ILE:HG23	2.14	0.47
1:A:177:ILE:HG22	1:A:184:TYR:CG	2.50	0.47
1:D:79:GLY:HA2	1:D:136:TYR:OH	2.15	0.47
1:B:79:GLY:HA2	1:B:136:TYR:OH	2.15	0.47
1:C:233:HIS:HA	5:C:623:HOH:O	2.15	0.47
1:D:316:CYS:O	1:D:317:ASN:ND2	2.47	0.47
1:A:459:ILE:HG22	1:B:335:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:SER:O	1:C:389:LEU:HD13	2.16	0.46
1:A:146:ASN:C	1:A:146:ASN:HD22	2.18	0.46
1:B:341:GLU:OE2	1:B:398:GLN:NE2	2.48	0.46
1:D:23:ASP:O	1:D:27:THR:HB	2.14	0.46
1:A:225:SER:HA	1:A:228:LEU:HD22	1.98	0.46
1:A:101:SER:HB3	1:A:104:ASP:OD1	2.15	0.46
1:A:344:ILE:HD13	1:A:395:LEU:HD23	1.97	0.46
1:A:86:ARG:HB2	1:A:421:TYR:HB2	1.97	0.46
1:A:384:ILE:O	1:A:387:VAL:HG12	2.16	0.46
1:B:381:GLN:NE2	1:B:382:LEU:HD12	2.31	0.46
1:D:198:PHE:CE2	1:D:438:LEU:HA	2.50	0.46
1:C:124:ILE:HD12	1:C:124:ILE:N	2.30	0.46
1:B:195:LEU:CD2	1:B:205:ILE:HD13	2.45	0.46
1:C:320:THR:N	3:C:503:PO4:O2	2.45	0.46
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.29	0.46
1:D:146:ASN:O	1:D:148:ASP:N	2.39	0.46
1:D:433:LYS:HA	5:D:612:HOH:O	2.16	0.46
1:A:13:ASN:HD21	1:A:15:ARG:HB2	1.80	0.46
1:D:364:ARG:NH2	1:D:373:TYR:OH	2.49	0.46
1:A:441:SER:O	1:A:444:THR:CG2	2.48	0.46
1:B:316:CYS:O	1:B:317:ASN:ND2	2.49	0.46
1:A:356:GLN:OE1	1:B:5:LYS:NZ	2.49	0.45
1:C:406:TRP:O	1:C:407:GLU:CG	2.63	0.45
1:A:185:VAL:HG22	1:A:222:TYR:HE2	1.81	0.45
1:D:311:ARG:NH1	1:D:311:ARG:CG	2.70	0.45
1:A:286:LYS:HD2	5:A:633:HOH:O	2.17	0.45
1:C:137:GLY:O	1:C:140:VAL:HG22	2.16	0.45
1:A:229:ASP:HA	1:C:230:LYS:HG3	1.97	0.45
1:B:173:LEU:O	1:B:177:ILE:HG23	2.16	0.45
1:A:102:PHE:CE2	1:A:106:LYS:HE3	2.52	0.45
1:C:102:PHE:CE2	1:C:106:LYS:HE3	2.51	0.45
1:D:19:LEU:HD11	1:D:291:LEU:HD22	1.98	0.45
1:C:359:VAL:C	1:C:361:LEU:H	2.20	0.45
1:B:241:VAL:HG11	1:B:278:VAL:HG22	1.98	0.45
1:A:376:GLU:HA	1:A:376:GLU:OE2	2.15	0.45
1:A:97:THR:O	1:A:97:THR:HG22	2.17	0.45
1:C:102:PHE:O	1:C:106:LYS:HG2	2.17	0.45
1:B:257:PHE:CE1	1:B:282:GLY:HA3	2.52	0.45
1:A:316:CYS:O	1:A:317:ASN:CB	2.65	0.45
1:C:393:ARG:CB	1:C:393:ARG:NH2	2.80	0.45
1:C:357:LYS:O	1:C:360:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:HG22	1:A:222:TYR:CE2	2.52	0.45
1:B:435:SER:O	1:B:439:GLU:HB2	2.17	0.45
1:C:340:ILE:O	1:C:344:ILE:HG13	2.16	0.45
1:C:43:LEU:HB3	1:C:167:VAL:HG21	1.99	0.45
1:A:43:LEU:HB3	1:A:167:VAL:HG21	1.99	0.45
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.76	0.45
1:D:198:PHE:O	1:D:203:LYS:HB2	2.17	0.45
1:B:86:ARG:HA	1:B:418:TYR:HA	1.99	0.45
1:C:124:ILE:CD1	1:C:124:ILE:H	2.24	0.44
1:A:34:LYS:HE3	1:A:65:PHE:HB2	1.98	0.44
1:D:183:LYS:HG2	1:D:183:LYS:O	2.17	0.44
1:D:305:ILE:HD12	1:D:305:ILE:N	2.33	0.44
1:C:146:ASN:OD1	1:C:149:LYS:HG2	2.17	0.44
1:B:374:ASP:HA	1:B:377:ILE:HG12	1.99	0.44
1:A:375:GLN:O	1:A:378:HIS:HB3	2.17	0.44
1:D:257:PHE:CE1	1:D:282:GLY:HA3	2.52	0.44
1:C:13:ASN:HD21	1:C:15:ARG:HB2	1.82	0.44
1:C:344:ILE:HD13	1:C:395:LEU:HD23	2.00	0.44
1:C:245:ALA:O	1:C:250:PHE:HB2	2.17	0.44
1:D:344:ILE:HD12	1:D:344:ILE:C	2.36	0.44
1:A:62:LYS:HG2	1:A:63:PHE:N	2.32	0.44
1:C:94:TYR:CZ	1:C:405:LYS:HG3	2.52	0.44
1:C:128:PHE:CE1	1:C:164:VAL:HG11	2.53	0.44
1:C:6:VAL:HG22	1:C:431:MET:CE	2.48	0.44
1:A:205:ILE:HG22	1:A:238:PHE:CD1	2.50	0.44
1:B:344:ILE:O	1:B:348:MET:HG3	2.17	0.44
1:B:177:ILE:HD12	1:B:181:LEU:HD23	1.99	0.44
1:D:287:PHE:CE1	1:D:291:LEU:HD13	2.53	0.44
1:C:154:GLN:O	1:C:158:GLN:HG3	2.18	0.44
1:C:78:ASN:HB2	1:C:80:ASN:ND2	2.32	0.44
1:A:102:PHE:O	1:A:106:LYS:HG2	2.18	0.44
1:A:213:TYR:CE2	1:A:217:LYS:HD2	2.53	0.44
1:D:312:LEU:O	1:D:312:LEU:HD23	2.17	0.44
1:A:128:PHE:CE1	1:A:164:VAL:HG11	2.53	0.44
1:A:146:ASN:CG	1:A:149:LYS:HG2	2.38	0.44
1:D:312:LEU:C	1:D:312:LEU:HD23	2.38	0.44
1:A:392:SER:HB3	1:B:447:ARG:NH2	2.33	0.44
1:C:145:THR:O	1:C:146:ASN:HB2	2.18	0.44
1:A:104:ASP:O	1:A:108:ILE:HG13	2.18	0.44
1:C:253:ASP:OD2	1:C:254:ASN:N	2.47	0.44
1:D:152:SER:O	1:D:156:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:CD2	1:B:425:ARG:HG3	2.52	0.43
1:A:182:LYS:HZ2	1:A:182:LYS:HB3	1.82	0.43
1:D:377:ILE:HG13	1:D:378:HIS:N	2.33	0.43
1:A:408:ARG:HH21	1:A:408:ARG:CG	2.31	0.43
1:A:145:THR:O	1:A:146:ASN:HB2	2.18	0.43
1:C:34:LYS:HE3	1:C:65:PHE:HB2	2.00	0.43
1:C:312:LEU:O	1:C:312:LEU:HD23	2.18	0.43
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.80	0.43
1:A:452:LEU:O	1:A:452:LEU:HD13	2.17	0.43
1:D:14:MET:O	1:D:203:LYS:NZ	2.46	0.43
1:B:305:ILE:HD12	1:B:305:ILE:N	2.32	0.43
1:B:152:SER:O	1:B:156:ILE:HG13	2.18	0.43
1:D:15:ARG:HD3	1:D:443:MET:SD	2.58	0.43
1:D:254:ASN:HD22	1:D:254:ASN:N	2.12	0.43
1:C:146:ASN:CG	1:C:149:LYS:HG2	2.39	0.43
1:A:154:GLN:O	1:A:158:GLN:HG3	2.18	0.43
1:D:354:LEU:HB3	1:D:384:ILE:HG13	2.01	0.43
1:B:39:LEU:HD13	1:B:173:LEU:HD23	2.00	0.43
1:A:78:ASN:HB2	1:A:80:ASN:ND2	2.33	0.43
1:D:43:LEU:HB3	1:D:167:VAL:HG21	1.99	0.43
1:C:97:THR:HG22	1:C:97:THR:O	2.19	0.43
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.19	0.43
1:C:135:LEU:O	1:C:139:LEU:HD13	2.18	0.43
1:A:449:ASN:C	1:A:451:ARG:H	2.21	0.43
1:C:358:TYR:CE2	1:D:441:SER:HA	2.54	0.43
1:C:62:LYS:HG2	1:C:63:PHE:N	2.34	0.43
1:C:393:ARG:HB3	1:C:393:ARG:HH21	1.83	0.43
1:C:354:LEU:HD23	1:C:357:LYS:HD2	2.00	0.43
1:C:178:ILE:HD12	1:C:181:LEU:HD21	2.01	0.43
1:A:30:ARG:NH1	1:A:30:ARG:HG2	2.31	0.43
1:A:182:LYS:HZ3	1:A:182:LYS:HB3	1.84	0.43
1:D:10:ARG:HH11	1:D:10:ARG:HG3	1.84	0.43
1:A:253:ASP:OD2	1:A:254:ASN:N	2.47	0.43
1:A:146:ASN:OD1	1:A:149:LYS:HG2	2.18	0.43
1:B:330:GLU:O	1:B:334:GLN:HG3	2.19	0.43
1:B:103:SER:O	1:B:107:LYS:HG2	2.19	0.43
1:C:356:GLN:NE2	1:C:359:VAL:HG21	2.34	0.43
1:D:39:LEU:HD13	1:D:173:LEU:HD23	2.01	0.43
1:B:254:ASN:HD22	1:B:254:ASN:N	2.10	0.43
1:A:368:GLU:O	1:A:369:SER:C	2.57	0.43
1:B:25:ASP:O	1:B:26:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:TYR:CE2	1:C:217:LYS:HD2	2.54	0.43
1:B:45:LYS:HD2	1:B:61:PHE:HB2	2.01	0.42
1:D:47:ARG:NH2	1:D:170:ASP:OD2	2.48	0.42
1:A:178:ILE:HA	1:A:178:ILE:HD12	1.93	0.42
1:A:178:ILE:HD12	1:A:181:LEU:HD21	2.00	0.42
1:B:340:ILE:O	1:B:344:ILE:HG13	2.20	0.42
1:A:241:VAL:HG11	1:A:278:VAL:HG22	2.00	0.42
1:A:94:TYR:CZ	1:A:99:GLN:HB2	2.54	0.42
1:C:401:PHE:N	1:C:401:PHE:CD1	2.88	0.42
1:D:177:ILE:HD12	1:D:181:LEU:HD23	2.01	0.42
1:D:243:THR:O	1:D:280:GLN:HA	2.20	0.42
1:B:340:ILE:HD12	1:B:397:GLU:HG2	2.00	0.42
1:D:349:ALA:O	1:D:353:GLU:HG3	2.19	0.42
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.84	0.42
1:C:308:ASP:OD2	1:C:311:ARG:HB2	2.19	0.42
1:A:19:LEU:CD2	1:A:291:LEU:HD13	2.49	0.42
1:D:333:SER:HB3	1:D:401:PHE:O	2.19	0.42
1:C:185:VAL:HG22	1:C:222:TYR:HE2	1.84	0.42
1:D:450:ARG:HG3	1:D:450:ARG:O	2.19	0.42
1:D:338:LEU:N	1:D:339:PRO:HD2	2.35	0.42
1:B:340:ILE:CD1	1:B:397:GLU:HG2	2.50	0.42
1:C:146:ASN:C	1:C:148:ASP:H	2.23	0.42
1:B:41:TYR:CE1	1:B:63:PHE:HB2	2.54	0.42
1:D:241:VAL:HG13	1:D:278:VAL:HG22	1.99	0.42
1:C:243:THR:O	1:C:280:GLN:HA	2.20	0.42
1:B:357:LYS:HD2	1:B:380:LEU:HD11	2.01	0.42
1:D:225:SER:HB2	1:D:226:PRO:HD3	2.02	0.42
1:B:47:ARG:NH2	1:B:170:ASP:OD2	2.50	0.42
1:D:58:ILE:HG13	1:D:59:LYS:N	2.35	0.42
1:B:380:LEU:O	1:B:384:ILE:HG13	2.20	0.42
1:C:185:VAL:HG22	1:C:222:TYR:CE2	2.55	0.41
1:C:346:GLU:O	1:C:350:ILE:HG12	2.20	0.41
1:B:110:ARG:O	1:B:111:SER:HB2	2.20	0.41
1:B:312:LEU:C	1:B:312:LEU:HD23	2.40	0.41
1:A:146:ASN:C	1:A:148:ASP:H	2.23	0.41
1:D:57:GLU:HA	1:D:57:GLU:OE1	2.20	0.41
1:B:12:ILE:HG23	1:B:12:ILE:O	2.20	0.41
1:D:154:GLN:HB2	1:D:154:GLN:HE21	1.65	0.41
1:D:290:ASP:HA	5:D:652:HOH:O	2.20	0.41
1:D:103:SER:O	1:D:107:LYS:HG2	2.19	0.41
1:A:124:ILE:CD1	1:A:124:ILE:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD21	1:B:234:TRP:HA	2.03	0.41
1:B:243:THR:O	1:B:280:GLN:HA	2.20	0.41
1:C:37:GLU:OE2	1:C:128:PHE:HA	2.20	0.41
1:D:12:ILE:O	1:D:12:ILE:HG23	2.20	0.41
1:A:245:ALA:O	1:A:250:PHE:HB2	2.19	0.41
1:D:41:TYR:CE1	1:D:63:PHE:HB2	2.55	0.41
1:B:58:ILE:HG13	1:B:59:LYS:N	2.36	0.41
1:D:316:CYS:O	1:D:317:ASN:CB	2.68	0.41
1:C:104:ASP:O	1:C:108:ILE:HG13	2.20	0.41
1:A:76:SER:HB2	1:A:154:GLN:HA	2.02	0.41
1:C:322:LEU:O	1:C:430:TYR:HA	2.20	0.41
1:C:13:ASN:HB2	1:C:445:TYR:CE2	2.55	0.41
1:D:228:LEU:HD21	1:D:234:TRP:HA	2.03	0.41
1:D:327:LEU:HD11	1:D:430:TYR:CE2	2.55	0.41
1:A:312:LEU:O	1:A:312:LEU:HD23	2.20	0.41
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.89	0.41
1:A:190:GLU:H	1:A:190:GLU:CD	2.24	0.41
1:A:135:LEU:O	1:A:139:LEU:HD13	2.19	0.41
1:B:254:ASN:ND2	1:B:254:ASN:N	2.69	0.41
1:C:94:TYR:CZ	1:C:99:GLN:HB2	2.55	0.41
1:C:76:SER:HB2	1:C:154:GLN:HA	2.03	0.41
1:B:10:ARG:NH1	1:B:10:ARG:HG3	2.36	0.41
1:B:376:GLU:O	1:B:380:LEU:HD23	2.21	0.41
1:D:351:LYS:NZ	1:D:355:GLU:OE2	2.54	0.41
1:A:228:LEU:HD21	1:A:234:TRP:CA	2.49	0.41
1:A:452:LEU:HA	1:A:452:LEU:HD22	1.75	0.41
1:B:404:PRO:HG2	5:B:625:HOH:O	2.21	0.41
1:C:194:GLY:HA3	1:C:438:LEU:HB3	2.02	0.41
1:C:326:GLU:OE1	1:C:326:GLU:N	2.45	0.40
1:D:330:GLU:OE2	1:D:409:VAL:N	2.51	0.40
1:B:146:ASN:C	1:B:148:ASP:H	2.24	0.40
1:D:146:ASN:OD1	1:D:149:LYS:HG2	2.21	0.40
1:B:6:VAL:HG13	1:B:431:MET:CE	2.51	0.40
1:A:373:TYR:CZ	1:A:376:GLU:HG2	2.56	0.40
1:D:30:ARG:HG2	1:D:30:ARG:HH11	1.86	0.40
1:A:229:ASP:OD1	1:C:230:LYS:HE3	2.22	0.40
1:C:393:ARG:HB2	1:C:393:ARG:NH2	2.36	0.40
1:A:452:LEU:O	1:A:455:HIS:HB3	2.21	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	451/470 (96%)	419 (93%)	25 (6%)	7 (2%)	12	20
1	B	456/470 (97%)	429 (94%)	22 (5%)	5 (1%)	17	30
1	C	434/470 (92%)	401 (92%)	28 (6%)	5 (1%)	16	28
1	D	454/470 (97%)	426 (94%)	23 (5%)	5 (1%)	17	30
All	All	1795/1880 (96%)	1675 (93%)	98 (6%)	22 (1%)	16	28

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	PRO
1	A	368	GLU
1	C	151	PRO
1	A	50	GLU
1	A	229	ASP
1	D	450	ARG
1	B	147	PRO
1	B	317	ASN
1	C	50	GLU
1	C	65	PHE
1	D	147	PRO
1	D	317	ASN
1	A	65	PHE
1	B	151	PRO
1	B	452	LEU
1	D	151	PRO
1	A	146	ASN
1	C	146	ASN
1	C	147	PRO
1	A	147	PRO
1	B	276	PRO
1	D	276	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/421 (97%)	375 (92%)	34 (8%)	14	25
1	B	411/421 (98%)	381 (93%)	30 (7%)	17	31
1	C	392/421 (93%)	363 (93%)	29 (7%)	17	30
1	D	410/421 (97%)	381 (93%)	29 (7%)	18	33
All	All	1622/1684 (96%)	1500 (92%)	122 (8%)	17	30

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	39	LEU
1	A	56	GLU
1	A	86	ARG
1	A	91	ARG
1	A	110	ARG
1	A	116	LEU
1	A	124	ILE
1	A	132	PHE
1	A	141	ASP
1	A	146	ASN
1	A	168	HIS
1	A	179	LYS
1	A	180	ASN
1	A	182	LYS
1	A	218	LEU
1	A	235	GLN
1	A	246	ASN
1	A	303	ASP
1	A	306	TYR
1	A	311	ARG
1	A	317	ASN
1	A	323	VAL
1	A	338	LEU

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Mol	Chain	Res	Type
1	A	363	THR
1	A	373	TYR
1	A	388	ASP
1	A	408	ARG
1	A	416	GLU
1	A	431	MET
1	A	437	LEU
1	A	444	THR
1	A	449	ASN
1	A	452	LEU
1	B	23	ASP
1	B	30	ARG
1	B	34	LYS
1	B	39	LEU
1	B	69	ILE
1	B	84	LEU
1	B	86	ARG
1	B	124	ILE
1	B	132	PHE
1	B	146	ASN
1	B	172	THR
1	B	173	LEU
1	B	177	ILE
1	B	180	ASN
1	B	185	VAL
1	B	218	LEU
1	B	228	LEU
1	B	235	GLN
1	B	246	ASN
1	B	254	ASN
1	B	291	LEU
1	B	303	ASP
1	B	317	ASN
1	B	341	GLU
1	B	383	GLN
1	B	385	SER
1	B	393	ARG
1	B	415	GLU
1	B	421	TYR
1	B	431	MET
1	C	5	LYS
1	C	39	LEU

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Mol	Chain	Res	Type
1	C	56	GLU
1	C	86	ARG
1	C	110	ARG
1	C	116	LEU
1	C	124	ILE
1	C	132	PHE
1	C	141	ASP
1	C	146	ASN
1	C	168	HIS
1	C	179	LYS
1	C	180	ASN
1	C	182	LYS
1	C	218	LEU
1	C	235	GLN
1	C	246	ASN
1	C	303	ASP
1	C	306	TYR
1	C	311	ARG
1	C	317	ASN
1	C	323	VAL
1	C	408	ARG
1	C	411	ARG
1	C	416	GLU
1	C	431	MET
1	C	437	LEU
1	C	444	THR
1	C	451	ARG
1	D	23	ASP
1	D	30	ARG
1	D	34	LYS
1	D	39	LEU
1	D	69	ILE
1	D	86	ARG
1	D	124	ILE
1	D	132	PHE
1	D	146	ASN
1	D	172	THR
1	D	173	LEU
1	D	177	ILE
1	D	180	ASN
1	D	185	VAL
1	D	218	LEU

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Mol	Chain	Res	Type
1	D	228	LEU
1	D	235	GLN
1	D	246	ASN
1	D	254	ASN
1	D	291	LEU
1	D	317	ASN
1	D	372	GLN
1	D	375	GLN
1	D	377	ILE
1	D	382	LEU
1	D	431	MET
1	D	449	ASN
1	D	451	ARG
1	D	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	ASN
1	A	64	ASN
1	A	154	GLN
1	A	180	ASN
1	A	246	ASN
1	A	390	GLN
1	A	455	HIS
1	B	154	GLN
1	B	235	GLN
1	B	246	ASN
1	B	254	ASN
1	B	317	ASN
1	B	381	GLN
1	B	399	ASN
1	B	449	ASN
1	C	13	ASN
1	C	35	ASN
1	C	64	ASN
1	C	154	GLN
1	C	180	ASN
1	C	246	ASN
1	C	334	GLN
1	C	356	GLN

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Mol	Chain	Res	Type
1	C	383	GLN
1	C	390	GLN
1	D	154	GLN
1	D	235	GLN
1	D	246	ASN
1	D	254	ASN
1	D	317	ASN
1	D	375	GLN
1	D	381	GLN
1	D	383	GLN
1	D	390	GLN
1	D	449	ASN

### 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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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	5GP	A	501	-	21,26,26	1.55	3 (14%)	25,40,40	2.11	7 (28%)
3	PO4	A	502	-	4,4,4	1.24	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	503	-	4,4,4	1.10	0	6,6,6	0.27	0
3	PO4	B	501	4	4,4,4	1.17	0	6,6,6	0.27	0
3	PO4	B	502	-	4,4,4	1.19	0	6,6,6	0.27	0
2	5GP	C	501	-	21,26,26	1.41	3 (14%)	25,40,40	2.32	6 (24%)
3	PO4	C	502	4	4,4,4	1.27	0	6,6,6	0.27	0
3	PO4	C	503	-	4,4,4	1.21	0	6,6,6	0.27	0
3	PO4	D	501	4	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	D	502	-	4,4,4	1.01	0	6,6,6	0.27	0

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	5GP	A	501	-	-	0/6/26/26	0/3/3/3
3	PO4	A	502	-	-	0/0/0/0	0/0/0/0
3	PO4	A	503	-	-	0/0/0/0	0/0/0/0
3	PO4	B	501	4	-	0/0/0/0	0/0/0/0
3	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	5GP	C	501	-	-	0/6/26/26	0/3/3/3
3	PO4	C	502	4	-	0/0/0/0	0/0/0/0
3	PO4	C	503	-	-	0/0/0/0	0/0/0/0
3	PO4	D	501	4	-	0/0/0/0	0/0/0/0
3	PO4	D	502	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	5GP	O2'-C2'	2.07	1.47	1.43
2	A	501	5GP	O2'-C2'	2.13	1.48	1.43
2	C	501	5GP	C6-N1	3.02	1.38	1.33
2	A	501	5GP	C6-N1	3.23	1.39	1.33
2	C	501	5GP	O4'-C1'	3.93	1.46	1.41
2	A	501	5GP	O4'-C1'	4.84	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	5GP	C4'-O4'-C1'	-7.27	101.73	109.72
2	A	501	5GP	C4'-O4'-C1'	-5.24	103.96	109.72
2	A	501	5GP	N3-C2-N1	-4.84	120.07	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	5GP	N3-C2-N1	-4.62	120.41	127.44
2	A	501	5GP	C5-C6-N1	-2.99	119.50	123.59
2	C	501	5GP	C5-C6-N1	-2.95	119.55	123.59
2	A	501	5GP	C6-C5-C4	-2.83	117.51	120.90
2	C	501	5GP	C6-C5-C4	-2.68	117.69	120.90
2	A	501	5GP	C4-C5-N7	-2.08	107.57	109.48
2	C	501	5GP	O4'-C4'-C5'	2.03	116.59	109.32
2	A	501	5GP	O4'-C4'-C5'	2.18	117.12	109.32
2	C	501	5GP	C6-N1-C2	4.17	121.72	115.94
2	A	501	5GP	C6-N1-C2	4.26	121.85	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	PO4	1	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	455/470 (96%)	0.55	47 (10%) 9 9	37, 57, 100, 109	0
1	B	458/470 (97%)	0.62	29 (6%) 23 26	32, 53, 81, 92	0
1	C	438/470 (93%)	0.63	49 (11%) 7 7	36, 62, 98, 119	0
1	D	456/470 (97%)	0.56	41 (8%) 12 13	35, 56, 83, 97	0
All	All	1807/1880 (96%)	0.59	166 (9%) 11 12	32, 56, 93, 119	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	MET	6.4
1	C	149	LYS	6.0
1	A	150	MET	5.8
1	D	228	LEU	5.7
1	D	100	ILE	5.6
1	D	140	VAL	5.6
1	B	150	MET	5.2
1	C	358	TYR	5.2
1	C	55	PRO	5.0
1	C	384	ILE	4.8
1	A	453	LEU	4.7
1	B	149	LYS	4.7
1	D	201	TYR	4.7
1	D	230	LYS	4.7
1	A	53	HIS	4.6
1	A	231	GLY	4.5
1	C	401	PHE	4.5
1	A	367	ASP	4.5
1	A	306	TYR	4.5
1	A	149	LYS	4.5
1	A	145	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	395	LEU	4.4
1	B	377	ILE	4.4
1	A	54	TYR	4.3
1	C	381	GLN	4.1
1	B	142	LEU	4.1
1	C	98	LYS	4.1
1	A	62	LYS	4.0
1	C	147	PRO	3.9
1	A	366	ILE	3.9
1	A	50	GLU	3.8
1	A	460	LEU	3.8
1	C	100	ILE	3.8
1	C	380	LEU	3.8
1	A	48	LEU	3.8
1	A	373	TYR	3.7
1	C	306	TYR	3.7
1	A	230	LYS	3.7
1	C	49	ALA	3.7
1	B	51	SER	3.7
1	D	147	PRO	3.7
1	A	157	ALA	3.7
1	A	459	ILE	3.6
1	B	382	LEU	3.6
1	B	53	HIS	3.6
1	C	148	ASP	3.5
1	C	357	LYS	3.5
1	D	54	TYR	3.5
1	A	142	LEU	3.5
1	A	58	ILE	3.5
1	D	150	MET	3.4
1	D	101	SER	3.4
1	C	142	LEU	3.4
1	B	52	PHE	3.4
1	D	306	TYR	3.4
1	D	144	ASP	3.4
1	B	54	TYR	3.4
1	A	154	GLN	3.4
1	C	59	LYS	3.3
1	D	49	ALA	3.3
1	D	98	LYS	3.3
1	D	58	ILE	3.2
1	B	128	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	LEU	3.2
1	D	149	LYS	3.2
1	A	450	ARG	3.2
1	A	146	ASN	3.1
1	A	140	VAL	3.1
1	A	369	SER	3.1
1	A	52	PHE	3.1
1	A	148	ASP	3.0
1	D	377	ILE	3.0
1	A	63	PHE	3.0
1	C	359	VAL	2.9
1	A	139	LEU	2.9
1	A	155	ALA	2.9
1	C	402	TYR	2.9
1	B	354	LEU	2.9
1	B	306	TYR	2.8
1	D	218	LEU	2.8
1	D	366	ILE	2.8
1	D	146	ASN	2.8
1	C	361	LEU	2.7
1	C	48	LEU	2.7
1	A	363	THR	2.7
1	C	63	PHE	2.7
1	D	50	GLU	2.7
1	A	307	GLY	2.7
1	C	136	TYR	2.7
1	B	148	ASP	2.7
1	C	166	LYS	2.7
1	D	229	ASP	2.7
1	C	354	LEU	2.7
1	D	4	HIS	2.7
1	C	201	TYR	2.7
1	B	47	ARG	2.7
1	C	50	GLU	2.6
1	C	398	GLN	2.6
1	C	153	TYR	2.6
1	A	152	SER	2.6
1	A	156	ILE	2.6
1	C	382	LEU	2.6
1	C	54	TYR	2.6
1	A	310	LEU	2.6
1	A	136	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	450	ARG	2.5
1	D	200	ARG	2.5
1	D	310	LEU	2.5
1	B	301	ILE	2.5
1	C	58	ILE	2.5
1	C	52	PHE	2.4
1	A	362	CYS	2.4
1	B	380	LEU	2.4
1	B	321	ALA	2.4
1	A	147	PRO	2.4
1	D	128	PHE	2.4
1	D	93	SER	2.4
1	B	357	LYS	2.3
1	C	62	LYS	2.3
1	A	49	ALA	2.3
1	C	60	LYS	2.3
1	C	356	GLN	2.3
1	D	57	GLU	2.3
1	D	48	LEU	2.3
1	C	383	GLN	2.3
1	A	59	LYS	2.3
1	C	51	SER	2.3
1	D	139	LEU	2.3
1	C	351	LYS	2.3
1	D	61	PHE	2.3
1	D	231	GLY	2.3
1	C	61	PHE	2.3
1	D	102	PHE	2.3
1	C	393	ARG	2.3
1	B	21	GLY	2.2
1	B	387	VAL	2.2
1	D	94	TYR	2.2
1	B	147	PRO	2.2
1	A	61	PHE	2.2
1	D	177	ILE	2.2
1	A	461	GLU	2.2
1	C	102	PHE	2.2
1	B	139	LEU	2.2
1	C	310	LEU	2.2
1	B	55	PRO	2.2
1	D	69	ILE	2.1
1	D	454	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	110	ARG	2.1
1	A	314	LYS	2.1
1	C	307	GLY	2.1
1	B	358	TYR	2.1
1	C	338	LEU	2.1
1	D	148	ASP	2.1
1	D	108	ILE	2.1
1	B	378	HIS	2.1
1	A	60	LYS	2.1
1	A	229	ASP	2.1
1	C	145	THR	2.1
1	A	316	CYS	2.1
1	B	305	ILE	2.0
1	C	344	ILE	2.0
1	D	60	LYS	2.0
1	A	177	ILE	2.0
1	B	146	ASN	2.0
1	B	48	LEU	2.0
1	B	5	LYS	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(Å <sup>2</sup> )	Q<0.9
2	5GP	C	501	24/24	0.87	0.22	0.51	78,91,106,106	0
2	5GP	A	501	24/24	0.87	0.21	0.39	78,90,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	503	5/5	0.97	0.18	0.34	83,84,85,85	0
3	PO4	C	503	5/5	0.98	0.18	0.29	75,76,78,78	0
3	PO4	A	502	5/5	0.99	0.17	0.08	49,49,52,53	0
3	PO4	D	501	5/5	0.99	0.16	-0.28	52,54,56,56	0
3	PO4	C	502	5/5	0.99	0.14	-0.48	46,48,50,50	0
3	PO4	B	502	5/5	0.97	0.17	-0.66	66,68,70,71	0
3	PO4	B	501	5/5	0.99	0.16	-0.68	38,41,42,45	0
4	MG	D	503	1/1	0.88	0.13	-0.87	62,62,62,62	0
3	PO4	D	502	5/5	0.96	0.14	-1.39	69,69,71,72	0
4	MG	B	503	1/1	0.83	0.13	-1.91	44,44,44,44	0
4	MG	C	504	1/1	0.98	0.04	-5.97	69,69,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.