



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MX0  
Title : Structure of topoisomerase subunit  
Authors : Corbett, K.D.; Berger, J.M.  
Deposited on : 2002-10-01  
Resolution : 2.30 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

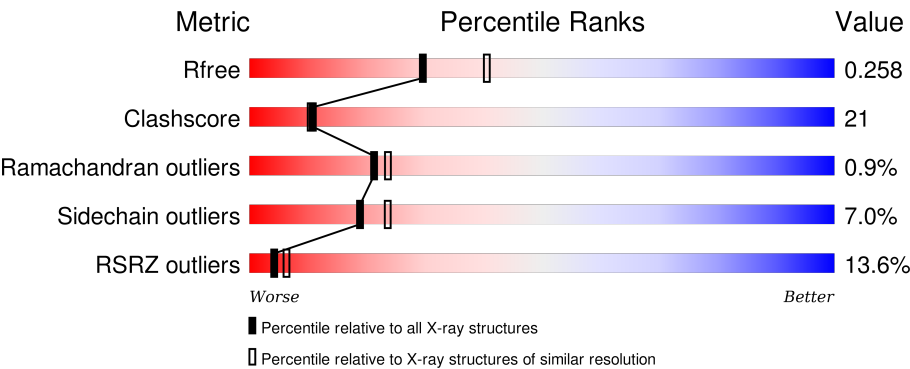
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 <sub>free</sub>	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	472	<div><div>10%</div><div>63%</div><div>31%</div><div>• •</div></div>
1	B	472	<div><div>8%</div><div>64%</div><div>30%</div><div>• •</div></div>
1	C	472	<div><div>8%</div><div>67%</div><div>29%</div><div>• •</div></div>
1	D	472	<div><div>6%</div><div>71%</div><div>24%</div><div>• •</div></div>
1	E	472	<div><div>10%</div><div>63%</div><div>30%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
1	F	472	<p>37% 40% 44% 11%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	D	901	-	-	-	X
4	ANP	A	900	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23057 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 Type II DNA topoisomerase VI subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3704	2384	620	694	1	5			
1	B	455	Total	C	N	O	S	Se	0	0	0
			3651	2352	608	685	1	5			
1	C	466	Total	C	N	O	S	Se	0	0	0
			3738	2404	626	702	1	5			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3687	2374	615	692	1	5			
1	E	456	Total	C	N	O	S	Se	0	0	0
			3677	2368	614	689	1	5			
1	F	454	Total	C	N	O	S	Se	0	0	0
			3596	2316	598	676	1	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP O05207
A	0	ALA	-	EXPRESSION TAG	UNP O05207
A	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
A	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
A	303	TYR	ASP	SEE REMARK 999	UNP O05207
A	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
A	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
A	435	ASP	ASN	SEE REMARK 999	UNP O05207
A	445	MSE	MET	MODIFIED RESIDUE	UNP O05207
B	-1	GLY	-	EXPRESSION TAG	UNP O05207
B	0	ALA	-	EXPRESSION TAG	UNP O05207
B	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
B	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
B	303	TYR	ASP	SEE REMARK 999	UNP O05207
B	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
B	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
B	435	ASP	ASN	SEE REMARK 999	UNP O05207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	MSE	MET	MODIFIED RESIDUE	UNP O05207
C	-1	GLY	-	EXPRESSION TAG	UNP O05207
C	0	ALA	-	EXPRESSION TAG	UNP O05207
C	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
C	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
C	303	TYR	ASP	SEE REMARK 999	UNP O05207
C	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
C	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
C	435	ASP	ASN	SEE REMARK 999	UNP O05207
C	445	MSE	MET	MODIFIED RESIDUE	UNP O05207
D	-1	GLY	-	EXPRESSION TAG	UNP O05207
D	0	ALA	-	EXPRESSION TAG	UNP O05207
D	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
D	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
D	303	TYR	ASP	SEE REMARK 999	UNP O05207
D	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
D	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
D	435	ASP	ASN	SEE REMARK 999	UNP O05207
D	445	MSE	MET	MODIFIED RESIDUE	UNP O05207
E	-1	GLY	-	EXPRESSION TAG	UNP O05207
E	0	ALA	-	EXPRESSION TAG	UNP O05207
E	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
E	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
E	303	TYR	ASP	SEE REMARK 999	UNP O05207
E	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
E	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
E	435	ASP	ASN	SEE REMARK 999	UNP O05207
E	445	MSE	MET	MODIFIED RESIDUE	UNP O05207
F	-1	GLY	-	EXPRESSION TAG	UNP O05207
F	0	ALA	-	EXPRESSION TAG	UNP O05207
F	107	MSE	MET	MODIFIED RESIDUE	UNP O05207
F	121	MSE	MET	MODIFIED RESIDUE	UNP O05207
F	303	TYR	ASP	SEE REMARK 999	UNP O05207
F	409	MSE	MET	MODIFIED RESIDUE	UNP O05207
F	412	MSE	MET	MODIFIED RESIDUE	UNP O05207
F	435	ASP	ASN	SEE REMARK 999	UNP O05207
F	445	MSE	MET	MODIFIED RESIDUE	UNP O05207

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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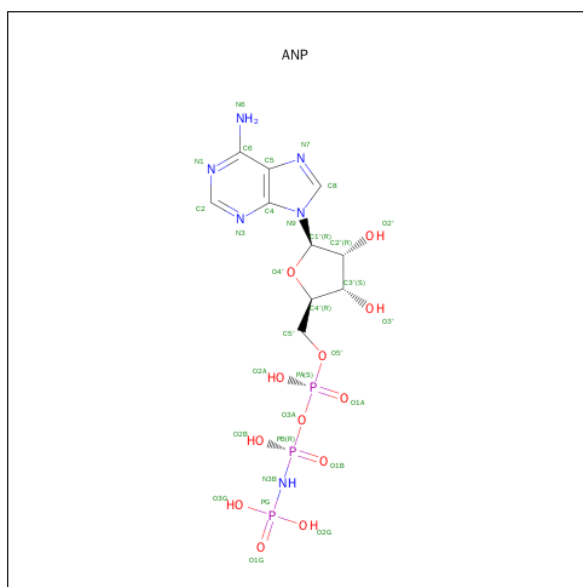
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

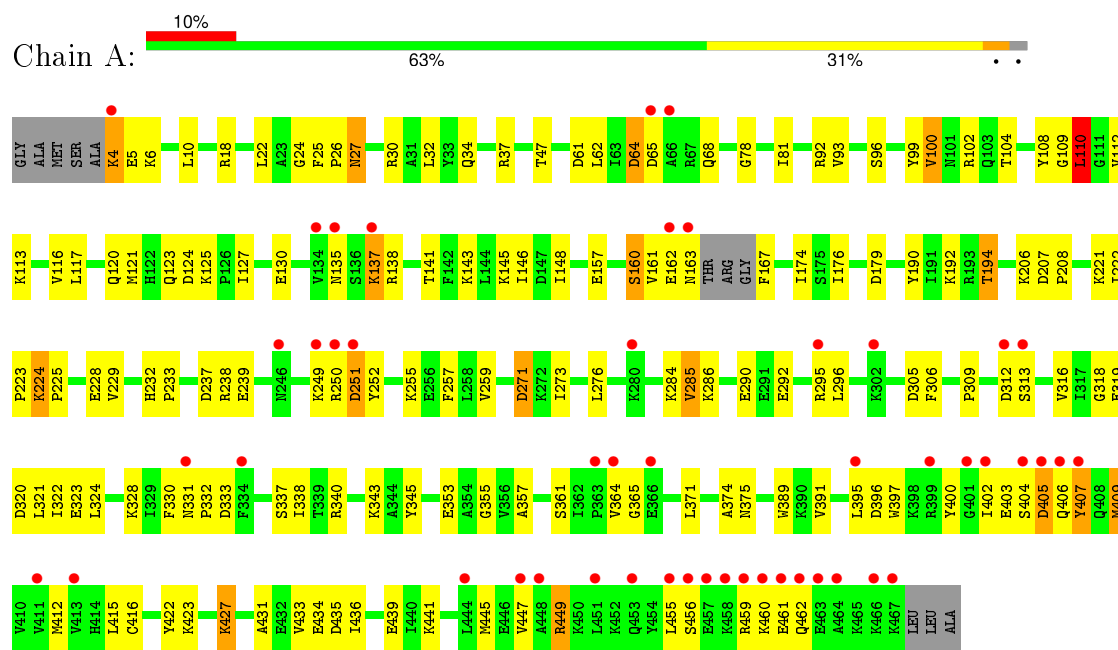
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		
5	B	145	Total	O	0	0
			145	145		
5	C	140	Total	O	0	0
			140	140		
5	D	160	Total	O	0	0
			160	160		
5	E	125	Total	O	0	0
			125	125		
5	F	81	Total	O	0	0
			81	81		

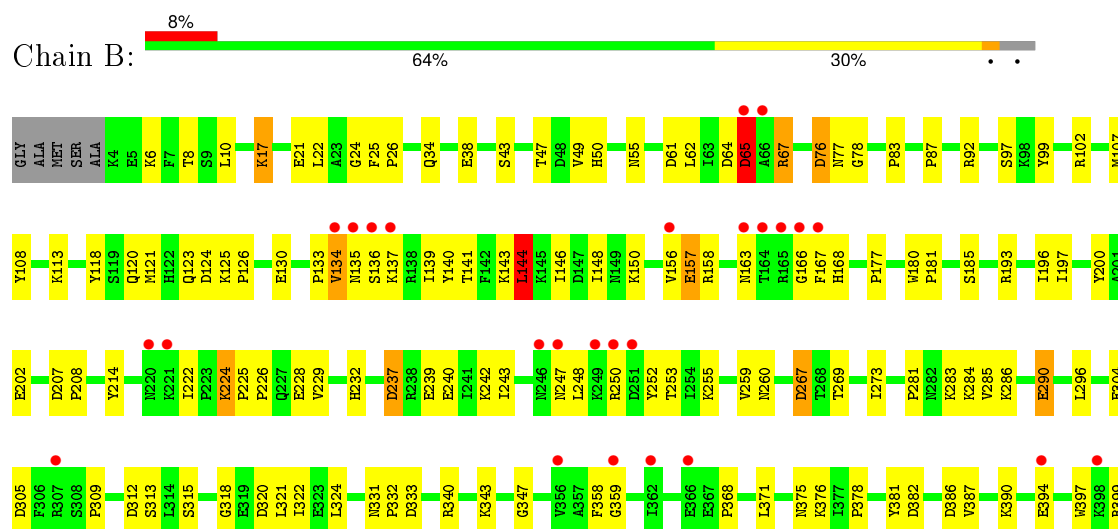
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

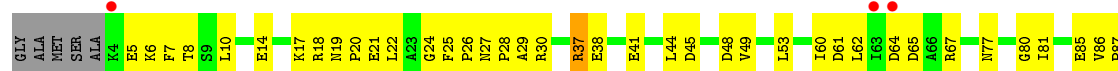
#### • Molecule 1: Type II DNA topoisomerase VI subunit B

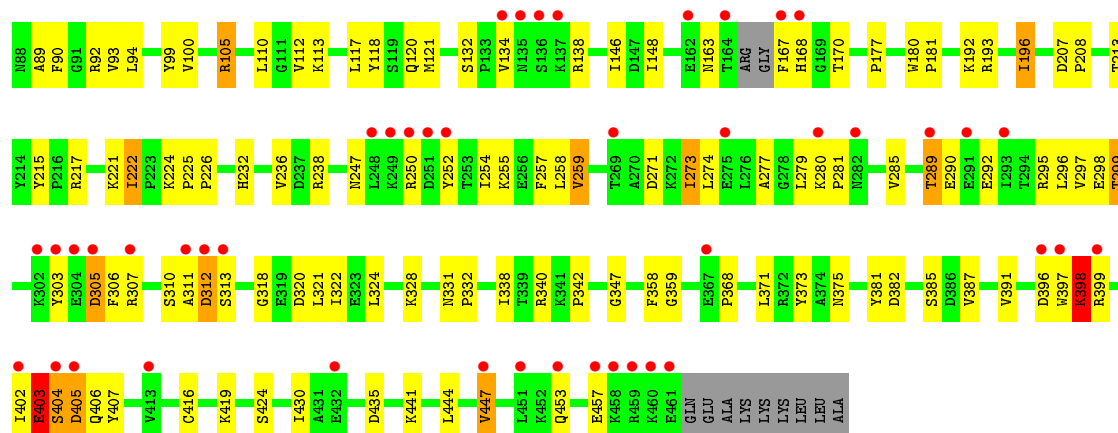


#### • Molecule 1: Type II DNA topoisomerase VI subunit B

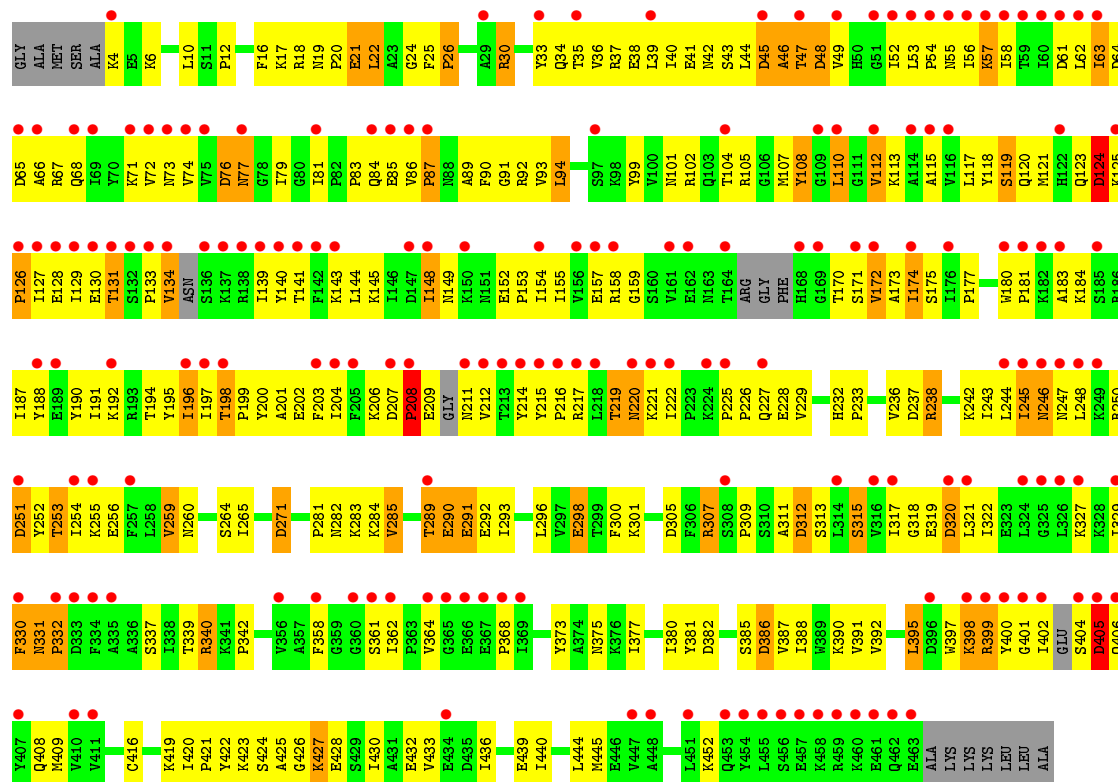








• Molecule 1: Type II DNA topoisomerase VI subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.66Å 219.19Å 106.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 22.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.30) 98.1 (22.40-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.214 , 0.263 0.216 , 0.258	Depositor DCC
$R_{free}$ test set	12535 reflections (9.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.3	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 150048 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: NA, MG, ANP

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	0.62	0/3779	0.81	13/5104 (0.3%)
1	B	0.64	0/3727	0.81	13/5038 (0.3%)
1	C	0.60	0/3814	0.79	16/5152 (0.3%)
1	D	0.62	0/3763	0.81	11/5087 (0.2%)
1	E	0.60	0/3752	0.81	14/5067 (0.3%)
1	F	0.48	1/3666 (0.0%)	0.80	16/4955 (0.3%)
All	All	0.59	1/22501 (0.0%)	0.81	83/30403 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	TYR	CB-CG	-5.04	1.44	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	C	105	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	271	ASP	CB-CG-OD2	6.95	124.56	118.30
1	D	382	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	251	ASP	CB-CG-OD2	6.82	124.44	118.30
1	D	320	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	124	ASP	CB-CG-OD2	6.74	124.37	118.30
1	F	330	PHE	N-CA-C	-6.70	92.92	111.00
1	F	76	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	267	ASP	CB-CG-OD2	6.65	124.29	118.30
1	F	382	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	435	ASP	CB-CG-OD2	6.36	124.03	118.30
1	D	267	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	61	ASP	CB-CG-OD2	6.30	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	320	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	207	ASP	CB-CG-OD2	6.23	123.91	118.30
1	E	61	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	271	ASP	CB-CG-OD2	5.92	123.63	118.30
1	F	386	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	65	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	396	ASP	CB-CG-OD2	5.86	123.57	118.30
1	F	305	ASP	CB-CG-OD2	5.82	123.53	118.30
1	E	65	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	61	ASP	CB-CG-OD2	5.79	123.51	118.30
1	E	405	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	271	ASP	CB-CG-OD2	5.76	123.48	118.30
1	E	435	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	105	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	435	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	405	ASP	CB-CG-OD2	5.70	123.42	118.30
1	C	320	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	64	ASP	CB-CG-OD2	5.66	123.39	118.30
1	E	271	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	271	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	405	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	65	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	320	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	124	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	76	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	110	LEU	CA-CB-CG	5.39	127.70	115.30
1	E	105	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	F	61	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	65	ASP	CB-CG-OD2	5.35	123.12	118.30
1	F	45	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	386	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	76	ASP	CB-CG-OD2	5.35	123.11	118.30
1	F	48	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	305	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	305	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	237	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	396	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	124	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	237	ASP	CB-CG-OD2	5.27	123.04	118.30
1	F	251	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	179	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	305	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	312	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	320	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	64	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	403	GLU	CB-CA-C	5.21	120.81	110.40
1	C	147	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	64	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	305	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	405	ASP	CB-CG-OD2	5.17	122.96	118.30
1	E	396	ASP	CB-CG-OD2	5.17	122.96	118.30
1	F	108	TYR	CB-CA-C	-5.16	100.09	110.40
1	B	312	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	108	TYR	N-CA-C	5.13	124.84	111.00
1	C	251	ASP	CB-CG-OD2	5.11	122.90	118.30
1	E	45	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	144	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	61	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	65	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	333	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	333	ASP	CB-CG-OD2	5.08	122.88	118.30
1	D	251	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	179	ASP	CB-CG-OD2	5.07	122.87	118.30
1	E	382	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	305	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	124	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	382	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	405	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	312	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3704	0	3760	155	0
1	B	3651	0	3704	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3738	0	3792	136	0
1	D	3687	0	3735	98	0
1	E	3677	0	3746	136	0
1	F	3596	0	3605	330	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	0	0
4	D	31	0	13	1	0
4	E	31	0	13	1	0
4	F	31	0	13	4	0
5	A	160	0	0	22	0
5	B	145	0	0	19	0
5	C	140	0	0	17	0
5	D	160	0	0	22	0
5	E	125	0	0	18	0
5	F	81	0	0	34	0
All	All	23057	0	22420	941	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 21.

All (941) 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:C:107:MSE:SE	1:C:107:MSE:CE	2.16	1.43
1:C:127:ILE:HD11	1:C:144:LEU:CD1	1.56	1.34
1:A:4:LYS:HD2	1:A:4:LYS:O	1.16	1.33
1:C:127:ILE:CD1	1:C:144:LEU:HD11	1.64	1.27
1:E:402:ILE:HG22	1:E:403:GLU:O	1.30	1.25
1:D:358:PHE:O	1:D:358:PHE:CD2	2.02	1.12
1:F:180:TRP:CG	1:F:208:PRO:HG2	1.84	1.12
1:F:203:PHE:HB2	1:F:215:TYR:HB2	1.31	1.10
1:F:53:LEU:HD23	1:F:222:ILE:HD11	1.25	1.10
1:C:238:ARG:HH22	1:C:290:GLU:HG3	1.04	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG2	5:B:962:HOH:O	1.53	1.06
1:A:239:GLU:HG3	5:A:1044:HOH:O	1.54	1.06
1:F:119:SER:O	1:F:123:GLN:HG3	1.56	1.05
1:F:117:LEU:HD22	1:F:148:ILE:HD13	1.36	1.04
1:F:53:LEU:CD2	1:F:222:ILE:HD11	1.87	1.04
1:B:441:LYS:HE2	1:B:445:MSE:HE3	1.10	1.04
1:C:322:ILE:HG23	1:C:412:MSE:HE3	1.39	1.03
1:D:250:ARG:HH11	1:D:250:ARG:CG	1.69	1.02
1:C:238:ARG:NH2	1:C:290:GLU:HG3	1.73	1.02
1:E:192:LYS:HG3	5:E:1044:HOH:O	1.58	1.02
1:E:120:GLN:NE2	1:E:146:ILE:H	1.58	1.01
1:F:198:THR:O	1:F:198:THR:HG23	1.56	1.01
1:A:313:SER:HA	5:A:1031:HOH:O	1.59	1.00
1:F:364:VAL:HG22	1:F:408:GLN:OE1	1.63	0.98
1:A:4:LYS:CD	1:A:4:LYS:O	2.11	0.98
1:E:120:GLN:HE22	1:E:146:ILE:N	1.60	0.97
1:A:409:MSE:SE	5:A:1021:HOH:O	2.31	0.96
1:E:37:ARG:CG	1:E:37:ARG:HH11	1.79	0.96
1:A:120:GLN:HE22	1:A:146:ILE:H	1.14	0.96
1:A:403:GLU:HG2	1:A:404:SER:H	1.30	0.95
1:F:143:LYS:HG3	1:F:157:GLU:HB3	1.45	0.95
1:C:322:ILE:HG23	1:C:412:MSE:CE	1.96	0.94
1:B:120:GLN:NE2	1:B:146:ILE:H	1.66	0.94
1:E:312:ASP:HB3	5:E:1047:HOH:O	1.66	0.94
1:B:120:GLN:HE22	1:B:146:ILE:N	1.66	0.93
1:D:358:PHE:O	1:D:358:PHE:CG	2.21	0.93
1:F:180:TRP:CD2	1:F:208:PRO:HG2	2.04	0.93
1:A:37:ARG:HH22	1:A:427:LYS:HB2	1.33	0.92
1:B:121:MSE:HE2	5:B:941:HOH:O	1.70	0.92
1:B:441:LYS:HE2	1:B:445:MSE:CE	1.98	0.92
1:B:441:LYS:CE	1:B:445:MSE:HE3	1.98	0.91
1:F:253:THR:CG2	1:F:256:GLU:HG3	2.01	0.91
1:C:120:GLN:HE22	1:C:146:ILE:H	1.13	0.91
1:C:453:GLN:HE21	1:C:457:GLU:HG3	1.32	0.91
1:F:53:LEU:HD23	1:F:222:ILE:CD1	2.00	0.90
1:C:134:VAL:HG23	5:C:1000:HOH:O	1.72	0.90
1:D:250:ARG:HG2	1:D:250:ARG:HH11	1.35	0.90
1:B:139:ILE:HG13	1:B:163:ASN:HB3	1.53	0.89
1:F:92:ARG:O	1:F:113:LYS:HE2	1.71	0.89
1:F:141:THR:OG1	1:F:159:GLY:HA3	1.72	0.89
1:A:137:LYS:CD	1:A:137:LYS:H	1.83	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:THR:HG22	1:E:215:TYR:CE2	2.08	0.88
1:F:83:PRO:HG3	1:F:140:TYR:CE2	2.07	0.88
1:F:154:ILE:HG12	5:F:978:HOH:O	1.72	0.88
1:A:4:LYS:HD2	1:A:4:LYS:C	1.94	0.88
1:F:55:ASN:H	1:F:77:ASN:HD21	1.22	0.88
1:C:135:ASN:HB2	5:C:969:HOH:O	1.71	0.87
1:E:163:ASN:HD21	1:E:167:PHE:HB3	1.38	0.87
1:A:37:ARG:NH2	1:A:427:LYS:HB2	1.90	0.87
1:C:453:GLN:NE2	1:C:457:GLU:HG3	1.89	0.87
1:F:124:ASP:O	1:F:126:PRO:HD3	1.75	0.86
1:B:136:SER:HB2	5:B:1008:HOH:O	1.74	0.86
1:A:163:ASN:HB2	5:A:1024:HOH:O	1.75	0.86
1:E:213:THR:HG21	1:E:215:TYR:OH	1.75	0.86
1:B:340:ARG:HD3	1:B:439:GLU:OE2	1.76	0.86
1:F:207:ASP:OD2	1:F:211:ASN:CB	2.23	0.86
1:A:229:VAL:HG11	1:A:313:SER:HB3	1.58	0.86
1:F:198:THR:CG2	1:F:198:THR:O	2.22	0.85
1:A:138:ARG:HH21	1:A:160:SER:HB3	1.40	0.85
1:F:330:PHE:C	1:F:332:PRO:HD3	1.97	0.85
1:E:311:ALA:HB2	1:E:342:PRO:CG	2.07	0.85
1:A:397:TRP:CD2	1:A:409:MSE:HE1	2.12	0.84
1:B:130:GLU:HG2	1:B:141:THR:HG22	1.59	0.84
1:F:127:ILE:HD12	1:F:174:ILE:HD13	1.58	0.84
1:C:458:LYS:HD2	5:C:1008:HOH:O	1.76	0.84
1:F:229:VAL:HG11	1:F:313:SER:HB3	1.59	0.84
1:E:213:THR:CG2	1:E:215:TYR:CZ	2.60	0.84
1:F:381:TYR:HB2	1:F:428:GLU:HG3	1.60	0.83
1:D:179:ASP:OD2	1:D:182:LYS:HD2	1.78	0.83
1:C:17:LYS:NZ	1:C:121:MSE:HE3	1.93	0.83
1:F:206:LYS:HG3	1:F:211:ASN:O	1.77	0.83
1:C:277:ALA:O	1:C:295:ARG:HD2	1.76	0.83
1:A:137:LYS:HD2	1:A:137:LYS:H	1.44	0.83
1:A:316:VAL:HG13	1:A:353:GLU:CD	2.00	0.82
1:F:155:ILE:HG22	5:F:1013:HOH:O	1.80	0.82
1:A:123:GLN:NE2	1:A:125:LYS:H	1.77	0.82
1:E:295:ARG:CZ	5:E:1054:HOH:O	2.26	0.82
1:C:424:SER:HB2	5:C:1057:HOH:O	1.80	0.81
1:A:316:VAL:HG13	1:A:353:GLU:OE2	1.80	0.81
1:F:245:ILE:HG22	1:F:246:ASN:N	1.95	0.81
1:B:250:ARG:HH11	1:B:252:TYR:HE1	1.29	0.81
1:E:257:PHE:HB2	1:E:285:VAL:HG21	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ALA:HB2	1:F:342:PRO:CG	2.10	0.81
1:E:295:ARG:O	1:E:299:THR:HG22	1.81	0.81
1:B:322:ILE:HG23	1:B:412:MSE:HE3	1.64	0.80
1:B:239:GLU:O	1:B:243:ILE:HD13	1.80	0.80
1:F:183:ALA:O	1:F:187:ILE:HG13	1.82	0.80
1:B:445:MSE:HE2	5:B:1048:HOH:O	1.80	0.79
1:C:322:ILE:CG2	1:C:412:MSE:HE3	2.11	0.79
1:F:206:LYS:HA	1:F:211:ASN:O	1.82	0.79
1:E:132:SER:O	1:E:168:HIS:HA	1.81	0.79
1:E:311:ALA:HB2	1:E:342:PRO:HG2	1.63	0.79
1:E:37:ARG:HG3	1:E:37:ARG:HH11	1.47	0.79
1:F:327:LYS:HA	1:F:332:PRO:HD2	1.62	0.79
1:C:249:LYS:HA	1:C:249:LYS:HE2	1.63	0.79
1:D:250:ARG:HH11	1:D:250:ARG:HG3	1.44	0.78
1:C:120:GLN:HE22	1:C:146:ILE:N	1.80	0.78
1:A:331:ASN:N	1:A:332:PRO:HD3	1.98	0.78
1:C:127:ILE:CD1	1:C:144:LEU:CD1	2.39	0.78
1:F:253:THR:HG23	1:F:256:GLU:HB2	1.65	0.78
4:F:950:ANP:H2'	5:F:951:HOH:O	1.83	0.78
1:A:130:GLU:HG2	1:A:141:THR:HG22	1.65	0.78
1:F:117:LEU:HD22	1:F:148:ILE:CD1	2.12	0.78
1:F:207:ASP:OD2	1:F:211:ASN:HB3	1.84	0.77
1:E:213:THR:HG22	1:E:215:TYR:CZ	2.19	0.77
1:F:127:ILE:HD12	1:F:174:ILE:CD1	2.15	0.77
1:F:77:ASN:HD22	1:F:77:ASN:H	1.31	0.77
1:C:407:TYR:HB3	5:C:1004:HOH:O	1.84	0.77
1:A:338:ILE:HG22	1:A:447:VAL:CG1	2.15	0.77
1:C:116:VAL:HG22	1:C:127:ILE:HG21	1.65	0.76
1:D:127:ILE:CG2	5:D:1080:HOH:O	2.33	0.76
1:F:55:ASN:H	1:F:77:ASN:ND2	1.82	0.76
1:F:126:PRO:HG3	1:F:145:LYS:HE3	1.65	0.76
1:C:453:GLN:HE21	1:C:457:GLU:CG	1.98	0.76
1:F:196:ILE:HG12	1:F:329:ILE:HD11	1.68	0.76
1:A:397:TRP:CE3	1:A:409:MSE:HE1	2.20	0.76
1:E:213:THR:HG21	1:E:215:TYR:CZ	2.20	0.75
1:F:131:THR:HG22	1:F:170:THR:OG1	1.85	0.75
1:F:311:ALA:HB2	1:F:342:PRO:HG3	1.67	0.75
1:F:53:LEU:CD2	1:F:222:ILE:CD1	2.60	0.75
1:F:39:LEU:HB3	1:F:74:VAL:HG21	1.68	0.75
1:E:60:ILE:HB	1:E:208:PRO:HD3	1.68	0.75
1:D:59:THR:HG23	5:D:1038:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASP:OD2	1:F:211:ASN:HB2	1.87	0.74
1:F:117:LEU:CD2	1:F:148:ILE:HD13	2.14	0.74
1:F:127:ILE:CD1	1:F:174:ILE:HD13	2.18	0.74
1:E:221:LYS:HE2	5:E:1045:HOH:O	1.86	0.74
1:A:224:LYS:HD2	5:A:1026:HOH:O	1.88	0.74
1:D:280:LYS:HG3	5:D:1089:HOH:O	1.88	0.74
1:C:390:LYS:HE2	1:C:437:GLU:OE2	1.88	0.74
1:F:58:ILE:HG12	1:F:74:VAL:HG22	1.70	0.74
1:B:381:TYR:HB2	1:B:428:GLU:HG3	1.69	0.73
1:A:338:ILE:HG22	1:A:447:VAL:HG13	1.70	0.73
1:F:422:TYR:CG	1:F:427:LYS:HB3	2.22	0.73
1:D:127:ILE:HG23	5:D:1080:HOH:O	1.87	0.73
1:C:127:ILE:CG1	1:C:144:LEU:HD12	2.19	0.73
1:F:207:ASP:HB2	1:F:208:PRO:HD2	1.70	0.73
1:F:117:LEU:CD2	1:F:148:ILE:CD1	2.66	0.73
1:A:120:GLN:HE22	1:A:146:ILE:N	1.86	0.73
1:E:38:GLU:OE2	5:E:976:HOH:O	2.06	0.73
1:D:338:ILE:HG12	1:D:447:VAL:HG13	1.70	0.73
1:C:127:ILE:CG1	1:C:144:LEU:CD1	2.66	0.73
1:F:422:TYR:CD1	1:F:427:LYS:HB3	2.23	0.73
1:F:253:THR:HG23	1:F:256:GLU:CB	2.19	0.72
1:C:120:GLN:NE2	1:C:146:ILE:H	1.85	0.72
1:B:390:LYS:HE3	1:B:394:GLU:OE2	1.89	0.72
1:C:332:PRO:HA	1:C:359:GLY:O	1.89	0.72
1:E:37:ARG:HG2	1:E:37:ARG:HH11	1.54	0.72
1:F:245:ILE:HG22	1:F:246:ASN:H	1.54	0.72
5:C:950:HOH:O	1:D:6:LYS:HD3	1.89	0.72
1:F:358:PHE:CG	1:F:358:PHE:O	2.41	0.72
1:B:226:PRO:HG3	1:B:315:SER:HB2	1.72	0.72
1:F:37:ARG:HG3	1:F:190:TYR:CE1	2.23	0.72
1:E:192:LYS:CE	5:E:1044:HOH:O	2.38	0.72
1:C:441:LYS:HE2	1:C:445:MSE:CE	2.20	0.72
1:C:207:ASP:HB2	1:C:208:PRO:CD	2.19	0.72
1:F:192:LYS:HG3	5:F:985:HOH:O	1.89	0.72
1:F:66:ALA:C	1:F:68:GLN:H	1.93	0.71
1:F:253:THR:CG2	1:F:256:GLU:CG	2.67	0.71
1:C:123:GLN:HE22	1:C:125:LYS:HB2	1.55	0.71
1:C:107:MSE:HE1	1:C:420:ILE:H	1.56	0.71
1:A:192:LYS:HE2	5:A:1033:HOH:O	1.90	0.71
1:B:453:GLN:HE21	1:B:457:GLU:HG3	1.56	0.71
1:D:368:PRO:HG3	1:D:409:MSE:HE3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:PRO:HB2	1:F:201:ALA:HB1	1.73	0.71
1:F:36:VAL:O	1:F:40:ILE:HD13	1.91	0.71
1:C:229:VAL:HG11	1:C:313:SER:HB3	1.72	0.71
1:F:264:SER:HA	1:F:307:ARG:HH11	1.55	0.71
1:A:137:LYS:HD2	1:A:137:LYS:N	2.02	0.71
1:C:368:PRO:HG3	1:C:409:MSE:HE3	1.71	0.70
1:F:130:GLU:HB2	1:F:171:SER:HB3	1.71	0.70
1:E:37:ARG:HG3	1:E:37:ARG:NH1	2.06	0.70
1:D:116:VAL:HG22	1:D:127:ILE:HG21	1.74	0.70
1:F:245:ILE:O	1:F:247:ASN:N	2.24	0.70
1:F:398:LYS:O	1:F:400:TYR:N	2.25	0.70
1:F:195:TYR:HA	1:F:198:THR:HG22	1.74	0.70
1:E:167:PHE:HA	5:E:1062:HOH:O	1.90	0.70
1:C:17:LYS:HZ2	1:C:121:MSE:HE3	1.56	0.70
1:F:340:ARG:HD3	1:F:439:GLU:OE2	1.90	0.70
1:B:240:GLU:HA	5:B:1054:HOH:O	1.91	0.70
1:E:163:ASN:ND2	1:E:167:PHE:HB3	2.06	0.69
1:C:127:ILE:HD11	1:C:144:LEU:HD11	0.75	0.69
1:F:86:VAL:N	1:F:87:PRO:CD	2.56	0.69
1:A:27:ASN:ND2	1:A:30:ARG:H	1.89	0.69
1:B:77:ASN:O	1:B:168:HIS:CE1	2.46	0.69
1:F:194:THR:CG2	5:F:975:HOH:O	2.41	0.69
1:F:42:ASN:ND2	5:F:982:HOH:O	2.16	0.69
1:F:296:LEU:HD21	1:F:300:PHE:CZ	2.28	0.69
1:F:207:ASP:O	1:F:209:GLU:N	2.26	0.69
1:C:407:TYR:CD2	1:C:409:MSE:HE2	2.28	0.69
1:F:110:LEU:HD13	1:F:110:LEU:N	2.08	0.69
1:F:141:THR:OG1	1:F:159:GLY:CA	2.41	0.68
1:F:289:THR:HG22	1:F:292:GLU:CD	2.13	0.68
1:C:330:PHE:HA	5:C:945:HOH:O	1.92	0.68
1:F:408:GLN:HB3	5:F:1015:HOH:O	1.92	0.68
1:F:83:PRO:CG	1:F:140:TYR:CE2	2.75	0.68
1:A:4:LYS:CG	5:B:962:HOH:O	2.23	0.68
1:A:252:TYR:O	1:A:285:VAL:HG23	1.93	0.68
1:F:110:LEU:N	1:F:110:LEU:CD1	2.56	0.68
1:F:24:GLY:C	1:F:26:PRO:HD3	2.14	0.68
1:D:252:TYR:O	1:D:285:VAL:HG23	1.94	0.68
1:E:192:LYS:HE3	5:E:1044:HOH:O	1.93	0.68
1:E:279:LEU:HD21	1:E:292:GLU:HB3	1.76	0.68
1:B:387:VAL:HG11	1:B:432:GLU:HA	1.74	0.68
1:D:30:ARG:HD2	5:D:1022:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ILE:CD1	1:F:174:ILE:CD1	2.72	0.67
1:F:4:LYS:HG3	5:F:1016:HOH:O	1.94	0.67
1:F:54:PRO:HB2	1:F:201:ALA:CB	2.25	0.67
1:D:364:VAL:HG12	1:D:406:GLN:HG2	1.76	0.67
1:D:340:ARG:HD3	1:D:439:GLU:OE2	1.95	0.67
1:B:322:ILE:HG23	1:B:412:MSE:CE	2.25	0.67
1:E:405:ASP:OD1	1:E:406:GLN:N	2.27	0.67
1:F:226:PRO:HG3	1:F:315:SER:HB3	1.74	0.67
1:C:251:ASP:OD1	1:C:284:LYS:HD2	1.95	0.67
1:F:425:ALA:C	1:F:427:LYS:H	1.97	0.66
1:B:107:MSE:HE2	1:B:108:TYR:CE1	2.30	0.66
1:F:203:PHE:HB2	1:F:215:TYR:CB	2.20	0.66
1:F:253:THR:CG2	1:F:256:GLU:HB2	2.25	0.66
1:F:289:THR:HG23	1:F:292:GLU:H	1.59	0.66
1:F:83:PRO:HG3	1:F:140:TYR:CD2	2.30	0.66
1:C:249:LYS:HA	1:C:249:LYS:CE	2.25	0.66
1:F:54:PRO:O	1:F:202:GLU:N	2.26	0.66
1:C:229:VAL:HG11	1:C:313:SER:CB	2.25	0.66
1:B:150:LYS:HE3	5:B:996:HOH:O	1.95	0.66
1:F:358:PHE:CD2	1:F:358:PHE:O	2.49	0.66
1:F:53:LEU:HD21	1:F:222:ILE:HG13	1.78	0.65
1:B:259:VAL:HG23	1:B:260:ASN:OD1	1.96	0.65
1:D:348:HIS:HB3	1:D:418:THR:HG22	1.77	0.65
1:A:125:LYS:HD3	5:A:1023:HOH:O	1.95	0.65
1:F:243:ILE:O	1:F:247:ASN:HB2	1.97	0.65
1:E:277:ALA:HB2	1:E:299:THR:HG21	1.78	0.65
1:A:92:ARG:O	1:A:113:LYS:HE3	1.97	0.65
1:C:121:MSE:CE	1:D:237:ASP:OD2	2.45	0.65
1:C:407:TYR:CE2	1:C:409:MSE:CE	2.80	0.65
1:E:453:GLN:HE21	1:E:457:GLU:HG3	1.60	0.65
1:F:219:THR:CG2	1:F:221:LYS:HB3	2.26	0.65
1:D:21:GLU:CD	1:D:21:GLU:H	1.99	0.65
1:A:123:GLN:HE22	1:A:125:LYS:HB2	1.60	0.65
1:F:86:VAL:H	1:F:87:PRO:CD	2.10	0.65
1:E:391:VAL:HG13	1:E:441:LYS:HG2	1.79	0.65
1:F:39:LEU:CB	1:F:74:VAL:HG21	2.27	0.64
1:F:391:VAL:HG11	1:F:440:ILE:HG22	1.79	0.64
1:C:453:GLN:NE2	1:C:457:GLU:CG	2.60	0.64
1:B:134:VAL:HG12	1:B:134:VAL:O	1.96	0.64
1:F:255:LYS:HE2	5:F:970:HOH:O	1.98	0.64
1:A:330:PHE:O	1:A:361:SER:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:PRO:O	1:C:224:LYS:C	2.35	0.64
1:F:245:ILE:O	1:F:246:ASN:C	2.35	0.64
1:F:387:VAL:HG12	1:F:430:ILE:HB	1.79	0.64
1:D:280:LYS:CG	5:D:1089:HOH:O	2.44	0.64
1:A:345:TYR:CG	1:A:436:ILE:HD11	2.33	0.64
1:D:89:ALA:O	1:D:113:LYS:HE3	1.98	0.64
1:A:403:GLU:HG2	1:A:404:SER:N	2.07	0.64
1:D:364:VAL:CG1	1:D:406:GLN:HG2	2.28	0.64
1:F:118:TYR:HA	1:F:121:MSE:HE2	1.81	0.64
1:D:250:ARG:HG2	1:D:250:ARG:NH1	2.07	0.63
1:E:192:LYS:HD2	5:E:1050:HOH:O	1.97	0.63
1:D:257:PHE:HB2	1:D:285:VAL:HG21	1.81	0.63
1:F:180:TRP:HB3	1:F:181:PRO:HD3	1.79	0.63
1:D:179:ASP:OD2	1:D:182:LYS:CD	2.45	0.63
1:A:123:GLN:NE2	1:A:125:LYS:HB2	2.14	0.63
1:C:441:LYS:HE2	1:C:445:MSE:HE1	1.81	0.63
1:C:121:MSE:HE3	1:D:237:ASP:OD2	1.98	0.63
4:F:950:ANP:C2'	5:F:951:HOH:O	2.43	0.63
1:F:58:ILE:HA	1:F:73:ASN:O	1.97	0.63
1:E:53:LEU:HD23	1:E:222:ILE:HG13	1.79	0.63
1:E:324:LEU:HD21	1:E:328:LYS:HE3	1.80	0.63
1:C:17:LYS:HZ3	1:C:121:MSE:HE3	1.64	0.63
1:A:206:LYS:HE2	5:A:981:HOH:O	1.98	0.63
1:B:248:LEU:HD22	1:B:252:TYR:CE2	2.34	0.63
1:D:207:ASP:HB2	1:D:208:PRO:CD	2.28	0.63
1:A:460:LYS:HD2	5:A:998:HOH:O	1.99	0.63
1:E:120:GLN:HE22	1:E:146:ILE:H	0.77	0.62
1:F:207:ASP:CG	1:F:211:ASN:HB2	2.20	0.62
1:F:34:GLN:O	1:F:38:GLU:HG2	1.99	0.62
1:F:35:THR:O	1:F:39:LEU:HG	1.98	0.62
1:A:120:GLN:NE2	1:A:146:ILE:H	1.92	0.62
1:D:4:LYS:N	5:D:997:HOH:O	2.31	0.62
1:F:368:PRO:HG3	1:F:409:MSE:HE3	1.81	0.62
1:F:57:LYS:HB3	1:F:204:ILE:HB	1.82	0.62
1:D:255:LYS:NZ	1:D:267:ASP:OD1	2.32	0.62
1:A:167:PHE:N	5:A:1054:HOH:O	2.32	0.62
1:C:240:GLU:HG3	1:D:17:LYS:HE3	1.82	0.62
1:F:408:GLN:CA	5:F:1015:HOH:O	2.47	0.62
1:B:387:VAL:CG1	1:B:432:GLU:HA	2.29	0.62
1:C:221:LYS:HD2	1:C:222:ILE:N	2.14	0.62
1:A:222:ILE:HG13	1:A:223:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:ILE:C	1:F:199:PRO:HD3	2.20	0.62
1:F:149:ASN:N	5:F:969:HOH:O	2.31	0.62
1:A:292:GLU:HG2	1:A:295:ARG:HH21	1.64	0.62
1:F:139:ILE:O	1:F:139:ILE:HG22	2.00	0.62
1:F:53:LEU:CG	1:F:222:ILE:HD11	2.30	0.61
1:F:289:THR:OG1	1:F:291:GLU:HG2	2.00	0.61
1:B:139:ILE:CG1	1:B:163:ASN:HB3	2.26	0.61
1:B:240:GLU:CA	5:B:1054:HOH:O	2.48	0.61
1:D:92:ARG:O	1:D:113:LYS:HE2	2.00	0.61
1:C:127:ILE:HG12	1:C:144:LEU:HD12	1.81	0.61
1:C:340:ARG:HD3	1:C:439:GLU:OE2	2.00	0.61
1:E:318:GLY:O	1:E:322:ILE:HG13	1.98	0.61
1:D:292:GLU:HG2	1:D:295:ARG:NH2	2.16	0.61
1:E:398:LYS:HD2	5:E:1005:HOH:O	1.99	0.61
1:F:53:LEU:HD23	1:F:222:ILE:CG1	2.30	0.61
1:F:33:TYR:O	1:F:33:TYR:CD2	2.54	0.61
1:B:232:HIS:O	1:B:347:GLY:HA2	1.99	0.61
1:C:123:GLN:NE2	1:C:125:LYS:HB2	2.16	0.61
1:E:14:GLU:CG	1:E:148:ILE:HG22	2.31	0.61
1:A:403:GLU:CG	1:A:404:SER:H	2.07	0.61
1:A:26:PRO:HD2	1:A:30:ARG:HG2	1.83	0.61
1:F:206:LYS:CG	1:F:211:ASN:O	2.48	0.60
1:F:53:LEU:CD2	1:F:222:ILE:CG1	2.79	0.60
1:F:4:LYS:HE3	5:F:991:HOH:O	2.01	0.60
1:F:253:THR:HG23	1:F:256:GLU:H	1.65	0.60
1:F:227:GLN:HB2	5:F:976:HOH:O	2.01	0.60
1:C:390:LYS:O	1:C:394:GLU:HG3	2.01	0.60
1:E:419:LYS:NZ	1:F:18:ARG:O	2.31	0.60
1:C:238:ARG:HH22	1:C:290:GLU:CG	1.97	0.60
1:A:343:LYS:HE2	5:A:950:HOH:O	2.00	0.60
1:B:269:THR:O	1:B:273:ILE:HG12	2.01	0.60
1:F:339:THR:O	1:F:339:THR:HG22	2.01	0.60
1:C:50:HIS:CD2	1:C:79:ILE:HD13	2.36	0.60
1:F:86:VAL:N	1:F:87:PRO:HD2	2.16	0.60
1:A:6:LYS:O	1:B:97:SER:HA	2.01	0.60
1:F:253:THR:OG1	1:F:282:ASN:HA	2.01	0.60
1:F:408:GLN:C	5:F:1015:HOH:O	2.40	0.60
1:F:245:ILE:O	1:F:248:LEU:N	2.31	0.60
1:A:400:TYR:OH	1:A:445:MSE:HG2	2.01	0.60
1:A:445:MSE:O	1:A:449:ARG:HD3	2.01	0.60
1:E:48:ASP:OD1	1:E:105:ARG:NH2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:ILE:CG1	1:F:329:ILE:HD11	2.32	0.60
1:F:86:VAL:H	1:F:87:PRO:HD2	1.66	0.60
1:A:316:VAL:CG1	1:A:353:GLU:OE2	2.50	0.60
1:F:253:THR:HG23	1:F:256:GLU:HG3	1.84	0.59
1:E:295:ARG:NH1	5:E:1054:HOH:O	2.33	0.59
1:E:8:THR:HG23	1:F:99:TYR:HD2	1.67	0.59
1:B:43:SER:HB3	1:B:76:ASP:HB3	1.84	0.59
1:A:123:GLN:NE2	1:A:125:LYS:N	2.49	0.59
1:F:37:ARG:HG3	1:F:190:TYR:CZ	2.37	0.59
1:F:433:VAL:HB	1:F:436:ILE:HD12	1.85	0.59
1:B:453:GLN:HE21	1:B:457:GLU:CG	2.16	0.59
1:F:289:THR:HG23	1:F:292:GLU:N	2.18	0.59
1:F:400:TYR:OH	1:F:445:MSE:HG2	2.03	0.59
1:B:240:GLU:HB3	5:B:1054:HOH:O	2.03	0.59
1:D:366:GLU:HG2	5:D:1058:HOH:O	2.02	0.59
1:A:322:ILE:HG12	1:A:412:MSE:HE2	1.84	0.59
1:C:407:TYR:HE2	1:C:409:MSE:HE1	1.68	0.58
1:D:100:VAL:HG13	1:D:228:GLU:CD	2.23	0.58
1:F:228:GLU:HB2	5:F:999:HOH:O	2.02	0.58
1:A:4:LYS:NZ	5:A:992:HOH:O	2.27	0.58
1:F:18:ARG:C	1:F:20:PRO:HD3	2.24	0.58
1:F:30:ARG:HD2	1:F:381:TYR:CE1	2.39	0.57
1:F:311:ALA:HB2	1:F:342:PRO:HG2	1.86	0.57
1:C:207:ASP:HB2	1:C:208:PRO:HD3	1.86	0.57
1:E:5:GLU:N	5:E:1037:HOH:O	2.36	0.57
1:F:77:ASN:HD22	1:F:77:ASN:N	1.96	0.57
1:C:123:GLN:NE2	1:C:125:LYS:H	2.02	0.57
1:D:399:ARG:CD	5:D:1018:HOH:O	2.53	0.57
1:A:207:ASP:HB2	1:A:208:PRO:CD	2.34	0.57
1:F:212:VAL:HG11	1:F:214:TYR:HE1	1.68	0.57
1:D:250:ARG:NH1	1:D:250:ARG:HG3	2.11	0.57
1:F:426:GLY:C	1:F:427:LYS:HG3	2.24	0.57
1:D:301:LYS:HG3	5:D:1064:HOH:O	2.03	0.57
1:F:214:TYR:HB3	1:F:216:PRO:HD3	1.87	0.57
1:C:226:PRO:HA	5:C:1058:HOH:O	2.03	0.57
1:F:238:ARG:HG2	1:F:293:ILE:HG22	1.87	0.57
1:F:330:PHE:C	1:F:332:PRO:CD	2.71	0.57
1:B:375:ASN:O	1:B:376:LYS:HB2	2.04	0.57
1:F:217:ARG:NH2	1:F:220:ASN:HD21	2.02	0.57
1:D:17:LYS:HD3	1:D:17:LYS:C	2.25	0.57
1:A:320:ASP:O	1:A:324:LEU:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:PRO:O	1:F:134:VAL:HG13	2.05	0.56
1:F:158:ARG:HG3	5:F:1013:HOH:O	2.05	0.56
1:B:134:VAL:CG1	1:B:134:VAL:O	2.53	0.56
1:A:250:ARG:HB2	1:A:252:TYR:CE1	2.40	0.56
1:C:423:LYS:HZ1	1:D:382:ASP:CG	2.08	0.56
1:D:192:LYS:HD2	5:D:1056:HOH:O	2.04	0.56
1:C:322:ILE:CG2	1:C:412:MSE:CE	2.76	0.56
1:C:365:GLY:O	1:C:407:TYR:HB2	2.05	0.56
1:D:383:GLU:HB2	5:D:983:HOH:O	2.05	0.56
1:E:86:VAL:HB	1:E:87:PRO:HD3	1.88	0.56
1:F:198:THR:N	1:F:199:PRO:HD3	2.20	0.56
1:F:89:ALA:O	1:F:113:LYS:HE3	2.06	0.56
1:F:386:ASP:OD1	1:F:388:ILE:N	2.31	0.56
1:D:276:LEU:HD22	5:D:991:HOH:O	2.05	0.56
1:F:126:PRO:HB3	1:F:144:LEU:O	2.05	0.56
1:B:126:PRO:HD2	5:B:1047:HOH:O	2.05	0.56
1:B:120:GLN:HE22	1:B:146:ILE:H	0.81	0.56
1:F:194:THR:O	1:F:198:THR:HB	2.06	0.56
1:F:33:TYR:OH	1:F:380:ILE:HG12	2.05	0.56
1:F:66:ALA:C	1:F:68:GLN:N	2.58	0.56
1:A:337:SER:HA	1:A:355:GLY:HA2	1.88	0.56
1:F:242:LYS:NZ	1:F:290:GLU:OE2	2.33	0.56
1:F:236:VAL:CG1	1:F:300:PHE:HD2	2.19	0.55
1:F:375:ASN:OD1	1:F:416:CYS:HA	2.05	0.55
1:F:49:VAL:O	1:F:49:VAL:HG12	2.07	0.55
1:F:327:LYS:HA	1:F:332:PRO:CD	2.32	0.55
1:B:242:LYS:NZ	1:B:290:GLU:OE2	2.38	0.55
1:B:250:ARG:NH1	1:B:252:TYR:CE1	2.73	0.55
1:C:249:LYS:HE2	1:C:249:LYS:CA	2.18	0.55
1:F:81:ILE:HD13	1:F:90:PHE:HE2	1.72	0.55
1:E:24:GLY:C	1:E:26:PRO:HD3	2.27	0.55
1:E:30:ARG:NH1	5:E:1016:HOH:O	2.34	0.55
1:F:215:TYR:N	1:F:216:PRO:HD3	2.22	0.55
1:F:77:ASN:ND2	1:F:77:ASN:H	2.03	0.55
1:C:385:SER:HB3	1:D:385:SER:OG	2.06	0.55
1:A:143:LYS:HB2	1:A:157:GLU:HB2	1.88	0.55
1:F:330:PHE:O	1:F:332:PRO:CD	2.54	0.55
1:C:407:TYR:HD2	1:C:409:MSE:HE2	1.71	0.55
1:F:264:SER:HA	1:F:307:ARG:NH1	2.20	0.55
1:D:193:ARG:HD2	5:D:1081:HOH:O	2.06	0.55
1:B:102:ARG:HA	5:B:1034:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ILE:HD12	1:C:129:ILE:HD11	1.89	0.55
1:F:215:TYR:N	1:F:216:PRO:CD	2.70	0.55
1:C:441:LYS:HE2	1:C:445:MSE:HE3	1.88	0.55
1:F:19:ASN:HB2	1:F:22:LEU:HD22	1.88	0.55
1:D:19:ASN:HB3	1:D:22:LEU:HD22	1.87	0.55
1:B:202:GLU:OE2	1:B:214:TYR:OH	2.24	0.55
1:A:117:LEU:O	1:A:121:MSE:HG3	2.06	0.55
1:F:253:THR:CG2	1:F:256:GLU:CB	2.84	0.55
1:F:330:PHE:CD2	1:F:330:PHE:N	2.74	0.55
1:E:295:ARG:HG3	1:F:67:ARG:HH22	1.72	0.55
1:C:93:VAL:HG12	1:C:94:LEU:HG	1.89	0.55
1:B:180:TRP:HB3	1:B:181:PRO:HD3	1.88	0.55
1:B:150:LYS:NZ	5:B:996:HOH:O	2.34	0.54
1:A:332:PRO:HG2	1:A:357:ALA:HB1	1.88	0.54
1:E:121:MSE:O	1:F:237:ASP:HB2	2.07	0.54
1:A:328:LYS:HG3	5:A:1059:HOH:O	2.07	0.54
1:B:83:PRO:HG3	1:B:140:TYR:CE2	2.42	0.54
1:B:25:PHE:N	1:B:26:PRO:HD3	2.22	0.54
1:C:99:TYR:CE2	1:D:10:LEU:HG	2.42	0.54
1:F:130:GLU:O	1:F:170:THR:HA	2.07	0.54
1:A:395:LEU:HD11	1:A:445:MSE:HE3	1.90	0.54
1:D:158:ARG:HG2	1:D:159:GLY:N	2.21	0.54
1:C:407:TYR:HE2	1:C:409:MSE:CE	2.18	0.54
1:F:110:LEU:HD13	1:F:110:LEU:H	1.72	0.54
1:C:221:LYS:HD2	1:C:221:LYS:C	2.27	0.54
1:E:14:GLU:HG2	1:E:148:ILE:HG22	1.89	0.54
1:A:99:TYR:HD2	1:B:8:THR:HG23	1.72	0.54
1:B:250:ARG:NH1	1:B:252:TYR:OH	2.41	0.54
1:D:404:SER:C	1:D:406:GLN:H	2.11	0.54
1:C:143:LYS:HB2	1:C:157:GLU:HB2	1.90	0.54
1:E:402:ILE:CG2	1:E:403:GLU:O	2.27	0.54
1:A:167:PHE:HB3	5:A:1036:HOH:O	2.06	0.54
1:E:30:ARG:HG3	5:E:1016:HOH:O	2.08	0.54
1:A:284:LYS:HD3	1:A:286:LYS:HE2	1.89	0.54
1:F:54:PRO:HD2	1:F:200:TYR:O	2.08	0.53
1:E:250:ARG:HD3	1:E:252:TYR:HE1	1.72	0.53
1:D:334:PHE:HA	5:D:1057:HOH:O	2.08	0.53
1:F:362:ILE:CB	5:F:1015:HOH:O	2.56	0.53
1:B:150:LYS:CE	5:B:996:HOH:O	2.53	0.53
1:B:358:PHE:CG	1:B:358:PHE:O	2.61	0.53
1:E:14:GLU:HG3	1:E:148:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:LYS:O	1:F:259:VAL:HG13	2.08	0.53
1:F:318:GLY:O	1:F:322:ILE:HG13	2.09	0.53
1:E:397:TRP:C	1:E:399:ARG:H	2.11	0.53
1:A:190:TYR:O	1:A:194:THR:HG22	2.08	0.53
1:D:255:LYS:CE	1:D:267:ASP:OD1	2.56	0.53
1:A:161:VAL:CG1	1:A:162:GLU:N	2.71	0.53
1:B:441:LYS:CE	1:B:445:MSE:CE	2.73	0.53
1:F:127:ILE:HD11	1:F:172:VAL:HG12	1.90	0.53
1:A:340:ARG:HD3	1:A:439:GLU:OE2	2.09	0.53
1:A:135:ASN:CG	5:A:978:HOH:O	2.47	0.53
1:A:331:ASN:H	1:A:332:PRO:HD3	1.73	0.53
1:E:93:VAL:HG12	1:E:94:LEU:HG	1.91	0.53
1:C:21:GLU:CD	1:C:21:GLU:H	2.12	0.53
1:F:42:ASN:HB3	4:F:950:ANP:N7	2.24	0.53
1:B:331:ASN:N	1:B:332:PRO:HD3	2.24	0.53
1:F:245:ILE:CG2	1:F:246:ASN:N	2.68	0.52
1:F:42:ASN:O	5:F:1029:HOH:O	2.19	0.52
1:A:257:PHE:HB2	1:A:285:VAL:HG21	1.91	0.52
1:E:89:ALA:O	1:E:113:LYS:HE2	2.09	0.52
1:F:401:GLY:O	1:F:402:ILE:C	2.47	0.52
1:D:326:LEU:HD21	1:D:412:MSE:HG2	1.90	0.52
1:F:253:THR:HG23	1:F:256:GLU:CG	2.37	0.52
1:A:331:ASN:N	1:A:332:PRO:CD	2.71	0.52
1:C:161:VAL:HG12	1:C:162:GLU:N	2.24	0.52
1:F:301:LYS:HD3	5:F:1001:HOH:O	2.08	0.52
1:C:322:ILE:HG23	1:C:412:MSE:HE1	1.85	0.52
1:B:207:ASP:HB2	1:B:208:PRO:CD	2.39	0.52
1:E:180:TRP:HB3	1:E:181:PRO:HD3	1.92	0.52
1:C:71:LYS:NZ	5:C:979:HOH:O	2.40	0.52
1:E:311:ALA:CB	1:E:342:PRO:CG	2.82	0.52
1:D:112:VAL:HG12	4:D:930:ANP:O2A	2.10	0.52
1:A:4:LYS:CD	1:A:4:LYS:C	2.67	0.52
1:F:194:THR:HG21	5:F:975:HOH:O	2.09	0.52
1:E:10:LEU:HG	1:F:99:TYR:CE2	2.44	0.52
1:A:10:LEU:HG	1:B:99:TYR:CE2	2.45	0.52
1:C:45:ASP:O	1:C:49:VAL:HB	2.10	0.52
1:D:34:GLN:O	1:D:38:GLU:HG2	2.10	0.52
1:F:253:THR:OG1	1:F:281:PRO:O	2.27	0.52
1:F:141:THR:HG1	1:F:159:GLY:HA3	1.70	0.52
1:F:229:VAL:HG11	1:F:313:SER:CB	2.37	0.52
1:F:192:LYS:HE2	5:F:1011:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HD11	1:A:306:PHE:CE1	2.44	0.52
1:A:47:THR:HG22	1:A:78:GLY:HA2	1.92	0.52
1:A:436:ILE:HD12	1:A:436:ILE:N	2.24	0.52
1:C:92:ARG:O	1:C:113:LYS:HD2	2.10	0.52
1:B:64:ASP:OD2	1:B:67:ARG:HD2	2.10	0.52
1:C:453:GLN:NE2	1:C:457:GLU:OE2	2.43	0.51
1:F:330:PHE:O	1:F:332:PRO:HD3	2.10	0.51
1:F:327:LYS:HA	1:F:332:PRO:HG2	1.92	0.51
1:E:311:ALA:CB	1:E:342:PRO:HG3	2.40	0.51
1:E:77:ASN:O	1:E:168:HIS:CE1	2.63	0.51
1:A:24:GLY:C	1:A:26:PRO:HD3	2.30	0.51
1:B:34:GLN:O	1:B:38:GLU:HG2	2.10	0.51
1:E:324:LEU:CD2	1:E:328:LYS:HE3	2.41	0.51
1:B:248:LEU:HD22	1:B:252:TYR:CD2	2.46	0.51
1:C:407:TYR:CE2	1:C:409:MSE:HE2	2.43	0.51
1:B:358:PHE:CD2	1:B:358:PHE:O	2.64	0.51
1:D:400:TYR:O	1:D:452:LYS:HG3	2.10	0.51
1:F:404:SER:C	1:F:406:GLN:H	2.14	0.51
1:A:232:HIS:CG	1:A:233:PRO:HD2	2.46	0.51
1:F:194:THR:HG23	5:F:975:HOH:O	2.06	0.51
1:F:395:LEU:HD22	1:F:444:LEU:HD13	1.92	0.51
1:C:132:SER:O	1:C:168:HIS:HA	2.10	0.51
1:F:219:THR:HG23	1:F:221:LYS:H	1.76	0.51
1:B:427:LYS:NZ	5:B:998:HOH:O	2.44	0.51
1:E:303:TYR:CE2	1:E:305:ASP:HB2	2.46	0.51
1:E:258:LEU:HD11	1:E:274:LEU:HD21	1.92	0.51
1:E:192:LYS:HE2	5:E:996:HOH:O	2.09	0.50
1:D:127:ILE:HG22	5:D:1080:HOH:O	2.06	0.50
1:D:130:GLU:HG2	1:D:141:THR:HG22	1.92	0.50
1:A:5:GLU:OE2	1:B:50:HIS:NE2	2.45	0.50
1:A:422:TYR:CD2	1:A:427:LYS:HD2	2.47	0.50
1:F:21:GLU:H	1:F:21:GLU:CD	2.15	0.50
1:C:232:HIS:O	1:C:347:GLY:HA2	2.11	0.50
1:D:263:GLN:O	1:D:264:SER:HB2	2.10	0.50
1:A:312:ASP:OD1	1:A:312:ASP:C	2.50	0.50
1:A:93:VAL:HG13	1:A:110:LEU:HD23	1.94	0.50
1:E:254:ILE:O	1:E:258:LEU:HG	2.12	0.50
1:F:148:ILE:C	5:F:969:HOH:O	2.49	0.50
1:F:253:THR:HG22	1:F:256:GLU:OE1	2.11	0.50
1:F:25:PHE:N	1:F:26:PRO:HD3	2.27	0.50
1:A:375:ASN:OD1	1:A:416:CYS:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:THR:HG21	1:F:256:GLU:HG3	1.89	0.50
1:C:331:ASN:N	1:C:332:PRO:HD3	2.27	0.50
1:E:250:ARG:HD3	1:E:252:TYR:CE1	2.47	0.50
1:F:233:PRO:HG3	1:F:265:ILE:HD11	1.94	0.50
1:A:391:VAL:HG13	1:A:441:LYS:HG2	1.93	0.50
1:A:407:TYR:CD2	1:A:407:TYR:N	2.80	0.50
1:E:398:LYS:HG2	1:E:402:ILE:O	2.12	0.49
1:A:409:MSE:HB2	5:A:1021:HOH:O	2.10	0.49
1:A:6:LYS:NZ	1:B:228:GLU:OE1	2.42	0.49
1:D:96:SER:HB2	1:D:109:GLY:CA	2.42	0.49
1:F:180:TRP:CD1	1:F:208:PRO:HG2	2.44	0.49
1:A:123:GLN:HE22	1:A:125:LYS:CB	2.25	0.49
1:F:4:LYS:CG	5:F:1016:HOH:O	2.55	0.49
1:A:232:HIS:ND1	1:A:233:PRO:HD2	2.27	0.49
1:F:232:HIS:CD2	1:F:309:PRO:HG3	2.47	0.49
1:A:402:ILE:HD12	1:A:455:LEU:HD11	1.94	0.49
1:A:365:GLY:O	1:A:406:GLN:HA	2.12	0.49
1:D:193:ARG:CD	5:D:1081:HOH:O	2.59	0.49
1:A:127:ILE:HG13	1:A:174:ILE:HG12	1.93	0.49
1:E:398:LYS:HG3	1:E:404:SER:HB2	1.94	0.49
1:F:57:LYS:HA	1:F:204:ILE:O	2.13	0.49
1:B:207:ASP:HB2	1:B:208:PRO:HD2	1.95	0.49
1:F:53:LEU:CD2	1:F:222:ILE:HG13	2.42	0.49
1:A:403:GLU:CG	1:A:404:SER:N	2.73	0.49
1:E:193:ARG:O	1:E:196:ILE:HG13	2.13	0.49
1:B:92:ARG:O	1:B:113:LYS:HE3	2.13	0.49
1:F:188:TYR:HD1	5:F:985:HOH:O	1.95	0.49
1:C:427:LYS:NZ	5:C:955:HOH:O	2.24	0.49
1:B:196:ILE:HG23	1:B:197:ILE:HG23	1.94	0.49
1:D:255:LYS:HE2	1:D:267:ASP:OD1	2.13	0.49
1:F:381:TYR:HB2	1:F:428:GLU:CG	2.37	0.49
1:B:453:GLN:NE2	1:B:457:GLU:HG3	2.25	0.49
1:C:207:ASP:HB2	1:C:208:PRO:HD2	1.95	0.49
1:B:167:PHE:HA	5:B:1050:HOH:O	2.12	0.49
1:A:459:ARG:O	1:A:462:GLN:N	2.46	0.49
1:B:284:LYS:HD3	1:B:286:LYS:HE2	1.94	0.49
1:F:423:LYS:NZ	1:F:432:GLU:OE2	2.37	0.49
1:F:52:ILE:O	1:F:54:PRO:HD3	2.13	0.48
1:E:207:ASP:OD1	1:E:207:ASP:C	2.51	0.48
1:E:92:ARG:O	1:E:113:LYS:HD3	2.13	0.48
1:D:370:VAL:O	1:D:371:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ILE:HD12	1:E:402:ILE:N	2.28	0.48
1:E:289:THR:HG23	1:E:292:GLU:HG3	1.94	0.48
1:F:128:GLU:HB2	1:F:173:ALA:HB3	1.94	0.48
1:A:461:GLU:OE1	1:A:461:GLU:HA	2.13	0.48
1:C:205:PHE:O	1:C:212:VAL:HA	2.13	0.48
1:D:441:LYS:HZ1	1:D:445:MSE:HE1	1.79	0.48
1:D:383:GLU:HG3	5:D:1035:HOH:O	2.14	0.48
1:D:441:LYS:NZ	1:D:445:MSE:HE1	2.29	0.48
1:C:65:ASP:C	1:C:65:ASP:OD1	2.52	0.48
1:F:196:ILE:HG12	1:F:329:ILE:CD1	2.40	0.48
1:A:26:PRO:CD	1:A:30:ARG:HG2	2.42	0.48
1:F:255:LYS:NZ	1:F:271:ASP:OD1	2.45	0.48
1:C:254:ILE:HA	1:C:285:VAL:HG13	1.95	0.48
1:A:148:ILE:N	1:A:148:ILE:HD13	2.29	0.48
1:F:400:TYR:O	1:F:452:LYS:HG3	2.13	0.48
1:B:87:PRO:HA	1:B:144:LEU:HD21	1.96	0.48
1:F:214:TYR:C	1:F:216:PRO:HD3	2.33	0.48
1:F:283:LYS:HG2	1:F:284:LYS:N	2.27	0.48
1:C:331:ASN:CG	1:C:331:ASN:O	2.52	0.48
1:D:399:ARG:NE	5:D:1018:HOH:O	2.47	0.48
1:C:196:ILE:HG22	1:C:197:ILE:HG23	1.95	0.48
1:F:236:VAL:CG1	1:F:300:PHE:CD2	2.97	0.48
1:A:402:ILE:HG22	5:A:977:HOH:O	2.13	0.48
1:B:397:TRP:C	1:B:399:ARG:H	2.17	0.48
1:E:444:LEU:O	1:E:447:VAL:HG23	2.14	0.48
1:F:33:TYR:CG	1:F:33:TYR:O	2.67	0.48
1:A:207:ASP:HB2	1:A:208:PRO:HD3	1.94	0.48
1:C:136:SER:HA	5:C:1044:HOH:O	2.13	0.48
1:E:21:GLU:CD	1:E:21:GLU:H	2.17	0.48
1:E:21:GLU:OE2	1:F:419:LYS:NZ	2.44	0.48
1:B:123:GLN:OE1	1:B:125:LYS:HB2	2.14	0.48
1:A:229:VAL:HG11	1:A:313:SER:CB	2.38	0.47
1:C:340:ARG:CD	1:C:439:GLU:OE2	2.61	0.47
1:C:34:GLN:O	1:C:38:GLU:HG2	2.14	0.47
1:A:338:ILE:CG2	1:A:447:VAL:HG13	2.40	0.47
1:A:96:SER:HB2	1:A:109:GLY:CA	2.44	0.47
1:B:193:ARG:O	1:B:196:ILE:HG22	2.13	0.47
1:F:317:ILE:O	1:F:321:LEU:HD12	2.14	0.47
1:C:124:ASP:HB2	5:C:983:HOH:O	2.14	0.47
1:E:49:VAL:O	1:E:49:VAL:HG12	2.13	0.47
1:F:33:TYR:CD2	1:F:381:TYR:HE2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:HG12	1:A:318:GLY:N	2.29	0.47
1:F:219:THR:CG2	1:F:221:LYS:H	2.27	0.47
1:E:30:ARG:HD3	1:E:381:TYR:CE1	2.48	0.47
1:C:44:LEU:HB3	1:C:105:ARG:CZ	2.43	0.47
1:A:255:LYS:NZ	1:A:271:ASP:OD1	2.32	0.47
1:F:53:LEU:HD21	1:F:222:ILE:CG1	2.43	0.47
1:C:453:GLN:HE21	1:C:457:GLU:CD	2.17	0.47
1:A:161:VAL:HG12	1:A:162:GLU:N	2.29	0.47
1:F:373:TYR:HA	1:F:377:ILE:O	2.14	0.47
1:B:65:ASP:OD2	1:B:65:ASP:N	2.46	0.47
1:E:37:ARG:NH1	1:E:41:GLU:OE1	2.47	0.47
1:A:190:TYR:O	1:A:194:THR:CG2	2.63	0.47
1:F:117:LEU:HD23	1:F:148:ILE:HD11	1.97	0.47
1:B:17:LYS:HG2	1:B:148:ILE:HD13	1.97	0.47
1:F:311:ALA:CB	1:F:342:PRO:HG3	2.43	0.47
1:F:131:THR:HG22	1:F:170:THR:HG1	1.76	0.47
1:B:390:LYS:HG3	1:B:394:GLU:OE2	2.15	0.47
1:F:4:LYS:HE2	5:F:1016:HOH:O	2.14	0.47
1:A:99:TYR:CE2	1:B:10:LEU:HG	2.49	0.47
1:B:400:TYR:O	1:B:452:LYS:HA	2.15	0.47
1:F:149:ASN:CA	5:F:969:HOH:O	2.62	0.47
1:F:253:THR:HG22	1:F:256:GLU:CG	2.43	0.47
1:A:123:GLN:NE2	1:A:125:LYS:CB	2.78	0.47
1:A:26:PRO:HD2	1:A:30:ARG:CG	2.43	0.47
1:F:444:LEU:HA	1:F:444:LEU:HD23	1.64	0.47
1:F:232:HIS:CG	1:F:233:PRO:HD2	2.49	0.47
1:C:254:ILE:HG22	1:C:274:LEU:HD21	1.97	0.47
1:B:333:ASP:H	1:B:359:GLY:HA3	1.79	0.47
1:A:102:ARG:HD3	1:A:104:THR:CG2	2.44	0.47
1:E:221:LYS:CE	5:E:1045:HOH:O	2.55	0.47
1:A:423:LYS:HG2	1:A:431:ALA:HB2	1.95	0.47
1:B:47:THR:HG22	1:B:78:GLY:HA2	1.97	0.47
1:F:43:SER:O	1:F:46:ALA:N	2.48	0.47
1:E:358:PHE:CD2	1:E:359:GLY:N	2.83	0.47
1:E:7:PHE:CD2	1:F:85:GLU:OE1	2.68	0.46
1:F:405:ASP:OD1	1:F:405:ASP:N	2.40	0.46
1:F:395:LEU:O	1:F:397:TRP:CD1	2.69	0.46
1:F:20:PRO:HD2	1:F:21:GLU:OE2	2.14	0.46
1:A:100:VAL:HG13	1:A:228:GLU:HG3	1.96	0.46
1:D:180:TRP:HB3	1:D:181:PRO:HD3	1.96	0.46
1:A:324:LEU:HD23	5:A:1059:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:LYS:HA	1:F:332:PRO:CG	2.45	0.46
1:D:207:ASP:HB2	1:D:208:PRO:HD3	1.97	0.46
1:F:18:ARG:O	1:F:20:PRO:HD3	2.15	0.46
1:A:309:PRO:HG2	1:A:343:LYS:O	2.15	0.46
1:B:83:PRO:HG3	1:B:140:TYR:CZ	2.51	0.46
1:C:33:TYR:O	1:C:37:ARG:HB2	2.16	0.46
1:D:324:LEU:CD2	1:D:328:LYS:HG3	2.45	0.46
1:C:10:LEU:HG	1:D:99:TYR:CE2	2.50	0.46
1:C:144:LEU:C	1:C:144:LEU:HD12	2.36	0.46
1:F:206:LYS:CA	1:F:211:ASN:O	2.59	0.46
1:F:330:PHE:O	1:F:332:PRO:HD2	2.15	0.46
1:B:237:ASP:OD1	1:B:240:GLU:HG3	2.16	0.46
1:F:225:PRO:HA	1:F:226:PRO:HD3	1.79	0.46
1:F:253:THR:HA	1:F:283:LYS:O	2.16	0.46
1:D:371:LEU:HB2	1:D:412:MSE:HB3	1.97	0.46
1:A:112:VAL:O	1:A:116:VAL:HG23	2.15	0.46
1:F:212:VAL:CG1	1:F:214:TYR:HE1	2.28	0.46
1:E:311:ALA:HB2	1:E:342:PRO:HG3	1.91	0.46
1:F:112:VAL:HG22	4:F:950:ANP:O2A	2.16	0.46
1:C:71:LYS:HE3	1:C:173:ALA:HB1	1.97	0.46
1:B:427:LYS:NZ	4:B:910:ANP:O3G	2.26	0.46
1:D:186:ARG:HG2	1:D:380:ILE:HG21	1.98	0.46
1:B:250:ARG:NH1	1:B:252:TYR:HE1	2.04	0.46
1:C:161:VAL:CG1	1:C:162:GLU:N	2.78	0.46
1:D:86:VAL:N	1:D:87:PRO:CD	2.79	0.46
1:F:254:ILE:CD1	1:F:285:VAL:HA	2.46	0.45
1:F:102:ARG:HB2	1:F:228:GLU:HA	1.98	0.45
1:F:81:ILE:HD13	1:F:90:PHE:CE2	2.50	0.45
1:B:143:LYS:HB2	1:B:157:GLU:H	1.81	0.45
1:E:81:ILE:HD12	1:E:90:PHE:HE2	1.81	0.45
1:A:422:TYR:CE2	1:A:427:LYS:HD2	2.51	0.45
1:F:58:ILE:CG2	1:F:74:VAL:HG22	2.46	0.45
1:E:22:LEU:CD2	1:F:424:SER:HA	2.46	0.45
1:E:27:ASN:HB2	1:E:28:PRO:CD	2.46	0.45
1:E:295:ARG:O	1:E:299:THR:CG2	2.57	0.45
1:C:71:LYS:CE	1:C:173:ALA:HB1	2.46	0.45
1:C:257:PHE:CG	1:C:285:VAL:HG11	2.51	0.45
1:D:230:LYS:HE2	1:D:260:ASN:O	2.16	0.45
1:F:198:THR:CG2	1:F:203:PHE:HE1	2.30	0.45
1:C:249:LYS:CE	1:C:249:LYS:CA	2.88	0.45
1:C:127:ILE:O	1:C:127:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:THR:O	1:E:292:GLU:N	2.49	0.45
1:F:45:ASP:OD2	1:F:104:THR:HB	2.16	0.45
1:D:45:ASP:O	1:D:49:VAL:HB	2.16	0.45
1:F:180:TRP:CZ2	1:F:184:LYS:HG3	2.50	0.45
1:F:254:ILE:HD13	1:F:285:VAL:HA	1.97	0.45
1:B:130:GLU:CG	1:B:141:THR:HG22	2.38	0.45
1:E:295:ARG:HG3	1:F:67:ARG:NH2	2.32	0.45
1:F:296:LEU:CD2	1:F:300:PHE:CZ	2.99	0.45
1:A:433:VAL:CG1	1:A:436:ILE:HD13	2.47	0.45
1:B:17:LYS:O	1:B:17:LYS:HD2	2.16	0.45
5:D:1032:HOH:O	1:E:221:LYS:HE3	2.17	0.45
1:B:255:LYS:NZ	1:B:267:ASP:OD1	2.49	0.45
1:A:345:TYR:CD2	1:A:436:ILE:HD11	2.52	0.45
1:A:251:ASP:OD2	1:A:284:LYS:HD3	2.16	0.45
1:E:232:HIS:O	1:E:347:GLY:HA2	2.17	0.45
1:F:37:ARG:HG2	1:F:41:GLU:OE2	2.16	0.45
1:B:255:LYS:CE	1:B:267:ASP:OD1	2.65	0.45
1:E:44:LEU:HB3	1:E:105:ARG:CZ	2.46	0.45
1:E:196:ILE:HD11	1:E:373:TYR:OH	2.17	0.45
1:F:207:ASP:HB2	1:F:208:PRO:CD	2.43	0.45
1:F:148:ILE:O	1:F:148:ILE:HG22	2.17	0.45
1:F:155:ILE:HG12	5:F:980:HOH:O	2.16	0.45
1:A:102:ARG:HB2	1:A:228:GLU:HA	1.99	0.45
1:E:331:ASN:N	1:E:332:PRO:HD3	2.32	0.45
1:B:248:LEU:HD22	1:B:252:TYR:HE2	1.79	0.44
1:F:392:VAL:HG22	1:F:444:LEU:HD11	1.98	0.44
1:F:105:ARG:HB3	1:F:377:ILE:HD11	1.98	0.44
1:E:280:LYS:HA	1:E:281:PRO:HD3	1.79	0.44
1:C:87:PRO:HB3	1:C:155:ILE:HD11	1.99	0.44
1:E:375:ASN:OD1	1:E:416:CYS:HA	2.17	0.44
1:F:83:PRO:HD3	1:F:133:PRO:HG3	1.99	0.44
1:A:102:ARG:HD3	1:A:104:THR:HG23	1.99	0.44
1:F:6:LYS:HE2	5:F:1026:HOH:O	2.17	0.44
1:B:441:LYS:NZ	1:B:445:MSE:HE1	2.31	0.44
1:F:253:THR:H	1:F:256:GLU:HB2	1.83	0.44
1:A:137:LYS:CE	1:A:137:LYS:H	2.29	0.44
1:E:213:THR:CG2	1:E:215:TYR:OH	2.53	0.44
1:C:326:LEU:HD13	1:C:357:ALA:HB2	2.00	0.44
1:E:118:TYR:CE2	1:E:177:PRO:HD2	2.53	0.44
1:F:58:ILE:HG23	1:F:74:VAL:HG22	1.98	0.44
1:E:453:GLN:NE2	1:E:457:GLU:HG3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:GLU:O	1:E:18:ARG:HG3	2.18	0.44
1:E:30:ARG:CG	5:E:1016:HOH:O	2.64	0.44
1:A:96:SER:HB3	1:A:99:TYR:CE2	2.53	0.44
1:E:402:ILE:CG2	1:E:403:GLU:N	2.80	0.44
1:D:100:VAL:CG1	1:D:228:GLU:CD	2.86	0.44
1:E:27:ASN:HB2	1:E:28:PRO:HD2	2.00	0.44
1:E:385:SER:HB3	1:F:385:SER:HB3	1.99	0.44
1:A:221:LYS:HD3	5:A:1047:HOH:O	2.17	0.44
1:A:319:GLU:O	1:A:323:GLU:HG3	2.18	0.44
1:E:25:PHE:N	1:E:26:PRO:HD3	2.33	0.44
1:B:118:TYR:CE2	1:B:177:PRO:HD2	2.52	0.44
1:F:93:VAL:HG12	1:F:94:LEU:HG	1.99	0.44
1:A:108:TYR:CE2	1:A:427:LYS:HD3	2.53	0.44
1:C:121:MSE:HE2	1:D:237:ASP:OD2	2.18	0.44
1:F:35:THR:HG23	1:F:115:ALA:HB1	1.98	0.44
1:F:291:GLU:HG2	1:F:291:GLU:H	1.40	0.44
1:C:423:LYS:NZ	1:D:382:ASP:OD1	2.50	0.44
1:A:18:ARG:O	1:B:419:LYS:HE3	2.17	0.44
1:D:161:VAL:CG1	1:D:162:GLU:N	2.81	0.44
1:F:289:THR:HG22	1:F:292:GLU:CG	2.47	0.44
1:E:255:LYS:O	1:E:259:VAL:HG12	2.18	0.44
1:F:87:PRO:O	1:F:91:GLY:N	2.49	0.44
1:F:118:TYR:CE2	1:F:177:PRO:HD2	2.53	0.44
1:E:27:ASN:ND2	1:E:30:ARG:H	2.16	0.44
1:A:10:LEU:HD12	1:B:99:TYR:CZ	2.52	0.44
1:D:196:ILE:CD1	1:D:329:ILE:HD11	2.48	0.44
1:C:144:LEU:O	1:C:144:LEU:HD12	2.17	0.43
1:C:207:ASP:CB	1:C:208:PRO:CD	2.88	0.43
1:B:200:TYR:OH	1:B:376:LYS:NZ	2.51	0.43
1:F:12:PRO:O	1:F:16:PHE:HD2	2.01	0.43
1:A:207:ASP:CB	1:A:208:PRO:CD	2.94	0.43
1:B:255:LYS:O	1:B:259:VAL:HG13	2.19	0.43
1:C:254:ILE:CG2	1:C:274:LEU:HD21	2.48	0.43
1:F:53:LEU:HD11	1:F:220:ASN:OD1	2.18	0.43
1:F:127:ILE:CD1	1:F:174:ILE:HD11	2.48	0.43
1:D:207:ASP:CB	1:D:208:PRO:CD	2.94	0.43
1:A:96:SER:HB2	1:A:109:GLY:HA2	2.00	0.43
1:A:306:PHE:HB2	5:A:932:HOH:O	2.18	0.43
1:C:338:ILE:HG22	1:C:447:VAL:HG13	2.00	0.43
1:F:56:ILE:HD12	1:F:203:PHE:HE2	1.83	0.43
1:C:48:ASP:OD1	1:C:105:ARG:NH2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:VAL:O	1:F:94:LEU:HB2	2.18	0.43
1:F:207:ASP:OD1	1:F:211:ASN:HB2	2.18	0.43
1:F:127:ILE:HD12	1:F:174:ILE:HD11	1.97	0.43
1:F:386:ASP:OD1	1:F:387:VAL:N	2.51	0.43
1:F:180:TRP:CD2	1:F:208:PRO:CG	2.91	0.43
1:C:318:GLY:O	1:C:322:ILE:HG13	2.18	0.43
1:E:60:ILE:HG22	1:E:208:PRO:HG3	2.00	0.43
1:C:148:ILE:HG13	1:C:149:ASN:N	2.34	0.43
1:F:250:ARG:CB	5:F:1023:HOH:O	2.66	0.43
1:B:21:GLU:HG3	1:B:26:PRO:HA	2.00	0.43
1:A:323:GLU:OE2	5:A:948:HOH:O	2.21	0.43
1:D:157:GLU:HG3	5:D:1002:HOH:O	2.17	0.43
1:C:29:ALA:HB2	1:C:179:ASP:HB3	2.01	0.43
1:C:96:SER:HB2	1:C:109:GLY:CA	2.48	0.43
1:D:93:VAL:O	1:D:94:LEU:HB2	2.19	0.43
1:B:49:VAL:O	1:B:49:VAL:HG12	2.19	0.43
1:F:319:GLU:HA	1:F:337:SER:OG	2.19	0.43
1:D:116:VAL:CG2	1:D:127:ILE:HD13	2.49	0.43
1:F:37:ARG:HD2	5:F:983:HOH:O	2.18	0.43
1:C:123:GLN:NE2	1:C:175:SER:HB2	2.34	0.43
1:A:25:PHE:N	1:A:26:PRO:HD3	2.33	0.43
1:B:157:GLU:HG2	5:B:1038:HOH:O	2.17	0.43
1:F:19:ASN:CB	1:F:22:LEU:HD22	2.48	0.42
1:B:253:THR:HB	1:B:281:PRO:O	2.18	0.42
1:D:227:GLN:NE2	5:D:965:HOH:O	2.52	0.42
1:B:6:LYS:CE	5:B:1051:HOH:O	2.66	0.42
1:A:34:GLN:NE2	1:A:37:ARG:NH1	2.67	0.42
1:F:289:THR:CG2	1:F:292:GLU:CG	2.96	0.42
1:E:387:VAL:HG12	1:E:430:ILE:HB	2.01	0.42
1:F:284:LYS:O	1:F:285:VAL:C	2.57	0.42
1:F:129:ILE:HD12	1:F:144:LEU:HD12	2.01	0.42
1:A:224:LYS:HA	1:A:225:PRO:HD3	1.95	0.42
1:F:388:ILE:O	1:F:392:VAL:HG23	2.20	0.42
1:B:397:TRP:HB3	1:B:402:ILE:HD12	2.00	0.42
1:B:397:TRP:C	1:B:399:ARG:N	2.73	0.42
1:B:253:THR:HA	1:B:283:LYS:O	2.18	0.42
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.88	0.42
1:F:331:ASN:HA	1:F:331:ASN:HD22	1.52	0.42
1:F:253:THR:HG1	1:F:282:ASN:HA	1.83	0.42
1:E:311:ALA:CB	1:E:342:PRO:HG2	2.43	0.42
1:F:398:LYS:O	1:F:399:ARG:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ILE:CG1	1:F:174:ILE:HD13	2.50	0.42
1:F:34:GLN:NE2	1:F:38:GLU:OE1	2.49	0.42
1:C:304:GLU:OE2	1:E:307:ARG:NH2	2.53	0.42
1:A:27:ASN:HD21	1:A:30:ARG:H	1.62	0.42
1:F:57:LYS:HD3	1:F:204:ILE:HD12	2.00	0.42
1:B:229:VAL:HG11	1:B:313:SER:HB3	2.01	0.42
1:B:368:PRO:HB3	1:B:409:MSE:HE3	2.00	0.42
1:A:32:LEU:HA	1:A:176:ILE:HD11	2.01	0.42
1:E:402:ILE:HG22	1:E:403:GLU:N	2.33	0.42
1:F:214:TYR:C	1:F:216:PRO:CD	2.87	0.42
1:A:146:ILE:HG22	1:A:148:ILE:HD13	2.02	0.42
1:F:33:TYR:OH	1:F:380:ILE:CG1	2.66	0.42
1:E:273:ILE:HD11	1:E:306:PHE:CZ	2.55	0.42
1:E:67:ARG:HG2	1:F:298:GLU:OE1	2.20	0.42
1:A:64:ASP:O	1:A:68:GLN:N	2.52	0.42
1:C:247:ASN:HD22	1:C:247:ASN:N	2.16	0.42
1:A:117:LEU:CD2	1:A:148:ILE:HD12	2.50	0.42
1:C:120:GLN:NE2	1:C:146:ILE:N	2.56	0.42
1:F:398:LYS:C	1:F:400:TYR:N	2.73	0.42
1:E:117:LEU:C	1:E:121:MSE:HE3	2.40	0.42
1:F:92:ARG:O	1:F:113:LYS:CE	2.55	0.42
1:C:206:LYS:HA	1:C:211:ASN:O	2.19	0.42
1:C:356:VAL:HG13	1:C:356:VAL:O	2.19	0.42
1:C:53:LEU:HA	1:C:54:PRO:HD3	1.86	0.42
1:C:332:PRO:HD2	5:C:1026:HOH:O	2.20	0.42
1:E:27:ASN:HD22	1:E:29:ALA:H	1.68	0.42
1:E:193:ARG:HD2	1:E:193:ARG:HH11	1.71	0.42
1:B:343:LYS:HE2	5:B:1020:HOH:O	2.19	0.42
1:C:438:LYS:HE2	5:C:959:HOH:O	2.19	0.42
1:E:37:ARG:HG3	1:E:41:GLU:OE2	2.20	0.41
1:F:307:ARG:NH2	5:F:1031:HOH:O	2.52	0.41
1:F:233:PRO:HG3	1:F:265:ILE:CD1	2.50	0.41
1:A:423:LYS:HG2	1:A:431:ALA:CA	2.50	0.41
1:F:63:ILE:HD11	1:F:71:LYS:HD2	2.02	0.41
1:F:117:LEU:HD23	1:F:148:ILE:CD1	2.45	0.41
1:B:318:GLY:O	1:B:322:ILE:HG13	2.20	0.41
1:B:24:GLY:C	1:B:26:PRO:HD3	2.40	0.41
1:F:320:ASP:OD1	1:F:321:LEU:HG	2.20	0.41
1:A:100:VAL:HG13	1:A:228:GLU:CG	2.50	0.41
1:F:48:ASP:C	1:F:48:ASP:OD1	2.58	0.41
1:B:133:PRO:O	1:B:135:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ASN:N	1:E:20:PRO:HD3	2.36	0.41
1:D:96:SER:HB2	1:D:109:GLY:HA2	2.02	0.41
1:E:99:TYR:CE2	1:F:10:LEU:HG	2.55	0.41
1:E:277:ALA:CB	1:E:299:THR:HG21	2.48	0.41
1:C:25:PHE:N	1:C:26:PRO:CD	2.83	0.41
1:B:441:LYS:NZ	1:B:445:MSE:CE	2.83	0.41
1:F:30:ARG:NH2	1:F:34:GLN:OE1	2.52	0.41
1:E:22:LEU:HD22	1:F:424:SER:HA	2.01	0.41
1:A:374:ALA:HA	1:A:415:LEU:O	2.20	0.41
1:A:222:ILE:HA	1:A:223:PRO:HD3	1.93	0.41
1:B:167:PHE:CA	5:B:1050:HOH:O	2.67	0.41
1:F:44:LEU:O	1:F:45:ASP:C	2.59	0.41
1:F:107:MSE:HE2	1:F:108:TYR:CE1	2.56	0.41
1:D:312:ASP:OD1	1:D:312:ASP:N	2.51	0.41
1:F:152:GLU:HA	1:F:153:PRO:HD3	1.86	0.41
1:F:212:VAL:CG1	1:F:214:TYR:CE1	3.04	0.41
1:A:237:ASP:OD2	1:B:17:LYS:NZ	2.53	0.41
1:C:330:PHE:CA	5:C:945:HOH:O	2.62	0.41
1:F:72:VAL:O	1:F:173:ALA:HA	2.21	0.41
1:A:238:ARG:NH1	1:A:290:GLU:O	2.53	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.94	0.41
1:A:237:ASP:OD2	1:B:121:MSE:HE3	2.21	0.41
1:F:55:ASN:HA	1:F:202:GLU:HB3	2.02	0.41
1:F:187:ILE:O	1:F:191:ILE:HG12	2.21	0.41
1:F:4:LYS:N	5:F:974:HOH:O	2.53	0.41
1:B:232:HIS:CD2	1:B:309:PRO:HG3	2.56	0.41
1:A:145:LYS:NZ	1:B:290:GLU:HG3	2.36	0.41
1:A:273:ILE:HD11	1:A:306:PHE:HE1	1.85	0.41
1:A:389:TRP:CE3	5:A:1058:HOH:O	2.74	0.41
1:B:222:ILE:HG23	1:B:222:ILE:O	2.21	0.41
1:E:112:VAL:HG12	4:E:940:ANP:O2A	2.21	0.41
1:E:224:LYS:HA	1:E:225:PRO:HD3	1.87	0.41
1:F:420:ILE:HA	1:F:421:PRO:HD3	1.92	0.41
1:F:34:GLN:O	1:F:38:GLU:CG	2.67	0.41
1:F:64:ASP:CG	1:F:67:ARG:HB2	2.41	0.41
1:F:424:SER:O	1:F:427:LYS:HA	2.20	0.41
1:B:64:ASP:CG	1:B:67:ARG:CG	2.89	0.41
1:D:196:ILE:HD11	1:D:329:ILE:HD11	2.03	0.41
1:D:232:HIS:CG	1:D:233:PRO:HD2	2.56	0.41
1:C:9:SER:HB3	1:D:95:TYR:CD1	2.56	0.41
1:F:236:VAL:HG13	1:F:236:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:HA	1:B:196:ILE:HD12	1.83	0.40
1:C:12:PRO:HG3	1:D:12:PRO:HG3	2.03	0.40
1:D:407:TYR:CD1	1:D:409:MSE:HE2	2.56	0.40
1:E:134:VAL:HB	5:E:1049:HOH:O	2.21	0.40
1:D:420:ILE:HA	1:D:421:PRO:HD3	1.88	0.40
1:D:335:ALA:HA	1:D:356:VAL:O	2.22	0.40
1:F:180:TRP:CB	1:F:208:PRO:HG2	2.48	0.40
1:F:256:GLU:O	1:F:260:ASN:HB2	2.21	0.40
1:F:381:TYR:N	1:F:428:GLU:OE1	2.46	0.40
1:E:48:ASP:CG	1:E:105:ARG:HH22	2.23	0.40
1:F:43:SER:O	1:F:44:LEU:C	2.59	0.40
1:E:225:PRO:HA	1:E:226:PRO:HD3	1.92	0.40
1:C:192:LYS:HE3	5:C:970:HOH:O	2.20	0.40
1:D:226:PRO:HG3	1:D:315:SER:HB2	2.02	0.40
1:F:53:LEU:HG	1:F:222:ILE:HD11	2.02	0.40
1:A:284:LYS:CD	1:A:286:LYS:HE2	2.50	0.40
1:C:239:GLU:CG	5:C:936:HOH:O	2.68	0.40
1:C:411:VAL:HG13	1:C:444:LEU:HD21	2.03	0.40
1:D:438:LYS:HE3	1:D:438:LYS:HB2	1.84	0.40
1:F:117:LEU:CD2	1:F:148:ILE:HD11	2.50	0.40
1:F:47:THR:HG21	1:F:54:PRO:HA	2.04	0.40
1:E:207:ASP:HB2	1:E:208:PRO:HD2	2.03	0.40
1:F:296:LEU:CD2	1:F:300:PHE:CE2	3.04	0.40
1:E:358:PHE:C	1:E:358:PHE:CD2	2.95	0.40
1:E:368:PRO:HD3	1:E:407:TYR:CE2	2.56	0.40
1:D:222:ILE:HG13	1:D:223:PRO:HD2	2.03	0.40
1:E:80:GLY:HA2	1:E:170:THR:OG1	2.22	0.40
1:E:236:VAL:O	1:E:297:VAL:HG13	2.21	0.40
1:E:238:ARG:HG2	1:E:297:VAL:HG21	2.03	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	457/472 (97%)	440 (96%)	17 (4%)	0	100	100
1	B	453/472 (96%)	426 (94%)	24 (5%)	3 (1%)	26	31
1	C	464/472 (98%)	448 (97%)	15 (3%)	1 (0%)	52	64
1	D	459/472 (97%)	440 (96%)	19 (4%)	0	100	100
1	E	452/472 (96%)	427 (94%)	22 (5%)	3 (1%)	26	31
1	F	444/472 (94%)	379 (85%)	48 (11%)	17 (4%)	4	2
All	All	2729/2832 (96%)	2560 (94%)	145 (5%)	24 (1%)	21	24

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	208	PRO
1	F	245	ILE
1	F	246	ASN
1	F	332	PRO
1	F	399	ARG
1	C	166	GLY
1	E	290	GLU
1	F	26	PRO
1	F	63	ILE
1	F	148	ILE
1	F	340	ARG
1	B	166	GLY
1	E	247	ASN
1	F	65	ASP
1	B	134	VAL
1	F	94	LEU
1	F	126	PRO
1	F	398	LYS
1	E	398	LYS
1	F	46	ALA
1	F	87	PRO
1	F	101	ASN
1	B	156	VAL
1	F	125	LYS

### 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	407/412 (99%)	382 (94%)	25 (6%)	23	30
1	B	402/412 (98%)	380 (94%)	22 (6%)	27	36
1	C	410/412 (100%)	383 (93%)	27 (7%)	21	27
1	D	404/412 (98%)	384 (95%)	20 (5%)	30	41
1	E	407/412 (99%)	378 (93%)	29 (7%)	18	23
1	F	389/412 (94%)	343 (88%)	46 (12%)	6	7
All	All	2419/2472 (98%)	2250 (93%)	169 (7%)	19	23

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	22	LEU
1	A	27	ASN
1	A	62	LEU
1	A	81	ILE
1	A	100	VAL
1	A	110	LEU
1	A	137	LYS
1	A	160	SER
1	A	194	THR
1	A	224	LYS
1	A	249	LYS
1	A	259	VAL
1	A	285	VAL
1	A	296	LEU
1	A	321	LEU
1	A	364	VAL
1	A	371	LEU
1	A	405	ASP
1	A	407	TYR
1	A	409	MSE
1	A	427	LYS
1	A	434	GLU
1	A	449	ARG
1	A	456	SER
1	B	17	LYS
1	B	22	LEU

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Mol	Chain	Res	Type
1	B	55	ASN
1	B	62	LEU
1	B	65	ASP
1	B	67	ARG
1	B	137	LYS
1	B	144	LEU
1	B	157	GLU
1	B	158	ARG
1	B	185	SER
1	B	224	LYS
1	B	247	ASN
1	B	285	VAL
1	B	290	GLU
1	B	296	LEU
1	B	304	GLU
1	B	321	LEU
1	B	324	LEU
1	B	371	LEU
1	B	378	PRO
1	B	444	LEU
1	C	17	LYS
1	C	22	LEU
1	C	30	ARG
1	C	37	ARG
1	C	62	LEU
1	C	73	ASN
1	C	100	VAL
1	C	110	LEU
1	C	113	LYS
1	C	138	ARG
1	C	144	LEU
1	C	152	GLU
1	C	196	ILE
1	C	221	LYS
1	C	239	GLU
1	C	244	LEU
1	C	249	LYS
1	C	263	GLN
1	C	267	ASP
1	C	285	VAL
1	C	290	GLU
1	C	296	LEU

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Mol	Chain	Res	Type
1	C	321	LEU
1	C	371	LEU
1	C	395	LEU
1	C	405	ASP
1	C	460	LYS
1	D	22	LEU
1	D	30	ARG
1	D	37	ARG
1	D	62	LEU
1	D	85	GLU
1	D	138	ARG
1	D	250	ARG
1	D	276	LEU
1	D	285	VAL
1	D	291	GLU
1	D	296	LEU
1	D	312	ASP
1	D	321	LEU
1	D	324	LEU
1	D	371	LEU
1	D	385	SER
1	D	405	ASP
1	D	418	THR
1	D	444	LEU
1	D	458	LYS
1	E	6	LYS
1	E	17	LYS
1	E	37	ARG
1	E	62	LEU
1	E	85	GLU
1	E	100	VAL
1	E	110	LEU
1	E	138	ARG
1	E	196	ILE
1	E	217	ARG
1	E	222	ILE
1	E	259	VAL
1	E	273	ILE
1	E	289	THR
1	E	296	LEU
1	E	298	GLU
1	E	299	THR

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Mol	Chain	Res	Type
1	E	310	SER
1	E	312	ASP
1	E	313	SER
1	E	321	LEU
1	E	338	ILE
1	E	340	ARG
1	E	371	LEU
1	E	398	LYS
1	E	403	GLU
1	E	404	SER
1	E	424	SER
1	E	447	VAL
1	F	17	LYS
1	F	21	GLU
1	F	22	LEU
1	F	30	ARG
1	F	47	THR
1	F	57	LYS
1	F	62	LEU
1	F	76	ASP
1	F	77	ASN
1	F	79	ILE
1	F	84	GLN
1	F	110	LEU
1	F	112	VAL
1	F	119	SER
1	F	120	GLN
1	F	124	ASP
1	F	131	THR
1	F	134	VAL
1	F	172	VAL
1	F	174	ILE
1	F	175	SER
1	F	196	ILE
1	F	198	THR
1	F	208	PRO
1	F	219	THR
1	F	220	ASN
1	F	238	ARG
1	F	244	LEU
1	F	251	ASP
1	F	252	TYR

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Mol	Chain	Res	Type
1	F	253	THR
1	F	259	VAL
1	F	285	VAL
1	F	289	THR
1	F	290	GLU
1	F	291	GLU
1	F	298	GLU
1	F	307	ARG
1	F	312	ASP
1	F	315	SER
1	F	331	ASN
1	F	361	SER
1	F	390	LYS
1	F	395	LEU
1	F	405	ASP
1	F	427	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	101	ASN
1	A	120	GLN
1	A	123	GLN
1	A	247	ASN
1	A	408	GLN
1	B	120	GLN
1	B	408	GLN
1	B	453	GLN
1	C	101	ASN
1	C	120	GLN
1	C	123	GLN
1	C	247	ASN
1	C	348	HIS
1	C	408	GLN
1	C	453	GLN
1	D	247	ASN
1	E	27	ASN
1	E	88	ASN
1	E	101	ASN
1	E	120	GLN
1	E	247	ASN

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Mol	Chain	Res	Type
1	E	408	GLN
1	E	453	GLN
1	F	27	ASN
1	F	73	ASN
1	F	77	ASN
1	F	120	GLN
1	F	220	ASN
1	F	227	GLN
1	F	331	ASN
1	F	453	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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$
4	ANP	A	900	2	27,33,33	1.86	7 (25%)	30,52,52	1.81	7 (23%)
4	ANP	B	910	2	27,33,33	2.02	7 (25%)	30,52,52	2.00	5 (16%)
4	ANP	C	920	2	27,33,33	2.10	7 (25%)	30,52,52	1.85	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ANP	D	930	2	27,33,33	2.08	6 (22%)	30,52,52	1.86	5 (16%)
4	ANP	E	940	2	27,33,33	2.03	9 (33%)	30,52,52	1.75	5 (16%)
4	ANP	F	950	2	27,33,33	1.99	7 (25%)	30,52,52	2.17	7 (23%)

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
4	ANP	A	900	2	-	0/12/38/38	0/3/3/3
4	ANP	B	910	2	-	1/12/38/38	0/3/3/3
4	ANP	C	920	2	-	1/12/38/38	0/3/3/3
4	ANP	D	930	2	-	1/12/38/38	0/3/3/3
4	ANP	E	940	2	-	0/12/38/38	0/3/3/3
4	ANP	F	950	2	-	0/12/38/38	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	920	ANP	PB-O3A	-7.80	1.49	1.59
4	F	950	ANP	PB-O3A	-6.32	1.51	1.59
4	D	930	ANP	PB-O3A	-6.23	1.51	1.59
4	B	910	ANP	PB-O3A	-5.89	1.51	1.59
4	A	900	ANP	PB-O3A	-5.36	1.52	1.59
4	E	940	ANP	PB-O3A	-5.19	1.52	1.59
4	B	910	ANP	PG-O2G	-3.32	1.47	1.56
4	D	930	ANP	PG-O2G	-3.11	1.48	1.56
4	B	910	ANP	PB-O2B	-3.00	1.48	1.56
4	A	900	ANP	PG-O2G	-2.99	1.48	1.56
4	E	940	ANP	PG-O3G	-2.93	1.48	1.56
4	A	900	ANP	PB-O2B	-2.86	1.48	1.56
4	C	920	ANP	PB-O2B	-2.74	1.49	1.56
4	E	940	ANP	PG-O2G	-2.71	1.49	1.56
4	E	940	ANP	PB-O2B	-2.59	1.49	1.56
4	B	910	ANP	PG-O3G	-2.54	1.49	1.56
4	A	900	ANP	PG-O3G	-2.51	1.49	1.56
4	C	920	ANP	PG-O2G	-2.48	1.49	1.56
4	F	950	ANP	PG-O3G	-2.34	1.50	1.56
4	F	950	ANP	PG-O2G	-2.32	1.50	1.56
4	D	930	ANP	PB-O2B	-2.28	1.50	1.56
4	E	940	ANP	C4-N3	-2.28	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	910	ANP	C5-N7	-2.27	1.31	1.39
4	E	940	ANP	C5-N7	-2.07	1.32	1.39
4	C	920	ANP	PG-O3G	-2.01	1.51	1.56
4	F	950	ANP	O4'-C1'	2.08	1.43	1.41
4	A	900	ANP	PB-O1B	2.46	1.48	1.46
4	D	930	ANP	C5-C4	2.63	1.46	1.40
4	C	920	ANP	C5-C4	2.63	1.46	1.40
4	C	920	ANP	PG-O1G	2.80	1.49	1.46
4	E	940	ANP	C5-C4	2.82	1.46	1.40
4	C	920	ANP	PB-O1B	2.88	1.49	1.46
4	A	900	ANP	C5-C4	2.89	1.47	1.40
4	F	950	ANP	PB-O1B	2.91	1.49	1.46
4	F	950	ANP	PG-O1G	3.03	1.49	1.46
4	A	900	ANP	PG-O1G	3.09	1.49	1.46
4	F	950	ANP	C5-C4	3.22	1.47	1.40
4	E	940	ANP	PB-O1B	3.28	1.49	1.46
4	B	910	ANP	PG-O1G	3.42	1.50	1.46
4	B	910	ANP	PB-O1B	3.46	1.50	1.46
4	D	930	ANP	PB-O1B	3.93	1.50	1.46
4	D	930	ANP	PG-O1G	4.07	1.50	1.46
4	E	940	ANP	PG-O1G	4.45	1.51	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	920	ANP	N3-C2-N1	-7.21	123.37	128.89
4	A	900	ANP	N3-C2-N1	-6.77	123.71	128.89
4	D	930	ANP	N3-C2-N1	-6.68	123.78	128.89
4	B	910	ANP	N3-C2-N1	-6.32	124.06	128.89
4	F	950	ANP	N3-C2-N1	-5.94	124.35	128.89
4	E	940	ANP	N3-C2-N1	-5.79	124.46	128.89
4	B	910	ANP	C4-C5-N7	-4.41	105.42	109.48
4	F	950	ANP	O1G-PG-N3B	-4.39	105.16	111.90
4	F	950	ANP	C2'-C1'-N9	-4.08	108.06	114.29
4	D	930	ANP	C4-C5-N7	-3.87	105.92	109.48
4	B	910	ANP	C2'-C1'-N9	-3.41	109.08	114.29
4	E	940	ANP	C4-C5-N7	-3.26	106.48	109.48
4	C	920	ANP	O1G-PG-N3B	-3.22	106.96	111.90
4	A	900	ANP	PA-O3A-PB	-3.00	122.59	132.67
4	F	950	ANP	C4-C5-N7	-2.78	106.92	109.48
4	C	920	ANP	C4-C5-N7	-2.75	106.95	109.48
4	D	930	ANP	O1G-PG-N3B	-2.46	108.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	930	ANP	C2'-C1'-N9	-2.41	110.61	114.29
4	F	950	ANP	PA-O3A-PB	-2.37	124.70	132.67
4	A	900	ANP	C1'-N9-C4	-2.26	123.53	126.94
4	A	900	ANP	C4-C5-N7	-2.09	107.55	109.48
4	C	920	ANP	PA-O3A-PB	-2.09	125.67	132.67
4	E	940	ANP	PA-O3A-PB	-2.05	125.79	132.67
4	B	910	ANP	PA-O3A-PB	-2.05	125.80	132.67
4	A	900	ANP	C2-N1-C6	2.18	122.66	118.77
4	A	900	ANP	C4'-O4'-C1'	2.54	112.51	109.72
4	A	900	ANP	O3A-PA-O5'	2.73	110.17	102.94
4	E	940	ANP	O3A-PA-O5'	2.88	110.58	102.94
4	C	920	ANP	C4'-O4'-C1'	2.88	112.89	109.72
4	D	930	ANP	C4'-O4'-C1'	3.35	113.41	109.72
4	E	940	ANP	C4'-O4'-C1'	3.77	113.86	109.72
4	F	950	ANP	O4'-C1'-N9	3.91	116.28	108.10
4	B	910	ANP	C4'-O4'-C1'	4.09	114.21	109.72
4	F	950	ANP	C4'-O4'-C1'	4.30	114.45	109.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	910	ANP	O1G-PG-N3B-PB
4	C	920	ANP	O1G-PG-N3B-PB
4	D	930	ANP	O1G-PG-N3B-PB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	910	ANP	1	0
4	D	930	ANP	1	0
4	E	940	ANP	1	0
4	F	950	ANP	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	456/472 (96%)	0.62	49 (10%)	8 12	4, 16, 48, 94	0
1	B	450/472 (95%)	0.51	37 (8%)	14 20	4, 16, 40, 56	0
1	C	461/472 (97%)	0.58	36 (7%)	16 22	7, 18, 39, 52	0
1	D	456/472 (96%)	0.45	27 (5%)	26 34	4, 15, 37, 71	0
1	E	451/472 (95%)	0.67	48 (10%)	8 12	4, 18, 50, 72	0
1	F	449/472 (95%)	1.87	174 (38%)	0 0	18, 46, 72, 98	0
All	All	2723/2832 (96%)	0.78	371 (13%)	4 6	4, 19, 59, 98	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	136	SER	9.5
1	F	401	GLY	9.4
1	C	164	THR	9.2
1	A	464	ALA	9.1
1	F	405	ASP	8.3
1	D	164	THR	8.0
1	D	403	GLU	7.8
1	F	461	GLU	7.4
1	F	62	LEU	7.2
1	F	156	VAL	7.1
1	F	56	ILE	7.0
1	F	75	VAL	7.0
1	C	165	ARG	6.8
1	A	467	LYS	6.8
1	F	333	ASP	6.7
1	F	320	ASP	6.6
1	F	157	GLU	6.6
1	F	161	VAL	6.4
1	D	463	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	462	GLN	6.3
1	B	404	SER	6.3
1	F	217	ARG	6.2
1	F	364	VAL	6.1
1	F	462	GLN	6.0
1	A	135	ASN	6.0
1	F	362	ILE	6.0
1	F	463	GLU	6.0
1	F	162	GLU	5.9
1	F	203	PHE	5.9
1	E	311	ALA	5.8
1	B	457	GLU	5.8
1	B	135	ASN	5.8
1	F	321	LEU	5.7
1	A	405	ASP	5.7
1	B	164	THR	5.7
1	F	139	ILE	5.6
1	F	213	THR	5.6
1	C	166	GLY	5.5
1	E	402	ILE	5.5
1	F	246	ASN	5.5
1	E	304	GLU	5.5
1	A	312	ASP	5.5
1	F	132	SER	5.4
1	B	167	PHE	5.3
1	F	129	ILE	5.3
1	A	463	GLU	5.3
1	F	453	GLN	5.2
1	E	167	PHE	5.2
1	A	406	GLN	5.2
1	E	4	LYS	5.2
1	F	208	PRO	5.1
1	A	460	LYS	5.1
1	F	212	VAL	5.1
1	B	137	LYS	5.0
1	C	167	PHE	4.9
1	F	400	TYR	4.9
1	E	250	ARG	4.9
1	B	251	ASP	4.8
1	F	356	VAL	4.8
1	F	127	ILE	4.8
1	F	360	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	365	GLY	4.8
1	E	399	ARG	4.8
1	F	53	LEU	4.7
1	F	358	PHE	4.7
1	C	65	ASP	4.7
1	F	361	SER	4.6
1	E	282	ASN	4.6
1	D	461	GLU	4.6
1	B	403	GLU	4.6
1	F	185	SER	4.6
1	D	166	GLY	4.5
1	F	61	ASP	4.5
1	F	222	ILE	4.5
1	A	134	VAL	4.5
1	F	154	ILE	4.4
1	F	174	ILE	4.4
1	A	366	GLU	4.4
1	C	168	HIS	4.4
1	A	459	ARG	4.3
1	D	405	ASP	4.3
1	C	403	GLU	4.3
1	C	406	GLN	4.2
1	F	72	VAL	4.2
1	F	183	ALA	4.2
1	F	399	ARG	4.2
1	F	137	LYS	4.2
1	E	251	ASP	4.1
1	B	165	ARG	4.1
1	F	168	HIS	4.1
1	C	135	ASN	4.1
1	F	224	LYS	4.1
1	F	138	ARG	4.1
1	E	404	SER	4.1
1	F	411	VAL	4.0
1	A	407	TYR	4.0
1	F	74	VAL	4.0
1	F	221	LYS	4.0
1	A	401	GLY	4.0
1	D	311	ALA	4.0
1	D	399	ARG	4.0
1	B	166	GLY	3.9
1	F	180	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	211	ASN	3.9
1	E	458	LYS	3.9
1	F	455	LEU	3.9
1	F	402	ILE	3.9
1	F	125	LYS	3.9
1	A	402	ILE	3.9
1	D	162	GLU	3.9
1	F	87	PRO	3.9
1	F	214	TYR	3.9
1	F	164	THR	3.8
1	F	65	ASP	3.8
1	F	216	PRO	3.8
1	E	396	ASP	3.8
1	F	396	ASP	3.8
1	A	458	LYS	3.8
1	F	150	LYS	3.8
1	F	81	ILE	3.8
1	F	77	ASN	3.8
1	F	456	SER	3.7
1	A	404	SER	3.7
1	A	457	GLU	3.7
1	F	406	GLN	3.7
1	E	459	ARG	3.7
1	D	402	ILE	3.7
1	F	459	ARG	3.7
1	F	324	LEU	3.7
1	F	366	GLU	3.7
1	F	134	VAL	3.7
1	E	249	LYS	3.7
1	F	63	ILE	3.6
1	F	66	ALA	3.6
1	F	54	PRO	3.6
1	F	368	PRO	3.6
1	B	136	SER	3.6
1	E	135	ASN	3.6
1	F	225	PRO	3.6
1	F	325	GLY	3.6
1	C	329	ILE	3.6
1	D	459	ARG	3.6
1	E	134	VAL	3.6
1	F	130	GLU	3.6
1	A	4	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	405	ASP	3.6
1	F	182	LYS	3.5
1	F	460	LYS	3.5
1	F	131	THR	3.5
1	F	85	GLU	3.5
1	E	312	ASP	3.5
1	F	60	ILE	3.5
1	E	164	THR	3.5
1	F	133	PRO	3.5
1	F	148	ILE	3.5
1	F	204	ILE	3.5
1	F	33	TYR	3.4
1	F	39	LEU	3.4
1	E	457	GLU	3.4
1	A	163	ASN	3.4
1	C	331	ASN	3.4
1	F	189	GLU	3.4
1	F	58	ILE	3.4
1	E	137	LYS	3.4
1	C	407	TYR	3.4
1	F	335	ALA	3.4
1	B	65	ASP	3.4
1	C	267	ASP	3.4
1	F	176	ILE	3.4
1	F	257	PHE	3.3
1	E	367	GLU	3.3
1	F	329	ILE	3.3
1	D	406	GLN	3.3
1	B	447	VAL	3.3
1	E	303	TYR	3.3
1	D	464	ALA	3.3
1	F	141	THR	3.2
1	A	162	GLU	3.2
1	B	453	GLN	3.2
1	B	456	SER	3.2
1	A	395	LEU	3.2
1	A	251	ASP	3.2
1	A	411	VAL	3.2
1	F	188	TYR	3.2
1	F	104	THR	3.2
1	F	326	LEU	3.1
1	B	221	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	249	LYS	3.1
1	E	136	SER	3.1
1	C	250	ARG	3.1
1	A	448	ALA	3.1
1	B	66	ALA	3.1
1	B	249	LYS	3.1
1	F	314	LEU	3.1
1	E	252	TYR	3.1
1	B	163	ASN	3.1
1	A	461	GLU	3.0
1	F	334	PHE	3.0
1	F	109	GLY	3.0
1	A	249	LYS	3.0
1	F	57	LYS	3.0
1	F	454	TYR	3.0
1	F	51	GLY	3.0
1	F	205	PHE	3.0
1	D	304	GLU	3.0
1	F	457	GLU	3.0
1	E	302	LYS	3.0
1	E	461	GLU	3.0
1	D	462	GLN	3.0
1	E	63	ILE	3.0
1	E	451	LEU	3.0
1	F	218	LEU	3.0
1	B	458	LYS	2.9
1	E	162	GLU	2.9
1	B	134	VAL	2.9
1	F	410	VAL	2.9
1	E	305	ASP	2.9
1	D	302	LYS	2.9
1	F	248	LEU	2.9
1	A	451	LEU	2.9
1	F	367	GLU	2.9
1	A	453	GLN	2.9
1	F	327	LYS	2.8
1	F	55	ASN	2.8
1	F	35	THR	2.8
1	E	453	GLN	2.8
1	F	247	ASN	2.8
1	A	444	LEU	2.8
1	B	451	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	197	ILE	2.8
1	B	247	ASN	2.8
1	E	460	LYS	2.8
1	A	66	ALA	2.8
1	F	447	VAL	2.7
1	B	246	ASN	2.7
1	B	359	GLY	2.7
1	C	394	GLU	2.7
1	A	302	LYS	2.7
1	C	155	ILE	2.7
1	F	245	ILE	2.7
1	B	250	ARG	2.7
1	F	4	LYS	2.7
1	B	366	GLU	2.7
1	C	363	PRO	2.7
1	C	361	SER	2.7
1	A	250	ARG	2.7
1	E	293	ILE	2.6
1	B	406	GLN	2.6
1	F	181	PRO	2.6
1	F	172	VAL	2.6
1	C	268	THR	2.6
1	F	398	LYS	2.6
1	A	447	VAL	2.6
1	F	142	PHE	2.6
1	C	312	ASP	2.6
1	F	289	THR	2.6
1	A	466	LYS	2.6
1	C	324	LEU	2.6
1	F	143	LYS	2.6
1	D	167	PHE	2.5
1	F	86	VAL	2.5
1	C	405	ASP	2.5
1	F	332	PRO	2.5
1	F	404	SER	2.5
1	B	307	ARG	2.5
1	B	407	TYR	2.5
1	F	215	TYR	2.5
1	F	251	ASP	2.5
1	A	363	PRO	2.5
1	D	341	LYS	2.5
1	A	399	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	455	LEU	2.5
1	D	165	ARG	2.5
1	C	413	VAL	2.5
1	C	162	GLU	2.5
1	C	459	ARG	2.5
1	F	158	ARG	2.5
1	F	227	GLN	2.5
1	F	308	SER	2.5
1	F	220	ASN	2.5
1	E	64	ASP	2.5
1	F	254	ILE	2.4
1	C	354	ALA	2.4
1	E	291	GLU	2.4
1	F	84	GLN	2.4
1	E	248	LEU	2.4
1	F	369	ILE	2.4
1	F	47	THR	2.4
1	F	126	PRO	2.4
1	B	156	VAL	2.4
1	A	65	ASP	2.4
1	C	359	GLY	2.4
1	A	413	VAL	2.4
1	E	168	HIS	2.4
1	B	398	LYS	2.3
1	E	307	ARG	2.3
1	E	269	THR	2.3
1	E	275	GLU	2.3
1	F	73	ASN	2.3
1	F	97	SER	2.3
1	C	63	ILE	2.3
1	C	355	GLY	2.3
1	D	361	SER	2.3
1	E	447	VAL	2.3
1	D	4	LYS	2.3
1	D	163	ASN	2.3
1	B	405	ASP	2.3
1	A	280	LYS	2.3
1	F	255	LYS	2.3
1	D	135	ASN	2.3
1	F	69	ILE	2.2
1	D	249	LYS	2.2
1	E	280	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	112	VAL	2.2
1	F	140	TYR	2.2
1	B	394	GLU	2.2
1	A	456	SER	2.2
1	A	246	ASN	2.2
1	F	196	ILE	2.2
1	F	68	GLN	2.2
1	F	169	GLY	2.2
1	F	59	THR	2.2
1	C	137	LYS	2.2
1	B	356	VAL	2.2
1	E	413	VAL	2.2
1	F	316	VAL	2.2
1	E	432	GLU	2.2
1	F	128	GLU	2.2
1	F	207	ASP	2.2
1	F	458	LYS	2.2
1	D	134	VAL	2.2
1	B	220	ASN	2.2
1	F	122	HIS	2.2
1	F	114	ALA	2.2
1	F	192	LYS	2.1
1	C	356	VAL	2.1
1	F	330	PHE	2.1
1	C	469	LEU	2.1
1	F	451	LEU	2.1
1	F	115	ALA	2.1
1	F	448	ALA	2.1
1	F	52	ILE	2.1
1	F	317	ILE	2.1
1	F	434	GLU	2.1
1	A	334	PHE	2.1
1	E	289	THR	2.1
1	F	116	VAL	2.1
1	C	251	ASP	2.1
1	F	407	TYR	2.1
1	D	404	SER	2.1
1	F	244	LEU	2.1
1	C	247	ASN	2.1
1	B	362	ILE	2.1
1	D	310	SER	2.1
1	F	147	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	71	LYS	2.1
1	A	331	ASN	2.1
1	E	397	TRP	2.1
1	A	364	VAL	2.1
1	F	110	LEU	2.0
1	A	137	LYS	2.0
1	C	302	LYS	2.0
1	A	313	SER	2.0
1	E	313	SER	2.0
1	F	171	SER	2.0
1	F	49	VAL	2.0
1	C	462	GLN	2.0
1	F	45	ASP	2.0
1	F	198	THR	2.0
1	F	29	ALA	2.0
1	A	295	ARG	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
4	ANP	A	900	31/31	0.95	0.19	2.94	40,45,47,47	0
3	NA	D	901	1/1	0.87	0.22	2.52	78,78,78,78	0
4	ANP	B	910	31/31	0.95	0.20	1.80	38,43,46,47	0
4	ANP	D	930	31/31	0.94	0.19	1.76	41,45,48,48	0
4	ANP	C	920	31/31	0.92	0.20	1.49	42,48,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	E	501	1/1	0.70	0.20	1.36	51,51,51,51	0
4	ANP	E	940	31/31	0.95	0.19	1.24	43,47,49,49	0
4	ANP	F	950	31/31	0.83	0.23	0.20	59,76,78,78	0
2	MG	B	501	1/1	0.82	0.14	-0.11	42,42,42,42	0
2	MG	C	501	1/1	0.88	0.13	-0.73	49,49,49,49	0
2	MG	D	501	1/1	0.86	0.11	-1.11	45,45,45,45	0
2	MG	A	501	1/1	0.91	0.12	-1.57	43,43,43,43	0
2	MG	F	501	1/1	0.80	0.12	-2.39	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.