



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:37 AM GMT

PDB ID : 3F5M  
Title : Crystal Structure of ATP-Bound Phosphofructokinase from Trypanosoma brucei  
Authors : McNae, I.W.; Martinez-Oyanedel, J.; Keillor, J.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.  
Deposited on : 2008-11-04  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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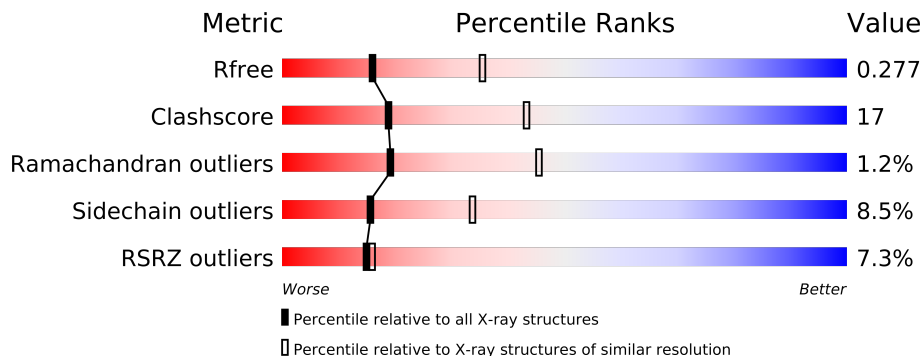
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	487	
1	B	487	
1	C	487	
1	D	487	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	A	490	-	X
5	NA	B	488	-	X

## 2 Entry composition i

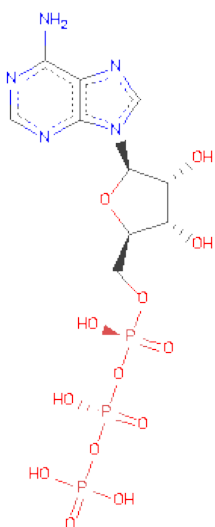
There are 7 unique types of molecules in this entry. The entry contains 14783 atoms, of which 0 are hydrogen and 0 are deuterium.

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 6-phospho-1-fructokinase(ATP-dependent phosphofructokinase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3536	2218	652	649	17			
1	B	462	Total	C	N	O	S	0	0	0
			3569	2234	659	659	17			
1	C	461	Total	C	N	O	S	0	0	0
			3562	2233	658	654	17			
1	D	458	Total	C	N	O	S	0	0	0
			3540	2219	655	649	17			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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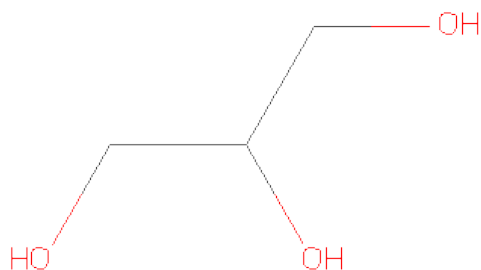
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

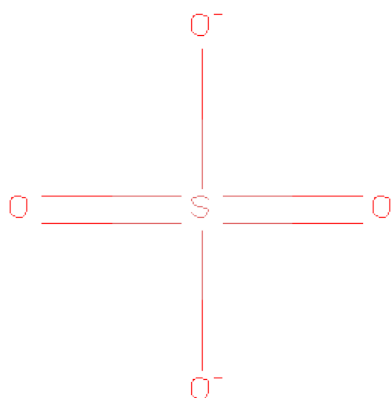


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Na 1	0	0
5	A	2	Total 2	Na 2	0	0
5	C	1	Total 1	Na 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 5	O 4	S 1	0	0

- Molecule 7 is water.

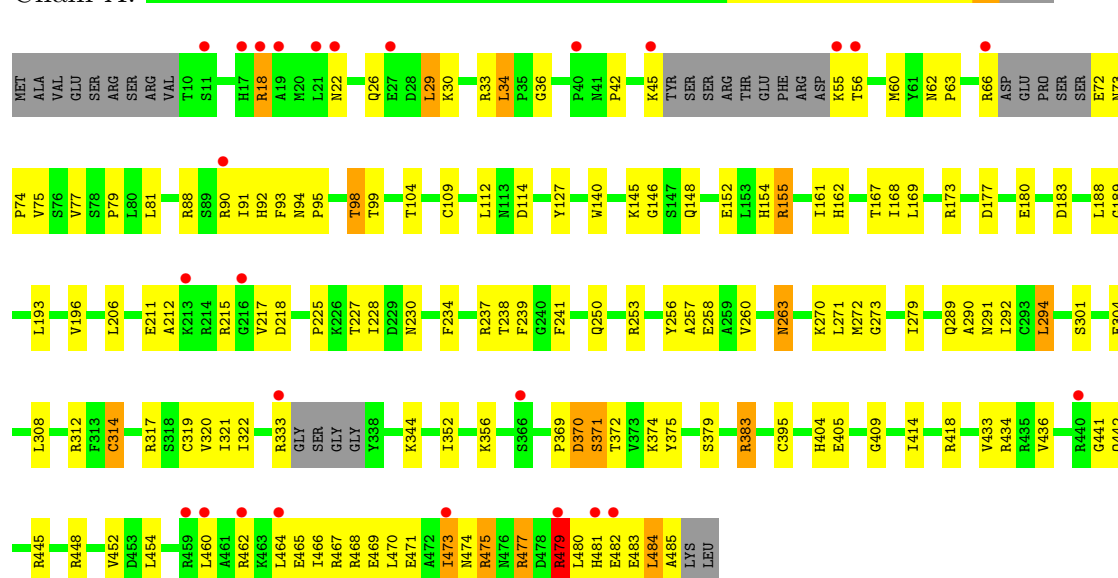
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total 102	O 102	0	0
7	B	103	Total 103	O 103	0	0
7	C	100	Total 100	O 100	0	0
7	D	123	Total 123	O 123	0	0

### 3 Residue-property plots

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

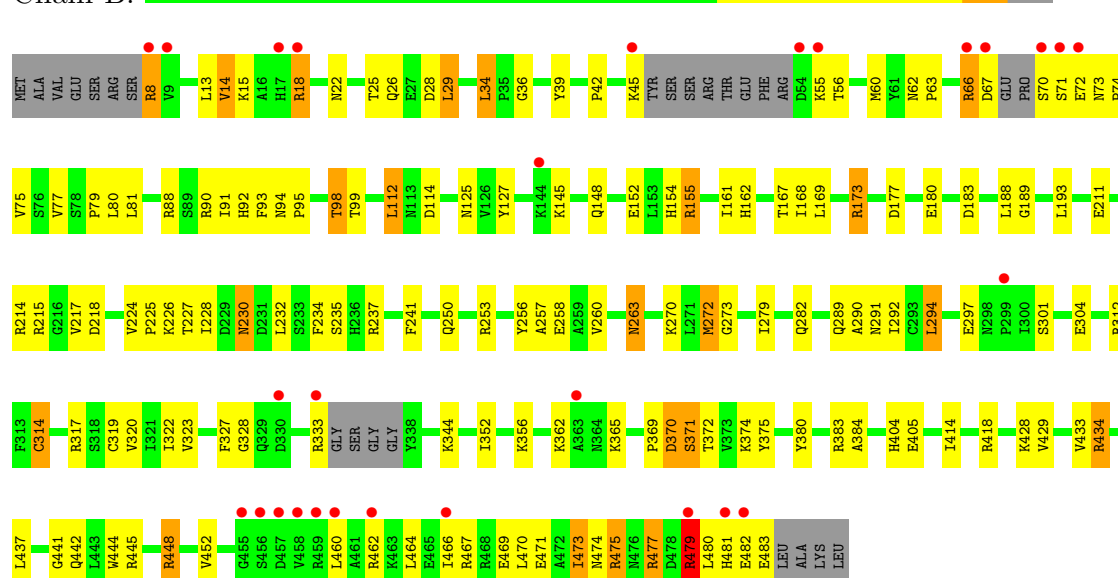
- Molecule 1: 6-phospho-1-fructokinase(ATP-dependent phosphofructokinase)

Chain A:

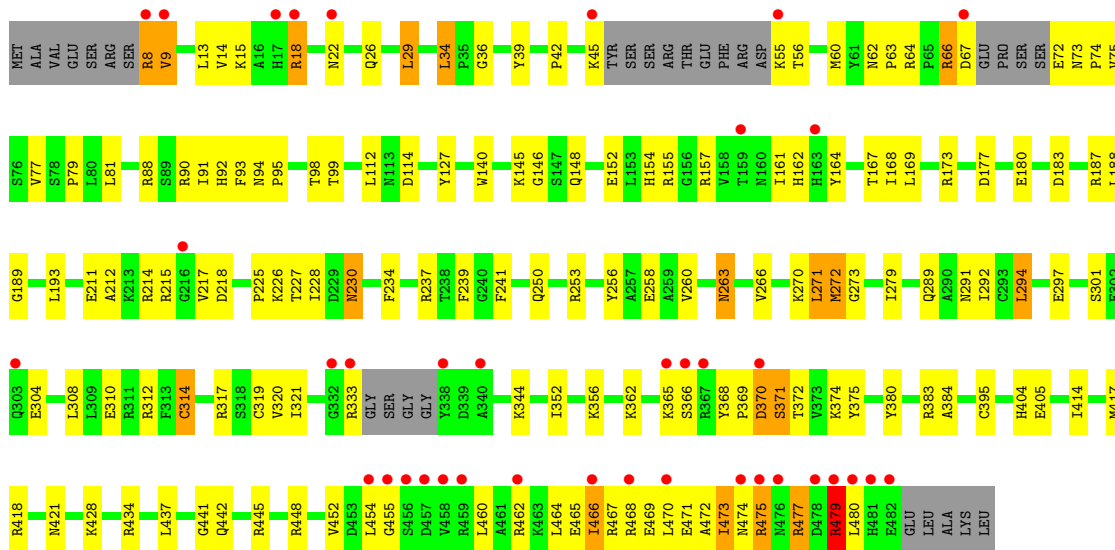


- Molecule 1: 6-phospho-1-fructokinase(ATP-dependent phosphofructokinase)

Chain B:



- Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.58Å 117.57Å 176.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.88 – 2.70 15.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.88-2.70) 97.9 (15.88-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.224 , 0.286 0.213 , 0.277	Depositor DCC
$R_{free}$ test set	2775 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	7 of 54492 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2323e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SO4, ATP, NA

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	0.47	0/3593	0.80	17/4856 (0.4%)
1	B	0.48	0/3626	1.14	22/4900 (0.4%)
1	C	0.46	0/3619	0.73	13/4891 (0.3%)
1	D	0.47	0/3597	0.73	16/4861 (0.3%)
All	All	0.47	0/14435	0.87	68/19508 (0.3%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH1	-20.03	110.28	120.30
1	B	383	ARG	NE-CZ-NH1	-19.32	110.64	120.30
1	B	155	ARG	NE-CZ-NH2	18.89	129.75	120.30
1	B	383	ARG	NE-CZ-NH2	18.87	129.74	120.30
1	B	18	ARG	NE-CZ-NH2	-18.76	110.92	120.30
1	B	434	ARG	NE-CZ-NH1	-17.78	111.41	120.30
1	B	434	ARG	NE-CZ-NH2	17.59	129.09	120.30
1	A	479	ARG	NE-CZ-NH2	17.48	129.04	120.30
1	B	18	ARG	NE-CZ-NH1	17.47	129.04	120.30
1	B	448	ARG	NE-CZ-NH2	17.24	128.92	120.30
1	B	448	ARG	NE-CZ-NH1	-16.96	111.82	120.30
1	A	479	ARG	NE-CZ-NH1	-15.69	112.45	120.30
1	B	467	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	B	467	ARG	NE-CZ-NH2	14.25	127.42	120.30
1	B	66	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	C	66	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	D	66	ARG	NE-CZ-NH1	-11.67	114.46	120.30
1	C	66	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	B	66	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	66	ARG	NE-CZ-NH1	-11.40	114.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ARG	NE-CZ-NH2	10.80	125.70	120.30
1	A	66	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	B	155	ARG	CD-NE-CZ	9.29	136.61	123.60
1	B	434	ARG	CD-NE-CZ	8.98	136.17	123.60
1	B	18	ARG	CD-NE-CZ	8.72	135.80	123.60
1	B	448	ARG	CD-NE-CZ	8.64	135.69	123.60
1	B	383	ARG	CD-NE-CZ	8.62	135.67	123.60
1	C	383	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	383	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	D	383	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	434	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	383	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	479	ARG	CD-NE-CZ	6.99	133.38	123.60
1	C	383	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	434	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	434	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	C	155	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	155	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	18	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	D	434	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	18	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	A	155	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	434	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	434	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	155	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	155	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	467	ARG	CD-NE-CZ	6.12	132.17	123.60
1	C	18	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	A	18	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	D	18	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	18	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	D	155	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	479	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	479	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	271	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	448	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	479	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	66	ARG	CD-NE-CZ	5.59	131.42	123.60
1	A	66	ARG	CD-NE-CZ	5.57	131.39	123.60
1	B	66	ARG	CD-NE-CZ	5.55	131.37	123.60
1	D	383	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	66	ARG	CD-NE-CZ	5.53	131.33	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	448	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	448	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	448	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	467	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	467	ARG	NE-CZ-NH2	-5.11	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3536	0	3608	145	0
1	B	3569	0	3632	142	1
1	C	3562	0	3634	148	1
1	D	3540	0	3612	135	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	C	5	0	0	0	0
7	A	102	0	0	5	0
7	B	103	0	0	7	0
7	C	100	0	0	5	0
7	D	123	0	0	12	0
All	All	14783	0	14550	479	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (479) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:ILE:HG13	1:C:477:ARG:HG2	1.40	1.03
1:A:477:ARG:HG2	1:C:473:ILE:HG13	1.38	1.02
1:B:477:ARG:HG3	1:D:477:ARG:HG3	1.44	0.98
1:C:258:GLU:HG2	1:C:374:LYS:HG3	1.45	0.97
1:C:475:ARG:HH22	1:C:479:ARG:HH11	1.00	0.97
1:B:258:GLU:HG2	1:B:374:LYS:HG3	1.43	0.97
1:A:291:ASN:ND2	1:A:320:VAL:H	1.62	0.96
1:C:291:ASN:HD22	1:C:320:VAL:H	1.02	0.95
1:D:475:ARG:HH22	1:D:479:ARG:HH11	0.96	0.95
1:A:258:GLU:HG2	1:A:374:LYS:HG3	1.47	0.95
1:B:475:ARG:HH22	1:B:479:ARG:HH11	0.97	0.94
1:B:291:ASN:HD22	1:B:320:VAL:H	1.09	0.93
1:C:291:ASN:ND2	1:C:320:VAL:H	1.67	0.92
1:D:291:ASN:HD22	1:D:320:VAL:H	1.11	0.92
1:A:474:ASN:HD21	1:C:477:ARG:HE	1.13	0.91
1:A:291:ASN:HD22	1:A:320:VAL:H	1.03	0.91
1:D:291:ASN:ND2	1:D:320:VAL:H	1.68	0.91
1:A:477:ARG:HE	1:C:474:ASN:HD21	1.18	0.89
1:B:291:ASN:ND2	1:B:320:VAL:H	1.68	0.89
1:A:75:VAL:HG22	1:B:75:VAL:HG22	1.51	0.89
1:D:56:THR:HG22	1:D:88:ARG:HH21	1.35	0.89
1:B:480:LEU:HB2	1:D:473:ILE:HD12	1.54	0.89
1:D:475:ARG:HH22	1:D:479:ARG:NH1	1.70	0.89
1:C:56:THR:HG22	1:C:88:ARG:HH21	1.37	0.89
1:B:475:ARG:HH22	1:B:479:ARG:NH1	1.71	0.88
1:D:258:GLU:HG2	1:D:374:LYS:HG3	1.55	0.87
1:C:75:VAL:HG22	1:D:75:VAL:HG22	1.55	0.87
1:A:56:THR:HG22	1:A:88:ARG:HH21	1.40	0.86
1:B:473:ILE:HD12	1:D:480:LEU:HB2	1.54	0.86
1:D:428:LYS:HD2	7:D:601:HOH:O	1.77	0.85
1:D:475:ARG:NH2	1:D:479:ARG:HH11	1.75	0.85
1:A:474:ASN:ND2	1:C:477:ARG:HE	1.75	0.85
1:A:484:LEU:HB2	1:C:470:LEU:HD11	1.59	0.84
1:C:475:ARG:HH22	1:C:479:ARG:NH1	1.74	0.84
1:A:481:HIS:HA	1:C:470:LEU:HD21	1.57	0.84
1:B:56:THR:HG22	1:B:88:ARG:HH21	1.42	0.84
1:A:477:ARG:HE	1:C:474:ASN:ND2	1.75	0.83
1:B:475:ARG:NH2	1:B:479:ARG:HH11	1.76	0.83
1:A:291:ASN:HD22	1:A:320:VAL:N	1.76	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:475:ARG:HH22	1:A:479:ARG:HH11	1.23	0.82
1:A:470:LEU:HD21	1:C:481:HIS:HA	1.60	0.81
1:C:291:ASN:HD22	1:C:320:VAL:N	1.77	0.81
1:C:475:ARG:NH2	1:C:479:ARG:HH11	1.78	0.81
1:B:291:ASN:HD22	1:B:320:VAL:N	1.80	0.78
1:B:480:LEU:HD13	1:D:473:ILE:CG2	2.13	0.78
1:B:473:ILE:CG2	1:D:480:LEU:HD13	2.12	0.78
1:D:291:ASN:HD22	1:D:320:VAL:N	1.82	0.77
1:B:263:ASN:HD21	1:B:317:ARG:HH11	1.31	0.77
1:D:66:ARG:HG2	1:D:67:ASP:H	1.50	0.76
1:B:8:ARG:HA	1:B:8:ARG:CZ	2.16	0.75
1:D:263:ASN:HD21	1:D:317:ARG:HH11	1.34	0.74
1:C:263:ASN:HD21	1:C:317:ARG:HH11	1.35	0.74
1:B:26:GLN:HE22	1:B:81:LEU:H	1.36	0.74
1:A:474:ASN:HD21	1:C:477:ARG:NE	1.85	0.74
1:D:475:ARG:NH2	1:D:479:ARG:NH1	2.35	0.73
1:B:480:LEU:HD13	1:D:473:ILE:HG22	1.70	0.73
1:B:473:ILE:HG22	1:D:480:LEU:HD13	1.69	0.73
1:A:483:GLU:HG2	1:C:466:ILE:HG21	1.71	0.72
1:B:477:ARG:CG	1:D:477:ARG:HG3	2.19	0.72
1:A:263:ASN:HD21	1:A:317:ARG:HH11	1.32	0.72
1:A:477:ARG:NE	1:C:474:ASN:HD21	1.88	0.72
1:C:475:ARG:NH2	1:C:479:ARG:NH1	2.37	0.72
1:B:475:ARG:NH2	1:B:479:ARG:NH1	2.35	0.72
1:C:270:LYS:HE2	1:C:375:TYR:OH	1.90	0.72
1:D:469:GLU:O	1:D:473:ILE:HG23	1.90	0.71
1:A:26:GLN:HE22	1:A:81:LEU:H	1.39	0.71
1:A:127:TYR:OH	1:A:404:HIS:HD2	1.74	0.71
1:B:88:ARG:NH1	1:B:405:GLU:OE1	2.24	0.70
1:D:26:GLN:HE22	1:D:81:LEU:H	1.38	0.70
1:C:64:ARG:NH1	7:C:586:HOH:O	2.23	0.70
1:A:469:GLU:O	1:A:473:ILE:HG23	1.92	0.70
1:D:56:THR:HG22	1:D:88:ARG:NH2	2.07	0.70
1:B:477:ARG:HG3	1:D:477:ARG:CG	2.19	0.70
1:D:88:ARG:NH1	1:D:405:GLU:OE1	2.25	0.69
1:D:291:ASN:ND2	1:D:319:CYS:HA	2.06	0.69
1:B:469:GLU:O	1:B:473:ILE:HG23	1.91	0.69
1:C:66:ARG:HG2	1:C:67:ASP:H	1.56	0.69
1:B:291:ASN:ND2	1:B:319:CYS:HA	2.07	0.68
1:A:473:ILE:CG2	1:C:480:LEU:HD13	2.23	0.68
1:C:469:GLU:O	1:C:473:ILE:HG23	1.94	0.68
1:B:215:ARG:HB2	1:B:217:VAL:HG23	1.76	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:480:LEU:HD23	1:C:483:GLU:OE1	1.92	0.68
1:C:8:ARG:CZ	1:C:8:ARG:HA	2.22	0.67
1:C:26:GLN:HE22	1:C:81:LEU:H	1.39	0.67
1:A:480:LEU:HD13	1:C:473:ILE:CG2	2.24	0.67
1:A:291:ASN:ND2	1:A:319:CYS:HA	2.10	0.67
1:C:215:ARG:HB2	1:C:217:VAL:HG23	1.77	0.66
1:C:370:ASP:O	1:C:371:SER:HB3	1.96	0.66
1:B:370:ASP:O	1:B:371:SER:HB3	1.96	0.65
1:B:66:ARG:HG2	1:B:67:ASP:H	1.61	0.65
1:C:56:THR:HG22	1:C:88:ARG:NH2	2.11	0.65
1:D:215:ARG:HB2	1:D:217:VAL:HG23	1.79	0.65
1:B:301:SER:OG	1:B:304:GLU:HG3	1.97	0.64
1:A:88:ARG:NH1	1:A:405:GLU:OE1	2.29	0.64
1:A:370:ASP:O	1:A:371:SER:HB3	1.94	0.64
1:A:473:ILE:HG21	1:C:480:LEU:CD1	2.28	0.64
1:D:301:SER:OG	1:D:304:GLU:HG3	1.97	0.64
1:C:127:TYR:OH	1:C:404:HIS:HD2	1.79	0.64
1:A:475:ARG:NH2	1:A:479:ARG:HH11	1.93	0.64
1:A:480:LEU:CD1	1:C:473:ILE:HG21	2.28	0.64
1:B:480:LEU:HB2	1:D:473:ILE:CD1	2.28	0.64
1:D:127:TYR:OH	1:D:404:HIS:HD2	1.80	0.63
1:D:291:ASN:HD22	1:D:319:CYS:HA	1.63	0.63
1:A:263:ASN:ND2	1:A:317:ARG:HD3	2.14	0.63
1:B:127:TYR:OH	1:B:404:HIS:HD2	1.82	0.63
1:D:177:ASP:HB3	1:D:180:GLU:HG3	1.78	0.63
1:D:8:ARG:HA	1:D:8:ARG:CZ	2.28	0.63
1:A:215:ARG:HB2	1:A:217:VAL:HG23	1.80	0.62
1:B:270:LYS:HE2	1:B:375:TYR:OH	1.99	0.62
1:B:460:LEU:O	1:B:464:LEU:HG	1.99	0.62
1:D:270:LYS:HE2	1:D:375:TYR:OH	1.98	0.62
1:A:177:ASP:HB3	1:A:180:GLU:HG3	1.80	0.62
1:C:312:ARG:HB2	1:C:452:VAL:HG21	1.80	0.62
1:C:291:ASN:ND2	1:C:319:CYS:HA	2.15	0.62
1:A:270:LYS:HE2	1:A:375:TYR:OH	1.99	0.62
1:B:258:GLU:CG	1:B:374:LYS:HG3	2.26	0.62
1:A:475:ARG:HH22	1:A:479:ARG:NH1	1.95	0.62
1:A:250:GLN:HE22	1:D:250:GLN:HE22	1.45	0.62
1:A:30:LYS:HG3	7:A:530:HOH:O	1.98	0.62
1:A:473:ILE:HG21	1:C:480:LEU:HD13	1.82	0.62
1:B:258:GLU:HG2	1:B:374:LYS:CG	2.27	0.61
1:B:473:ILE:CD1	1:D:480:LEU:HB2	2.29	0.61
1:A:301:SER:OG	1:A:304:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:481:HIS:C	1:B:483:GLU:H	2.02	0.61
1:D:263:ASN:ND2	1:D:317:ARG:HD3	2.15	0.61
1:C:88:ARG:NH1	1:C:405:GLU:OE1	2.32	0.61
1:B:250:GLN:HE22	1:C:250:GLN:HE22	1.49	0.61
1:A:74:PRO:HD3	1:B:79:PRO:HA	1.83	0.61
1:A:93:PHE:O	1:A:95:PRO:HD3	2.00	0.61
1:B:177:ASP:HB3	1:B:180:GLU:HG3	1.81	0.61
1:D:460:LEU:O	1:D:464:LEU:HG	2.01	0.60
1:C:93:PHE:O	1:C:95:PRO:HD3	2.01	0.60
1:A:312:ARG:HB2	1:A:452:VAL:HG21	1.83	0.60
1:A:145:LYS:O	1:A:148:GLN:HG2	2.02	0.60
1:A:481:HIS:HA	1:C:470:LEU:CD2	2.31	0.60
1:A:475:ARG:NH1	1:B:152:GLU:H	1.99	0.60
1:A:91:ILE:HD11	1:A:95:PRO:HG3	1.84	0.60
1:A:460:LEU:O	1:A:464:LEU:HG	2.02	0.60
1:C:74:PRO:HD3	1:D:79:PRO:HA	1.84	0.59
1:B:56:THR:HG22	1:B:88:ARG:NH2	2.16	0.59
1:C:460:LEU:O	1:C:464:LEU:HG	2.02	0.59
1:B:441:GLY:O	1:B:445:ARG:HG3	2.02	0.59
1:D:145:LYS:O	1:D:148:GLN:HG2	2.02	0.59
1:A:56:THR:HG22	1:A:88:ARG:NH2	2.13	0.59
1:B:263:ASN:ND2	1:B:317:ARG:HD3	2.17	0.59
1:B:145:LYS:O	1:B:148:GLN:HG2	2.02	0.59
1:D:258:GLU:CG	1:D:374:LYS:HG3	2.28	0.58
1:B:473:ILE:HG21	1:D:480:LEU:CB	2.33	0.58
1:B:480:LEU:CB	1:D:473:ILE:HG21	2.32	0.58
1:C:66:ARG:CG	1:C:67:ASP:H	2.15	0.58
1:C:145:LYS:O	1:C:148:GLN:HG2	2.02	0.58
1:C:154:HIS:HB2	7:C:562:HOH:O	2.03	0.58
1:B:291:ASN:HD22	1:B:319:CYS:HA	1.67	0.58
1:D:91:ILE:HD11	1:D:95:PRO:HG3	1.86	0.58
1:A:258:GLU:HG2	1:A:374:LYS:CG	2.30	0.58
1:B:480:LEU:HD13	1:D:473:ILE:HG21	1.85	0.58
1:C:301:SER:OG	1:C:304:GLU:HG3	2.03	0.58
1:D:312:ARG:HB2	1:D:452:VAL:HG21	1.86	0.58
1:D:370:ASP:O	1:D:371:SER:HB3	2.02	0.58
1:B:91:ILE:HD11	1:B:95:PRO:HG3	1.84	0.58
1:C:215:ARG:HB2	1:C:217:VAL:CG2	2.34	0.57
1:A:230:ASN:HD21	1:A:237:ARG:HA	1.70	0.57
1:B:312:ARG:HB2	1:B:452:VAL:HG21	1.87	0.57
1:A:215:ARG:HB2	1:A:217:VAL:CG2	2.36	0.56
1:D:66:ARG:O	1:D:67:ASP:HB2	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:PRO:HA	1:B:74:PRO:HD3	1.88	0.56
1:C:177:ASP:HB3	1:C:180:GLU:HG3	1.86	0.56
1:A:26:GLN:HG2	1:B:70:SER:HB3	1.87	0.56
1:C:475:ARG:HG2	7:D:600:HOH:O	2.05	0.56
1:A:475:ARG:NH2	1:A:479:ARG:HE	2.04	0.55
1:C:263:ASN:ND2	1:C:317:ARG:HD3	2.22	0.55
1:D:441:GLY:O	1:D:445:ARG:HG3	2.06	0.55
1:C:481:HIS:C	1:C:483:GLU:H	2.08	0.55
1:B:473:ILE:HG21	1:D:480:LEU:HD13	1.86	0.55
1:A:480:LEU:HD13	1:C:473:ILE:HG21	1.84	0.55
1:A:473:ILE:CG2	1:C:480:LEU:CD1	2.85	0.55
1:A:258:GLU:CG	1:A:374:LYS:HG3	2.31	0.54
1:C:258:GLU:CG	1:C:374:LYS:HG3	2.29	0.54
1:C:475:ARG:NH1	1:D:152:GLU:H	2.06	0.54
1:D:258:GLU:HG2	1:D:374:LYS:CG	2.33	0.54
1:A:481:HIS:CA	1:C:470:LEU:HD21	2.34	0.54
1:D:187:ARG:NH1	7:D:499:HOH:O	2.41	0.54
1:A:291:ASN:ND2	1:A:320:VAL:N	2.43	0.53
1:A:475:ARG:NH2	1:A:479:ARG:NH1	2.55	0.53
1:A:473:ILE:HG22	1:C:480:LEU:HD13	1.89	0.53
1:A:470:LEU:CD2	1:C:481:HIS:HA	2.35	0.53
1:A:480:LEU:CD1	1:C:473:ILE:CG2	2.86	0.53
1:C:91:ILE:HD11	1:C:95:PRO:HG3	1.90	0.53
1:A:234:PHE:HA	1:A:418:ARG:HD2	1.91	0.53
1:D:475:ARG:NH2	1:D:479:ARG:HD2	2.23	0.53
1:B:215:ARG:HB2	1:B:217:VAL:CG2	2.39	0.53
1:A:481:HIS:C	1:A:483:GLU:H	2.13	0.53
1:B:214:ARG:NH2	7:B:514:HOH:O	2.42	0.53
1:D:215:ARG:HB2	1:D:217:VAL:CG2	2.39	0.52
1:C:230:ASN:HD21	1:C:237:ARG:HA	1.74	0.52
1:A:480:LEU:HD13	1:C:473:ILE:HG22	1.90	0.52
1:A:477:ARG:NE	1:C:474:ASN:ND2	2.51	0.52
1:A:480:LEU:HD23	1:A:483:GLU:OE1	2.09	0.52
1:D:42:PRO:O	1:D:45:LYS:HG2	2.10	0.52
1:B:230:ASN:HD21	1:B:237:ARG:HA	1.75	0.52
1:C:441:GLY:O	1:C:445:ARG:HG3	2.10	0.52
1:C:475:ARG:NH2	1:C:479:ARG:HD2	2.24	0.52
1:D:93:PHE:O	1:D:95:PRO:HD3	2.09	0.52
1:D:230:ASN:HD21	1:D:237:ARG:HA	1.75	0.52
1:C:272:MET:HE3	1:C:272:MET:HA	1.92	0.52
1:A:291:ASN:HD22	1:A:319:CYS:HA	1.72	0.51
1:A:30:LYS:CG	7:A:530:HOH:O	2.56	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:LEU:HA	7:A:582:HOH:O	2.09	0.51
1:B:481:HIS:C	1:B:483:GLU:N	2.64	0.51
1:D:234:PHE:HA	1:D:418:ARG:HD2	1.93	0.51
1:A:477:ARG:HA	1:C:473:ILE:HD12	1.93	0.51
1:A:263:ASN:ND2	1:A:317:ARG:HH11	2.07	0.51
1:A:94:ASN:O	1:A:98:THR:HG22	2.11	0.51
1:B:180:GLU:O	1:B:183:ASP:HB2	2.10	0.51
1:C:234:PHE:HA	1:C:418:ARG:HD2	1.93	0.50
1:A:161:ILE:HG21	1:A:168:ILE:HD13	1.93	0.50
1:B:93:PHE:O	1:B:95:PRO:HD3	2.10	0.50
1:C:79:PRO:HA	1:D:74:PRO:HD3	1.94	0.50
1:B:480:LEU:O	1:D:470:LEU:HD21	2.12	0.50
1:B:66:ARG:CG	1:B:67:ASP:H	2.24	0.50
1:B:225:PRO:HG3	1:B:414:ILE:HB	1.93	0.50
1:A:470:LEU:HD21	1:C:481:HIS:CA	2.38	0.50
1:B:263:ASN:ND2	1:B:317:ARG:HH11	2.04	0.50
1:A:79:PRO:O	1:B:70:SER:HB2	2.12	0.50
1:C:258:GLU:HG2	1:C:374:LYS:CG	2.29	0.50
1:C:291:ASN:HD22	1:C:319:CYS:HA	1.75	0.50
1:B:161:ILE:HG21	1:B:168:ILE:HD13	1.94	0.50
1:B:234:PHE:HA	1:B:418:ARG:HD2	1.94	0.49
1:B:477:ARG:CB	1:D:477:ARG:HG3	2.42	0.49
1:B:475:ARG:NH2	1:B:479:ARG:HD2	2.27	0.49
1:D:13:LEU:O	1:D:14:VAL:HG23	2.11	0.49
1:A:26:GLN:CG	1:B:70:SER:HB3	2.42	0.49
1:D:60:MET:HA	1:D:81:LEU:HD23	1.94	0.49
1:C:8:ARG:HA	1:C:8:ARG:NH1	2.27	0.49
1:D:352:ILE:O	1:D:356:LYS:HG2	2.13	0.49
1:B:235:SER:HB3	7:B:565:HOH:O	2.12	0.49
1:B:477:ARG:HG3	1:D:477:ARG:CB	2.42	0.49
1:A:442:GLN:HE22	1:A:445:ARG:NH2	2.10	0.49
1:B:42:PRO:O	1:B:45:LYS:HG2	2.12	0.49
1:A:152:GLU:H	1:B:475:ARG:NH1	2.11	0.49
1:B:290:ALA:CB	1:B:322:ILE:HD13	2.42	0.49
1:A:475:ARG:HH22	1:A:479:ARG:HE	1.60	0.48
1:B:272:MET:HB2	1:B:279:ILE:HD12	1.95	0.48
1:D:26:GLN:NE2	1:D:81:LEU:H	2.07	0.48
1:A:60:MET:HA	1:A:81:LEU:HD23	1.96	0.48
1:C:162:HIS:H	1:C:162:HIS:CD2	2.31	0.48
1:A:238:THR:HB	7:A:563:HOH:O	2.13	0.48
1:A:34:LEU:HB3	1:A:92:HIS:NE2	2.29	0.48
1:A:477:ARG:CG	1:C:473:ILE:HG13	2.26	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:480:LEU:CD1	1:D:473:ILE:CG2	2.90	0.48
1:C:161:ILE:HG21	1:C:168:ILE:HD13	1.96	0.48
1:C:253:ARG:HG2	1:C:289:GLN:HE22	1.79	0.48
1:D:36:GLY:O	1:D:92:HIS:HD2	1.97	0.48
1:A:230:ASN:HB2	1:A:241:PHE:CD2	2.48	0.48
1:C:442:GLN:HE22	1:C:445:ARG:NH2	2.12	0.48
1:C:211:GLU:O	1:C:215:ARG:HG3	2.13	0.47
1:B:483:GLU:OE1	1:D:466:ILE:HG22	2.14	0.47
1:D:162:HIS:H	1:D:162:HIS:CD2	2.32	0.47
1:C:173:ARG:NH1	2:C:1001:ATP:O1G	2.48	0.47
1:C:314:CYS:HB3	1:C:462:ARG:HH21	1.79	0.47
1:B:13:LEU:O	1:B:14:VAL:HG23	2.15	0.47
1:B:60:MET:HA	1:B:81:LEU:HD23	1.95	0.47
1:A:473:ILE:HD12	1:C:477:ARG:HA	1.97	0.47
1:D:180:GLU:O	1:D:183:ASP:HB2	2.14	0.47
1:A:42:PRO:O	1:A:45:LYS:HG2	2.15	0.47
1:B:480:LEU:CD1	1:D:473:ILE:HG21	2.44	0.47
1:C:66:ARG:HG2	1:C:67:ASP:N	2.27	0.47
1:D:8:ARG:HA	1:D:8:ARG:NE	2.29	0.47
1:C:92:HIS:HE1	1:C:218:ASP:OD1	1.98	0.47
1:C:42:PRO:O	1:C:45:LYS:HG2	2.15	0.47
1:D:314:CYS:HB3	1:D:462:ARG:HH21	1.80	0.47
1:A:441:GLY:O	1:A:445:ARG:HG3	2.14	0.47
1:D:225:PRO:HG3	1:D:414:ILE:HB	1.95	0.47
1:C:481:HIS:C	1:C:483:GLU:N	2.68	0.47
1:A:484:LEU:HD13	1:A:485:ALA:N	2.30	0.47
1:C:99:THR:HB	1:C:189:GLY:O	2.14	0.47
1:B:314:CYS:HB3	1:B:462:ARG:HH21	1.79	0.47
1:A:225:PRO:HG3	1:A:414:ILE:HB	1.95	0.47
1:B:26:GLN:NE2	1:B:81:LEU:H	2.07	0.46
1:A:180:GLU:O	1:A:183:ASP:HB2	2.15	0.46
1:D:15:LYS:HE3	1:D:22:ASN:ND2	2.30	0.46
1:B:70:SER:OG	1:B:71:SER:N	2.48	0.46
1:C:60:MET:HA	1:C:81:LEU:HD23	1.96	0.46
1:C:140:TRP:O	1:C:146:GLY:HA3	2.15	0.46
1:B:442:GLN:HE22	1:B:445:ARG:NH2	2.13	0.46
1:D:442:GLN:HE22	1:D:445:ARG:NH2	2.13	0.46
1:C:79:PRO:HB3	1:D:73:ASN:ND2	2.30	0.46
1:B:272:MET:HA	1:B:272:MET:HE3	1.97	0.46
1:D:92:HIS:HE1	1:D:218:ASP:OD1	1.98	0.46
1:B:384:ALA:HB1	1:C:257:ALA:HB3	1.97	0.46
1:D:417:MET:HG2	1:D:421:ASN:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:448:ARG:NH1	7:B:523:HOH:O	2.47	0.46
1:C:292:ILE:HB	1:C:321:ILE:HG12	1.98	0.46
1:A:484:LEU:HD23	1:C:470:LEU:HD12	1.97	0.46
1:C:152:GLU:H	1:D:475:ARG:NH1	2.12	0.46
1:B:470:LEU:HD21	1:D:480:LEU:O	2.16	0.46
1:D:214:ARG:NH2	7:D:542:HOH:O	2.46	0.46
1:C:352:ILE:O	1:C:356:LYS:HG2	2.15	0.46
1:B:232:LEU:HB3	7:B:565:HOH:O	2.14	0.46
1:B:15:LYS:HE3	1:B:22:ASN:ND2	2.30	0.46
1:D:226:LYS:HA	7:D:553:HOH:O	2.15	0.46
1:B:66:ARG:O	1:B:67:ASP:HB2	2.15	0.46
1:D:366:SER:HB3	7:D:579:HOH:O	2.16	0.46
1:B:8:ARG:HA	1:B:8:ARG:NE	2.30	0.46
1:B:428:LYS:HG3	7:B:567:HOH:O	2.16	0.46
1:A:473:ILE:HG13	1:C:477:ARG:CG	2.29	0.46
1:C:12:LYS:HE2	7:C:542:HOH:O	2.15	0.46
1:C:365:LYS:HD3	7:C:499:HOH:O	2.15	0.46
1:D:211:GLU:O	1:D:215:ARG:HG3	2.16	0.45
1:A:253:ARG:NH2	7:A:522:HOH:O	2.48	0.45
1:C:36:GLY:O	1:C:92:HIS:HD2	1.98	0.45
1:B:444:TRP:O	1:B:448:ARG:HG3	2.16	0.45
1:B:162:HIS:H	1:B:162:HIS:CD2	2.35	0.45
1:A:162:HIS:H	1:A:162:HIS:CD2	2.33	0.45
1:A:212:ALA:O	1:A:217:VAL:HG23	2.16	0.45
1:B:36:GLY:O	1:B:92:HIS:HD2	1.99	0.45
1:B:39:TYR:CZ	1:B:94:ASN:HB2	2.52	0.45
1:B:473:ILE:HG21	1:D:480:LEU:CD1	2.46	0.45
1:B:127:TYR:OH	1:B:404:HIS:CD2	2.67	0.45
1:D:362:LYS:O	1:D:365:LYS:HG3	2.17	0.45
1:D:297:GLU:CD	1:D:437:LEU:HB2	2.37	0.45
1:C:225:PRO:HG3	1:C:414:ILE:HB	1.98	0.44
1:B:173:ARG:NH1	2:B:1001:ATP:O3G	2.50	0.44
1:C:62:ASN:HA	1:C:63:PRO:HD3	1.79	0.44
1:B:481:HIS:O	1:B:483:GLU:N	2.50	0.44
1:C:290:ALA:CB	1:C:322:ILE:HD13	2.47	0.44
1:A:62:ASN:HA	1:A:63:PRO:HD3	1.78	0.44
1:C:484:LEU:HG	1:C:485:ALA:N	2.32	0.44
1:A:484:LEU:CD1	1:A:484:LEU:C	2.86	0.44
1:B:34:LEU:HB3	1:B:92:HIS:NE2	2.32	0.44
1:A:104:THR:HG22	1:A:196:VAL:HB	1.99	0.44
1:A:379:SER:O	1:A:383:ARG:HG3	2.17	0.44
1:D:55:LYS:HB3	1:D:55:LYS:HE2	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:198:GLY:O	1:C:202:GLN:HG2	2.17	0.44
1:B:473:ILE:CG2	1:D:480:LEU:CD1	2.90	0.44
1:C:95:PRO:O	1:C:98:THR:HG23	2.17	0.44
1:B:473:ILE:HG21	1:D:480:LEU:HB3	1.99	0.44
1:D:263:ASN:ND2	1:D:317:ARG:HH11	2.10	0.44
1:A:480:LEU:O	1:C:470:LEU:HD21	2.18	0.44
1:C:226:LYS:HA	7:C:564:HOH:O	2.18	0.44
1:A:271:LEU:HD12	1:A:322:ILE:HG23	2.00	0.44
1:A:140:TRP:O	1:A:146:GLY:HA3	2.18	0.44
1:C:386:PRO:HA	1:C:387:PRO:HD3	1.83	0.44
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.83	0.43
1:C:34:LEU:HB3	1:C:92:HIS:NE2	2.34	0.43
1:A:352:ILE:O	1:A:356:LYS:HG2	2.18	0.43
1:D:140:TRP:O	1:D:146:GLY:HA3	2.17	0.43
1:A:314:CYS:HB3	1:A:462:ARG:HH21	1.83	0.43
1:A:154:HIS:O	1:A:155:ARG:C	2.56	0.43
1:A:481:HIS:C	1:A:483:GLU:N	2.71	0.43
1:B:480:LEU:HB3	1:D:473:ILE:HG21	1.99	0.43
1:B:473:ILE:HG12	1:B:474:ASN:N	2.33	0.43
1:D:212:ALA:O	1:D:217:VAL:HG23	2.18	0.43
1:D:230:ASN:HB2	1:D:241:PHE:CD2	2.53	0.43
1:C:22:ASN:HA	1:C:22:ASN:HD22	1.60	0.43
1:A:257:ALA:HB3	1:D:384:ALA:HB1	1.99	0.43
1:B:22:ASN:HA	1:B:22:ASN:HD22	1.63	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.80	0.43
1:B:73:ASN:HD22	1:B:73:ASN:N	2.16	0.43
1:C:34:LEU:HD23	1:C:93:PHE:CZ	2.52	0.43
1:B:352:ILE:O	1:B:356:LYS:HG2	2.18	0.43
1:D:256:TYR:CZ	1:D:260:VAL:HG21	2.53	0.43
1:C:33:ARG:HA	1:C:409:GLY:O	2.18	0.43
1:B:224:VAL:HA	1:B:225:PRO:HD3	1.84	0.43
1:C:197:GLY:HA2	1:C:226:LYS:HB3	2.00	0.43
1:A:484:LEU:O	1:A:485:ALA:HB3	2.18	0.43
1:B:477:ARG:HB2	1:D:477:ARG:HG3	2.01	0.43
1:A:211:GLU:O	1:A:215:ARG:HG3	2.19	0.43
1:B:290:ALA:HB2	1:B:322:ILE:HD13	1.99	0.43
1:B:297:GLU:CD	1:B:437:LEU:HB2	2.39	0.43
1:D:455:GLY:HA2	7:D:593:HOH:O	2.19	0.43
1:A:127:TYR:OH	1:A:404:HIS:CD2	2.63	0.43
1:C:230:ASN:HB2	1:C:241:PHE:CD2	2.53	0.43
1:D:99:THR:HB	1:D:189:GLY:O	2.19	0.43
1:B:477:ARG:HG3	1:D:477:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:HIS:HE1	1:B:218:ASP:OD1	2.01	0.43
1:C:228:ILE:O	1:C:279:ILE:HD11	2.19	0.43
1:A:473:ILE:HD12	1:C:480:LEU:HB2	2.00	0.42
1:A:95:PRO:O	1:A:98:THR:HG23	2.18	0.42
1:B:362:LYS:O	1:B:365:LYS:HG3	2.19	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.83	0.42
1:B:125:ASN:HD21	1:B:155:ARG:NH2	2.17	0.42
1:B:99:THR:HB	1:B:189:GLY:O	2.18	0.42
1:C:263:ASN:ND2	1:C:317:ARG:HH11	2.11	0.42
1:D:272:MET:HE3	1:D:272:MET:HA	2.01	0.42
1:A:470:LEU:HD21	1:C:480:LEU:O	2.20	0.42
1:B:154:HIS:HE1	7:B:580:HOH:O	2.01	0.42
1:C:13:LEU:O	1:C:14:VAL:HG23	2.20	0.42
1:D:127:TYR:OH	1:D:404:HIS:CD2	2.67	0.42
1:A:94:ASN:O	1:A:98:THR:CG2	2.67	0.42
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.81	0.42
1:A:239:PHE:HB2	1:A:395:CYS:SG	2.59	0.42
1:A:62:ASN:C	1:A:62:ASN:OD1	2.58	0.42
1:D:73:ASN:HA	1:D:74:PRO:HD3	1.78	0.42
1:B:256:TYR:CZ	1:B:260:VAL:HG21	2.55	0.42
1:B:292:ILE:HG22	1:B:294:LEU:HD13	2.02	0.42
1:D:465:GLU:O	1:D:468:ARG:HB2	2.20	0.42
1:D:292:ILE:HG22	1:D:294:LEU:HD13	2.01	0.42
1:B:380:TYR:CE1	1:C:374:LYS:HD2	2.55	0.42
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.78	0.42
1:A:253:ARG:HA	1:A:289:GLN:HE22	1.85	0.42
1:B:226:LYS:HA	7:B:511:HOH:O	2.19	0.42
1:A:230:ASN:HD21	1:A:237:ARG:CA	2.33	0.42
1:D:253:ARG:HA	1:D:289:GLN:HE22	1.83	0.42
1:D:161:ILE:HG21	1:D:168:ILE:HD13	2.02	0.42
1:B:270:LYS:HA	1:B:323:VAL:O	2.20	0.41
1:B:94:ASN:O	1:B:98:THR:HG22	2.19	0.41
1:C:17:HIS:CE1	1:C:434:ARG:CZ	3.03	0.41
1:A:33:ARG:HA	1:A:409:GLY:O	2.20	0.41
1:A:228:ILE:O	1:A:279:ILE:HD11	2.20	0.41
1:A:374:LYS:HD2	1:D:380:TYR:CE1	2.56	0.41
1:A:92:HIS:HE1	1:A:218:ASP:OD1	2.03	0.41
1:D:39:TYR:CZ	1:D:94:ASN:HB2	2.54	0.41
1:D:66:ARG:HG2	1:D:67:ASP:N	2.29	0.41
1:A:290:ALA:CB	1:A:322:ILE:HD13	2.50	0.41
1:D:292:ILE:HB	1:D:321:ILE:HG12	2.02	0.41
1:C:39:TYR:HA	1:C:40:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:474:ASN:ND2	1:C:477:ARG:NE	2.52	0.41
1:A:473:ILE:CD1	1:C:480:LEU:HB2	2.50	0.41
1:D:473:ILE:HG12	1:D:474:ASN:N	2.34	0.41
1:C:174:GLY:O	2:C:1001:ATP:O3'	2.37	0.41
1:D:228:ILE:O	1:D:279:ILE:HD11	2.21	0.41
1:B:257:ALA:HB3	1:C:384:ALA:HB1	2.02	0.41
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.83	0.41
1:D:34:LEU:HB3	1:D:92:HIS:NE2	2.35	0.41
1:D:164:TYR:HB3	7:D:493:HOH:O	2.19	0.41
1:A:292:ILE:HB	1:A:321:ILE:HG12	2.03	0.41
1:D:239:PHE:HB2	1:D:395:CYS:SG	2.60	0.41
1:A:480:LEU:HB2	1:C:473:ILE:CD1	2.51	0.41
1:A:484:LEU:HB2	1:C:470:LEU:CD1	2.42	0.41
1:A:26:GLN:NE2	1:B:70:SER:HB3	2.35	0.41
1:C:180:GLU:O	1:C:183:ASP:HB2	2.19	0.41
1:C:173:ARG:HG3	1:C:341:SER:OG	2.20	0.41
1:D:253:ARG:HG2	1:D:289:GLN:HE22	1.86	0.41
1:A:308:LEU:HD21	1:A:454:LEU:HG	2.03	0.41
1:D:308:LEU:HD21	1:D:454:LEU:HG	2.03	0.41
1:C:26:GLN:NE2	1:C:81:LEU:H	2.13	0.41
1:C:212:ALA:O	1:C:217:VAL:HG23	2.21	0.41
1:D:310:GLU:HG3	1:D:368:TYR:OH	2.20	0.41
1:A:465:GLU:O	1:A:468:ARG:HB2	2.21	0.41
1:D:9:VAL:HG13	1:D:64:ARG:NH2	2.36	0.41
1:C:483:GLU:O	1:C:485:ALA:O	2.38	0.41
1:B:228:ILE:O	1:B:279:ILE:HD11	2.20	0.41
1:D:272:MET:HB2	1:D:279:ILE:HD12	2.02	0.41
1:D:64:ARG:NH1	7:D:522:HOH:O	2.39	0.41
1:B:253:ARG:HA	1:B:289:GLN:HE22	1.85	0.41
1:B:62:ASN:HA	1:B:63:PRO:HD3	1.78	0.41
1:B:282:GLN:HE21	1:B:282:GLN:HB3	1.67	0.41
1:B:25:THR:O	1:B:28:ASP:HB2	2.21	0.41
1:A:99:THR:HB	1:A:189:GLY:O	2.20	0.41
1:D:154:HIS:CD2	7:D:600:HOH:O	2.73	0.40
1:D:266:VAL:HA	1:D:319:CYS:O	2.21	0.40
1:D:73:ASN:HD22	1:D:73:ASN:N	2.17	0.40
1:C:465:GLU:O	1:C:468:ARG:HB2	2.21	0.40
1:A:29:LEU:HA	1:A:29:LEU:HD12	1.96	0.40
1:D:62:ASN:HA	1:D:63:PRO:HD3	1.78	0.40
1:A:473:ILE:HG12	1:A:474:ASN:N	2.35	0.40
1:B:112:LEU:HD12	1:B:112:LEU:HA	1.94	0.40
1:B:327:PHE:CG	1:B:328:GLY:N	2.89	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:GLU:O	1:B:215:ARG:HG3	2.21	0.40
1:C:94:ASN:O	1:C:98:THR:HG22	2.21	0.40
1:A:36:GLY:O	1:A:92:HIS:HD2	2.04	0.40
1:C:417:MET:HG2	1:C:421:ASN:O	2.21	0.40
1:C:73:ASN:N	1:C:73:ASN:HD22	2.19	0.40
1:D:472:ALA:HB3	7:D:563:HOH:O	2.22	0.40
1:C:43:SER:HB2	1:C:126:VAL:CG1	2.52	0.40
1:B:26:GLN:NE2	1:B:80:LEU:HA	2.36	0.40
1:B:230:ASN:HB2	1:B:241:PHE:CD2	2.56	0.40
1:B:272:MET:CE	1:B:272:MET:HA	2.50	0.40
1:C:62:ASN:OD1	1:C:62:ASN:C	2.60	0.40
1:C:15:LYS:HE3	1:C:22:ASN:ND2	2.37	0.40
1:A:256:TYR:CZ	1:A:260:VAL:HG21	2.56	0.40
1:B:29:LEU:HD12	1:B:429:VAL:HG21	2.04	0.40
1:D:157:ARG:HG3	7:D:595:HOH:O	2.22	0.40
1:D:29:LEU:HA	1:D:29:LEU:HD12	1.96	0.40
1:A:22:ASN:HA	1:A:22:ASN:HD22	1.59	0.40
1:A:480:LEU:HB2	1:C:473:ILE:HD12	2.03	0.40
1:A:79:PRO:HB3	1:B:73:ASN:ND2	2.36	0.40
1:C:125:ASN:HD21	1:C:155:ARG:HH21	1.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:474:ASN:ND2	1:C:477:ARG:NH2[2_554]	2.12	0.08

## 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	450/487 (92%)	425 (94%)	20 (4%)	5 (1%)	21 49
1	B	454/487 (93%)	426 (94%)	23 (5%)	5 (1%)	21 49
1	C	453/487 (93%)	425 (94%)	22 (5%)	6 (1%)	18 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	450/487 (92%)	425 (94%)	20 (4%)	5 (1%)	21 49
All	All	1807/1948 (93%)	1701 (94%)	85 (5%)	21 (1%)	19 45

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	GLU
1	A	273	GLY
1	A	371	SER
1	B	371	SER
1	C	273	GLY
1	C	482	GLU
1	D	371	SER
1	A	369	PRO
1	A	482	GLU
1	B	369	PRO
1	C	369	PRO
1	C	371	SER
1	D	369	PRO
1	A	471	GLU
1	B	273	GLY
1	B	471	GLU
1	C	471	GLU
1	D	273	GLY
1	D	471	GLU
1	D	9	VAL
1	C	95	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	380/405 (94%)	348 (92%)	32 (8%)	16 34
1	B	385/405 (95%)	352 (91%)	33 (9%)	15 33
1	C	383/405 (95%)	349 (91%)	34 (9%)	14 31
1	D	381/405 (94%)	350 (92%)	31 (8%)	17 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1529/1620 (94%)	1399 (92%)	130 (8%)	15	34

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	29	LEU
1	A	34	LEU
1	A	72	GLU
1	A	77	VAL
1	A	90	ARG
1	A	98	THR
1	A	109	CYS
1	A	112	LEU
1	A	114	ASP
1	A	167	THR
1	A	169	LEU
1	A	173	ARG
1	A	188	LEU
1	A	193	LEU
1	A	227	THR
1	A	263	ASN
1	A	272	MET
1	A	294	LEU
1	A	314	CYS
1	A	333	ARG
1	A	344	LYS
1	A	370	ASP
1	A	372	THR
1	A	433	VAL
1	A	436	VAL
1	A	466	ILE
1	A	473	ILE
1	A	475	ARG
1	A	477	ARG
1	A	479	ARG
1	A	484	LEU
1	B	8	ARG
1	B	14	VAL
1	B	18	ARG
1	B	29	LEU
1	B	34	LEU

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Mol	Chain	Res	Type
1	B	72	GLU
1	B	77	VAL
1	B	90	ARG
1	B	98	THR
1	B	112	LEU
1	B	114	ASP
1	B	167	THR
1	B	169	LEU
1	B	173	ARG
1	B	188	LEU
1	B	193	LEU
1	B	227	THR
1	B	230	ASN
1	B	263	ASN
1	B	272	MET
1	B	294	LEU
1	B	314	CYS
1	B	333	ARG
1	B	344	LYS
1	B	370	ASP
1	B	372	THR
1	B	433	VAL
1	B	434	ARG
1	B	466	ILE
1	B	473	ILE
1	B	475	ARG
1	B	477	ARG
1	B	479	ARG
1	C	8	ARG
1	C	9	VAL
1	C	11	SER
1	C	18	ARG
1	C	29	LEU
1	C	34	LEU
1	C	72	GLU
1	C	77	VAL
1	C	90	ARG
1	C	98	THR
1	C	109	CYS
1	C	112	LEU
1	C	114	ASP
1	C	167	THR

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Mol	Chain	Res	Type
1	C	169	LEU
1	C	173	ARG
1	C	188	LEU
1	C	193	LEU
1	C	227	THR
1	C	263	ASN
1	C	272	MET
1	C	294	LEU
1	C	314	CYS
1	C	333	ARG
1	C	344	LYS
1	C	370	ASP
1	C	372	THR
1	C	433	VAL
1	C	436	VAL
1	C	466	ILE
1	C	473	ILE
1	C	475	ARG
1	C	477	ARG
1	C	479	ARG
1	D	8	ARG
1	D	18	ARG
1	D	29	LEU
1	D	34	LEU
1	D	72	GLU
1	D	77	VAL
1	D	90	ARG
1	D	98	THR
1	D	112	LEU
1	D	114	ASP
1	D	167	THR
1	D	169	LEU
1	D	173	ARG
1	D	188	LEU
1	D	193	LEU
1	D	227	THR
1	D	230	ASN
1	D	263	ASN
1	D	271	LEU
1	D	272	MET
1	D	294	LEU
1	D	314	CYS

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Mol	Chain	Res	Type
1	D	333	ARG
1	D	344	LYS
1	D	370	ASP
1	D	372	THR
1	D	466	ILE
1	D	473	ILE
1	D	475	ARG
1	D	477	ARG
1	D	479	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	26	GLN
1	A	73	ASN
1	A	92	HIS
1	A	94	ASN
1	A	128	ASN
1	A	162	HIS
1	A	163	HIS
1	A	176	GLN
1	A	210	GLN
1	A	230	ASN
1	A	242	GLN
1	A	250	GLN
1	A	263	ASN
1	A	282	GLN
1	A	289	GLN
1	A	291	ASN
1	A	298	ASN
1	A	404	HIS
1	A	421	ASN
1	A	442	GLN
1	A	474	ASN
1	B	22	ASN
1	B	26	GLN
1	B	73	ASN
1	B	92	HIS
1	B	94	ASN
1	B	128	ASN
1	B	154	HIS

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Mol	Chain	Res	Type
1	B	162	HIS
1	B	176	GLN
1	B	210	GLN
1	B	230	ASN
1	B	242	GLN
1	B	250	GLN
1	B	263	ASN
1	B	282	GLN
1	B	289	GLN
1	B	291	ASN
1	B	298	ASN
1	B	404	HIS
1	B	419	HIS
1	B	442	GLN
1	B	474	ASN
1	B	481	HIS
1	C	22	ASN
1	C	26	GLN
1	C	73	ASN
1	C	92	HIS
1	C	94	ASN
1	C	128	ASN
1	C	162	HIS
1	C	176	GLN
1	C	210	GLN
1	C	230	ASN
1	C	242	GLN
1	C	250	GLN
1	C	263	ASN
1	C	282	GLN
1	C	289	GLN
1	C	291	ASN
1	C	298	ASN
1	C	404	HIS
1	C	419	HIS
1	C	442	GLN
1	C	474	ASN
1	D	22	ASN
1	D	26	GLN
1	D	73	ASN
1	D	92	HIS
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	148	GLN
1	D	154	HIS
1	D	162	HIS
1	D	176	GLN
1	D	210	GLN
1	D	230	ASN
1	D	242	GLN
1	D	250	GLN
1	D	263	ASN
1	D	282	GLN
1	D	289	GLN
1	D	291	ASN
1	D	298	ASN
1	D	404	HIS
1	D	419	HIS
1	D	442	GLN
1	D	474	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	ATP	A	1001	-	33,33,33	0.98	1 (3%)	52,52,52	1.90	9 (17%)
4	GOL	A	488	-	5,5,5	0.35	0	5,5,5	0.92	0
2	ATP	B	1001	3	33,33,33	1.03	3 (9%)	52,52,52	1.92	12 (23%)
2	ATP	C	1001	-	33,33,33	1.00	2 (6%)	52,52,52	1.83	10 (19%)
4	GOL	C	488	-	5,5,5	0.18	0	5,5,5	1.19	1 (20%)
6	SO4	C	489	-	4,4,4	0.09	0	6,6,6	0.25	0
2	ATP	D	1001	3	33,33,33	1.10	2 (6%)	52,52,52	1.85	11 (21%)

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	ATP	A	1001	-	-	0/22/38/38	0/1/3/3
4	GOL	A	488	-	-	0/4/4/4	0/0/0/0
2	ATP	B	1001	3	-	0/22/38/38	0/1/3/3
2	ATP	C	1001	-	-	0/22/38/38	0/1/3/3
4	GOL	C	488	-	-	0/4/4/4	0/0/0/0
6	SO4	C	489	-	-	0/0/0/0	0/0/0/0
2	ATP	D	1001	3	-	0/22/38/38	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	C5-C4	3.58	1.48	1.40
2	C	1001	ATP	C5-C4	3.23	1.47	1.40
2	A	1001	ATP	C5-C4	3.04	1.47	1.40
2	B	1001	ATP	C5-C4	3.02	1.47	1.40
2	B	1001	ATP	C4-N9	-2.39	1.34	1.37
2	D	1001	ATP	C4-N9	-2.18	1.34	1.37
2	B	1001	ATP	O4'-C1'	2.04	1.44	1.41
2	C	1001	ATP	C4-N9	-2.01	1.34	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ATP	N3-C2-N1	-6.78	123.04	128.71
2	B	1001	ATP	N3-C2-N1	-6.66	123.14	128.71
2	D	1001	ATP	N3-C2-N1	-6.48	123.29	128.71
2	A	1001	ATP	O4'-C1'-N9	6.35	114.34	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ATP	N3-C4-N9	6.02	136.31	125.43
2	A	1001	ATP	N3-C2-N1	-5.74	123.91	128.71
2	D	1001	ATP	N3-C4-N9	5.70	135.72	125.43
2	C	1001	ATP	N3-C4-N9	5.56	135.47	125.43
2	A	1001	ATP	N3-C4-N9	5.37	135.13	125.43
2	D	1001	ATP	O4'-C1'-N9	4.79	112.90	108.44
2	C	1001	ATP	O4'-C1'-N9	4.25	112.39	108.44
2	A	1001	ATP	C5-C4-N3	-3.44	118.22	125.70
2	B	1001	ATP	C8-N9-C4	3.36	109.47	106.90
2	A	1001	ATP	C4-C5-N7	-3.26	106.73	109.52
2	B	1001	ATP	O4'-C1'-N9	3.16	111.38	108.44
2	C	1001	ATP	C5-C4-N3	-3.12	118.90	125.70
2	D	1001	ATP	O3A-PB-O3B	-3.10	95.36	101.66
2	D	1001	ATP	C5-C4-N3	-3.04	119.08	125.70
2	B	1001	ATP	N6-C6-N1	3.03	125.32	119.36
2	B	1001	ATP	C5-C4-N3	-2.98	119.21	125.70
2	C	1001	ATP	PB-O3B-PG	-2.82	123.43	131.68
2	A	1001	ATP	PB-O3B-PG	-2.69	123.80	131.68
2	B	1001	ATP	PB-O3B-PG	-2.61	124.02	131.68
2	B	1001	ATP	O3'-C3'-C4'	-2.51	103.70	111.08
2	B	1001	ATP	O3A-PB-O3B	-2.50	96.59	101.66
2	A	1001	ATP	C2-N3-C4	2.41	120.89	114.01
2	B	1001	ATP	PA-O3A-PB	-2.41	124.62	131.68
2	A	1001	ATP	PA-O3A-PB	-2.39	124.67	131.68
2	C	1001	ATP	C2-N3-C4	2.38	120.80	114.01
2	D	1001	ATP	C8-N9-C4	2.37	108.71	106.90
2	D	1001	ATP	O3'-C3'-C4'	-2.35	104.15	111.08
2	A	1001	ATP	C3'-C2'-C1'	2.30	104.51	100.91
2	D	1001	ATP	N6-C6-N1	2.28	123.84	119.36
2	D	1001	ATP	C2-N1-C6	2.27	122.87	118.77
2	B	1001	ATP	C2-N3-C4	2.22	120.32	114.01
2	D	1001	ATP	C2-N3-C4	2.21	120.31	114.01
2	C	1001	ATP	C8-N9-C4	2.20	108.58	106.90
2	C	1001	ATP	C4-C5-N7	-2.17	107.66	109.52
4	C	488	GOL	C3-C2-C1	-2.13	101.85	111.26
2	C	1001	ATP	C2-N1-C6	2.06	122.50	118.77
2	B	1001	ATP	C2-N1-C6	2.04	122.46	118.77
2	D	1001	ATP	C4-C5-N7	-2.02	107.79	109.52
2	C	1001	ATP	N6-C6-N1	2.01	123.31	119.36

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

## 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	458/487 (94%)	-0.08	26 (5%)	23	25	12, 29, 77, 111	0
1	B	462/487 (94%)	-0.09	28 (6%)	21	22	12, 28, 80, 111	0
1	C	461/487 (94%)	0.01	43 (9%)	9	9	12, 29, 80, 111	0
1	D	458/487 (94%)	-0.05	38 (8%)	11	12	12, 28, 81, 113	0
All	All	1839/1948 (94%)	-0.05	135 (7%)	15	16	12, 29, 80, 113	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	LYS	6.1
1	D	455	GLY	5.9
1	D	45	LYS	5.8
1	D	480	LEU	5.7
1	D	457	ASP	5.2
1	C	55	LYS	5.1
1	C	22	ASN	5.1
1	C	482	GLU	5.1
1	C	459	ARG	5.0
1	C	17	HIS	4.8
1	A	45	LYS	4.6
1	C	473	ILE	4.5
1	B	482	GLU	4.4
1	B	455	GLY	4.3
1	C	45	LYS	4.2
1	D	458	VAL	4.2
1	A	482	GLU	4.2
1	C	27	GLU	4.1
1	B	9	VAL	4.1
1	D	459	ARG	4.0
1	A	366	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	55	LYS	4.0
1	C	457	ASP	3.9
1	A	459	ARG	3.9
1	C	480	LEU	3.9
1	D	8	ARG	3.9
1	B	54	ASP	3.8
1	A	55	LYS	3.6
1	C	460	LEU	3.6
1	C	9	VAL	3.6
1	B	457	ASP	3.5
1	C	483	GLU	3.5
1	D	340	ALA	3.5
1	C	8	ARG	3.5
1	A	17	HIS	3.5
1	D	163	HIS	3.4
1	C	478	ASP	3.4
1	B	462	ARG	3.3
1	C	18	ARG	3.3
1	B	17	HIS	3.3
1	B	458	VAL	3.2
1	A	333	ARG	3.2
1	D	481	HIS	3.2
1	B	456	SER	3.2
1	B	363	ALA	3.2
1	C	481	HIS	3.2
1	D	9	VAL	3.1
1	C	366	SER	3.1
1	A	460	LEU	3.1
1	C	471	GLU	3.1
1	A	19	ALA	3.1
1	A	216	GLY	3.0
1	C	479	ARG	3.0
1	A	18	ARG	3.0
1	C	474	ASN	3.0
1	B	460	LEU	3.0
1	D	476	ASN	2.9
1	C	38	ASP	2.9
1	B	67	ASP	2.8
1	D	67	ASP	2.8
1	A	440	ARG	2.8
1	D	466	ILE	2.8
1	C	90	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	18	ARG	2.8
1	D	468	ARG	2.8
1	D	462	ARG	2.7
1	C	333	ARG	2.7
1	A	462	ARG	2.7
1	B	8	ARG	2.7
1	C	72	GLU	2.7
1	D	333	ARG	2.7
1	C	463	LYS	2.7
1	A	464	LEU	2.6
1	A	22	ASN	2.6
1	B	333	ARG	2.6
1	A	473	ILE	2.6
1	A	479	ARG	2.6
1	C	462	ARG	2.6
1	D	365	LYS	2.6
1	C	21	LEU	2.6
1	A	90	ARG	2.6
1	B	330	ASP	2.6
1	B	466	ILE	2.6
1	C	440	ARG	2.6
1	B	299	PRO	2.6
1	B	459	ARG	2.5
1	D	456	SER	2.5
1	A	11	SER	2.5
1	D	17	HIS	2.5
1	C	214	ARG	2.5
1	A	27	GLU	2.5
1	C	469	GLU	2.5
1	D	22	ASN	2.5
1	C	466	ILE	2.4
1	B	71	SER	2.4
1	D	478	ASP	2.4
1	C	19	ALA	2.4
1	D	366	SER	2.4
1	A	40	PRO	2.4
1	B	66	ARG	2.4
1	D	367	ARG	2.4
1	C	32	ASP	2.4
1	D	474	ASN	2.4
1	A	56	THR	2.4
1	A	66	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	481	HIS	2.3
1	D	370	ASP	2.3
1	C	470	LEU	2.3
1	D	332	GLY	2.3
1	B	144	LYS	2.3
1	D	303	GLN	2.3
1	C	97	GLU	2.3
1	B	18	ARG	2.3
1	B	70	SER	2.2
1	D	479	ARG	2.2
1	D	454	LEU	2.2
1	C	56	THR	2.2
1	C	458	VAL	2.2
1	D	216	GLY	2.2
1	C	369	PRO	2.2
1	C	57	ASP	2.2
1	B	479	ARG	2.2
1	C	67	ASP	2.2
1	D	470	LEU	2.2
1	A	481	HIS	2.1
1	D	159	THR	2.1
1	B	55	LYS	2.1
1	D	338	TYR	2.1
1	C	315	HIS	2.1
1	D	475	ARG	2.1
1	B	72	GLU	2.1
1	D	482	GLU	2.1
1	A	21	LEU	2.1
1	C	340	ALA	2.0
1	A	213	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	A	490	1/1	0.22	7.41	43,43,43,43	0
5	NA	B	488	1/1	0.19	2.08	45,45,45,45	0
3	MG	A	1002	1/1	0.20	1.68	49,49,49,49	0
5	NA	C	490	1/1	0.20	1.45	34,34,34,34	0
6	SO4	C	489	5/5	0.14	0.43	33,41,48,91	0
5	NA	A	489	1/1	0.15	0.42	30,30,30,30	0
3	MG	D	1002	1/1	0.16	0.08	45,45,45,45	0
3	MG	B	1002	1/1	0.14	-0.33	51,51,51,51	0
4	GOL	A	488	6/6	0.11	-0.41	5,19,35,41	0
2	ATP	C	1001	31/31	0.12	-0.59	17,32,43,62	0
2	ATP	D	1001	31/31	0.12	-0.76	15,29,39,71	0
2	ATP	B	1001	31/31	0.10	-0.79	14,25,38,66	0
2	ATP	A	1001	31/31	0.12	-0.80	19,40,62,73	0
4	GOL	C	488	6/6	0.09	-0.84	9,14,28,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.