



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 10:05 AM EST

PDB ID : 4II3  
Title : Crystal structure of *S. pombe* Ubiquitin activating enzyme 1 (Uba1) in complex with ubiquitin and ATP/Mg  
Authors : Olsen, S.K.; Lima, C.D.  
Deposited on : unknown  
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

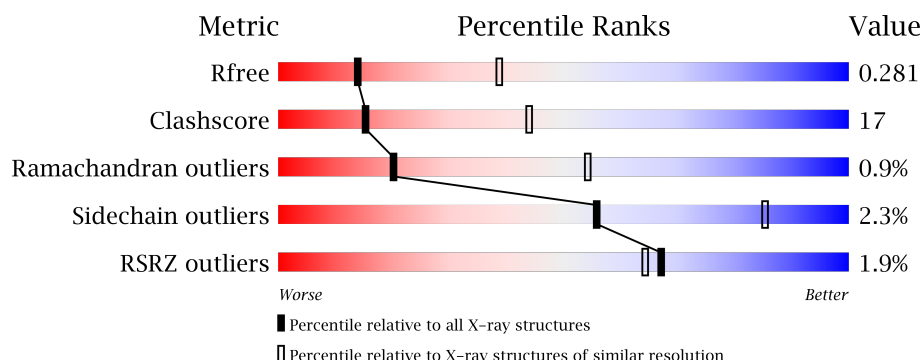
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	1001	
1	C	1001	
2	B	96	
2	D	96	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16848 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total	C	N	O	S	0	0	0
			7745	4953	1266	1487	39			
1	C	977	Total	C	N	O	S	0	0	0
			7676	4904	1257	1476	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	EXPRESSION TAG	UNP O94609
C	12	SER	-	EXPRESSION TAG	UNP O94609

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			601	375	105	120	1			
2	D	76	Total	C	N	O	S	0	0	0
			601	375	105	120	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP P0CH07
B	-18	GLY	-	EXPRESSION TAG	UNP P0CH07
B	-17	SER	-	EXPRESSION TAG	UNP P0CH07
B	-16	SER	-	EXPRESSION TAG	UNP P0CH07
B	-15	HIS	-	EXPRESSION TAG	UNP P0CH07
B	-14	HIS	-	EXPRESSION TAG	UNP P0CH07
B	-13	HIS	-	EXPRESSION TAG	UNP P0CH07
B	-12	HIS	-	EXPRESSION TAG	UNP P0CH07
B	-11	HIS	-	EXPRESSION TAG	UNP P0CH07
B	-10	HIS	-	EXPRESSION TAG	UNP P0CH07

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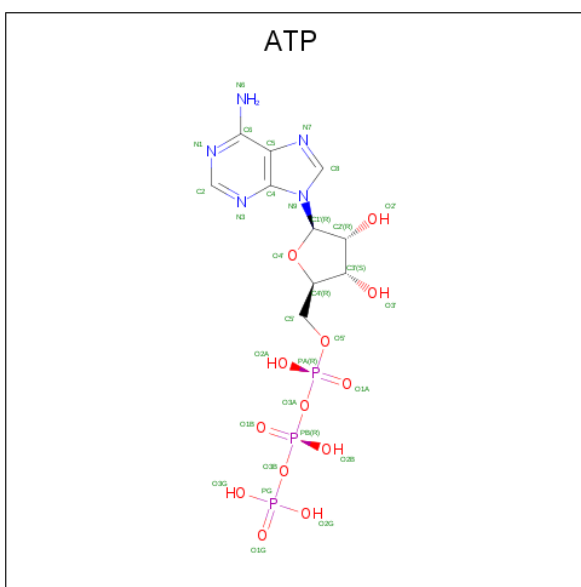
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	EXPRESSION TAG	UNP P0CH07
B	-8	SER	-	EXPRESSION TAG	UNP P0CH07
B	-7	GLY	-	EXPRESSION TAG	UNP P0CH07
B	-6	LEU	-	EXPRESSION TAG	UNP P0CH07
B	-5	VAL	-	EXPRESSION TAG	UNP P0CH07
B	-4	PRO	-	EXPRESSION TAG	UNP P0CH07
B	-3	ARG	-	EXPRESSION TAG	UNP P0CH07
B	-2	GLY	-	EXPRESSION TAG	UNP P0CH07
B	-1	SER	-	EXPRESSION TAG	UNP P0CH07
B	0	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-19	MET	-	EXPRESSION TAG	UNP P0CH07
D	-18	GLY	-	EXPRESSION TAG	UNP P0CH07
D	-17	SER	-	EXPRESSION TAG	UNP P0CH07
D	-16	SER	-	EXPRESSION TAG	UNP P0CH07
D	-15	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-14	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-13	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-12	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-11	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-10	HIS	-	EXPRESSION TAG	UNP P0CH07
D	-9	SER	-	EXPRESSION TAG	UNP P0CH07
D	-8	SER	-	EXPRESSION TAG	UNP P0CH07
D	-7	GLY	-	EXPRESSION TAG	UNP P0CH07
D	-6	LEU	-	EXPRESSION TAG	UNP P0CH07
D	-5	VAL	-	EXPRESSION TAG	UNP P0CH07
D	-4	PRO	-	EXPRESSION TAG	UNP P0CH07
D	-3	ARG	-	EXPRESSION TAG	UNP P0CH07
D	-2	GLY	-	EXPRESSION TAG	UNP P0CH07
D	-1	SER	-	EXPRESSION TAG	UNP P0CH07
D	0	HIS	-	EXPRESSION TAG	UNP P0CH07

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Ca 4 4	0	0
5	C	6	Total Ca 6 6	0	0

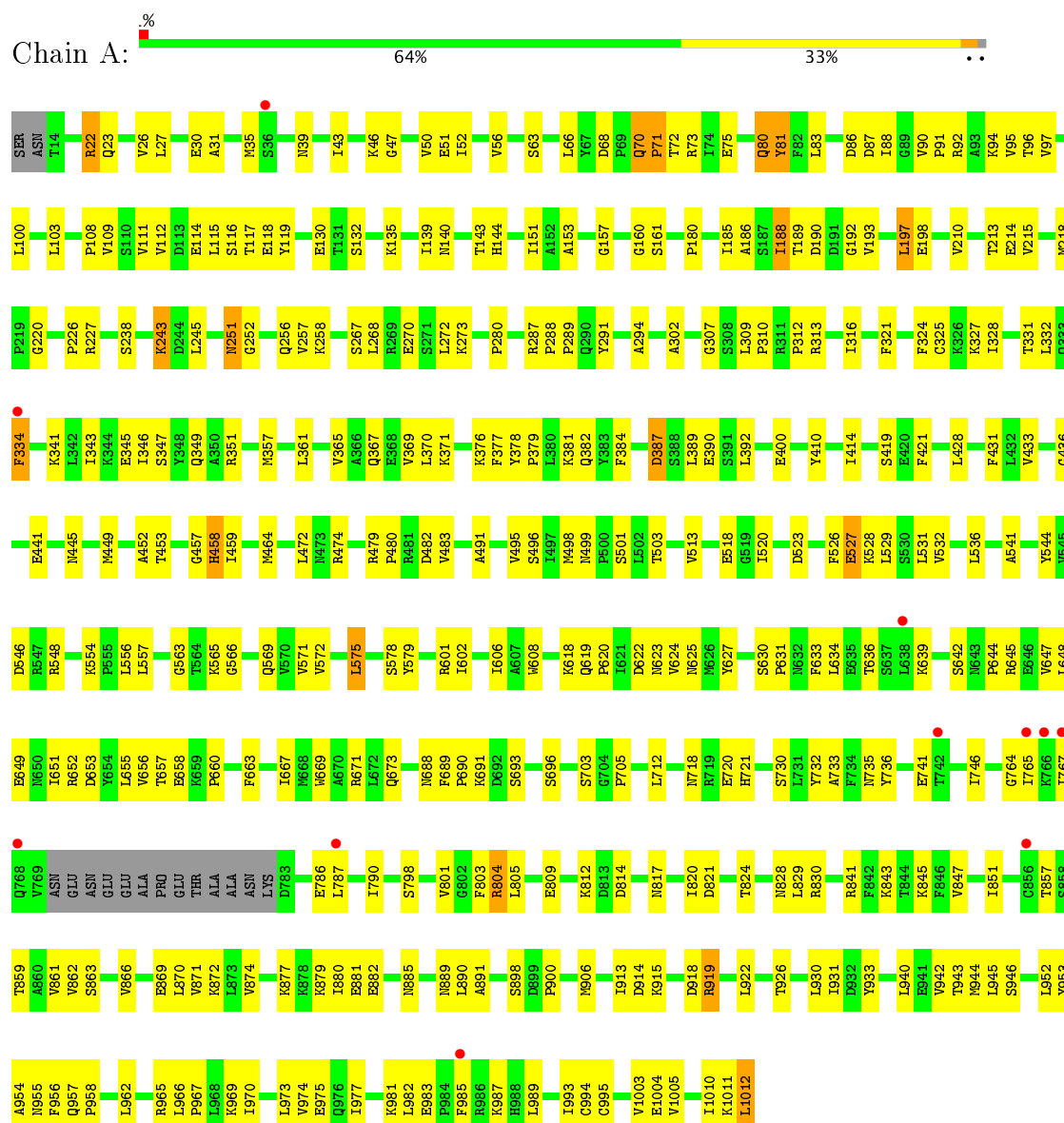
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 78 78	0	0
6	B	12	Total O 12 12	0	0
6	C	47	Total O 47 47	0	0
6	D	12	Total O 12 12	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 the various outlier classes 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: Ubiquitin-activating enzyme E1 1



#### • Molecule 1: Ubiquitin-activating enzyme E1 1





## 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, $\alpha$ , $\beta$ , $\gamma$	180.50 Å   113.30 Å   126.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.90 39.80 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.90) 95.2 (39.80-2.91)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.90 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239   ,   0.283 0.240   ,   0.281	Depositor DCC
$R_{free}$ test set	2770 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.31	0/7916	0.51	0/10713
1	C	0.31	0/7842	0.51	0/10608
2	B	0.31	0/606	0.56	0/812
2	D	0.30	0/606	0.55	0/812
All	All	0.31	0/16970	0.51	0/22945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	7745	0	7688	270	0
1	C	7676	0	7612	277	0
2	B	601	0	625	9	0
2	D	601	0	625	12	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	31	0	12	2	0
4	C	31	0	12	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	0	0	0
6	A	78	0	0	4	0
6	B	12	0	0	1	0
6	C	47	0	0	1	0
6	D	12	0	0	0	0
All	All	16848	0	16574	555	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 17.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PRO:HD3	1:A:351:ARG:HD2	1.41	1.03
1:C:312:PRO:HD3	1:C:351:ARG:HD2	1.46	0.98
1:C:80:GLN:HE22	1:C:96:THR:HG21	1.29	0.97
1:A:80:GLN:HE22	1:A:96:THR:HG21	1.32	0.92
1:A:436:GLY:HA3	4:A:1103:ATP:H5'2	1.52	0.91
1:A:197:LEU:HG	1:A:198:GLU:H	1.40	0.86
1:A:634:LEU:HD12	1:A:634:LEU:H	1.41	0.84
2:D:45:PHE:HB2	2:D:67:LEU:HD22	1.57	0.84
1:A:623:ASN:HD22	1:A:647:VAL:HG13	1.43	0.83
1:C:197:LEU:HG	1:C:198:GLU:H	1.42	0.83
1:C:653:ASP:HA	1:C:657:THR:HB	1.60	0.83
1:A:433:VAL:HG12	1:A:536:LEU:HD21	1.61	0.83
1:A:803:PHE:O	1:A:804:ARG:HD3	1.79	0.82
1:A:87:ASP:O	1:A:90:VAL:HG22	1.82	0.80
1:C:634:LEU:HD12	1:C:634:LEU:H	1.45	0.80
1:A:653:ASP:HA	1:A:657:THR:HB	1.63	0.79
1:C:87:ASP:O	1:C:90:VAL:HG22	1.82	0.79
1:C:623:ASN:HD22	1:C:647:VAL:HG13	1.49	0.78
2:B:45:PHE:HB2	2:B:67:LEU:HD22	1.66	0.78
1:C:433:VAL:HG12	1:C:536:LEU:HD21	1.65	0.77
1:C:565:LYS:HG2	1:C:889:ASN:ND2	2.02	0.75
1:A:71:PRO:HD2	1:A:73:ARG:NH1	2.02	0.74
1:C:433:VAL:HG13	1:C:513:VAL:HG21	1.70	0.74
1:C:71:PRO:HD2	1:C:73:ARG:NH1	2.03	0.73
1:C:22:ARG:HG3	1:C:474:ARG:NH1	2.04	0.72
1:A:316:ILE:H	1:A:316:ILE:HD12	1.53	0.72
1:C:942:VAL:HA	1:C:995:CYS:HB3	1.72	0.72
1:C:441:GLU:HG3	1:C:859:THR:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ILE:HD12	1:C:316:ILE:H	1.55	0.70
1:A:160:GLY:HA3	1:A:361:LEU:HD11	1.74	0.70
1:C:410:TYR:O	1:C:414:ILE:HG13	1.92	0.69
1:A:267:SER:OG	1:A:270:GLU:HG2	1.92	0.69
1:A:520:ILE:HD12	1:A:520:ILE:N	2.08	0.69
1:A:433:VAL:HG13	1:A:513:VAL:HG21	1.76	0.68
1:A:80:GLN:NE2	1:A:96:THR:HG21	2.06	0.68
1:C:520:ILE:H	1:C:520:ILE:HD12	1.60	0.67
1:C:268:LEU:O	1:C:272:LEU:HB2	1.93	0.67
1:A:410:TYR:O	1:A:414:ILE:HG13	1.94	0.67
1:C:520:ILE:N	1:C:520:ILE:HD12	2.10	0.67
2:D:7:THR:HG22	2:D:69:LEU:HB3	1.76	0.67
1:C:267:SER:OG	1:C:270:GLU:HG2	1.95	0.67
1:A:157:GLY:O	1:A:357:MET:HG3	1.94	0.66
1:A:814:ASP:HB3	1:A:817:ASN:ND2	2.11	0.66
1:A:942:VAL:HA	1:A:995:CYS:HB3	1.76	0.66
1:A:268:LEU:O	1:A:272:LEU:HB2	1.96	0.66
1:C:630:SER:HB2	1:C:633:PHE:HB2	1.76	0.66
1:A:630:SER:HB2	1:A:633:PHE:HB2	1.78	0.65
1:C:814:ASP:HB3	1:C:817:ASN:ND2	2.11	0.65
1:A:798:SER:O	1:A:801:VAL:HG23	1.95	0.65
1:C:624:VAL:HG11	1:C:805:LEU:HD12	1.77	0.65
1:C:812:LYS:O	1:C:845:LYS:HE3	1.98	0.64
1:C:80:GLN:NE2	1:C:96:THR:HG21	2.08	0.64
1:C:213:THR:HG22	1:C:214:GLU:HG3	1.80	0.63
1:C:602:ILE:O	1:C:606:ILE:HG13	1.97	0.63
1:A:245:LEU:HD23	1:A:245:LEU:O	1.98	0.63
1:C:846:PHE:HE1	1:C:853:PRO:HD3	1.64	0.62
1:C:220:GLY:N	1:C:245:LEU:HD21	2.15	0.62
1:C:25:TYR:CE1	1:C:846:PHE:HB2	2.35	0.62
1:A:520:ILE:HD12	1:A:520:ILE:H	1.64	0.61
1:C:72:THR:HB	1:C:88:ILE:HA	1.81	0.61
1:C:71:PRO:HD2	1:C:73:ARG:HH12	1.65	0.61
1:C:245:LEU:O	1:C:245:LEU:HD23	2.00	0.61
1:C:906:MET:SD	1:C:913:ILE:HD11	2.40	0.61
1:A:931:ILE:HG12	1:A:942:VAL:HG11	1.83	0.61
1:A:623:ASN:ND2	1:A:647:VAL:HG13	2.13	0.61
1:C:572:VAL:HG13	1:C:575:LEU:HB3	1.83	0.61
1:C:889:ASN:OD1	1:C:891:ALA:HB3	2.01	0.61
1:A:71:PRO:HD2	1:A:73:ARG:HH12	1.63	0.60
1:A:565:LYS:HG2	1:A:889:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:GLU:HG2	1:C:652:ARG:HH21	1.67	0.60
1:C:669:TRP:O	1:C:673:GLN:HG2	2.01	0.60
1:C:922:LEU:HD21	1:C:933:TYR:CE2	2.36	0.60
1:A:213:THR:HG22	1:A:214:GLU:HG3	1.84	0.60
1:C:671:ARG:HG3	1:C:671:ARG:HH11	1.66	0.60
1:C:566:GLY:HA2	2:D:73:LEU:HD12	1.82	0.60
1:A:72:THR:HG23	1:A:83:LEU:HD13	1.83	0.60
1:C:536:LEU:O	2:D:76:GLY:HA3	2.02	0.60
1:A:556:LEU:HB3	1:A:571:VAL:HG13	1.84	0.60
1:A:66:LEU:HD11	1:A:100:LEU:HD12	1.83	0.60
1:C:66:LEU:HD11	1:C:100:LEU:HD12	1.82	0.60
1:C:606:ILE:HG21	1:C:847:VAL:HG13	1.83	0.59
1:C:499:ASN:OD1	1:C:501:SER:HB2	2.01	0.59
1:C:160:GLY:HA3	1:C:361:LEU:HD11	1.83	0.59
1:C:421:PHE:CZ	1:C:874:VAL:HG23	2.38	0.59
1:A:421:PHE:CZ	1:A:874:VAL:HG23	2.37	0.59
1:A:218:MET:HB3	1:A:245:LEU:HD22	1.85	0.59
1:C:791:ALA:O	1:C:794:LEU:HD22	2.03	0.58
1:A:220:GLY:N	1:A:245:LEU:HD21	2.18	0.58
1:C:556:LEU:HB3	1:C:571:VAL:HG13	1.85	0.58
1:A:316:ILE:N	1:A:316:ILE:HD12	2.18	0.58
1:A:889:ASN:OD1	1:A:891:ALA:HB3	2.04	0.58
2:B:18:GLU:HB2	2:B:21:ASP:OD1	2.03	0.58
1:C:316:ILE:HD12	1:C:316:ILE:N	2.18	0.58
1:C:428:LEU:HD21	1:C:874:VAL:HG12	1.86	0.58
1:A:71:PRO:O	1:A:92:ARG:HG3	2.04	0.58
1:C:210:VAL:HG12	1:C:256:GLN:HA	1.86	0.58
1:C:367:GLN:HG2	1:C:890:LEU:HB3	1.84	0.58
1:C:116:SER:HB3	1:C:119:TYR:HB2	1.85	0.57
1:A:280:PRO:HB3	1:A:384:PHE:CE1	2.40	0.57
2:D:18:GLU:HB2	2:D:21:ASP:OD1	2.04	0.57
1:A:634:LEU:CD1	1:A:634:LEU:H	2.15	0.57
1:C:71:PRO:O	1:C:92:ARG:HG3	2.04	0.57
1:C:115:LEU:O	1:C:115:LEU:HD23	2.04	0.57
1:A:215:VAL:HG22	1:A:252:GLY:HA3	1.86	0.57
1:C:480:PRO:O	1:C:483:VAL:HG23	2.05	0.57
1:C:975:GLU:OE2	1:C:981:LYS:HG3	2.05	0.57
1:A:566:GLY:HA2	2:B:73:LEU:HD12	1.87	0.56
2:B:7:THR:HG22	2:B:69:LEU:HB3	1.86	0.56
1:C:26:VAL:HG23	1:C:27:LEU:HG	1.87	0.56
1:A:606:ILE:HG21	1:A:847:VAL:HG13	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PRO:HB3	1:C:384:PHE:CE1	2.40	0.56
1:C:140:ASN:HA	1:C:143:THR:OG1	2.06	0.56
1:C:943:THR:HG23	1:C:995:CYS:HA	1.87	0.56
1:A:22:ARG:HG3	1:A:474:ARG:NH1	2.21	0.56
1:A:480:PRO:O	1:A:483:VAL:HG23	2.05	0.56
1:A:92:ARG:HA	1:A:95:VAL:HG12	1.86	0.56
1:A:496:SER:HB3	1:A:503:THR:HG22	1.86	0.56
1:A:922:LEU:HD21	1:A:933:TYR:CE2	2.40	0.56
1:A:880:ILE:HD11	1:A:900:PRO:O	2.06	0.56
1:C:536:LEU:HD13	1:C:541:ALA:CB	2.35	0.56
1:C:428:LEU:HD11	1:C:874:VAL:HG11	1.88	0.56
1:A:606:ILE:HD13	1:A:847:VAL:HG11	1.87	0.56
1:A:441:GLU:HG3	1:A:859:THR:HG22	1.87	0.55
1:A:428:LEU:HD11	1:A:874:VAL:HG11	1.87	0.55
1:C:496:SER:HB3	1:C:503:THR:HG22	1.88	0.55
1:C:634:LEU:CD1	1:C:634:LEU:H	2.19	0.55
1:C:608:TRP:CE3	1:C:830:ARG:HD2	2.41	0.55
1:A:72:THR:HB	1:A:88:ILE:HA	1.87	0.55
1:C:814:ASP:HB3	1:C:817:ASN:HD21	1.69	0.55
1:A:140:ASN:ND2	1:A:144:HIS:HB2	2.22	0.55
1:A:624:VAL:HG11	1:A:805:LEU:HD12	1.87	0.55
1:C:623:ASN:ND2	1:C:647:VAL:HG13	2.18	0.55
1:A:602:ILE:O	1:A:606:ILE:HG13	2.07	0.55
1:C:651:ILE:HG22	1:C:655:LEU:HD12	1.88	0.55
1:C:72:THR:HG23	1:C:83:LEU:HD13	1.87	0.55
1:C:321:PHE:CD2	1:C:347:SER:HB2	2.42	0.55
1:C:92:ARG:HA	1:C:95:VAL:HG12	1.88	0.55
1:A:115:LEU:O	1:A:115:LEU:HD23	2.06	0.55
1:A:491:ALA:O	1:A:495:VAL:HG23	2.06	0.55
1:A:765:ILE:N	1:A:765:ILE:HD12	2.22	0.55
1:C:518:GLU:HG2	1:C:548:ARG:NH1	2.22	0.55
1:A:190:ASP:HB2	1:A:243:LYS:HB3	1.87	0.55
1:A:499:ASN:OD1	1:A:501:SER:HB2	2.07	0.55
1:A:880:ILE:HG22	1:A:881:GLU:OE2	2.07	0.55
1:C:606:ILE:HD13	1:C:847:VAL:HG11	1.88	0.55
1:A:814:ASP:HB3	1:A:817:ASN:HD21	1.71	0.55
1:C:636:THR:HA	1:C:639:LYS:HD2	1.89	0.55
1:A:857:THR:O	1:A:861:VAL:HG23	2.07	0.54
1:A:906:MET:CE	1:A:915:LYS:HE2	2.37	0.54
1:A:906:MET:HE1	1:A:915:LYS:HE2	1.88	0.54
1:A:479:ARG:HB3	1:A:480:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:N	1:A:634:LEU:HD12	2.16	0.54
1:A:957:GLN:HB2	1:A:962:LEU:HD21	1.88	0.54
1:C:273:LYS:HA	1:C:332:LEU:HD21	1.90	0.54
1:C:556:LEU:HD12	1:C:557:LEU:N	2.23	0.54
1:C:518:GLU:HG3	1:C:544:TYR:OH	2.07	0.54
1:A:436:GLY:CA	4:A:1103:ATP:H5'2	2.33	0.54
1:A:46:LYS:HD3	1:A:130:GLU:HG2	1.89	0.54
1:A:943:THR:HG23	1:A:995:CYS:HA	1.88	0.54
1:C:970:ILE:O	1:C:974:VAL:HG23	2.08	0.54
1:A:140:ASN:HA	1:A:143:THR:OG1	2.07	0.53
1:A:696:SER:OG	1:C:198:GLU:HB3	2.07	0.53
1:C:544:TYR:CZ	1:C:548:ARG:HD2	2.43	0.53
1:A:227:ARG:HH22	1:C:949:VAL:CG1	2.21	0.53
1:A:601:ARG:HD3	6:A:1224:HOH:O	2.08	0.53
1:C:94:LYS:O	1:C:97:VAL:HG12	2.08	0.53
1:A:618:LYS:HE2	1:A:809:GLU:OE2	2.08	0.53
1:A:153:ALA:HA	1:A:161:SER:O	2.09	0.53
1:A:325:CYS:SG	1:A:343:ILE:HG21	2.49	0.53
1:A:608:TRP:CE3	1:A:830:ARG:HD2	2.44	0.53
1:A:881:GLU:H	1:A:881:GLU:CD	2.11	0.53
1:C:634:LEU:N	1:C:634:LEU:HD12	2.20	0.53
1:A:390:GLU:O	1:A:877:LYS:HE3	2.09	0.53
1:A:671:ARG:HH11	1:A:671:ARG:HG3	1.72	0.53
1:C:644:PRO:O	1:C:648:LEU:HG	2.09	0.53
1:A:556:LEU:HD12	1:A:557:LEU:N	2.24	0.53
1:C:550:VAL:HA	1:C:917:TRP:CZ3	2.44	0.53
1:C:857:THR:O	1:C:861:VAL:HG23	2.08	0.53
1:A:954:ALA:HB3	1:A:957:GLN:HG3	1.91	0.53
1:A:544:TYR:CZ	1:A:548:ARG:HD2	2.44	0.52
1:A:116:SER:HB3	1:A:119:TYR:HB2	1.90	0.52
1:A:518:GLU:HG3	1:A:544:TYR:OH	2.09	0.52
1:A:332:LEU:HD22	1:A:334:PHE:CD1	2.44	0.52
1:A:227:ARG:HH22	1:C:949:VAL:HG12	1.73	0.52
1:A:830:ARG:HH11	1:A:830:ARG:HG3	1.73	0.52
1:C:180:PRO:HG3	1:C:258:LYS:HG3	1.92	0.52
1:C:663:PHE:O	1:C:667:ILE:HG13	2.10	0.52
1:A:544:TYR:OH	1:A:548:ARG:HD2	2.10	0.52
1:A:824:THR:HG22	1:A:828:ASN:ND2	2.25	0.52
1:C:983:GLU:HG3	1:C:985:PHE:CZ	2.45	0.52
1:A:46:LYS:O	1:A:50:VAL:HG12	2.09	0.52
1:A:944:MET:HB3	1:A:994:CYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:931:ILE:HG12	1:C:942:VAL:HG11	1.92	0.52
1:C:125:CYS:HA	1:C:149:ALA:HB3	1.91	0.51
1:C:786:GLU:O	1:C:790:ILE:HG13	2.10	0.51
1:C:218:MET:HB3	1:C:245:LEU:HD22	1.92	0.51
1:C:491:ALA:O	1:C:495:VAL:HG23	2.09	0.51
1:C:111:VAL:HG12	1:C:112:VAL:N	2.26	0.51
1:C:190:ASP:HB2	1:C:243:LYS:HB3	1.91	0.51
1:A:975:GLU:OE2	1:A:981:LYS:HG3	2.09	0.51
1:C:703:SER:O	1:C:705:PRO:HD2	2.11	0.51
1:C:765:ILE:N	1:C:765:ILE:HD12	2.26	0.51
1:A:712:LEU:HD21	1:A:721:HIS:HE2	1.76	0.51
1:C:843:LYS:O	1:C:847:VAL:HG12	2.10	0.51
1:A:688:ASN:ND2	1:A:767:ILE:HG13	2.26	0.51
1:A:983:GLU:HG3	1:A:985:PHE:CZ	2.46	0.51
1:C:762:LYS:H	1:C:762:LYS:HD2	1.75	0.51
1:A:531:LEU:HD21	1:A:870:LEU:HD11	1.92	0.51
1:A:518:GLU:HG2	1:A:548:ARG:NH1	2.26	0.51
1:C:215:VAL:HG22	1:C:252:GLY:HA3	1.93	0.51
1:C:869:GLU:OE2	1:C:872:LYS:HD2	2.11	0.51
1:A:367:GLN:O	1:A:371:LYS:HG3	2.10	0.51
1:A:619:GLN:N	1:A:620:PRO:HD2	2.26	0.51
1:C:103:LEU:HD23	1:C:479:ARG:HH21	1.75	0.51
1:C:453:THR:HG23	1:C:501:SER:HB3	1.92	0.51
1:C:881:GLU:H	1:C:881:GLU:CD	2.15	0.51
1:A:919:ARG:HG3	1:A:919:ARG:HH11	1.76	0.50
1:C:556:LEU:HD12	1:C:557:LEU:H	1.75	0.50
1:C:687:PHE:HE2	1:C:763:SER:HB3	1.77	0.50
1:A:421:PHE:HZ	1:A:874:VAL:HG23	1.74	0.50
1:A:556:LEU:HB3	1:A:571:VAL:CG1	2.40	0.50
1:A:367:GLN:HG2	1:A:890:LEU:HB3	1.93	0.50
1:A:536:LEU:O	2:B:76:GLY:HA3	2.11	0.50
1:A:843:LYS:O	1:A:847:VAL:HG12	2.11	0.50
1:A:94:LYS:O	1:A:97:VAL:HG12	2.11	0.50
1:C:23:GLN:O	1:C:26:VAL:HG22	2.11	0.50
1:C:324:PHE:O	1:C:327:LYS:HB3	2.12	0.50
1:A:862:VAL:O	1:A:866:VAL:HG23	2.11	0.50
1:C:824:THR:HG22	1:C:828:ASN:ND2	2.27	0.50
1:C:192:GLY:O	1:C:238:SER:HA	2.12	0.50
1:C:732:TYR:HA	1:C:735:ASN:HD22	1.77	0.50
1:C:943:THR:O	1:C:954:ALA:HA	2.12	0.50
1:C:975:GLU:CD	1:C:981:LYS:HG3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:VAL:HG13	1:A:575:LEU:HB3	1.94	0.50
1:A:569:GLN:HA	1:A:885:ASN:OD1	2.12	0.50
1:A:962:LEU:O	1:A:966:LEU:HG	2.12	0.50
1:C:619:GLN:N	1:C:620:PRO:HD2	2.27	0.50
1:C:316:ILE:CD1	1:C:316:ILE:H	2.24	0.50
1:C:862:VAL:O	1:C:866:VAL:HG23	2.12	0.50
1:C:919:ARG:HH11	1:C:919:ARG:HG3	1.77	0.50
2:B:22:THR:HG22	2:B:55:THR:HG22	1.94	0.50
1:C:220:GLY:C	1:C:245:LEU:HD11	2.32	0.50
1:C:962:LEU:O	1:C:966:LEU:HG	2.12	0.50
1:C:140:ASN:ND2	1:C:144:HIS:HB2	2.26	0.49
1:C:153:ALA:HA	1:C:161:SER:O	2.11	0.49
1:A:321:PHE:CD2	1:A:347:SER:HB2	2.47	0.49
1:A:965:ARG:C	1:A:967:PRO:HD2	2.32	0.49
1:C:46:LYS:HD3	1:C:130:GLU:HG2	1.94	0.49
1:A:656:VAL:HG13	1:A:657:THR:H	1.77	0.49
1:C:946:SER:HB2	1:C:950:SER:O	2.12	0.49
1:C:946:SER:HA	1:C:952:LEU:HD13	1.94	0.49
1:C:966:LEU:N	1:C:967:PRO:HD2	2.28	0.49
1:A:73:ARG:HB3	1:A:75:GLU:OE1	2.13	0.49
1:C:457:GLY:O	1:C:458:HIS:HB2	2.12	0.49
1:C:957:GLN:HB3	1:C:958:PRO:HD2	1.94	0.49
1:A:197:LEU:HG	1:A:198:GLU:N	2.18	0.49
1:A:316:ILE:H	1:A:316:ILE:CD1	2.23	0.49
1:A:92:ARG:HA	1:A:95:VAL:CG1	2.42	0.49
1:A:428:LEU:HD21	1:A:874:VAL:HG12	1.94	0.49
1:A:81:TYR:HB2	1:A:498:MET:CE	2.42	0.49
1:A:812:LYS:O	1:A:845:LYS:HE3	2.11	0.49
1:C:157:GLY:O	1:C:357:MET:HG3	2.12	0.49
1:C:431:PHE:HB2	1:C:529:LEU:HD22	1.95	0.49
1:C:871:VAL:HA	1:C:874:VAL:HG22	1.94	0.49
1:C:618:LYS:HE2	1:C:809:GLU:OE2	2.13	0.49
1:C:880:ILE:HG22	1:C:881:GLU:OE2	2.12	0.49
1:C:569:GLN:HA	1:C:885:ASN:OD1	2.13	0.49
1:A:192:GLY:O	1:A:238:SER:HA	2.13	0.48
1:C:46:LYS:O	1:C:50:VAL:HG12	2.13	0.48
1:C:70:GLN:O	1:C:91:PRO:HA	2.12	0.48
1:A:644:PRO:O	1:A:648:LEU:HG	2.13	0.48
1:C:97:VAL:HG23	1:C:109:VAL:HG12	1.95	0.48
1:C:987:LYS:O	1:C:1012:LEU:HD12	2.13	0.48
1:C:26:VAL:HG11	1:C:563:GLY:HA2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:ALA:HB3	1:C:957:GLN:HG3	1.94	0.48
1:A:111:VAL:HG12	1:A:112:VAL:N	2.28	0.48
1:A:140:ASN:HD21	1:A:144:HIS:HB2	1.78	0.48
1:A:431:PHE:HB2	1:A:529:LEU:HD22	1.95	0.48
1:C:520:ILE:CD1	1:C:520:ILE:H	2.24	0.48
1:C:197:LEU:HG	1:C:198:GLU:N	2.20	0.48
1:C:479:ARG:O	1:C:482:ASP:HB2	2.13	0.48
1:C:821:ASP:OD1	1:C:841:ARG:NH1	2.47	0.48
1:C:390:GLU:O	1:C:877:LYS:HE3	2.13	0.48
1:A:946:SER:HA	1:A:952:LEU:HD13	1.96	0.48
1:C:954:ALA:HB1	1:C:956:PHE:CE1	2.48	0.48
1:A:871:VAL:HA	1:A:874:VAL:HG22	1.96	0.48
1:A:210:VAL:HG12	1:A:256:GLN:HA	1.95	0.48
1:A:906:MET:SD	1:A:913:ILE:HD11	2.53	0.48
1:C:186:ALA:HB2	1:C:197:LEU:HA	1.96	0.48
1:A:414:ILE:HG23	1:A:419:SER:N	2.29	0.47
1:A:556:LEU:HD12	1:A:557:LEU:H	1.78	0.47
1:A:830:ARG:HG3	1:A:830:ARG:NH1	2.29	0.47
1:A:966:LEU:N	1:A:967:PRO:HD2	2.29	0.47
1:C:135:LYS:O	1:C:139:ILE:HG13	2.14	0.47
1:C:544:TYR:OH	1:C:548:ARG:HD2	2.13	0.47
1:C:72:THR:O	1:C:88:ILE:HG23	2.13	0.47
1:A:703:SER:O	1:A:705:PRO:HD2	2.14	0.47
1:C:63:SER:HB2	1:C:108:PRO:HG2	1.96	0.47
1:A:649:GLU:HG2	1:A:652:ARG:HH21	1.77	0.47
1:A:975:GLU:CD	1:A:981:LYS:HG3	2.35	0.47
1:A:606:ILE:CD1	1:A:847:VAL:HG11	2.44	0.47
1:C:220:GLY:CA	1:C:245:LEU:HD21	2.45	0.47
1:C:925:CYS:O	1:C:970:ILE:HG12	2.15	0.47
1:C:627:TYR:HE1	1:C:634:LEU:HD21	1.80	0.47
2:D:22:THR:HG22	2:D:55:THR:HG22	1.97	0.47
1:A:453:THR:HG23	1:A:501:SER:HB3	1.96	0.47
1:C:463:ASP:O	1:C:510:GLN:HA	2.13	0.47
1:C:671:ARG:HG3	1:C:671:ARG:NH1	2.29	0.47
1:C:792:ASP:O	1:C:794:LEU:HD23	2.15	0.47
1:A:324:PHE:O	1:A:327:LYS:HB3	2.13	0.47
1:A:345:GLU:HG3	1:A:349:GLN:NE2	2.30	0.47
1:C:452:ALA:CB	1:C:459:ILE:HG13	2.45	0.47
1:C:690:PRO:HB2	1:C:693:SER:HB3	1.96	0.47
1:A:135:LYS:O	1:A:139:ILE:HG13	2.13	0.47
1:A:313:ARG:HB3	1:A:400:GLU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HD12	1:A:43:ILE:N	2.30	0.47
1:A:80:GLN:HE22	1:A:96:THR:CG2	2.15	0.47
1:C:1003:VAL:HG22	1:C:1004:GLU:N	2.29	0.47
1:C:651:ILE:CG2	1:C:655:LEU:HD12	2.45	0.47
1:C:656:VAL:HG13	1:C:657:THR:H	1.79	0.47
1:A:457:GLY:O	1:A:458:HIS:HB2	2.14	0.47
1:A:669:TRP:O	1:A:673:GLN:HG2	2.14	0.47
1:A:690:PRO:HB2	1:A:693:SER:HB3	1.96	0.47
1:C:197:LEU:HD21	1:C:705:PRO:HD3	1.97	0.47
1:A:68:ASP:OD2	1:A:92:ARG:NE	2.48	0.47
1:C:52:ILE:O	1:C:56:VAL:HG23	2.13	0.47
1:A:226:PRO:HG3	1:A:257:VAL:HG21	1.97	0.47
1:C:313:ARG:HB3	1:C:400:GLU:HA	1.97	0.47
1:C:584:ASP:C	2:D:40:GLN:HG2	2.34	0.47
1:A:973:LEU:O	1:A:977:ILE:HG12	2.15	0.46
1:C:940:LEU:HD13	1:C:1005:VAL:HG11	1.96	0.46
1:C:367:GLN:O	1:C:371:LYS:HG3	2.15	0.46
1:C:556:LEU:HB3	1:C:571:VAL:CG1	2.45	0.46
1:C:92:ARG:HA	1:C:95:VAL:CG1	2.45	0.46
1:A:645:ARG:HG2	1:A:787:LEU:HD13	1.98	0.46
1:A:954:ALA:HB1	1:A:956:PHE:CE1	2.50	0.46
1:C:197:LEU:CG	1:C:198:GLU:H	2.16	0.46
1:A:970:ILE:O	1:A:974:VAL:HG23	2.16	0.46
1:C:650:ASN:O	1:C:654:TYR:HB2	2.15	0.46
1:C:103:LEU:HD23	1:C:479:ARG:NH2	2.29	0.46
1:C:115:LEU:HD13	1:C:135:LYS:NZ	2.30	0.46
1:A:47:GLY:O	1:A:50:VAL:HG12	2.16	0.46
1:A:636:THR:HA	1:A:639:LYS:HD2	1.96	0.46
1:A:957:GLN:HB3	1:A:958:PRO:HD2	1.96	0.46
1:C:421:PHE:HZ	1:C:874:VAL:HG23	1.79	0.46
1:C:291:TYR:CD1	1:C:346:ILE:HD11	2.51	0.46
1:A:1003:VAL:HG22	1:A:1004:GLU:N	2.31	0.46
1:A:52:ILE:O	1:A:56:VAL:HG23	2.16	0.46
1:C:294:ALA:CB	1:C:346:ILE:HD12	2.46	0.46
1:C:565:LYS:HG2	1:C:889:ASN:HD22	1.75	0.46
1:A:943:THR:HA	1:A:955:ASN:ND2	2.31	0.46
1:A:327:LYS:O	1:A:331:THR:HG23	2.15	0.45
1:C:144:HIS:ND1	1:C:267:SER:HB3	2.31	0.45
1:C:657:THR:HG22	1:C:658:GLU:HG2	1.97	0.45
1:C:794:LEU:H	1:C:794:LEU:HD23	1.81	0.45
1:C:943:THR:HA	1:C:955:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ILE:HG23	1:C:419:SER:N	2.30	0.45
1:C:579:TYR:CD1	2:D:72:ARG:NH1	2.85	0.45
1:A:63:SER:HB2	1:A:108:PRO:HG2	1.98	0.45
1:A:520:ILE:CD1	1:A:520:ILE:N	2.77	0.45
1:A:663:PHE:O	1:A:667:ILE:HG13	2.17	0.45
1:C:327:LYS:HE3	1:C:327:LYS:HA	1.97	0.45
1:C:830:ARG:HG3	1:C:830:ARG:HH11	1.79	0.45
1:A:198:GLU:OE1	1:A:198:GLU:HA	2.16	0.45
1:A:821:ASP:OD1	1:A:841:ARG:NH1	2.50	0.45
1:C:176:ASP:HB2	1:C:178:ASN:OD1	2.17	0.45
1:A:627:TYR:HE1	1:A:634:LEU:HD21	1.82	0.45
1:C:926:THR:HA	1:C:969:LYS:HA	1.99	0.45
1:A:479:ARG:O	1:A:482:ASP:HB2	2.17	0.45
1:A:579:TYR:CD1	2:B:72:ARG:NH1	2.85	0.45
1:C:179:GLU:OE2	1:C:179:GLU:O	2.34	0.45
1:C:526:PHE:C	1:C:528:LYS:H	2.20	0.45
1:A:288:PRO:HB2	1:A:289:PRO:HD3	1.99	0.45
1:A:30:GLU:HG2	6:A:1268:HOH:O	2.16	0.45
1:A:361:LEU:O	1:A:365:VAL:HG23	2.16	0.45
1:A:689:PHE:HE2	1:A:767:ILE:HG21	1.82	0.45
1:C:536:LEU:HD13	1:C:541:ALA:HB1	1.97	0.45
1:A:139:ILE:O	1:A:143:THR:HG23	2.17	0.45
1:A:70:GLN:O	1:A:91:PRO:HA	2.17	0.45
1:A:820:ILE:HB	1:A:841:ARG:NH2	2.32	0.45
1:A:879:LYS:HB2	1:A:882:GLU:OE1	2.16	0.45
1:C:43:ILE:N	1:C:43:ILE:HD12	2.32	0.45
1:A:97:VAL:HG23	1:A:109:VAL:HG12	1.99	0.45
1:C:185:ILE:HG22	1:C:186:ALA:N	2.32	0.45
1:A:71:PRO:HD2	1:A:73:ARG:CZ	2.47	0.45
1:A:975:GLU:HG2	1:A:982:LEU:H	1.81	0.45
1:C:502:LEU:HD13	1:C:506:ILE:HD11	1.99	0.45
1:C:681:ASN:HA	6:C:1245:HOH:O	2.17	0.45
1:C:898:SER:HA	2:D:47:GLY:O	2.17	0.45
1:C:360:PHE:CE1	1:C:865:LEU:HD21	2.53	0.44
1:C:730:SER:O	1:C:733:ALA:HB3	2.17	0.44
1:C:762:LYS:HD2	1:C:762:LYS:N	2.32	0.44
1:A:115:LEU:HD13	1:A:135:LYS:NZ	2.32	0.44
1:C:930:LEU:HD23	1:C:930:LEU:C	2.37	0.44
1:A:930:LEU:HD23	1:A:930:LEU:C	2.37	0.44
1:A:953:TYR:CG	1:A:954:ALA:N	2.85	0.44
1:C:117:THR:HG23	1:C:118:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:CYS:SG	1:C:343:ILE:HG21	2.57	0.44
1:C:879:LYS:HB2	1:C:882:GLU:OE1	2.18	0.44
1:A:660:PRO:HD2	1:A:736:TYR:CE2	2.52	0.44
1:A:943:THR:O	1:A:954:ALA:HA	2.17	0.44
1:C:361:LEU:O	1:C:365:VAL:HG23	2.17	0.44
1:C:820:ILE:HB	1:C:841:ARG:NH2	2.33	0.44
1:A:764:GLY:C	1:A:765:ILE:HD12	2.38	0.44
1:C:378:TYR:HA	1:C:379:PRO:HD3	1.82	0.44
1:A:26:VAL:HG23	1:A:27:LEU:HG	1.99	0.44
1:A:345:GLU:HG2	1:A:389:LEU:HD11	1.99	0.44
1:A:953:TYR:HE1	1:A:962:LEU:HD22	1.83	0.44
1:C:942:VAL:HG13	1:C:942:VAL:O	2.18	0.44
1:A:523:ASP:O	1:A:527:GLU:HG3	2.17	0.44
1:A:536:LEU:HD13	1:A:541:ALA:CB	2.47	0.44
1:A:433:VAL:CG1	1:A:536:LEU:HD21	2.42	0.44
1:A:732:TYR:HA	1:A:735:ASN:HD22	1.82	0.44
1:C:944:MET:HB3	1:C:994:CYS:HB2	2.00	0.44
1:A:520:ILE:H	1:A:520:ILE:CD1	2.28	0.44
1:A:656:VAL:HG13	1:A:657:THR:N	2.32	0.44
1:C:23:GLN:HG2	1:C:27:LEU:HD12	1.99	0.44
1:C:376:LYS:O	1:C:377:PHE:HB2	2.17	0.44
1:A:378:TYR:HA	1:A:379:PRO:HD3	1.81	0.43
1:C:862:VAL:HG23	1:C:863:SER:N	2.33	0.43
1:C:957:GLN:HB2	1:C:962:LEU:HD21	2.00	0.43
1:A:898:SER:HB3	2:B:44:ILE:HD13	2.01	0.43
1:A:381:LYS:HA	1:A:382:GLN:HA	1.75	0.43
1:C:741:GLU:HB3	1:C:746:ILE:HD12	2.00	0.43
1:C:606:ILE:CD1	1:C:847:VAL:HG11	2.47	0.43
1:A:940:LEU:HD13	1:A:1005:VAL:HG11	1.99	0.43
1:A:914:ASP:HB3	1:A:918:ASP:H	1.84	0.43
1:A:919:ARG:HG3	1:A:919:ARG:NH1	2.33	0.43
1:A:302:ALA:O	1:A:307:GLY:N	2.51	0.43
1:A:23:GLN:O	1:A:26:VAL:HG22	2.19	0.43
1:C:29:HIS:HE1	1:C:842:PHE:CE2	2.36	0.43
1:C:919:ARG:HG3	1:C:919:ARG:NH1	2.33	0.43
1:A:786:GLU:O	1:A:790:ILE:HG13	2.17	0.43
1:A:953:TYR:CE1	1:A:962:LEU:HD22	2.54	0.43
2:D:50:LEU:HD22	2:D:59:TYR:CD2	2.54	0.43
1:A:273:LYS:HA	1:A:332:LEU:HD21	2.00	0.43
1:A:376:LYS:O	1:A:377:PHE:HB2	2.19	0.43
1:A:671:ARG:NH1	1:A:671:ARG:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:SER:O	1:A:733:ALA:HB3	2.19	0.43
1:A:645:ARG:HG2	1:A:787:LEU:HD22	2.01	0.43
1:A:851:ILE:HD12	1:A:851:ILE:N	2.33	0.43
1:C:523:ASP:O	1:C:527:GLU:HG3	2.19	0.43
1:C:712:LEU:HD21	1:C:721:HIS:HE2	1.83	0.43
1:A:294:ALA:CB	1:A:346:ILE:HD12	2.49	0.43
1:A:942:VAL:O	1:A:942:VAL:HG13	2.19	0.42
1:A:117:THR:HG23	1:A:118:GLU:N	2.33	0.42
1:C:428:LEU:O	1:C:457:GLY:HA2	2.19	0.42
1:A:987:LYS:O	1:A:1012:LEU:HD12	2.19	0.42
1:A:309:LEU:HB3	1:A:310:PRO:HD2	2.02	0.42
1:A:606:ILE:HD13	1:A:847:VAL:CG1	2.49	0.42
1:A:645:ARG:HG2	1:A:787:LEU:CD1	2.49	0.42
1:C:608:TRP:CD2	1:C:830:ARG:HD2	2.54	0.42
1:C:830:ARG:HG3	1:C:830:ARG:NH1	2.34	0.42
1:C:885:ASN:ND2	1:C:900:PRO:HA	2.33	0.42
1:C:961:LYS:HD2	1:C:965:ARG:NH2	2.35	0.42
1:C:345:GLU:HG3	1:C:349:GLN:NE2	2.35	0.42
1:C:47:GLY:HA3	1:C:79:SER:OG	2.19	0.42
1:C:50:VAL:HG13	1:C:51:GLU:N	2.35	0.42
1:C:906:MET:CE	1:C:915:LYS:HE2	2.49	0.42
1:A:332:LEU:HD22	1:A:334:PHE:HD1	1.84	0.42
1:C:229:VAL:HG13	1:C:237:PHE:HB2	2.01	0.42
1:C:755:ASN:HA	1:C:756:PRO:HD2	1.93	0.42
1:A:341:LYS:HB2	1:A:341:LYS:HE2	1.93	0.42
1:A:35:MET:CE	1:A:370:LEU:HD22	2.49	0.42
1:A:618:LYS:HD3	1:A:622:ASP:OD2	2.19	0.42
1:A:970:ILE:HG21	1:A:1010:ILE:HG13	2.02	0.42
1:A:220:GLY:C	1:A:245:LEU:HD11	2.39	0.42
1:A:50:VAL:HG13	1:A:51:GLU:N	2.35	0.42
1:C:30:GLU:HG3	1:C:31:ALA:N	2.35	0.42
1:C:526:PHE:O	1:C:528:LYS:N	2.53	0.42
1:C:953:TYR:CE1	1:C:962:LEU:HD22	2.54	0.42
1:A:185:ILE:O	1:A:251:ASN:HA	2.20	0.42
1:A:26:VAL:HG11	1:A:563:GLY:HA2	2.01	0.42
1:A:287:ARG:N	1:A:288:PRO:CD	2.83	0.42
1:A:103:LEU:HD23	1:A:479:ARG:HH21	1.83	0.42
1:C:918:ASP:O	1:C:1006:PRO:HB3	2.19	0.42
1:C:288:PRO:HB2	1:C:289:PRO:HD3	2.02	0.42
1:C:381:LYS:HG3	1:C:382:GLN:HG3	2.01	0.42
1:C:600:ASN:OD1	1:C:601:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:LYS:HE2	6:A:1257:HOH:O	2.19	0.42
1:A:185:ILE:HG22	1:A:186:ALA:N	2.34	0.42
1:A:180:PRO:HG3	1:A:258:LYS:HD2	2.00	0.42
1:C:128:VAL:HG21	1:C:150:TYR:HE1	1.83	0.42
1:C:73:ARG:HG2	1:C:73:ARG:HH21	1.85	0.42
1:A:625:ASN:OD1	1:A:804:ARG:HG3	2.20	0.41
1:A:651:ILE:HG22	1:A:655:LEU:HD12	2.02	0.41
1:C:332:LEU:HD22	1:C:334:PHE:CD1	2.54	0.41
1:A:862:VAL:HG23	1:A:863:SER:N	2.35	0.41
1:A:945:LEU:HD13	1:A:993:ILE:HG22	2.02	0.41
1:C:139:ILE:O	1:C:143:THR:HG23	2.20	0.41
1:C:656:VAL:HG13	1:C:657:THR:N	2.36	0.41
1:C:71:PRO:HD2	1:C:73:ARG:CZ	2.49	0.41
1:C:975:GLU:HG2	1:C:982:LEU:H	1.85	0.41
1:A:472:LEU:HD11	1:A:480:PRO:HA	2.02	0.41
1:A:630:SER:HA	1:A:631:PRO:HD3	1.92	0.41
1:A:720:GLU:HB3	1:A:829:LEU:CD2	2.49	0.41
1:C:115:LEU:HD13	1:C:135:LYS:HZ1	1.85	0.41
1:C:651:ILE:O	1:C:655:LEU:HB2	2.20	0.41
1:A:313:ARG:HG3	1:A:313:ARG:O	2.20	0.41
1:C:287:ARG:N	1:C:288:PRO:CD	2.84	0.41
1:C:720:GLU:HB3	1:C:829:LEU:CD2	2.50	0.41
1:C:953:TYR:CG	1:C:954:ALA:N	2.88	0.41
1:A:651:ILE:CG2	1:A:655:LEU:HD12	2.50	0.41
1:A:926:THR:HA	1:A:969:LYS:HA	2.02	0.41
2:B:63:LYS:HE3	6:B:105:HOH:O	2.20	0.41
1:C:62:LYS:O	1:C:108:PRO:HD2	2.20	0.41
1:C:846:PHE:CE1	1:C:853:PRO:HD3	2.50	0.41
1:C:965:ARG:C	1:C:967:PRO:HD2	2.40	0.41
1:A:526:PHE:O	1:A:554:LYS:HE2	2.21	0.41
1:A:532:VAL:O	1:A:556:LEU:HA	2.20	0.41
1:A:642:SER:C	1:A:644:PRO:HD3	2.41	0.41
1:A:657:THR:HG22	1:A:658:GLU:HG2	2.02	0.41
1:A:989:LEU:HB3	1:A:1010:ILE:HB	2.02	0.41
1:C:536:LEU:HD13	1:C:541:ALA:HB3	2.01	0.41
1:A:452:ALA:CB	1:A:459:ILE:HG13	2.51	0.41
1:C:327:LYS:O	1:C:331:THR:HG23	2.21	0.41
1:C:445:ASN:O	1:C:449:MET:HG3	2.21	0.41
1:C:660:PRO:HD2	1:C:736:TYR:CE2	2.56	0.41
1:C:663:PHE:CE2	1:C:667:ILE:HD11	2.55	0.41
1:A:227:ARG:HG2	1:A:227:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TYR:CD1	1:A:346:ILE:HD11	2.56	0.41
1:A:608:TRP:CD2	1:A:830:ARG:HD2	2.55	0.41
1:A:741:GLU:HB3	1:A:746:ILE:HD12	2.01	0.41
1:C:302:ALA:O	1:C:307:GLY:N	2.54	0.41
1:A:387:ASP:OD1	1:A:387:ASP:C	2.59	0.41
1:C:198:GLU:OE1	1:C:198:GLU:HA	2.20	0.41
1:C:482:ASP:O	1:C:483:VAL:C	2.59	0.41
1:C:952:LEU:HD12	1:C:952:LEU:N	2.35	0.41
1:C:299:SER:O	1:C:302:ALA:HB3	2.21	0.41
1:C:904:PRO:HD2	1:C:916:ILE:CD1	2.51	0.41
1:A:188:ILE:O	1:A:188:ILE:HG23	2.21	0.41
1:A:70:GLN:HA	1:A:71:PRO:HD3	1.88	0.41
1:C:529:LEU:O	1:C:554:LYS:HE3	2.20	0.41
1:C:433:VAL:CG1	1:C:536:LEU:HD21	2.44	0.41
1:C:676:LYS:HG2	1:C:676:LYS:O	2.21	0.41
1:C:953:TYR:HE1	1:C:962:LEU:HD22	1.86	0.41
1:A:132:SER:HB2	6:A:1267:HOH:O	2.20	0.40
1:C:266:LYS:HB2	1:C:271:SER:HB3	2.02	0.40
1:A:445:ASN:O	1:A:449:MET:HG3	2.20	0.40
1:A:546:ASP:OD1	1:A:578:SER:HB2	2.22	0.40
1:C:906:MET:HE3	1:C:915:LYS:HE2	2.03	0.40
1:A:151:ILE:HD12	1:A:369:VAL:HG22	2.04	0.40
1:A:328:ILE:O	1:A:332:LEU:HB2	2.22	0.40
1:A:526:PHE:C	1:A:528:LYS:H	2.24	0.40
1:C:81:TYR:HB2	1:C:498:MET:CE	2.51	0.40
1:C:546:ASP:O	1:C:550:VAL:HG23	2.22	0.40
1:C:898:SER:HB3	2:D:44:ILE:HD13	2.01	0.40
2:D:56:LEU:CD2	2:D:61:ILE:HD12	2.51	0.40
1:A:30:GLU:HG3	1:A:31:ALA:N	2.36	0.40
1:A:869:GLU:OE2	1:A:872:LYS:HD2	2.22	0.40
1:A:189:THR:OG1	1:A:193:VAL:HB	2.21	0.40
1:A:428:LEU:O	1:A:457:GLY:HA2	2.21	0.40
1:C:120:LEU:C	1:C:122:ASN:H	2.24	0.40
1:C:292:HIS:HA	1:C:385:TYR:CZ	2.57	0.40
1:C:479:ARG:HB3	1:C:480:PRO:HD2	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	982/1001 (98%)	869 (88%)	104 (11%)	9 (1%)	20	54
1	C	971/1001 (97%)	862 (89%)	99 (10%)	10 (1%)	18	51
2	B	74/96 (77%)	73 (99%)	1 (1%)	0	100	100
2	D	74/96 (77%)	73 (99%)	1 (1%)	0	100	100
All	All	2101/2194 (96%)	1877 (89%)	205 (10%)	19 (1%)	20	54

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	251	ASN
1	C	71	PRO
1	C	251	ASN
1	C	197	LEU
1	A	197	LEU
1	C	527	GLU
1	A	188	ILE
1	C	121	LYS
1	A	458	HIS
1	A	527	GLU
1	A	691	LYS
1	C	458	HIS
1	A	81	TYR
1	C	70	GLN
1	C	188	ILE
1	C	764	GLY
1	A	70	GLN
1	C	483	VAL



### 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	865/877 (99%)	850 (98%)	15 (2%)	66	89
1	C	855/877 (98%)	835 (98%)	20 (2%)	56	85
2	B	69/86 (80%)	65 (94%)	4 (6%)	23	56
2	D	69/86 (80%)	66 (96%)	3 (4%)	33	68
All	All	1858/1926 (96%)	1816 (98%)	42 (2%)	56	85

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	39	ASN
1	A	80	GLN
1	A	86	ASP
1	A	114	GLU
1	A	243	LYS
1	A	334	PHE
1	A	387	ASP
1	A	392	LEU
1	A	464	MET
1	A	575	LEU
1	A	718	ASN
1	A	804	ARG
1	A	919	ARG
1	A	1012	LEU
2	B	21	ASP
2	B	24	ASP
2	B	52	ASP
2	B	64	GLU
1	C	22	ARG
1	C	39	ASN
1	C	80	GLN
1	C	86	ASP
1	C	114	GLU

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Mol	Chain	Res	Type
1	C	178	ASN
1	C	179	GLU
1	C	243	LYS
1	C	334	PHE
1	C	387	ASP
1	C	392	LEU
1	C	464	MET
1	C	571	VAL
1	C	575	LEU
1	C	593	CYS
1	C	718	ASN
1	C	762	LYS
1	C	919	ARG
1	C	995	CYS
1	C	1012	LEU
2	D	24	ASP
2	D	52	ASP
2	D	64	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	136	GLN
1	A	251	ASN
1	A	471	ASN
1	A	510	GLN
1	A	623	ASN
1	A	650	ASN
1	A	680	ASN
1	A	688	ASN
1	A	699	GLN
1	A	718	ASN
1	A	735	ASN
2	B	31	GLN
1	C	80	GLN
1	C	136	GLN
1	C	251	ASN
1	C	471	ASN
1	C	510	GLN
1	C	623	ASN
1	C	650	ASN

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Mol	Chain	Res	Type
1	C	680	ASN
1	C	688	ASN
1	C	717	HIS
1	C	718	ASN
1	C	735	ASN
1	C	833	ASN
2	D	25	ASN
2	D	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	ATP	A	1103	3	27,33,33	1.21	3 (11%)	25,52,52	2.07	5 (20%)
4	ATP	C	1103	3	27,33,33	1.23	3 (11%)	25,52,52	2.03	4 (16%)

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	ATP	A	1103	3	-	0/18/38/38	0/3/3/3
4	ATP	C	1103	3	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1103	ATP	PG-O3B	2.11	1.63	1.60
4	A	1103	ATP	PG-O3B	2.21	1.63	1.60
4	C	1103	ATP	C2-N3	2.65	1.36	1.32
4	A	1103	ATP	C2-N3	2.68	1.36	1.32
4	A	1103	ATP	C5-C4	3.33	1.48	1.40
4	C	1103	ATP	C5-C4	3.37	1.48	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1103	ATP	N3-C2-N1	-8.12	121.78	128.86
4	A	1103	ATP	N3-C2-N1	-7.97	121.92	128.86
4	A	1103	ATP	C4'-O4'-C1'	-3.75	105.77	109.77
4	A	1103	ATP	C4-C5-N7	-2.64	106.86	109.41
4	C	1103	ATP	C1'-N9-C4	-2.61	122.13	126.64
4	C	1103	ATP	C4-C5-N7	-2.33	107.16	109.41
4	A	1103	ATP	C1'-N9-C4	-2.04	123.11	126.64
4	A	1103	ATP	C2-N1-C6	2.05	122.36	118.77
4	C	1103	ATP	C2-N1-C6	2.32	122.83	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	ATP	2	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	986/1001 (98%)	-0.08	11 (1%) 80 79	26, 57, 96, 133	0
1	C	977/1001 (97%)	0.14	29 (2%) 51 44	27, 65, 101, 135	0
2	B	76/96 (79%)	-0.24	0 100 100	29, 44, 62, 68	0
2	D	76/96 (79%)	-0.29	0 100 100	35, 48, 65, 71	0
All	All	2115/2194 (96%)	0.01	40 (1%) 67 64	26, 60, 97, 135	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	PHE	6.5
1	A	767	ILE	6.3
1	A	768	GLN	5.8
1	C	747	TYR	4.4
1	C	335	ASP	4.2
1	C	656	VAL	4.0
1	C	634	LEU	3.9
1	A	766	LYS	3.6
1	C	765	ILE	3.6
1	C	120	LEU	3.5
1	C	788	LYS	3.4
1	C	779	ALA	3.2
1	C	661	LEU	3.2
1	C	209	PHE	3.1
1	C	336	VAL	2.9
1	C	638	LEU	2.9
1	C	751	LEU	2.8
1	C	793	SER	2.8
1	A	985	PHE	2.7
1	C	115	LEU	2.6
1	C	332	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	651	ILE	2.5
1	C	818	HIS	2.5
1	A	638	LEU	2.4
1	A	742	THR	2.4
1	C	962	LEU	2.4
1	C	219	PRO	2.4
1	A	334	PHE	2.4
1	C	627	TYR	2.3
1	A	36	SER	2.2
1	C	664	GLU	2.2
1	C	745	ALA	2.2
1	C	742	THR	2.2
1	A	787	LEU	2.1
1	C	628	LEU	2.1
1	C	781	ASN	2.1
1	A	856	CYS	2.1
1	A	765	ILE	2.1
1	C	749	ARG	2.1
1	C	655	LEU	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
5	CA	A	1107	1/1	0.91	0.21	1.27	73,73,73,73	0
4	ATP	A	1103	31/31	0.95	0.21	0.23	41,45,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	C	1103	31/31	0.91	0.18	0.04	46,53,83,84	0
5	CA	C	1107	1/1	0.97	0.09	-3.09	52,52,52,52	0
5	CA	A	1105	1/1	0.98	0.06	-9.65	60,60,60,60	0
5	CA	C	1104	1/1	0.95	0.12	-	57,57,57,57	0
3	MG	C	1101	1/1	0.85	0.29	-	42,42,42,42	0
3	MG	A	1102	1/1	0.92	0.26	-	28,28,28,28	0
3	MG	A	1101	1/1	0.96	0.20	-	2,2,2,2	0
3	MG	C	1102	1/1	0.94	0.15	-	29,29,29,29	0
5	CA	A	1104	1/1	0.97	0.19	-	46,46,46,46	0
5	CA	C	1108	1/1	0.96	0.06	-	46,46,46,46	0
5	CA	C	1106	1/1	0.88	0.07	-	81,81,81,81	0
5	CA	A	1106	1/1	0.96	0.13	-	60,60,60,60	0
5	CA	C	1109	1/1	0.69	0.13	-	72,72,72,72	0
5	CA	C	1105	1/1	0.95	0.16	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.