



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 02:03 AM JST

PDB ID : 6KID
Title : Crystal structure of human leucyl-tRNA synthetase, ATP-bound form
Authors : Kim, S.; Son, J.; Kim, S.; Hwang, K.Y.
Deposited on : 2019-07-18
Resolution : 3.15 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

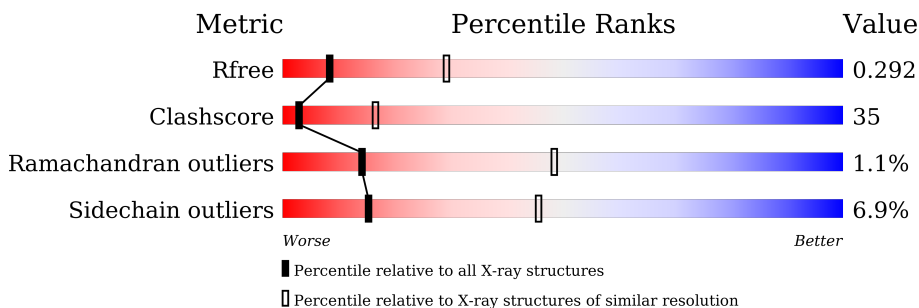
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1188	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8353 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.

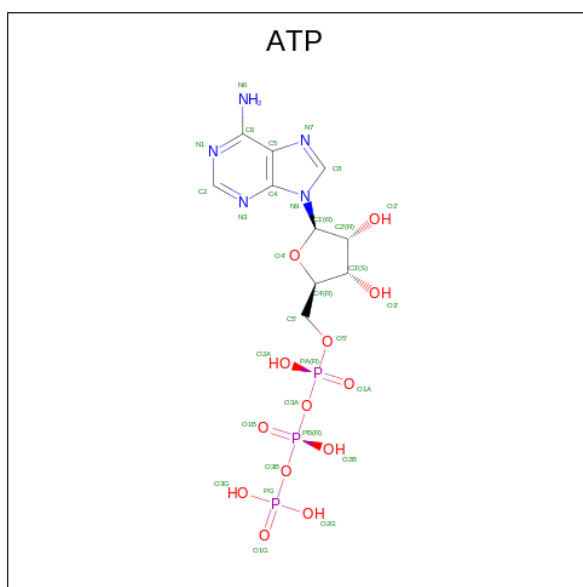
- Molecule 1 is a protein called Leucine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1004	8103	5213	1346	1491	53	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

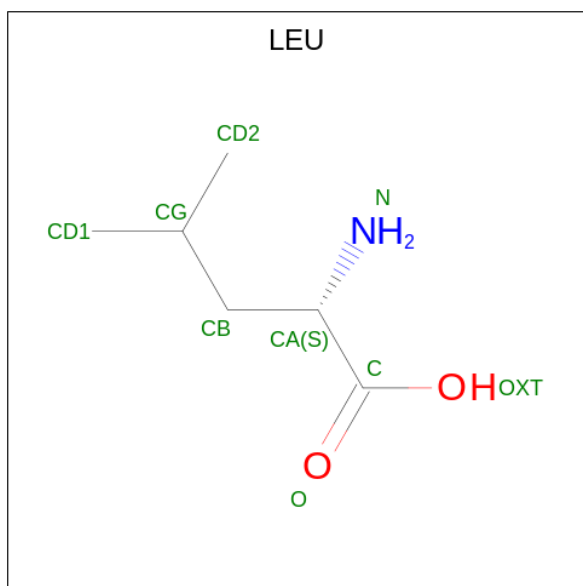
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9P2J5
A	-10	ARG	-	expression tag	UNP Q9P2J5
A	-9	GLY	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	HIS	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	HIS	-	expression tag	UNP Q9P2J5
A	-4	HIS	-	expression tag	UNP Q9P2J5
A	-3	HIS	-	expression tag	UNP Q9P2J5
A	-2	HIS	-	expression tag	UNP Q9P2J5
A	-1	GLY	-	expression tag	UNP Q9P2J5
A	0	SER	-	expression tag	UNP Q9P2J5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



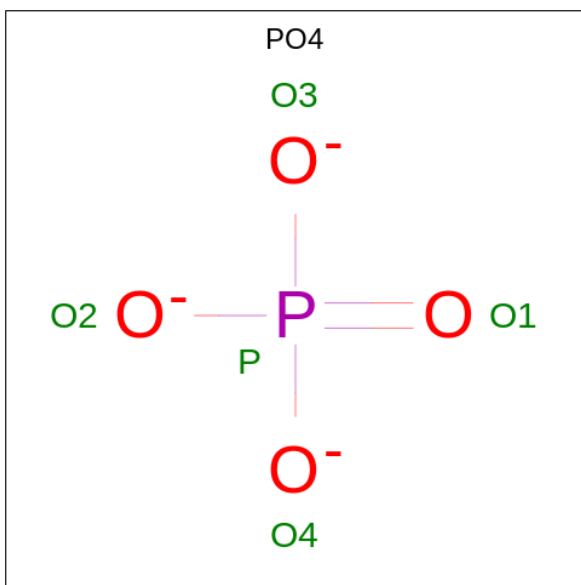
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	9	6	1	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

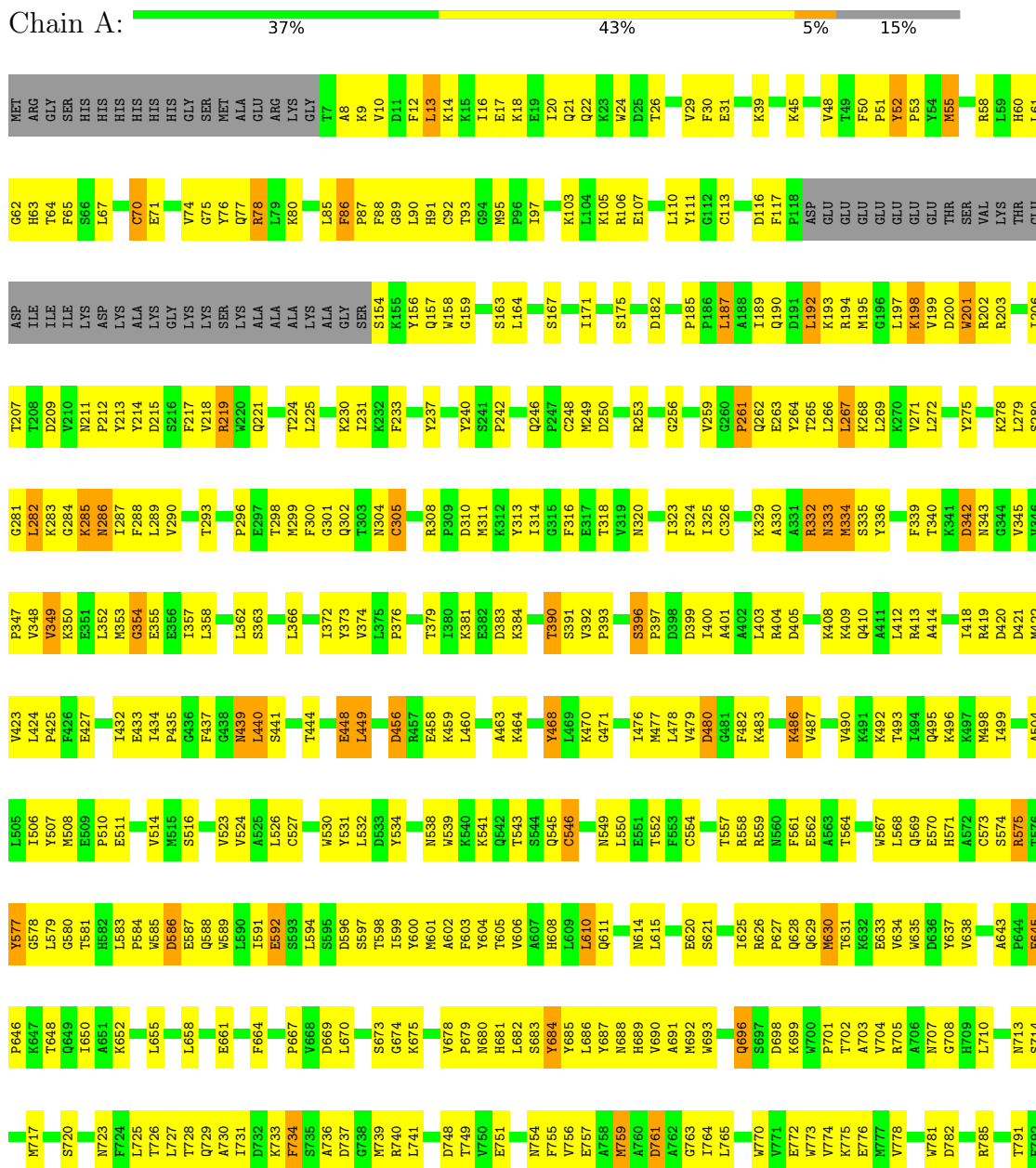
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	200	Total O 200 200	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Leucine-tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.22Å 137.22Å 433.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.89 – 3.15 49.01 – 2.97	Depositor EDS
% Data completeness (in resolution range)	91.0 (42.89-3.15) 88.2 (49.01-2.97)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.245 , 0.293 0.246 , 0.292	Depositor DCC
R_{free} test set	1832 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, 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	0.81	6/8303 (0.1%)	0.98	21/11222 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	CYS	CB-SG	-10.06	1.65	1.82
1	A	305	CYS	CB-SG	-8.84	1.67	1.82
1	A	326	CYS	CB-SG	-6.48	1.71	1.82
1	A	546	CYS	CB-SG	-6.41	1.71	1.82
1	A	201	TRP	CB-CG	5.20	1.59	1.50
1	A	427	GLU	CB-CG	5.19	1.62	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	MET	CG-SD-CE	10.73	117.38	100.20
1	A	847	LEU	CA-CB-CG	8.86	135.69	115.30
1	A	282	LEU	CA-CB-CG	-8.23	96.36	115.30
1	A	575	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	A	249	MET	CB-CG-SD	7.01	133.44	112.40
1	A	267	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	A	761	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	610	LEU	CA-CB-CG	-6.50	100.35	115.30
1	A	249	MET	CA-CB-CG	6.36	124.10	113.30
1	A	978	SER	C-N-CA	-6.30	105.96	121.70
1	A	192	LEU	CB-CG-CD2	6.04	121.27	111.00
1	A	881	MET	CG-SD-CE	6.03	109.85	100.20
1	A	440	LEU	CA-CB-CG	-6.01	101.47	115.30
1	A	358	LEU	CA-CB-CG	-5.85	101.83	115.30
1	A	261	PRO	N-CA-C	-5.85	96.90	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	741	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	A	809	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	1000	LEU	CB-CG-CD1	5.32	120.05	111.00
1	A	349	VAL	CG1-CB-CG2	5.23	119.27	110.90
1	A	1027	LEU	CA-CB-CG	-5.17	103.40	115.30

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	8103	0	8062	562	0
2	A	31	0	11	4	0
3	A	9	0	10	0	0
4	A	10	0	0	0	0
5	A	200	0	0	22	0
All	All	8353	0	8083	564	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 35.

All (564) 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:1017:LYS:NZ	1:A:1038:VAL:CG1	1.68	1.55
1:A:1017:LYS:NZ	1:A:1038:VAL:HG12	1.03	1.36
1:A:1017:LYS:CE	1:A:1038:VAL:HG12	1.70	1.19
1:A:629:GLN:HE21	1:A:650:ILE:HD11	0.99	1.14
1:A:629:GLN:NE2	1:A:650:ILE:HD11	1.65	1.11
1:A:1017:LYS:CE	1:A:1038:VAL:CG1	2.29	1.09
1:A:1017:LYS:HZ3	1:A:1038:VAL:CG1	1.42	1.08
1:A:629:GLN:HE21	1:A:650:ILE:CD1	1.66	1.07
1:A:268:LYS:HE3	1:A:288:PHE:CE2	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:MET:HG2	1:A:1007:ILE:HD11	1.37	1.03
1:A:954:VAL:O	1:A:957:LYS:HB2	1.63	0.96
1:A:940:VAL:HG21	1:A:1017:LYS:CD	1.96	0.95
1:A:9:LYS:HE3	1:A:765:LEU:HD22	1.46	0.95
1:A:1017:LYS:HZ3	1:A:1038:VAL:HG13	1.32	0.94
1:A:629:GLN:NE2	1:A:650:ILE:CD1	2.30	0.91
1:A:267:LEU:HD21	1:A:498:MET:SD	2.11	0.90
1:A:237:TYR:CZ	1:A:526:LEU:HD22	2.07	0.89
1:A:92:CYS:SG	1:A:206:ILE:HD12	2.15	0.87
1:A:629:GLN:HG2	1:A:650:ILE:CD1	2.05	0.86
1:A:1017:LYS:HZ2	1:A:1038:VAL:CG1	1.55	0.85
1:A:751:GLU:O	5:A:1301:HOH:O	1.94	0.85
1:A:320:ASN:OD1	5:A:1302:HOH:O	1.95	0.84
1:A:972:ILE:HD12	1:A:990:MET:HG2	1.58	0.84
1:A:1017:LYS:HE3	1:A:1038:VAL:HG11	1.59	0.83
1:A:949:HIS:O	1:A:953:SER:HB2	1.79	0.83
1:A:940:VAL:HG21	1:A:1017:LYS:HD3	1.61	0.82
1:A:1017:LYS:NZ	1:A:1038:VAL:HG13	1.89	0.81
1:A:942:LYS:HG3	1:A:943:ASN:H	1.44	0.81
1:A:976:LEU:HD13	1:A:982:LEU:HD12	1.63	0.80
1:A:434:ILE:HG12	1:A:471:GLY:HA2	1.61	0.80
1:A:213:TYR:HD2	1:A:611:GLN:HG2	1.46	0.80
1:A:10:VAL:HG22	1:A:764:ILE:HD13	1.62	0.80
1:A:586:ASP:HB3	1:A:589:TRP:CD1	2.17	0.80
1:A:629:GLN:CG	1:A:650:ILE:HD11	2.12	0.80
1:A:941:ALA:HB3	1:A:1054:PRO:HD3	1.63	0.80
1:A:774:VAL:HG13	1:A:852:ILE:HD13	1.64	0.79
1:A:1017:LYS:CE	1:A:1038:VAL:HG11	2.11	0.78
1:A:1017:LYS:HE3	1:A:1038:VAL:CG1	2.13	0.78
1:A:761:ASP:OD2	5:A:1303:HOH:O	2.01	0.78
1:A:954:VAL:O	1:A:957:LYS:N	2.15	0.78
1:A:1049:ARG:HH11	1:A:1050:GLU:HG3	1.50	0.77
1:A:330:ALA:O	1:A:334:MET:HG2	1.86	0.76
1:A:799:SER:HB3	1:A:892:ASN:H	1.51	0.76
1:A:940:VAL:HG12	1:A:941:ALA:H	1.51	0.76
1:A:770:TRP:HE1	1:A:870:ILE:HD11	1.49	0.76
1:A:837:GLU:HG2	1:A:1026:TYR:OH	1.86	0.76
1:A:569:GLN:HG2	1:A:570:GLU:H	1.51	0.76
1:A:31:GLU:OE1	1:A:202:ARG:NH1	2.19	0.75
1:A:605:THR:O	1:A:661:GLU:HG2	1.87	0.75
1:A:261:PRO:HG2	5:A:1360:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:GLY:HA2	1:A:986:MET:HG3	1.69	0.74
1:A:16:ILE:O	1:A:20:ILE:HG12	1.88	0.73
1:A:538:ASN:ND2	5:A:1307:HOH:O	2.18	0.73
1:A:24:TRP:CH2	1:A:864:PRO:HB2	2.25	0.72
1:A:78:ARG:HD2	1:A:881:MET:HE2	1.69	0.72
1:A:586:ASP:HB3	1:A:589:TRP:HD1	1.55	0.71
1:A:268:LYS:HE3	1:A:288:PHE:CD2	2.25	0.71
1:A:282:LEU:HD11	1:A:349:VAL:HG21	1.72	0.71
1:A:892:ASN:HB3	1:A:895:LEU:HB2	1.73	0.71
2:A:1201:ATP:H5'1	2:A:1201:ATP:O1B	1.91	0.71
1:A:990:MET:HA	1:A:993:VAL:HB	1.74	0.70
1:A:602:ALA:O	1:A:605:THR:OG1	2.09	0.69
1:A:645:PHE:HZ	1:A:652:LYS:HA	1.56	0.69
1:A:940:VAL:CG2	1:A:1017:LYS:NZ	2.56	0.69
1:A:287:ILE:HG23	1:A:323:ILE:HB	1.73	0.69
1:A:629:GLN:CG	1:A:650:ILE:CD1	2.71	0.69
1:A:947:TRP:HZ3	1:A:989:VAL:HA	1.58	0.69
1:A:471:GLY:O	1:A:487:VAL:HG21	1.94	0.68
1:A:366:LEU:HD21	1:A:498:MET:HG3	1.75	0.68
1:A:60:HIS:HA	1:A:726:THR:HA	1.75	0.68
1:A:439:ASN:HB2	1:A:440:LEU:HG	1.77	0.67
1:A:200:ASP:OD2	1:A:202:ARG:NH2	2.27	0.67
1:A:203:ARG:HG3	1:A:608:HIS:HB3	1.76	0.67
1:A:335:SER:HA	1:A:340:THR:HG23	1.76	0.67
1:A:949:HIS:O	1:A:949:HIS:ND1	2.28	0.67
1:A:167:SER:O	1:A:171:ILE:HG13	1.94	0.67
1:A:10:VAL:HG22	1:A:764:ILE:CD1	2.25	0.66
1:A:573:CYS:HA	1:A:592:GLU:HG2	1.77	0.66
1:A:614:ASN:OD1	1:A:615:LEU:N	2.27	0.66
1:A:1056:LYS:NZ	5:A:1312:HOH:O	2.28	0.66
1:A:259:VAL:HG13	1:A:511:GLU:HB2	1.76	0.66
1:A:423:VAL:HG23	1:A:424:LEU:HG	1.78	0.66
1:A:940:VAL:HG21	1:A:1017:LYS:HD2	1.77	0.66
1:A:530:TRP:H	1:A:574:SER:HB3	1.61	0.66
1:A:736:ALA:O	1:A:740:ARG:N	2.26	0.66
1:A:1000:LEU:HD22	1:A:1004:GLY:O	1.96	0.66
1:A:55:MET:SD	1:A:90:LEU:HD22	2.37	0.65
1:A:237:TYR:CE2	1:A:526:LEU:HD22	2.31	0.65
1:A:733:LYS:NZ	1:A:757:GLU:OE2	2.25	0.65
1:A:10:VAL:CG2	1:A:764:ILE:HD13	2.26	0.65
1:A:1049:ARG:NH1	1:A:1050:GLU:HG3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:HA	1:A:17:GLU:HB2	1.78	0.65
1:A:629:GLN:CD	1:A:650:ILE:HD11	2.16	0.65
1:A:859:LEU:HB3	1:A:867:CYS:SG	2.38	0.64
1:A:282:LEU:CD1	1:A:349:VAL:HG21	2.28	0.64
1:A:1053:CYS:HB2	1:A:1054:PRO:HD2	1.80	0.64
1:A:893:GLU:OE2	5:A:1304:HOH:O	2.14	0.64
1:A:409:LYS:HB2	1:A:412:LEU:HD13	1.80	0.64
1:A:965:LYS:HD3	1:A:966:LEU:O	1.97	0.64
1:A:969:ASN:HA	1:A:972:ILE:HG23	1.78	0.64
1:A:60:HIS:O	1:A:63:HIS:HB2	1.98	0.64
1:A:977:GLY:HA2	1:A:986:MET:CG	2.28	0.63
1:A:22:GLN:O	1:A:26:THR:HG22	1.99	0.63
1:A:601:MET:O	1:A:604:TYR:HB2	1.98	0.63
1:A:280:SER:O	1:A:283:LYS:HE3	1.97	0.63
1:A:673:SER:OG	1:A:674:GLY:N	2.32	0.63
1:A:12:PHE:HB3	5:A:1305:HOH:O	1.99	0.62
1:A:61:LEU:O	1:A:64:THR:N	2.29	0.62
1:A:947:TRP:CE3	1:A:989:VAL:HG12	2.34	0.62
1:A:77:GLN:O	1:A:80:LYS:N	2.33	0.62
1:A:194:ARG:O	1:A:731:ILE:HD13	1.98	0.62
1:A:940:VAL:CG2	1:A:1017:LYS:HD3	2.28	0.62
1:A:158:TRP:CH2	1:A:171:ILE:HD12	2.35	0.62
1:A:185:PRO:HG3	1:A:206:ILE:HD11	1.81	0.62
1:A:256:GLY:O	1:A:259:VAL:HG23	1.98	0.62
1:A:271:VAL:HG23	1:A:287:ILE:O	1.99	0.62
1:A:648:THR:HG21	1:A:655:LEU:HD12	1.82	0.62
1:A:299:MET:HE1	1:A:302:GLN:OE1	1.99	0.62
1:A:413:ARG:HD3	1:A:423:VAL:HG21	1.82	0.62
1:A:267:LEU:HD11	1:A:299:MET:HG3	1.82	0.62
1:A:995:MET:SD	1:A:996:ILE:HG12	2.40	0.62
1:A:282:LEU:HD22	1:A:285:LYS:HE3	1.82	0.61
1:A:9:LYS:O	5:A:1305:HOH:O	2.16	0.61
1:A:314:ILE:HG23	1:A:348:VAL:HG13	1.82	0.61
1:A:629:GLN:HE21	1:A:650:ILE:CG1	2.12	0.61
1:A:948:GLN:HA	1:A:951:THR:OG1	2.01	0.61
1:A:93:THR:HG21	1:A:596:ASP:OD2	2.01	0.61
1:A:916:TYR:HE1	1:A:1061:PHE:HD2	1.46	0.61
1:A:650:ILE:HD12	1:A:650:ILE:N	2.16	0.61
1:A:199:VAL:HB	1:A:201:TRP:CD1	2.36	0.61
1:A:557:THR:HG22	1:A:561:PHE:HE1	1.66	0.60
1:A:939:TYR:HB3	1:A:1041:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:HG23	1:A:424:LEU:N	2.16	0.60
1:A:39:LYS:O	5:A:1306:HOH:O	2.17	0.60
1:A:940:VAL:HG23	1:A:1017:LYS:NZ	2.16	0.60
1:A:1024:ILE:HA	1:A:1027:LEU:HD12	1.83	0.60
1:A:569:GLN:HG2	1:A:570:GLU:N	2.15	0.60
1:A:631:THR:O	1:A:634:VAL:N	2.34	0.60
1:A:982:LEU:O	1:A:986:MET:HG2	2.01	0.60
1:A:213:TYR:CD2	1:A:611:GLN:HG2	2.33	0.60
1:A:267:LEU:CD1	1:A:299:MET:HG3	2.31	0.60
1:A:281:GLY:O	1:A:283:LYS:N	2.31	0.60
1:A:316:PHE:HB2	1:A:347:PRO:HD2	1.83	0.60
1:A:190:GLN:O	1:A:193:LYS:HB3	2.01	0.60
1:A:564:THR:HG21	1:A:679:PRO:HA	1.84	0.60
1:A:737:ASP:OD1	1:A:865:HIS:ND1	2.26	0.60
1:A:268:LYS:CE	1:A:288:PHE:CE2	2.80	0.59
1:A:558:ARG:O	1:A:562:GLU:HB2	2.03	0.59
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.84	0.59
1:A:263:GLU:HA	1:A:508:MET:HG2	1.84	0.59
1:A:559:ARG:NH1	5:A:1318:HOH:O	2.34	0.59
1:A:626:ARG:NH2	5:A:1321:HOH:O	2.35	0.59
1:A:972:ILE:HG13	1:A:973:ALA:H	1.67	0.59
1:A:770:TRP:HZ3	1:A:851:PHE:CE2	2.21	0.59
1:A:214:TYR:O	1:A:218:VAL:HG23	2.03	0.58
1:A:266:LEU:O	1:A:504:ALA:HB1	2.03	0.58
1:A:543:THR:HG21	1:A:687:TYR:CD1	2.38	0.58
1:A:731:ILE:HG23	1:A:736:ALA:HB2	1.85	0.58
1:A:606:VAL:HG11	1:A:658:LEU:HB3	1.85	0.58
1:A:1023:ASN:O	1:A:1027:LEU:HG	2.03	0.58
1:A:64:THR:HG21	1:A:727:LEU:HD13	1.85	0.58
1:A:266:LEU:CG	1:A:290:VAL:HG13	2.33	0.58
1:A:539:TRP:O	1:A:543:THR:HG23	2.03	0.58
1:A:24:TRP:HH2	1:A:864:PRO:HB2	1.66	0.58
1:A:1006:ARG:O	1:A:1008:LEU:N	2.36	0.58
1:A:9:LYS:HB3	1:A:764:ILE:HD12	1.86	0.58
1:A:942:LYS:HG3	1:A:943:ASN:N	2.18	0.58
1:A:262:GLN:HG3	1:A:511:GLU:HG2	1.84	0.58
1:A:278:LYS:O	1:A:279:LEU:HD23	2.03	0.58
1:A:959:PHE:HA	1:A:962:ASN:HB2	1.86	0.58
1:A:543:THR:HG21	1:A:687:TYR:HD1	1.70	0.57
1:A:458:GLU:HG3	1:A:459:LYS:HG3	1.85	0.57
1:A:21:GLN:OE1	1:A:194:ARG:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:HIS:NE2	1:A:592:GLU:OE2	2.38	0.57
1:A:625:ILE:HG21	1:A:630:MET:HE2	1.85	0.57
1:A:821:LEU:HD12	1:A:862:PHE:CD2	2.39	0.57
1:A:10:VAL:HG11	1:A:734:PHE:HA	1.86	0.57
1:A:85:LEU:HG	1:A:87:PRO:HD3	1.85	0.56
1:A:675:LYS:HD2	1:A:708:GLY:HA2	1.87	0.56
1:A:189:ILE:HD11	1:A:201:TRP:CD1	2.40	0.56
1:A:266:LEU:HG	1:A:290:VAL:HG13	1.86	0.56
1:A:976:LEU:HD13	1:A:982:LEU:CD1	2.35	0.56
1:A:1017:LYS:HZ2	1:A:1038:VAL:HG12	0.73	0.56
1:A:78:ARG:HD2	1:A:881:MET:CE	2.36	0.56
1:A:637:TYR:HA	1:A:643:ALA:HB3	1.86	0.56
1:A:954:VAL:C	1:A:957:LYS:H	2.07	0.56
1:A:798:ALA:HB2	1:A:847:LEU:HD11	1.88	0.56
1:A:13:LEU:O	1:A:16:ILE:HG12	2.06	0.56
1:A:93:THR:HG23	1:A:207:THR:HB	1.86	0.56
1:A:308:ARG:HD3	1:A:310:ASP:OD1	2.06	0.56
1:A:397:PRO:HA	1:A:400:ILE:CG2	2.36	0.56
1:A:971:VAL:HA	1:A:974:SER:HB3	1.86	0.56
1:A:821:LEU:HB2	1:A:862:PHE:CE2	2.41	0.56
1:A:954:VAL:O	1:A:957:LYS:CB	2.46	0.56
1:A:242:PRO:HG2	1:A:332:ARG:NH2	2.20	0.56
1:A:418:ILE:HG22	1:A:422:MET:HB2	1.87	0.56
1:A:437:PHE:HE2	1:A:470:LYS:HD3	1.69	0.56
1:A:269:LEU:HD12	1:A:289:LEU:O	2.07	0.55
1:A:905:VAL:O	1:A:908:ASP:HB3	2.06	0.55
1:A:449:LEU:CD1	1:A:463:ALA:HB2	2.37	0.55
1:A:947:TRP:CZ3	1:A:989:VAL:HG12	2.40	0.55
1:A:1025:VAL:HA	1:A:1028:THR:OG1	2.07	0.55
1:A:1017:LYS:O	1:A:1020:LEU:N	2.31	0.55
1:A:58:ARG:NH1	1:A:728:THR:HG21	2.23	0.55
1:A:978:SER:O	1:A:978:SER:OG	2.16	0.55
1:A:192:LEU:HD22	1:A:197:LEU:HD12	1.90	0.54
1:A:669:ASP:HA	1:A:702:THR:OG1	2.07	0.54
1:A:103:LYS:HD3	1:A:157:GLN:HB2	1.88	0.54
1:A:266:LEU:HD21	1:A:290:VAL:CG1	2.38	0.54
1:A:397:PRO:HA	1:A:400:ILE:HG22	1.90	0.54
1:A:586:ASP:O	1:A:588:GLN:N	2.41	0.54
1:A:50:PHE:CD1	1:A:51:PRO:HD2	2.43	0.54
1:A:71:GLU:HG3	1:A:740:ARG:NH2	2.23	0.54
1:A:854:VAL:O	1:A:858:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ASN:ND2	1:A:841:GLU:OE2	2.40	0.53
1:A:845:ARG:O	1:A:848:VAL:N	2.32	0.53
1:A:947:TRP:NE1	1:A:1051:ASP:OD1	2.41	0.53
1:A:195:MET:CE	1:A:197:LEU:HD21	2.39	0.53
1:A:597:SER:O	1:A:681:HIS:HE1	1.91	0.53
1:A:770:TRP:HE1	1:A:870:ILE:CD1	2.18	0.53
1:A:250:ASP:OD2	1:A:680:ASN:HB3	2.08	0.53
1:A:383:ASP:OD1	1:A:384:LYS:HG2	2.08	0.53
1:A:773:TRP:CD2	1:A:832:LYS:HE2	2.43	0.53
1:A:940:VAL:HG21	1:A:1017:LYS:NZ	2.23	0.53
1:A:52:TYR:HE1	1:A:91:HIS:CE1	2.26	0.53
1:A:195:MET:HE2	1:A:197:LEU:HD21	1.91	0.53
1:A:583:LEU:HD11	1:A:585:TRP:CZ2	2.44	0.53
1:A:761:ASP:HA	1:A:764:ILE:HG12	1.91	0.53
1:A:940:VAL:HG11	1:A:1016:GLU:HG2	1.90	0.53
1:A:432:ILE:HD11	1:A:477:MET:SD	2.49	0.53
1:A:678:VAL:HB	1:A:679:PRO:HD3	1.91	0.53
1:A:600:TYR:HE1	1:A:604:TYR:CE2	2.27	0.52
1:A:717:MET:HA	1:A:723:ASN:O	2.09	0.52
1:A:21:GLN:CD	1:A:194:ARG:HA	2.29	0.52
1:A:770:TRP:HZ3	1:A:851:PHE:HE2	1.56	0.52
1:A:305:CYS:HB3	1:A:374:VAL:HA	1.92	0.52
1:A:354:GLY:HA2	1:A:357:ILE:HD12	1.90	0.52
1:A:594:LEU:HD13	1:A:684:TYR:HE2	1.75	0.52
1:A:785:ARG:HB3	1:A:785:ARG:CZ	2.39	0.52
1:A:545:GLN:NE2	5:A:1325:HOH:O	2.43	0.52
1:A:65:PHE:HB2	1:A:710:LEU:HD22	1.91	0.52
1:A:221:GLN:HG3	1:A:692:MET:SD	2.49	0.52
1:A:601:MET:CE	1:A:685:TYR:HE1	2.23	0.52
1:A:956:ARG:O	1:A:959:PHE:N	2.41	0.51
1:A:967:PRO:HB2	1:A:971:VAL:HG11	1.92	0.51
1:A:985:TYR:O	1:A:989:VAL:HG13	2.09	0.51
1:A:480:ASP:OD1	1:A:483:LYS:HE2	2.10	0.51
1:A:335:SER:O	1:A:343:ASN:ND2	2.43	0.51
1:A:933:PRO:HG3	1:A:1061:PHE:CD1	2.46	0.51
1:A:972:ILE:C	1:A:974:SER:H	2.14	0.51
1:A:419:ARG:H	1:A:422:MET:CE	2.24	0.51
1:A:793:ASN:HA	1:A:796:VAL:HB	1.91	0.51
1:A:263:GLU:HG3	1:A:264:TYR:N	2.24	0.51
1:A:70:CYS:O	1:A:74:VAL:HG22	2.10	0.51
1:A:92:CYS:O	1:A:97:ILE:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:MET:O	1:A:994:ALA:N	2.43	0.51
1:A:856:THR:OG1	1:A:870:ILE:HG21	2.10	0.51
1:A:938:ILE:HD11	1:A:1036:ILE:HG21	1.93	0.51
1:A:966:LEU:HD12	1:A:966:LEU:H	1.76	0.51
1:A:52:TYR:CE1	1:A:91:HIS:CG	2.99	0.51
1:A:266:LEU:HD11	1:A:290:VAL:CG1	2.41	0.51
1:A:979:MET:HG3	1:A:980:PRO:HD2	1.91	0.51
1:A:282:LEU:HA	5:A:1346:HOH:O	2.10	0.50
1:A:396:SER:HB2	1:A:468:TYR:HE1	1.76	0.50
1:A:48:VAL:HG21	1:A:70:CYS:HB2	1.94	0.50
1:A:332:ARG:O	1:A:335:SER:OG	2.30	0.50
1:A:756:VAL:O	1:A:759:MET:N	2.42	0.50
1:A:947:TRP:CH2	1:A:992:PHE:HD2	2.30	0.50
1:A:1025:VAL:HG22	1:A:1025:VAL:O	2.11	0.50
1:A:106:ARG:NH2	5:A:1327:HOH:O	2.45	0.50
1:A:288:PHE:N	1:A:323:ILE:O	2.30	0.50
1:A:111:TYR:HB3	1:A:116:ASP:H	1.76	0.49
1:A:253:ARG:HD3	1:A:514:VAL:HG11	1.94	0.49
1:A:334:MET:HB3	1:A:339:PHE:CD2	2.47	0.49
1:A:763:GLY:O	1:A:765:LEU:N	2.44	0.49
1:A:266:LEU:HD21	1:A:290:VAL:HG11	1.93	0.49
1:A:448:GLU:O	1:A:448:GLU:HG3	2.12	0.49
1:A:199:VAL:CG1	1:A:201:TRP:HD1	2.24	0.49
1:A:568:LEU:HD21	1:A:684:TYR:HE1	1.78	0.49
1:A:224:THR:HG21	1:A:692:MET:HE3	1.93	0.49
1:A:293:THR:HB	1:A:390:THR:HG21	1.94	0.49
1:A:336:TYR:HA	1:A:343:ASN:HD21	1.77	0.49
1:A:568:LEU:HD21	1:A:684:TYR:CE1	2.47	0.49
1:A:65:PHE:CB	1:A:710:LEU:HD22	2.43	0.49
1:A:674:GLY:N	2:A:1201:ATP:O2'	2.42	0.49
1:A:275:TYR:CE2	1:A:287:ILE:HD12	2.48	0.49
1:A:482:PHE:O	1:A:483:LYS:C	2.49	0.49
1:A:24:TRP:HD1	1:A:29:VAL:HG21	1.77	0.49
1:A:412:LEU:C	1:A:414:ALA:H	2.16	0.49
1:A:819:GLU:O	1:A:823:THR:HG23	2.12	0.49
1:A:67:LEU:HD11	1:A:195:MET:HE2	1.95	0.49
1:A:881:MET:HA	1:A:881:MET:HE3	1.93	0.49
1:A:804:GLY:HA3	1:A:828:PHE:HE1	1.78	0.49
1:A:857:LEU:HD13	1:A:886:PRO:HD3	1.94	0.48
1:A:1027:LEU:O	1:A:1031:LEU:HB2	2.13	0.48
1:A:999:ASN:O	1:A:1003:MET:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LYS:HZ3	1:A:1038:VAL:HG11	1.62	0.48
1:A:53:PRO:HA	2:A:1201:ATP:O5'	2.13	0.48
1:A:103:LYS:HE2	1:A:107:GLU:OE2	2.13	0.48
1:A:569:GLN:HG2	1:A:570:GLU:HG3	1.93	0.48
1:A:967:PRO:HB2	1:A:971:VAL:CG1	2.43	0.48
2:A:1201:ATP:H3'	2:A:1201:ATP:O3A	2.14	0.48
1:A:265:THR:HG21	1:A:296:PRO:HB3	1.96	0.48
1:A:804:GLY:O	1:A:805:ILE:C	2.51	0.48
1:A:421:ASP:O	1:A:425:PRO:HD2	2.14	0.48
1:A:867:CYS:HB3	1:A:880:ILE:HD13	1.95	0.48
1:A:486:LYS:O	1:A:490:VAL:HG22	2.12	0.48
1:A:999:ASN:HA	1:A:1002:LYS:HB2	1.95	0.48
1:A:75:GLY:HA2	1:A:198:LYS:HE2	1.95	0.48
1:A:209:ASP:N	1:A:580:GLY:O	2.47	0.48
1:A:495:GLN:O	1:A:499:ILE:HG13	2.13	0.48
1:A:158:TRP:CZ3	1:A:171:ILE:HB	2.49	0.48
1:A:329:LYS:NZ	5:A:1330:HOH:O	2.46	0.48
1:A:608:HIS:HD2	5:A:1326:HOH:O	1.95	0.48
1:A:726:THR:HG22	1:A:729:GLN:HB2	1.95	0.48
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.42	0.48
1:A:821:LEU:HB2	1:A:862:PHE:HE2	1.77	0.48
1:A:211:ASN:O	1:A:215:ASP:HB2	2.14	0.48
1:A:366:LEU:HD21	1:A:498:MET:CG	2.43	0.48
1:A:635:TRP:O	1:A:638:VAL:N	2.47	0.48
1:A:333:ASN:O	1:A:334:MET:C	2.52	0.47
1:A:311:MET:HB3	1:A:313:TYR:CE1	2.49	0.47
1:A:92:CYS:N	1:A:207:THR:OG1	2.42	0.47
1:A:693:TRP:HB3	1:A:696:GLN:HG3	1.95	0.47
1:A:951:THR:HA	1:A:976:LEU:HD11	1.97	0.47
1:A:61:LEU:HD21	1:A:755:PHE:CD2	2.50	0.47
1:A:433:GLU:HB3	1:A:478:LEU:HD11	1.96	0.47
1:A:713:ASN:HD21	1:A:757:GLU:CD	2.18	0.47
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.80	0.47
1:A:107:GLU:OE2	1:A:156:TYR:HD1	1.97	0.47
1:A:192:LEU:HD22	1:A:197:LEU:CD1	2.44	0.47
1:A:324:PHE:O	1:A:325:ILE:HG12	2.15	0.47
1:A:940:VAL:CG1	1:A:1016:GLU:HG2	2.45	0.47
1:A:543:THR:HA	1:A:690:VAL:HG21	1.97	0.47
1:A:675:LYS:HE2	5:A:1442:HOH:O	2.13	0.47
1:A:892:ASN:O	1:A:895:LEU:N	2.47	0.47
1:A:18:LYS:HE3	1:A:194:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLY:O	1:A:285:LYS:HG3	2.14	0.47
1:A:976:LEU:O	1:A:979:MET:N	2.47	0.47
1:A:1021:MET:SD	1:A:1038:VAL:HG21	2.54	0.47
1:A:250:ASP:O	1:A:253:ARG:HG3	2.15	0.47
1:A:50:PHE:HD1	1:A:51:PRO:HD2	1.79	0.46
1:A:916:TYR:HE1	1:A:1061:PHE:CD2	2.31	0.46
1:A:158:TRP:CZ2	1:A:171:ILE:HD12	2.50	0.46
1:A:353:MET:O	1:A:355:GLU:N	2.48	0.46
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.34	0.46
1:A:405:ASP:HA	1:A:408:LYS:HB2	1.98	0.46
1:A:541:LYS:O	1:A:541:LYS:HG3	2.15	0.46
1:A:1024:ILE:HD12	1:A:1025:VAL:N	2.30	0.46
1:A:253:ARG:HD3	1:A:514:VAL:CG1	2.46	0.46
1:A:629:GLN:HG2	1:A:650:ILE:HD12	1.91	0.46
1:A:940:VAL:HG12	1:A:941:ALA:N	2.24	0.46
1:A:58:ARG:HD3	1:A:187:LEU:HD13	1.98	0.46
1:A:362:LEU:HD22	1:A:374:VAL:HG22	1.96	0.46
1:A:449:LEU:HD12	1:A:463:ALA:HB2	1.96	0.46
1:A:224:THR:HG21	1:A:692:MET:CE	2.46	0.46
1:A:304:ASN:ND2	1:A:391:SER:OG	2.43	0.46
1:A:1041:ALA:HA	1:A:1044:ALA:HB2	1.98	0.46
1:A:225:LEU:HB2	1:A:231:ILE:HD11	1.98	0.46
1:A:300:PHE:N	1:A:300:PHE:CD1	2.83	0.46
1:A:318:THR:HG21	1:A:320:ASN:OD1	2.16	0.46
1:A:379:THR:O	1:A:379:THR:OG1	2.34	0.46
1:A:749:THR:HB	1:A:751:GLU:H	1.80	0.46
1:A:947:TRP:O	1:A:951:THR:HG23	2.16	0.46
1:A:24:TRP:HZ3	1:A:865:HIS:NE2	2.14	0.46
1:A:476:ILE:HG13	1:A:476:ILE:O	2.15	0.46
1:A:606:VAL:HG12	1:A:658:LEU:HD22	1.98	0.46
1:A:730:ALA:O	1:A:733:LYS:N	2.47	0.46
1:A:773:TRP:CE2	1:A:832:LYS:HE2	2.50	0.46
1:A:510:PRO:HD3	1:A:524:VAL:HG23	1.97	0.46
1:A:951:THR:OG1	1:A:952:LEU:N	2.49	0.46
1:A:278:LYS:HE2	1:A:350:LYS:NZ	2.31	0.45
1:A:916:TYR:CE1	1:A:1061:PHE:HD2	2.30	0.45
1:A:45:LYS:HD3	1:A:664:PHE:O	2.16	0.45
1:A:476:ILE:HA	1:A:486:LYS:HA	1.98	0.45
1:A:610:LEU:CD1	1:A:630:MET:HE1	2.45	0.45
1:A:629:GLN:CD	1:A:650:ILE:CD1	2.82	0.45
1:A:678:VAL:O	1:A:683:SER:OG	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLN:OE1	1:A:599:ILE:HG12	2.16	0.45
1:A:403:LEU:O	1:A:403:LEU:HD12	2.17	0.45
1:A:774:VAL:HG13	1:A:852:ILE:CD1	2.41	0.45
1:A:972:ILE:HG13	1:A:973:ALA:N	2.30	0.45
1:A:71:GLU:HG2	1:A:197:LEU:HD22	1.99	0.45
1:A:579:LEU:HA	1:A:579:LEU:HD23	1.40	0.45
1:A:599:ILE:CG2	1:A:688:ASN:HB3	2.46	0.45
1:A:1007:ILE:N	1:A:1007:ILE:HD12	2.32	0.45
1:A:67:LEU:HD11	1:A:195:MET:CE	2.47	0.45
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.52	0.45
1:A:947:TRP:CZ3	1:A:989:VAL:HA	2.44	0.45
1:A:230:LYS:HG3	1:A:691:ALA:HB1	1.99	0.45
1:A:506:ILE:HD13	1:A:506:ILE:HA	1.68	0.45
1:A:675:LYS:HB3	1:A:707:ASN:O	2.16	0.45
1:A:698:ASP:OD1	1:A:698:ASP:N	2.46	0.45
1:A:772:GLU:OE2	1:A:775:LYS:HD2	2.16	0.45
1:A:1019:VAL:HG13	1:A:1020:LEU:CD2	2.46	0.45
1:A:201:TRP:NE1	5:A:1322:HOH:O	2.36	0.45
1:A:71:GLU:OE2	1:A:198:LYS:HG3	2.16	0.45
1:A:833:ASP:O	5:A:1308:HOH:O	2.21	0.45
1:A:1008:LEU:HD12	1:A:1008:LEU:HA	1.58	0.45
1:A:8:ALA:HB1	5:A:1422:HOH:O	2.17	0.45
1:A:456:ASP:O	1:A:460:LEU:HB2	2.17	0.45
1:A:726:THR:HG22	1:A:729:GLN:CG	2.47	0.45
1:A:795:ARG:NH2	1:A:895:LEU:HD11	2.32	0.45
1:A:892:ASN:HD22	1:A:895:LEU:HD12	1.82	0.45
1:A:601:MET:SD	1:A:685:TYR:HE1	2.40	0.45
1:A:831:ALA:O	1:A:832:LYS:C	2.55	0.45
1:A:539:TRP:CE2	1:A:691:ALA:HB2	2.51	0.44
1:A:550:LEU:CD2	1:A:552:THR:HG22	2.47	0.44
1:A:316:PHE:O	1:A:323:ILE:HA	2.16	0.44
1:A:487:VAL:H	1:A:487:VAL:HG22	1.56	0.44
1:A:492:LYS:HE3	1:A:492:LYS:HB3	1.56	0.44
1:A:956:ARG:O	1:A:958:HIS:N	2.50	0.44
1:A:543:THR:O	1:A:546:CYS:N	2.48	0.44
1:A:703:ALA:O	1:A:704:VAL:HG23	2.18	0.44
1:A:977:GLY:C	1:A:979:MET:H	2.21	0.44
1:A:105:LYS:CE	1:A:175:SER:HB3	2.47	0.44
1:A:246:GLN:OE1	1:A:575:ARG:HB3	2.17	0.44
1:A:373:TYR:CD2	1:A:422:MET:HA	2.53	0.44
1:A:440:LEU:O	1:A:444:THR:OG1	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:GLN:O	1:A:570:GLU:C	2.55	0.44
1:A:630:MET:HE2	1:A:630:MET:HB2	1.85	0.44
1:A:736:ALA:O	1:A:740:ARG:HB2	2.18	0.44
1:A:230:LYS:HD2	1:A:539:TRP:CE3	2.52	0.44
1:A:726:THR:HG22	1:A:729:GLN:CB	2.48	0.44
1:A:947:TRP:HB2	1:A:982:LEU:HD22	1.99	0.44
1:A:482:PHE:CD1	1:A:490:VAL:HG11	2.53	0.44
1:A:30:PHE:CE1	1:A:881:MET:HG3	2.53	0.44
1:A:214:TYR:HA	1:A:603:PHE:CE2	2.52	0.44
1:A:1000:LEU:HD13	1:A:1000:LEU:O	2.17	0.44
1:A:1006:ARG:O	1:A:1009:ASP:N	2.50	0.44
1:A:682:LEU:O	1:A:685:TYR:HB3	2.18	0.44
1:A:936:CYS:HB2	1:A:1033:LEU:HD13	2.00	0.44
1:A:95:MET:HE3	1:A:95:MET:HB3	1.66	0.44
1:A:185:PRO:CG	1:A:206:ILE:HD11	2.47	0.44
1:A:197:LEU:O	1:A:199:VAL:N	2.51	0.44
1:A:206:ILE:HD13	1:A:206:ILE:HA	1.87	0.44
1:A:301:GLY:O	1:A:393:PRO:HD2	2.17	0.44
1:A:410:GLN:HA	1:A:413:ARG:HH21	1.83	0.44
1:A:493:THR:O	1:A:496:LYS:HB3	2.17	0.44
1:A:60:HIS:CD2	1:A:63:HIS:CE1	3.06	0.43
1:A:539:TRP:NE1	1:A:691:ALA:HB2	2.33	0.43
1:A:316:PHE:CE1	1:A:324:PHE:HB2	2.53	0.43
1:A:892:ASN:O	1:A:895:LEU:HB2	2.17	0.43
1:A:224:THR:HG22	1:A:225:LEU:HD23	2.00	0.43
1:A:202:ARG:HE	1:A:202:ARG:HB2	1.43	0.43
1:A:464:LYS:HE3	1:A:468:TYR:CZ	2.53	0.43
1:A:648:THR:HG21	1:A:655:LEU:CD1	2.48	0.43
1:A:958:HIS:O	1:A:966:LEU:HG	2.18	0.43
1:A:977:GLY:HA2	1:A:986:MET:SD	2.59	0.43
1:A:1060:VAL:O	1:A:1061:PHE:CD1	2.71	0.43
1:A:266:LEU:HD22	1:A:507:TYR:HB2	2.00	0.43
1:A:585:TRP:HB3	5:A:1352:HOH:O	2.19	0.43
1:A:626:ARG:HE	1:A:628:GLN:HG3	1.83	0.43
1:A:24:TRP:CZ3	1:A:865:HIS:CD2	3.07	0.43
1:A:76:TYR:CE2	1:A:77:GLN:NE2	2.85	0.43
1:A:106:ARG:HG2	1:A:110:LEU:HD12	1.99	0.43
1:A:434:ILE:HD12	1:A:441:SER:OG	2.19	0.43
1:A:225:LEU:HD21	1:A:692:MET:SD	2.58	0.43
1:A:298:THR:OG1	1:A:392:VAL:HG21	2.19	0.43
1:A:333:ASN:O	1:A:335:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:O	1:A:549:ASN:HB2	2.19	0.43
1:A:669:ASP:O	1:A:703:ALA:HB3	2.18	0.43
1:A:105:LYS:HE2	1:A:175:SER:HB3	2.00	0.43
1:A:263:GLU:HG3	1:A:264:TYR:H	1.82	0.43
1:A:601:MET:CE	1:A:685:TYR:CE1	3.01	0.43
1:A:969:ASN:C	1:A:972:ILE:HG12	2.39	0.43
1:A:400:ILE:O	1:A:404:ARG:HG2	2.18	0.43
1:A:689:HIS:HD1	1:A:701:PRO:HD3	1.83	0.43
1:A:342:ASP:O	1:A:345:VAL:HG23	2.19	0.42
1:A:391:SER:HA	1:A:399:ASP:OD1	2.18	0.42
1:A:667:PRO:HB3	1:A:699:LYS:O	2.19	0.42
1:A:731:ILE:HG12	1:A:739:MET:SD	2.58	0.42
1:A:795:ARG:HB3	1:A:895:LEU:HD11	2.01	0.42
1:A:577:TYR:HD1	1:A:578:GLY:N	2.17	0.42
1:A:614:ASN:O	1:A:615:LEU:HD23	2.18	0.42
1:A:791:THR:OG1	1:A:794:ASP:OD1	2.33	0.42
1:A:947:TRP:HH2	1:A:992:PHE:HD2	1.67	0.42
1:A:413:ARG:HH11	1:A:423:VAL:HG21	1.83	0.42
1:A:620:GLU:HG3	1:A:621:SER:N	2.34	0.42
1:A:763:GLY:C	1:A:765:LEU:N	2.71	0.42
1:A:933:PRO:HG3	1:A:1061:PHE:CG	2.55	0.42
1:A:333:ASN:OD1	1:A:523:VAL:HB	2.20	0.42
1:A:686:LEU:CD2	1:A:701:PRO:HG2	2.49	0.42
1:A:834:LYS:HD3	1:A:838:LEU:HD22	2.01	0.42
1:A:105:LYS:HB2	1:A:105:LYS:HE3	1.72	0.42
1:A:154:SER:HB3	1:A:159:GLY:O	2.20	0.42
1:A:305:CYS:HB3	1:A:374:VAL:HG13	2.01	0.42
1:A:87:PRO:HA	1:A:199:VAL:HG13	2.02	0.42
1:A:304:ASN:CA	1:A:372:ILE:HD12	2.50	0.42
1:A:418:ILE:HA	1:A:422:MET:HE3	2.02	0.42
1:A:571:HIS:CE1	1:A:592:GLU:OE2	2.72	0.42
1:A:803:ALA:HB2	1:A:891:VAL:CG1	2.49	0.42
1:A:419:ARG:H	1:A:422:MET:HE3	1.85	0.42
1:A:381:LYS:HD2	1:A:381:LYS:HA	1.82	0.42
1:A:773:TRP:CE3	1:A:832:LYS:HE2	2.54	0.42
1:A:48:VAL:HG22	1:A:86:PHE:HB2	2.01	0.41
1:A:199:VAL:CG1	1:A:201:TRP:CD1	3.03	0.41
1:A:212:PRO:HB2	1:A:627:PRO:HB3	2.00	0.41
1:A:434:ILE:HA	1:A:435:PRO:HD3	1.94	0.41
1:A:977:GLY:C	1:A:979:MET:N	2.74	0.41
1:A:1017:LYS:O	1:A:1019:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:OE1	1:A:264:TYR:HE1	2.03	0.41
1:A:286:ASN:OD1	1:A:286:ASN:N	2.54	0.41
1:A:313:TYR:HB2	1:A:352:LEU:HD21	2.02	0.41
1:A:499:ILE:HA	1:A:504:ALA:O	2.20	0.41
1:A:1002:LYS:HA	1:A:1002:LYS:HD2	1.89	0.41
1:A:598:THR:OG1	1:A:688:ASN:OD1	2.32	0.41
1:A:637:TYR:HA	1:A:643:ALA:CB	2.50	0.41
1:A:268:LYS:HE2	1:A:268:LYS:HB3	1.78	0.41
1:A:420:ASP:HB3	1:A:424:LEU:HD12	2.02	0.41
1:A:670:LEU:HD12	1:A:670:LEU:HA	1.86	0.41
1:A:424:LEU:HB2	1:A:425:PRO:HD3	2.01	0.41
1:A:532:LEU:O	1:A:534:TYR:N	2.52	0.41
1:A:568:LEU:HD12	1:A:568:LEU:HA	1.78	0.41
1:A:774:VAL:O	1:A:778:VAL:HG23	2.20	0.41
1:A:964:GLY:O	1:A:965:LYS:HB2	2.20	0.41
1:A:976:LEU:HD22	1:A:976:LEU:HA	1.78	0.41
1:A:266:LEU:HD11	1:A:290:VAL:HG12	2.02	0.41
1:A:314:ILE:O	1:A:325:ILE:HA	2.20	0.41
1:A:413:ARG:HB3	1:A:418:ILE:O	2.19	0.41
1:A:52:TYR:CD1	1:A:91:HIS:CG	3.09	0.41
1:A:52:TYR:HB3	1:A:89:GLY:O	2.20	0.41
1:A:171:ILE:HG13	1:A:171:ILE:H	1.52	0.41
1:A:316:PHE:HZ	1:A:334:MET:HE3	1.86	0.41
1:A:633:GLU:HB3	1:A:646:PRO:HB3	2.03	0.41
1:A:770:TRP:CZ3	1:A:851:PHE:CE2	3.07	0.41
1:A:1007:ILE:N	1:A:1007:ILE:CD1	2.83	0.41
1:A:75:GLY:CA	1:A:198:LYS:HE2	2.51	0.41
1:A:335:SER:HB3	1:A:340:THR:HG21	2.02	0.41
1:A:401:ALA:O	1:A:404:ARG:HB2	2.21	0.41
1:A:581:THR:HB	1:A:591:ILE:HD12	2.02	0.41
1:A:773:TRP:O	1:A:776:GLU:HB3	2.21	0.41
1:A:799:SER:CB	1:A:892:ASN:H	2.27	0.41
1:A:48:VAL:HA	1:A:670:LEU:HB3	2.03	0.41
1:A:61:LEU:O	1:A:63:HIS:N	2.54	0.41
1:A:311:MET:HB3	1:A:313:TYR:CZ	2.56	0.41
1:A:311:MET:O	1:A:353:MET:HA	2.21	0.41
1:A:630:MET:HG3	1:A:634:VAL:CG1	2.51	0.41
1:A:714:SER:HG	1:A:754:ASN:HD21	1.68	0.41
1:A:725:LEU:HD13	1:A:730:ALA:HB2	2.03	0.41
1:A:827:GLU:O	1:A:830:ALA:HB3	2.21	0.41
1:A:92:CYS:HA	1:A:97:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:O	1:A:218:VAL:C	2.60	0.41
1:A:810:GLN:O	1:A:814:LYS:HG3	2.21	0.41
1:A:199:VAL:HG11	1:A:201:TRP:HD1	1.86	0.40
1:A:242:PRO:HB3	1:A:336:TYR:CZ	2.56	0.40
1:A:803:ALA:HB2	1:A:891:VAL:HG13	2.03	0.40
1:A:413:ARG:H	1:A:413:ARG:HG3	1.67	0.40
1:A:1027:LEU:HB3	1:A:1031:LEU:HD12	2.02	0.40
1:A:269:LEU:O	1:A:288:PHE:HD1	2.02	0.40
1:A:354:GLY:HA2	1:A:357:ILE:CD1	2.52	0.40
1:A:434:ILE:CG1	1:A:471:GLY:HA2	2.40	0.40
1:A:493:THR:HA	1:A:496:LYS:CB	2.51	0.40
1:A:737:ASP:OD2	1:A:863:CYS:HB3	2.22	0.40
1:A:996:ILE:HG23	1:A:1007:ILE:HG21	2.03	0.40
1:A:1007:ILE:O	1:A:1007:ILE:HG22	2.22	0.40
1:A:117:PHE:CE2	1:A:156:TYR:CD1	3.09	0.40
1:A:219:ARG:HG2	1:A:584:PRO:HG3	2.02	0.40
1:A:479:VAL:HG22	1:A:480:ASP:N	2.37	0.40
1:A:645:PHE:HA	1:A:646:PRO:HD3	1.83	0.40
1:A:705:ARG:HH22	1:A:748:ASP:HB2	1.86	0.40
1:A:240:TYR:HB3	1:A:523:VAL:O	2.22	0.40
1:A:423:VAL:CG2	1:A:424:LEU:N	2.83	0.40
1:A:1060:VAL:HG12	1:A:1061:PHE:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	998/1188 (84%)	810 (81%)	177 (18%)	11 (1%)	14 48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	GLU
1	A	978	SER
1	A	62	GLY
1	A	164	LEU
1	A	354	GLY
1	A	198	LYS
1	A	334	MET
1	A	390	THR
1	A	720	SER
1	A	951	THR
1	A	376	PRO

5.3.2 Protein sidechains [i](#)

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	885/1047 (84%)	825 (93%)	60 (7%)	16 46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	52	TYR
1	A	55	MET
1	A	70	CYS
1	A	78	ARG
1	A	86	PHE
1	A	88	PHE
1	A	113	CYS
1	A	163	SER
1	A	187	LEU
1	A	219	ARG
1	A	233	PHE
1	A	285	LYS
1	A	286	ASN
1	A	332	ARG
1	A	333	ASN

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Mol	Chain	Res	Type
1	A	342	ASP
1	A	363	SER
1	A	396	SER
1	A	439	ASN
1	A	448	GLU
1	A	449	LEU
1	A	456	ASP
1	A	468	TYR
1	A	480	ASP
1	A	486	LYS
1	A	516	SER
1	A	527	CYS
1	A	531	TYR
1	A	554	CYS
1	A	567	TRP
1	A	577	TYR
1	A	586	ASP
1	A	592	GLU
1	A	630	MET
1	A	645	PHE
1	A	684	TYR
1	A	696	GLN
1	A	734	PHE
1	A	759	MET
1	A	781	TRP
1	A	782	ASP
1	A	812	TYR
1	A	828	PHE
1	A	832	LYS
1	A	833	ASP
1	A	866	LEU
1	A	876	LYS
1	A	902	LEU
1	A	916	TYR
1	A	934	SER
1	A	968	ASP
1	A	970	LYS
1	A	976	LEU
1	A	978	SER
1	A	995	MET
1	A	1014	PHE
1	A	1047	LYS

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Mol	Chain	Res	Type
1	A	1049	ARG
1	A	1052	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	343	ASN
1	A	513	GLN
1	A	629	GLN
1	A	729	GLN
1	A	793	ASN
1	A	892	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	1203	-	4,4,4	0.97	0	6,6,6	0.85	0
3	LEU	A	1202	-	7,8,8	1.05	1 (14%)	9,10,10	1.34	2 (22%)
2	ATP	A	1201	1	26,33,33	1.22	4 (15%)	31,52,52	1.78	7 (22%)
4	PO4	A	1204	-	4,4,4	0.71	0	6,6,6	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LEU	A	1202	-	-	2/8/8/8	-
2	ATP	A	1201	1	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ATP	C5-C4	2.63	1.47	1.40
2	A	1201	ATP	C2-N3	2.62	1.36	1.32
3	A	1202	LEU	OXT-C	-2.30	1.23	1.30
2	A	1201	ATP	C2'-C1'	-2.12	1.50	1.53
2	A	1201	ATP	O4'-C1'	2.09	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ATP	N6-C6-N1	4.30	127.49	118.57
2	A	1201	ATP	N3-C2-N1	-3.34	123.47	128.68
2	A	1201	ATP	C5-C6-N6	-3.27	115.39	120.35
2	A	1201	ATP	C2'-C3'-C4'	3.11	108.69	102.64
2	A	1201	ATP	O3'-C3'-C2'	-3.06	101.91	111.82
2	A	1201	ATP	O2'-C2'-C3'	-2.73	103.00	111.82
3	A	1202	LEU	OXT-C-O	-2.47	118.48	124.09
2	A	1201	ATP	O3G-PG-O3B	2.29	112.31	104.64
3	A	1202	LEU	CB-CA-C	-2.02	103.99	110.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

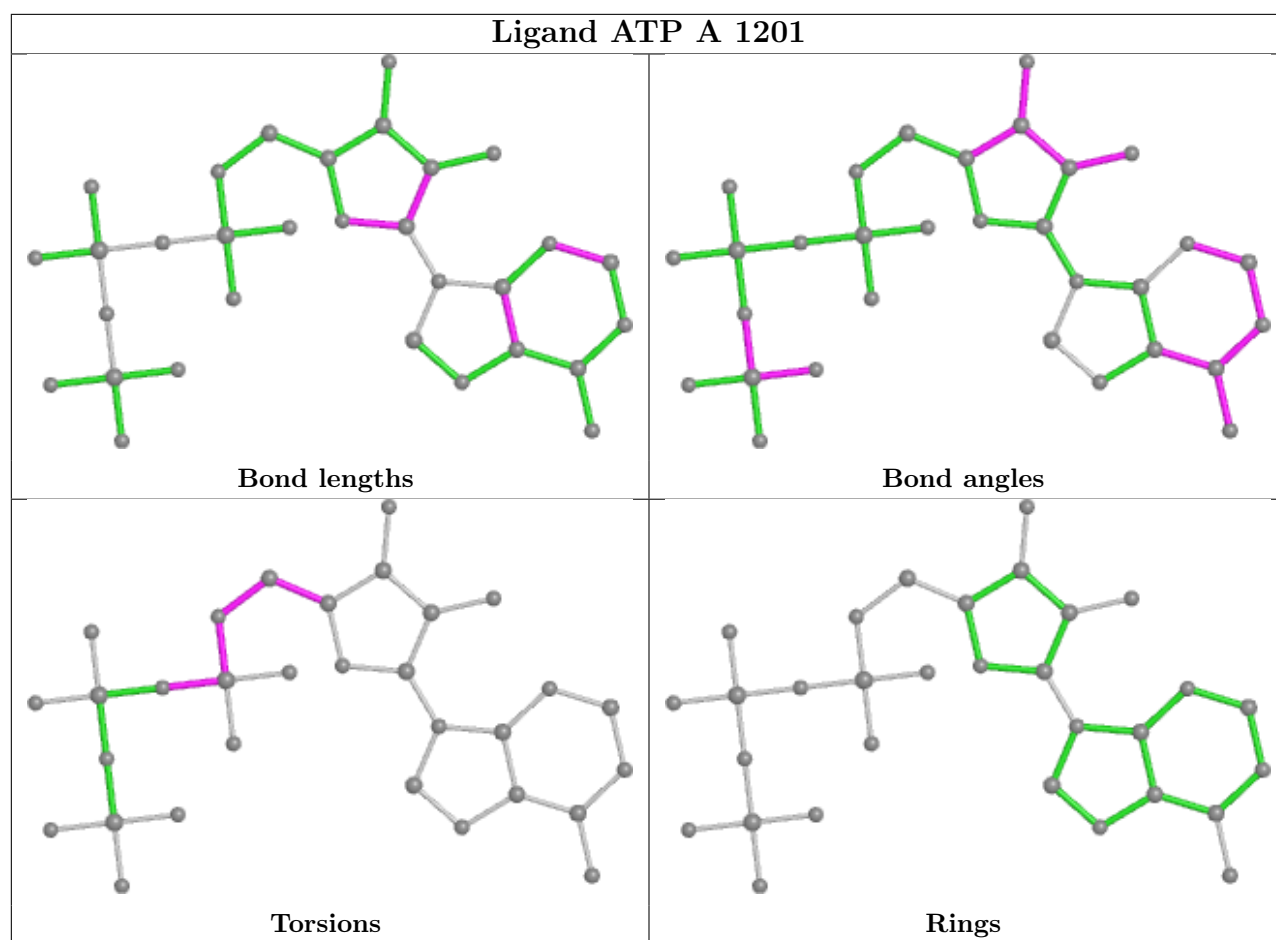
Mol	Chain	Res	Type	Atoms
2	A	1201	ATP	C5'-O5'-PA-O1A
2	A	1201	ATP	C5'-O5'-PA-O2A
2	A	1201	ATP	C5'-O5'-PA-O3A
3	A	1202	LEU	CA-CB-CG-CD1
3	A	1202	LEU	CA-CB-CG-CD2
2	A	1201	ATP	C4'-C5'-O5'-PA
2	A	1201	ATP	PB-O3A-PA-O2A
2	A	1201	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

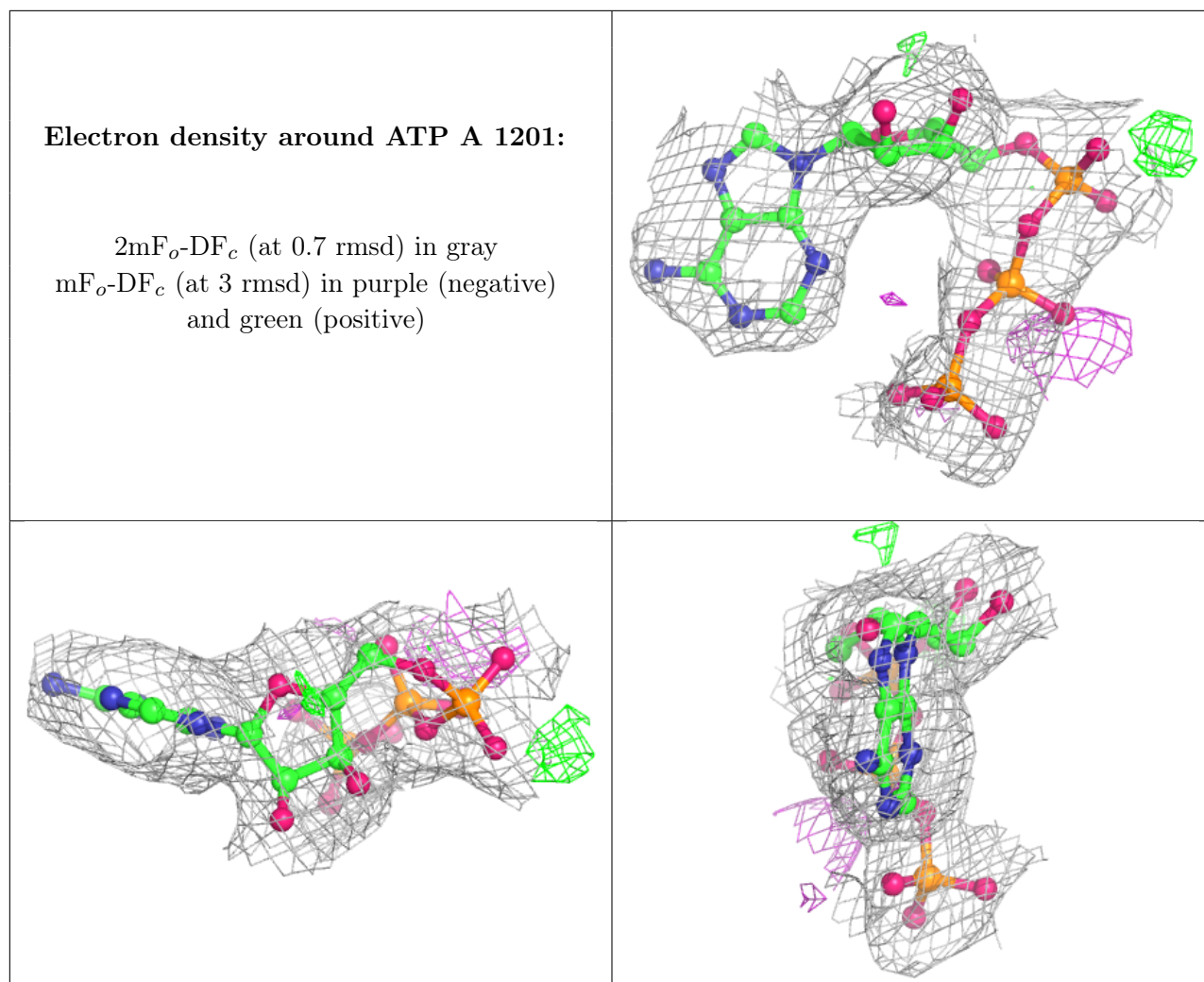
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.