



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:42 pm BST

PDB ID : 2V7Z
Title : Crystal structure of the 70-kDa heat shock cognate protein from *Rattus norvegicus* in post-ATP hydrolysis state
Authors : Chang, Y.-W.; Sun, Y.-J.; Wang, C.; Hsiao, C.-D.
Deposited on : 2007-08-02
Resolution : 3.50 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 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 : 2.11
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) : 2.11

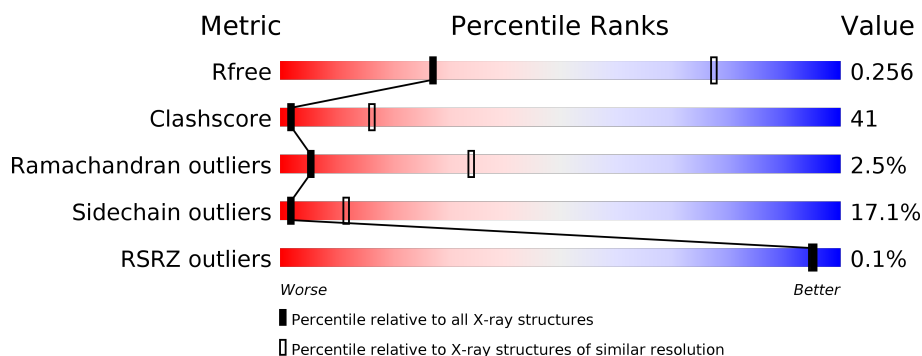
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 ≥ 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 $\leq 5\%$. 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	543	
1	B	543	

2 Entry composition [i](#)

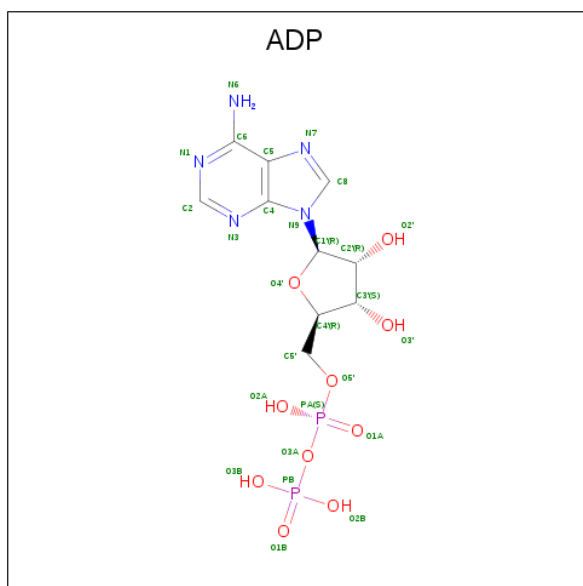
There are 4 unique types of molecules in this entry. The entry contains 6062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEAT SHOCK COGNATE 71 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	1
			2952	1851	522	571	8			
1	B	382	Total	C	N	O	S	0	0	1
			2952	1851	522	571	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





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

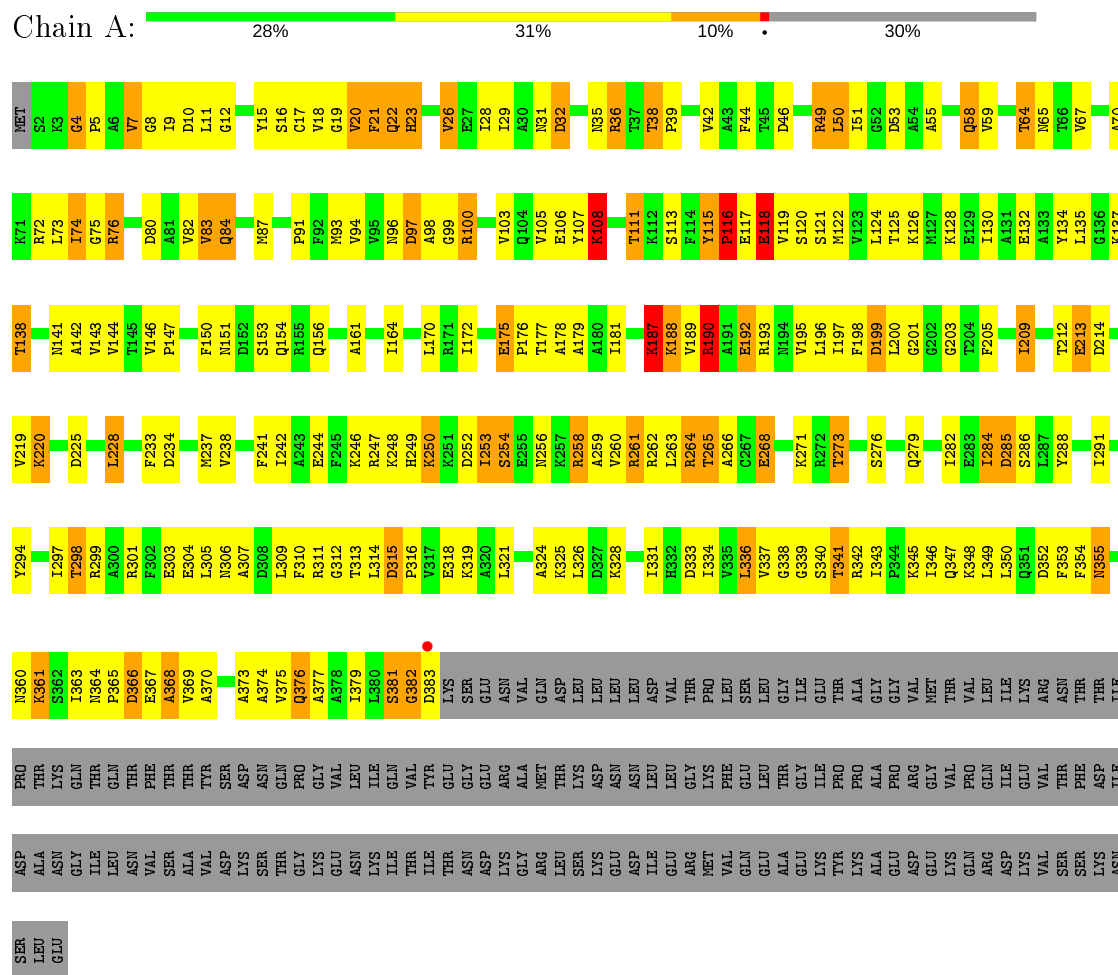
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	43	Total	O	0	0
			43	43		

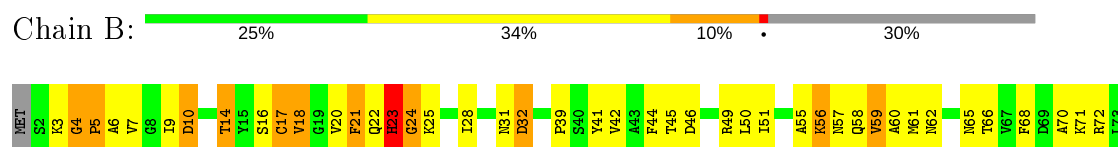
3 Residue-property plots

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: HEAT SHOCK COGNATE 71 KDA PROTEIN



• Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.85Å 94.79Å 78.23Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	29.01 – 3.50 29.01 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.01-3.50) 87.7 (29.01-3.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.47Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.257 , 0.279 0.235 , 0.256	Depositor DCC
R_{free} test set	816 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	1.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ADP

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	0.69	1/2997 (0.0%)	1.19	19/4046 (0.5%)
1	B	0.72	3/2998 (0.1%)	1.23	39/4048 (1.0%)
All	All	0.71	4/5995 (0.1%)	1.21	58/8094 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	6
1	B	1	9
All	All	2	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	C-N	8.77	1.50	1.34
1	B	345	LYS	C-O	8.63	1.39	1.23
1	B	345	LYS	C-N	5.95	1.47	1.34
1	B	343	ILE	C-N	5.38	1.44	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	LYS	O-C-N	-12.45	102.78	122.70
1	B	24	GLY	O-C-N	10.98	140.26	122.70
1	B	24	GLY	CA-C-N	-10.41	94.30	117.20
1	B	344	PRO	C-N-CA	-10.25	96.08	121.70
1	B	87	MET	C-N-CA	-10.22	96.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ASP	N-CA-CB	9.28	127.30	110.60
1	A	285	ASP	CB-CG-OD1	8.96	126.37	118.30
1	A	38	THR	C-N-CD	8.89	147.08	128.40
1	A	190	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	B	220	LYS	CB-CA-C	8.02	126.45	110.40
1	B	345	LYS	CA-C-O	-7.62	104.09	120.10
1	B	144	VAL	O-C-N	-7.39	110.87	122.70
1	B	199	ASP	CB-CG-OD2	7.38	124.94	118.30
1	B	5	PRO	CA-C-N	-6.97	101.86	117.20
1	A	118	GLU	N-CA-CB	6.88	122.99	110.60
1	A	26	VAL	CB-CA-C	-6.86	98.36	111.40
1	A	190	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	4	GLY	C-N-CD	6.81	142.70	128.40
1	B	143	VAL	C-N-CA	-6.75	104.82	121.70
1	B	86	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	100	ARG	C-N-CD	6.65	142.36	128.40
1	A	116	PRO	O-C-N	-6.61	112.12	122.70
1	A	250	LYS	N-CA-CB	6.57	122.42	110.60
1	A	175	GLU	C-N-CD	6.54	142.14	128.40
1	B	175	GLU	C-N-CD	6.49	142.04	128.40
1	B	343	ILE	C-N-CD	6.48	142.00	128.40
1	A	4	GLY	N-CA-C	6.42	129.16	113.10
1	B	5	PRO	N-CA-C	6.37	128.65	112.10
1	B	88	LYS	N-CA-CB	6.22	121.79	110.60
1	A	382	GLY	N-CA-C	5.91	127.87	113.10
1	B	21	PHE	C-N-CA	-5.84	107.09	121.70
1	B	88	LYS	CA-C-O	-5.83	107.87	120.10
1	B	5	PRO	O-C-N	5.78	131.95	122.70
1	A	5	PRO	CA-N-CD	-5.71	103.51	111.50
1	B	89	HIS	CA-C-N	5.69	129.72	117.20
1	B	367	GLU	CB-CA-C	-5.65	99.09	110.40
1	B	23	HIS	CA-CB-CG	5.60	123.12	113.60
1	A	209	ILE	C-N-CA	5.54	135.54	121.70
1	B	344	PRO	O-C-N	5.49	131.49	122.70
1	A	209	ILE	O-C-N	5.43	131.39	122.70
1	A	58	GLN	CB-CA-C	5.42	121.24	110.40
1	B	146	VAL	C-N-CD	5.39	139.72	128.40
1	B	25	LYS	CB-CA-C	-5.39	99.63	110.40
1	B	88	LYS	C-N-CA	-5.37	108.29	121.70
1	B	354	PHE	CB-CG-CD2	5.37	124.56	120.80
1	A	187	LYS	CB-CA-C	5.36	121.11	110.40
1	B	285	ASP	CB-CA-C	-5.34	99.72	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	LYS	CB-CA-C	5.34	121.07	110.40
1	B	345	LYS	CB-CA-C	5.31	121.02	110.40
1	B	210	LEU	CB-CA-C	-5.30	100.12	110.20
1	B	346	ILE	O-C-N	-5.28	114.26	122.70
1	B	21	PHE	CA-C-N	-5.26	105.64	117.20
1	B	343	ILE	CA-C-N	-5.25	102.40	117.10
1	B	325	LYS	CB-CA-C	5.23	120.85	110.40
1	A	213	GLU	CA-CB-CG	5.17	124.77	113.40
1	B	88	LYS	N-CA-C	5.12	124.82	111.00
1	B	193	ARG	CB-CA-C	-5.06	100.28	110.40
1	B	125	THR	C-N-CA	-5.01	109.18	121.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	250	LYS	CA
1	B	199	ASP	CA

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Mainchain
1	A	116	PRO	Mainchain
1	A	187	LYS	Mainchain
1	A	22	GLN	Mainchain
1	A	276	SER	Mainchain
1	A	36	ARG	Mainchain
1	B	144	VAL	Mainchain
1	B	146	VAL	Mainchain
1	B	214	ASP	Mainchain
1	B	220	LYS	Mainchain
1	B	312	GLY	Mainchain
1	B	345	LYS	Mainchain,Peptide
1	B	70	ALA	Mainchain
1	B	88	LYS	Mainchain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2952	0	2958	246	4
1	B	2952	0	2958	253	4
2	A	27	0	12	1	0
2	B	27	0	12	2	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	51	0	0	3	0
4	B	43	0	0	6	0
All	All	6062	0	5940	494	4

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 41.

All (494) 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:B:141:ASN:ND2	1:B:170:LEU:HD21	1.34	1.41
1:B:211:THR:O	1:B:211:THR:HG22	1.39	1.19
1:A:74:ILE:HD13	1:A:116:PRO:HB2	1.30	1.12
1:A:21:PHE:HB2	1:A:26:VAL:HA	1.29	1.09
1:A:94:VAL:HG22	1:A:103:VAL:HG12	1.37	1.06
1:A:199:ASP:HA	1:A:337:VAL:O	1.56	1.05
1:A:188:LYS:HE3	1:A:190:ARG:H	1.18	1.03
1:A:84:GLN:NE2	1:A:84:GLN:HA	1.73	1.03
1:B:5:PRO:HB2	1:B:139:VAL:HG12	1.36	1.03
1:B:141:ASN:ND2	1:B:170:LEU:CD2	2.22	1.02
1:B:211:THR:CG2	1:B:211:THR:O	2.05	1.01
1:B:147:PRO:HD2	1:B:150:PHE:CE1	1.96	1.00
1:A:271:LYS:NZ	2:A:1383:ADP:O2'	1.94	1.00
1:B:246:LYS:O	1:B:250:LYS:HA	1.62	0.98
1:B:42:VAL:HG13	1:B:51:ILE:HG22	1.43	0.97
1:A:205:PHE:HB2	1:A:228:LEU:HD22	1.44	0.97
1:B:314:LEU:HD22	1:B:353:PHE:HD1	1.30	0.97
1:A:209:ILE:O	1:A:220:LYS:HB3	1.66	0.94
1:B:141:ASN:HD21	1:B:170:LEU:CD2	1.81	0.93
1:B:159:LYS:HG3	1:B:172:ILE:HD11	1.48	0.92
1:A:21:PHE:HB2	1:A:26:VAL:CA	1.99	0.92
1:A:382:GLY:C	1:A:383:ASP:N	2.24	0.91
1:A:253:ILE:HD13	1:A:288:TYR:CD1	2.06	0.91
1:B:192:GLU:HB2	1:B:213:GLU:HB2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HB2	1:B:88:LYS:NZ	1.85	0.89
1:A:313:THR:O	1:A:316:PRO:HD2	1.72	0.88
1:A:196:LEU:HD12	1:A:331:ILE:HD13	1.55	0.88
1:B:284:ILE:HG13	1:B:293:PHE:HB3	1.56	0.88
1:B:284:ILE:HD12	1:B:287:LEU:HD13	1.56	0.88
1:B:301:ARG:HA	1:B:304:GLU:OE1	1.73	0.87
1:A:301:ARG:HA	1:A:304:GLU:OE1	1.72	0.87
1:B:141:ASN:HD21	1:B:170:LEU:HD21	0.94	0.86
1:B:185:LEU:HD12	1:B:195:VAL:CG1	2.04	0.86
1:A:76:ARG:CZ	1:A:82:VAL:HG21	2.06	0.85
1:B:299:ARG:O	1:B:303:GLU:HG3	1.78	0.84
1:A:205:PHE:HB2	1:A:228:LEU:CD2	2.07	0.83
1:A:175:GLU:HG2	1:A:369:VAL:HG21	1.60	0.83
1:A:188:LYS:HE3	1:A:190:ARG:N	1.91	0.83
1:A:118:GLU:HG2	1:A:121:SER:HB3	1.61	0.82
1:B:65:ASN:HD21	1:B:106:GLU:HB2	1.41	0.82
1:B:283:GLU:HG2	1:B:294:TYR:HD1	1.41	0.82
1:A:74:ILE:HD13	1:A:116:PRO:CB	2.09	0.82
1:B:343:ILE:HB	1:B:346:ILE:HG22	1.61	0.82
1:A:94:VAL:CG2	1:A:103:VAL:HG12	2.10	0.81
1:A:253:ILE:HD11	1:A:256:ASN:HB3	1.63	0.81
1:A:115:TYR:HE2	1:A:118:GLU:HB2	1.46	0.81
1:B:284:ILE:CG1	1:B:293:PHE:HB3	2.11	0.81
1:A:21:PHE:CB	1:A:26:VAL:HA	2.13	0.79
1:B:283:GLU:HG2	1:B:294:TYR:CD1	2.16	0.79
1:B:103:VAL:HG21	1:B:119:VAL:HG21	1.66	0.78
1:A:285:ASP:OD1	1:A:294:TYR:OH	2.03	0.77
1:B:334:ILE:O	1:B:360:ASN:HB2	1.84	0.77
1:B:59:VAL:HG23	1:B:66:THR:HG21	1.67	0.77
1:A:241:PHE:CE1	1:A:282:ILE:HD12	2.21	0.76
1:B:208:SER:HB3	1:B:222:THR:HG22	1.67	0.76
1:B:353:PHE:HD2	1:B:353:PHE:O	1.68	0.76
1:A:338:GLY:O	1:A:341:THR:OG1	2.02	0.76
1:B:159:LYS:HG3	1:B:172:ILE:CD1	2.14	0.76
1:B:141:ASN:HD22	1:B:170:LEU:HD21	1.51	0.76
1:A:253:ILE:HD11	1:A:259:ALA:HB3	1.69	0.75
1:A:29:ILE:CG2	1:A:130:ILE:HG22	2.17	0.75
1:A:188:LYS:HG2	1:A:189:VAL:N	2.00	0.74
1:A:115:TYR:CE2	1:A:118:GLU:HB2	2.22	0.74
1:B:41:TYR:CD1	1:B:56:LYS:HB2	2.22	0.74
1:A:106:GLU:OE2	1:A:111:THR:HB	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HG3	1:A:164:ILE:HG21	1.70	0.73
1:B:334:ILE:HD11	1:B:350:LEU:HD21	1.70	0.73
1:A:29:ILE:HG22	1:A:130:ILE:HG22	1.70	0.73
1:B:228:LEU:HD23	1:B:229:GLY:N	2.04	0.73
1:B:59:VAL:HG23	1:B:66:THR:CG2	2.19	0.73
1:A:31:ASN:HD22	1:A:35:ASN:HD22	1.37	0.73
1:B:185:LEU:HD12	1:B:195:VAL:HG11	1.70	0.72
1:B:274:LEU:HD21	1:B:299:ARG:HA	1.71	0.72
1:A:141:ASN:HB3	1:A:170:LEU:HD11	1.72	0.72
1:B:160:ASP:O	1:B:164:ILE:HG13	1.90	0.72
1:A:188:LYS:CE	1:A:190:ARG:H	2.00	0.71
1:A:94:VAL:HG22	1:A:103:VAL:CG1	2.17	0.71
1:B:42:VAL:HG13	1:B:51:ILE:CG2	2.20	0.71
1:B:192:GLU:HB2	1:B:213:GLU:CB	2.19	0.71
1:B:382:GLY:HA3	4:B:2042:HOH:O	1.91	0.71
1:A:366:ASP:N	1:A:366:ASP:OD1	2.24	0.71
1:A:285:ASP:HB3	1:B:216:ILE:HD12	1.73	0.70
1:A:31:ASN:HB3	1:A:35:ASN:H	1.56	0.70
1:B:51:ILE:HD12	1:B:122:MET:O	1.91	0.70
1:A:177:THR:HG22	1:A:181:ILE:HD11	1.73	0.69
1:A:28:ILE:HD13	1:A:367:GLU:HB3	1.74	0.69
1:B:314:LEU:HD22	1:B:353:PHE:CD1	2.21	0.69
1:A:301:ARG:O	1:A:304:GLU:HG2	1.91	0.69
1:B:237:MET:O	1:B:240:HIS:HB3	1.93	0.69
1:A:179:ALA:HB2	1:A:337:VAL:HG21	1.75	0.69
1:A:74:ILE:HD11	1:A:117:GLU:OE1	1.93	0.69
1:B:308:ASP:OD1	1:B:309:LEU:HD12	1.93	0.69
1:B:328:LYS:O	1:B:331:ILE:HD11	1.93	0.68
1:A:46:ASP:O	1:A:108:LYS:HA	1.92	0.68
1:A:29:ILE:HG13	1:A:134:TYR:CD2	2.28	0.68
1:A:179:ALA:CB	1:A:337:VAL:HG21	2.24	0.68
1:B:94:VAL:HG22	1:B:103:VAL:HA	1.75	0.68
1:B:185:LEU:HD12	1:B:195:VAL:HG12	1.75	0.68
1:A:285:ASP:HB3	1:B:216:ILE:CD1	2.24	0.68
1:A:84:GLN:HA	1:A:84:GLN:HE21	1.56	0.67
1:B:199:ASP:HB3	1:B:337:VAL:HB	1.76	0.67
1:B:6:ALA:HA	1:B:141:ASN:O	1.95	0.67
1:A:29:ILE:HG22	1:A:130:ILE:CG2	2.25	0.67
1:B:198:PHE:O	1:B:337:VAL:O	2.11	0.67
1:B:334:ILE:HD12	1:B:359:LEU:HD23	1.75	0.67
1:A:199:ASP:OD2	1:A:337:VAL:HG12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:CZ	1:A:284:ILE:HG22	2.24	0.67
1:B:334:ILE:HD12	1:B:359:LEU:CD2	2.24	0.67
1:B:345:LYS:HG2	1:B:348:LYS:HB3	1.77	0.67
1:A:253:ILE:CD1	1:A:256:ASN:HB3	2.23	0.67
1:B:328:LYS:HG2	1:B:353:PHE:HE2	1.60	0.67
1:A:64:THR:HA	1:A:91:PRO:O	1.94	0.67
1:A:12:GLY:HA3	1:A:15:TYR:O	1.95	0.67
1:A:196:LEU:CD1	1:A:354:PHE:HZ	2.08	0.67
1:B:185:LEU:HD11	1:B:333:ASP:CB	2.25	0.67
1:A:116:PRO:O	1:A:117:GLU:C	2.32	0.66
1:A:193:ARG:HB2	1:A:212:THR:HB	1.78	0.66
1:A:242:ILE:CD1	1:A:253:ILE:HG23	2.25	0.66
1:A:147:PRO:HG2	1:A:150:PHE:CD1	2.30	0.66
1:A:151:ASN:ND2	1:A:154:GLN:OE1	2.28	0.66
1:A:195:VAL:O	1:A:209:ILE:HD12	1.95	0.66
1:B:313:THR:O	1:B:316:PRO:HD2	1.97	0.65
1:A:321:LEU:HD21	1:A:331:ILE:HD11	1.78	0.65
1:A:73:LEU:HD11	1:A:94:VAL:HG21	1.77	0.65
1:A:253:ILE:HD13	1:A:288:TYR:CE1	2.31	0.65
1:B:88:LYS:CB	1:B:88:LYS:NZ	2.60	0.65
1:B:88:LYS:HZ1	1:B:88:LYS:HB2	1.59	0.65
1:A:246:LYS:O	1:A:250:LYS:HA	1.97	0.65
1:B:345:LYS:O	1:B:349:LEU:HG	1.97	0.65
1:A:76:ARG:NH2	1:A:82:VAL:HG21	2.12	0.65
1:B:17:CYS:SG	1:B:28:ILE:HG23	2.37	0.65
1:A:147:PRO:HG2	1:A:150:PHE:CE1	2.32	0.64
1:B:125:THR:O	1:B:129:GLU:HG3	1.97	0.64
1:B:78:PHE:H	1:B:101:PRO:HD3	1.62	0.64
1:B:273:THR:CG2	1:B:273:THR:O	2.44	0.64
1:B:303:GLU:O	1:B:307:ALA:N	2.30	0.64
1:A:200:LEU:O	1:A:340:SER:HB2	1.98	0.64
1:A:253:ILE:HD12	1:A:253:ILE:O	1.98	0.64
1:B:195:VAL:CG2	1:B:210:LEU:HB2	2.28	0.64
1:A:205:PHE:CB	1:A:228:LEU:HD22	2.25	0.64
1:A:247:ARG:HA	1:A:250:LYS:HG3	1.80	0.64
1:B:233:PHE:HB3	1:B:306:ASN:OD1	1.98	0.64
1:A:225:ASP:HB3	1:A:228:LEU:HB3	1.78	0.63
1:A:253:ILE:HD11	1:A:259:ALA:CB	2.27	0.63
1:A:21:PHE:CB	1:A:26:VAL:HG22	2.29	0.63
1:A:200:LEU:HG	1:A:340:SER:CB	2.29	0.63
1:A:21:PHE:HB3	1:A:26:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PRO:CB	1:B:139:VAL:HG12	2.21	0.63
1:B:159:LYS:HG2	1:B:169:VAL:CG2	2.28	0.63
1:B:345:LYS:HG2	1:B:348:LYS:CB	2.28	0.63
1:B:9:ILE:HG12	1:B:18:VAL:HB	1.79	0.63
1:A:196:LEU:HD13	1:A:354:PHE:CZ	2.33	0.63
1:B:100:ARG:HG3	1:B:101:PRO:HD2	1.79	0.63
1:A:234:ASP:OD2	1:A:268:GLU:HG2	1.97	0.63
1:A:346:ILE:HA	1:A:349:LEU:HD12	1.80	0.63
1:A:12:GLY:H	1:A:16:SER:HB3	1.64	0.62
1:B:334:ILE:HD13	1:B:334:ILE:C	2.20	0.62
1:A:196:LEU:CD1	1:A:354:PHE:CZ	2.82	0.62
1:B:16:SER:C	1:B:127:MET:HE1	2.20	0.62
1:B:308:ASP:CG	1:B:309:LEU:HD12	2.20	0.62
1:A:80:ASP:HB3	1:A:83:VAL:HG12	1.82	0.62
1:A:303:GLU:OE2	1:A:345:LYS:HB2	2.00	0.61
1:A:198:PHE:O	1:A:337:VAL:O	2.19	0.61
1:A:339:GLY:O	1:A:342:ARG:HG3	2.01	0.61
1:B:146:VAL:HG22	1:B:172:ILE:CG2	2.30	0.61
1:B:353:PHE:O	1:B:353:PHE:CD2	2.52	0.61
1:A:7:VAL:HA	1:A:20:VAL:HG23	1.83	0.60
1:A:200:LEU:HG	1:A:340:SER:HB2	1.83	0.60
1:B:159:LYS:HG2	1:B:169:VAL:HG21	1.82	0.60
1:B:173:ILE:HG22	4:B:2021:HOH:O	2.01	0.60
1:A:298:THR:HB	1:A:301:ARG:H	1.65	0.60
1:A:107:TYR:CZ	1:A:108:LYS:HD2	2.36	0.60
1:A:253:ILE:HD11	1:A:256:ASN:CB	2.32	0.60
1:A:246:LYS:HD3	1:A:252:ASP:OD1	2.01	0.60
1:B:20:VAL:HG22	1:B:22:GLN:HG3	1.84	0.60
1:A:310:PHE:CD1	1:A:346:ILE:HD11	2.36	0.60
1:B:45:THR:HG23	1:B:46:ASP:H	1.66	0.60
1:A:192:GLU:HG3	1:A:193:ARG:N	2.17	0.59
1:B:336:LEU:HD12	1:B:361:LYS:HB3	1.83	0.59
1:A:244:GLU:O	1:A:248:LYS:HG3	2.02	0.59
1:B:119:VAL:O	1:B:122:MET:HB2	2.02	0.59
1:B:21:PHE:HE1	1:B:24:GLY:O	1.85	0.59
1:B:65:ASN:ND2	1:B:106:GLU:HB2	2.14	0.59
1:A:132:GLU:OE2	1:A:138:THR:HA	2.02	0.59
1:A:328:LYS:HE2	1:A:353:PHE:CZ	2.37	0.59
1:B:195:VAL:HG23	1:B:210:LEU:HB2	1.85	0.59
1:B:32:ASP:HB3	4:B:2005:HOH:O	2.03	0.59
1:B:286:SER:OG	1:B:290:GLY:HA2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:O	1:A:172:ILE:HD12	2.02	0.58
1:A:299:ARG:O	1:A:303:GLU:HG3	2.03	0.58
1:B:42:VAL:HG11	1:B:122:MET:SD	2.43	0.58
1:B:177:THR:HG22	1:B:181:ILE:HD11	1.84	0.58
1:A:199:ASP:CA	1:A:337:VAL:O	2.44	0.58
1:B:274:LEU:CD2	1:B:299:ARG:HA	2.33	0.58
1:B:284:ILE:HD12	1:B:287:LEU:CD1	2.30	0.58
1:A:199:ASP:OD2	1:A:337:VAL:CG1	2.52	0.58
1:B:363:ILE:HG22	1:B:368:ALA:HB2	1.85	0.58
1:A:347:GLN:OE1	1:A:361:LYS:HD2	2.04	0.58
1:B:284:ILE:HD11	1:B:293:PHE:CD2	2.38	0.58
1:A:107:TYR:CE2	1:A:108:LYS:HD2	2.37	0.58
1:B:126:LYS:HG2	1:B:130:ILE:HD12	1.86	0.58
1:B:318:GLU:HA	1:B:321:LEU:HB2	1.85	0.57
1:A:9:ILE:HG12	1:A:18:VAL:HG23	1.86	0.57
1:B:151:ASN:OD1	1:B:154:GLN:HG3	2.04	0.57
1:A:196:LEU:HD12	1:A:331:ILE:CD1	2.33	0.57
1:B:171:ARG:C	1:B:172:ILE:HD12	2.24	0.57
1:A:118:GLU:HG2	1:A:121:SER:CB	2.33	0.57
1:A:273:THR:HG21	1:B:152:ASP:CB	2.34	0.57
1:A:146:VAL:HB	1:A:150:PHE:CD2	2.39	0.57
1:A:96:ASN:OD1	1:A:99:GLY:N	2.37	0.57
1:A:253:ILE:HD13	1:A:288:TYR:CG	2.39	0.57
1:A:273:THR:HG21	1:B:152:ASP:HB2	1.86	0.57
1:A:144:VAL:HB	1:A:172:ILE:CD1	2.35	0.56
1:B:357:LYS:HG2	1:B:358:GLU:N	2.20	0.56
1:A:8:GLY:HA3	1:A:373:ALA:C	2.24	0.56
1:B:210:LEU:HD23	1:B:217:PHE:CD2	2.41	0.56
1:B:56:LYS:HG3	4:B:2001:HOH:O	2.04	0.56
1:A:310:PHE:HD1	1:A:346:ILE:HD11	1.69	0.56
1:A:261:ARG:O	1:A:264:ARG:HB2	2.04	0.56
1:B:176:PRO:O	1:B:179:ALA:HB3	2.05	0.56
1:B:97:ASP:HB2	1:B:102:LYS:HE2	1.87	0.56
1:A:325:LYS:O	1:A:326:LEU:HD23	2.05	0.56
1:B:228:LEU:HD23	1:B:228:LEU:C	2.27	0.56
1:A:260:VAL:HG12	1:A:261:ARG:CD	2.36	0.55
1:B:41:TYR:CE2	1:B:68:PHE:HB3	2.40	0.55
1:A:196:LEU:HD23	1:A:197:ILE:N	2.21	0.55
1:A:260:VAL:HG12	1:A:261:ARG:HD2	1.88	0.55
1:B:239:ASN:HA	1:B:242:ILE:CD1	2.36	0.55
1:B:172:ILE:N	1:B:172:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HG2	1:A:353:PHE:HZ	1.72	0.54
1:B:284:ILE:CD1	1:B:287:LEU:HD22	2.36	0.54
1:A:17:CYS:SG	1:A:28:ILE:CG2	2.95	0.54
1:A:51:ILE:CD1	1:A:126:LYS:HB2	2.37	0.54
1:A:17:CYS:SG	1:A:28:ILE:HG21	2.48	0.54
1:A:253:ILE:CD1	1:A:256:ASN:CB	2.86	0.54
1:B:314:LEU:CD2	1:B:353:PHE:HD1	2.14	0.54
1:A:49:ARG:HB3	1:A:107:TYR:CE2	2.43	0.54
1:A:228:LEU:HD23	1:A:228:LEU:C	2.28	0.54
1:A:125:THR:O	1:A:128:LYS:HB3	2.08	0.53
1:A:262:ARG:NH2	1:A:284:ILE:HG22	2.23	0.53
1:A:370:ALA:O	1:A:373:ALA:HB3	2.08	0.53
1:B:284:ILE:HD11	1:B:287:LEU:HD22	1.90	0.53
1:A:118:GLU:O	1:A:122:MET:HG3	2.08	0.53
1:A:374:ALA:O	1:A:377:ALA:HB3	2.09	0.53
1:A:195:VAL:HG22	1:A:333:ASP:HB2	1.89	0.53
1:B:199:ASP:HB3	1:B:337:VAL:C	2.30	0.53
1:A:10:ASP:CG	1:A:369:VAL:HG13	2.29	0.53
1:B:194:ASN:HD22	1:B:326:LEU:HD13	1.74	0.53
1:A:44:PHE:CD2	1:A:105:VAL:HG21	2.44	0.52
1:B:315:ASP:HB3	1:B:316:PRO:HD3	1.91	0.52
1:A:84:GLN:CA	1:A:84:GLN:HE21	2.20	0.52
1:A:377:ALA:O	1:A:381:SER:N	2.42	0.52
1:A:241:PHE:CD1	1:A:282:ILE:HD12	2.45	0.52
1:B:368:ALA:O	1:B:371:TYR:HB3	2.10	0.52
1:B:148:ALA:C	1:B:150:PHE:H	2.13	0.52
1:A:7:VAL:O	1:A:142:ALA:HA	2.10	0.52
1:A:31:ASN:HB3	1:A:35:ASN:N	2.24	0.52
1:B:209:ILE:C	1:B:209:ILE:HD13	2.30	0.52
1:A:22:GLN:O	1:A:23:HIS:C	2.47	0.52
1:A:334:ILE:HD12	1:A:354:PHE:CE2	2.45	0.52
1:B:185:LEU:HD11	1:B:333:ASP:HB2	1.91	0.52
1:B:239:ASN:HA	1:B:242:ILE:HD11	1.93	0.51
1:B:143:VAL:CG2	1:B:377:ALA:HB2	2.41	0.51
1:B:45:THR:HG23	1:B:46:ASP:N	2.25	0.51
1:B:147:PRO:HD2	1:B:150:PHE:CD1	2.43	0.51
1:B:177:THR:HG22	1:B:181:ILE:CD1	2.40	0.51
1:B:241:PHE:CE1	1:B:282:ILE:HD12	2.45	0.51
1:B:314:LEU:O	1:B:317:VAL:HB	2.10	0.51
1:B:190:ARG:HB2	1:B:193:ARG:HH21	1.75	0.51
1:B:94:VAL:HG13	1:B:102:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HG21	1:A:130:ILE:HG22	1.92	0.51
1:A:42:VAL:HG11	1:A:122:MET:SD	2.51	0.51
1:B:147:PRO:O	1:B:150:PHE:HB2	2.10	0.51
1:B:353:PHE:C	1:B:353:PHE:CD2	2.84	0.51
1:B:353:PHE:HD2	1:B:353:PHE:C	2.14	0.51
1:B:188:LYS:NZ	1:B:214:ASP:HA	2.26	0.50
1:B:310:PHE:CD1	1:B:346:ILE:HD13	2.46	0.50
1:B:62:ASN:O	1:B:66:THR:HG22	2.10	0.50
1:A:219:VAL:CG1	4:A:2027:HOH:O	2.59	0.50
1:B:241:PHE:CZ	1:B:282:ILE:HD12	2.45	0.50
1:B:238:VAL:HG13	1:B:263:LEU:HD23	1.93	0.50
1:B:41:TYR:CE1	1:B:56:LYS:HB2	2.46	0.50
1:A:258:ARG:HH11	1:A:258:ARG:HG2	1.76	0.50
1:A:286:SER:HB3	1:B:216:ILE:CG1	2.41	0.50
1:B:7:VAL:O	1:B:142:ALA:HA	2.10	0.50
1:A:209:ILE:HG21	1:A:324:ALA:HB2	1.93	0.50
1:B:284:ILE:HG13	1:B:293:PHE:CB	2.33	0.50
1:B:74:ILE:HD11	1:B:117:GLU:HA	1.94	0.50
1:B:200:LEU:O	1:B:338:GLY:HA3	2.11	0.50
1:A:67:VAL:HG11	1:A:103:VAL:HG21	1.93	0.50
1:B:372:GLY:O	1:B:373:ALA:C	2.49	0.50
1:A:219:VAL:HG12	4:A:2027:HOH:O	2.12	0.49
1:A:249:HIS:CE1	1:A:291:ILE:HG21	2.47	0.49
1:A:151:ASN:OD1	1:A:153:SER:HB3	2.12	0.49
1:A:200:LEU:HG	1:A:340:SER:HB3	1.93	0.49
1:B:238:VAL:C	1:B:240:HIS:N	2.66	0.49
1:A:75:GLY:HA3	1:A:154:GLN:HG2	1.94	0.49
1:A:318:GLU:HG2	1:A:353:PHE:CZ	2.47	0.49
1:A:80:ASP:O	1:A:83:VAL:HG13	2.12	0.49
1:A:304:GLU:HA	1:A:307:ALA:HB2	1.95	0.49
1:A:143:VAL:CG2	1:A:377:ALA:HB2	2.42	0.49
1:A:117:GLU:H	1:A:117:GLU:CD	2.16	0.49
1:A:348:LYS:NZ	1:A:352:ASP:OD2	2.46	0.49
1:A:36:ARG:HD3	1:A:367:GLU:OE2	2.13	0.49
1:B:284:ILE:HD11	1:B:293:PHE:HD2	1.78	0.49
1:B:3:LYS:HD2	1:B:3:LYS:HA	1.70	0.49
1:A:29:ILE:HG13	1:A:134:TYR:HD2	1.77	0.49
1:A:31:ASN:HD22	1:A:35:ASN:ND2	2.06	0.48
1:B:72:ARG:HD3	1:B:86:ASP:OD2	2.13	0.48
1:A:107:TYR:CZ	1:A:108:LYS:CD	2.96	0.48
1:A:263:LEU:O	1:A:266:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:CB	1:B:213:GLU:HB2	2.34	0.48
1:A:156:GLN:NE2	4:A:2019:HOH:O	2.47	0.48
1:A:367:GLU:O	1:A:369:VAL:N	2.47	0.48
1:B:334:ILE:HD13	1:B:335:VAL:N	2.28	0.48
1:B:207:VAL:HB	1:B:223:ALA:O	2.14	0.48
1:B:58:GLN:C	1:B:60:ALA:H	2.17	0.48
1:B:46:ASP:O	1:B:108:LYS:HG2	2.14	0.48
1:B:195:VAL:O	1:B:209:ILE:HG12	2.13	0.48
1:B:253:ILE:HG22	1:B:288:TYR:CD2	2.48	0.48
1:B:378:ALA:HA	1:B:381:SER:OG	2.14	0.48
1:B:58:GLN:C	1:B:60:ALA:N	2.67	0.48
1:A:175:GLU:O	1:A:176:PRO:C	2.49	0.48
1:A:242:ILE:HD13	1:A:253:ILE:CG2	2.43	0.48
1:B:3:LYS:HG3	1:B:4:GLY:H	1.79	0.48
1:B:325:LYS:HA	1:B:325:LYS:HD3	1.47	0.47
1:B:151:ASN:O	1:B:155:ARG:HG3	2.14	0.47
1:B:100:ARG:CG	1:B:101:PRO:HD2	2.44	0.47
1:A:124:LEU:O	1:A:128:LYS:N	2.45	0.47
1:A:142:ALA:O	1:A:170:LEU:HD12	2.14	0.47
1:B:103:VAL:HG22	1:B:114:PHE:O	2.15	0.47
1:B:76:ARG:HG2	1:B:80:ASP:OD2	2.14	0.47
1:A:228:LEU:HD23	1:A:228:LEU:O	2.15	0.47
1:A:376:GLN:O	1:A:376:GLN:HG3	2.15	0.47
1:A:107:TYR:CE1	1:A:108:LYS:HD3	2.49	0.47
1:A:336:LEU:HB3	1:A:341:THR:HG21	1.96	0.47
1:B:97:ASP:HB2	1:B:102:LYS:CE	2.44	0.47
1:A:118:GLU:CG	1:A:121:SER:HB3	2.40	0.47
1:A:143:VAL:HG23	1:A:377:ALA:HB2	1.96	0.47
1:A:50:LEU:O	1:A:55:ALA:HB2	2.15	0.47
1:B:14:THR:OG1	2:B:1383:ADP:O3B	2.32	0.47
1:B:162:GLY:O	1:B:165:ALA:HB3	2.15	0.47
1:A:74:ILE:CD1	1:A:117:GLU:OE1	2.63	0.46
1:B:273:THR:O	1:B:273:THR:HG23	2.15	0.46
1:B:337:VAL:HG11	1:B:369:VAL:HG23	1.98	0.46
1:A:314:LEU:HD13	1:A:353:PHE:HD1	1.81	0.46
1:A:151:ASN:OD1	1:A:153:SER:CB	2.64	0.46
1:A:151:ASN:OD1	1:A:153:SER:N	2.48	0.46
1:B:56:LYS:HD3	1:B:57:ASN:OD1	2.15	0.46
1:B:58:GLN:OE1	1:B:62:ASN:HB3	2.15	0.46
1:A:237:MET:CE	1:A:297:ILE:HG21	2.46	0.46
1:B:261:ARG:HD2	1:B:261:ARG:HA	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:HD13	1:A:253:ILE:HG23	1.96	0.46
1:B:159:LYS:CG	1:B:169:VAL:HG21	2.45	0.46
1:B:39:PRO:HB2	1:B:41:TYR:HD1	1.81	0.46
1:A:234:ASP:O	1:A:238:VAL:HG23	2.16	0.46
1:A:31:ASN:OD1	1:A:32:ASP:N	2.49	0.46
1:A:19:GLY:O	1:A:374:ALA:HB2	2.15	0.46
1:B:284:ILE:HG12	1:B:293:PHE:HB3	1.95	0.46
1:A:193:ARG:CB	1:A:212:THR:HB	2.45	0.45
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.80	0.45
1:A:209:ILE:CD1	1:A:331:ILE:HG12	2.46	0.45
1:A:334:ILE:O	1:A:360:ASN:HB2	2.16	0.45
1:B:44:PHE:CD2	1:B:105:VAL:HG21	2.51	0.45
2:B:1383:ADP:O2B	3:B:1384:PO4:O3	2.34	0.45
1:B:190:ARG:CB	1:B:193:ARG:HH21	2.30	0.45
1:A:253:ILE:CD1	1:A:288:TYR:CD1	2.91	0.45
1:A:306:ASN:O	1:A:309:LEU:N	2.46	0.45
1:B:302:PHE:HA	1:B:305:LEU:HD12	1.98	0.45
1:B:357:LYS:CG	1:B:358:GLU:N	2.80	0.45
1:A:116:PRO:O	1:A:118:GLU:N	2.49	0.45
1:B:150:PHE:HA	1:B:154:GLN:NE2	2.31	0.45
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.69	0.45
1:B:41:TYR:CE2	1:B:68:PHE:CB	2.99	0.45
1:B:190:ARG:HA	1:B:190:ARG:HD3	1.61	0.45
1:B:338:GLY:O	1:B:365:PRO:HB2	2.16	0.45
1:B:273:THR:O	1:B:273:THR:HG22	2.14	0.45
1:B:364:ASN:C	1:B:366:ASP:H	2.20	0.45
1:B:71:LYS:HE2	1:B:150:PHE:HZ	1.82	0.45
1:B:318:GLU:O	1:B:321:LEU:N	2.50	0.45
1:A:15:TYR:HA	1:A:38:THR:O	2.17	0.45
1:A:11:LEU:HA	1:A:16:SER:HB2	1.99	0.45
1:A:261:ARG:HH11	1:A:261:ARG:CB	2.30	0.45
1:B:44:PHE:HB3	1:B:107:TYR:CD1	2.51	0.45
1:B:242:ILE:HG13	1:B:243:ALA:N	2.31	0.45
1:A:261:ARG:O	1:A:265:THR:HG22	2.16	0.44
1:A:70:ALA:HB2	1:A:119:VAL:CG1	2.47	0.44
1:B:198:PHE:CE1	1:B:205:PHE:CE1	3.05	0.44
1:A:273:THR:HG21	1:B:152:ASP:HB3	1.99	0.44
1:B:197:ILE:HG23	1:B:337:VAL:CG2	2.48	0.44
1:B:239:ASN:HA	1:B:242:ILE:HG12	2.00	0.44
1:A:147:PRO:CG	1:A:150:PHE:CE1	2.99	0.44
1:A:188:LYS:HG2	1:A:189:VAL:H	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HH11	1:A:261:ARG:HB3	1.82	0.44
1:A:350:LEU:HD11	1:A:354:PHE:CE2	2.52	0.44
1:B:238:VAL:O	1:B:242:ILE:HG12	2.17	0.44
1:A:285:ASP:O	1:A:286:SER:C	2.54	0.44
1:B:303:GLU:O	1:B:307:ALA:HB2	2.18	0.44
1:B:278:THR:OG1	1:B:279:GLN:NE2	2.51	0.44
1:A:328:LYS:HE2	1:A:353:PHE:CE2	2.53	0.44
1:A:118:GLU:HA	1:A:121:SER:HB3	2.00	0.44
1:A:144:VAL:HB	1:A:172:ILE:HD12	1.99	0.44
1:A:70:ALA:HB2	1:A:119:VAL:HG11	2.00	0.43
1:A:80:ASP:OD1	1:A:82:VAL:HG22	2.18	0.43
1:B:210:LEU:HD23	1:B:217:PHE:HD2	1.81	0.43
1:B:252:ASP:OD2	1:B:253:ILE:N	2.51	0.43
1:B:285:ASP:OD2	1:B:294:TYR:OH	2.18	0.43
1:A:21:PHE:HB2	1:A:26:VAL:CG2	2.48	0.43
1:B:50:LEU:O	1:B:55:ALA:HB2	2.18	0.43
1:A:199:ASP:HA	1:A:337:VAL:C	2.33	0.43
1:A:178:ALA:HA	1:A:181:ILE:HD12	2.00	0.43
1:A:97:ASP:O	1:A:98:ALA:C	2.57	0.43
1:B:195:VAL:HG12	1:B:333:ASP:HB2	2.00	0.43
1:A:260:VAL:HG12	1:A:261:ARG:HD3	2.01	0.43
1:B:117:GLU:O	1:B:121:SER:HB3	2.18	0.43
1:B:17:CYS:SG	1:B:28:ILE:CG2	3.05	0.43
1:B:235:ASN:CG	1:B:264:ARG:HH22	2.21	0.43
1:B:334:ILE:CD1	1:B:350:LEU:HD21	2.45	0.43
1:B:103:VAL:CG2	1:B:114:PHE:HB2	2.49	0.43
1:B:31:ASN:HB2	1:B:130:ILE:HD13	2.00	0.43
1:B:310:PHE:HD1	1:B:346:ILE:HD13	1.83	0.43
1:A:21:PHE:HB2	1:A:26:VAL:HG22	2.01	0.43
1:B:129:GLU:HG2	4:B:2019:HOH:O	2.18	0.43
1:B:143:VAL:HG22	1:B:170:LEU:HB2	2.01	0.43
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.75	0.43
1:B:14:THR:HG21	1:B:202:GLY:HA3	2.01	0.43
1:B:278:THR:HA	1:B:299:ARG:HB2	2.00	0.43
1:A:376:GLN:HA	1:A:379:ILE:HD12	2.00	0.43
1:A:126:LYS:HG3	1:A:130:ILE:CD1	2.48	0.42
1:A:364:ASN:HB2	1:A:367:GLU:HG3	2.01	0.42
1:B:229:GLY:O	1:B:233:PHE:CZ	2.72	0.42
1:B:318:GLU:O	1:B:322:ARG:N	2.49	0.42
1:B:39:PRO:HB2	1:B:41:TYR:CD1	2.54	0.42
1:A:64:THR:HG22	1:A:65:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ASP:OD2	1:B:319:LYS:HD2	2.18	0.42
1:B:121:SER:HB2	1:B:161:ALA:O	2.18	0.42
1:B:144:VAL:HG23	1:B:172:ILE:HG13	2.02	0.42
1:B:302:PHE:O	1:B:305:LEU:HB2	2.19	0.42
1:A:246:LYS:HG3	1:A:252:ASP:HA	2.01	0.42
1:B:238:VAL:C	1:B:240:HIS:H	2.22	0.42
1:B:334:ILE:C	1:B:334:ILE:CD1	2.88	0.42
1:B:77:ARG:NH2	1:B:79:ASP:OD1	2.53	0.42
1:B:345:LYS:HG2	1:B:348:LYS:HB2	2.01	0.42
1:B:58:GLN:O	1:B:60:ALA:N	2.51	0.42
1:B:28:ILE:N	1:B:28:ILE:HD12	2.34	0.42
1:B:41:TYR:CD2	1:B:68:PHE:HB3	2.55	0.42
1:A:124:LEU:HD12	1:A:161:ALA:HB1	2.01	0.42
1:A:200:LEU:CD2	1:A:346:ILE:HD12	2.50	0.42
1:A:179:ALA:HB1	1:A:337:VAL:HG21	1.98	0.42
1:B:6:ALA:HA	1:B:141:ASN:C	2.40	0.42
1:A:303:GLU:O	1:A:307:ALA:HB2	2.20	0.42
1:A:310:PHE:CD1	1:A:346:ILE:CD1	3.02	0.42
1:A:336:LEU:CD2	1:A:350:LEU:HD23	2.50	0.42
1:B:58:GLN:HB3	4:B:2010:HOH:O	2.19	0.42
1:A:367:GLU:O	1:A:368:ALA:C	2.58	0.41
1:B:370:ALA:O	1:B:373:ALA:HB3	2.20	0.41
1:A:310:PHE:CE1	1:A:343:ILE:HD13	2.56	0.41
1:B:308:ASP:OD2	1:B:309:LEU:HD12	2.20	0.41
1:B:364:ASN:O	1:B:366:ASP:N	2.53	0.41
1:A:15:TYR:CE2	1:A:39:PRO:HG3	2.55	0.41
1:B:148:ALA:C	1:B:150:PHE:N	2.74	0.41
1:B:185:LEU:HD11	1:B:333:ASP:CG	2.40	0.41
1:B:209:ILE:HD13	1:B:210:LEU:N	2.35	0.41
1:A:20:VAL:HG11	1:A:135:LEU:HD21	2.03	0.41
1:B:328:LYS:H	1:B:328:LYS:HD3	1.85	0.41
1:B:199:ASP:HB3	1:B:337:VAL:O	2.21	0.41
1:B:297:ILE:HG13	1:B:301:ARG:HG2	2.03	0.41
1:B:200:LEU:O	1:B:338:GLY:CA	2.69	0.41
1:B:41:TYR:CD1	1:B:56:LYS:CB	3.00	0.41
1:A:261:ARG:HD2	1:A:261:ARG:HA	1.74	0.41
1:A:312:GLY:O	1:A:315:ASP:HB3	2.20	0.41
1:A:343:ILE:HG22	1:A:345:LYS:H	1.86	0.41
1:B:210:LEU:HD23	1:B:217:PHE:CE2	2.56	0.41
1:B:344:PRO:O	1:B:347:GLN:HB2	2.20	0.41
1:A:382:GLY:CA	1:A:383:ASP:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:CB	1:B:337:VAL:O	2.69	0.41
1:B:325:LYS:O	1:B:326:LEU:HD23	2.21	0.41
1:A:375:VAL:C	1:A:377:ALA:N	2.75	0.41
1:A:379:ILE:H	1:A:379:ILE:HG13	1.61	0.41
1:B:178:ALA:O	1:B:372:GLY:HA3	2.21	0.41
1:A:233:PHE:HA	1:A:306:ASN:ND2	2.36	0.40
1:A:316:PRO:HA	1:A:319:LYS:HB3	2.03	0.40
1:B:177:THR:O	1:B:181:ILE:HG13	2.20	0.40
1:B:280:ALA:O	1:B:296:SER:HB2	2.21	0.40
1:B:10:ASP:C	1:B:10:ASP:OD1	2.60	0.40
1:B:71:LYS:HE2	1:B:150:PHE:CZ	2.57	0.40
1:A:74:ILE:HD11	1:A:117:GLU:CD	2.41	0.40
1:B:137:LYS:H	1:B:137:LYS:HG2	1.75	0.40
1:B:185:LEU:CD1	1:B:195:VAL:HG12	2.48	0.40
1:B:324:ALA:O	1:B:326:LEU:HG	2.21	0.40
1:A:144:VAL:HB	1:A:172:ILE:HD13	2.02	0.40
1:A:242:ILE:HD12	1:A:253:ILE:HG23	2.03	0.40
1:B:200:LEU:HD12	1:B:200:LEU:HA	1.96	0.40
1:B:75:GLY:HA3	1:B:154:GLN:HA	2.04	0.40

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:ND2	1:B:355:ASN:OD1[4_546]	1.19	1.01
1:A:355:ASN:CG	1:B:355:ASN:OD1[4_546]	1.60	0.60
1:A:355:ASN:OD1	1:B:355:ASN:OD1[4_546]	1.85	0.35
1:A:355:ASN:ND2	1:B:355:ASN:CG[4_546]	1.96	0.24

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	379/543 (70%)	329 (87%)	39 (10%)	11 (3%)	4	31
1	B	380/543 (70%)	326 (86%)	46 (12%)	8 (2%)	7	38
All	All	759/1086 (70%)	655 (86%)	85 (11%)	19 (2%)	5	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	368	ALA
1	A	4	GLY
1	A	23	HIS
1	A	59	VAL
1	A	365	PRO
1	B	59	VAL
1	B	78	PHE
1	B	170	LEU
1	B	220	LYS
1	B	32	ASP
1	A	214	ASP
1	A	203	GLY
1	A	220	LYS
1	A	355	ASN
1	B	23	HIS
1	B	365	PRO
1	A	201	GLY
1	B	312	GLY

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	315/459 (69%)	263 (84%)	52 (16%)	2	13
1	B	315/459 (69%)	259 (82%)	56 (18%)	2	10
All	All	630/918 (69%)	522 (83%)	108 (17%)	2	12

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	20	VAL
1	A	21	PHE
1	A	32	ASP
1	A	49	ARG
1	A	50	LEU
1	A	53	ASP
1	A	58	GLN
1	A	64	THR
1	A	72	ARG
1	A	74	ILE
1	A	76	ARG
1	A	83	VAL
1	A	84	GLN
1	A	87	MET
1	A	93	MET
1	A	97	ASP
1	A	100	ARG
1	A	108	LYS
1	A	111	THR
1	A	113	SER
1	A	116	PRO
1	A	118	GLU
1	A	120	SER
1	A	137	LYS
1	A	138	THR
1	A	187	LYS
1	A	188	LYS
1	A	190	ARG
1	A	192	GLU
1	A	199	ASP
1	A	213	GLU
1	A	228	LEU
1	A	253	ILE
1	A	254	SER
1	A	258	ARG
1	A	261	ARG
1	A	264	ARG
1	A	265	THR
1	A	268	GLU
1	A	273	THR
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	284	ILE
1	A	298	THR
1	A	315	ASP
1	A	336	LEU
1	A	341	THR
1	A	361	LYS
1	A	363	ILE
1	A	366	ASP
1	A	376	GLN
1	A	381	SER
1	B	10	ASP
1	B	14	THR
1	B	17	CYS
1	B	18	VAL
1	B	23	HIS
1	B	49	ARG
1	B	56	LYS
1	B	61	MET
1	B	79	ASP
1	B	87	MET
1	B	88	LYS
1	B	93	MET
1	B	95	VAL
1	B	102	LYS
1	B	112	LYS
1	B	113	SER
1	B	120	SER
1	B	121	SER
1	B	137	LYS
1	B	159	LYS
1	B	164	ILE
1	B	185	LEU
1	B	189	VAL
1	B	190	ARG
1	B	192	GLU
1	B	193	ARG
1	B	198	PHE
1	B	208	SER
1	B	209	ILE
1	B	211	THR
1	B	213	GLU
1	B	214	ASP

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Mol	Chain	Res	Type
1	B	216	ILE
1	B	247	ARG
1	B	248	LYS
1	B	257	LYS
1	B	261	ARG
1	B	262	ARG
1	B	268	GLU
1	B	269	ARG
1	B	273	THR
1	B	274	LEU
1	B	277	SER
1	B	279	GLN
1	B	315	ASP
1	B	328	LYS
1	B	331	ILE
1	B	334	ILE
1	B	337	VAL
1	B	340	SER
1	B	352	ASP
1	B	353	PHE
1	B	360	ASN
1	B	366	ASP
1	B	367	GLU
1	B	376	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	35	ASN
1	A	84	GLN
1	A	89	HIS
1	A	249	HIS
1	A	306	ASN
1	A	376	GLN
1	B	22	GLN
1	B	84	GLN
1	B	141	ASN
1	B	239	ASN
1	B	249	HIS
1	B	279	GLN
1	B	360	ASN

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Mol	Chain	Res	Type
1	B	376	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](#)

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	$\# Z > 2$
2	ADP	A	1383	-	24,29,29	0.96	1 (4%)	29,45,45	1.83	7 (24%)
2	ADP	B	1383	-	24,29,29	0.93	2 (8%)	29,45,45	1.88	6 (20%)
3	PO4	A	1384	-	4,4,4	1.44	1 (25%)	6,6,6	1.60	1 (16%)
3	PO4	B	1384	-	4,4,4	1.32	1 (25%)	6,6,6	1.47	1 (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
2	ADP	A	1383	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1383	-	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1384	PO4	P-O3	-2.63	1.46	1.54
3	B	1384	PO4	P-O3	-2.49	1.47	1.54
2	B	1383	ADP	C2'-C1'	2.34	1.57	1.53
2	B	1383	ADP	C5-C4	2.12	1.46	1.40
2	A	1383	ADP	C5-C4	2.01	1.46	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1383	ADP	PA-O3A-PB	-5.42	114.23	132.83
2	B	1383	ADP	PA-O3A-PB	-5.28	114.71	132.83
2	B	1383	ADP	N3-C2-N1	-4.15	122.19	128.68
2	A	1383	ADP	N3-C2-N1	-3.70	122.89	128.68
2	A	1383	ADP	C4-C5-N7	-2.79	106.50	109.40
3	A	1384	PO4	O4-P-O1	-2.70	101.02	110.89
2	A	1383	ADP	C2'-C3'-C4'	2.65	107.79	102.64
2	B	1383	ADP	C3'-C2'-C1'	2.61	104.90	100.98
2	B	1383	ADP	O2B-PB-O3A	-2.52	96.19	104.64
2	A	1383	ADP	O3B-PB-O2B	2.50	117.19	107.64
3	B	1384	PO4	O4-P-O1	-2.28	102.56	110.89
2	A	1383	ADP	O2B-PB-O3A	-2.23	97.16	104.64
2	A	1383	ADP	C5'-C4'-C3'	-2.22	106.87	115.18
2	B	1383	ADP	O3B-PB-O2B	2.06	115.50	107.64
2	B	1383	ADP	O2A-PA-O1A	2.04	122.31	112.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

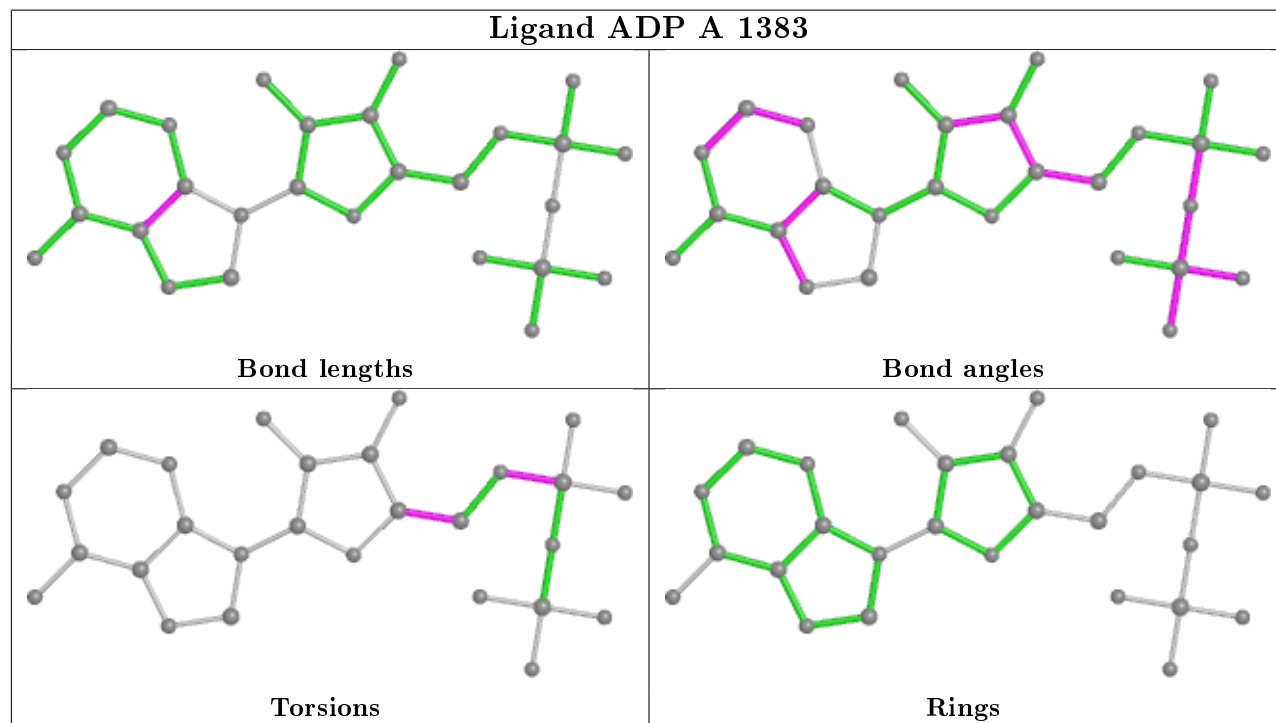
Mol	Chain	Res	Type	Atoms
2	B	1383	ADP	C5'-O5'-PA-O1A
2	A	1383	ADP	C3'-C4'-C5'-O5'
2	A	1383	ADP	O4'-C4'-C5'-O5'
2	B	1383	ADP	C5'-O5'-PA-O3A
2	A	1383	ADP	C5'-O5'-PA-O1A

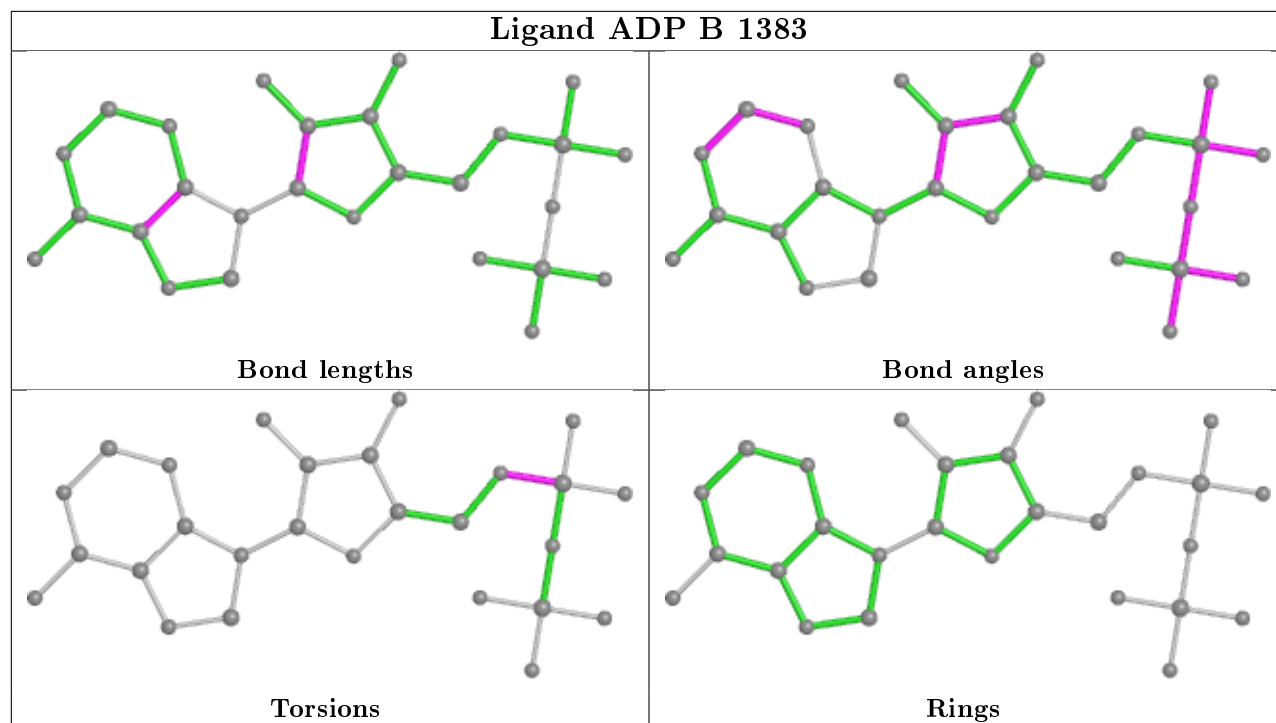
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1383	ADP	1	0
2	B	1383	ADP	2	0
3	B	1384	PO4	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	382:GLY	C	383:ASP	N	2.24

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	382/543 (70%)	-0.47	1 (0%) 94 91	20, 67, 119, 163	0
1	B	382/543 (70%)	-0.47	0 100 100	14, 68, 112, 147	0
All	All	764/1086 (70%)	-0.47	1 (0%) 95 95	14, 68, 116, 163	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	4.1

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](#)

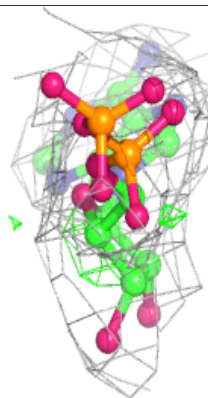
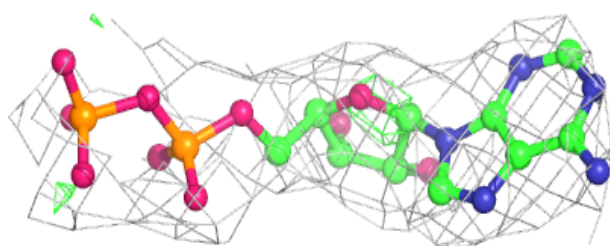
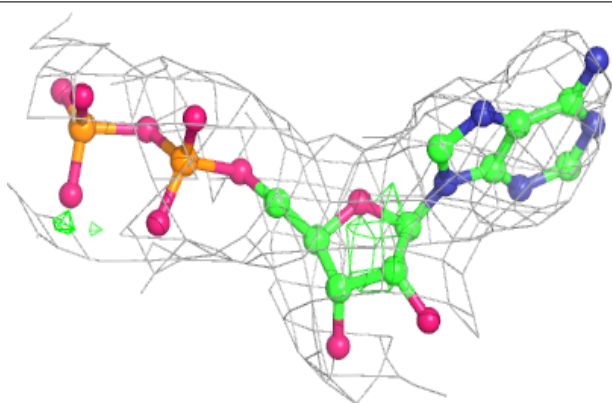
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

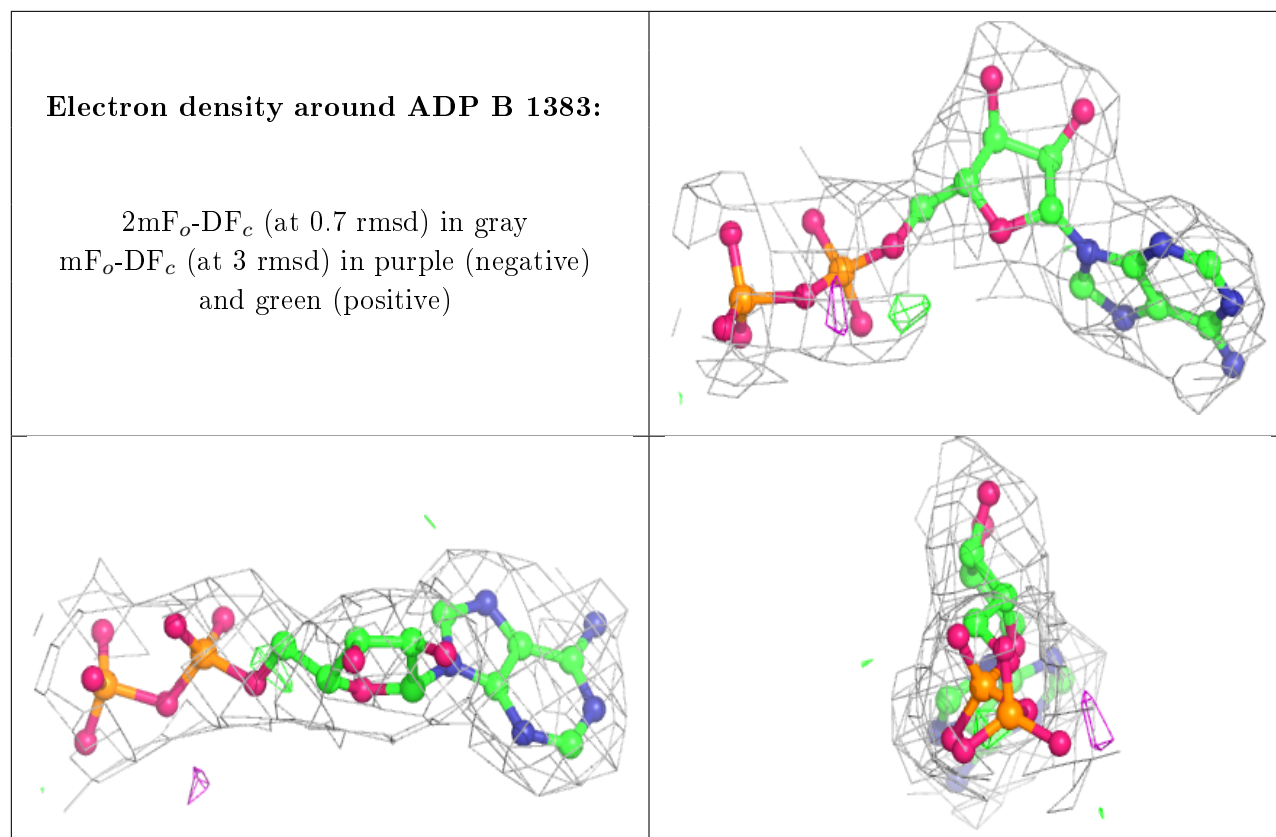
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	1383	27/27	0.95	0.21	77,77,77,77	0
2	ADP	B	1383	27/27	0.96	0.18	61,61,61,61	0
3	PO4	A	1384	5/5	0.96	0.17	74,101,101,101	0
3	PO4	B	1384	5/5	0.98	0.11	37,37,37,165	0

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.

Electron density around ADP A 1383:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.