



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:21 AM UTC

PDB ID : 2V7Z / pdb_00002v7z
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

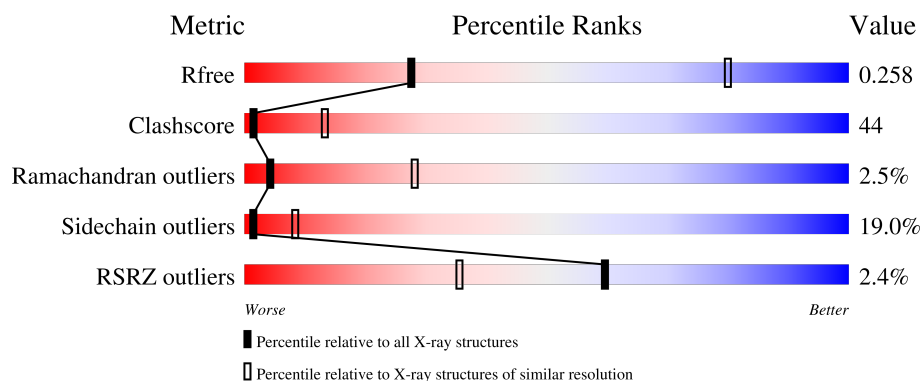
1 Overall quality at a glance

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	2% 24% 32% 12% 30%
1	B	543	2% 24% 32% 12% 30%

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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		



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 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.01-3.50) 90.5 (29.01-3.50)	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 , 0.258	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 , 83.7	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	0.99	7/2997 (0.2%)	1.68	81/4046 (2.0%)
1	B	1.04	17/2998 (0.6%)	1.77	80/4048 (2.0%)
All	All	1.01	24/5995 (0.4%)	1.73	161/8094 (2.0%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	C-N	15.41	1.50	1.33
1	B	345	LYS	C-N	12.02	1.47	1.33
1	B	345	LYS	C-O	11.81	1.39	1.23
1	B	88	LYS	N-CA	-8.65	1.36	1.46
1	B	344	PRO	C-N	8.11	1.45	1.33
1	B	343	ILE	C-N	7.62	1.44	1.33
1	B	89	HIS	CA-C	7.55	1.63	1.52
1	B	87	MET	C-O	7.09	1.32	1.24
1	B	88	LYS	C-O	-6.75	1.14	1.24
1	A	70	ALA	N-CA	6.21	1.53	1.46
1	B	175	GLU	C-N	6.06	1.41	1.33
1	A	37	THR	CA-CB	6.06	1.63	1.53
1	A	38	THR	C-N	5.89	1.40	1.33
1	A	118	GLU	CA-CB	-5.86	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	ALA	CA-C	5.77	1.59	1.52
1	A	116	PRO	C-O	-5.50	1.16	1.24
1	B	189	VAL	CA-CB	5.45	1.61	1.54
1	A	4	GLY	CA-C	5.41	1.59	1.51
1	B	125	THR	C-O	5.20	1.30	1.24
1	B	382	GLY	C-N	-5.20	1.26	1.33
1	B	25	LYS	N-CA	-5.09	1.39	1.45
1	B	343	ILE	C-O	-5.06	1.18	1.24
1	B	21	PHE	CA-C	-5.01	1.46	1.53
1	B	198	PHE	N-CA	-5.01	1.40	1.46

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	PRO	CA-C-N	-18.18	96.08	123.17
1	B	344	PRO	C-N-CA	-18.18	96.08	123.17
1	B	87	MET	CA-C-N	-16.26	96.16	122.66
1	B	87	MET	C-N-CA	-16.26	96.16	122.66
1	B	345	LYS	O-C-N	-14.21	102.78	121.97
1	B	345	LYS	CA-C-O	-13.78	104.09	121.17
1	B	24	GLY	O-C-N	13.51	140.26	122.70
1	A	26	VAL	CB-CA-C	-11.91	98.36	111.23
1	A	38	THR	CA-C-N	-11.82	106.77	120.13
1	A	38	THR	C-N-CA	-11.82	106.77	120.13
1	B	13	THR	N-CA-C	-11.59	98.37	111.82
1	B	144	VAL	O-C-N	-11.31	110.87	122.97
1	B	88	LYS	N-CA-C	11.18	124.82	112.97
1	B	143	VAL	CA-C-N	-10.76	104.82	122.57
1	B	143	VAL	C-N-CA	-10.76	104.82	122.57
1	B	199	ASP	N-CA-CB	10.26	127.30	110.37
1	B	199	ASP	CA-CB-CG	10.17	122.77	112.60
1	B	90	TRP	N-CA-C	10.11	123.54	110.39
1	B	21	PHE	CA-C-N	-10.01	107.09	122.81
1	B	21	PHE	C-N-CA	-10.01	107.09	122.81
1	A	175	GLU	CA-C-N	-9.53	108.46	119.32
1	A	175	GLU	C-N-CA	-9.53	108.46	119.32
1	A	20	VAL	CA-C-N	-9.40	109.51	122.86
1	A	20	VAL	C-N-CA	-9.40	109.51	122.86
1	B	23	HIS	CA-CB-CG	9.32	123.12	113.80
1	A	209	ILE	CA-C-N	9.29	135.54	122.72
1	A	209	ILE	C-N-CA	9.29	135.54	122.72
1	B	343	ILE	CA-C-N	-9.13	109.74	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ILE	C-N-CA	-9.13	109.74	119.24
1	A	100	ARG	CA-C-N	-9.10	108.47	119.84
1	A	100	ARG	C-N-CA	-9.10	108.47	119.84
1	B	4	GLY	CA-C-N	-9.02	108.56	119.84
1	B	4	GLY	C-N-CA	-9.02	108.56	119.84
1	B	175	GLU	CA-C-N	-8.93	110.45	119.56
1	B	175	GLU	C-N-CA	-8.93	110.45	119.56
1	B	88	LYS	CA-C-O	-8.91	107.87	119.80
1	B	344	PRO	O-C-N	8.62	131.49	122.18
1	A	168	ASN	CA-C-N	-8.39	111.54	122.37
1	A	168	ASN	C-N-CA	-8.39	111.54	122.37
1	A	4	GLY	N-CA-C	8.24	129.16	112.34
1	A	173	ILE	N-CA-C	8.12	120.82	109.29
1	A	364	ASN	CA-C-N	8.09	129.95	119.84
1	A	364	ASN	C-N-CA	8.09	129.95	119.84
1	B	220	LYS	CB-CA-C	8.05	126.45	110.42
1	A	118	GLU	N-CA-CB	8.04	122.99	110.44
1	A	209	ILE	O-C-N	7.89	131.39	123.18
1	B	5	PRO	N-CA-C	7.85	128.65	112.47
1	B	88	LYS	N-CA-CB	7.84	121.79	110.65
1	B	71	LYS	N-CA-C	7.83	120.71	111.71
1	A	116	PRO	O-C-N	-7.79	112.12	122.64
1	B	5	PRO	CA-C-N	7.49	132.41	122.30
1	B	5	PRO	C-N-CA	7.49	132.41	122.30
1	B	88	LYS	CA-C-N	-7.41	108.29	122.06
1	B	88	LYS	C-N-CA	-7.41	108.29	122.06
1	A	92	PHE	CA-C-N	-7.39	112.57	123.00
1	A	92	PHE	C-N-CA	-7.39	112.57	123.00
1	B	211	THR	CB-CA-C	-7.37	98.99	110.78
1	B	87	MET	CA-C-O	-7.35	112.69	120.55
1	A	299	ARG	N-CA-C	-7.18	103.46	111.28
1	A	114	PHE	CA-C-N	7.17	130.40	120.65
1	A	114	PHE	C-N-CA	7.17	130.40	120.65
1	B	12	GLY	N-CA-C	7.17	121.68	110.71
1	A	93	MET	CA-C-N	-7.04	113.89	122.90
1	A	93	MET	C-N-CA	-7.04	113.89	122.90
1	A	8	GLY	CA-C-N	-7.02	114.05	123.10
1	A	8	GLY	C-N-CA	-7.02	114.05	123.10
1	B	343	ILE	O-C-N	7.00	129.08	121.10
1	B	199	ASP	CA-C-O	6.99	127.80	120.54
1	A	250	LYS	N-CA-CB	6.92	122.42	111.91
1	B	125	THR	CA-C-O	-6.91	111.64	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	PRO	O-C-N	6.89	131.95	122.64
1	B	125	THR	CA-C-N	-6.83	109.18	121.14
1	B	125	THR	C-N-CA	-6.83	109.18	121.14
1	A	187	LYS	CA-C-N	-6.75	110.62	123.32
1	A	187	LYS	C-N-CA	-6.75	110.62	123.32
1	A	188	LYS	CA-C-N	-6.72	109.87	121.97
1	A	188	LYS	C-N-CA	-6.72	109.87	121.97
1	A	71	LYS	N-CA-C	6.69	119.41	111.71
1	A	199	ASP	N-CA-C	-6.67	98.76	109.96
1	A	13	THR	N-CA-C	-6.60	103.28	112.45
1	A	21	PHE	CB-CA-C	6.46	120.38	110.62
1	A	69	ASP	CA-C-N	6.40	129.38	120.29
1	A	69	ASP	C-N-CA	6.40	129.38	120.29
1	A	187	LYS	CB-CA-C	6.40	121.11	110.88
1	B	285	ASP	CB-CA-C	-6.36	99.72	109.89
1	B	172	ILE	CA-C-N	-6.20	113.89	122.69
1	B	172	ILE	C-N-CA	-6.20	113.89	122.69
1	B	89	HIS	CA-C-O	-6.17	111.84	119.18
1	B	94	VAL	CB-CA-C	6.14	119.19	110.84
1	B	37	THR	CB-CA-C	-6.12	106.75	114.40
1	B	367	GLU	CB-CA-C	-6.12	99.09	109.38
1	B	343	ILE	CA-C-O	6.12	128.15	119.95
1	B	197	ILE	CA-C-O	6.11	127.93	120.84
1	A	118	GLU	CA-C-O	-6.10	112.13	119.27
1	A	5	PRO	CA-N-CD	-6.06	103.51	112.00
1	B	21	PHE	CA-C-O	6.04	127.58	120.70
1	A	175	GLU	CA-C-O	6.03	124.63	118.73
1	B	199	ASP	CA-C-N	-6.02	114.76	122.77
1	B	199	ASP	C-N-CA	-6.02	114.76	122.77
1	A	58	GLN	CB-CA-C	6.00	121.24	109.72
1	A	250	LYS	CB-CA-C	5.98	119.88	111.86
1	B	169	VAL	N-CA-C	5.98	115.22	106.55
1	A	69	ASP	CB-CA-C	5.95	120.33	111.89
1	A	114	PHE	N-CA-C	5.89	119.12	108.69
1	A	4	GLY	CA-C-O	-5.88	113.12	121.52
1	B	98	ALA	CA-C-O	5.87	128.65	121.84
1	B	146	VAL	CA-C-N	-5.87	112.50	119.84
1	B	146	VAL	C-N-CA	-5.87	112.50	119.84
1	B	94	VAL	CA-C-N	-5.86	114.63	122.77
1	B	94	VAL	C-N-CA	-5.86	114.63	122.77
1	A	117	GLU	CA-C-N	-5.85	111.37	121.66
1	A	117	GLU	C-N-CA	-5.85	111.37	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	CA-C-O	5.82	126.62	120.63
1	B	199	ASP	N-CA-C	5.79	118.10	108.20
1	B	25	LYS	CB-CA-C	-5.78	99.63	109.51
1	B	345	LYS	CB-CA-C	5.76	121.02	111.23
1	B	346	ILE	O-C-N	-5.70	114.26	122.12
1	B	325	LYS	CB-CA-C	5.69	120.85	112.09
1	A	62	ASN	O-C-N	-5.67	114.79	121.32
1	A	249	HIS	CA-C-N	5.64	130.18	122.34
1	A	249	HIS	C-N-CA	5.64	130.18	122.34
1	A	281	SER	CB-CA-C	5.59	118.79	110.62
1	A	198	PHE	CA-CB-CG	5.58	119.38	113.80
1	B	4	GLY	N-CA-C	5.52	123.59	112.34
1	B	88	LYS	CB-CA-C	-5.46	102.81	111.17
1	A	38	THR	C-N-CD	5.38	147.08	125.00
1	A	28	ILE	CB-CA-C	5.38	118.84	111.31
1	A	108	LYS	CB-CA-C	5.35	121.07	110.42
1	B	251	LYS	O-C-N	-5.34	116.92	122.96
1	A	213	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	275	SER	CA-C-N	-5.31	113.77	122.79
1	A	275	SER	C-N-CA	-5.31	113.77	122.79
1	B	220	LYS	CA-C-O	-5.30	112.93	120.51
1	B	95	VAL	CA-C-N	-5.30	115.25	122.93
1	B	95	VAL	C-N-CA	-5.30	115.25	122.93
1	A	219	VAL	N-CA-CB	5.29	117.69	111.66
1	B	233	PHE	N-CA-C	-5.29	104.95	111.40
1	A	204	THR	N-CA-C	5.28	117.69	108.76
1	A	71	LYS	N-CA-CB	5.26	118.32	110.22
1	B	22	GLN	CA-C-N	5.22	131.50	121.54
1	B	22	GLN	C-N-CA	5.22	131.50	121.54
1	B	147	PRO	CA-C-N	5.21	127.69	120.29
1	B	147	PRO	C-N-CA	5.21	127.69	120.29
1	A	186	ASP	N-CA-C	-5.21	107.06	113.41
1	A	141	ASN	CA-C-N	-5.20	114.04	122.36
1	A	141	ASN	C-N-CA	-5.20	114.04	122.36
1	B	334	ILE	CB-CA-C	5.17	118.52	110.96
1	A	115	TYR	O-C-N	5.15	125.88	121.30
1	A	76	ARG	CB-CA-C	-5.13	100.73	109.51
1	B	144	VAL	CA-C-N	-5.11	114.78	122.81
1	B	144	VAL	C-N-CA	-5.11	114.78	122.81
1	A	287	LEU	O-C-N	-5.09	115.82	122.59
1	A	25	LYS	CA-C-N	-5.09	114.78	122.01
1	A	25	LYS	C-N-CA	-5.09	114.78	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	VAL	CA-C-N	-5.07	112.76	121.17
1	A	18	VAL	C-N-CA	-5.07	112.76	121.17
1	A	24	GLY	CA-C-N	-5.06	115.35	122.94
1	A	24	GLY	C-N-CA	-5.06	115.35	122.94
1	A	117	GLU	CA-C-O	-5.04	114.56	120.20
1	A	382	GLY	N-CA-C	5.02	127.87	113.30
1	A	223	ALA	N-CA-C	5.01	115.80	107.73

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 [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	2952	0	2958	258	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2952	0	2958	266	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	519	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 44.

All (519) 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:HG22	1:B:211:THR:O	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:84:GLN:HA	1:A:84:GLN:NE2	1.73	1.03
1:A:188:LYS:HE3	1:A:190:ARG:H	1.18	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:O	1:B:211:THR:CG2	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:382:GLY:C	1:A:383:ASP:N	2.24	0.96
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:MET:HE1	1:A:93:MET:HE2	1.72	0.72
1:A:141:ASN:HB3	1:A:170:LEU:HD11	1.72	0.72
1:A:87:MET:HE1	1:A:93:MET:CE	2.19	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:A:116:PRO:O	1:A:117:GLU:C	2.32	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:74:ILE:HD11	1:A:117:GLU:OE1	1.93	0.69
1:A:179:ALA:HB2	1:A:337:VAL:HG21	1.75	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:29:ILE:HG13	1:A:134:TYR:CD2	2.28	0.68
1:A:46:ASP:O	1:A:108:LYS:HA	1.92	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:6:ALA:HA	1:B:141:ASN:O	1.95	0.67
1:B:199:ASP:HB3	1:B:337:VAL:HB	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:OD2	1:A:337:VAL:HG12	1.95	0.67
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:B:308:ASP:CG	1:B:309:LEU:HD12	2.20	0.67
1:B:334:ILE:C	1:B:334:ILE:HD13	2.20	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: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:NZ	1:B:88:LYS:CB	2.60	0.65
1:B:88:LYS:HB2	1:B:88:LYS:HZ1	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:21:PHE:CB	1:A:26:VAL:HG22	2.29	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:HB3	1:A:26:VAL:HG22	1.81	0.63
1:A:200:LEU:HG	1:A:340:SER:CB	2.29	0.63
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:A:196:LEU:CD1	1:A:354:PHE:CZ	2.82	0.62
1:B:171:ARG:C	1:B:172:ILE:HD12	2.24	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:8:GLY:HA3	1:A:373:ALA:C	2.24	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:B:228:LEU:HD23	1:B:228:LEU:C	2.27	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:21:PHE:HE1	1:B:24:GLY:O	1.85	0.59
1:B:119:VAL:O	1:B:122:MET:HB2	2.02	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:32:ASP:HB3	4:B:2005:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG23	1:B:210:LEU:HB2	1.85	0.59
1:B:286:SER:OG	1:B:290:GLY:HA2	2.02	0.59
1:A:144:VAL:O	1:A:172:ILE:HD12	2.02	0.58
1:A:228:LEU:C	1:A:228:LEU:HD23	2.28	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:B:199:ASP:HB3	1:B:337:VAL:C	2.30	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: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:96:ASN:OD1	1:A:99:GLY:N	2.37	0.57
1:A:146:VAL:HB	1:A:150:PHE:CD2	2.39	0.57
1:A:253:ILE:HD13	1:A:288:TYR:CG	2.39	0.57
1:A:10:ASP:CG	1:A:369:VAL:HG13	2.29	0.57
1:B:148:ALA:C	1:B:150:PHE:H	2.13	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:209:ILE:HD13	1:B:209:ILE:C	2.30	0.56
1:B:357:LYS:HG2	1:B:358:GLU:N	2.20	0.56
1:A:22:GLN:O	1:A:23:HIS:C	2.47	0.56
1:B:56:LYS:HG3	4:B:2001:HOH:O	2.04	0.56
1:B:210:LEU:HD23	1:B:217:PHE:CD2	2.41	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:97:ASP:HB2	1:B:102:LYS:HE2	1.87	0.56
1:B:176:PRO:O	1:B:179:ALA:HB3	2.05	0.56
1:A:325:LYS:O	1:A:326:LEU:HD23	2.05	0.56
1:A:260:VAL:HG12	1:A:261:ARG:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:PHE:HD2	1:B:353:PHE:C	2.14	0.55
1:B:353:PHE:CD2	1:B:353:PHE:C	2.84	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:HD12	1:B:172:ILE:N	2.21	0.55
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:B:372:GLY:O	1:B:373:ALA:C	2.49	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: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:B:238:VAL:C	1:B:240:HIS:N	2.66	0.53
1:A:374:ALA:O	1:A:377:ALA:HB3	2.09	0.53
1:A:117:GLU:CD	1:A:117:GLU:H	2.16	0.53
1:B:16:SER:CB	1:B:127:MET:HE2	2.39	0.53
1:A:195:VAL:HG22	1:A:333:ASP:HB2	1.89	0.53
1:B:58:GLN:C	1:B:60:ALA:N	2.67	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:HE21	1:A:84:GLN:CA	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: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:58:GLN:C	1:B:60:ALA:H	2.17	0.52
1:A:175:GLU:O	1:A:176:PRO:C	2.49	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:45:THR:HG23	1:B:46:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:CG2	1:B:377:ALA:HB2	2.41	0.51
1:B:239:ASN:HA	1:B:242:ILE:HD11	1.93	0.51
1:B:16:SER:HB3	1:B:127:MET:HE2	1.91	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:94:VAL:HG13	1:B:102:LYS:O	2.10	0.51
1:B:190:ARG:HB2	1:B:193:ARG:HH21	1.75	0.51
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:62:ASN:O	1:B:66:THR:HG22	2.10	0.50
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:A:219:VAL:CG1	4:A:2027:HOH:O	2.59	0.50
1:B:41:TYR:CE1	1:B:56:LYS:HB2	2.46	0.50
1:B:238:VAL:HG13	1:B:263:LEU:HD23	1.93	0.50
1:B:241:PHE:CZ	1:B:282:ILE:HD12	2.45	0.50
1:A:258:ARG:HG2	1:A:258:ARG:HH11	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:364:ASN:C	1:B:366:ASP:H	2.20	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:199:ASP:HA	1:A:337:VAL:C	2.33	0.49
1:A:200:LEU:HG	1:A:340:SER:HB3	1.93	0.49
1:A:75:GLY:HA3	1:A:154:GLN:HG2	1.94	0.49
1:A:80:ASP:O	1:A:83:VAL:HG13	2.12	0.49
1:A:318:GLU:HG2	1:A:353:PHE:CZ	2.47	0.49
1:A:143:VAL:CG2	1:A:377:ALA:HB2	2.42	0.49
1:A:304:GLU:HA	1:A:307:ALA:HB2	1.95	0.49
1:A:36:ARG:HD3	1:A:367:GLU:OE2	2.13	0.49
1:A:348:LYS:NZ	1:A:352:ASP:OD2	2.46	0.49
1:A:285:ASP:O	1:A:286:SER:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HA	1:B:3:LYS:HD2	1.70	0.49
1:B:284:ILE:HD11	1:B:293:PHE:HD2	1.78	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
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:A:97:ASP:O	1:A:98:ALA:C	2.57	0.48
1:B:207:VAL:HB	1:B:223:ALA:O	2.14	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: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:235:ASN:CG	1:B:264:ARG:HH22	2.21	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:76:ARG:HG2	1:B:80:ASP:OD2	2.14	0.47
1:B:103:VAL:HG22	1:B:114:PHE:O	2.15	0.47
1:A:107:TYR:CE1	1:A:108:LYS:HD3	2.49	0.47
1:A:228:LEU:HD23	1:A:228:LEU:O	2.15	0.47
1:A:336:LEU:HB3	1:A:341:THR:HG21	1.96	0.47
1:A:376:GLN:O	1:A:376:GLN:HG3	2.15	0.47
1:B:97:ASP:HB2	1:B:102:LYS:CE	2.44	0.47
1:B:185:LEU:HD11	1:B:333:ASP:CG	2.40	0.47
1:A:50:LEU:O	1:A:55:ALA:HB2	2.15	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:B:14:THR:OG1	2:B:1383:ADP:O3B	2.32	0.47
1:B:6:ALA:HA	1:B:141:ASN:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:367:GLU:O	1:A:368:ALA:C	2.58	0.46
1:B:238:VAL:C	1:B:240:HIS:H	2.22	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:16:SER:C	1:B:127:MET:HE1	2.41	0.46
1:B:261:ARG:HA	1:B:261:ARG:HD2	1.62	0.46
1:A:242:ILE:HD13	1:A:253:ILE:HG23	1.96	0.46
1:B:39:PRO:HB2	1:B:41:TYR:HD1	1.81	0.46
1:B:159:LYS:CG	1:B:169:VAL:HG21	2.45	0.46
1:A:31:ASN:OD1	1:A:32:ASP:N	2.49	0.46
1:A:234:ASP:O	1:A:238:VAL:HG23	2.16	0.46
1:B:334:ILE:C	1:B:334:ILE:CD1	2.88	0.46
1:A:19:GLY:O	1:A:374:ALA:HB2	2.15	0.46
1:B:148:ALA:C	1:B:150:PHE:N	2.74	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:209:ILE:CD1	1:A:331:ILE:HG12	2.46	0.45
1:A:311:ARG:HG3	1:A:311:ARG:HH11	1.80	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
1:B:190:ARG:CB	1:B:193:ARG:HH21	2.30	0.45
2:B:1383:ADP:O2B	3:B:1384:PO4:O3	2.34	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:A:375:VAL:C	1:A:377:ALA:N	2.75	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:10:ASP:OD1	1:B:10:ASP:C	2.60	0.45
1:B:150:PHE:HA	1:B:154:GLN:NE2	2.31	0.45
1:B:341:THR:C	1:B:343:ILE:H	2.24	0.45
1:A:74:ILE:HD11	1:A:117:GLU:CD	2.41	0.45
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.69	0.45
1:B:12:GLY:C	1:B:14:THR:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLY:O	1:B:365:PRO:HB2	2.16	0.45
1:B:71:LYS:HE2	1:B:150:PHE:HZ	1.82	0.45
1:B:273:THR:O	1:B:273:THR:HG22	2.14	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:36:ARG:HD3	1:A:367:GLU:CD	2.43	0.44
1:A:70:ALA:HB2	1:A:119:VAL:CG1	2.47	0.44
1:A:261:ARG:O	1:A:265:THR:HG22	2.16	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
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:102:LYS:HE2	1:A:113:SER:C	2.42	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:150:PHE:HA	1:B:154:GLN:CD	2.43	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:A:306:ASN:O	1:A:307:ALA:C	2.60	0.43
1:A:353:PHE:C	1:A:353:PHE:CD2	2.95	0.43
1:B:50:LEU:O	1:B:55:ALA:HB2	2.18	0.43
1:B:300:ALA:O	1:B:301:ARG:C	2.60	0.43
1:A:178:ALA:HA	1:A:181:ILE:HD12	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:CYS:SG	1:B:28:ILE:CG2	3.05	0.43
1:B:117:GLU:O	1:B:121:SER:HB3	2.18	0.43
1:B:334:ILE:CD1	1:B:350:LEU:HD21	2.45	0.43
1:B:31:ASN:HB2	1:B:130:ILE:HD13	2.00	0.43
1:B:103:VAL:CG2	1:B:114:PHE:HB2	2.49	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:17:CYS:HA	1:B:127:MET:HE1	2.00	0.42
1:B:39:PRO:HB2	1:B:41:TYR:CD1	2.54	0.42
1:B:228:LEU:C	1:B:228:LEU:CD2	2.92	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:A:64:THR:HG22	1:A:65:ASN:ND2	2.34	0.42
1:A:126:LYS:O	1:A:127:MET:C	2.62	0.42
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:77:ARG:NH2	1:B:79:ASP:OD1	2.53	0.42
1:B:58:GLN:O	1:B:60:ALA:N	2.51	0.42
1:B:345:LYS:HG2	1:B:348:LYS:HB2	2.01	0.42
1:B:28:ILE:HD12	1:B:28:ILE:N	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:179:ALA:HB1	1:A:337:VAL:HG21	1.98	0.42
1:A:200:LEU:CD2	1:A:346:ILE:HD12	2.50	0.42
1:A:340:SER:C	1:A:342:ARG:H	2.26	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:348:LYS:O	1:A:349:LEU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:THR:C	1:B:343:ILE:N	2.78	0.41
1:B:370:ALA:O	1:B:373:ALA:HB3	2.20	0.41
1:B:313:THR:O	1:B:314:LEU:C	2.63	0.41
1:B:364:ASN:C	1:B:366:ASP:N	2.78	0.41
1:A:177:THR:O	1:A:178:ALA:C	2.63	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:367:GLU:O	1:B:368:ALA:C	2.62	0.41
1:B:213:GLU:C	1:B:215:GLY:H	2.28	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:41:TYR:CD1	1:B:56:LYS:CB	3.00	0.41
1:B:199:ASP:HB3	1:B:337:VAL:O	2.21	0.41
1:B:200:LEU:O	1:B:338:GLY:CA	2.69	0.41
1:B:297:ILE:HG13	1:B:301:ARG:HG2	2.03	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:338:GLY:C	1:A:365:PRO:O	2.64	0.41
1:A:343:ILE:HG22	1:A:345:LYS:H	1.86	0.41
1:A:375:VAL:C	1:A:377:ALA:H	2.29	0.41
1:A:382:GLY:CA	1:A:383:ASP:N	2.84	0.41
1:B:199:ASP:CB	1:B:337:VAL:O	2.69	0.41
1:B:210:LEU:HD23	1:B:217:PHE:CE2	2.56	0.41
1:B:325:LYS:O	1:B:326:LEU:HD23	2.21	0.41
1:B:344:PRO:O	1:B:347:GLN:HB2	2.20	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:71:LYS:HE2	1:B:150:PHE:CZ	2.57	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:75:GLY:HA3	1:B:154:GLN:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD12	1:B:200:LEU:HA	1.96	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%)	3	26
1	B	380/543 (70%)	326 (86%)	46 (12%)	8 (2%)	5	31
All	All	759/1086 (70%)	655 (86%)	85 (11%)	19 (2%)	4	28

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

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Mol	Chain	Res	Type
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 [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	315/459 (69%)	257 (82%)	58 (18%)	1	9
1	B	315/459 (69%)	253 (80%)	62 (20%)	1	8
All	All	630/918 (69%)	510 (81%)	120 (19%)	1	8

All (120) 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	47	THR
1	A	49	ARG
1	A	50	LEU
1	A	53	ASP
1	A	56	LYS
1	A	64	THR
1	A	71	LYS
1	A	72	ARG
1	A	74	ILE

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Mol	Chain	Res	Type
1	A	83	VAL
1	A	84	GLN
1	A	87	MET
1	A	93	MET
1	A	100	ARG
1	A	108	LYS
1	A	111	THR
1	A	113	SER
1	A	116	PRO
1	A	117	GLU
1	A	120	SER
1	A	125	THR
1	A	137	LYS
1	A	138	THR
1	A	143	VAL
1	A	172	ILE
1	A	187	LYS
1	A	188	LYS
1	A	192	GLU
1	A	199	ASP
1	A	200	LEU
1	A	213	GLU
1	A	228	LEU
1	A	242	ILE
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
1	A	284	ILE
1	A	297	ILE
1	A	298	THR
1	A	315	ASP
1	A	335	VAL
1	A	336	LEU
1	A	341	THR
1	A	361	LYS
1	A	363	ILE

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Mol	Chain	Res	Type
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	20	VAL
1	B	23	HIS
1	B	49	ARG
1	B	56	LYS
1	B	74	ILE
1	B	79	ASP
1	B	87	MET
1	B	88	LYS
1	B	93	MET
1	B	95	VAL
1	B	112	LYS
1	B	113	SER
1	B	120	SER
1	B	121	SER
1	B	137	LYS
1	B	138	THR
1	B	141	ASN
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	208	SER
1	B	209	ILE
1	B	211	THR
1	B	212	THR
1	B	213	GLU
1	B	214	ASP
1	B	216	ILE
1	B	248	LYS
1	B	250	LYS
1	B	251	LYS
1	B	257	LYS

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Mol	Chain	Res	Type
1	B	261	ARG
1	B	262	ARG
1	B	265	THR
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	297	ILE
1	B	315	ASP
1	B	325	LYS
1	B	326	LEU
1	B	331	ILE
1	B	334	ILE
1	B	337	VAL
1	B	340	SER
1	B	353	PHE
1	B	360	ASN
1	B	366	ASP
1	B	367	GLU
1	B	375	VAL
1	B	376	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	35	ASN
1	A	84	GLN
1	A	141	ASN
1	A	239	ASN
1	A	249	HIS
1	A	306	ASN
1	A	360	ASN
1	A	376	GLN
1	B	22	GLN
1	B	33	GLN
1	B	84	GLN
1	B	141	ASN
1	B	194	ASN
1	B	249	HIS

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Mol	Chain	Res	Type
1	B	279	GLN
1	B	360	ASN
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 oligosaccharides 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	$\# Z > 2$
3	PO4	A	1384	-	4,4,4	1.49	1 (25%)	6,6,6	1.65	1 (16%)
2	ADP	B	1383	-	28,29,29	1.19	1 (3%)	43,45,45	2.07	11 (25%)
3	PO4	B	1384	-	4,4,4	1.37	1 (25%)	6,6,6	1.52	2 (33%)
2	ADP	A	1383	-	28,29,29	1.27	3 (10%)	43,45,45	2.01	13 (30%)

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	B	1383	-	-	1/16/32/32	0/3/3/3
2	ADP	A	1383	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1383	ADP	C5-C4	4.18	1.46	1.39
2	A	1383	ADP	C5-C4	4.02	1.46	1.39
3	A	1384	PO4	P-O3	-2.73	1.46	1.54
3	B	1384	PO4	P-O3	-2.59	1.47	1.54
2	A	1383	ADP	C5-C6	2.28	1.47	1.41
2	A	1383	ADP	C5-N7	-2.18	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1383	ADP	C5-C4-N3	-5.59	119.02	126.72
2	B	1383	ADP	C5-C4-N3	-5.49	119.16	126.72
2	B	1383	ADP	N3-C4-N9	4.38	134.62	127.17
2	B	1383	ADP	N3-C2-N1	-4.22	122.19	128.58
2	A	1383	ADP	N3-C4-N9	4.06	134.07	127.17
2	B	1383	ADP	C2-N3-C4	3.90	121.37	111.83
2	A	1383	ADP	C2-N3-C4	3.85	121.24	111.83
2	A	1383	ADP	N3-C2-N1	-3.76	122.89	128.58
2	B	1383	ADP	C2'-C1'-N9	-3.74	104.02	113.30
2	A	1383	ADP	C4-C5-N7	-3.57	106.50	110.58
2	B	1383	ADP	O4'-C1'-N9	3.48	114.78	108.09
2	A	1383	ADP	O4'-C1'-N9	3.41	114.64	108.09
3	A	1384	PO4	O4-P-O1	-2.81	101.02	110.95
2	A	1383	ADP	C2'-C3'-C4'	2.68	107.79	102.61
2	A	1383	ADP	C5-N7-C8	2.65	107.61	103.45
2	B	1383	ADP	C4-C5-N7	-2.58	107.63	110.58
2	B	1383	ADP	O2B-PB-O3A	-2.52	96.19	104.64
2	A	1383	ADP	O3B-PB-O2B	2.50	117.19	107.80
3	B	1384	PO4	O4-P-O1	-2.37	102.56	110.95
2	A	1383	ADP	C5'-C4'-C3'	-2.32	106.87	115.21
2	A	1383	ADP	C6-C5-N7	2.25	136.43	132.09
2	A	1383	ADP	O2B-PB-O3A	-2.23	97.16	104.64
2	A	1383	ADP	C2'-C1'-N9	-2.20	107.85	113.30
2	B	1383	ADP	C5-N7-C8	2.19	106.89	103.45
2	B	1383	ADP	O2A-PA-O1A	2.12	122.31	112.44
2	B	1383	ADP	O3B-PB-O2B	2.05	115.50	107.80
3	B	1384	PO4	O3-P-O2	2.04	114.26	107.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

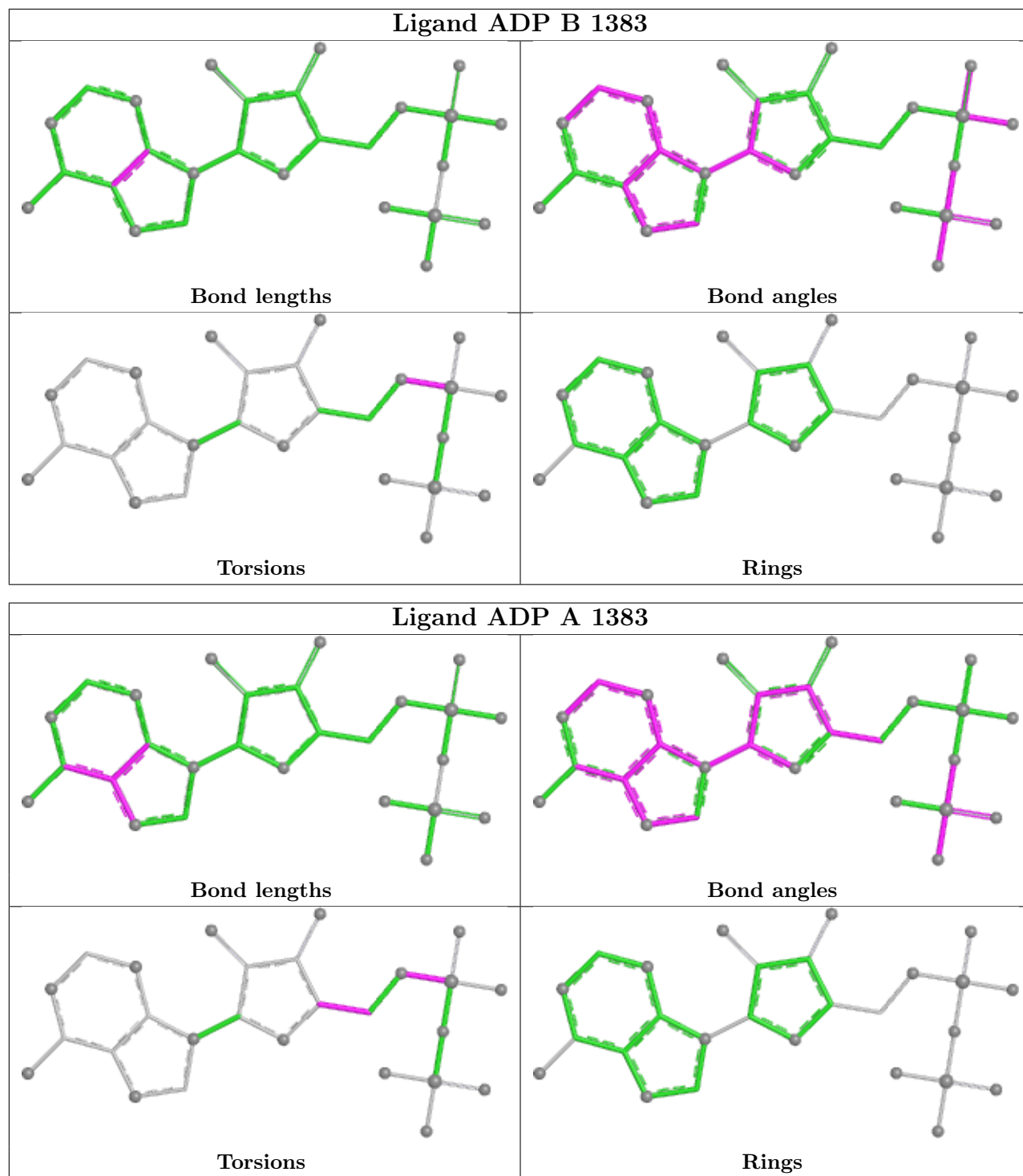
Mol	Chain	Res	Type	Atoms
2	B	1383	ADP	C5'-O5'-PA-O1A
2	A	1383	ADP	C3'-C4'-C5'-O5'
2	A	1383	ADP	C5'-O5'-PA-O1A
2	A	1383	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1383	ADP	2	0
3	B	1384	PO4	1	0
2	A	1383	ADP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.34	9 (2%) 59 35	20, 67, 119, 163	0
1	B	382/543 (70%)	0.35	9 (2%) 59 35	14, 68, 112, 147	0
All	All	764/1086 (70%)	0.34	18 (2%) 59 35	14, 68, 116, 163	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	3.7
1	A	258	ARG	3.5
1	A	382	GLY	3.1
1	B	130	ILE	3.0
1	A	383	ASP	3.0
1	B	218	GLU	2.9
1	A	215	GLY	2.8
1	A	69	ASP	2.8
1	B	367	GLU	2.8
1	B	93	MET	2.6
1	A	66	THR	2.5
1	B	67	VAL	2.5
1	B	102	LYS	2.5
1	A	175	GLU	2.4
1	B	189	VAL	2.3
1	A	201	GLY	2.3
1	B	45	THR	2.2
1	A	93	MET	2.1

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](#)

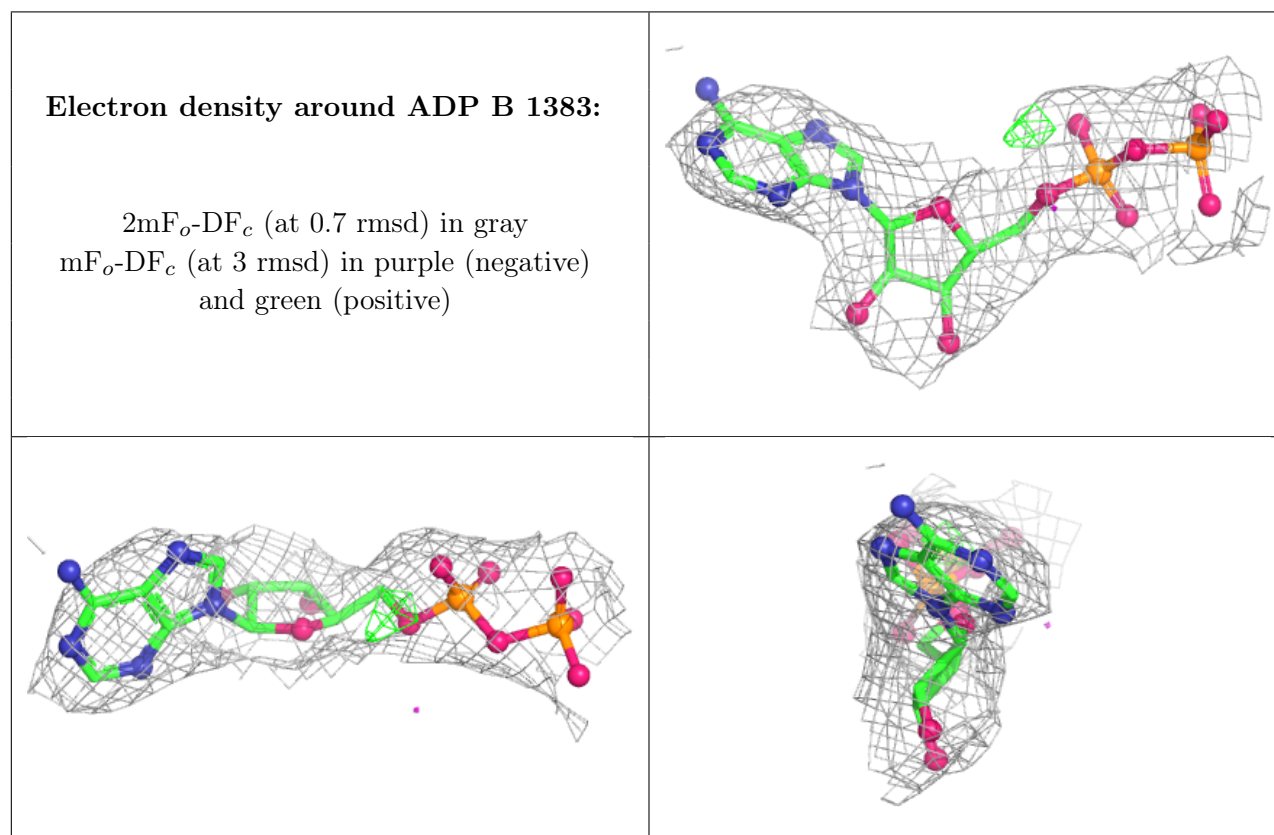
There are no oligosaccharides in this entry.

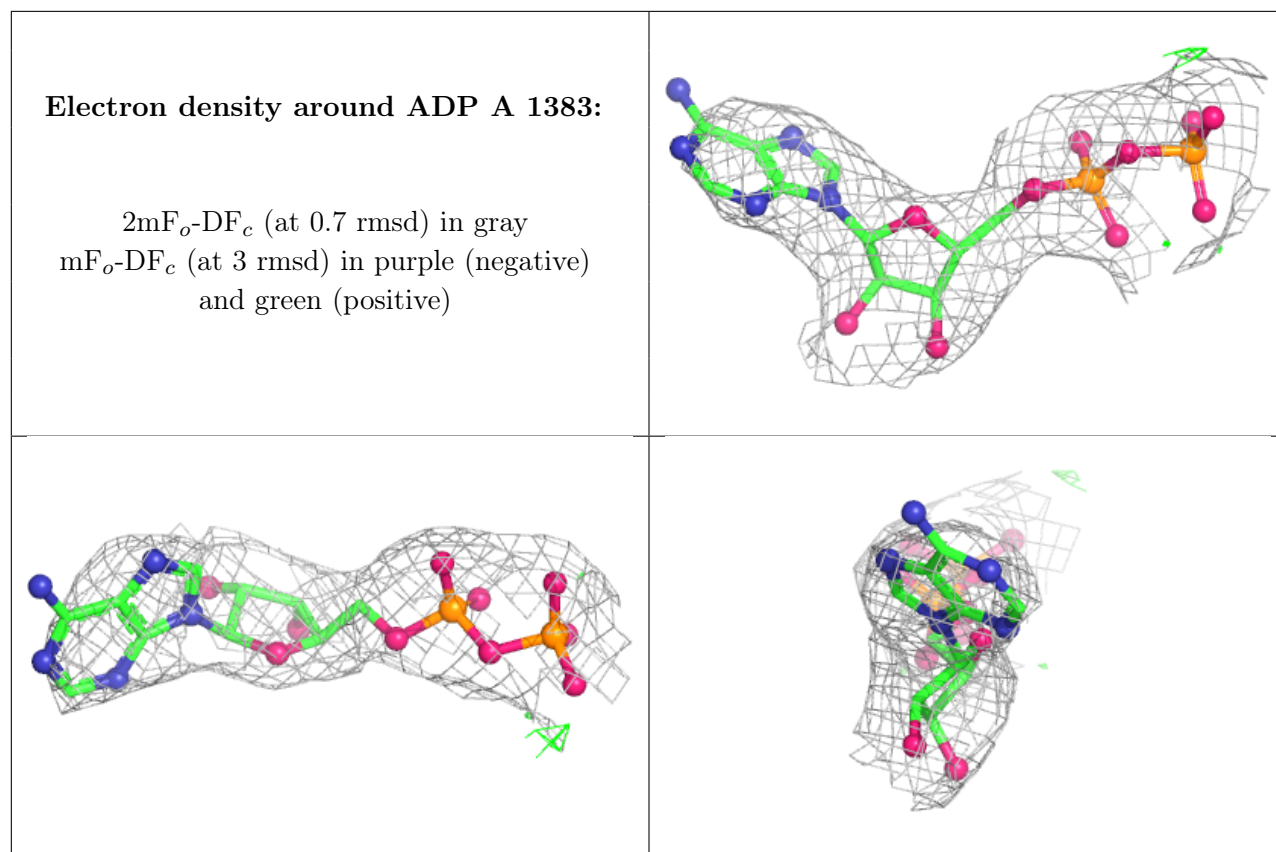
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	PO4	A	1384	5/5	0.86	0.15	74,101,101,101	0
3	PO4	B	1384	5/5	0.90	0.12	37,37,37,165	0
2	ADP	B	1383	27/27	0.93	0.12	61,61,61,61	0
2	ADP	A	1383	27/27	0.94	0.13	77,77,77,77	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.