



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

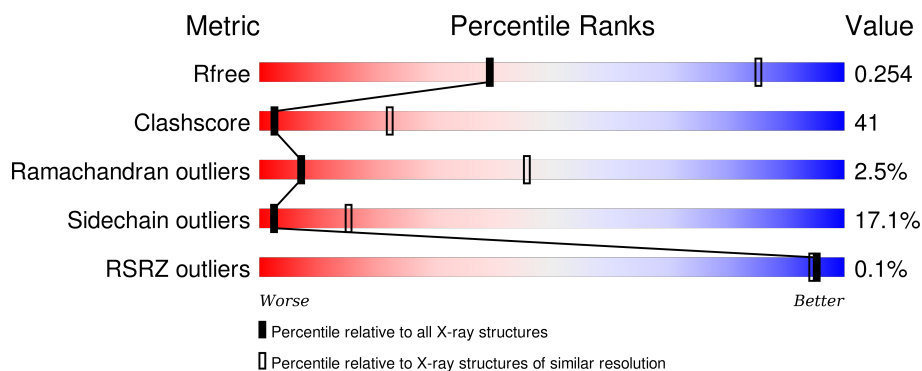
1 Overall quality at a glance

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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. 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	 28% 31% 10% • 30%
1	B	543	 25% 34% 10% • 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 (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		

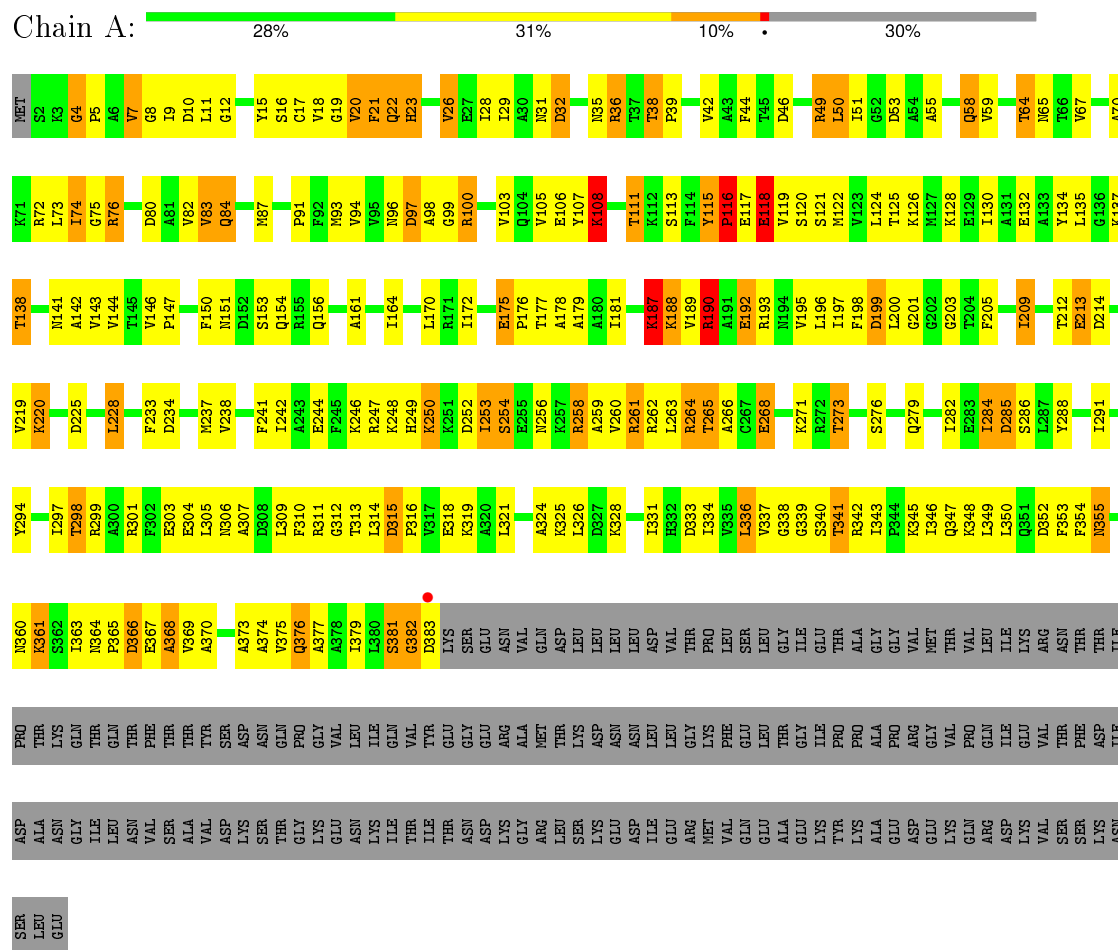
- Molecule 4 is water.

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

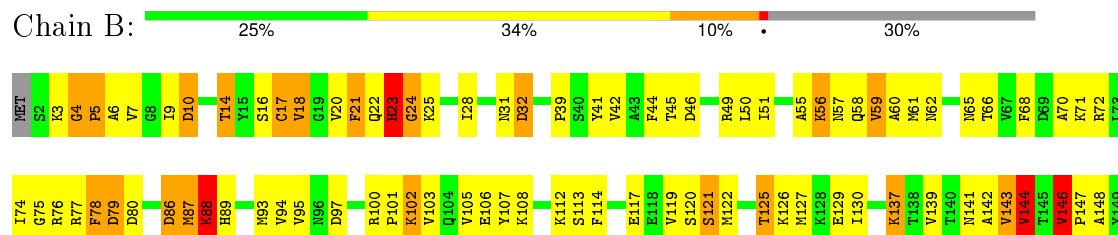
3 Residue-property plots

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

• Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



• Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



LYS	ASN	SER	LEU	GLU	THR	ILE	ASP	THR	K357	T295	K220	F150
ASN	SER	LEU	GLU	GLY	THR	ILE	ILE	THR	E358	S296	S221	N151
SER	LEU	ALA	ALA	ASN	THR	THR	PRO	THR	N360	T297	T222	D152
GLU	GLY	GLN	LYS	GLN	LYS	LYS	LYS	LYS	K361	R299	A223	Q154
	ILE	THR	THR	THR	THR	THR	THR	THR	S362	A300		R155
	LEU	GLN	THR	GLN	THR	GLN	THR	THR	I363	R301	L228	K159
	ASN	THR	THR	THR	THR	THR	THR	THR	N364	F302	G229	D160
	VAL	THR	THR	THR	THR	THR	THR	THR	P365	E303		A161
	SER	THR	THR	THR	THR	THR	THR	THR	D366	E304	F233	G162
	VAL	THR	THR	THR	THR	THR	THR	THR	E367	L305	D234	I163
	VAL	THR	THR	THR	THR	THR	THR	THR	A368	N306	N235	T163
	ASP	THR	THR	THR	THR	THR	THR	THR	V369	A307	R236	I164
	LYS	ASP	THR	THR	THR	THR	THR	THR	A370	D308	M237	A165
	SER	ASN	THR	THR	THR	THR	THR	THR	Y371	L309	V238	
	SER	ASN	THR	THR	THR	THR	THR	THR	G372	F310	N239	V169
	THR	GLN	THR	THR	THR	THR	THR	THR	A373	G311	H240	R170
	GLY	PRO	GLY	PRO	GLY	GLY	GLY	GLY		T312	F241	R171
	LYS	LYS	GLU	LYS	VAL	VAL	VAL	VAL	Q376	T313	I242	I172
	ASN	ASN	LEU	LEU	LEU	LEU	LEU	LEU	A377	L314	A243	I173
	ILE	ILE	LYS	ILE	ILE	ILE	ILE	ILE	A378	D315		R174
	THR	THR	THR	THR	THR	THR	THR	THR	S381	P316	K246	E175
	THR	THR	THR	THR	THR	THR	THR	THR	E318	V317	R247	P176
	THR	THR	THR	THR	THR	THR	THR	THR	G382	E318	K248	T177
	THR	THR	THR	THR	THR	THR	THR	THR	D383	K319	H249	A178
	ASN	ASN	ASP	GLY	GLY	GLY	GLY	GLY	LYS	A320	K250	A179
	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	SER	L321	R251	A180
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLU	R322	D252	I181
	ARG	ARG	GLY	GLY	GLY	GLY	GLY	GLY	ASN	D323	I253	
	LEU	LEU	ARG	MET	GLN	THR	THR	THR	VAL	A324	K257	L185
	SER	SER	LEU	THR	THR	THR	THR	THR	ASP	K325		
	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LEU	L326	R261	K188
	GLU	GLU	GLU	ASN	ASN	ASN	ASN	ASN	LEU	D327	R262	V189
	ASP	ASP	ASP	ASN	ASN	ASN	ASN	ASN	LEU	K328	L263	R190
	ILE	ILE	ILE	LEU	LEU	LEU	LEU	LEU	LEU	I331	R264	A191
	GLU	GLU	GLU	LEU	LEU	LEU	LEU	LEU	ASP	H332		E192
	ARG	ARG	ARG	GLY	GLY	GLY	GLY	GLY	VAL	D333	R193	R194
	MET	MET	VAL	THR	THR	THR	THR	THR	THR	I334	V195	
	VAL	VAL	VAL	PHE	LYS	LYS	LYS	LYS	PRO	V335	L196	
	GLN	GLN	GLN	GLU	GLU	GLU	GLU	GLU	LEU	L336	T273	F198
	ALA	ALA	ALA	THR	THR	THR	THR	THR	LEU	V337	L274	D199
	LYS	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	G338		L200
	TYR	TYR	TYR	ILE	ILE	ILE	ILE	ILE	ILE	S340	S277	G201
	LYS	LYS	LYS	PRO	PRO	PRO	PRO	PRO	THR		I278	G202
	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	A280	A280	
	GLU	GLU	GLU	PRO	PRO	PRO	PRO	PRO	GLY	S281		F205
	ASP	ASP	ASP	ARG	ARG	ARG	ARG	ARG	GLY	D282	D206	
	GLU	GLU	GLU	GLY	GLY	GLY	GLY	GLY	VAL	E283	V207	
	LYS	LYS	LYS	VAL	VAL	VAL	VAL	VAL	MET	I284	S208	
	GLN	GLN	GLN	PRO	PRO	PRO	PRO	PRO	THR	D285	I209	
	ARG	ARG	ARG	ILE	ILE	ILE	ILE	ILE	VAL	S286	L210	
	ASP	ASP	ASP	ILE	ILE	ILE	ILE	ILE	LEU	L287	T211	
	LYS	LYS	LYS	GLU	GLU	GLU	GLU	GLU	ILE	Y288	T212	
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	D352	P289	E213	
	SER	SER	SER	THR	THR	THR	THR	THR	LYS	F353	D214	
									ARG	F354	G215	
									ASN	N355	I216	
									THR		F217	
											Y294	

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 0.234 , 0.254	Depositor DCC
R_{free} test set	800 reflections (5.56%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16673 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:84:GLN:NE2	1:A:84:GLN:HA	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: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

Continued on next page...

Continued from previous page...

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:283:GLU:HG2	1:B:294:TYR:HD1	1.41	0.82
1:B:65:ASN:HD21	1:B:106:GLU:HB2	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

Continued on next page...

Continued from previous page...

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:B:51:ILE:HD12	1:B:122:MET:O	1.91	0.70
1:A:31:ASN:HB3	1:A:35:ASN:H	1.56	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:B:6:ALA:HA	1:B:141:ASN:O	1.95	0.67
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:334:ILE:HD12	1:B:359:LEU:HD23	1.75	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:A:199:ASP:OD2	1:A:337:VAL:HG12	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:HD12	1:B:359:LEU:CD2	2.24	0.67
1:A:262:ARG:CZ	1:A:284:ILE:HG22	2.24	0.67
1:B:345:LYS:HG2	1:B:348:LYS:HB3	1.77	0.67
1:B:328:LYS:HG2	1:B:353:PHE:HE2	1.60	0.67
1:A:253:ILE:CD1	1:A:256:ASN:HB3	2.23	0.67
1:A:64:THR:HA	1:A:91:PRO:O	1.94	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:12:GLY:HA3	1:A:15:TYR:O	1.95	0.67
1:A:116:PRO:O	1:A:117:GLU:C	2.32	0.66
1:A:242:ILE:CD1	1:A:253:ILE:HG23	2.25	0.66
1:A:193:ARG:HB2	1:A:212:THR:HB	1.78	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:B:345:LYS:O	1:B:349:LEU:HG	1.97	0.65
1:A:246:LYS:O	1:A:250:LYS:HA	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:303:GLU:O	1:B:307:ALA:N	2.30	0.64
1:B:273:THR:O	1:B:273:THR:CG2	2.44	0.64
1:A:253:ILE:HD12	1:A:253:ILE:O	1.98	0.64
1:A:200:LEU:O	1:A:340:SER:HB2	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:B:233:PHE:HB3	1:B:306:ASN:OD1	1.98	0.64
1:A:247:ARG:HA	1:A:250:LYS:HG3	1.80	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
1:A:21:PHE:HB3	1:A:26:VAL:HG22	1.81	0.63
1:B:5:PRO:CB	1:B:139:VAL:HG12	2.21	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HG2	1:B:169:VAL:CG2	2.28	0.63
1:A:200:LEU:HG	1:A:340:SER:CB	2.29	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:B:334:ILE:HD13	1:B:334:ILE:C	2.20	0.62
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: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:B:353:PHE:O	1:B:353:PHE:CD2	2.52	0.61
1:B:146:VAL:HG22	1:B:172:ILE:CG2	2.30	0.61
1:A:339:GLY:O	1:A:342:ARG:HG3	2.01	0.61
1:A:7:VAL:HA	1:A:20:VAL:HG23	1.83	0.60
1:B:159:LYS:HG2	1:B:169:VAL:HG21	1.82	0.60
1:A:200:LEU:HG	1:A:340:SER:HB2	1.83	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:253:ILE:HD11	1:A:256:ASN:CB	2.32	0.60
1:A:107:TYR:CZ	1:A:108:LYS:HD2	2.36	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:B:119:VAL:O	1:B:122:MET:HB2	2.02	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: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:B:195:VAL:HG23	1:B:210:LEU:HB2	1.85	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
1:B:286:SER:OG	1:B:290:GLY:HA2	2.02	0.59

Continued on next page...

Continued from previous page...

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:B:42:VAL:HG11	1:B:122:MET:SD	2.43	0.58
1:A:299:ARG:O	1:A:303:GLU:HG3	2.03	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:284:ILE:HD12	1:B:287:LEU:CD1	2.30	0.58
1:B:274:LEU:CD2	1:B:299:ARG:HA	2.33	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:B:284:ILE:HD11	1:B:293:PHE:CD2	2.38	0.58
1:A:347:GLN:OE1	1:A:361:LYS:HD2	2.04	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:151:ASN:OD1	1:B:154:GLN:HG3	2.04	0.57
1:A:9:ILE:HG12	1:A:18:VAL:HG23	1.86	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: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:8:GLY:HA3	1:A:373:ALA:C	2.24	0.56
1:A:310:PHE:HD1	1:A:346:ILE:HD11	1.69	0.56
1:B:97:ASP:HB2	1:B:102:LYS:HE2	1.87	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:A:325:LYS:O	1:A:326:LEU:HD23	2.05	0.56
1:B:228:LEU:C	1:B:228:LEU:HD23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:CD1	1:B:287:LEU:HD22	2.36	0.54
1:A:318:GLU:HG2	1:A:353:PHE:HZ	1.72	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:B:314:LEU:CD2	1:B:353:PHE:HD1	2.14	0.54
1:A:253:ILE:CD1	1:A:256:ASN:CB	2.86	0.54
1:A:17:CYS:SG	1:A:28:ILE:HG21	2.48	0.54
1:A:228:LEU:HD23	1:A:228:LEU:C	2.28	0.54
1:A:49:ARG:HB3	1:A:107:TYR:CE2	2.43	0.54
1:A:262:ARG:NH2	1:A:284:ILE:HG22	2.23	0.53
1:A:125:THR:O	1:A:128:LYS:HB3	2.08	0.53
1:B:284:ILE:HD11	1:B:287:LEU:HD22	1.90	0.53
1:A:370:ALA:O	1:A:373:ALA:HB3	2.08	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:B:315:ASP:HB3	1:B:316:PRO:HD3	1.91	0.52
1:A:44:PHE:CD2	1:A:105:VAL:HG21	2.44	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:B:209:ILE:C	1:B:209:ILE:HD13	2.30	0.52
1:A:31:ASN:HB3	1:A:35:ASN:N	2.24	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:A:22:GLN:O	1:A:23:HIS:C	2.47	0.52
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: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: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

Continued on next page...

Continued from previous page...

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: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:B:188:LYS:NZ	1:B:214:ASP:HA	2.26	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: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:258:ARG:HH11	1:A:258:ARG:HG2	1.76	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:200:LEU:O	1:B:338:GLY:HA3	2.11	0.50
1:B:74:ILE:HD11	1:B:117:GLU:HA	1.94	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:200:LEU:HG	1:A:340:SER:HB3	1.93	0.49
1:A:151:ASN:OD1	1:A:153:SER:HB3	2.12	0.49
1:B:238:VAL:C	1:B:240:HIS:N	2.66	0.49
1:A:80:ASP:O	1:A:83:VAL:HG13	2.12	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: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: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: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:B:192:GLU:CB	1:B:213:GLU:HB2	2.34	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:O	1:A:266:ALA:HB3	2.12	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:156:GLN:NE2	4:A:2019:HOH:O	2.47	0.48
1:B:58:GLN:C	1:B:60:ALA:H	2.17	0.48
1:B:207:VAL:HB	1:B:223:ALA:O	2.14	0.48
1:B:195:VAL:O	1:B:209:ILE:HG12	2.13	0.48
1:B:46:ASP:O	1:B:108:LYS:HG2	2.14	0.48
1:B:58:GLN:C	1:B:60:ALA:N	2.67	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:A:175:GLU:O	1:A:176:PRO:C	2.49	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:B:103:VAL:HG22	1:B:114:PHE:O	2.15	0.47
1:A:142:ALA:O	1:A:170:LEU:HD12	2.14	0.47
1:A:124:LEU:O	1:A:128:LYS:N	2.45	0.47
1:B:76:ARG:HG2	1:B:80:ASP:OD2	2.14	0.47
1:B:97:ASP:HB2	1:B:102:LYS:CE	2.44	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:107:TYR:CE1	1:A:108:LYS:HD3	2.49	0.47
1:A:376:GLN:O	1:A:376:GLN:HG3	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: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:337:VAL:HG11	1:B:369:VAL:HG23	1.98	0.46
1:B:273:THR:HG23	1:B:273:THR:O	2.15	0.46
1:A:314:LEU:HD13	1:A:353:PHE:HD1	1.81	0.46
1:B:58:GLN:OE1	1:B:62:ASN:HB3	2.15	0.46
1:B:56:LYS:HD3	1:B:57:ASN:OD1	2.15	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:CG	1:B:169:VAL:HG21	2.45	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: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: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: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:A:193:ARG:CB	1:A:212:THR:HB	2.45	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:311:ARG:HG3	1:A:311:ARG:HH11	1.80	0.45
1:B:44:PHE:CD2	1:B:105:VAL:HG21	2.51	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:357:LYS:CG	1:B:358:GLU:N	2.80	0.45
1:B:302:PHE:HA	1:B:305:LEU:HD12	1.98	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:B:41:TYR:CE2	1:B:68:PHE:CB	2.99	0.45
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.69	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: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:364:ASN:C	1:B:366:ASP:H	2.20	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:B:242:ILE:HG13	1:B:243:ALA:N	2.31	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:198:PHE:CE1	1:B:205:PHE:CE1	3.05	0.44
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:239:ASN:HA	1:B:242:ILE:HG12	2.00	0.44
1:B:197:ILE:HG23	1:B:337:VAL:CG2	2.48	0.44
1:A:273:THR:HG21	1:B:152:ASP:HB3	1.99	0.44
1:A:188:LYS:HG2	1:A:189:VAL:H	1.79	0.44
1:A:350:LEU:HD11	1:A:354:PHE:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:VAL:O	1:B:242:ILE:HG12	2.17	0.44
1:A:147:PRO:CG	1:A:150:PHE:CE1	2.99	0.44
1:A:261:ARG:HH11	1:A:261:ARG:HB3	1.82	0.44
1:B:303:GLU:O	1:B:307:ALA:HB2	2.18	0.44
1:A:285:ASP:O	1:A:286:SER:C	2.54	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:B:210:LEU:HD23	1:B:217:PHE:HD2	1.81	0.43
1:A:80:ASP:OD1	1:A:82:VAL:HG22	2.18	0.43
1:B:285:ASP:OD2	1:B:294:TYR:OH	2.18	0.43
1:B:252:ASP:OD2	1:B:253:ILE:N	2.51	0.43
1:A:70:ALA:HB2	1:A:119:VAL:HG11	2.00	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:B:195:VAL:HG12	1:B:333:ASP:HB2	2.00	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:334:ILE:CD1	1:B:350:LEU:HD21	2.45	0.43
1:B:17:CYS:SG	1:B:28:ILE:CG2	3.05	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:235:ASN:CG	1:B:264:ARG:HH22	2.21	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:B:31:ASN:HB2	1:B:130:ILE:HD13	2.00	0.43
1:B:143:VAL:HG22	1:B:170:LEU:HB2	2.01	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:278:THR:HA	1:B:299:ARG:HB2	2.00	0.43
1:B:14:THR:HG21	1:B:202:GLY:HA3	2.01	0.43
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.75	0.43
1:A:376:GLN:HA	1:A:379:ILE:HD12	2.00	0.43
1:A:364:ASN:HB2	1:A:367:GLU:HG3	2.01	0.42
1:A:126:LYS:HG3	1:A:130:ILE:CD1	2.48	0.42
1:B:39:PRO:HB2	1:B:41:TYR:CD1	2.54	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

Continued on next page...

Continued from previous page...

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:144:VAL:HG23	1:B:172:ILE:HG13	2.02	0.42
1:B:121:SER:HB2	1:B:161:ALA:O	2.18	0.42
1:B:302:PHE:O	1:B:305:LEU:HB2	2.19	0.42
1:B:334:ILE:C	1:B:334:ILE:CD1	2.88	0.42
1:B:238:VAL:C	1:B:240:HIS:H	2.22	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:41:TYR:CD2	1:B:68:PHE:HB3	2.55	0.42
1:B:28:ILE:HD12	1:B:28:ILE:N	2.34	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:124:LEU:HD12	1:A:161:ALA:HB1	2.01	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:B:328:LYS:H	1:B:328:LYS:HD3	1.85	0.41
1:A:20:VAL:HG11	1:A:135:LEU:HD21	2.03	0.41
1:B:297:ILE:HG13	1:B:301:ARG:HG2	2.03	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:A:382:GLY:CA	1:A:383:ASP:N	2.84	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:199:ASP:CB	1:B:337:VAL:O	2.69	0.41
1:A:261:ARG:HD2	1:A:261:ARG:HA	1.74	0.41
1:B:325:LYS:O	1:B:326:LEU:HD23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLY:O	1:A:315:ASP:HB3	2.20	0.41
1:B:344:PRO:O	1:B:347:GLN:HB2	2.20	0.41
1:A:375:VAL:C	1:A:377:ALA:N	2.75	0.41
1:B:178:ALA:O	1:B:372:GLY:HA3	2.21	0.41
1:A:379:ILE:H	1:A:379:ILE:HG13	1.61	0.41
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:A:233:PHE:HA	1:A:306:ASN:ND2	2.36	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:10:ASP:C	1:B:10:ASP:OD1	2.60	0.40
1:A:74:ILE:HD11	1:A:117:GLU:CD	2.41	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:B:137:LYS:H	1:B:137:LYS:HG2	1.75	0.40
1:A:144:VAL:HB	1:A:172:ILE:HD13	2.02	0.40
1:B:75:GLY:HA3	1:B:154:GLN:HA	2.04	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

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%)	6	42
1	B	380/543 (70%)	326 (86%)	46 (12%)	8 (2%)	9	50
All	All	759/1086 (70%)	655 (86%)	85 (11%)	19 (2%)	7	46

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%)	3	16
1	B	315/459 (69%)	259 (82%)	56 (18%)	2	13
All	All	630/918 (69%)	522 (83%)	108 (17%)	2	15

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	376	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	22,29,29	0.97	1 (4%)	27,45,45	2.50	9 (33%)
3	PO4	A	1384	-	4,4,4	1.12	0	6,6,6	0.35	0
2	ADP	B	1383	-	22,29,29	0.88	1 (4%)	27,45,45	2.79	8 (29%)
3	PO4	B	1384	-	4,4,4	1.03	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1383	-	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1384	-	-	0/0/0/0	0/0/0/0
2	ADP	B	1383	-	-	0/12/32/32	0/3/3/3
3	PO4	B	1384	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1383	ADP	C5-C4	2.55	1.46	1.40
2	B	1383	ADP	C5-C4	2.68	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1383	ADP	N3-C2-N1	-8.76	122.19	128.89
2	A	1383	ADP	N3-C2-N1	-7.84	122.89	128.89
2	B	1383	ADP	C2'-C1'-N9	-6.72	104.02	114.29
2	A	1383	ADP	PA-O3A-PB	-5.50	114.23	132.67
2	B	1383	ADP	PA-O3A-PB	-5.36	114.71	132.67
2	A	1383	ADP	C2'-C1'-N9	-4.22	107.85	114.29
2	A	1383	ADP	C4-C5-N7	-3.24	106.50	109.48
2	A	1383	ADP	C5'-C4'-C3'	-2.10	106.87	115.21
2	B	1383	ADP	C4-C5-N7	-2.01	107.63	109.48
2	A	1383	ADP	O3B-PB-O1B	2.00	117.03	110.58
2	B	1383	ADP	O3B-PB-O2B	2.13	115.50	107.38
2	B	1383	ADP	O3B-PB-O1B	2.22	117.73	110.58
2	A	1383	ADP	C2'-C3'-C4'	2.52	107.79	102.61
2	B	1383	ADP	O3A-PA-O5'	2.53	109.65	102.94
2	A	1383	ADP	O3B-PB-O2B	2.58	117.19	107.38
2	A	1383	ADP	O4'-C1'-N9	3.12	114.64	108.10
2	B	1383	ADP	O4'-C1'-N9	3.19	114.78	108.10

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.45	1 (0%) 94 91	20, 67, 119, 163	0
1	B	382/543 (70%)	-0.44	0 100 100	14, 68, 112, 147	0
All	All	764/1086 (70%)	-0.44	1 (0%) 95 94	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	A	1383	27/27	0.95	0.21	0.34	77,77,77,77	0
2	ADP	B	1383	27/27	0.96	0.18	-0.29	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	A	1384	5/5	0.96	0.17	-0.80	74,101,101,101	0
3	PO4	B	1384	5/5	0.98	0.11	-2.88	37,37,37,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.