



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:55 PM UTC

PDB ID : 1JM6 / pdb_00001jm6
Title : Pyruvate dehydrogenase kinase, isozyme 2, containing ADP
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Deposited on : 2001-07-17
Resolution : 2.50 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

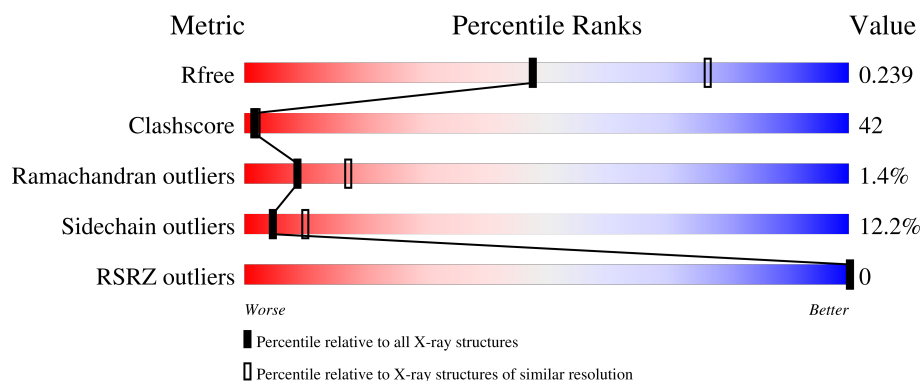
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	407	
1	B	407	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	3510	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5677 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.

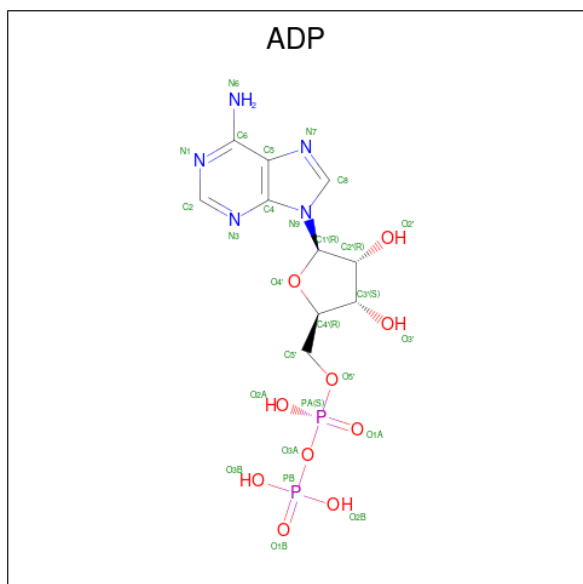
- Molecule 1 is a protein called Pyruvate dehydrogenase kinase, isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2709	1743	444	505	17			
1	B	336	Total	C	N	O	S	0	0	0
			2684	1728	441	498	17			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

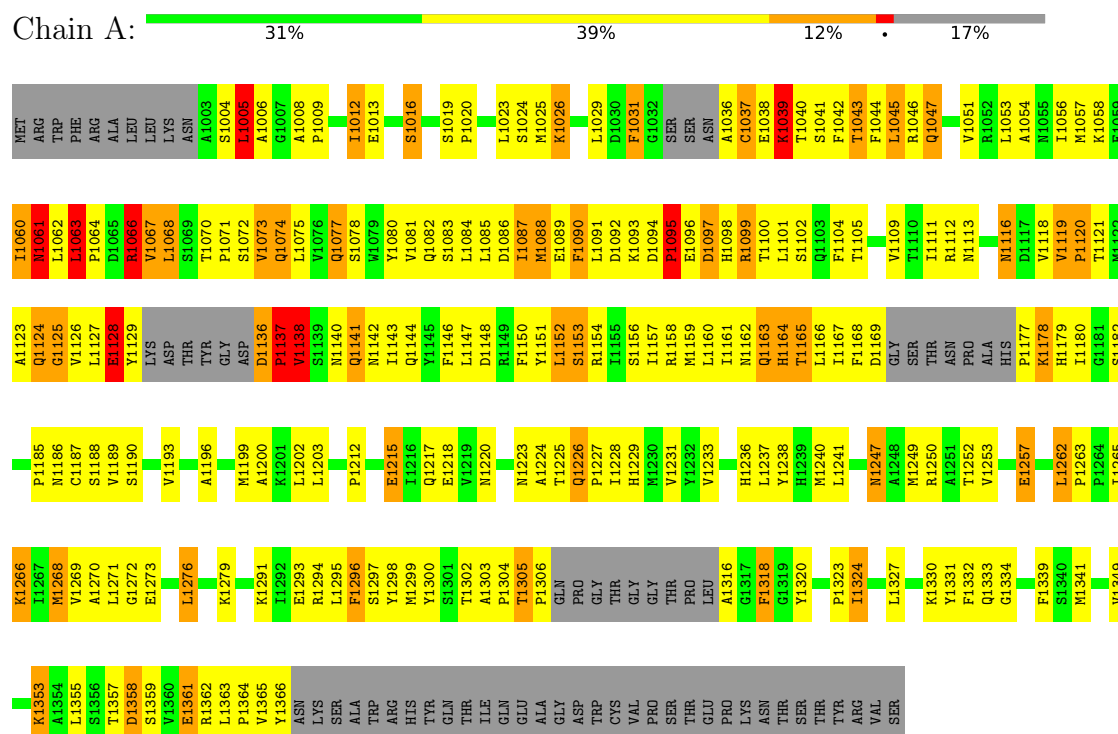
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	109	Total	O	0	0
			109	109		

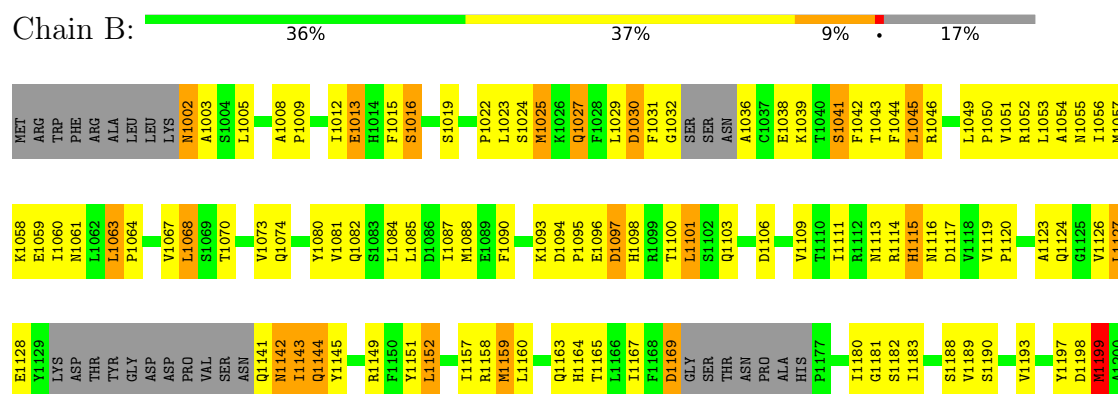
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Pyruvate dehydrogenase kinase, isozyme 2



• Molecule 1: Pyruvate dehydrogenase kinase, isozyme 2



V1360	K1201
E1361	L1202
R1362	L1203
L1363	C1204
P1364	D1205
V1365	K1206
TYR	Y1207
ASN	Y1208
LYS	L1209
SER	M1209
ALA	
TRP	P1212
ARG	
HIS	Q1217
TYR	E1218
GLN	V1219
THR	N1220
ILE	N1223
GLN	A1224
GLU	T1225
ALA	Q1226
GLY	P1227
ASP	I1228
TRP	
CYS	Y1232
VAL	V1233
PRO	P1234
SER	S1235
THR	H1236
GLU	L1237
PRO	Y1238
LYS	
ASN	F1245
THR	K1246
SER	N1247
THR	A1248
TYR	M1249
ARG	R1250
VAL	
SER	V1253
	S1258
	T1261
	L1262
	P1263
	P1264
	I1265
	K1266
	I1267
	M1268
	V1269
	A1270
	L1271
	L1276
	K1279
	R1283

V1287
R1290
K1291
R1294
L1295
F1296
S1297
Y1298
T1302
A1303
P1304
T1305
P1306
GLN
PRO
GLY
THR
GLY
GLY
THR
P1314
L1315
A1316
G1317
F1318
G1319
Y1320
G1321
L1322
P1323
I1324
S1325
R1326
L1327
K1330
Y1331
F1332
Q1333
G1334
D1335
L1338
F1339
S1340
M1341
E1342
G1343
F1344
G1345
T1346
D1347
T1357
D1358
S1359

V1360
E1361
R1362
L1363
P1364
V1365
TYR
ASN
LYS
SER
ALA
TRP
ARG
HIS
TYR
GLN
THR
ILE
GLN
GLU
ALA
GLY
ASP
TRP
CYS
VAL
PRO
SER
THR
GLU
PRO
LYS
ASN
THR
SER
THR
TYR
ARG
VAL
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.42Å 109.87Å 71.41Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 6.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.2 (6.00-2.50) 88.4 (6.00-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.202 , 0.262 0.187 , 0.239	Depositor DCC
R_{free} test set	1626 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: MG, 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	1.07	24/2771 (0.9%)	1.66	72/3752 (1.9%)
1	B	0.85	12/2745 (0.4%)	1.34	26/3715 (0.7%)
All	All	0.96	36/5516 (0.7%)	1.51	98/7467 (1.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1178	LYS	C-N	-12.33	1.16	1.33
1	B	1115	HIS	CA-C	-9.02	1.40	1.52
1	A	1096	GLU	C-O	8.29	1.34	1.24
1	B	1027	GLN	C-N	-7.50	1.23	1.33
1	A	1090	PHE	C-N	-7.48	1.14	1.33
1	A	1165	THR	N-CA	-7.32	1.37	1.46
1	B	1306	PRO	CA-C	6.97	1.67	1.52
1	A	1164	HIS	C-N	-6.89	1.24	1.34
1	B	1302	THR	CB-OG1	6.82	1.54	1.43
1	B	1115	HIS	C-N	-6.53	1.25	1.34
1	A	1095	PRO	CA-C	6.53	1.61	1.52
1	A	1031	PHE	CA-C	6.51	1.61	1.52
1	B	1143	ILE	CA-C	6.47	1.60	1.52
1	B	1142	ASN	CA-C	-6.28	1.44	1.52
1	A	1005	LEU	CA-C	6.21	1.60	1.53
1	A	1126	VAL	C-O	6.18	1.31	1.24
1	A	1087	ILE	C-N	6.16	1.43	1.33
1	A	1066	ARG	C-N	6.14	1.42	1.33
1	A	1097	ASP	N-CA	5.97	1.53	1.45
1	B	1306	PRO	C-O	5.86	1.35	1.23
1	A	1026	LYS	C-N	-5.83	1.25	1.33
1	A	1305	THR	CA-C	5.82	1.60	1.52
1	A	1006	ALA	CA-C	-5.67	1.45	1.52
1	B	1142	ASN	C-N	-5.60	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1109	VAL	C-N	-5.58	1.26	1.33
1	A	1037	CYS	CA-C	5.52	1.59	1.52
1	B	1262	LEU	C-N	5.50	1.39	1.33
1	A	1296	PHE	CA-C	-5.38	1.45	1.52
1	A	1137	PRO	C-N	5.37	1.41	1.33
1	A	1074	GLN	C-N	-5.33	1.27	1.33
1	A	1296	PHE	C-N	-5.27	1.26	1.33
1	B	1228	ILE	N-CA	-5.26	1.40	1.46
1	A	1138	VAL	N-CA	5.26	1.52	1.46
1	A	1119	VAL	CA-C	5.17	1.58	1.52
1	A	1088	MET	N-CA	5.09	1.52	1.46
1	A	1087	ILE	CA-C	5.08	1.59	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	O-C-N	-15.69	102.73	122.34
1	A	1137	PRO	CA-C-N	14.68	148.39	121.97
1	A	1137	PRO	C-N-CA	14.68	148.39	121.97
1	A	1138	VAL	N-CA-C	13.88	138.22	109.34
1	A	1077	GLN	OE1-CD-NE2	-10.78	111.82	122.60
1	A	1006	ALA	CA-C-N	-10.58	102.27	120.79
1	A	1006	ALA	C-N-CA	-10.58	102.27	120.79
1	A	1226	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	A	1061	ASN	CA-CB-CG	10.33	122.93	112.60
1	A	1141	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	1124	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	1074	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	1247	ASN	OD1-CG-ND2	9.57	132.17	122.60
1	A	1082	GLN	OE1-CD-NE2	-9.38	113.22	122.60
1	B	1141	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	B	1027	GLN	OE1-CD-NE2	-9.33	113.27	122.60
1	B	1144	GLN	OE1-CD-NE2	-9.32	113.28	122.60
1	A	1163	GLN	OE1-CD-NE2	-9.11	113.50	122.60
1	B	1226	GLN	OE1-CD-NE2	-9.09	113.52	122.60
1	B	1223	ASN	N-CA-C	-8.99	93.99	108.55
1	A	1137	PRO	N-CA-C	8.50	129.98	112.47
1	A	1061	ASN	N-CA-C	-8.05	103.54	112.72
1	B	1115	HIS	CA-CB-CG	-7.99	105.81	113.80
1	A	1026	LYS	CA-C-N	-7.92	107.22	120.68
1	A	1026	LYS	C-N-CA	-7.92	107.22	120.68
1	B	1224	ALA	N-CA-C	7.89	123.02	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1096	GLU	O-C-N	-7.51	113.12	122.35
1	B	1318	PHE	CA-CB-CG	-7.46	106.34	113.80
1	B	1223	ASN	N-CA-CB	7.33	123.97	110.99
1	A	1127	LEU	N-CA-C	7.02	120.33	111.69
1	B	1141	GLN	CG-CD-NE2	6.89	126.73	116.40
1	A	1125	GLY	N-CA-C	-6.72	106.33	114.66
1	A	1094	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	1124	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	1074	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	1077	GLN	CG-CD-NE2	6.61	126.32	116.40
1	B	1027	GLN	CG-CD-NE2	6.60	126.30	116.40
1	B	1005	LEU	CA-C-N	-6.58	110.87	122.26
1	B	1005	LEU	C-N-CA	-6.58	110.87	122.26
1	A	1226	GLN	CG-CD-NE2	6.58	126.27	116.40
1	B	1144	GLN	CG-CD-NE2	6.53	126.19	116.40
1	B	1199	MET	CA-C-O	-6.50	111.21	120.51
1	A	1082	GLN	CG-CD-NE2	6.49	126.14	116.40
1	A	1063	LEU	O-C-N	6.44	128.43	121.60
1	A	1031	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	1270	ALA	CA-C-N	-6.37	114.20	123.00
1	A	1270	ALA	C-N-CA	-6.37	114.20	123.00
1	A	1227	PRO	CB-CA-C	6.34	119.51	111.39
1	A	1163	GLN	CG-CD-NE2	6.31	125.86	116.40
1	A	1141	GLN	CG-CD-NE2	6.30	125.85	116.40
1	A	1127	LEU	O-C-N	6.23	130.33	122.23
1	B	1226	GLN	CG-CD-NE2	6.23	125.74	116.40
1	A	1236	HIS	CA-CB-CG	6.20	120.00	113.80
1	A	1125	GLY	CA-C-N	-6.19	112.86	121.77
1	A	1125	GLY	C-N-CA	-6.19	112.86	121.77
1	A	1060	ILE	CA-C-N	-6.15	112.83	122.73
1	A	1060	ILE	C-N-CA	-6.15	112.83	122.73
1	A	1127	LEU	CA-C-N	6.14	131.39	122.85
1	A	1127	LEU	C-N-CA	6.14	131.39	122.85
1	A	1127	LEU	N-CA-CB	-6.13	101.06	110.20
1	A	1215	GLU	CB-CG-CD	-6.11	102.22	112.60
1	A	1138	VAL	N-CA-CB	-6.06	101.23	111.23
1	A	1024	SER	O-C-N	-6.05	115.20	122.65
1	B	1364	PRO	CB-CA-C	5.93	118.72	110.95
1	A	1128	GLU	N-CA-C	-5.74	97.07	107.75
1	A	1116	ASN	CA-C-N	-5.73	114.09	122.86
1	A	1116	ASN	C-N-CA	-5.73	114.09	122.86
1	A	1097	ASP	CA-CB-CG	5.68	118.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1263	PRO	CA-N-CD	-5.57	104.20	112.00
1	A	1137	PRO	O-C-N	5.57	130.16	122.64
1	A	1006	ALA	N-CA-C	-5.44	99.22	110.80
1	B	1115	HIS	CA-C-N	-5.43	112.46	120.28
1	B	1115	HIS	C-N-CA	-5.43	112.46	120.28
1	A	1099	ARG	CA-C-O	-5.39	114.01	120.10
1	A	1236	HIS	CB-CG-ND1	5.38	130.77	122.70
1	A	1136	ASP	CA-C-N	5.36	126.53	119.84
1	A	1136	ASP	C-N-CA	5.36	126.53	119.84
1	A	1138	VAL	CB-CA-C	-5.34	102.53	111.29
1	B	1236	HIS	CB-CG-CD2	5.33	138.13	131.20
1	A	1073	VAL	CA-C-N	-5.33	113.19	120.44
1	A	1073	VAL	C-N-CA	-5.33	113.19	120.44
1	A	1236	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	1090	PHE	CA-C-N	5.30	140.33	122.20
1	A	1090	PHE	C-N-CA	5.30	140.33	122.20
1	A	1119	VAL	N-CA-CB	-5.28	103.81	111.21
1	A	1305	THR	O-C-N	5.25	127.36	121.32
1	B	1142	ASN	CA-C-N	-5.24	112.54	121.97
1	B	1142	ASN	C-N-CA	-5.24	112.54	121.97
1	B	1142	ASN	N-CA-C	-5.22	106.75	113.01
1	A	1087	ILE	CA-C-N	5.22	130.28	121.14
1	A	1087	ILE	C-N-CA	5.22	130.28	121.14
1	A	1303	ALA	N-CA-C	5.15	117.77	110.40
1	A	1123	ALA	O-C-N	-5.08	116.27	122.22
1	A	1039	LYS	CA-C-N	5.07	127.34	120.44
1	A	1039	LYS	C-N-CA	5.07	127.34	120.44
1	B	1097	ASP	CA-C-N	5.05	127.29	120.38
1	B	1097	ASP	C-N-CA	5.05	127.29	120.38
1	A	1120	PRO	CA-N-CD	-5.01	104.98	112.00

There are no chirality outliers.

There are no planarity outliers.

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	2709	0	2692	263	0
1	B	2684	0	2679	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	9	0
4	A	119	0	0	19	0
4	B	109	0	0	16	0
All	All	5677	0	5395	455	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:PHE:CE2	1:A:1095:PRO:HG3	1.64	1.33
1:A:1138:VAL:O	1:A:1138:VAL:CG1	1.75	1.29
1:A:1223:ASN:HD22	1:A:1226:GLN:CB	1.58	1.16
1:A:1031:PHE:HA	1:A:1036:ALA:N	1.60	1.15
1:A:1177:PRO:HD2	1:A:1179:HIS:NE2	1.62	1.14
1:A:1070:THR:HG21	1:A:1125:GLY:HA2	1.30	1.13
1:A:1005:LEU:HG	1:A:1005:LEU:O	1.36	1.12
1:B:1306:PRO:O	1:B:1317:GLY:HA3	1.49	1.11
1:A:1225:THR:O	1:A:1225:THR:HG22	1.44	1.10
1:A:1138:VAL:O	1:A:1138:VAL:HG12	1.30	1.10
1:A:1112:ARG:HH12	1:A:1165:THR:HG21	0.95	1.08
1:A:1038:GLU:HG2	1:A:1168:PHE:CD2	1.89	1.07
1:A:1223:ASN:HD22	1:A:1226:GLN:HB3	0.96	1.06
1:B:1218:GLU:HG2	1:B:1269:VAL:HB	1.39	1.05
1:A:1177:PRO:CD	1:A:1179:HIS:NE2	2.23	1.01
1:A:1112:ARG:NH1	1:A:1165:THR:HG21	1.74	0.99
1:A:1223:ASN:ND2	1:A:1226:GLN:HB3	1.76	0.99
1:A:1042:PHE:HE2	1:A:1095:PRO:CG	1.73	0.99
1:A:1085:LEU:HA	1:A:1088:MET:HE3	1.45	0.98
1:A:1066:ARG:HG2	1:A:1136:ASP:OD2	1.64	0.96
1:A:1042:PHE:HE2	1:A:1095:PRO:HG3	0.81	0.96
1:B:1144:GLN:HE22	1:B:1297:SER:HA	1.31	0.95
1:A:1005:LEU:O	1:A:1005:LEU:CG	2.15	0.94
1:A:1225:THR:O	1:A:1225:THR:CG2	2.16	0.94
1:A:1177:PRO:HD2	1:A:1179:HIS:CE1	2.02	0.94
1:A:1271:LEU:HD13	1:A:1276:LEU:HD22	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:LYS:O	1:A:1178:LYS:HG3	1.65	0.93
1:A:1138:VAL:O	1:A:1138:VAL:HG13	1.69	0.92
1:B:1144:GLN:NE2	1:B:1297:SER:HA	1.85	0.91
1:A:1084:LEU:HG	1:A:1088:MET:HE2	1.50	0.90
1:B:1152:LEU:HD13	1:B:1364:PRO:CD	2.02	0.90
1:A:1031:PHE:CA	1:A:1036:ALA:N	2.35	0.89
1:B:1346:THR:HG21	3:B:3510:ADP:N6	1.86	0.89
1:B:1258:SER:O	1:B:1262:LEU:CD1	2.21	0.88
1:A:1041:SER:O	1:A:1045:LEU:HB2	1.74	0.88
1:A:1093:LYS:O	1:A:1095:PRO:HD3	1.73	0.88
1:B:1061:ASN:HA	1:B:1068:LEU:HD11	1.54	0.87
1:A:1084:LEU:HG	1:A:1088:MET:CE	2.06	0.86
1:B:1095:PRO:HD3	4:B:6192:HOH:O	1.75	0.84
1:B:1113:ASN:HA	1:B:1116:ASN:HD22	1.41	0.84
1:A:1306:PRO:HG2	4:A:6188:HOH:O	1.77	0.84
1:A:1038:GLU:HG2	1:A:1168:PHE:CE2	2.13	0.83
1:B:1013:GLU:HG3	4:B:6051:HOH:O	1.78	0.83
1:B:1152:LEU:CD1	1:B:1364:PRO:HD3	2.09	0.82
1:A:1223:ASN:ND2	1:A:1226:GLN:CB	2.38	0.82
1:A:1086:ASP:O	1:A:1089:GLU:HG2	1.79	0.81
1:A:1074:GLN:O	1:A:1075:LEU:C	2.20	0.81
1:B:1025:MET:O	1:B:1029:LEU:HD13	1.81	0.80
1:B:1024:SER:H	1:B:1027:GLN:HE21	1.30	0.80
1:B:1002:ASN:HB3	1:B:1082:GLN:HE22	1.48	0.79
1:A:1148:ASP:HA	1:A:1327:LEU:HD11	1.64	0.79
1:B:1152:LEU:HD13	1:B:1364:PRO:HD3	1.64	0.78
1:A:1302:THR:HG22	1:A:1302:THR:O	1.83	0.78
1:A:1067:VAL:O	1:A:1073:VAL:HG21	1.85	0.77
1:A:1084:LEU:O	1:A:1088:MET:HE2	1.84	0.77
1:B:1022:PRO:HB3	1:B:1361:GLU:O	1.84	0.77
1:A:1084:LEU:C	1:A:1088:MET:HE2	2.09	0.77
1:B:1097:ASP:O	1:B:1100:THR:HG22	1.85	0.76
1:A:1177:PRO:CG	1:A:1179:HIS:NE2	2.48	0.76
1:A:1178:LYS:O	1:A:1178:LYS:CG	2.33	0.76
1:A:1012:ILE:HG23	1:A:1054:ALA:HB1	1.67	0.76
1:A:1237:LEU:HA	1:A:1240:MET:HE3	1.66	0.76
1:B:1142:ASN:O	1:B:1143:ILE:C	2.28	0.76
1:A:1042:PHE:CE2	1:A:1095:PRO:CG	2.58	0.75
1:A:1163:GLN:NE2	1:A:1182:SER:H	1.85	0.75
1:A:1093:LYS:O	1:A:1095:PRO:CD	2.35	0.74
1:B:1258:SER:O	1:B:1262:LEU:HD13	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1306:PRO:O	1:B:1317:GLY:CA	2.32	0.74
1:A:1228:ILE:HD13	1:A:1269:VAL:HG12	1.69	0.74
1:A:1012:ILE:O	1:A:1016:SER:HB3	1.88	0.74
1:A:1037:CYS:HB3	1:A:1040:THR:HG23	1.68	0.74
1:A:1085:LEU:HD23	1:A:1088:MET:CE	2.18	0.74
1:A:1119:VAL:HG12	1:A:1120:PRO:HD3	1.69	0.74
1:B:1012:ILE:O	1:B:1016:SER:HB3	1.87	0.73
1:B:1250:ARG:NH2	1:B:1303:ALA:HB2	2.03	0.73
1:A:1138:VAL:HG22	1:A:1141:GLN:NE2	2.03	0.73
1:B:1152:LEU:HD13	1:B:1364:PRO:HD2	1.69	0.73
1:A:1105:THR:O	1:A:1109:VAL:HG23	1.89	0.73
1:B:1029:LEU:HD11	1:B:1183:ILE:HG21	1.69	0.73
1:A:1041:SER:OG	1:A:1164:HIS:HD2	1.72	0.73
1:A:1089:GLU:OE2	1:A:1090:PHE:CE1	2.42	0.72
1:B:1182:SER:O	1:B:1234:PRO:HD2	1.89	0.72
1:A:1089:GLU:OE2	1:A:1090:PHE:HE1	1.71	0.72
1:B:1271:LEU:HD13	1:B:1276:LEU:HD22	1.70	0.72
1:A:1177:PRO:HB2	1:A:1179:HIS:CD2	2.24	0.72
1:A:1163:GLN:HE22	1:A:1182:SER:H	1.35	0.71
1:A:1257:GLU:HG3	4:A:6020:HOH:O	1.90	0.71
1:A:1158:ARG:HD2	4:A:6149:HOH:O	1.91	0.71
1:A:1212:PRO:HG3	1:A:1252:THR:HG21	1.71	0.71
1:B:1038:GLU:OE1	1:B:1101:LEU:HD12	1.90	0.71
1:A:1088:MET:HA	1:A:1091:LEU:HD12	1.72	0.71
1:A:1070:THR:HG23	1:A:1071:PRO:HD2	1.73	0.71
1:B:1319:GLY:N	3:B:3510:ADP:O1B	2.20	0.70
1:A:1299:MET:HG2	4:A:6187:HOH:O	1.91	0.70
1:B:1152:LEU:CD1	1:B:1364:PRO:CD	2.69	0.70
1:A:1063:LEU:CD2	1:A:1067:VAL:HG21	2.22	0.69
1:A:1085:LEU:HD23	1:A:1088:MET:HE3	1.73	0.69
1:B:1346:THR:HG21	3:B:3510:ADP:HN62	1.56	0.69
1:B:1094:ASP:O	1:B:1100:THR:HG21	1.92	0.69
1:B:1249:MET:O	1:B:1253:VAL:HG23	1.93	0.69
1:A:1138:VAL:HG22	1:A:1141:GLN:HE22	1.57	0.69
1:A:1020:PRO:HD2	1:A:1366:TYR:HB2	1.74	0.69
1:B:1038:GLU:CD	1:B:1101:LEU:HD12	2.18	0.69
1:B:1220:ASN:CG	1:B:1223:ASN:O	2.35	0.68
1:A:1112:ARG:HH12	1:A:1165:THR:CG2	1.90	0.68
1:A:1199:MET:HG3	1:A:1238:TYR:OH	1.93	0.68
1:A:1063:LEU:CD2	1:A:1067:VAL:CG2	2.72	0.68
1:A:1020:PRO:HD2	1:A:1366:TYR:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:CYS:HB3	1:A:1040:THR:CG2	2.23	0.67
1:A:1066:ARG:NE	1:A:1136:ASP:OD1	2.28	0.67
1:A:1083:SER:OG	1:A:1111:ILE:HG23	1.94	0.67
1:B:1346:THR:CG2	3:B:3510:ADP:HN62	2.08	0.66
1:B:1106:ASP:HA	4:B:6193:HOH:O	1.93	0.66
1:B:1142:ASN:OD1	1:B:1145:TYR:HB3	1.95	0.66
1:B:1159:MET:HE3	1:B:1233:VAL:HG21	1.78	0.66
1:A:1113:ASN:HA	1:A:1116:ASN:ND2	2.11	0.66
1:B:1022:PRO:HG3	1:B:1363:LEU:HD12	1.78	0.65
1:B:1295:LEU:HD22	3:B:3510:ADP:O4'	1.97	0.65
1:A:1220:ASN:OD1	1:A:1223:ASN:N	2.25	0.65
1:A:1112:ARG:HD2	1:A:1162:ASN:HD21	1.61	0.65
1:A:1088:MET:HG2	1:A:1091:LEU:CD1	2.27	0.65
1:B:1068:LEU:O	1:B:1074:GLN:HG3	1.97	0.65
1:B:1163:GLN:OE1	1:B:1181:GLY:HA3	1.97	0.65
1:B:1291:LYS:HG2	1:B:1294:ARG:NH1	2.12	0.65
1:A:1118:VAL:HG21	4:A:6148:HOH:O	1.95	0.64
1:B:1123:ALA:O	1:B:1126:VAL:HG22	1.96	0.64
1:A:1165:THR:HG22	4:A:6183:HOH:O	1.97	0.64
1:B:1116:ASN:ND2	4:B:6234:HOH:O	2.30	0.64
1:A:1089:GLU:HG3	1:A:1090:PHE:CD1	2.33	0.64
1:A:1279:LYS:NZ	4:A:6186:HOH:O	2.31	0.64
1:A:1084:LEU:CG	1:A:1088:MET:HE2	2.27	0.63
1:A:1088:MET:HA	1:A:1091:LEU:CD1	2.28	0.63
1:A:1053:LEU:HD22	1:A:1080:TYR:CD2	2.33	0.63
1:B:1119:VAL:HG22	1:B:1151:TYR:CE2	2.34	0.63
1:B:1093:LYS:NZ	1:B:1103:GLN:OE1	2.31	0.62
1:B:1331:TYR:CE1	1:B:1361:GLU:HB2	2.34	0.62
1:B:1346:THR:HG21	3:B:3510:ADP:C6	2.34	0.62
1:A:1112:ARG:O	1:A:1116:ASN:ND2	2.32	0.62
1:A:1272:GLY:HA3	1:B:1342:GLU:HG2	1.82	0.62
1:A:1296:PHE:O	1:A:1323:PRO:HG3	1.99	0.62
1:B:1113:ASN:HA	1:B:1116:ASN:ND2	2.13	0.62
1:B:1197:TYR:CE2	1:B:1201:LYS:HD3	2.34	0.62
1:A:1097:ASP:O	1:A:1098:HIS:C	2.41	0.61
1:A:1153:SER:O	1:A:1157:ILE:HD12	2.01	0.61
1:A:1084:LEU:O	1:A:1088:MET:CE	2.49	0.61
1:B:1261:THR:O	1:B:1263:PRO:HD3	2.00	0.61
1:A:1025:MET:HE3	1:A:1231:VAL:HG12	1.82	0.60
1:A:1031:PHE:C	1:A:1036:ALA:N	2.59	0.60
1:A:1156:SER:O	1:A:1160:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1290:ARG:HH11	1:B:1294:ARG:HH22	1.47	0.60
1:B:1326:ARG:HD2	4:B:6042:HOH:O	2.01	0.60
1:A:1152:LEU:CD1	1:A:1364:PRO:HD3	2.31	0.60
1:A:1316:ALA:HB3	4:A:4603:HOH:O	2.02	0.60
1:B:1038:GLU:CG	1:B:1101:LEU:HD12	2.31	0.60
1:A:1320:TYR:O	1:A:1323:PRO:HD2	2.02	0.60
1:A:1063:LEU:HD11	1:A:1146:PHE:CD2	2.37	0.60
1:A:1168:PHE:O	1:A:1169:ASP:C	2.46	0.59
1:A:1228:ILE:CD1	1:A:1269:VAL:HG12	2.32	0.59
1:B:1023:LEU:HD11	1:B:1044:PHE:HZ	1.67	0.59
1:B:1059:GLU:CD	1:B:1149:ARG:HH21	2.10	0.59
1:B:1266:LYS:HD2	4:B:6090:HOH:O	2.01	0.59
1:A:1089:GLU:CG	1:A:1090:PHE:CD1	2.86	0.59
1:B:1207:TYR:CD1	1:B:1314:PRO:HB3	2.37	0.59
1:B:1057:MET:SD	1:B:1080:TYR:HB3	2.43	0.59
1:A:1063:LEU:HD22	1:A:1067:VAL:HG22	1.83	0.59
1:A:1067:VAL:HG12	1:A:1129:TYR:CE1	2.38	0.59
1:B:1144:GLN:HE22	1:B:1297:SER:CA	2.12	0.59
1:A:1294:ARG:C	1:A:1296:PHE:H	2.11	0.59
1:A:1163:GLN:O	1:A:1167:ILE:HG13	2.01	0.58
1:A:1302:THR:O	1:A:1302:THR:CG2	2.51	0.58
1:B:1063:LEU:HG	1:B:1064:PRO:HD2	1.86	0.58
1:B:1258:SER:HB3	4:B:6012:HOH:O	2.02	0.58
1:A:1331:TYR:CE1	1:A:1361:GLU:HG2	2.39	0.58
1:A:1250:ARG:HD3	4:A:6072:HOH:O	2.03	0.58
1:A:1116:ASN:ND2	4:A:6081:HOH:O	2.29	0.58
1:A:1020:PRO:CD	1:A:1366:TYR:HB2	2.34	0.57
1:A:1112:ARG:HD2	1:A:1162:ASN:ND2	2.19	0.57
1:A:1341:MET:HE2	1:B:1279:LYS:HE2	1.87	0.57
1:B:1159:MET:HG3	1:B:1331:TYR:OH	2.04	0.57
1:A:1019:SER:OG	1:A:1366:TYR:C	2.48	0.57
1:A:1025:MET:HG3	1:A:1029:LEU:HD12	1.86	0.57
1:A:1088:MET:HG2	1:A:1091:LEU:HD11	1.86	0.57
1:B:1038:GLU:HG2	1:B:1101:LEU:CD1	2.34	0.57
1:A:1152:LEU:HD12	1:A:1364:PRO:HD3	1.87	0.57
1:A:1249:MET:O	1:A:1253:VAL:HG23	2.05	0.57
1:A:1215:GLU:OE1	1:A:1266:LYS:HD2	2.05	0.57
1:A:1294:ARG:O	1:A:1296:PHE:N	2.37	0.57
1:A:1039:LYS:O	1:A:1043:THR:HB	2.05	0.56
1:A:1072:SER:HB3	1:A:1121:THR:O	2.05	0.56
1:B:1250:ARG:HH12	1:B:1302:THR:HG22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:HD22	1:A:1067:VAL:CG2	2.36	0.56
1:A:1141:GLN:HG2	1:A:1299:MET:HE2	1.88	0.56
1:A:1293:GLU:HG3	4:A:6221:HOH:O	2.04	0.56
1:B:1250:ARG:NH1	1:B:1302:THR:HG22	2.21	0.56
1:A:1046:ARG:O	1:A:1091:LEU:HD21	2.06	0.56
1:B:1084:LEU:O	1:B:1088:MET:HG3	2.04	0.56
1:B:1063:LEU:HD23	1:B:1067:VAL:HG13	1.87	0.56
1:B:1144:GLN:HE22	1:B:1298:TYR:H	1.54	0.56
1:A:1042:PHE:CD2	1:A:1095:PRO:HG3	2.34	0.56
1:A:1099:ARG:O	1:A:1100:THR:C	2.46	0.56
1:A:1045:LEU:HB3	1:A:1104:PHE:HZ	1.70	0.55
1:A:1099:ARG:HA	1:A:1102:SER:OG	2.07	0.55
1:A:1143:ILE:HG22	1:A:1147:LEU:HD22	1.88	0.55
1:B:1002:ASN:CB	1:B:1082:GLN:HE22	2.18	0.55
1:A:1063:LEU:HD23	1:A:1067:VAL:CG2	2.35	0.55
1:A:1177:PRO:HB2	1:A:1179:HIS:HD2	1.70	0.55
1:B:1207:TYR:CE1	1:B:1314:PRO:HB3	2.41	0.55
1:A:1146:PHE:CD2	1:A:1147:LEU:HD12	2.41	0.55
1:A:1146:PHE:HD2	1:A:1147:LEU:HD12	1.70	0.55
1:B:1228:ILE:CD1	1:B:1269:VAL:HG12	2.36	0.55
1:A:1113:ASN:HA	1:A:1116:ASN:HD22	1.70	0.55
1:B:1039:LYS:NZ	1:B:1096:GLU:OE1	2.30	0.55
1:B:1117:ASP:O	1:B:1120:PRO:HD2	2.07	0.55
1:A:1167:ILE:O	1:A:1167:ILE:HG22	2.05	0.55
1:A:1085:LEU:HD23	1:A:1088:MET:HE1	1.88	0.55
1:A:1186:ASN:O	1:A:1186:ASN:ND2	2.40	0.55
1:A:1353:LYS:HG2	1:A:1358:ASP:HB2	1.89	0.54
1:B:1029:LEU:HA	1:B:1180:ILE:HG21	1.88	0.54
1:B:1228:ILE:HD13	1:B:1269:VAL:HG12	1.88	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:HZ	1.72	0.54
1:B:1064:PRO:HD2	1:B:1067:VAL:CG1	2.38	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:CZ	2.42	0.54
1:A:1038:GLU:CG	1:A:1168:PHE:CD2	2.77	0.54
1:B:1022:PRO:HG3	1:B:1363:LEU:CD1	2.36	0.54
1:B:1081:VAL:O	1:B:1085:LEU:HG	2.08	0.54
1:B:1346:THR:CG2	3:B:3510:ADP:N6	2.62	0.54
1:A:1063:LEU:HD23	1:A:1067:VAL:HG21	1.89	0.54
1:B:1061:ASN:CB	4:B:6231:HOH:O	2.56	0.54
1:B:1320:TYR:HB2	1:B:1324:ILE:CD1	2.37	0.54
1:B:1100:THR:CG2	1:B:1101:LEU:HD23	2.38	0.54
1:A:1279:LYS:HG3	1:A:1349:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:CD2	1:A:1067:VAL:HG22	2.38	0.53
1:A:1152:LEU:HD13	1:A:1363:LEU:HA	1.91	0.53
1:B:1100:THR:HG23	1:B:1101:LEU:HD23	1.91	0.53
1:B:1304:PRO:CB	1:B:1306:PRO:HD2	2.39	0.53
1:A:1084:LEU:C	1:A:1088:MET:CE	2.81	0.53
1:A:1297:SER:HB3	1:A:1300:TYR:CB	2.38	0.53
1:B:1246:LYS:HD2	1:B:1315:LEU:HD22	1.91	0.53
1:B:1304:PRO:O	1:B:1317:GLY:CA	2.56	0.53
1:A:1212:PRO:HG3	1:A:1252:THR:CG2	2.37	0.53
1:A:1294:ARG:C	1:A:1296:PHE:N	2.66	0.53
1:B:1119:VAL:HG22	1:B:1151:TYR:HE2	1.73	0.53
1:A:1364:PRO:O	1:A:1366:TYR:HD2	1.92	0.53
1:B:1041:SER:HB3	1:B:1164:HIS:CE1	2.44	0.53
1:B:1302:THR:HB	3:B:3510:ADP:O2'	2.10	0.52
1:A:1177:PRO:HG2	1:A:1179:HIS:NE2	2.22	0.52
1:B:1070:THR:HG23	1:B:1128:GLU:HG3	1.90	0.52
1:A:1063:LEU:HD11	1:A:1146:PHE:CE2	2.43	0.52
1:A:1229:HIS:NE2	4:A:6144:HOH:O	2.34	0.52
1:B:1058:LYS:NZ	4:B:6230:HOH:O	2.42	0.52
1:A:1025:MET:HG3	1:A:1029:LEU:CD1	2.39	0.52
1:A:1037:CYS:O	1:A:1040:THR:OG1	2.23	0.52
1:A:1200:ALA:C	1:A:1249:MET:HE1	2.35	0.52
1:A:1355:LEU:HB2	1:A:1358:ASP:OD2	2.09	0.52
1:A:1129:TYR:C	1:A:1136:ASP:HB3	2.35	0.52
1:B:1152:LEU:HD12	1:B:1364:PRO:HD3	1.89	0.52
1:A:1038:GLU:HB3	1:A:1101:LEU:HD13	1.91	0.51
1:A:1163:GLN:NE2	1:A:1182:SER:OG	2.42	0.51
1:A:1223:ASN:ND2	1:A:1226:GLN:HB2	2.24	0.51
1:B:1159:MET:HG3	1:B:1331:TYR:CE2	2.45	0.51
1:A:1020:PRO:HG2	1:A:1366:TYR:HB3	1.93	0.51
1:A:1038:GLU:O	1:A:1041:SER:N	2.43	0.51
1:B:1024:SER:HB3	1:B:1027:GLN:HG3	1.93	0.51
1:B:1070:THR:CG2	1:B:1128:GLU:HG3	2.40	0.51
1:B:1051:VAL:O	1:B:1055:ASN:OD1	2.29	0.51
1:B:1165:THR:O	1:B:1169:ASP:OD2	2.28	0.51
1:B:1220:ASN:OD1	1:B:1223:ASN:O	2.28	0.51
1:A:1320:TYR:C	1:A:1323:PRO:HD2	2.36	0.50
1:B:1119:VAL:HB	1:B:1120:PRO:HD3	1.93	0.50
1:A:1193:VAL:HA	1:A:1241:LEU:HD13	1.92	0.50
1:B:1163:GLN:O	1:B:1167:ILE:HG13	2.11	0.50
1:A:1061:ASN:HD22	1:A:1061:ASN:H	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:ARG:HB2	1:A:1161:ILE:HG21	1.93	0.50
1:B:1038:GLU:CG	1:B:1101:LEU:CD1	2.89	0.50
1:A:1042:PHE:O	1:A:1043:THR:C	2.54	0.50
1:A:1146:PHE:CZ	1:A:1150:PHE:HB2	2.47	0.50
1:B:1189:VAL:O	1:B:1193:VAL:HG23	2.12	0.49
1:B:1316:ALA:HB2	4:B:6087:HOH:O	2.11	0.49
1:A:1061:ASN:HD22	1:A:1061:ASN:N	2.10	0.49
1:A:1247:ASN:ND2	3:A:3500:ADP:O2A	2.45	0.49
1:B:1031:PHE:O	1:B:1032:GLY:O	2.30	0.49
1:A:1020:PRO:HB3	1:A:1363:LEU:HD13	1.95	0.49
1:A:1167:ILE:O	1:A:1167:ILE:CG2	2.60	0.49
1:A:1190:SER:OG	1:A:1218:GLU:OE2	2.29	0.49
1:A:1318:PHE:HE1	4:A:6218:HOH:O	1.94	0.49
1:B:1008:ALA:HB3	1:B:1009:PRO:HD3	1.94	0.49
1:A:1180:ILE:HD12	1:A:1185:PRO:HG3	1.95	0.49
1:A:1212:PRO:HB3	1:A:1263:PRO:O	2.12	0.49
1:B:1111:ILE:O	1:B:1115:HIS:HD2	1.96	0.49
1:B:1144:GLN:HE22	1:B:1298:TYR:N	2.10	0.49
1:A:1019:SER:OG	1:A:1366:TYR:HB2	2.13	0.49
1:A:1053:LEU:CD1	1:A:1083:SER:O	2.61	0.49
1:B:1197:TYR:O	1:B:1201:LYS:HB2	2.13	0.48
1:A:1066:ARG:CG	1:A:1136:ASP:OD2	2.50	0.48
1:A:1038:GLU:CB	1:A:1101:LEU:HD13	2.43	0.48
1:B:1159:MET:HE1	1:B:1182:SER:OG	2.14	0.48
1:A:1067:VAL:HG12	1:A:1129:TYR:HE1	1.77	0.48
1:A:1042:PHE:CE2	1:A:1046:ARG:NH1	2.81	0.48
1:A:1119:VAL:HG22	1:A:1151:TYR:CE2	2.49	0.48
1:A:1148:ASP:OD1	1:A:1327:LEU:HD21	2.14	0.48
1:B:1250:ARG:CZ	1:B:1303:ALA:HB2	2.44	0.48
1:A:1268:MET:HE2	1:B:1344:PHE:CD2	2.49	0.47
1:B:1003:ALA:H	1:B:1085:LEU:HB3	1.79	0.47
1:A:1188:SER:O	1:A:1189:VAL:C	2.55	0.47
1:A:1341:MET:CE	1:B:1279:LYS:HE2	2.43	0.47
1:A:1363:LEU:HB2	1:A:1366:TYR:CE2	2.49	0.47
1:A:1136:ASP:N	1:A:1137:PRO:CD	2.76	0.47
1:B:1012:ILE:HG23	1:B:1054:ALA:HB1	1.95	0.47
1:B:1046:ARG:NH1	1:B:1090:PHE:O	2.45	0.47
1:B:1061:ASN:HB2	4:B:6231:HOH:O	2.12	0.47
1:B:1149:ARG:HH22	1:B:1365:VAL:HB	1.78	0.47
1:A:1081:VAL:O	1:A:1085:LEU:HG	2.13	0.47
1:B:1346:THR:HG22	4:B:6060:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:ARG:HH22	1:A:1302:THR:C	2.22	0.47
1:A:1075:LEU:HD23	1:A:1121:THR:HG21	1.96	0.47
1:B:1258:SER:HB3	1:B:1261:THR:OG1	2.15	0.47
1:A:1058:LYS:O	1:A:1062:LEU:HD13	2.14	0.47
1:A:1163:GLN:HE22	1:A:1182:SER:N	2.08	0.47
1:A:1092:ASP:OD1	1:A:1093:LYS:N	2.48	0.47
1:A:1042:PHE:CZ	1:A:1046:ARG:NH1	2.82	0.47
1:B:1038:GLU:O	1:B:1041:SER:N	2.48	0.47
1:B:1199:MET:HG3	1:B:1238:TYR:OH	2.15	0.46
1:A:1305:THR:HG23	1:A:1306:PRO:HD2	1.96	0.46
1:B:1304:PRO:O	1:B:1317:GLY:HA3	2.16	0.46
1:A:1042:PHE:CZ	1:A:1046:ARG:HD3	2.51	0.46
1:B:1060:ILE:O	1:B:1063:LEU:HB2	2.15	0.46
1:B:1002:ASN:HB3	1:B:1082:GLN:NE2	2.25	0.46
1:B:1044:PHE:CD2	1:B:1045:LEU:HD13	2.51	0.46
1:A:1070:THR:HG23	1:A:1071:PRO:CD	2.45	0.46
1:A:1339:PHE:CE1	1:B:1339:PHE:HB3	2.51	0.46
1:B:1052:ARG:CZ	1:B:1160:LEU:HD11	2.46	0.46
1:B:1267:ILE:HA	1:B:1279:LYS:O	2.16	0.46
1:A:1143:ILE:O	1:A:1147:LEU:HB2	2.16	0.46
1:A:1353:LYS:HG2	1:A:1358:ASP:CB	2.46	0.46
1:B:1061:ASN:HA	1:B:1068:LEU:CD1	2.38	0.45
1:B:1198:ASP:O	1:B:1199:MET:O	2.33	0.45
1:B:1332:PHE:O	1:B:1333:GLN:HB2	2.16	0.45
1:A:1053:LEU:CD2	1:A:1080:TYR:CD2	2.99	0.45
1:B:1025:MET:HE2	1:B:1183:ILE:CD1	2.46	0.45
1:B:1263:PRO:HB3	1:B:1283:ARG:NE	2.32	0.45
1:B:1094:ASP:OD2	1:B:1097:ASP:HB2	2.16	0.45
1:B:1098:HIS:HB2	4:B:6117:HOH:O	2.16	0.45
1:B:1025:MET:HE3	1:B:1025:MET:HA	1.99	0.45
1:A:1196:ALA:HA	1:A:1238:TYR:CE1	2.51	0.45
1:B:1245:PHE:O	1:B:1249:MET:HG3	2.17	0.45
1:A:1012:ILE:HG23	1:A:1054:ALA:CB	2.41	0.45
1:A:1020:PRO:CD	1:A:1366:TYR:CB	2.92	0.44
1:A:1089:GLU:CG	1:A:1090:PHE:CE1	3.00	0.44
1:A:1084:LEU:HG	1:A:1088:MET:HE1	1.95	0.44
1:B:1333:GLN:HG2	1:B:1360:VAL:O	2.18	0.44
1:A:1045:LEU:HD12	1:A:1045:LEU:HA	1.78	0.44
1:A:1158:ARG:NH1	4:A:6082:HOH:O	2.51	0.44
1:A:1318:PHE:HB2	1:A:1320:TYR:CE2	2.53	0.44
1:B:1212:PRO:HD2	1:B:1249:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:VAL:HG11	1:B:1236:HIS:CD2	2.53	0.44
1:B:1320:TYR:C	1:B:1323:PRO:HD2	2.43	0.44
1:A:1152:LEU:HD13	1:A:1364:PRO:HD3	2.00	0.44
1:A:1200:ALA:HB1	1:A:1249:MET:CE	2.47	0.44
1:A:1297:SER:HB3	1:A:1300:TYR:HB3	1.98	0.44
1:A:1330:LYS:HA	1:A:1334:GLY:O	2.17	0.44
1:B:1106:ASP:CA	4:B:6193:HOH:O	2.59	0.44
1:A:1053:LEU:O	1:A:1057:MET:HG3	2.18	0.44
1:A:1223:ASN:ND2	1:A:1226:GLN:OE1	2.50	0.44
1:A:1141:GLN:C	1:A:1143:ILE:H	2.26	0.44
1:B:1023:LEU:HD11	1:B:1044:PHE:CZ	2.49	0.44
1:B:1324:ILE:O	1:B:1327:LEU:HB2	2.18	0.43
1:A:1143:ILE:O	1:A:1147:LEU:HD13	2.18	0.43
1:A:1166:LEU:HD23	1:A:1166:LEU:HA	1.87	0.43
1:B:1068:LEU:HA	1:B:1073:VAL:HG11	2.00	0.43
1:B:1203:LEU:HB3	1:B:1315:LEU:HD23	1.99	0.43
1:B:1322:LEU:N	3:B:3510:ADP:O1A	2.43	0.43
1:B:1331:TYR:O	1:B:1361:GLU:HA	2.18	0.43
1:A:1177:PRO:CB	1:A:1179:HIS:CD2	3.00	0.43
4:A:6186:HOH:O	1:B:1344:PHE:HE2	2.01	0.43
1:B:1015:PHE:HB3	1:B:1051:VAL:HA	2.00	0.43
1:A:1072:SER:OG	1:A:1124:GLN:HB3	2.18	0.43
1:A:1158:ARG:NH2	4:A:6153:HOH:O	2.45	0.43
1:A:1199:MET:CG	1:A:1238:TYR:OH	2.64	0.43
1:B:1038:GLU:HG2	1:B:1101:LEU:HD13	1.99	0.43
1:A:1070:THR:HG21	1:A:1125:GLY:CA	2.22	0.43
1:B:1043:THR:O	4:B:6190:HOH:O	2.21	0.43
1:B:1012:ILE:O	1:B:1016:SER:N	2.50	0.43
1:B:1059:GLU:OE1	1:B:1149:ARG:NH2	2.50	0.43
1:A:1060:ILE:C	1:A:1062:LEU:H	2.27	0.43
1:A:1074:GLN:O	1:A:1077:GLN:N	2.52	0.42
1:B:1082:GLN:HB3	1:B:1114:ARG:NH1	2.33	0.42
1:B:1318:PHE:HB3	1:B:1320:TYR:CE2	2.54	0.42
1:B:1041:SER:HB3	1:B:1164:HIS:ND1	2.34	0.42
1:B:1057:MET:HA	1:B:1060:ILE:HD12	2.01	0.42
1:B:1330:LYS:HE2	1:B:1335:ASP:OD2	2.19	0.42
1:A:1291:LYS:O	1:A:1294:ARG:HB2	2.19	0.42
1:A:1297:SER:HB3	1:A:1300:TYR:HB2	2.01	0.42
1:B:1124:GLN:HE22	1:B:1127:LEU:HD23	1.85	0.42
1:B:1049:LEU:HB3	1:B:1087:ILE:HD13	2.01	0.42
1:B:1164:HIS:NE2	4:B:6027:HOH:O	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:VAL:HG12	1:B:1291:LYS:HB2	2.02	0.42
1:A:1067:VAL:N	1:A:1129:TYR:HE1	2.18	0.42
1:B:1023:LEU:HD12	1:B:1023:LEU:N	2.35	0.42
1:B:1202:LEU:O	1:B:1206:LYS:HG3	2.20	0.42
1:A:1159:MET:O	1:A:1163:GLN:HG2	2.19	0.42
1:B:1128:GLU:OE1	1:B:1128:GLU:HA	2.20	0.42
1:A:1060:ILE:O	1:A:1060:ILE:CG2	2.68	0.42
1:B:1250:ARG:HB2	1:B:1315:LEU:HD12	2.02	0.42
1:A:1070:THR:HG23	1:A:1128:GLU:OE1	2.20	0.41
1:A:1020:PRO:HD2	1:A:1366:TYR:HB3	2.00	0.41
1:A:1029:LEU:HD23	1:A:1180:ILE:HD13	2.02	0.41
1:A:1068:LEU:HA	1:A:1073:VAL:HG11	2.02	0.41
1:A:1193:VAL:HG22	1:A:1241:LEU:HD13	2.01	0.41
1:B:1044:PHE:HD2	1:B:1045:LEU:HD13	1.85	0.41
1:B:1202:LEU:HD12	1:B:1202:LEU:HA	1.87	0.41
1:A:1129:TYR:O	1:A:1136:ASP:HB3	2.20	0.41
1:A:1353:LYS:NZ	4:A:6085:HOH:O	2.48	0.41
1:A:1262:LEU:HA	1:A:1263:PRO:HD3	1.90	0.41
1:B:1290:ARG:NH1	1:B:1294:ARG:HH22	2.16	0.41
1:A:1265:ILE:HD13	1:A:1265:ILE:HG21	1.90	0.41
1:B:1339:PHE:CD1	1:B:1347:ASP:HB2	2.55	0.41
1:B:1049:LEU:HB2	1:B:1050:PRO:HD3	2.03	0.41
1:B:1096:GLU:OE1	1:B:1096:GLU:HA	2.20	0.41
1:B:1190:SER:OG	1:B:1218:GLU:OE1	2.31	0.41
1:B:1218:GLU:HA	1:B:1269:VAL:O	2.20	0.41
1:B:1357:THR:O	1:B:1357:THR:HG23	2.21	0.41
1:B:1364:PRO:O	1:B:1365:VAL:C	2.62	0.41
1:A:1144:GLN:OE1	1:A:1298:TYR:CD1	2.74	0.41
1:A:1187:CYS:O	1:A:1229:HIS:HA	2.20	0.41
1:A:1332:PHE:O	1:A:1333:GLN:HB2	2.21	0.41
1:B:1159:MET:HG3	1:B:1331:TYR:CZ	2.56	0.41
1:A:1039:LYS:O	1:A:1043:THR:CB	2.68	0.41
1:A:1324:ILE:CG2	4:A:6096:HOH:O	2.68	0.41
1:B:1030:ASP:O	1:B:1036:ALA:N	2.54	0.41
1:A:1008:ALA:HB3	1:A:1009:PRO:HD3	2.02	0.41
1:A:1086:ASP:O	1:A:1089:GLU:CG	2.59	0.41
1:A:1154:ARG:HD2	4:A:6148:HOH:O	2.21	0.41
1:A:1220:ASN:HB3	1:A:1223:ASN:O	2.21	0.41
1:A:1331:TYR:OH	1:A:1361:GLU:OE2	2.39	0.41
1:B:1197:TYR:CZ	1:B:1201:LYS:HD3	2.56	0.41
1:B:1296:PHE:O	1:B:1323:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:PHE:HE1	1:B:1090:PHE:HB3	1.86	0.41
1:A:1140:ASN:HB3	1:A:1142:ASN:ND2	2.36	0.40
1:B:1111:ILE:O	1:B:1115:HIS:CD2	2.74	0.40
1:B:1205:ASP:O	1:B:1209:MET:HA	2.21	0.40
1:B:1304:PRO:O	1:B:1317:GLY:HA2	2.20	0.40
1:A:1047:GLN:O	1:A:1051:VAL:HG23	2.21	0.40
1:B:1203:LEU:HD23	1:B:1203:LEU:HA	1.78	0.40
1:B:1296:PHE:C	1:B:1323:PRO:HG3	2.47	0.40
1:A:1012:ILE:HD11	1:A:1057:MET:SD	2.61	0.40
1:A:1085:LEU:HA	1:A:1088:MET:CE	2.32	0.40
1:A:1161:ILE:O	1:A:1165:THR:OG1	2.36	0.40
1:B:1002:ASN:OD1	1:B:1082:GLN:NE2	2.54	0.40
1:B:1248:ALA:CB	1:B:1265:ILE:HD12	2.51	0.40
1:A:1203:LEU:N	1:A:1203:LEU:HD23	2.36	0.40
1:A:1250:ARG:NH2	1:A:1302:THR:O	2.54	0.40
1:B:1053:LEU:HD23	1:B:1080:TYR:CD2	2.56	0.40
1:B:1063:LEU:HG	1:B:1064:PRO:CD	2.52	0.40
1:B:1232:TYR:O	1:B:1234:PRO:HD3	2.21	0.40
1:A:1182:SER:O	1:A:1233:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/407 (81%)	290 (88%)	32 (10%)	7 (2%)	5	9
1	B	326/407 (80%)	306 (94%)	18 (6%)	2 (1%)	21	38
All	All	655/814 (80%)	596 (91%)	50 (8%)	9 (1%)	9	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1138	VAL
1	A	1224	ALA
1	A	1295	LEU
1	A	1039	LYS
1	B	1199	MET
1	A	1137	PRO
1	A	1304	PRO
1	B	1304	PRO
1	A	1095	PRO

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	305/363 (84%)	266 (87%)	39 (13%)	4	9
1	B	302/363 (83%)	267 (88%)	35 (12%)	5	11
All	All	607/726 (84%)	533 (88%)	74 (12%)	5	10

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	SER
1	A	1005	LEU
1	A	1012	ILE
1	A	1013	GLU
1	A	1016	SER
1	A	1026	LYS
1	A	1043	THR
1	A	1045	LEU
1	A	1047	GLN
1	A	1056	ILE
1	A	1061	ASN
1	A	1063	LEU
1	A	1064	PRO
1	A	1066	ARG
1	A	1067	VAL

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Mol	Chain	Res	Type
1	A	1068	LEU
1	A	1078	SER
1	A	1087	ILE
1	A	1128	GLU
1	A	1138	VAL
1	A	1152	LEU
1	A	1153	SER
1	A	1202	LEU
1	A	1217	GLN
1	A	1257	GLU
1	A	1262	LEU
1	A	1266	LYS
1	A	1268	MET
1	A	1273	GLU
1	A	1276	LEU
1	A	1318	PHE
1	A	1324	ILE
1	A	1353	LYS
1	A	1357	THR
1	A	1358	ASP
1	A	1359	SER
1	A	1361	GLU
1	A	1362	ARG
1	A	1365	VAL
1	B	1002	ASN
1	B	1013	GLU
1	B	1016	SER
1	B	1019	SER
1	B	1025	MET
1	B	1030	ASP
1	B	1041	SER
1	B	1045	LEU
1	B	1056	ILE
1	B	1063	LEU
1	B	1068	LEU
1	B	1101	LEU
1	B	1127	LEU
1	B	1152	LEU
1	B	1157	ILE
1	B	1158	ARG
1	B	1159	MET
1	B	1169	ASP

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Mol	Chain	Res	Type
1	B	1188	SER
1	B	1202	LEU
1	B	1217	GLN
1	B	1265	ILE
1	B	1276	LEU
1	B	1302	THR
1	B	1306	PRO
1	B	1315	LEU
1	B	1318	PHE
1	B	1338	LEU
1	B	1339	PHE
1	B	1340	SER
1	B	1357	THR
1	B	1359	SER
1	B	1360	VAL
1	B	1362	ARG
1	B	1365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN
1	A	1061	ASN
1	A	1116	ASN
1	A	1162	ASN
1	A	1163	GLN
1	A	1164	HIS
1	A	1186	ASN
1	A	1217	GLN
1	A	1223	ASN
1	A	1236	HIS
1	B	1002	ASN
1	B	1027	GLN
1	B	1055	ASN
1	B	1082	GLN
1	B	1115	HIS
1	B	1116	ASN
1	B	1144	GLN
1	B	1162	ASN
1	B	1256	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	3510	2	28,29,29	1.58	6 (21%)	43,45,45	2.25	11 (25%)
3	ADP	A	3500	2	28,29,29	1.57	5 (17%)	43,45,45	2.25	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	3510	2	-	7/16/32/32	0/3/3/3
3	ADP	A	3500	2	-	7/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500	ADP	PA-O3A	-3.87	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3510	ADP	PA-O3A	-3.85	1.55	1.59
3	B	3510	ADP	C5-N7	-2.80	1.34	1.39
3	A	3500	ADP	C5-N7	-2.78	1.34	1.39
3	B	3510	ADP	PB-O2B	2.77	1.65	1.54
3	A	3500	ADP	PB-O2B	2.77	1.65	1.54
3	A	3500	ADP	C4-N9	-2.77	1.31	1.37
3	B	3510	ADP	C4-N9	-2.75	1.32	1.37
3	B	3510	ADP	C5-C4	2.75	1.44	1.39
3	A	3500	ADP	C5-C4	2.74	1.44	1.39
3	B	3510	ADP	C8-N7	2.02	1.35	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3510	ADP	C5-C4-N3	-6.42	117.87	126.72
3	A	3500	ADP	C5-C4-N3	-6.41	117.89	126.72
3	A	3500	ADP	N3-C2-N1	-6.15	119.27	128.58
3	B	3510	ADP	N3-C2-N1	-6.15	119.27	128.58
3	A	3500	ADP	C4-C5-N7	-5.12	104.73	110.58
3	B	3510	ADP	C4-C5-N7	-5.11	104.74	110.58
3	B	3510	ADP	C2-N3-C4	5.02	124.10	111.83
3	A	3500	ADP	C2-N3-C4	5.02	124.09	111.83
3	B	3510	ADP	N9-C8-N7	-4.18	108.00	113.94
3	A	3500	ADP	N9-C8-N7	-4.18	108.01	113.94
3	B	3510	ADP	N3-C4-N9	3.92	133.83	127.17
3	A	3500	ADP	N3-C4-N9	3.91	133.82	127.17
3	A	3500	ADP	C5-N7-C8	3.37	108.75	103.45
3	B	3510	ADP	C5-N7-C8	3.37	108.75	103.45
3	B	3510	ADP	O4'-C1'-N9	3.15	114.14	108.09
3	A	3500	ADP	O4'-C1'-N9	3.14	114.12	108.09
3	A	3500	ADP	C6-C5-N7	2.34	136.61	132.09
3	B	3510	ADP	C6-C5-N7	2.33	136.59	132.09
3	B	3510	ADP	C5-C4-N9	2.14	108.14	105.81
3	A	3500	ADP	C4-N9-C8	2.14	107.98	105.74
3	B	3510	ADP	C4-N9-C8	2.14	107.98	105.74
3	A	3500	ADP	C5-C4-N9	2.14	108.14	105.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3500	ADP	PA-O3A-PB-O3B

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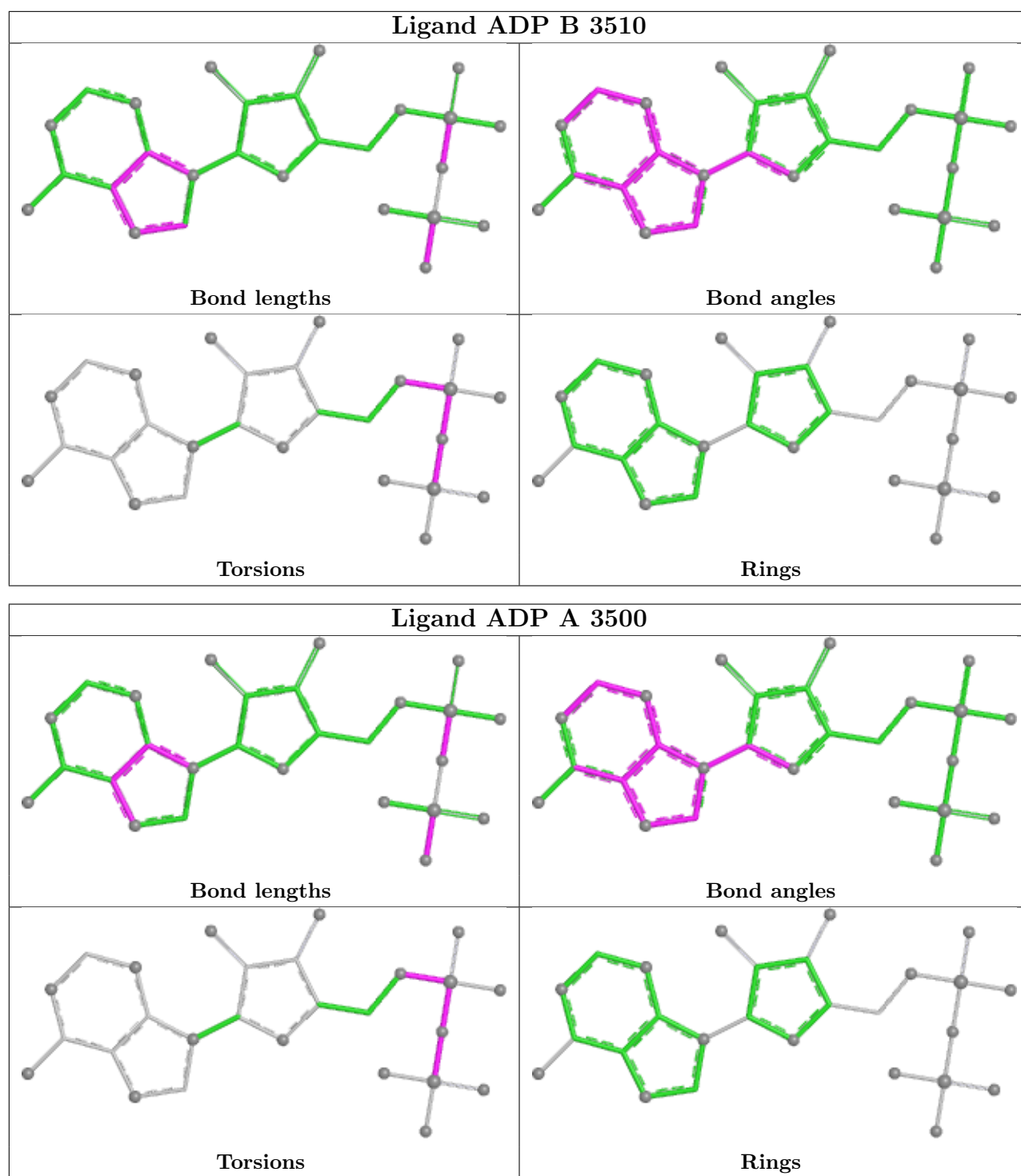
Mol	Chain	Res	Type	Atoms
3	A	3500	ADP	C5'-O5'-PA-O1A
3	A	3500	ADP	C5'-O5'-PA-O3A
3	B	3510	ADP	PA-O3A-PB-O3B
3	B	3510	ADP	C5'-O5'-PA-O1A
3	B	3510	ADP	C5'-O5'-PA-O3A
3	A	3500	ADP	PB-O3A-PA-O1A
3	B	3510	ADP	PB-O3A-PA-O1A
3	A	3500	ADP	C5'-O5'-PA-O2A
3	B	3510	ADP	C5'-O5'-PA-O2A
3	A	3500	ADP	PB-O3A-PA-O2A
3	B	3510	ADP	PB-O3A-PA-O2A
3	A	3500	ADP	PA-O3A-PB-O1B
3	B	3510	ADP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3510	ADP	9	0
3	A	3500	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	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1178:LYS	C	1179:HIS	N	1.16
1	A	1090:PHE	C	1091:LEU	N	1.14

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	339/407 (83%)	-1.37	0 100 100	19, 41, 80, 117	0
1	B	336/407 (82%)	-1.41	0 100 100	20, 40, 70, 107	0
All	All	675/814 (82%)	-1.39	0 100 100	19, 41, 74, 117	0

There are no RSRZ outliers to report.

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.

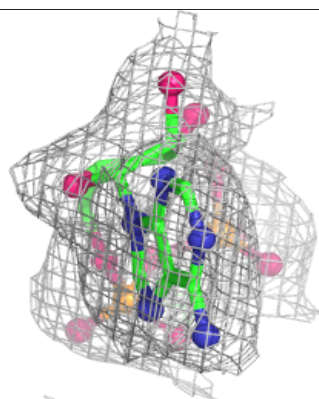
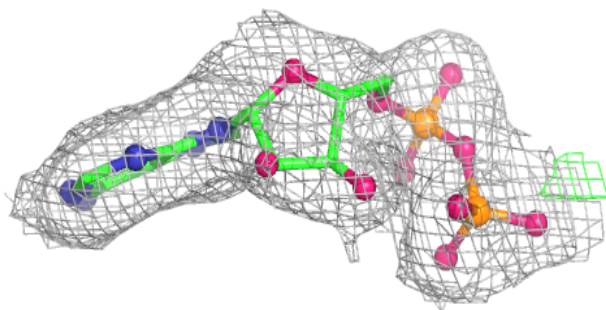
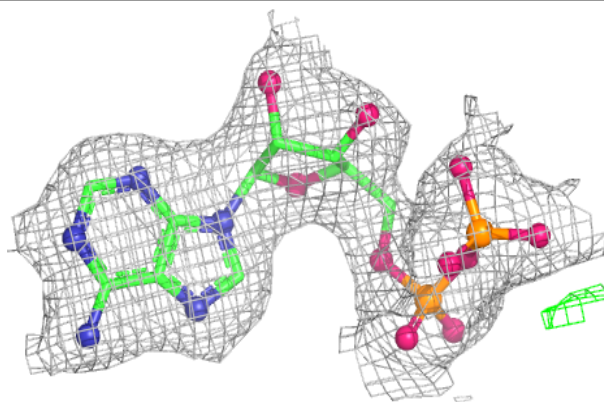
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	4601	1/1	0.99	0.02	44,44,44,44	0
2	MG	B	4611	1/1	0.99	0.04	47,47,47,47	0
3	ADP	A	3500	27/27	1.00	0.02	16,26,35,38	0
3	ADP	B	3510	27/27	1.00	0.02	16,26,35,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

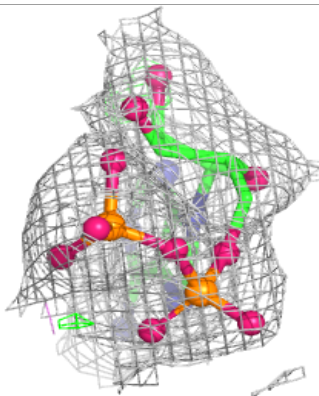
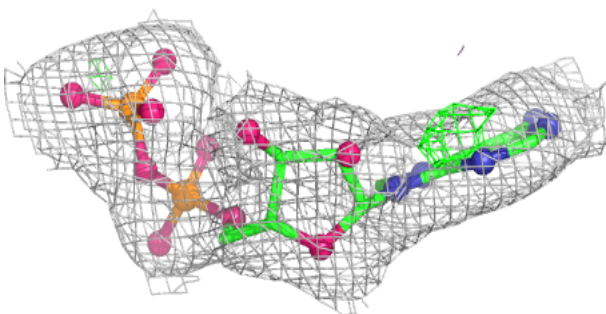
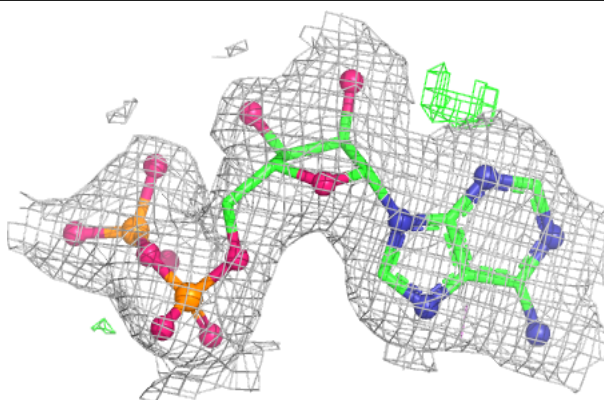
Electron density around ADP A 3500:

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



Electron density around ADP B 3510:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.