



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3UDS
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with ADP.
Authors : Gosein, V.; Leung, T.-F.; Krajden, O.; Miller, G.J.
Deposited on : 2011-10-28
Resolution : 3.10 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

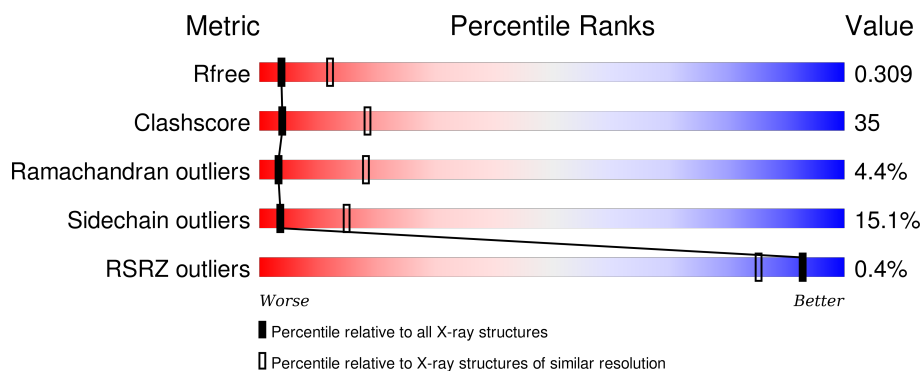
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	493	 31% 35% 7% 26%
1	B	493	 28% 35% 8% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5796 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 Inositol-pentakisphosphate 2-kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2919	1876	489	543	11			
1	B	352	Total	C	N	O	S	0	0	0
			2821	1816	474	522	9			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	EXPRESSION TAG	UNP Q93YN9
A	-32	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-31	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-30	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-29	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-28	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-27	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-26	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-25	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-24	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-23	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-22	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-21	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-20	LEU	-	EXPRESSION TAG	UNP Q93YN9
A	-19	VAL	-	EXPRESSION TAG	UNP Q93YN9
A	-18	PRO	-	EXPRESSION TAG	UNP Q93YN9
A	-17	ARG	-	EXPRESSION TAG	UNP Q93YN9
A	-16	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-15	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-14	HIS	-	EXPRESSION TAG	UNP Q93YN9
A	-13	MET	-	EXPRESSION TAG	UNP Q93YN9
A	-12	ALA	-	EXPRESSION TAG	UNP Q93YN9
A	-11	SER	-	EXPRESSION TAG	UNP Q93YN9
A	-10	MET	-	EXPRESSION TAG	UNP Q93YN9
A	-9	THR	-	EXPRESSION TAG	UNP Q93YN9

Continued on next page...

Continued from previous page...

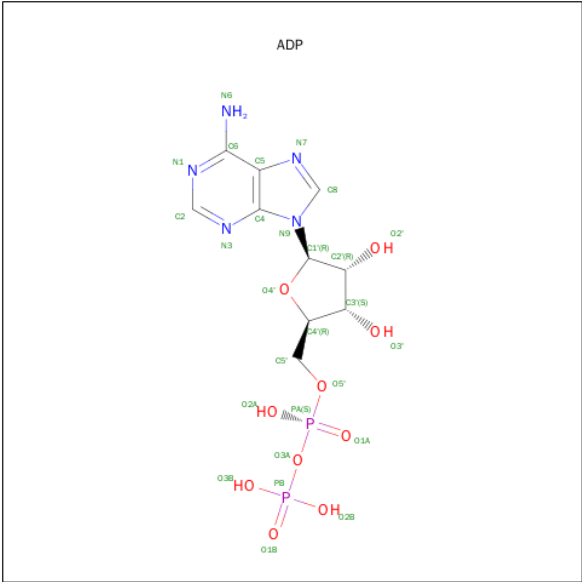
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-7	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-6	GLN	-	EXPRESSION TAG	UNP Q93YN9
A	-5	GLN	-	EXPRESSION TAG	UNP Q93YN9
A	-4	MET	-	EXPRESSION TAG	UNP Q93YN9
A	-3	GLY	-	EXPRESSION TAG	UNP Q93YN9
A	-2	ARG	-	EXPRESSION TAG	UNP Q93YN9
A	-1	ILE	-	EXPRESSION TAG	UNP Q93YN9
A	0	LEU	-	EXPRESSION TAG	UNP Q93YN9
A	54	SER	ALA	CONFLICT	UNP Q93YN9
A	90	GLN	LYS	CONFLICT	UNP Q93YN9
A	157	THR	SER	CONFLICT	UNP Q93YN9
A	185	ILE	MET	CONFLICT	UNP Q93YN9
A	204	ILE	ASN	CONFLICT	UNP Q93YN9
A	224	ARG	SER	CONFLICT	UNP Q93YN9
A	321	CYS	SER	CONFLICT	UNP Q93YN9
A	325	ILE	LEU	CONFLICT	UNP Q93YN9
A	337	ARG	LYS	CONFLICT	UNP Q93YN9
A	452	ASP	-	EXPRESSION TAG	UNP Q93YN9
A	453	TYR	-	EXPRESSION TAG	UNP Q93YN9
A	454	LYS	-	EXPRESSION TAG	UNP Q93YN9
A	455	ASP	-	EXPRESSION TAG	UNP Q93YN9
A	456	ASP	-	EXPRESSION TAG	UNP Q93YN9
A	457	ASP	-	EXPRESSION TAG	UNP Q93YN9
A	458	ASP	-	EXPRESSION TAG	UNP Q93YN9
A	459	LYS	-	EXPRESSION TAG	UNP Q93YN9
B	-33	MET	-	EXPRESSION TAG	UNP Q93YN9
B	-32	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-31	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-30	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-29	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-28	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-27	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-26	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-25	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-24	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-23	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-22	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-21	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-20	LEU	-	EXPRESSION TAG	UNP Q93YN9
B	-19	VAL	-	EXPRESSION TAG	UNP Q93YN9
B	-18	PRO	-	EXPRESSION TAG	UNP Q93YN9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ARG	-	EXPRESSION TAG	UNP Q93YN9
B	-16	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-15	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-14	HIS	-	EXPRESSION TAG	UNP Q93YN9
B	-13	MET	-	EXPRESSION TAG	UNP Q93YN9
B	-12	ALA	-	EXPRESSION TAG	UNP Q93YN9
B	-11	SER	-	EXPRESSION TAG	UNP Q93YN9
B	-10	MET	-	EXPRESSION TAG	UNP Q93YN9
B	-9	THR	-	EXPRESSION TAG	UNP Q93YN9
B	-8	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-7	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-6	GLN	-	EXPRESSION TAG	UNP Q93YN9
B	-5	GLN	-	EXPRESSION TAG	UNP Q93YN9
B	-4	MET	-	EXPRESSION TAG	UNP Q93YN9
B	-3	GLY	-	EXPRESSION TAG	UNP Q93YN9
B	-2	ARG	-	EXPRESSION TAG	UNP Q93YN9
B	-1	ILE	-	EXPRESSION TAG	UNP Q93YN9
B	0	LEU	-	EXPRESSION TAG	UNP Q93YN9
B	54	SER	ALA	CONFLICT	UNP Q93YN9
B	90	GLN	LYS	CONFLICT	UNP Q93YN9
B	157	THR	SER	CONFLICT	UNP Q93YN9
B	185	ILE	MET	CONFLICT	UNP Q93YN9
B	204	ILE	ASN	CONFLICT	UNP Q93YN9
B	224	ARG	SER	CONFLICT	UNP Q93YN9
B	321	CYS	SER	CONFLICT	UNP Q93YN9
B	325	ILE	LEU	CONFLICT	UNP Q93YN9
B	337	ARG	LYS	CONFLICT	UNP Q93YN9
B	452	ASP	-	EXPRESSION TAG	UNP Q93YN9
B	453	TYR	-	EXPRESSION TAG	UNP Q93YN9
B	454	LYS	-	EXPRESSION TAG	UNP Q93YN9
B	455	ASP	-	EXPRESSION TAG	UNP Q93YN9
B	456	ASP	-	EXPRESSION TAG	UNP Q93YN9
B	457	ASP	-	EXPRESSION TAG	UNP Q93YN9
B	458	ASP	-	EXPRESSION TAG	UNP Q93YN9
B	459	LYS	-	EXPRESSION TAG	UNP Q93YN9

- 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

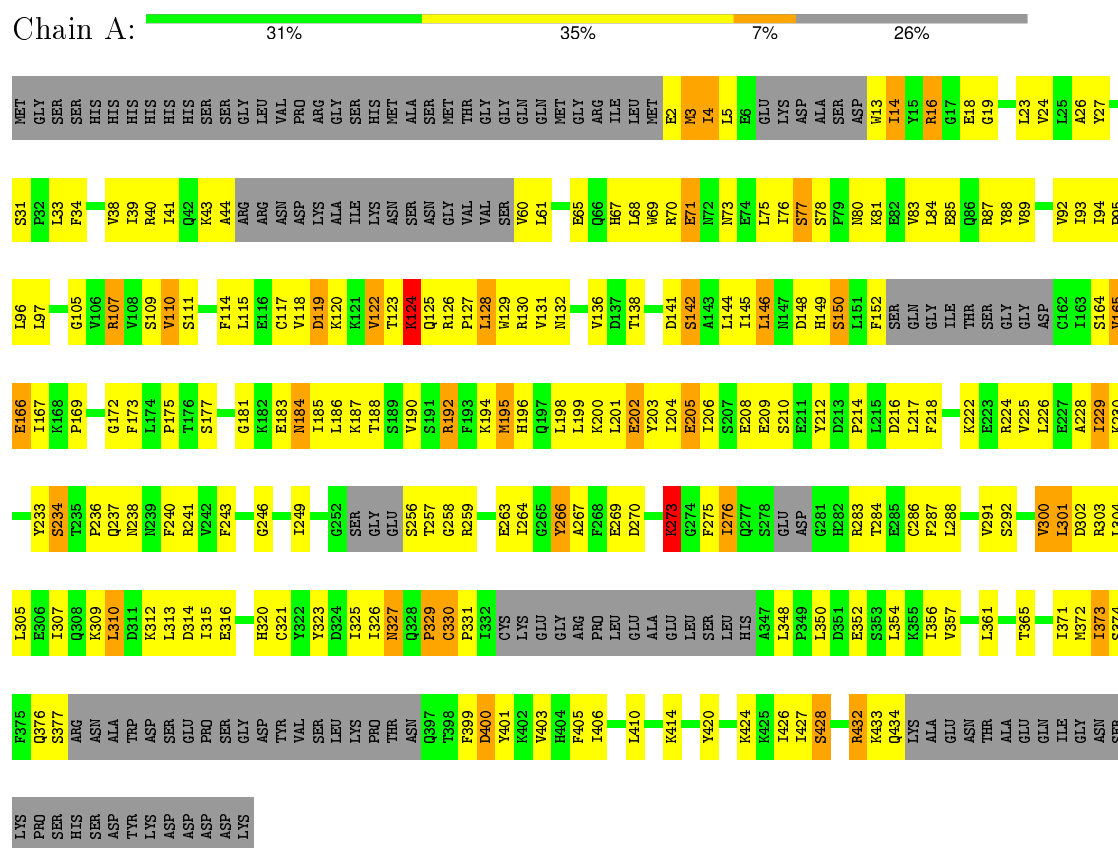
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

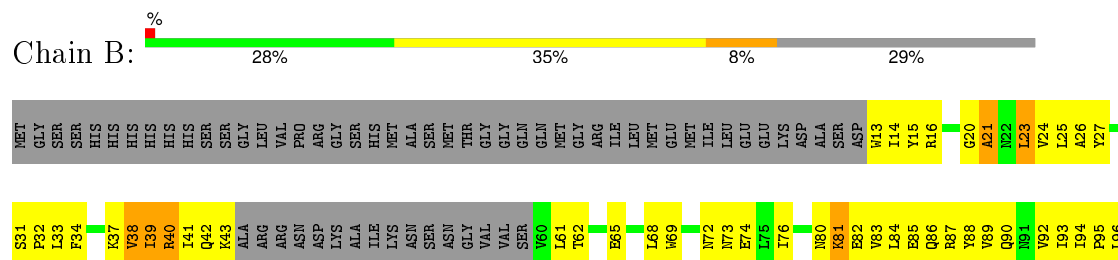
3 Residue-property plots

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: Inositol-pentakisphosphate 2-kinase



• Molecule 1: Inositol-pentakisphosphate 2-kinase



PRO	SER	HIS	SER	ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS
GLU	PRO	HIS	GLY	ASP	TYR	VAL	SER	LEU	LYS	PRO	THR
										ASN	Q397
											T398
											F399
											D400
											Y401
											K402
											V403
											R404
											F406
											D407
											L408
											S409
											L410
											K411
											K414
											R415
											S418
											Y419
											L422
											D423
											I426
											I427
											S428
											F429
											Y430
											M431
											R432
											K433
											Q434
											LYS
											ALA
											GLU
											ASN
											THR
											ALA
											GLU
											GLN
											ILE
											GLY
											ASN
											SER
											LYS
D314	I315	E316	G317	Y323	D324	I325	I326	F329	CYS	PRO	ILE
											CYS
											S261
											LYS
											GLU
											GLY
											ARG
											PRO
											LEU
											ALA
											GLU
											LEU
											SER
											HIS
											A347
											P349
											E352
											S353
											L354
											K355
											I356
											V357
											K358
											E359
											Y360
											A363
											K367
											D368
											C369
											LYS
											M372
											I373
											S374
											F375
											GLN
											SER
											ARG
											ASN
											ALA
											TRP
											K312
											ASP
											SER
											LYS
R241	I249	L250	G251	SER	GLY	SER	T257	G258	R259	T260	S261
											L262
											E263
											I264
											A267
											D270
											A271
											L272
											F275
											I276
											GLN
											SER
											GLU
											ASP
											G281
											H282
											R283
											T284
											F287
											L288
											Q289
											L290
											V291
											S292
											D293
											Y296
											G297
											S298
											G299
											V300
											I301
											D302
											R303
											E306
											I307
											L310
											D311
											K312
											ASP
											SER
I163	S164	V165	E166	P169	K170	L174	T175	S177	R178	K182	E183
											M184
											I185
											L186
											K187
											T188
											R192
											M195
											H196
											L199
											K200
											L201
											E202
											Y203
											I204
											E205
											I206
											S207
											Y212
											D213
											D216
											L217
											F218
											K222
											E223
											R224
											V225
											L226
											E227
											A228
											I229
											K230
											A231
											L232
											Q237
											M238
											M239
											F240
L97	K100	H101	V106	R107	V108	S109	V110	S111	K112	E113	F114
											L115
											G117
											V118
											D119
											K120
											K121
											V122
											T123
											K124
											Q125
											R126
											P127
											L128
											M129
											R130
											V131
											H132
											A133
											M134
											N135
											V136
											H140
											D141
											S142
											A143
											L144
											I145
											L146
											N147
											D148
											H149
											S150
											L151
											F152
											S153
											GLN
											ILE
											THR
											SER
											GLY
											ASP
											C162

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.29Å 59.88Å 82.91Å 83.40° 89.40° 65.30°	Depositor
Resolution (Å)	42.82 – 3.10 42.82 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.2 (42.82-3.10) 83.2 (42.82-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.237 , 0.312 0.221 , 0.309	Depositor DCC
R_{free} test set	875 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27678 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5796	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2970	0.65	0/3999
1	B	0.46	0/2872	0.62	0/3868
All	All	0.47	0/5842	0.64	0/7867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2919	0	2962	191	0
1	B	2821	0	2866	221	0
2	A	27	0	12	2	0
2	B	27	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5796	0	5852	404	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (404) 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:70:ARG:HA	1:A:76:ILE:HD13	1.41	0.99
1:B:43:LYS:HG2	1:B:136:VAL:HA	1.46	0.95
1:B:74:GLU:HB3	1:B:87:ARG:HH11	1.32	0.94
1:B:80:ASN:OD1	1:B:82:GLU:HB2	1.73	0.88
1:B:16:ARG:HH22	1:B:150:SER:HB3	1.39	0.86
1:B:312:LYS:O	1:B:313:LEU:HB2	1.73	0.86
1:A:70:ARG:HH11	1:A:70:ARG:HG2	1.41	0.86
1:A:325:ILE:HD13	1:A:354:LEU:HD23	1.58	0.85
1:B:307:ILE:O	1:B:310:LEU:HB2	1.76	0.85
1:B:74:GLU:HB3	1:B:87:ARG:NH1	1.93	0.84
1:B:148:ASP:OD1	1:B:151:LEU:HG	1.82	0.80
1:A:184:ASN:HB3	1:A:427:ILE:HG12	1.63	0.80
1:B:128:LEU:HA	1:B:131:VAL:HG22	1.64	0.79
1:A:329:PRO:O	1:A:331:PRO:HD3	1.81	0.79
1:B:229:ILE:HD11	1:B:288:LEU:HB3	1.65	0.78
1:B:422:LEU:HD11	1:B:426:ILE:HD11	1.64	0.78
1:A:304:LEU:HD13	1:A:405:PHE:HE2	1.48	0.78
1:A:304:LEU:HD13	1:A:405:PHE:CE2	2.19	0.78
1:A:110:VAL:HG22	1:A:141:ASP:HA	1.67	0.76
1:A:185:ILE:HG12	1:A:185:ILE:O	1.84	0.76
1:B:415:ARG:HG2	1:B:419:TYR:CZ	2.19	0.76
1:A:85:GLU:O	1:A:89:VAL:HG23	1.85	0.76
1:A:61:LEU:HD22	1:A:65:GLU:HB3	1.67	0.76
1:B:300:VAL:HG22	1:B:405:PHE:CZ	2.22	0.75
1:A:60:VAL:HG22	1:A:78:SER:O	1.87	0.74
1:A:19:GLY:HA3	2:A:600:ADP:O2B	1.88	0.74
1:B:373:ILE:HG22	1:B:403:VAL:HG22	1.68	0.74
1:B:110:VAL:HG22	1:B:141:ASP:HA	1.68	0.74
1:B:122:VAL:HG23	1:B:123:THR:H	1.52	0.74
1:B:13:TRP:HA	1:B:26:ALA:O	1.88	0.73
1:A:320:HIS:ND1	1:A:330:CYS:SG	2.60	0.73
1:A:217:LEU:HG	1:A:301:LEU:HD21	1.70	0.72
1:B:374:SER:O	1:B:401:TYR:HA	1.90	0.72
1:B:355:LYS:O	1:B:359:GLU:HG3	1.90	0.71
1:B:429:PHE:HA	1:B:432:ARG:CD	2.21	0.71
1:A:216:ASP:HB2	1:A:228:ALA:HB2	1.72	0.71
1:B:100:LYS:HD3	1:B:101:HIS:NE2	2.07	0.70
1:A:300:VAL:HG11	1:A:403:VAL:HG11	1.72	0.70
1:A:276:ILE:HG23	1:A:283:ARG:HD2	1.71	0.70
1:B:80:ASN:HD21	1:B:83:VAL:HG23	1.56	0.70
1:B:83:VAL:O	1:B:87:ARG:HG3	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:OE2	1:A:283:ARG:HB2	1.91	0.70
1:B:325:ILE:HD12	1:B:357:VAL:HG21	1.73	0.70
1:A:96:LEU:HB3	1:A:307:ILE:HD11	1.74	0.70
1:A:270:ASP:O	1:A:273:LYS:HD2	1.91	0.69
1:B:429:PHE:HA	1:B:432:ARG:HD3	1.74	0.69
1:A:287:PHE:HD2	1:A:288:LEU:HD23	1.58	0.69
1:B:119:ASP:OD2	1:B:136:VAL:HG21	1.93	0.69
1:B:120:LYS:O	1:B:123:THR:HG23	1.93	0.69
1:A:305:LEU:HG	1:A:309:LYS:HD2	1.76	0.68
1:A:184:ASN:HB3	1:A:427:ILE:CG1	2.23	0.68
1:B:348:LEU:HD12	1:B:349:PRO:HD2	1.76	0.68
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.29	0.68
1:B:284:THR:O	1:B:284:THR:HG22	1.93	0.68
1:B:166:GLU:HB3	1:B:241:ARG:HB2	1.76	0.68
1:B:163:ILE:O	1:B:375:PHE:HD1	1.77	0.67
1:A:129:TRP:CE2	1:A:130:ARG:HG2	2.29	0.67
1:B:83:VAL:HG12	1:B:87:ARG:HE	1.60	0.67
1:A:60:VAL:HG11	1:A:80:ASN:HA	1.74	0.66
1:B:106:VAL:O	1:B:144:LEU:HD23	1.95	0.66
1:A:123:THR:OG1	1:A:124:LYS:HD2	1.95	0.66
1:A:204:ILE:O	1:A:204:ILE:HG22	1.96	0.66
1:A:128:LEU:HA	1:A:131:VAL:HG12	1.77	0.66
1:A:131:VAL:O	1:B:182:LYS:HE2	1.96	0.66
1:B:201:LEU:HD12	1:B:206:ILE:HD11	1.78	0.66
1:B:20:GLY:O	1:B:21:ALA:HB2	1.96	0.65
1:B:422:LEU:O	1:B:426:ILE:HG12	1.95	0.65
1:B:122:VAL:HG23	1:B:123:THR:N	2.11	0.64
1:A:123:THR:N	1:A:126:ARG:HG3	2.12	0.64
1:B:107:ARG:HG2	1:B:142:SER:OG	1.98	0.64
1:B:222:LYS:HD3	1:B:296:TYR:CG	2.33	0.64
1:A:124:LYS:HE3	1:A:124:LYS:HA	1.79	0.64
1:A:23:LEU:HD22	1:A:43:LYS:HG2	1.79	0.63
1:A:307:ILE:O	1:A:310:LEU:HB2	1.98	0.63
1:A:199:LEU:HD11	1:A:203:TYR:HE2	1.64	0.63
1:B:16:ARG:NH2	1:B:150:SER:HB3	2.12	0.63
1:B:204:ILE:HG22	1:B:204:ILE:O	1.99	0.62
1:B:72:ASN:O	1:B:76:ILE:HG12	1.99	0.62
1:A:302:ASP:O	1:A:304:LEU:N	2.29	0.62
1:B:300:VAL:HG22	1:B:405:PHE:HZ	1.62	0.62
1:B:127:PRO:HD2	1:B:130:ARG:HB2	1.82	0.62
1:B:232:LEU:HB3	1:B:240:PHE:CD1	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB3	1:B:276:ILE:CG2	2.31	0.61
1:B:272:LEU:HB2	1:B:283:ARG:HD2	1.81	0.61
1:B:83:VAL:CG1	1:B:87:ARG:HE	2.13	0.61
1:A:111:SER:O	1:A:114:PHE:HB3	2.00	0.61
1:A:225:VAL:O	1:A:229:ILE:HG22	2.01	0.61
1:A:80:ASN:OD1	1:A:83:VAL:HG23	2.00	0.61
1:A:432:ARG:O	1:A:434:GLN:N	2.34	0.61
1:A:2:GLU:O	1:A:3:MET:HB2	2.01	0.60
1:A:229:ILE:CD1	1:A:291:VAL:HB	2.31	0.60
1:A:61:LEU:CD2	1:A:65:GLU:HB3	2.30	0.60
1:B:120:LYS:O	1:B:122:VAL:N	2.35	0.60
1:B:126:ARG:HE	1:B:131:VAL:HG12	1.67	0.59
1:B:373:ILE:HA	1:B:402:LYS:O	2.02	0.59
1:B:312:LYS:O	1:B:313:LEU:CB	2.46	0.59
1:B:422:LEU:CD1	1:B:426:ILE:HD11	2.30	0.59
1:B:80:ASN:ND2	1:B:83:VAL:HG23	2.16	0.59
1:B:24:VAL:HG21	2:B:600:ADP:C8	2.37	0.59
1:B:23:LEU:HD22	1:B:23:LEU:N	2.18	0.59
1:A:38:VAL:HG12	1:A:148:ASP:HB2	1.85	0.59
1:B:313:LEU:O	1:B:314:ASP:HB3	2.01	0.58
1:A:321:CYS:O	1:A:325:ILE:HG13	2.03	0.58
1:B:114:PHE:O	1:B:117:CYS:SG	2.60	0.58
1:B:113:GLU:H	1:B:115:LEU:HD23	1.68	0.58
1:B:81:LYS:O	1:B:84:LEU:HB3	2.03	0.58
1:A:68:LEU:HD23	1:A:69:TRP:CE2	2.38	0.58
1:A:325:ILE:HD12	1:A:357:VAL:HG21	1.86	0.58
1:B:226:LEU:HD12	1:B:229:ILE:CD1	2.34	0.57
1:B:276:ILE:HG23	1:B:283:ARG:HG2	1.86	0.57
1:A:313:LEU:O	1:A:314:ASP:HB3	2.05	0.57
1:A:195:MET:HE1	1:A:427:ILE:HA	1.85	0.57
1:A:276:ILE:HG12	1:A:283:ARG:HG2	1.87	0.57
1:A:70:ARG:NH1	1:A:70:ARG:HG2	2.14	0.57
1:B:222:LYS:HD3	1:B:296:TYR:CD2	2.40	0.57
1:A:127:PRO:HG2	1:A:130:ARG:HB2	1.87	0.57
1:B:16:ARG:HH22	1:B:150:SER:CB	2.13	0.56
1:B:199:LEU:HD22	1:B:426:ILE:HD13	1.87	0.56
1:A:226:LEU:HA	1:A:229:ILE:HG23	1.87	0.56
1:B:149:HIS:O	1:B:374:SER:OG	2.23	0.56
1:A:199:LEU:O	1:A:200:LYS:C	2.44	0.56
1:A:124:LYS:N	1:A:124:LYS:HD2	2.21	0.56
1:B:73:ASN:O	1:B:76:ILE:HG13	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PRO:O	1:A:331:PRO:CD	2.54	0.56
1:A:175:PRO:HD2	1:A:187:LYS:O	2.05	0.56
1:B:272:LEU:HB3	1:B:276:ILE:HG22	1.87	0.56
1:B:150:SER:O	1:B:162:CYS:HB3	2.06	0.55
1:A:81:LYS:HA	1:A:84:LEU:HB3	1.88	0.55
1:B:127:PRO:O	1:B:131:VAL:HG13	2.06	0.55
1:B:202:GLU:HG2	1:B:429:PHE:CE1	2.41	0.55
1:A:266:TYR:O	1:A:270:ASP:HB2	2.06	0.55
1:A:146:LEU:N	1:A:146:LEU:HD12	2.21	0.55
1:A:374:SER:O	1:A:401:TYR:HA	2.06	0.55
1:B:112:LYS:HA	1:B:115:LEU:HD23	1.87	0.55
1:A:150:SER:OG	1:A:246:GLY:HA2	2.07	0.55
1:A:212:TYR:CE2	1:A:214:PRO:HG3	2.41	0.55
1:B:429:PHE:HA	1:B:432:ARG:HD2	1.89	0.55
1:B:276:ILE:HG23	1:B:283:ARG:CG	2.37	0.55
1:B:229:ILE:HA	1:B:232:LEU:HD12	1.90	0.54
1:A:199:LEU:HD11	1:A:203:TYR:CE2	2.41	0.54
1:A:216:ASP:HB3	1:A:224:ARG:O	2.08	0.54
1:A:132:ASN:O	1:B:182:LYS:HG3	2.07	0.54
1:B:40:ARG:C	1:B:41:ILE:HD12	2.28	0.54
1:A:302:ASP:C	1:A:304:LEU:H	2.11	0.54
1:A:70:ARG:HH11	1:A:70:ARG:CG	2.17	0.54
1:A:276:ILE:CD1	1:A:283:ARG:HA	2.37	0.54
1:A:236:PRO:HB3	1:A:240:PHE:HB3	1.89	0.54
1:B:149:HIS:CE1	1:B:404:HIS:CG	2.96	0.54
1:A:123:THR:CA	1:A:126:ARG:HG3	2.37	0.54
1:A:203:TYR:CE1	1:B:312:LYS:HB3	2.42	0.54
1:A:2:GLU:OE2	1:A:3:MET:N	2.40	0.54
1:B:37:LYS:NZ	1:B:147:ASN:HD21	2.05	0.54
1:A:4:ILE:HA	1:A:109:SER:HB2	1.89	0.54
1:B:120:LYS:HD2	1:B:123:THR:HG21	1.90	0.54
1:A:125:GLN:H	1:A:125:GLN:CD	2.10	0.54
1:B:37:LYS:NZ	1:B:147:ASN:ND2	2.56	0.54
1:B:126:ARG:HH22	1:B:135:ASN:HA	1.73	0.54
1:B:16:ARG:HB3	1:B:24:VAL:O	2.08	0.54
1:B:276:ILE:HG23	1:B:283:ARG:CD	2.38	0.54
1:A:83:VAL:HG12	1:A:87:ARG:HD2	1.90	0.53
1:B:100:LYS:HG2	1:B:101:HIS:CD2	2.43	0.53
1:B:110:VAL:HG22	1:B:141:ASP:CA	2.36	0.53
1:B:373:ILE:CG2	1:B:403:VAL:HG22	2.37	0.53
1:A:23:LEU:HD22	1:A:43:LYS:CG	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:O	1:A:3:MET:CB	2.56	0.53
1:A:71:GLU:CD	1:A:71:GLU:H	2.11	0.53
1:B:226:LEU:HG	1:B:230:LYS:HE2	1.91	0.53
1:B:85:GLU:O	1:B:89:VAL:HG23	2.09	0.52
1:A:276:ILE:HD13	1:A:283:ARG:HA	1.92	0.52
1:A:373:ILE:HD13	1:A:403:VAL:HG22	1.90	0.52
1:B:275:PHE:CZ	1:B:399:PHE:CE2	2.98	0.52
1:A:119:ASP:OD2	1:A:136:VAL:HG13	2.09	0.52
1:B:80:ASN:HD21	1:B:83:VAL:CG2	2.22	0.52
1:B:225:VAL:HG21	1:B:296:TYR:HD1	1.75	0.52
1:B:15:TYR:HA	1:B:25:LEU:HD13	1.92	0.52
1:A:43:LYS:O	1:A:44:ALA:HB2	2.09	0.52
1:A:291:VAL:O	1:A:292:SER:C	2.48	0.52
1:A:195:MET:HE2	1:A:426:ILE:HG22	1.92	0.51
1:B:126:ARG:NH2	1:B:131:VAL:HA	2.25	0.51
1:A:188:THR:HG22	1:A:188:THR:O	2.10	0.51
1:B:73:ASN:ND2	1:B:74:GLU:OE2	2.42	0.51
1:B:82:GLU:HB3	1:B:107:ARG:HG3	1.93	0.51
1:A:93:ILE:O	1:A:96:LEU:N	2.32	0.51
1:B:20:GLY:O	1:B:21:ALA:CB	2.58	0.51
1:B:115:LEU:HD22	1:B:115:LEU:H	1.74	0.51
1:B:261:SER:OG	1:B:264:ILE:HG13	2.11	0.51
1:B:86:GLN:OE1	1:B:107:ARG:HB2	2.11	0.51
1:B:93:ILE:HG21	1:B:408:LEU:HD13	1.92	0.51
1:B:163:ILE:O	1:B:375:PHE:CD1	2.60	0.51
1:B:16:ARG:NH2	1:B:150:SER:CB	2.74	0.51
1:A:105:GLY:HA3	1:A:144:LEU:CD2	2.41	0.51
1:B:97:LEU:HD23	1:B:307:ILE:HD11	1.93	0.50
1:A:148:ASP:O	1:A:150:SER:N	2.44	0.50
1:B:24:VAL:C	1:B:25:LEU:HD22	2.32	0.50
1:B:287:PHE:O	1:B:290:LEU:HB3	2.11	0.50
1:A:226:LEU:HG	1:A:230:LYS:HE2	1.93	0.50
1:A:107:ARG:HD2	1:A:142:SER:OG	2.11	0.50
1:A:204:ILE:HD11	1:B:356:ILE:HD11	1.94	0.50
1:A:166:GLU:HA	1:A:371:ILE:O	2.12	0.50
1:A:39:ILE:O	1:A:39:ILE:HG23	2.11	0.50
1:A:315:ILE:HG23	1:A:316:GLU:N	2.25	0.50
1:B:212:TYR:CD1	1:B:213:ASP:N	2.79	0.50
1:B:275:PHE:HZ	1:B:375:PHE:HB2	1.77	0.50
1:B:201:LEU:CD1	1:B:206:ILE:HD11	2.41	0.50
1:A:81:LYS:O	1:A:84:LEU:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE2	1:A:406:ILE:HD11	2.11	0.50
1:B:126:ARG:NE	1:B:131:VAL:HG12	2.25	0.50
1:B:27:TYR:CE2	1:B:34:PHE:HB2	2.47	0.50
1:B:92:VAL:O	1:B:96:LEU:HD23	2.12	0.50
1:A:201:LEU:HD12	1:A:206:ILE:HG13	1.93	0.49
1:B:177:SER:HB2	1:B:313:LEU:HA	1.94	0.49
1:A:284:THR:O	1:A:288:LEU:HG	2.12	0.49
1:A:302:ASP:C	1:A:304:LEU:N	2.66	0.49
1:B:115:LEU:O	1:B:118:VAL:HG23	2.12	0.49
1:B:249:ILE:HG13	1:B:250:LEU:N	2.27	0.49
1:B:126:ARG:HB3	1:B:131:VAL:CG1	2.42	0.49
1:A:287:PHE:CD2	1:A:288:LEU:HD23	2.44	0.49
1:B:226:LEU:HD12	1:B:229:ILE:HD12	1.95	0.48
1:A:23:LEU:HD11	1:A:126:ARG:NH1	2.28	0.48
1:B:314:ASP:O	1:B:317:GLY:N	2.45	0.48
1:A:424:LYS:O	1:A:428:SER:HB3	2.13	0.48
1:A:123:THR:O	1:A:125:GLN:OE1	2.31	0.48
1:A:123:THR:H	1:A:126:ARG:HG3	1.77	0.48
1:B:39:ILE:CD1	1:B:41:ILE:HD11	2.44	0.48
1:A:129:TRP:CZ3	1:B:178:ARG:NH2	2.81	0.48
1:B:217:LEU:O	1:B:301:LEU:HD23	2.13	0.48
1:B:90:GLN:O	1:B:95:PRO:HD3	2.13	0.48
1:B:119:ASP:CG	1:B:136:VAL:HG11	2.33	0.48
1:B:121:LYS:HD3	1:B:122:VAL:N	2.28	0.48
1:B:264:ILE:HG22	1:B:264:ILE:O	2.13	0.48
1:B:287:PHE:O	1:B:291:VAL:HG23	2.14	0.48
1:B:430:TYR:O	1:B:431:ASN:C	2.50	0.48
1:B:237:GLN:HB3	1:B:238:ASN:H	1.48	0.47
1:B:415:ARG:HG2	1:B:419:TYR:CE2	2.49	0.47
1:A:92:VAL:O	1:A:96:LEU:HD23	2.13	0.47
1:B:128:LEU:HA	1:B:131:VAL:CG2	2.40	0.47
1:A:200:LYS:HB3	1:A:206:ILE:HG12	1.96	0.47
1:A:267:ALA:O	1:A:270:ASP:HB3	2.15	0.47
1:B:140:HIS:N	1:B:140:HIS:ND1	2.62	0.47
1:A:67:HIS:ND1	1:A:70:ARG:HD3	2.30	0.47
1:A:5:LEU:HB3	1:A:114:PHE:CE1	2.50	0.47
1:A:326:ILE:O	1:A:327:ASN:CB	2.62	0.47
1:A:263:GLU:HG2	1:A:264:ILE:H	1.78	0.47
1:B:122:VAL:CG2	1:B:123:THR:H	2.17	0.47
1:B:128:LEU:CA	1:B:131:VAL:HG22	2.42	0.47
1:A:273:LYS:O	1:A:273:LYS:CG	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLY:HA3	1:A:144:LEU:HD22	1.95	0.47
1:B:192:ARG:O	1:B:196:HIS:HB2	2.15	0.47
1:B:170:LYS:HA	1:B:170:LYS:HD2	1.75	0.47
1:B:149:HIS:CE1	1:B:404:HIS:ND1	2.83	0.47
1:A:39:ILE:HG13	1:A:145:ILE:HD13	1.97	0.47
1:B:115:LEU:H	1:B:115:LEU:CD2	2.28	0.47
1:B:117:CYS:SG	1:B:118:VAL:N	2.88	0.47
1:B:38:VAL:O	1:B:145:ILE:HG23	2.14	0.47
1:A:210:SER:HB2	1:A:237:GLN:NE2	2.30	0.46
1:B:97:LEU:CD2	1:B:307:ILE:HD11	2.45	0.46
1:B:291:VAL:O	1:B:292:SER:C	2.52	0.46
1:A:23:LEU:CD2	1:A:43:LYS:HG2	2.45	0.46
1:A:97:LEU:HD21	1:A:307:ILE:HD12	1.96	0.46
1:B:216:ASP:OD2	1:B:227:GLU:OE2	2.34	0.46
1:A:126:ARG:HH21	1:A:131:VAL:HG23	1.81	0.46
1:B:289:GLN:O	1:B:293:ASP:HB2	2.15	0.46
1:A:270:ASP:O	1:A:273:LYS:CD	2.61	0.46
1:B:276:ILE:HG23	1:B:283:ARG:HD2	1.98	0.46
1:B:115:LEU:HD22	1:B:115:LEU:N	2.30	0.46
1:A:263:GLU:HG2	1:A:264:ILE:N	2.31	0.46
1:B:363:ALA:O	1:B:367:LYS:HG3	2.16	0.46
1:B:428:SER:C	1:B:432:ARG:HD2	2.36	0.46
1:A:129:TRP:HB2	1:B:178:ARG:HB3	1.98	0.46
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.75	0.46
1:B:249:ILE:CG1	1:B:250:LEU:N	2.79	0.46
1:A:164:SER:HB2	1:A:243:PHE:HB2	1.97	0.46
1:A:195:MET:HE3	1:A:195:MET:HB3	1.90	0.46
1:B:152:PHE:O	1:B:153:SER:HB2	2.16	0.46
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.81	0.45
1:B:249:ILE:CG1	1:B:250:LEU:H	2.30	0.45
1:B:132:ASN:HB3	1:B:133:ALA:H	1.65	0.45
1:B:227:GLU:O	1:B:230:LYS:HB2	2.15	0.45
1:A:111:SER:OG	1:A:114:PHE:HB2	2.15	0.45
1:A:257:THR:HG22	1:A:258:GLY:N	2.32	0.45
1:B:112:LYS:O	1:B:113:GLU:HB2	2.17	0.45
1:B:90:GLN:OE1	1:B:94:ILE:HD12	2.16	0.45
1:B:232:LEU:CB	1:B:240:PHE:CD1	2.99	0.45
1:B:432:ARG:HB3	1:B:432:ARG:HH11	1.81	0.45
1:A:122:VAL:HG23	1:A:123:THR:N	2.31	0.45
1:B:110:VAL:HG13	1:B:142:SER:CA	2.46	0.45
1:A:218:PHE:CE1	1:A:304:LEU:HD23	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:CB	1:B:283:ARG:HD2	2.46	0.45
1:A:208:GLU:CD	1:A:259:ARG:HH21	2.19	0.45
1:A:218:PHE:HE1	1:A:304:LEU:HD23	1.82	0.45
1:A:190:VAL:CG1	1:A:195:MET:HG2	2.46	0.45
1:A:190:VAL:HG12	1:A:195:MET:HG2	1.99	0.45
1:A:372:MET:O	1:A:403:VAL:HA	2.17	0.45
1:B:39:ILE:HD13	1:B:41:ILE:HD11	1.98	0.45
1:B:310:LEU:O	1:B:312:LYS:N	2.49	0.45
1:A:323:TYR:CE2	1:A:331:PRO:HD2	2.52	0.45
1:A:273:LYS:O	1:A:273:LYS:HG2	2.17	0.45
1:B:323:TYR:HD1	1:B:326:ILE:HD11	1.81	0.45
1:A:118:VAL:O	1:A:120:LYS:N	2.50	0.45
1:B:299:GLY:HA2	1:B:302:ASP:OD2	2.16	0.45
1:A:229:ILE:HD12	1:A:291:VAL:CG1	2.47	0.44
1:B:88:TYR:CD1	1:B:410:LEU:HD13	2.52	0.44
1:A:19:GLY:HA3	2:A:600:ADP:PB	2.56	0.44
1:A:400:ASP:O	1:A:401:TYR:HB3	2.17	0.44
1:A:376:GLN:O	1:A:399:PHE:HA	2.18	0.44
1:A:119:ASP:C	1:A:122:VAL:HG22	2.37	0.44
1:A:167:ILE:O	1:A:169:PRO:HD3	2.18	0.44
1:A:128:LEU:O	1:A:131:VAL:HG12	2.17	0.44
1:A:16:ARG:HB3	1:A:24:VAL:O	2.18	0.44
1:A:14:ILE:HD12	1:A:26:ALA:HB3	1.99	0.44
1:B:128:LEU:O	1:B:132:ASN:HB2	2.18	0.44
1:A:60:VAL:CG2	1:A:78:SER:O	2.60	0.44
1:B:37:LYS:HZ2	1:B:147:ASN:ND2	2.16	0.44
1:B:177:SER:CB	1:B:313:LEU:O	2.66	0.44
1:B:68:LEU:HA	1:B:354:LEU:HD22	2.00	0.44
1:B:174:LEU:HD23	1:B:188:THR:O	2.17	0.44
1:B:23:LEU:HD23	1:B:41:ILE:HG22	2.01	0.43
1:A:110:VAL:HG22	1:A:141:ASP:CA	2.45	0.43
1:A:205:GLU:HG3	1:B:178:ARG:NH1	2.33	0.43
1:A:73:ASN:HA	1:A:76:ILE:HG12	2.01	0.43
1:A:88:TYR:CZ	1:A:93:ILE:HD11	2.53	0.43
1:A:27:TYR:OH	1:A:31:SER:HB3	2.18	0.43
1:B:135:ASN:O	1:B:136:VAL:CG1	2.67	0.43
1:B:423:ASP:O	1:B:427:ILE:HG22	2.18	0.43
1:A:73:ASN:O	1:A:77:SER:HB3	2.19	0.43
1:A:352:GLU:O	1:A:356:ILE:HG13	2.19	0.43
1:B:149:HIS:HD2	2:B:600:ADP:C6	2.37	0.43
1:B:110:VAL:HG22	1:B:141:ASP:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:C	1:A:122:VAL:N	2.72	0.43
1:A:238:ASN:N	1:A:256:SER:HB2	2.33	0.43
1:B:323:TYR:CD1	1:B:326:ILE:HD11	2.53	0.43
1:B:61:LEU:HD22	1:B:65:GLU:HB3	2.01	0.43
1:A:175:PRO:O	1:A:188:THR:HG23	2.19	0.43
1:B:31:SER:HA	1:B:32:PRO:HD3	1.93	0.43
1:B:107:ARG:NE	1:B:142:SER:OG	2.51	0.42
1:B:223:GLU:H	1:B:223:GLU:HG3	1.59	0.42
1:B:119:ASP:OD1	1:B:136:VAL:HG11	2.19	0.42
1:B:101:HIS:HB3	1:B:403:VAL:O	2.19	0.42
1:B:195:MET:CE	1:B:430:TYR:CD2	3.02	0.42
1:A:275:PHE:CZ	1:A:399:PHE:CE2	3.07	0.42
1:A:40:ARG:NH1	1:A:85:GLU:OE1	2.51	0.42
1:A:23:LEU:N	1:A:41:ILE:O	2.46	0.42
1:A:166:GLU:OE1	1:A:241:ARG:HD2	2.18	0.42
1:A:68:LEU:HD21	1:A:361:LEU:HD12	2.00	0.42
1:B:149:HIS:HE1	1:B:404:HIS:ND1	2.17	0.42
1:B:23:LEU:HD21	1:B:43:LYS:HG3	2.01	0.42
1:A:18:GLU:OE2	1:A:126:ARG:NH1	2.52	0.42
1:B:94:ILE:O	1:B:95:PRO:C	2.56	0.42
1:A:237:GLN:HB3	1:A:238:ASN:H	1.69	0.42
1:A:257:THR:HG22	1:A:258:GLY:H	1.84	0.42
1:B:122:VAL:CG2	1:B:123:THR:N	2.77	0.42
1:B:126:ARG:HB3	1:B:131:VAL:HG12	2.01	0.42
1:A:192:ARG:O	1:A:196:HIS:HB2	2.20	0.42
1:B:261:SER:HB2	1:B:262:PRO:HD2	2.01	0.42
1:A:23:LEU:HD23	1:A:136:VAL:HG12	2.01	0.42
1:B:369:CYS:HB2	1:B:406:ILE:O	2.20	0.42
1:A:27:TYR:CD2	1:A:34:PHE:O	2.73	0.41
1:B:169:PRO:HB2	1:B:218:PHE:HE2	1.85	0.41
1:B:267:ALA:O	1:B:270:ASP:HB3	2.20	0.41
1:A:69:TRP:HB2	1:A:76:ILE:HG22	2.02	0.41
1:B:287:PHE:HD2	1:B:288:LEU:HD23	1.84	0.41
1:B:414:LYS:HD2	1:B:414:LYS:HA	1.92	0.41
1:A:201:LEU:O	1:A:202:GLU:C	2.58	0.41
1:B:100:LYS:CD	1:B:101:HIS:NE2	2.80	0.41
1:B:13:TRP:CZ3	1:B:27:TYR:HB2	2.55	0.41
1:A:276:ILE:HD11	1:A:286:CYS:HB2	2.02	0.41
1:B:222:LYS:O	1:B:222:LYS:HD2	2.21	0.41
1:A:38:VAL:HG12	1:A:148:ASP:CB	2.48	0.41
1:A:94:ILE:N	1:A:95:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG23	1:A:373:ILE:HB	2.01	0.41
1:A:173:PHE:HB3	1:A:305:LEU:HD11	2.01	0.41
1:A:38:VAL:CG1	1:A:148:ASP:HA	2.50	0.41
1:A:315:ILE:HG12	1:A:420:TYR:HA	2.01	0.41
1:A:13:TRP:HA	1:A:26:ALA:O	2.21	0.41
1:A:194:LYS:NZ	1:A:209:GLU:OE2	2.53	0.41
1:B:258:GLY:O	1:B:259:ARG:C	2.58	0.41
1:B:69:TRP:O	1:B:76:ILE:HG23	2.20	0.41
1:A:132:ASN:HA	1:B:182:LYS:HB2	2.03	0.41
1:A:238:ASN:HB3	1:A:256:SER:HB3	2.02	0.41
1:B:187:LYS:HG3	1:B:427:ILE:HD13	2.01	0.41
1:B:314:ASP:O	1:B:316:GLU:N	2.54	0.41
1:B:111:SER:HG	1:B:114:PHE:HD2	1.65	0.41
1:B:37:LYS:HZ2	1:B:147:ASN:HD21	1.66	0.41
1:B:135:ASN:C	1:B:136:VAL:HG13	2.41	0.41
1:A:114:PHE:HD2	1:A:115:LEU:HD23	1.86	0.41
1:B:25:LEU:HB2	1:B:39:ILE:CG2	2.51	0.41
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.78	0.41
1:A:190:VAL:HG12	1:A:195:MET:CG	2.50	0.41
1:B:428:SER:O	1:B:432:ARG:HG3	2.21	0.41
1:A:273:LYS:O	1:A:273:LYS:HD3	2.20	0.41
1:B:398:THR:O	1:B:399:PHE:HB2	2.20	0.41
1:A:312:LYS:C	1:A:313:LEU:HD23	2.41	0.41
1:B:25:LEU:HB2	1:B:39:ILE:HG23	2.01	0.41
1:B:108:VAL:O	1:B:142:SER:HA	2.21	0.41
1:B:249:ILE:HG13	1:B:250:LEU:H	1.86	0.41
1:A:233:TYR:O	1:A:234:SER:C	2.59	0.41
1:B:229:ILE:O	1:B:229:ILE:HG12	2.21	0.41
1:B:226:LEU:HD13	1:B:292:SER:CB	2.51	0.41
1:A:38:VAL:HG23	1:A:39:ILE:N	2.36	0.41
1:B:360:TYR:C	1:B:360:TYR:CD2	2.95	0.40
1:B:149:HIS:CD2	2:B:600:ADP:N6	2.89	0.40
1:B:372:MET:O	1:B:403:VAL:HA	2.21	0.40
1:A:204:ILE:O	1:A:204:ILE:CG2	2.66	0.40
1:A:92:VAL:O	1:A:96:LEU:CD2	2.70	0.40

There are no symmetry-related clashes.

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	349/493 (71%)	297 (85%)	37 (11%)	15 (4%)	3	19
1	B	338/493 (69%)	269 (80%)	54 (16%)	15 (4%)	3	18
All	All	687/986 (70%)	566 (82%)	91 (13%)	30 (4%)	3	18

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	177	SER
1	A	303	ARG
1	A	330	CYS
1	A	433	LYS
1	B	21	ALA
1	B	113	GLU
1	B	121	LYS
1	B	122	VAL
1	B	132	ASN
1	B	311	ASP
1	B	313	LEU
1	A	3	MET
1	A	4	ILE
1	A	149	HIS
1	A	234	SER
1	A	327	ASN
1	B	112	LYS
1	B	123	THR
1	B	270	ASP
1	B	315	ILE
1	A	181	GLY
1	B	133	ALA
1	A	119	ASP
1	B	62	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	119	ASP
1	B	136	VAL
1	A	124	LYS
1	A	273	LYS
1	A	329	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	327/434 (75%)	282 (86%)	45 (14%)	4	19
1	B	315/434 (73%)	263 (84%)	52 (16%)	3	12
All	All	642/868 (74%)	545 (85%)	97 (15%)	3	15

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	16	ARG
1	A	33	LEU
1	A	71	GLU
1	A	75	LEU
1	A	77	SER
1	A	107	ARG
1	A	110	VAL
1	A	117	CYS
1	A	124	LYS
1	A	128	LEU
1	A	138	THR
1	A	142	SER
1	A	146	LEU
1	A	150	SER
1	A	152	PHE
1	A	165	VAL
1	A	166	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	GLU
1	A	184	ASN
1	A	186	LEU
1	A	192	ARG
1	A	195	MET
1	A	198	LEU
1	A	202	GLU
1	A	205	GLU
1	A	222	LYS
1	A	229	ILE
1	A	249	ILE
1	A	266	TYR
1	A	273	LYS
1	A	276	ILE
1	A	300	VAL
1	A	301	LEU
1	A	310	LEU
1	A	348	LEU
1	A	350	LEU
1	A	365	THR
1	A	373	ILE
1	A	377	SER
1	A	400	ASP
1	A	410	LEU
1	A	414	LYS
1	A	428	SER
1	A	432	ARG
1	B	14	ILE
1	B	23	LEU
1	B	33	LEU
1	B	38	VAL
1	B	39	ILE
1	B	40	ARG
1	B	42	GLN
1	B	81	LYS
1	B	97	LEU
1	B	107	ARG
1	B	108	VAL
1	B	112	LYS
1	B	126	ARG
1	B	129	TRP
1	B	132	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	135	ASN
1	B	140	HIS
1	B	144	LEU
1	B	152	PHE
1	B	165	VAL
1	B	176	THR
1	B	177	SER
1	B	178	ARG
1	B	183	GLU
1	B	185	ILE
1	B	186	LEU
1	B	192	ARG
1	B	195	MET
1	B	196	HIS
1	B	201	LEU
1	B	207	SER
1	B	217	LEU
1	B	223	GLU
1	B	229	ILE
1	B	237	GLN
1	B	241	ARG
1	B	257	THR
1	B	260	THR
1	B	298	SER
1	B	301	LEU
1	B	303	ARG
1	B	306	GLU
1	B	310	LEU
1	B	352	GLU
1	B	373	ILE
1	B	375	PHE
1	B	404	HIS
1	B	407	ASP
1	B	411	LYS
1	B	418	SER
1	B	432	ARG
1	B	434	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	HIS
1	A	196	HIS
1	B	22	ASN
1	B	80	ASN
1	B	147	ASN
1	B	149	HIS
1	B	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ADP	A	600	3	22,29,29	1.08	2 (9%)	27,45,45	2.15	4 (14%)
2	ADP	B	600	3	22,29,29	0.98	1 (4%)	27,45,45	1.91	4 (14%)

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	600	3	-	0/12/32/32	0/3/3/3
2	ADP	B	600	3	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ADP	C2-N3	2.06	1.35	1.32
2	B	600	ADP	C5-C4	3.08	1.47	1.40
2	A	600	ADP	C5-C4	3.35	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ADP	C2'-C1'-N9	-7.27	103.18	114.29
2	B	600	ADP	N3-C2-N1	-6.50	123.92	128.89
2	A	600	ADP	N3-C2-N1	-6.21	124.14	128.89
2	B	600	ADP	C2'-C1'-N9	-4.66	107.17	114.29
2	A	600	ADP	C4-C5-N7	-3.50	106.26	109.48
2	B	600	ADP	C4-C5-N7	-2.63	107.06	109.48
2	A	600	ADP	PA-O3A-PB	-2.37	124.72	132.67
2	B	600	ADP	O3B-PB-O2B	2.15	115.58	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ADP	2	0
2	B	600	ADP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	365/493 (74%)	-0.69	0	100 100	36, 58, 86, 103	0
1	B	352/493 (71%)	-0.59	3 (0%)	85 72	32, 65, 121, 139	0
All	All	717/986 (72%)	-0.64	3 (0%)	93 85	32, 60, 105, 139	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	LEU	4.3
1	B	133	ALA	4.0
1	B	124	LYS	2.2

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(\AA^2)	Q<0.9
2	ADP	B	600	27/27	0.95	0.15	-0.18	58,77,81,85	0
2	ADP	A	600	27/27	0.96	0.14	-0.24	47,53,63,64	0
3	MG	A	700	1/1	0.95	0.22	-	46,46,46,46	0
3	MG	B	700	1/1	0.95	0.29	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.