Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 08:59 AM EDT

PDB ID	:	4PKH
Title	:	Complex of ADP-actin With the N-terminal Actin-Binding Domain of Tropomodulin
Authors	:	Rao, J.N.; Dominguez, R.
Deposited on	:	2014-05-14
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

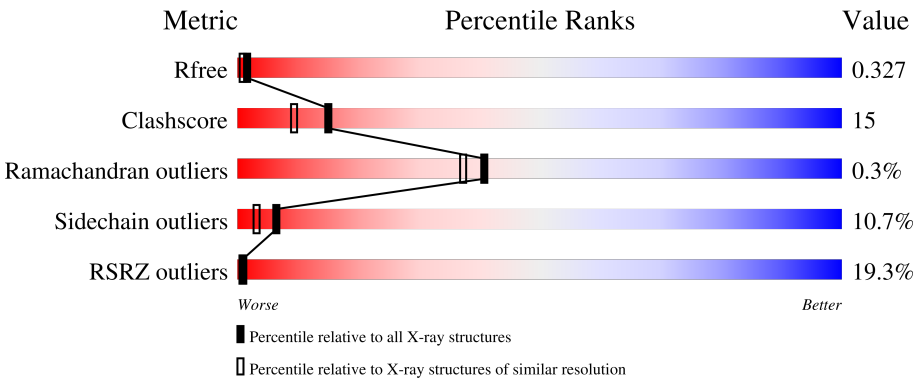
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	377	3%, 62%, 30%, •, 5%
1	D	377	2%, 71%, 22%, •, 5%
1	F	377	33%, 59%, 33%, 5%, •
1	I	377	37%, 52%, 37%, 6%, 5%
2	B	186	5%, 70%, 17%, •, 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	186	2% 48% 17% 33%
2	G	186	23% 41% 32% 23%
2	J	186	26% 40% 23% 5% 32%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31981 atoms, of which 15522 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	359	5592	1787	2775	469	541	20	0	2	0
1	D	360	5609	1790	2786	473	541	19	0	1	0
1	F	365	5678	1812	2821	481	544	20	0	0	0
1	I	360	5609	1790	2786	473	540	20	0	1	0

- Molecule 2 is a protein called Gelsolin,Tropomodulin-1 chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	165	2622	859	1291	225	246	1	0	0	0
2	E	125	1944	642	952	165	184	1	0	0	0
2	G	143	2245	738	1102	191	212	2	0	0	0
2	J	126	1970	650	965	166	187	2	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

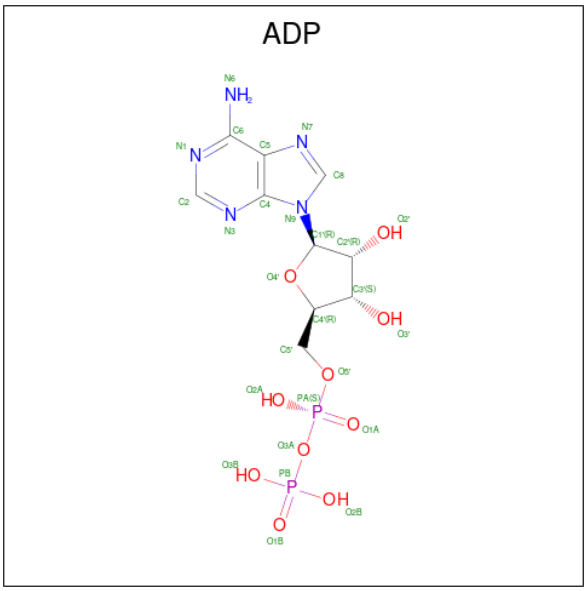
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	linker	UNP P06396
B	178	GLY	-	linker	UNP P06396
B	179	SER	-	linker	UNP P06396
B	180	GLY	-	linker	UNP P06396
B	181	GLY	-	linker	UNP P06396
B	182	SER	-	linker	UNP P06396
B	183	GLY	-	linker	UNP P06396
B	184	GLY	-	linker	UNP P06396

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	185	SER	-	linker	UNP P06396
E	177	GLY	-	linker	UNP P06396
E	178	GLY	-	linker	UNP P06396
E	179	SER	-	linker	UNP P06396
E	180	GLY	-	linker	UNP P06396
E	181	GLY	-	linker	UNP P06396
E	182	SER	-	linker	UNP P06396
E	183	GLY	-	linker	UNP P06396
E	184	GLY	-	linker	UNP P06396
E	185	SER	-	linker	UNP P06396
G	177	GLY	-	linker	UNP P06396
G	178	GLY	-	linker	UNP P06396
G	179	SER	-	linker	UNP P06396
G	180	GLY	-	linker	UNP P06396
G	181	GLY	-	linker	UNP P06396
G	182	SER	-	linker	UNP P06396
G	183	GLY	-	linker	UNP P06396
G	184	GLY	-	linker	UNP P06396
G	185	SER	-	linker	UNP P06396
J	177	GLY	-	linker	UNP P06396
J	178	GLY	-	linker	UNP P06396
J	179	SER	-	linker	UNP P06396
J	180	GLY	-	linker	UNP P06396
J	181	GLY	-	linker	UNP P06396
J	182	SER	-	linker	UNP P06396
J	183	GLY	-	linker	UNP P06396
J	184	GLY	-	linker	UNP P06396
J	185	SER	-	linker	UNP P06396

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	38	10	11	5	10	2	0	0
3	D	1	38	10	11	5	10	2	0	0
3	F	1	38	10	11	5	10	2	0	0
3	I	1	38	10	11	5	10	2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0
4	B	1	1	1	0	0
4	D	2	2	2	0	0
4	E	1	1	1	0	0
4	F	2	2	2	0	0
4	G	1	1	1	0	0
4	I	2	2	2	0	0
4	J	1	1	1	0	0

- Molecule 5 is water.

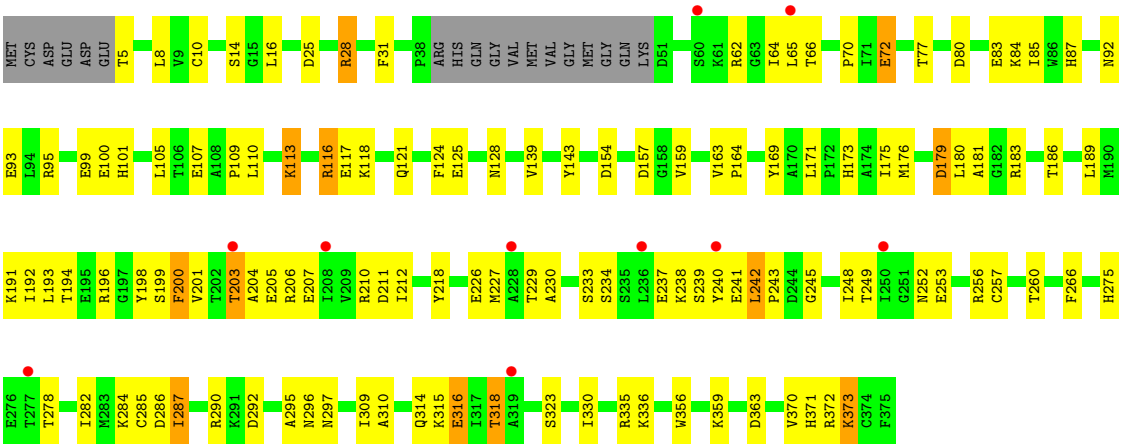
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	88	88	88	0	0
			Total	O		
5	B	82	82	82	0	0
			Total	O		
5	D	87	87	87	0	0
			Total	O		
5	E	77	77	77	0	0
			Total	O		
5	F	63	63	63	0	0
			Total	O		
5	G	49	49	49	0	0
			Total	O		
5	I	62	62	62	0	0
			Total	O		
5	J	40	40	40	0	0

3 Residue-property plots (i)

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.

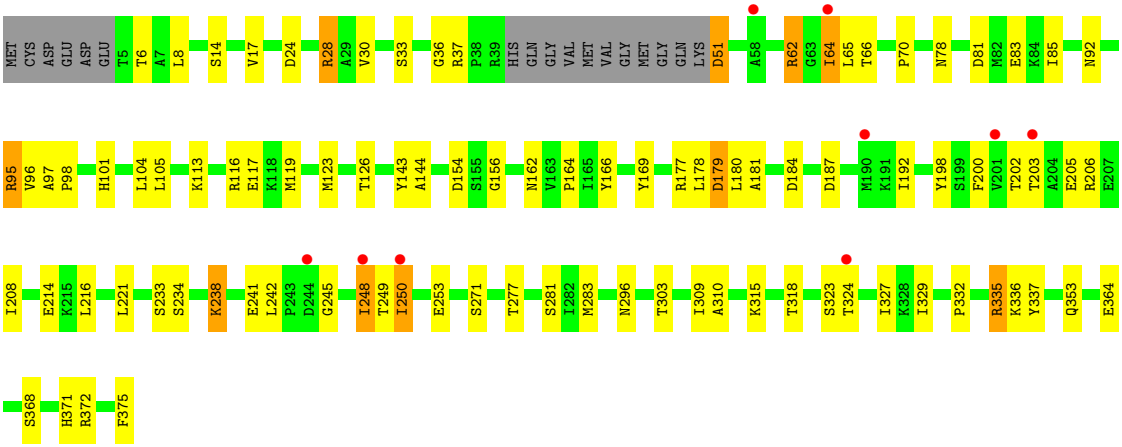
• Molecule 1: Actin, alpha skeletal muscle

Chain A:



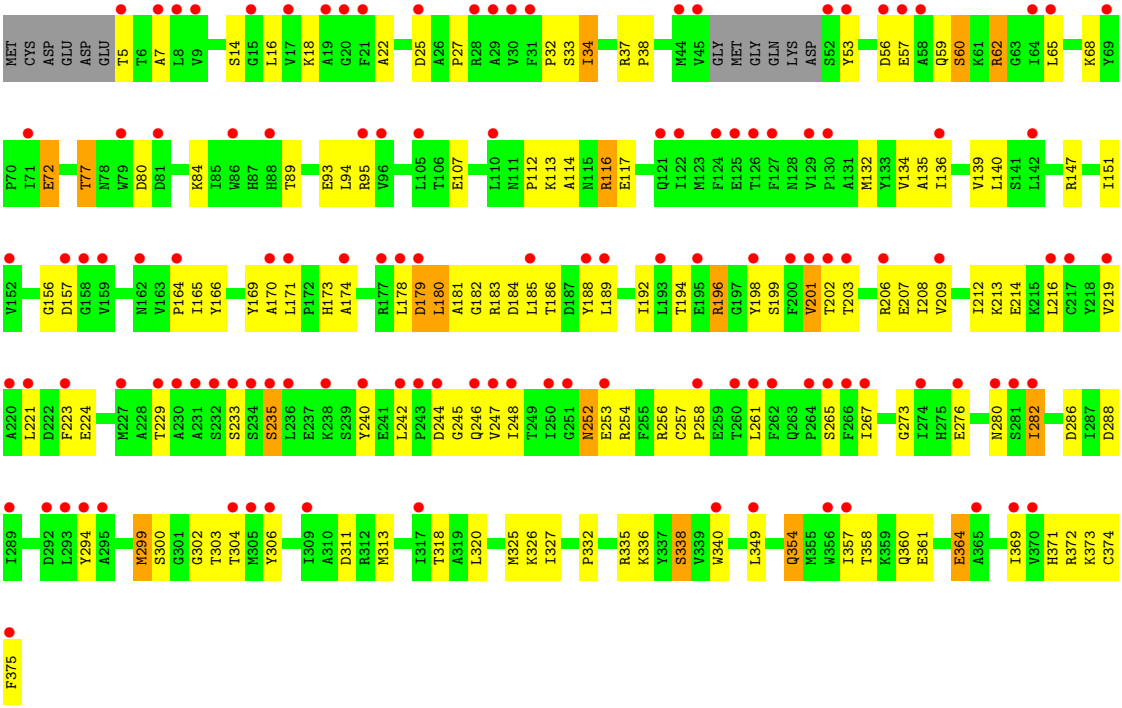
• Molecule 1: Actin, alpha skeletal muscle

Chain D:



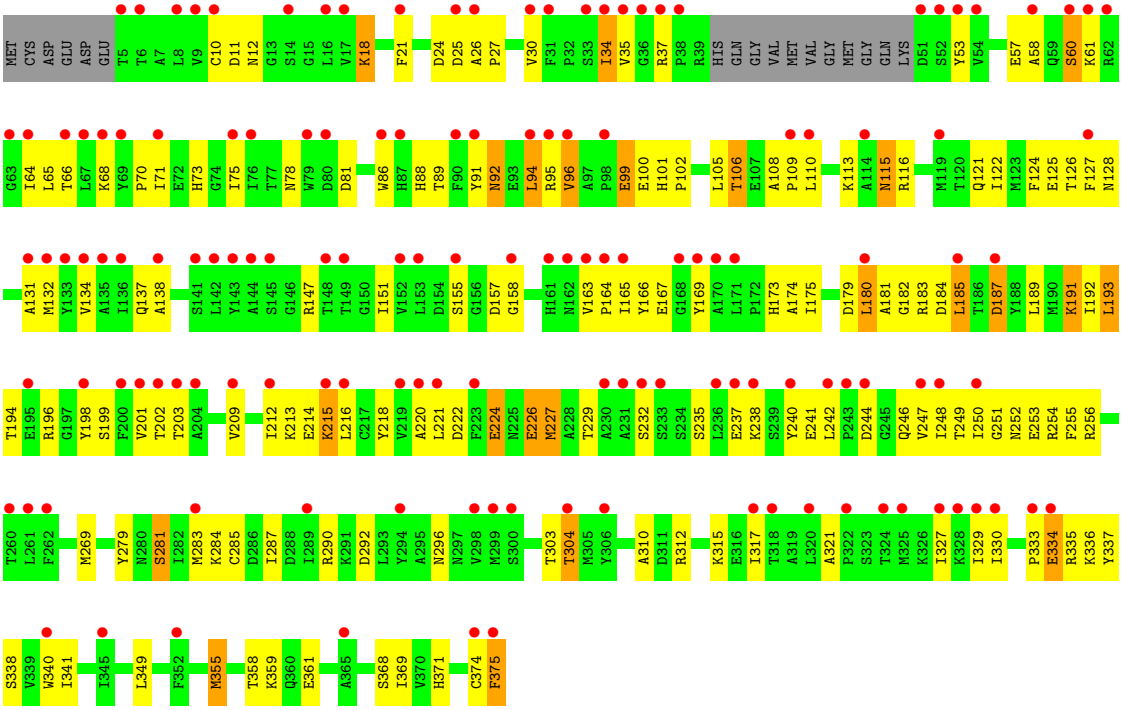
• Molecule 1: Actin, alpha skeletal muscle

Chain F:



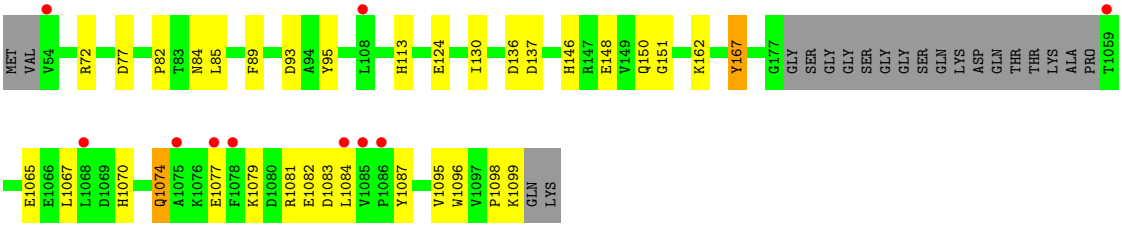
• Molecule 1: Actin, alpha skeletal muscle

Chain I:



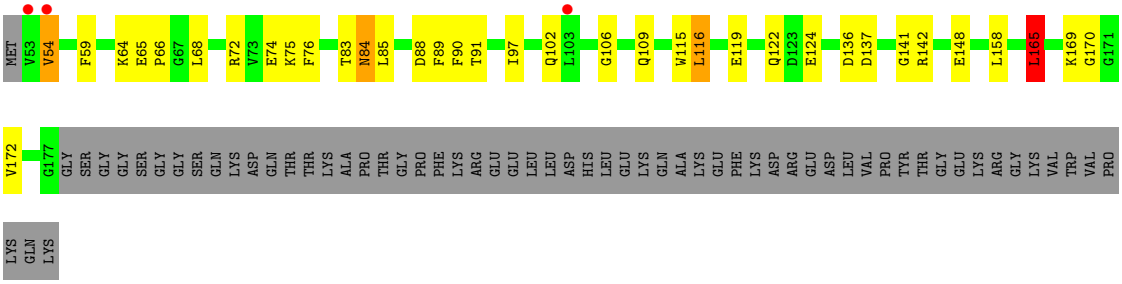
• Molecule 2: Gelsolin,Tropomodulin-1 chimera

Chain B:



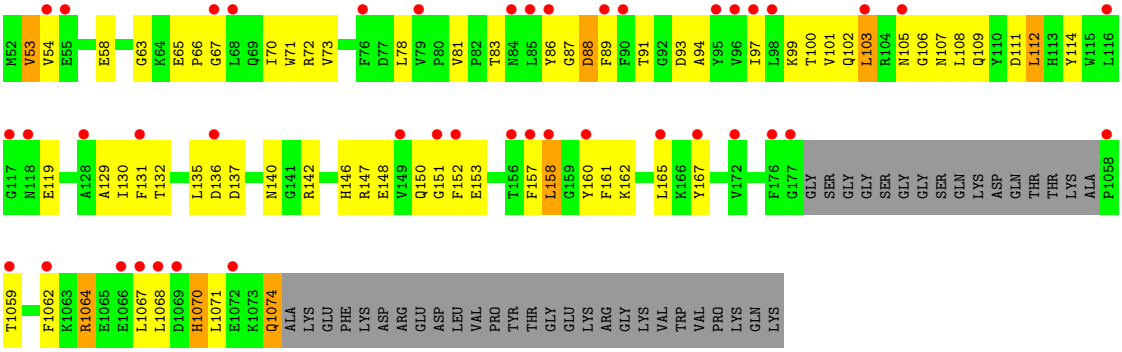
• Molecule 2: Gelsolin,Tropomodulin-1 chimera

Chain E:



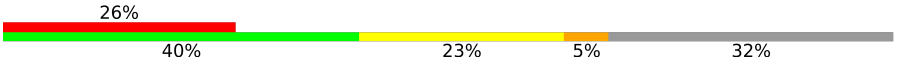
• Molecule 2: Gelsolin,Tropomodulin-1 chimera

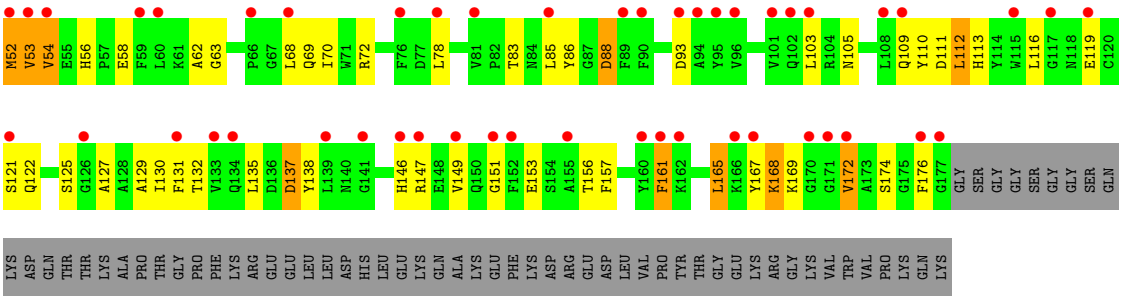
Chain G:



• Molecule 2: Gelsolin,Tropomodulin-1 chimera

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.22Å 135.14Å 140.55Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	44.90 – 2.15 44.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.90-2.15) 72.6 (44.91-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.274 , 0.326 0.280 , 0.327	Depositor DCC
R_{free} test set	2019 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	31981	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7803e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ADP, CA

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	0.95	2/2884 (0.1%)	0.92	4/3909 (0.1%)
1	D	0.99	2/2887 (0.1%)	0.95	5/3912 (0.1%)
1	F	0.63	0/2919	0.72	0/3955
1	I	0.59	0/2887	0.71	0/3912
2	B	1.07	3/1365 (0.2%)	0.92	1/1840 (0.1%)
2	E	1.29	3/1018 (0.3%)	1.05	5/1377 (0.4%)
2	G	0.73	0/1172	0.75	1/1581 (0.1%)
2	J	0.70	0/1035	0.76	0/1399
All	All	0.86	10/16167 (0.1%)	0.85	16/21885 (0.1%)

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	0	1
1	D	0	2
1	I	0	2
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	TYR	CD2-CE2	5.90	1.48	1.39
2	B	167	TYR	CE2-CZ	5.66	1.46	1.38
2	B	124	GLU	CG-CD	5.46	1.60	1.51
2	B	148	GLU	CB-CG	5.44	1.62	1.52
1	A	139	VAL	CA-CB	5.41	1.66	1.54
1	D	166	TYR	CD1-CE1	-5.39	1.31	1.39
1	A	370	VAL	CB-CG2	5.35	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	124	GLU	CG-CD	5.33	1.59	1.51
2	E	148	GLU	CB-CG	5.22	1.62	1.52
2	E	115	TRP	CB-CG	5.14	1.59	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	165	LEU	CA-CB-CG	8.16	134.08	115.30
2	B	77	ASP	CB-CG-OD2	7.65	125.19	118.30
2	E	142	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	25	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	154	ASP	CB-CG-OD1	6.46	124.12	118.30
1	D	372	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	116	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	E	136	ASP	CB-CG-OD2	-5.77	113.10	118.30
2	G	136	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	372	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	116	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	16	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	A	335	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	116	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	E	116	LEU	CB-CG-CD1	5.15	119.75	111.00
2	E	136	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ASN	Mainchain
1	D	179	ASP	Peptide
1	D	296	ASN	Mainchain
1	I	235	SER	Peptide
1	I	57	GLU	Peptide

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	2817	2775	2785	94	1
1	D	2823	2786	2794	57	0
1	F	2857	2821	2830	94	1
1	I	2823	2786	2794	121	1
2	B	1331	1291	1295	20	0
2	E	992	952	955	28	0
2	G	1143	1102	1106	52	0
2	J	1005	965	966	43	1
3	A	27	11	12	0	0
3	D	27	11	12	2	0
3	F	27	11	12	6	0
3	I	27	11	12	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
5	A	88	0	0	11	0
5	B	82	0	0	2	0
5	D	87	0	0	2	0
5	E	77	0	0	7	0
5	F	63	0	0	7	0
5	G	49	0	0	4	0
5	I	62	0	0	13	0
5	J	40	0	0	4	0
All	All	16459	15522	15573	476	2

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 15.

All (476) 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)
2:J:72:ARG:NH1	2:J:93:ASP:OD2	1.76	1.17
1:I:95:ARG:NH1	5:I:501:HOH:O	1.89	1.04
2:J:52:MET:SD	2:J:52:MET:N	2.33	1.01
2:J:88:ASP:OD2	2:J:168:LYS:NZ	1.96	0.98
1:I:226:GLU:OE2	5:I:526:HOH:O	1.86	0.92
1:A:83:GLU:OE2	2:B:1087:TYR:OH	1.88	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:HIS:NE2	1:I:284:LYS:O	2.03	0.91
3:I:401:ADP:O1A	5:I:514:HOH:O	1.89	0.89
1:D:178:LEU:HD21	1:D:277:THR:HG21	1.54	0.88
1:I:227:MET:SD	1:I:252:ASN:ND2	2.47	0.87
1:I:88:HIS:ND1	1:I:92:ASN:OD1	2.08	0.86
1:F:358:THR:N	1:F:361:GLU:OE2	2.08	0.86
1:D:24:ASP:OD2	1:D:28:ARG:NH1	2.10	0.85
1:A:169:TYR:OH	2:B:137:ASP:OD2	1.96	0.83
1:F:364:GLU:O	5:F:521:HOH:O	1.95	0.83
1:D:117:GLU:OE2	1:D:371:HIS:NE2	2.09	0.81
1:D:62:ARG:NH1	1:D:203:THR:OG1	2.14	0.81
2:G:91:THR:OG1	2:G:119:GLU:OE2	2.00	0.79
1:D:221:LEU:O	1:D:315:LYS:NZ	2.15	0.79
1:A:154:ASP:OD2	5:A:588:HOH:O	2.01	0.79
1:D:253:GLU:OE2	1:D:253:GLU:N	2.16	0.79
1:A:356:TRP:O	1:A:373:LYS:NZ	2.15	0.78
1:D:187:ASP:OD1	1:D:206:ARG:NH2	2.16	0.78
1:D:327:ILE:O	5:D:550:HOH:O	2.01	0.78
1:F:199:SER:O	2:G:1064:ARG:NH2	2.18	0.76
1:I:169:TYR:OH	2:J:137:ASP:OD1	2.04	0.75
2:J:116:LEU:HD12	2:J:147:ARG:NH1	2.03	0.74
1:A:295:ALA:O	5:A:551:HOH:O	2.06	0.74
2:G:148:GLU:OE1	5:G:1329:HOH:O	2.04	0.74
2:B:136:ASP:OD2	5:B:1374:HOH:O	2.06	0.73
2:G:67:GLY:N	2:G:100:THR:OG1	2.22	0.72
1:F:273:GLY:N	1:F:276:GLU:OE1	2.22	0.72
3:F:401:ADP:N1	5:F:531:HOH:O	2.21	0.71
1:I:174:ALA:O	1:I:281:SER:OG	2.07	0.71
1:I:252:ASN:HA	1:I:255:PHE:CE1	2.26	0.69
2:G:88:ASP:O	5:G:1311:HOH:O	2.09	0.69
2:G:1070:HIS:O	2:G:1074:GLN:N	2.24	0.69
1:F:117:GLU:OE2	5:F:562:HOH:O	2.08	0.69
1:F:156:GLY:O	1:F:303:THR:OG1	2.09	0.69
1:I:115:ASN:OD1	1:I:115:ASN:N	2.26	0.68
1:A:198:TYR:CZ	1:A:248:ILE:HG23	2.29	0.67
1:D:238:LYS:NZ	5:D:565:HOH:O	2.27	0.66
2:G:151:GLY:N	2:G:167:TYR:OH	2.28	0.66
2:G:137:ASP:OD2	5:G:1323:HOH:O	2.13	0.65
1:D:214:GLU:HG2	3:D:401:ADP:C5	2.32	0.65
1:I:212:ILE:HG23	1:I:216:LEU:HD12	1.78	0.65
2:B:162:LYS:NZ	5:B:1380:HOH:O	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:214:GLU:OE1	5:I:517:HOH:O	2.15	0.65
2:J:58:GLU:OE1	5:J:1317:HOH:O	2.15	0.65
1:A:95:ARG:O	5:A:530:HOH:O	2.14	0.64
1:F:72:GLU:OE1	1:F:77:THR:OG1	2.16	0.64
1:A:229:THR:O	1:A:233:SER:OG	2.04	0.64
1:A:186:THR:HG21	1:A:206:ARG:HE	1.63	0.64
2:E:74:GLU:OE1	5:E:1355:HOH:O	2.14	0.64
1:A:117:GLU:OE2	1:A:371:HIS:HE1	1.81	0.64
1:F:147:ARG:NH1	2:G:147:ARG:HH12	1.96	0.64
2:E:137:ASP:HA	5:E:1303:HOH:O	1.96	0.64
1:A:128:ASN:OD1	1:A:359:LYS:NZ	2.31	0.64
2:G:72:ARG:HD2	2:G:93:ASP:OD2	1.98	0.63
1:I:218:TYR:OH	1:I:226:GLU:OE1	2.15	0.63
1:A:100:GLU:HG2	1:A:101:HIS:CD2	2.33	0.63
1:D:169:TYR:OH	2:E:137:ASP:OD2	2.16	0.62
2:G:72:ARG:NH1	2:G:93:ASP:OD2	2.31	0.62
1:I:116:ARG:NH2	1:I:374:CYS:O	2.32	0.62
1:A:285:CYS:O	1:A:290:ARG:NH2	2.33	0.61
1:A:372:ARG:NH1	5:A:554:HOH:O	2.23	0.61
1:I:213:LYS:NZ	3:I:401:ADP:O2'	2.31	0.61
1:A:314:GLN:O	1:A:318:THR:OG1	2.14	0.61
1:D:178:LEU:CD2	1:D:277:THR:HG21	2.30	0.61
1:I:229:THR:O	1:I:232:SER:OG	2.09	0.61
1:F:114:ALA:HA	1:F:117:GLU:OE2	2.01	0.60
2:J:112:LEU:O	2:J:146:HIS:N	2.34	0.60
1:I:336:LYS:NZ	5:I:545:HOH:O	2.27	0.60
1:F:286:ASP:OD1	1:F:288:ASP:N	2.23	0.60
2:G:63:GLY:HA2	2:G:100:THR:HG21	1.83	0.60
2:E:72:ARG:NH1	2:E:172:VAL:HG23	2.17	0.59
1:I:355:MET:SD	5:I:543:HOH:O	2.57	0.59
1:A:194:THR:HG22	1:A:199:SER:HA	1.84	0.59
2:G:1068:LEU:O	2:G:1071:LEU:N	2.35	0.59
1:A:80:ASP:OD1	5:A:584:HOH:O	2.16	0.59
1:F:244:ASP:HB3	2:G:1067:LEU:HD12	1.84	0.59
2:G:83:THR:HA	2:G:86:TYR:CE1	2.37	0.59
1:A:196:ARG:NH2	1:A:249:THR:OG1	2.35	0.59
2:E:68:LEU:HD11	2:E:97:ILE:HG23	1.84	0.59
1:F:372:ARG:NH1	2:J:153[A]:GLU:OE2	2.36	0.59
1:D:95:ARG:HH21	1:D:95:ARG:HG3	1.68	0.59
2:E:141:GLY:N	5:E:1303:HOH:O	2.34	0.59
1:F:214:GLU:OE2	3:F:401:ADP:C4	2.55	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:OD2	1:A:183:ARG:NE	2.36	0.59
1:A:241:GLU:OE2	1:A:245:GLY:HA2	2.03	0.58
2:E:66:PRO:O	5:E:1349:HOH:O	2.17	0.58
1:I:220:ALA:O	1:I:312:ARG:NH2	2.35	0.58
2:J:78:LEU:HD13	2:J:131:PHE:CD2	2.38	0.58
1:I:96:VAL:HG11	1:I:101:HIS:CE1	2.38	0.58
1:I:253:GLU:HA	1:I:256:ARG:HB2	1.84	0.58
2:E:89:PHE:CD2	2:E:165:LEU:HD13	2.38	0.58
2:J:137:ASP:HB3	5:J:1301:HOH:O	2.03	0.58
2:G:140:ASN:O	2:J:119:GLU:OE1	2.22	0.58
2:E:91:THR:OG1	2:E:119:GLU:OE2	2.13	0.57
1:I:317:ILE:O	1:I:321:ALA:N	2.37	0.57
1:F:37:ARG:NH1	1:F:68:LYS:NZ	2.53	0.57
1:D:214:GLU:HG2	3:D:401:ADP:C4	2.40	0.57
1:D:318:THR:HA	1:D:327:ILE:CD1	2.34	0.56
1:F:179:ASP:OD1	1:F:179:ASP:N	2.37	0.56
1:A:117:GLU:OE2	1:A:371:HIS:CE1	2.58	0.56
1:D:113:LYS:HG3	1:D:371:HIS:CE1	2.40	0.56
1:F:135:ALA:HB3	1:F:140:LEU:HD11	1.88	0.56
1:A:128:ASN:OD1	1:A:359:LYS:CE	2.54	0.56
1:A:207:GLU:OE2	1:A:210:ARG:NH1	2.37	0.56
2:E:64:LYS:N	5:E:1369:HOH:O	2.38	0.56
1:D:105:LEU:HD11	1:D:123:MET:HG3	1.87	0.56
1:A:95:ARG:NH1	2:B:1083:ASP:OD2	2.27	0.56
1:F:180:LEU:HD12	1:F:181:ALA:N	2.20	0.56
1:F:240:TYR:C	1:F:247:VAL:HG13	2.26	0.56
1:F:214:GLU:OE2	3:F:401:ADP:C5	2.59	0.56
1:I:251:GLY:N	1:I:253:GLU:OE2	2.39	0.56
2:J:116:LEU:HD12	2:J:147:ARG:HH12	1.71	0.56
2:E:72:ARG:NH1	2:E:172:VAL:CG2	2.69	0.56
1:I:25:ASP:HA	2:J:176:PHE:CE1	2.41	0.56
1:I:121:GLN:CG	1:I:125:GLU:OE2	2.54	0.55
1:I:73:HIS:HB3	1:I:179:ASP:OD1	2.06	0.55
1:I:180:LEU:HD11	1:I:185:LEU:HD11	1.88	0.55
1:A:118:LYS:NZ	5:A:580:HOH:O	2.38	0.55
1:A:242:LEU:N	1:A:242:LEU:CD1	2.70	0.55
2:E:97:ILE:HD12	2:E:97:ILE:N	2.21	0.55
1:I:181:ALA:N	1:I:184:ASP:OD2	2.39	0.55
2:J:85:LEU:O	2:J:88:ASP:HB2	2.07	0.55
1:I:240:TYR:O	1:I:248:ILE:N	2.39	0.55
1:F:224:GLU:N	1:F:224:GLU:OE1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:103:LEU:HD23	2:G:105:ASN:H	1.71	0.54
1:A:200:PHE:HB3	1:A:205:GLU:HB3	1.89	0.54
1:D:28:ARG:HH11	1:D:28:ARG:CG	2.20	0.54
1:F:7:ALA:HB3	1:F:22:ALA:HB3	1.90	0.54
1:F:38:PRO:HA	1:F:65:LEU:HD23	1.90	0.54
1:I:349:LEU:HD11	2:J:130:ILE:HG21	1.90	0.54
1:D:51:ASP:OD1	1:D:51:ASP:N	2.40	0.54
2:E:89:PHE:HD2	2:E:165:LEU:HD13	1.71	0.54
1:A:198:TYR:CE1	1:A:248:ILE:HG23	2.43	0.54
1:I:180:LEU:HD12	1:I:181:ALA:N	2.22	0.54
1:A:157:ASP:OD2	1:A:183:ARG:NH1	2.41	0.53
1:A:200:PHE:HB3	1:A:205:GLU:CB	2.38	0.53
1:A:28:ARG:NH1	5:A:577:HOH:O	2.40	0.53
1:A:70:PRO:HG3	1:A:85:ILE:HD12	1.89	0.53
1:D:216:LEU:HD12	1:D:250:ILE:HD12	1.91	0.53
2:E:54:VAL:HG11	2:E:59:PHE:CD2	2.43	0.53
1:I:21:PHE:HB2	1:I:24:ASP:OD2	2.08	0.53
1:I:147:ARG:NH2	1:I:296:ASN:OD1	2.41	0.53
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.90	0.53
1:F:201:VAL:HG12	1:F:202:THR:H	1.74	0.53
1:F:216:LEU:N	1:F:216:LEU:HD22	2.23	0.53
1:F:372:ARG:CD	2:J:165:LEU:HD11	2.39	0.53
1:I:155:SER:OG	1:I:303:THR:HG23	2.09	0.53
2:E:102:GLN:HE22	2:E:106:GLY:C	2.11	0.53
1:I:218:TYR:HD1	1:I:254:ARG:NH1	2.05	0.53
1:I:355:MET:N	5:I:543:HOH:O	2.41	0.53
1:I:18:LYS:HG3	1:I:30:VAL:HG13	1.91	0.53
1:I:242:LEU:HD13	1:I:244:ASP:OD2	2.09	0.53
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.90	0.53
2:E:68:LEU:HD11	2:E:97:ILE:CG2	2.39	0.52
2:G:160:TYR:O	2:G:162:LYS:NZ	2.30	0.52
1:I:60:SER:O	1:I:60:SER:OG	2.25	0.52
1:I:99:GLU:OE2	1:I:100:GLU:HG3	2.10	0.52
1:A:84:LYS:NZ	5:A:560:HOH:O	2.30	0.52
1:F:357:ILE:HA	1:F:361:GLU:OE2	2.09	0.52
1:F:349:LEU:HD22	2:G:131:PHE:CE1	2.45	0.52
1:A:5:THR:HB	1:A:101:HIS:CE1	2.44	0.52
1:I:64:ILE:HG23	1:I:65:LEU:H	1.75	0.52
1:I:113:LYS:HG3	1:I:371:HIS:CE1	2.44	0.52
1:A:207:GLU:OE2	1:A:210:ARG:NE	2.42	0.52
1:F:372:ARG:NH1	2:J:153[B]:GLU:OE1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:ILE:HG23	1:I:169:TYR:C	2.30	0.52
2:G:71:TRP:HB3	2:G:78:LEU:HG	1.90	0.52
1:I:251:GLY:CA	1:I:253:GLU:OE2	2.59	0.51
1:F:233:SER:OG	1:F:235:SER:N	2.38	0.51
1:D:233:SER:OG	1:D:234:SER:N	2.44	0.51
2:G:1070:HIS:CG	2:G:1071:LEU:N	2.79	0.51
1:I:121:GLN:HG2	1:I:125:GLU:OE2	2.11	0.51
1:D:164:PRO:HG3	1:D:281:SER:OG	2.11	0.51
1:I:37:ARG:O	1:I:66:THR:OG1	2.26	0.51
1:I:26:ALA:HB3	5:I:540:HOH:O	2.11	0.51
1:I:182:GLY:CA	1:I:213:LYS:NZ	2.74	0.51
2:J:138:TYR:O	5:J:1325:HOH:O	2.19	0.51
1:F:252:ASN:OD1	1:F:252:ASN:N	2.37	0.51
1:F:302:GLY:HA2	1:F:336:LYS:CG	2.41	0.50
2:G:150:GLN:O	2:G:152:PHE:HD1	1.94	0.50
2:J:72:ARG:NH1	2:J:172:VAL:HB	2.26	0.50
1:I:215:LYS:HD3	1:I:216:LEU:HD23	1.94	0.50
2:J:62:ALA:HA	2:J:69:GLN:HE22	1.75	0.50
1:F:216:LEU:HD22	1:F:216:LEU:H	1.76	0.50
1:D:70:PRO:HG3	1:D:85:ILE:CD1	2.42	0.50
1:I:241:GLU:HA	1:I:247:VAL:HA	1.93	0.50
1:A:113:LYS:NZ	1:A:113:LYS:HB3	2.27	0.50
1:I:196:ARG:NH1	5:I:509:HOH:O	2.44	0.50
1:A:278:THR:O	1:A:282:ILE:HG13	2.11	0.49
1:F:93:GLU:HA	5:F:555:HOH:O	2.11	0.49
1:F:357:ILE:HG23	1:F:369:ILE:HD12	1.94	0.49
2:G:106:GLY:HA3	1:I:334:GLU:HG3	1.94	0.49
1:I:184:ASP:O	1:I:187:ASP:N	2.45	0.49
2:J:56:HIS:CE1	2:J:58:GLU:HB2	2.46	0.49
1:F:147:ARG:NH1	2:G:147:ARG:NH1	2.60	0.49
2:G:73:VAL:HB	2:G:94:ALA:HB3	1.93	0.49
1:D:216:LEU:HD12	1:D:250:ILE:CD1	2.42	0.49
1:A:31:PHE:CE1	1:A:93:GLU:HG3	2.48	0.49
1:F:209:VAL:O	1:F:213:LYS:N	2.44	0.49
1:D:198:TYR:CE1	1:D:248:ILE:HG13	2.48	0.49
1:A:207:GLU:O	1:A:211:ASP:N	2.42	0.49
1:D:64:ILE:HG12	1:D:65:LEU:HG	1.94	0.49
1:I:157:ASP:OD1	3:I:401:ADP:O3'	2.30	0.49
1:A:62:ARG:NH1	1:A:204:ALA:HA	2.28	0.49
2:E:158:LEU:HD23	2:E:165:LEU:HD23	1.94	0.49
1:F:116:ARG:NH2	1:F:371:HIS:HA	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:94:ALA:HB2	5:G:1327:HOH:O	2.12	0.49
2:B:1081:ARG:NH2	2:B:1083:ASP:OD1	2.46	0.48
1:D:17:VAL:O	1:D:30:VAL:HA	2.13	0.48
2:G:89:PHE:CD2	2:G:165:LEU:HD11	2.48	0.48
2:G:112:LEU:HD12	2:G:132:THR:HG23	1.94	0.48
1:I:189:LEU:HD23	1:I:209:VAL:HG13	1.94	0.48
1:A:363:ASP:O	2:B:1096:TRP:HD1	1.96	0.48
1:F:183:ARG:NE	5:F:539:HOH:O	2.37	0.48
1:I:285:CYS:O	1:I:290:ARG:NE	2.39	0.48
2:J:103:LEU:HD11	2:J:109:GLN:N	2.28	0.48
1:A:234:SER:OG	1:A:237:GLU:OE1	2.32	0.48
2:E:84:ASN:HD22	2:E:85:LEU:N	2.10	0.48
1:I:99:GLU:OE2	1:I:100:GLU:CG	2.62	0.48
1:I:287:ILE:HA	1:I:290:ARG:NE	2.28	0.48
1:F:32:PRO:HB2	1:F:34:ILE:HD12	1.96	0.48
2:J:157:PHE:CZ	2:J:161:PHE:HZ	2.31	0.48
2:G:129:ALA:O	2:G:132:THR:HB	2.14	0.48
1:A:62:ARG:NH1	1:A:203:THR:O	2.45	0.48
2:G:99:LYS:HB3	2:G:111:ASP:HB2	1.95	0.48
2:B:113:HIS:CE1	2:B:146:HIS:CD2	3.02	0.47
1:F:208:ILE:HG21	1:F:242:LEU:HD23	1.96	0.47
1:F:335:ARG:HA	1:F:338:SER:OG	2.13	0.47
2:J:72:ARG:HH12	2:J:172:VAL:HB	1.79	0.47
1:A:241:GLU:OE2	1:A:242:LEU:O	2.32	0.47
2:J:78:LEU:HD13	2:J:131:PHE:CG	2.48	0.47
1:D:303:THR:HG22	1:D:303:THR:O	2.13	0.47
1:A:189:LEU:HD21	1:A:212:ILE:HG22	1.97	0.47
1:D:6:THR:O	1:D:101:HIS:ND1	2.33	0.47
1:D:83:GLU:OE2	1:D:126:THR:HG21	2.14	0.47
1:I:166:TYR:CE2	1:I:167:GLU:OE2	2.67	0.47
1:F:185:LEU:HD11	1:F:261:LEU:HD21	1.96	0.47
1:F:299:MET:HG2	1:F:304:THR:HB	1.95	0.47
1:I:121:GLN:HG3	1:I:125:GLU:OE2	2.14	0.47
1:I:218:TYR:CD1	1:I:254:ARG:NH1	2.82	0.47
1:I:252:ASN:HA	1:I:255:PHE:CZ	2.49	0.47
1:I:317:ILE:HG21	1:I:327:ILE:HG21	1.96	0.47
1:A:242:LEU:HD21	1:A:248:ILE:HD12	1.97	0.47
1:A:252:ASN:ND2	1:A:256:ARG:HD2	2.30	0.47
1:D:70:PRO:HG3	1:D:85:ILE:HD12	1.95	0.47
2:J:174:SER:HA	5:J:1310:HOH:O	2.15	0.47
2:J:53:VAL:HG12	2:J:54:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASN:ND2	1:D:81:ASP:OD2	2.48	0.47
1:F:244:ASP:OD1	1:F:245:GLY:N	2.48	0.47
1:I:37:ARG:O	1:I:66:THR:N	2.42	0.47
1:I:108:ALA:HB1	1:I:109:PRO:HD2	1.96	0.47
1:I:157:ASP:O	1:I:181:ALA:HB3	2.15	0.47
1:I:187:ASP:OD1	1:I:191:LYS:HE3	2.14	0.47
1:D:318:THR:HA	1:D:327:ILE:HD12	1.97	0.46
1:I:287:ILE:HA	1:I:290:ARG:CD	2.45	0.46
2:J:147:ARG:HH12	2:J:149:VAL:HG22	1.79	0.46
1:F:258:PRO:HG3	1:F:306:TYR:CE1	2.50	0.46
1:F:282:ILE:HD12	1:F:294:TYR:CE1	2.50	0.46
1:F:113:LYS:HG3	1:F:114:ALA:N	2.30	0.46
1:D:28:ARG:NH1	1:D:28:ARG:CG	2.77	0.46
2:G:88:ASP:OD1	2:G:88:ASP:N	2.47	0.46
1:I:58:ALA:HB1	1:I:61:LYS:CG	2.45	0.46
1:A:10[A]:CYS:HB2	1:A:105:LEU:HD23	1.97	0.46
1:A:84:LYS:HG2	2:B:1087:TYR:CD2	2.50	0.46
2:J:70:ILE:HD12	2:J:86:TYR:CG	2.51	0.46
1:I:252:ASN:CG	1:I:256:ARG:HE	2.19	0.46
2:G:97:ILE:HG13	2:G:157:PHE:HE1	1.81	0.46
1:A:330:ILE:HD12	1:A:330:ILE:N	2.31	0.46
2:B:82:PRO:HG2	2:B:85:LEU:HD12	1.98	0.46
1:D:70:PRO:CG	1:D:85:ILE:CD1	2.94	0.46
1:F:166:TYR:N	1:F:169:TYR:O	2.45	0.46
1:A:87:HIS:CD2	2:B:1087:TYR:HB2	2.51	0.46
1:I:106:THR:HG21	1:I:137:GLN:HE21	1.80	0.46
1:I:180:LEU:HD11	1:I:185:LEU:CD1	2.46	0.46
1:I:349:LEU:CD1	2:J:130:ILE:HG21	2.45	0.46
1:I:237:GLU:HG2	1:I:251:GLY:HA2	1.97	0.45
1:I:310:ALA:HB1	5:I:535:HOH:O	2.17	0.45
2:B:1065:GLU:HA	2:B:1065:GLU:OE2	2.16	0.45
1:D:64:ILE:CG1	1:D:65:LEU:N	2.80	0.45
1:F:214:GLU:HA	3:F:401:ADP:C6	2.51	0.45
2:J:111:ASP:HB3	2:J:113:HIS:NE2	2.30	0.45
1:A:227:MET:O	1:A:230:ALA:HB3	2.17	0.45
1:F:147:ARG:CZ	2:G:147:ARG:NH1	2.79	0.45
1:I:304:THR:O	1:I:335:ARG:NH1	2.50	0.45
2:B:89:PHE:HD2	2:B:95:TYR:CD1	2.35	0.45
2:B:72:ARG:NH1	2:B:93:ASP:OD2	2.44	0.45
1:D:104:LEU:C	1:D:104:LEU:HD23	2.37	0.45
1:I:78:ASN:CG	1:I:81:ASP:HB3	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:C	2:B:1096:TRP:HD1	2.20	0.45
1:F:151:ILE:HB	1:F:164:PRO:HA	1.99	0.45
1:I:128:ASN:N	1:I:128:ASN:HD22	2.15	0.45
1:I:253:GLU:H	1:I:253:GLU:CD	2.20	0.45
1:D:332:PRO:O	1:D:335:ARG:NE	2.42	0.45
1:F:151:ILE:HD12	1:F:164:PRO:HD3	1.99	0.45
2:G:97:ILE:HG13	2:G:157:PHE:CE1	2.52	0.45
2:E:54:VAL:HG11	2:E:59:PHE:CE2	2.52	0.45
1:F:113:LYS:CG	1:F:114:ALA:N	2.80	0.45
1:F:372:ARG:HD2	2:J:165:LEU:HD11	1.98	0.45
1:I:192:ILE:CD1	1:I:253:GLU:HB3	2.47	0.45
1:I:216:LEU:HD22	1:I:238:LYS:HD3	1.98	0.45
1:F:72:GLU:CD	1:F:77:THR:OG1	2.55	0.44
2:G:70:ILE:HG23	2:G:97:ILE:CD1	2.47	0.44
2:G:108:LEU:HG	1:I:333:PRO:HB3	1.99	0.44
1:I:12:ASN:HD21	1:I:86:TRP:HE1	1.63	0.44
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.53	0.44
1:D:28:ARG:NH1	1:D:28:ARG:HG3	2.32	0.44
1:A:180:LEU:HD12	1:A:181:ALA:N	2.32	0.44
1:D:144:ALA:HB1	2:E:122:GLN:NE2	2.33	0.44
1:F:188:TYR:HB2	1:F:267:ILE:HD11	2.00	0.44
1:I:138:ALA:CB	1:I:163:VAL:HG11	2.48	0.44
1:I:151:ILE:HA	1:I:164:PRO:HA	2.00	0.44
1:I:222:ASP:OD1	1:I:222:ASP:C	2.55	0.44
1:D:156:GLY:O	1:D:181:ALA:HB1	2.17	0.44
2:J:129:ALA:O	2:J:132:THR:HB	2.18	0.44
1:A:100:GLU:CG	1:A:101:HIS:CD2	3.00	0.44
1:F:107:GLU:OE2	1:F:134:VAL:HG22	2.18	0.44
1:I:11:ASP:OD1	1:I:106:THR:HG21	2.17	0.44
1:A:92:ASN:N	1:A:92:ASN:HD22	2.14	0.44
1:D:180:LEU:HA	1:D:184:ASP:OD2	2.18	0.44
2:E:65:GLU:N	5:E:1369:HOH:O	2.46	0.44
1:F:372:ARG:HD3	2:J:165:LEU:HD11	1.99	0.44
1:D:309:ILE:HG23	1:D:310:ALA:N	2.33	0.44
1:F:354:GLN:HG3	2:G:54:VAL:HA	1.99	0.44
2:G:101:VAL:O	2:G:109:GLN:N	2.41	0.44
1:I:251:GLY:C	1:I:253:GLU:OE2	2.56	0.44
1:A:99:GLU:OE2	1:A:99:GLU:N	2.48	0.44
1:A:164:PRO:O	1:A:171:LEU:HD12	2.18	0.44
1:D:8:LEU:HD11	1:D:96:VAL:HG21	1.99	0.44
1:F:136:ILE:CG2	1:F:139:VAL:HG23	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.99	0.44
2:B:1074:GLN:NE2	2:B:1077:GLU:OE2	2.50	0.43
2:E:90:PHE:HB3	2:E:170:GLY:O	2.18	0.43
1:F:208:ILE:HG21	1:F:242:LEU:CD2	2.48	0.43
1:A:316:GLU:CA	1:A:316:GLU:OE2	2.66	0.43
1:F:165:ILE:HA	1:F:170:ALA:HA	2.00	0.43
1:I:35:VAL:CG2	1:I:81:ASP:OD1	2.66	0.43
1:A:113:LYS:HB3	1:A:113:LYS:HZ1	1.83	0.43
1:D:336:LYS:HE2	1:D:337:TYR:CE2	2.53	0.43
1:F:112:PRO:O	1:F:116:ARG:HG3	2.19	0.43
2:G:58:GLU:HB3	2:G:71:TRP:NE1	2.33	0.43
1:I:58:ALA:HB1	1:I:61:LYS:HG2	2.01	0.43
1:A:92:ASN:N	1:A:92:ASN:ND2	2.65	0.43
2:B:1070:HIS:NE2	2:B:1074:GLN:OE1	2.52	0.43
1:F:84:LYS:HA	5:F:550:HOH:O	2.18	0.43
1:F:219:VAL:CG2	1:F:258:PRO:HB2	2.48	0.43
2:G:53:VAL:HG22	2:G:54:VAL:N	2.33	0.43
1:I:122:ILE:CG2	1:I:127:PHE:HE2	2.32	0.43
1:I:155:SER:O	1:I:303:THR:HG22	2.18	0.43
1:A:171:LEU:HD12	1:A:171:LEU:N	2.33	0.43
1:F:354:GLN:HE21	2:G:54:VAL:HG23	1.84	0.43
1:I:221:LEU:HD12	1:I:315:LYS:HD3	2.00	0.43
1:A:121:GLN:O	1:A:125:GLU:HG3	2.19	0.43
1:D:303:THR:O	1:D:303:THR:CG2	2.67	0.43
2:E:75:LYS:O	2:E:76:PHE:HB2	2.18	0.43
1:F:196:ARG:HA	1:F:196:ARG:NE	2.34	0.43
1:I:158:GLY:HA2	1:I:183:ARG:HH22	1.84	0.43
1:F:37:ARG:NH1	1:F:68:LYS:HZ3	2.17	0.43
1:I:124:PHE:CE1	1:I:359:LYS:HA	2.53	0.43
1:I:196:ARG:NH1	1:I:251:GLY:HA3	2.33	0.43
1:A:248:ILE:CG2	1:A:249:THR:N	2.81	0.43
1:F:192:ILE:O	1:F:196:ARG:HG2	2.18	0.43
1:F:223:PHE:HZ	1:F:256:ARG:HG3	1.83	0.43
1:F:302:GLY:HA2	1:F:336:LYS:HD2	2.01	0.43
2:G:1068:LEU:HD12	2:G:1068:LEU:H	1.84	0.43
1:A:238:LYS:HG3	1:A:239:SER:H	1.84	0.43
1:D:178:LEU:HD21	1:D:277:THR:CG2	2.39	0.43
1:I:358:THR:HG23	1:I:361:GLU:OE2	2.19	0.43
1:F:372:ARG:HH12	2:J:151:GLY:HA2	1.84	0.42
1:A:196:ARG:NH2	5:A:567:HOH:O	2.51	0.42
1:D:192:ILE:HD12	1:D:253:GLU:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:PHE:HA	1:D:205:GLU:OE2	2.19	0.42
1:D:242:LEU:O	1:D:245:GLY:N	2.48	0.42
1:I:27:PRO:HD3	1:I:340:TRP:CE3	2.54	0.42
1:D:177:ARG:C	1:D:178:LEU:HD22	2.40	0.42
2:E:84:ASN:HD22	2:E:84:ASN:N	2.18	0.42
1:F:164:PRO:HG3	1:F:174:ALA:CB	2.49	0.42
2:G:87:GLY:HA2	2:G:161:PHE:CE1	2.55	0.42
1:I:349:LEU:HD21	2:J:127:ALA:HB2	2.00	0.42
2:J:122:GLN:HA	2:J:125:SER:OG	2.19	0.42
1:D:37:ARG:NH2	1:D:81:ASP:OD1	2.46	0.42
1:I:371:HIS:O	1:I:375:PHE:HB3	2.18	0.42
2:B:151:GLY:N	2:B:167:TYR:OH	2.45	0.42
1:F:157:ASP:N	3:F:401:ADP:H5'1	2.33	0.42
1:F:349:LEU:HD11	2:G:130:ILE:HG21	2.01	0.42
1:I:21:PHE:CD1	1:I:21:PHE:N	2.88	0.42
1:I:329:ILE:N	1:I:329:ILE:HD12	2.33	0.42
2:J:151:GLY:N	2:J:167:TYR:OH	2.52	0.42
1:A:8:LEU:HG	1:A:101:HIS:HB3	2.02	0.42
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.02	0.42
1:A:169:TYR:CD1	2:E:169:LYS:HE3	2.55	0.42
1:A:192:ILE:HD12	1:A:253:GLU:CB	2.48	0.42
1:F:37:ARG:NH1	1:F:68:LYS:HZ2	2.18	0.42
1:F:203:THR:O	1:F:203:THR:OG1	2.37	0.42
1:I:109:PRO:HB2	1:I:175:ILE:HD13	2.01	0.42
1:I:361:GLU:HB3	1:I:369:ILE:CD1	2.49	0.42
2:J:63:GLY:HA2	2:J:110:TYR:CE1	2.54	0.42
2:G:112:LEU:HD21	2:G:135:LEU:HD13	2.01	0.42
2:J:147:ARG:HG3	2:J:147:ARG:HH11	1.84	0.42
1:A:107:GLU:OE1	1:A:116:ARG:HD2	2.20	0.42
2:E:54:VAL:O	2:E:54:VAL:HG12	2.20	0.42
2:E:84:ASN:HD22	2:E:85:LEU:H	1.66	0.42
1:F:147:ARG:NH1	5:F:525:HOH:O	2.38	0.42
1:F:212:ILE:HG23	1:F:216:LEU:HD23	2.02	0.42
1:I:193:LEU:HD23	1:I:198:TYR:CD2	2.55	0.42
1:F:171:LEU:HB3	1:F:173:HIS:CE1	2.55	0.42
2:G:53:VAL:HG22	2:G:54:VAL:H	1.85	0.42
1:I:240:TYR:HD2	1:I:248:ILE:HD11	1.85	0.42
1:I:341:ILE:HD11	5:I:532:HOH:O	2.18	0.42
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.01	0.41
1:I:252:ASN:CB	1:I:255:PHE:CZ	3.02	0.41
1:A:64:ILE:C	1:A:65:LEU:HD12	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLY:HA2	1:D:66:THR:O	2.20	0.41
1:A:143:TYR:CD2	2:B:130:ILE:HG12	2.56	0.41
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.95	0.41
1:F:18:LYS:NZ	3:F:401:ADP:O1B	2.53	0.41
1:I:337:TYR:HA	5:I:525:HOH:O	2.20	0.41
1:F:223:PHE:CZ	1:F:256:ARG:HG3	2.55	0.41
1:F:372:ARG:HD3	2:J:165:LEU:CD1	2.50	0.41
1:D:202:THR:HB	1:D:205:GLU:HG3	2.03	0.41
1:F:182:GLY:HA2	1:F:185:LEU:HD12	2.01	0.41
1:I:102:PRO:HA	1:I:131:ALA:O	2.21	0.41
1:I:336:LYS:CE	5:I:545:HOH:O	2.67	0.41
1:A:212:ILE:HG13	1:A:240:TYR:CE2	2.56	0.41
1:A:286:ASP:OD1	1:A:287:ILE:N	2.54	0.41
2:B:1096:TRP:CH2	2:B:1098:PRO:HA	2.56	0.41
2:E:88:ASP:OD2	5:E:1354:HOH:O	2.22	0.41
1:F:202:THR:OG1	1:F:203:THR:N	2.51	0.41
1:A:233:SER:O	1:A:234:SER:CB	2.69	0.41
2:G:70:ILE:HG22	2:G:81:VAL:HG21	2.03	0.41
1:I:58:ALA:CB	1:I:61:LYS:HG3	2.51	0.41
1:A:10[B]:CYS:HB3	1:A:105:LEU:HD23	2.01	0.41
1:A:100:GLU:CG	1:A:101:HIS:NE2	2.84	0.41
1:A:124:PHE:O	1:A:128:ASN:HA	2.21	0.41
1:D:97:ALA:HA	1:D:98:PRO:HD3	1.94	0.41
1:D:202:THR:OG1	1:D:205:GLU:OE1	2.17	0.41
1:I:53:TYR:CD2	1:I:65:LEU:HD11	2.56	0.41
1:I:106:THR:HG23	1:I:137:GLN:CG	2.51	0.41
1:A:72:GLU:HG2	1:A:77:THR:HG21	2.03	0.41
1:A:193:LEU:O	1:A:198:TYR:N	2.44	0.41
1:A:336:LYS:HB2	5:A:503:HOH:O	2.21	0.41
1:F:56:ASP:HA	1:F:59:GLN:HB3	2.03	0.41
1:F:89:THR:O	1:F:94:LEU:HD13	2.21	0.41
2:G:87:GLY:CA	2:G:161:PHE:CE1	3.04	0.41
1:A:218:TYR:OH	1:A:226:GLU:OE2	2.20	0.41
1:A:309:ILE:HG23	1:A:310:ALA:N	2.36	0.41
1:F:354:GLN:HG3	2:G:53:VAL:O	2.21	0.41
1:I:10[B]:CYS:HB3	1:I:105:LEU:CD2	2.50	0.41
1:I:70:PRO:HG2	1:I:71:ILE:HD12	2.03	0.41
1:I:96:VAL:CG1	1:I:101:HIS:CE1	3.04	0.41
1:I:126:THR:O	1:I:128:ASN:ND2	2.54	0.41
1:D:310:ALA:HA	1:D:329:ILE:HG21	2.03	0.40
1:F:180:LEU:HA	1:F:184:ASP:OD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1064:ARG:O	2:G:1068:LEU:HD12	2.21	0.40
1:I:194:THR:HA	1:I:198:TYR:O	2.21	0.40
1:I:304:THR:O	1:I:335:ARG:CZ	2.69	0.40
2:J:147:ARG:NH1	2:J:147:ARG:HG3	2.36	0.40
1:A:316:GLU:OE2	1:A:316:GLU:HA	2.22	0.40
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.56	0.40
1:F:60:SER:HA	1:F:62:ARG:CZ	2.51	0.40
1:A:110:LEU:N	1:A:110:LEU:HD23	2.36	0.40
1:A:314:GLN:O	1:A:318:THR:N	2.48	0.40
2:G:66:PRO:HA	2:G:100:THR:OG1	2.22	0.40
2:G:153:GLU:HB2	2:G:158:LEU:HD23	2.03	0.40
2:J:68:LEU:CD2	2:J:70:ILE:HG13	2.51	0.40
1:A:62:ARG:HG2	1:A:62:ARG:HH21	1.87	0.40
1:F:198:TYR:CD2	1:F:248:ILE:HD12	2.56	0.40
1:I:279:TYR:CE1	1:I:283:MET:SD	3.14	0.40
1:F:357:ILE:HD11	1:F:373:LYS:HB2	2.03	0.40
1:I:89:THR:O	1:I:94:LEU:HG	2.21	0.40

All (2) 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:66:THR:OG1	1:I:224:GLU:OE2[2_557]	2.06	0.14
1:F:25:ASP:OD2	2:J:105:ASN:HD21[1_455]	1.57	0.03

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	357/377 (95%)	348 (98%)	9 (2%)	0	100	100
1	D	357/377 (95%)	349 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	361/377 (96%)	341 (94%)	19 (5%)	1 (0%)	41	37
1	I	357/377 (95%)	339 (95%)	17 (5%)	1 (0%)	41	37
2	B	161/186 (87%)	156 (97%)	5 (3%)	0	100	100
2	E	123/186 (66%)	118 (96%)	4 (3%)	1 (1%)	19	12
2	G	139/186 (75%)	135 (97%)	3 (2%)	1 (1%)	22	15
2	J	125/186 (67%)	122 (98%)	1 (1%)	2 (2%)	9	4
All	All	1980/2252 (88%)	1908 (96%)	66 (3%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	201	VAL
2	G	53	VAL
2	E	54	VAL
1	I	34	ILE
2	J	54	VAL
2	J	53	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/320 (96%)	284 (92%)	23 (8%)	13	8
1	D	307/320 (96%)	281 (92%)	26 (8%)	10	6
1	F	310/320 (97%)	260 (84%)	50 (16%)	2	1
1	I	307/320 (96%)	266 (87%)	41 (13%)	4	1
2	B	138/153 (90%)	129 (94%)	9 (6%)	17	12
2	E	102/153 (67%)	97 (95%)	5 (5%)	25	21
2	G	119/153 (78%)	104 (87%)	15 (13%)	4	1
2	J	104/153 (68%)	91 (88%)	13 (12%)	4	1
All	All	1694/1892 (90%)	1512 (89%)	182 (11%)	6	3

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	28	ARG
1	A	72	GLU
1	A	113	LYS
1	A	159	VAL
1	A	176	MET
1	A	179[A]	ASP
1	A	179[B]	ASP
1	A	200	PHE
1	A	201	VAL
1	A	203	THR
1	A	242	LEU
1	A	257	CYS
1	A	275	HIS
1	A	284	LYS
1	A	287	ILE
1	A	292	ASP
1	A	297	ASN
1	A	315	LYS
1	A	316	GLU
1	A	318	THR
1	A	323	SER
1	A	373	LYS
2	B	84	ASN
2	B	150	GLN
2	B	1067	LEU
2	B	1074	GLN
2	B	1079	LYS
2	B	1082	GLU
2	B	1084	LEU
2	B	1095	VAL
2	B	1099	LYS
1	D	14	SER
1	D	28	ARG
1	D	33	SER
1	D	51	ASP
1	D	62	ARG
1	D	64	ILE
1	D	92	ASN
1	D	95	ARG
1	D	119	MET
1	D	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	179	ASP
1	D	208	ILE
1	D	238	LYS
1	D	241	GLU
1	D	248	ILE
1	D	249	THR
1	D	250	ILE
1	D	271	SER
1	D	283	MET
1	D	323	SER
1	D	324	THR
1	D	335	ARG
1	D	353	GLN
1	D	364	GLU
1	D	368	SER
1	D	375	PHE
2	E	83	THR
2	E	84	ASN
2	E	109	GLN
2	E	116	LEU
2	E	165	LEU
1	F	5	THR
1	F	14	SER
1	F	16	LEU
1	F	33	SER
1	F	34	ILE
1	F	53	TYR
1	F	57	GLU
1	F	60	SER
1	F	62	ARG
1	F	72	GLU
1	F	77	THR
1	F	80	ASP
1	F	95	ARG
1	F	116	ARG
1	F	132	MET
1	F	178	LEU
1	F	179	ASP
1	F	180	LEU
1	F	186	THR
1	F	189	LEU
1	F	194	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	196	ARG
1	F	206	ARG
1	F	207	GLU
1	F	221	LEU
1	F	229	THR
1	F	235	SER
1	F	246	GLN
1	F	252	ASN
1	F	253	GLU
1	F	254	ARG
1	F	265	SER
1	F	280	ASN
1	F	282	ILE
1	F	299	MET
1	F	300	SER
1	F	311	ASP
1	F	313	MET
1	F	318	THR
1	F	320	LEU
1	F	325	MET
1	F	326	LYS
1	F	327	ILE
1	F	332	PRO
1	F	338	SER
1	F	354	GLN
1	F	360	GLN
1	F	364	GLU
1	F	374	CYS
1	F	375	PHE
2	G	65	GLU
2	G	88	ASP
2	G	102	GLN
2	G	103	LEU
2	G	107	ASN
2	G	112	LEU
2	G	114	TYR
2	G	142	ARG
2	G	146	HIS
2	G	158	LEU
2	G	1059	THR
2	G	1062	PHE
2	G	1064	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1070	HIS
2	G	1074	GLN
1	I	18	LYS
1	I	34	ILE
1	I	60	SER
1	I	68	LYS
1	I	75	ILE
1	I	91	TYR
1	I	92	ASN
1	I	94	LEU
1	I	96	VAL
1	I	99	GLU
1	I	106	THR
1	I	110	LEU
1	I	115	ASN
1	I	132	MET
1	I	134	VAL
1	I	180	LEU
1	I	185	LEU
1	I	187	ASP
1	I	191	LYS
1	I	193	LEU
1	I	199	SER
1	I	201	VAL
1	I	202	THR
1	I	203	THR
1	I	215	LYS
1	I	224	GLU
1	I	226	GLU
1	I	227	MET
1	I	246	GLN
1	I	249	THR
1	I	250	ILE
1	I	269	MET
1	I	281	SER
1	I	292	ASP
1	I	304	THR
1	I	330	ILE
1	I	334	GLU
1	I	338	SER
1	I	355	MET
1	I	368	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	375	PHE
2	J	52	MET
2	J	83	THR
2	J	88	ASP
2	J	112	LEU
2	J	121	SER
2	J	135	LEU
2	J	137	ASP
2	J	156	THR
2	J	161	PHE
2	J	165	LEU
2	J	168	LYS
2	J	169	LYS
2	J	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	121	GLN
1	A	161	HIS
1	A	371	HIS
2	B	134	GLN
1	D	92	ASN
1	D	115	ASN
1	D	297	ASN
1	D	353	GLN
2	E	84	ASN
2	E	102	GLN
2	E	134	GLN
2	E	145	GLN
1	F	41	GLN
1	F	73	HIS
1	F	161	HIS
1	F	162	ASN
1	F	280	ASN
1	F	371	HIS
2	G	134	GLN
2	G	146	HIS
1	I	111	ASN
1	I	128	ASN
1	I	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	162	ASN
1	I	225	ASN
1	I	371	HIS
2	J	69	GLN
2	J	107	ASN
2	J	140	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	F	401	-	24,29,29	1.10	3 (12%)	29,45,45	1.48	5 (17%)
3	ADP	I	401	4	24,29,29	1.18	3 (12%)	29,45,45	2.08	12 (41%)
3	ADP	A	401	4	24,29,29	1.34	5 (20%)	29,45,45	1.80	9 (31%)
3	ADP	D	401	4	24,29,29	1.08	3 (12%)	29,45,45	1.63	10 (34%)

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	F	401	-	-	5/12/32/32	0/3/3/3
3	ADP	I	401	4	-	0/12/32/32	0/3/3/3
3	ADP	A	401	4	-	2/12/32/32	0/3/3/3
3	ADP	D	401	4	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	O4'-C1'	2.90	1.45	1.41
3	A	401	ADP	C2-N3	2.84	1.36	1.32
3	I	401	ADP	C2'-C1'	-2.67	1.49	1.53
3	F	401	ADP	O4'-C1'	2.48	1.44	1.41
3	A	401	ADP	C6-C5	2.44	1.52	1.43
3	A	401	ADP	PB-O3B	-2.39	1.45	1.54
3	I	401	ADP	C5-C4	2.38	1.47	1.40
3	D	401	ADP	C5-C4	2.34	1.47	1.40
3	F	401	ADP	C5-C4	2.33	1.47	1.40
3	F	401	ADP	C2-N3	2.26	1.35	1.32
3	D	401	ADP	O4'-C1'	2.24	1.44	1.41
3	D	401	ADP	C2-N3	2.20	1.35	1.32
3	I	401	ADP	C8-N7	2.18	1.38	1.34
3	A	401	ADP	C5-C4	2.12	1.46	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ADP	C4-C5-N7	-4.73	104.47	109.40
3	I	401	ADP	PA-O3A-PB	-4.06	118.90	132.83
3	A	401	ADP	O3B-PB-O3A	-4.02	91.17	104.64
3	I	401	ADP	C1'-N9-C4	-3.95	119.70	126.64
3	I	401	ADP	O3'-C3'-C2'	-3.49	100.54	111.82
3	I	401	ADP	O4'-C1'-C2'	3.20	111.61	106.93
3	I	401	ADP	N3-C2-N1	-3.14	123.77	128.68
3	F	401	ADP	N3-C2-N1	-3.04	123.93	128.68
3	I	401	ADP	C2-N1-C6	2.87	123.67	118.75
3	D	401	ADP	O3B-PB-O1B	2.85	121.84	110.68
3	A	401	ADP	O3B-PB-O1B	2.83	121.75	110.68
3	D	401	ADP	C3'-C2'-C1'	2.78	105.16	100.98
3	F	401	ADP	C4-C5-N7	-2.76	106.52	109.40
3	I	401	ADP	C3'-C2'-C1'	2.66	104.98	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ADP	O4'-C1'-C2'	-2.60	103.12	106.93
3	F	401	ADP	O2B-PB-O3A	2.55	113.18	104.64
3	D	401	ADP	O3'-C3'-C4'	-2.53	103.74	111.05
3	I	401	ADP	O3B-PB-O2B	2.49	117.16	107.64
3	I	401	ADP	O3A-PB-O1B	-2.49	97.38	111.19
3	I	401	ADP	C4-C5-N7	-2.43	106.86	109.40
3	D	401	ADP	C5'-C4'-C3'	-2.39	106.23	115.18
3	D	401	ADP	C1'-N9-C4	-2.38	122.46	126.64
3	F	401	ADP	C1'-N9-C4	-2.32	122.56	126.64
3	I	401	ADP	O3B-PB-O1B	2.31	119.73	110.68
3	D	401	ADP	C4-C5-N7	-2.31	107.00	109.40
3	I	401	ADP	O4'-C4'-C3'	2.29	109.64	105.11
3	A	401	ADP	C2'-C3'-C4'	2.27	107.06	102.64
3	A	401	ADP	O2A-PA-O1A	2.25	123.35	112.24
3	D	401	ADP	N3-C2-N1	-2.23	125.19	128.68
3	D	401	ADP	PA-O3A-PB	-2.21	125.23	132.83
3	D	401	ADP	O4'-C4'-C3'	2.19	109.45	105.11
3	A	401	ADP	O3A-PB-O1B	-2.18	99.12	111.19
3	D	401	ADP	O3B-PB-O3A	-2.17	97.37	104.64
3	F	401	ADP	O5'-C5'-C4'	2.09	116.20	108.99
3	A	401	ADP	O3B-PB-O2B	2.08	115.58	107.64
3	A	401	ADP	N3-C2-N1	-2.05	125.47	128.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	ADP	C5'-O5'-PA-O3A
3	F	401	ADP	O4'-C4'-C5'-O5'
3	F	401	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	PA-O3A-PB-O3B
3	F	401	ADP	C5'-O5'-PA-O1A
3	F	401	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	ADP	6	0
3	I	401	ADP	3	0

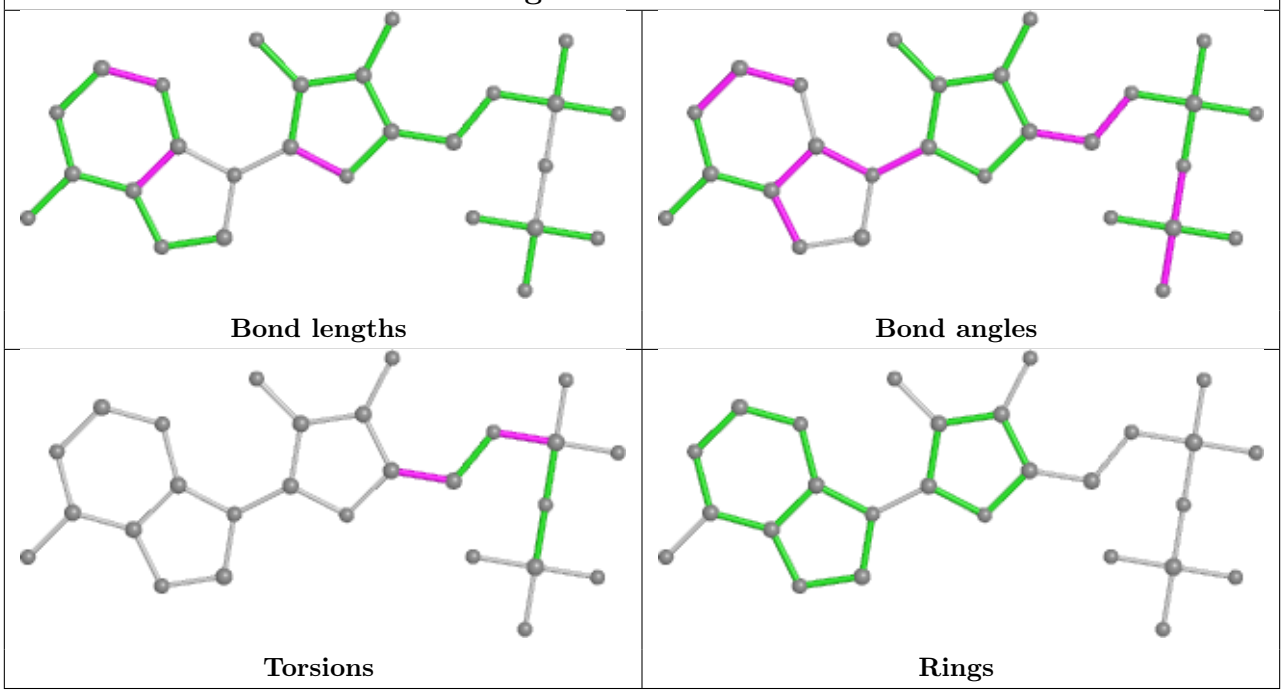
Continued on next page...

Continued from previous page...

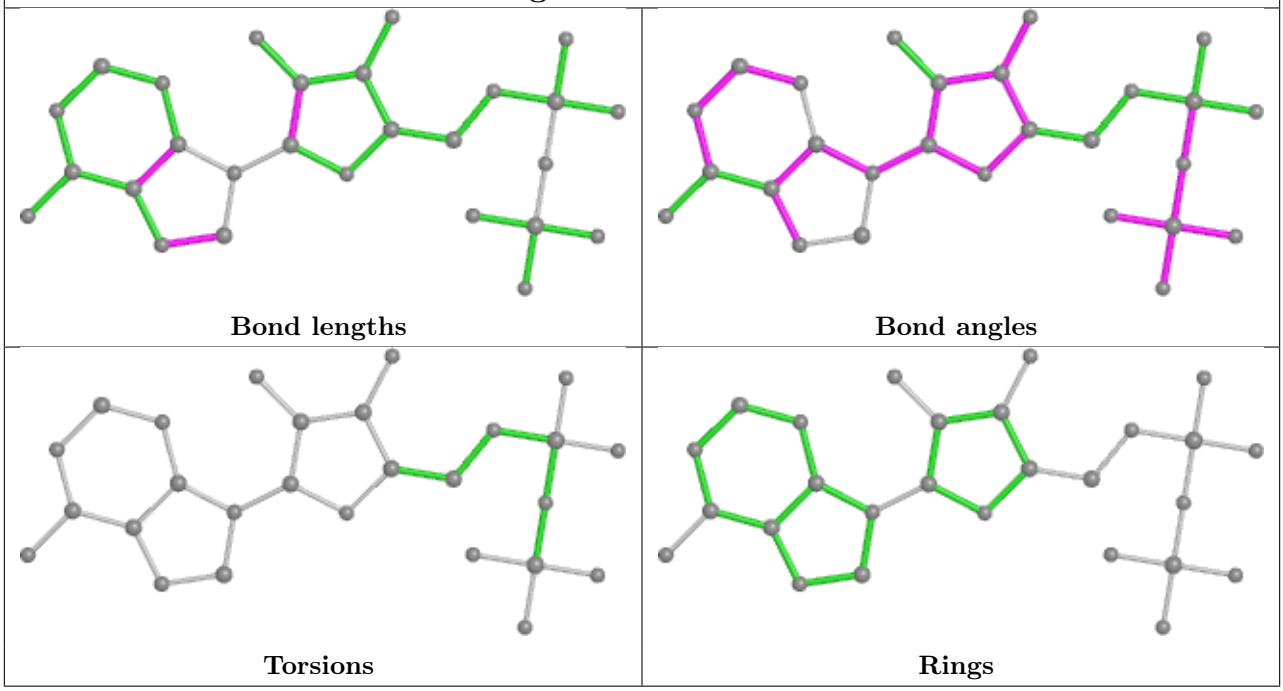
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0

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 then 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.

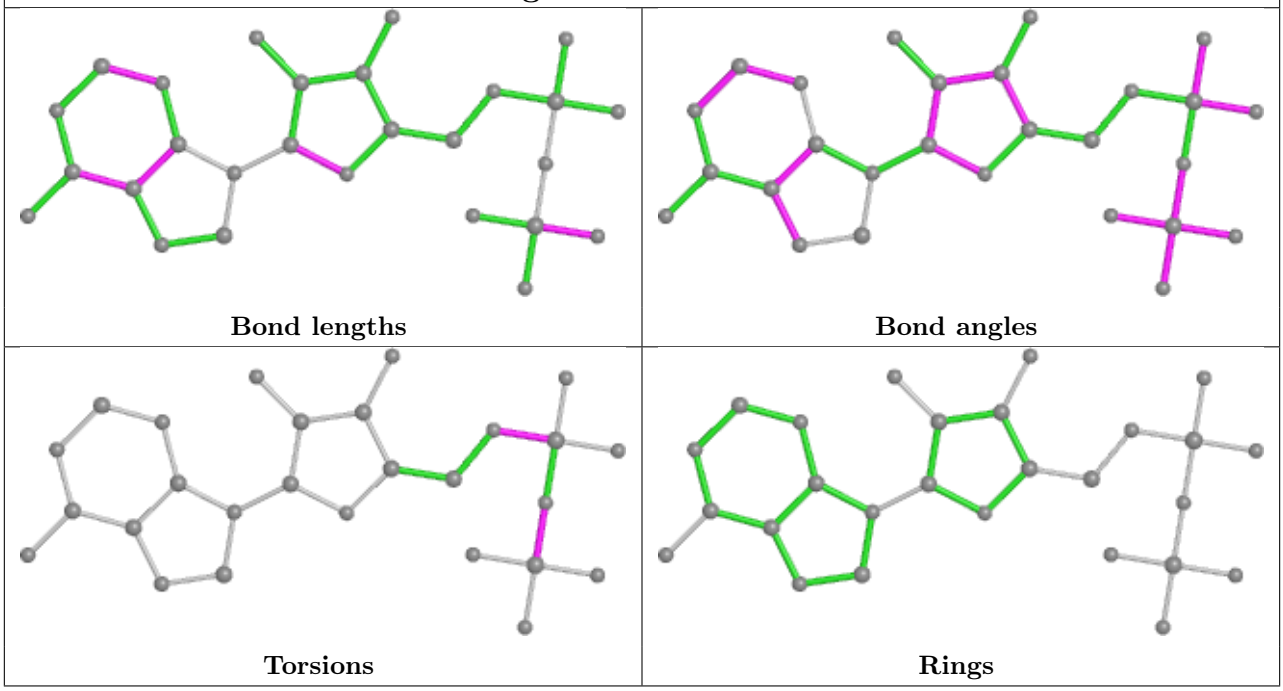
Ligand ADP F 401

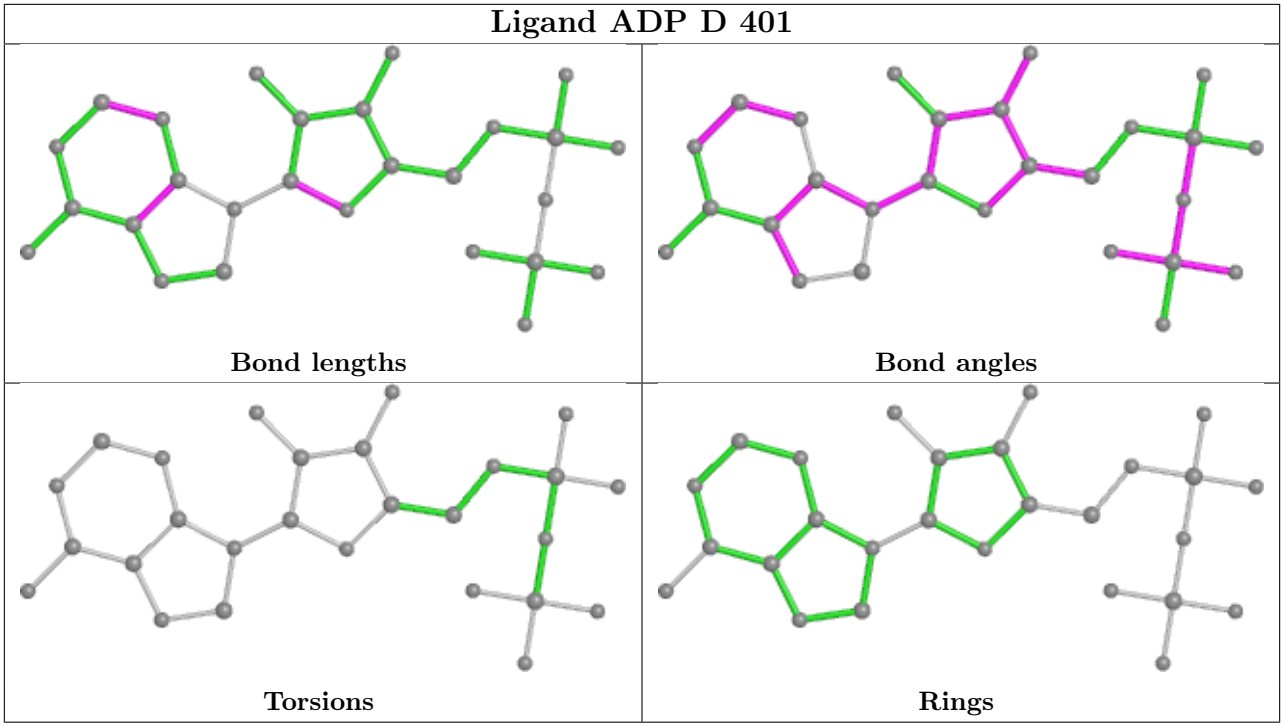


Ligand ADP I 401



Ligand ADP A 401





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	359/377 (95%)	0.29	10 (2%) 53 62	18, 46, 80, 120	1 (0%)
1	D	360/377 (95%)	0.19	9 (2%) 57 65	17, 38, 82, 116	0
1	F	365/377 (96%)	1.79	124 (33%) 0 0	56, 79, 127, 182	0
1	I	360/377 (95%)	1.97	139 (38%) 0 0	57, 81, 126, 166	0
2	B	165/186 (88%)	0.38	10 (6%) 21 28	18, 38, 101, 129	0
2	E	125/186 (67%)	0.01	3 (2%) 59 67	16, 29, 52, 95	0
2	G	143/186 (76%)	1.74	43 (30%) 0 0	57, 77, 110, 167	0
2	J	126/186 (67%)	1.87	48 (38%) 0 0	60, 80, 106, 142	0
All	All	2003/2252 (88%)	1.04	386 (19%) 1 1	16, 67, 111, 182	1 (0%)

All (386) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	327	ILE	14.0
1	F	209	VAL	10.2
2	G	55	GLU	9.1
1	I	91	TYR	8.2
1	I	54	VAL	8.1
2	J	53	VAL	8.0
1	I	203	THR	8.0
1	F	248	ILE	7.8
1	F	375	PHE	7.7
1	I	201	VAL	7.5
1	I	158	GLY	7.4
1	F	232	SER	7.4
2	J	108	LEU	7.2
1	F	58	ALA	7.0
1	F	178	LEU	6.9
1	F	53	TYR	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	276	GLU	6.7
2	G	54	VAL	6.3
1	I	202	THR	6.2
1	F	152	VAL	6.2
2	G	85	LEU	6.1
1	I	69	TYR	6.0
1	I	200	PHE	6.0
1	I	250	ILE	6.0
1	F	219	VAL	6.0
1	F	317	ILE	5.7
1	D	201	VAL	5.7
1	F	19	ALA	5.7
1	I	375	PHE	5.7
2	B	54	VAL	5.5
2	J	152	PHE	5.5
1	F	8	LEU	5.4
2	J	103	LEU	5.3
1	I	163	VAL	5.3
2	G	1062	PHE	5.3
1	I	58	ALA	5.2
1	I	317	ILE	5.2
1	F	251	GLY	5.1
1	F	306	TYR	5.1
2	B	1078	PHE	5.1
1	F	5	THR	5.0
1	I	324	THR	5.0
1	F	236	LEU	5.0
1	I	79	TRP	5.0
2	J	76	PHE	5.0
1	I	64	ILE	4.9
1	F	304	THR	4.9
2	J	171	GLY	4.8
1	F	200	PHE	4.7
1	I	333	PRO	4.7
1	I	60	SER	4.7
2	J	96	VAL	4.7
1	I	304	THR	4.6
1	I	63	GLY	4.6
1	I	127	PHE	4.4
1	I	138	ALA	4.4
2	J	59	PHE	4.4
1	F	233	SER	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	165	ILE	4.3
1	I	215	LYS	4.3
2	J	155	ALA	4.2
2	G	176	PHE	4.2
2	G	1067	LEU	4.2
1	I	36	GLY	4.2
1	F	88	HIS	4.1
1	I	26	ALA	4.1
2	J	54	VAL	4.1
1	F	238	LYS	4.1
1	F	20	GLY	4.0
1	I	365	ALA	4.0
1	A	240	TYR	3.9
1	F	242	LEU	3.9
2	G	103	LEU	3.9
2	G	98	LEU	3.9
2	J	90	PHE	3.9
2	J	149	VAL	3.9
1	F	230	ALA	3.9
1	D	64	ILE	3.9
1	F	289	ILE	3.8
1	I	164	PRO	3.8
1	I	195	GLU	3.8
1	F	17	VAL	3.8
2	G	152	PHE	3.8
1	D	203	THR	3.8
1	F	164	PRO	3.8
1	F	246	GLN	3.7
1	F	282	ILE	3.7
2	J	162	LYS	3.7
1	I	329	ILE	3.7
1	I	328	LYS	3.7
1	F	244	ASP	3.7
1	F	57	GLU	3.7
1	I	161	HIS	3.7
2	J	115	TRP	3.7
1	I	90	PHE	3.7
2	G	1069	ASP	3.6
2	J	146	HIS	3.6
1	I	143	TYR	3.6
1	F	198	TYR	3.6
1	I	261	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	67	GLY	3.6
1	F	262	PHE	3.5
1	F	247	VAL	3.5
2	B	1085	VAL	3.5
1	F	170	ALA	3.5
2	G	131	PHE	3.5
2	G	165	LEU	3.5
1	I	374	CYS	3.5
1	I	31	PHE	3.5
1	F	250	ILE	3.5
1	I	294	TYR	3.5
1	I	162	ASN	3.4
1	F	177	ARG	3.4
1	F	9	VAL	3.4
1	F	266	PHE	3.4
2	G	90	PHE	3.4
1	F	28	ARG	3.4
2	G	97	ILE	3.4
1	I	62	ARG	3.4
1	F	158	GLY	3.4
1	F	217	CYS	3.4
1	I	110	LEU	3.4
1	F	79	TRP	3.4
1	F	280	ASN	3.4
1	I	142	LEU	3.4
1	A	228	ALA	3.4
1	F	159	VAL	3.4
1	F	261	LEU	3.3
1	F	30	VAL	3.3
1	F	96	VAL	3.3
1	I	10[A]	CYS	3.3
2	G	95	TYR	3.3
2	E	53	VAL	3.3
2	G	177	GLY	3.3
1	I	171	LEU	3.3
1	I	68	LYS	3.3
2	B	1086	PRO	3.3
1	I	131	ALA	3.3
1	I	240	TYR	3.2
1	A	65	LEU	3.2
2	G	1072	GLU	3.2
1	F	234	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	340	TRP	3.2
2	G	167	TYR	3.2
1	F	188	TYR	3.2
2	J	167	TYR	3.2
1	I	153	LEU	3.2
1	I	148	THR	3.2
2	J	119	GLU	3.2
2	J	109	GLN	3.2
1	D	324	THR	3.2
1	D	58	ALA	3.1
2	B	1068	LEU	3.1
2	J	85	LEU	3.1
1	F	86	TRP	3.1
1	I	170	ALA	3.1
1	I	185	LEU	3.1
2	J	170	GLY	3.1
1	I	232	SER	3.1
1	F	174	ALA	3.1
1	I	180	LEU	3.1
2	E	54	VAL	3.1
2	G	68	LEU	3.1
2	G	1068	LEU	3.1
1	F	31	PHE	3.1
1	I	325	MET	3.0
2	G	1059	THR	3.0
2	G	149	VAL	3.0
1	A	277	THR	3.0
1	I	96	VAL	3.0
1	I	155	SER	3.0
1	I	5	THR	3.0
1	D	250	ILE	2.9
1	F	206	ARG	2.9
1	F	292	ASP	2.9
1	I	6	THR	2.9
1	I	198	TYR	2.9
2	G	84	ASN	2.9
2	G	116	LEU	2.9
1	I	71	ILE	2.9
1	F	294	TYR	2.9
1	I	306	TYR	2.9
2	J	95	TYR	2.9
1	F	25	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	185	LEU	2.9
1	A	250	ILE	2.9
1	F	64	ILE	2.9
1	I	52	SER	2.9
1	I	98	PRO	2.9
2	G	96	VAL	2.9
1	I	87	HIS	2.9
1	F	21	PHE	2.8
1	I	37	ARG	2.8
1	I	231	ALA	2.8
1	I	248	ILE	2.8
1	I	345	ILE	2.8
1	F	295	ALA	2.8
2	G	105	ASN	2.8
1	I	75	ILE	2.8
2	G	117	GLY	2.8
1	F	171	LEU	2.8
1	I	8	LEU	2.8
1	F	7	ALA	2.8
1	F	231	ALA	2.8
1	F	202	THR	2.8
1	F	309	ILE	2.8
1	I	67	LEU	2.7
1	I	330	ILE	2.7
1	I	86	TRP	2.7
1	I	223	PHE	2.7
1	F	265	SER	2.7
1	I	135	ALA	2.7
1	F	179	ASP	2.7
2	B	1077	GLU	2.7
1	I	238	LYS	2.7
2	B	1084	LEU	2.7
1	F	305	MET	2.7
1	I	9	VAL	2.7
1	D	248	ILE	2.7
2	G	128	ALA	2.7
2	J	151	GLY	2.6
1	F	357	ILE	2.6
1	I	352	PHE	2.6
2	G	76	PHE	2.6
1	I	236	LEU	2.6
1	I	38	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	ALA	2.6
1	A	203	THR	2.6
1	F	227	MET	2.6
1	F	56	ASP	2.6
2	J	172	VAL	2.6
1	I	262	PHE	2.6
1	I	144	ALA	2.6
2	J	102	GLN	2.6
1	F	203	THR	2.6
1	F	260	THR	2.6
1	I	243	PRO	2.6
2	J	66	PRO	2.6
1	I	53	TYR	2.6
2	G	136	ASP	2.6
1	F	281	SER	2.6
1	F	71	ILE	2.6
1	F	223	PHE	2.6
2	J	161	PHE	2.6
1	I	221	LEU	2.6
1	I	298	VAL	2.5
1	I	300	SER	2.5
2	J	176	PHE	2.5
1	I	216	LEU	2.5
2	J	60	LEU	2.5
1	F	201	VAL	2.5
1	I	318	THR	2.5
2	G	1066	GLU	2.5
1	F	235	SER	2.5
1	I	76	ILE	2.5
2	G	118	ASN	2.5
1	I	244	ASP	2.5
2	J	131	PHE	2.5
1	I	299	MET	2.4
2	J	78	LEU	2.4
1	F	243	PRO	2.4
1	F	264	PRO	2.4
1	I	109	PRO	2.4
1	F	369	ILE	2.4
2	B	1075	ALA	2.4
1	F	240	TYR	2.4
1	I	169	TYR	2.4
1	F	124	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	349	LEU	2.4
1	A	236	LEU	2.4
1	F	110	LEU	2.4
1	F	189	LEU	2.4
1	I	242	LEU	2.4
1	I	30	VAL	2.4
2	G	86	TYR	2.4
1	F	121	GLN	2.4
1	F	221	LEU	2.4
1	I	320	LEU	2.4
1	F	45	VAL	2.4
1	F	229	THR	2.4
1	I	187	ASP	2.4
1	F	127	PHE	2.3
2	G	158	LEU	2.3
1	I	230	ALA	2.3
2	J	94	ALA	2.3
1	F	69	TYR	2.3
1	F	130	PRO	2.3
1	I	94	LEU	2.3
2	J	89	PHE	2.3
1	I	119	MET	2.3
1	I	283	MET	2.3
1	F	195	GLU	2.3
1	F	274	ILE	2.3
1	I	80	ASP	2.3
2	G	1058	PRO	2.3
1	I	145	SER	2.3
2	G	160	TYR	2.3
1	I	152	VAL	2.3
1	I	209	VAL	2.3
2	J	133	VAL	2.3
1	F	29	ALA	2.3
1	I	260	THR	2.3
1	F	356	TRP	2.3
1	I	340	TRP	2.3
2	J	93	ASP	2.3
2	B	108	LEU	2.2
1	I	21	PHE	2.2
1	F	253	GLU	2.2
1	F	293	LEU	2.2
2	J	139	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	162	ASN	2.2
1	A	60	SER	2.2
1	F	52	SER	2.2
1	I	168	GLY	2.2
2	J	121	SER	2.2
2	J	166	LYS	2.2
1	F	220	ALA	2.2
2	G	156	THR	2.2
1	F	142	LEU	2.2
1	F	216	LEU	2.2
1	I	133	TYR	2.2
1	D	244	ASP	2.2
1	F	81	ASP	2.2
1	F	157	ASP	2.2
1	I	334	GLU	2.2
1	A	208	ILE	2.2
1	I	212	ILE	2.2
1	I	237	GLU	2.2
1	F	370	VAL	2.2
2	G	79	VAL	2.2
2	G	89	PHE	2.2
1	I	149	THR	2.2
1	F	95	ARG	2.2
2	J	52	MET	2.2
1	F	365	ALA	2.2
2	J	101	VAL	2.1
1	I	204	ALA	2.1
1	F	105	LEU	2.1
2	J	68	LEU	2.1
1	I	51	ASP	2.1
2	J	117	GLY	2.1
1	I	114	ALA	2.1
1	F	258	PRO	2.1
1	I	289	ILE	2.1
2	G	151	GLY	2.1
2	J	177	GLY	2.1
1	F	44	MET	2.1
1	F	126	THR	2.1
2	J	134	GLN	2.1
1	F	122	ILE	2.1
1	F	267	ILE	2.1
1	I	34	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	15	GLY	2.1
1	F	65	LEU	2.1
2	E	103	LEU	2.1
2	J	141	GLY	2.1
1	I	33	SER	2.1
1	I	141	SER	2.1
1	I	247	VAL	2.1
2	J	81	VAL	2.1
1	I	220	ALA	2.1
1	I	322	PRO	2.1
1	I	25	ASP	2.1
2	J	147	ARG	2.1
1	I	132	MET	2.1
1	F	125	GLU	2.1
2	G	157	PHE	2.1
2	J	160	TYR	2.1
1	F	136	ILE	2.0
1	D	190	MET	2.0
1	F	193	LEU	2.0
1	I	17	VAL	2.0
1	I	35	VAL	2.0
1	I	61	LYS	2.0
1	I	134	VAL	2.0
1	I	219	VAL	2.0
1	I	14	SER	2.0
1	I	95	ARG	2.0
1	I	233	SER	2.0
1	I	16	LEU	2.0
1	I	136	ILE	2.0
1	F	129	VAL	2.0
1	I	66	THR	2.0
2	B	1059	THR	2.0
2	G	172	VAL	2.0
2	J	126	GLY	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

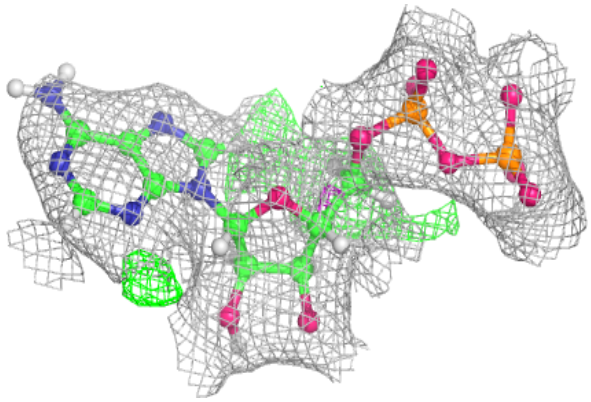
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

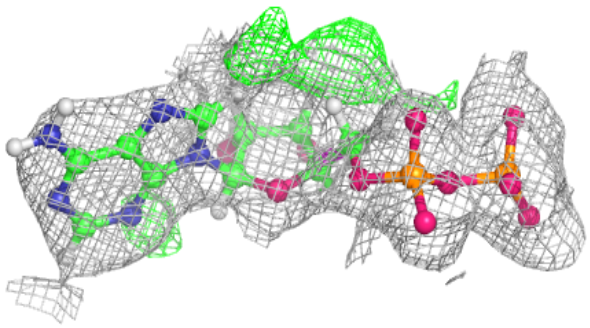
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	F	402	1/1	0.70	0.09	91,91,91,91	0
4	CA	I	402	1/1	0.77	0.12	81,81,81,81	0
4	CA	D	403	1/1	0.88	0.07	63,63,63,63	0
4	CA	D	402	1/1	0.91	0.10	64,64,64,64	0
4	CA	I	403	1/1	0.91	0.10	67,67,67,67	0
3	ADP	I	401	27/27	0.92	0.13	35,48,59,62	0
4	CA	J	1201	1/1	0.92	0.13	60,60,60,60	0
3	ADP	F	401	27/27	0.94	0.12	38,57,69,74	0
4	CA	A	402	1/1	0.94	0.07	63,63,63,63	0
4	CA	F	403	1/1	0.96	0.24	55,55,55,55	0
3	ADP	A	401	27/27	0.96	0.13	18,41,55,57	0
3	ADP	D	401	27/27	0.97	0.11	16,30,40,42	0
4	CA	A	403	1/1	0.98	0.05	40,40,40,40	0
4	CA	B	1201	1/1	0.99	0.06	26,26,26,26	0
4	CA	E	1201	1/1	0.99	0.06	24,24,24,24	0
4	CA	G	1201	1/1	0.99	0.13	56,56,56,56	0

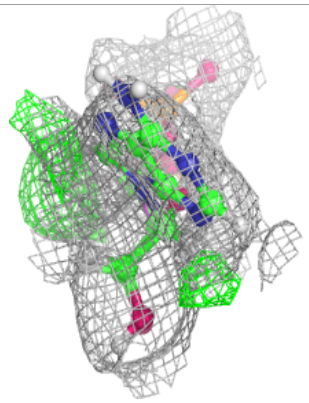
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP I 401:

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

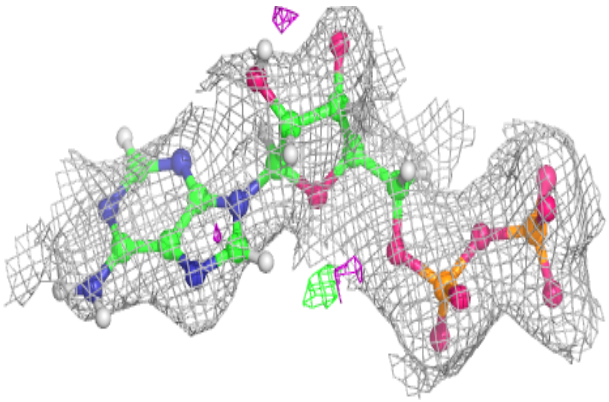


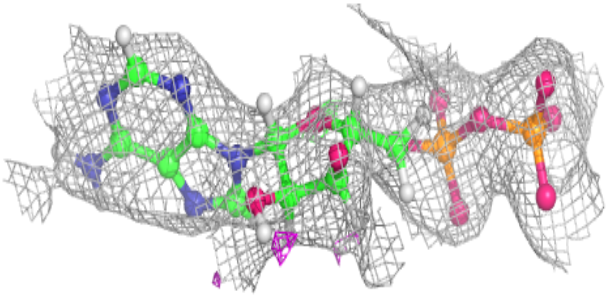


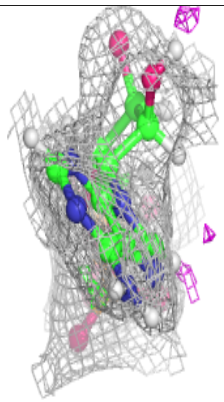


Electron density around ADP F 401:

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

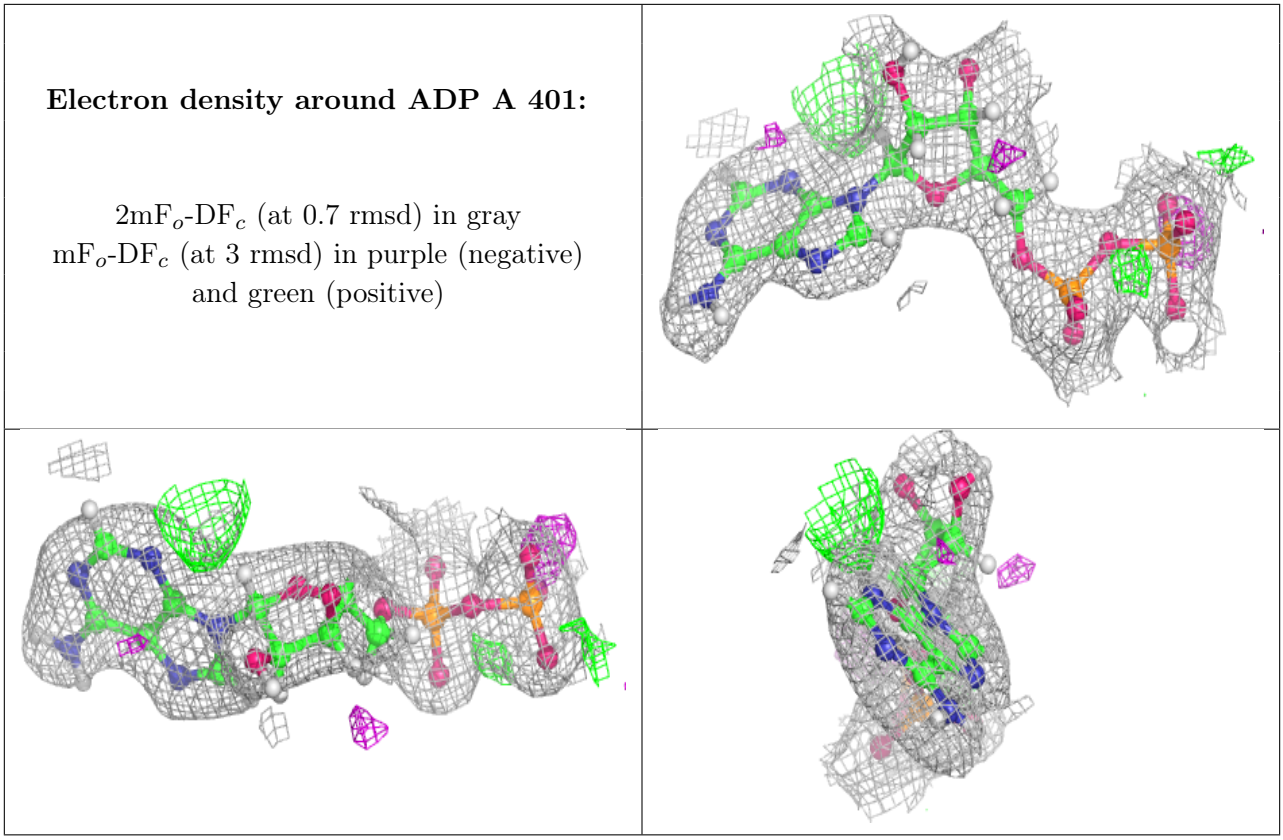






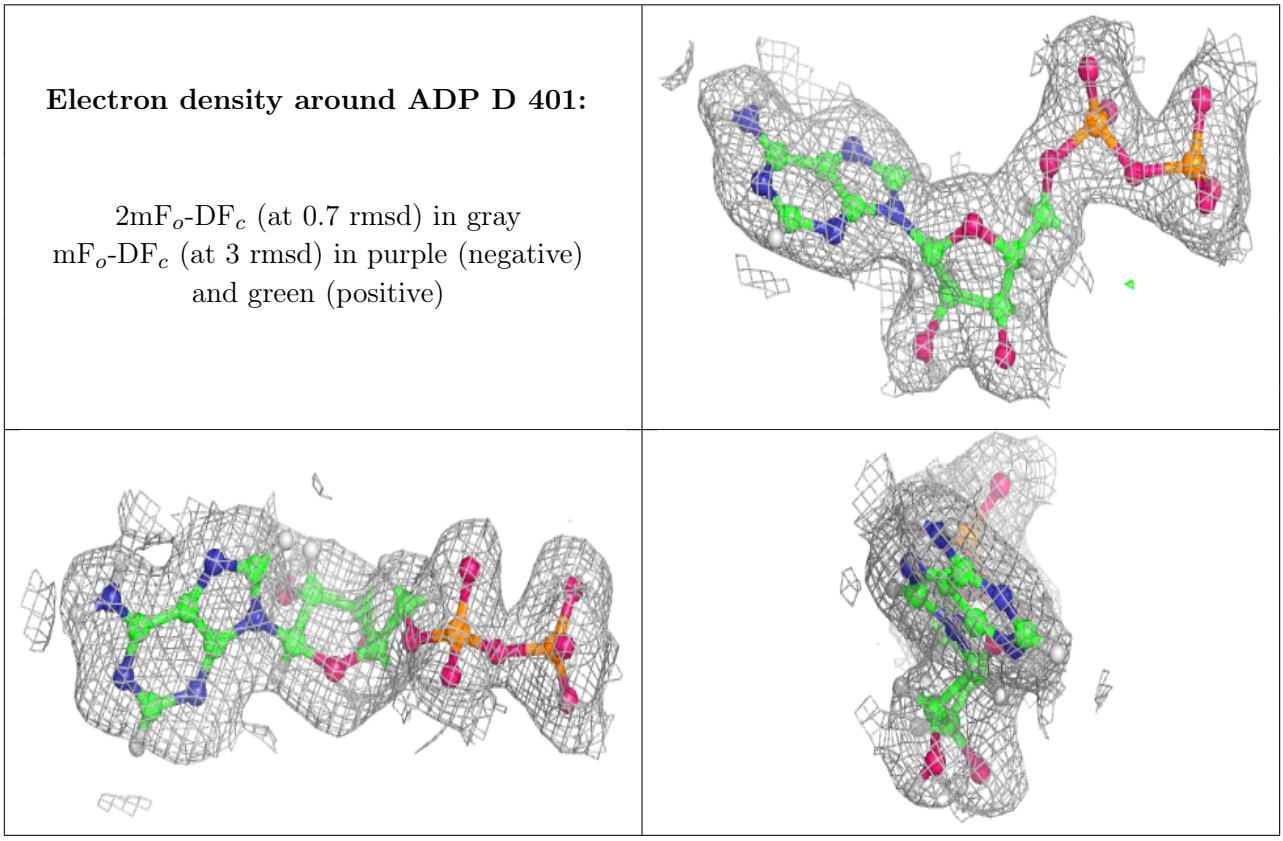
Electron density around ADP A 401:

$2mF_o$-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 D 401:

$2mF_o$-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.