Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:40 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

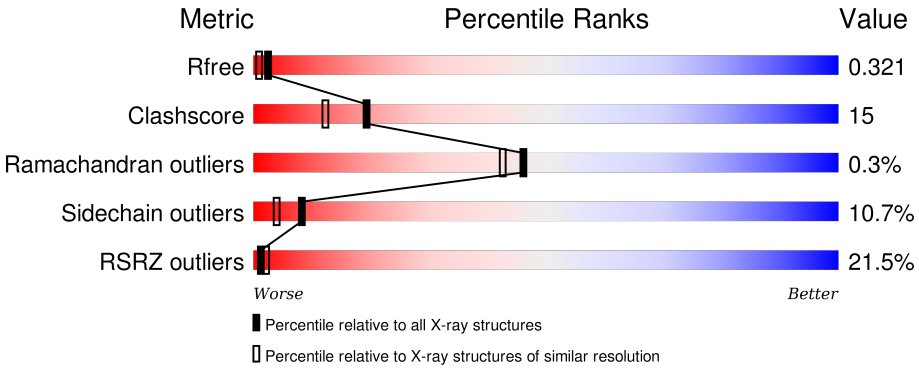
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 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 <=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	36% 59% 33% 5% •
1	I	377	41% 52% 37% 6% 5%
2	B	186	8% 70% 17% • 11%

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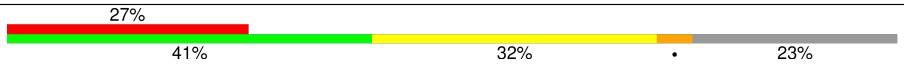
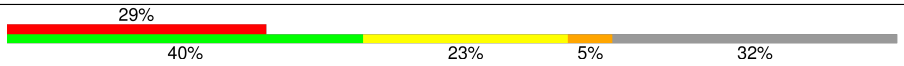
Mol	Chain	Length	Quality of chain
2	E	186	
2	G	186	
2	J	186	

2 Entry composition

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

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

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

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

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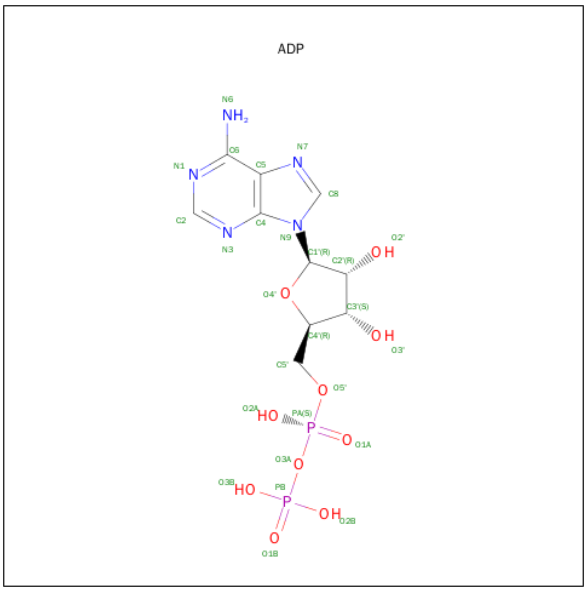
Chain	Residue	Modelled	Actual	Comment	Reference
B	185	SER	-	linker	UNP P06396
E	177	GLY	-	linker	UNP P06396
E	178	GLY	-	linker	UNP P06396
E	179	SER	-	linker	UNP P06396
E	180	GLY	-	linker	UNP P06396
E	181	GLY	-	linker	UNP P06396
E	182	SER	-	linker	UNP P06396
E	183	GLY	-	linker	UNP P06396
E	184	GLY	-	linker	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
3	A	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
3	D	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
3	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
3	I	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

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

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

- Molecule 5 is water.

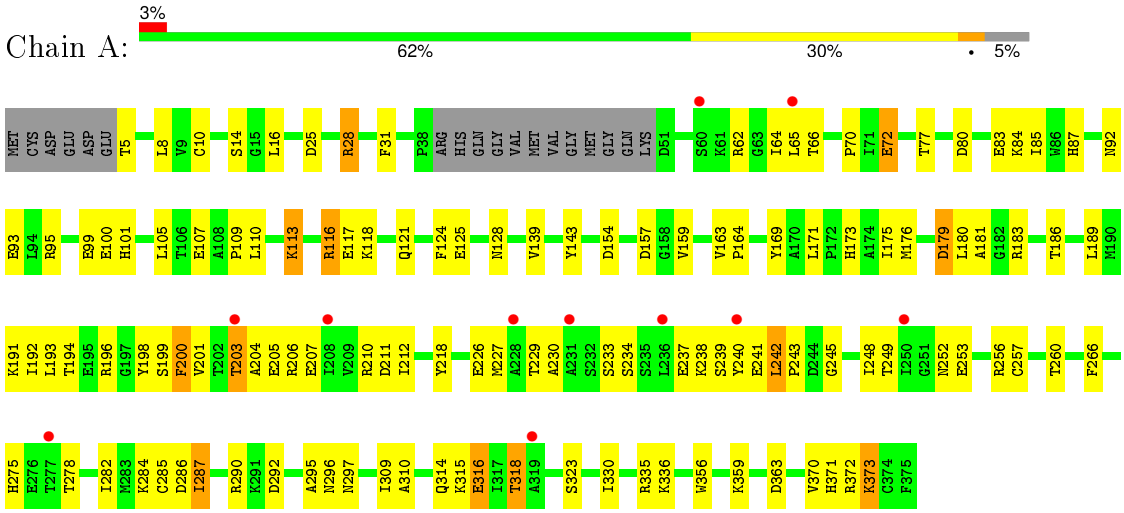
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0
5	B	82	Total O 82 82	0	0
5	D	87	Total O 87 87	0	0
5	E	77	Total O 77 77	0	0
5	F	63	Total O 63 63	0	0
5	G	49	Total O 49 49	0	0
5	I	62	Total O 62 62	0	0
5	J	40	Total O 40 40	0	0

3 Residue-property plots (i)

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.

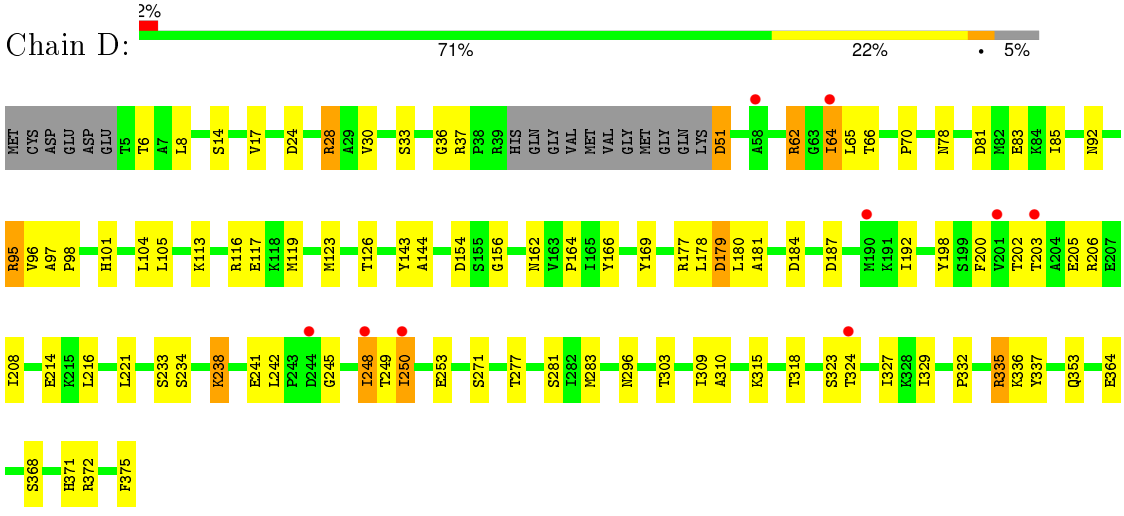
- Molecule 1: Actin, alpha skeletal muscle

Chain A:



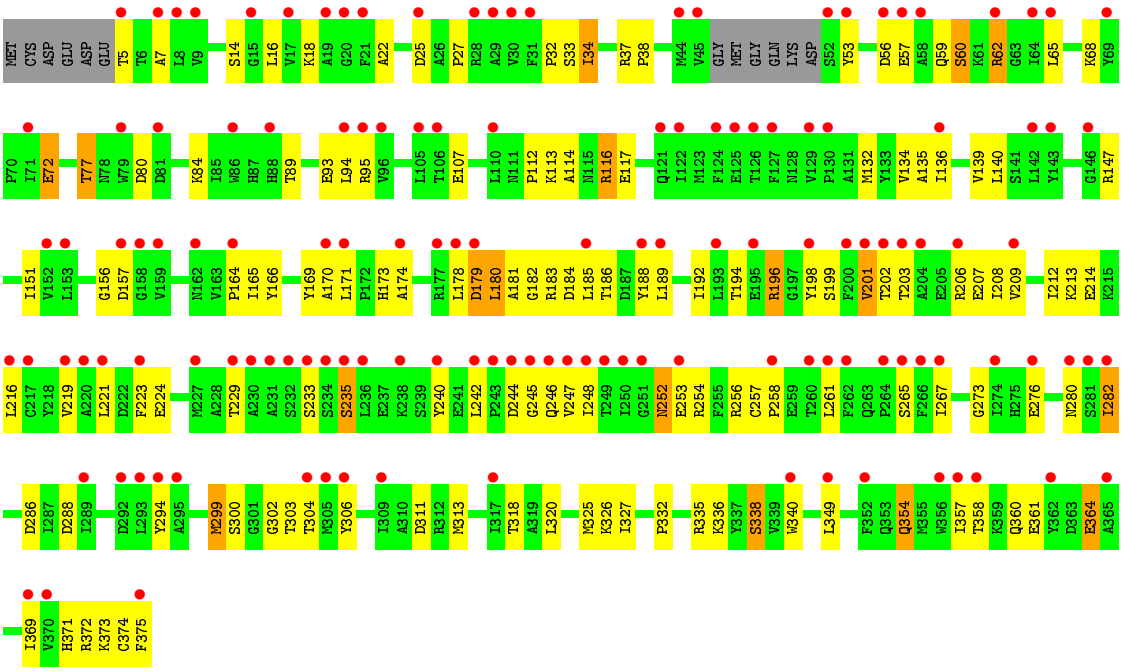
- Molecule 1: Actin, alpha skeletal muscle

Chain D:



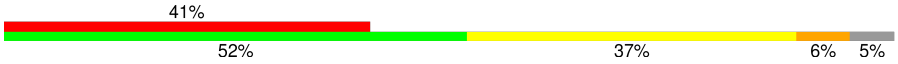
- Molecule 1: Actin, alpha skeletal muscle

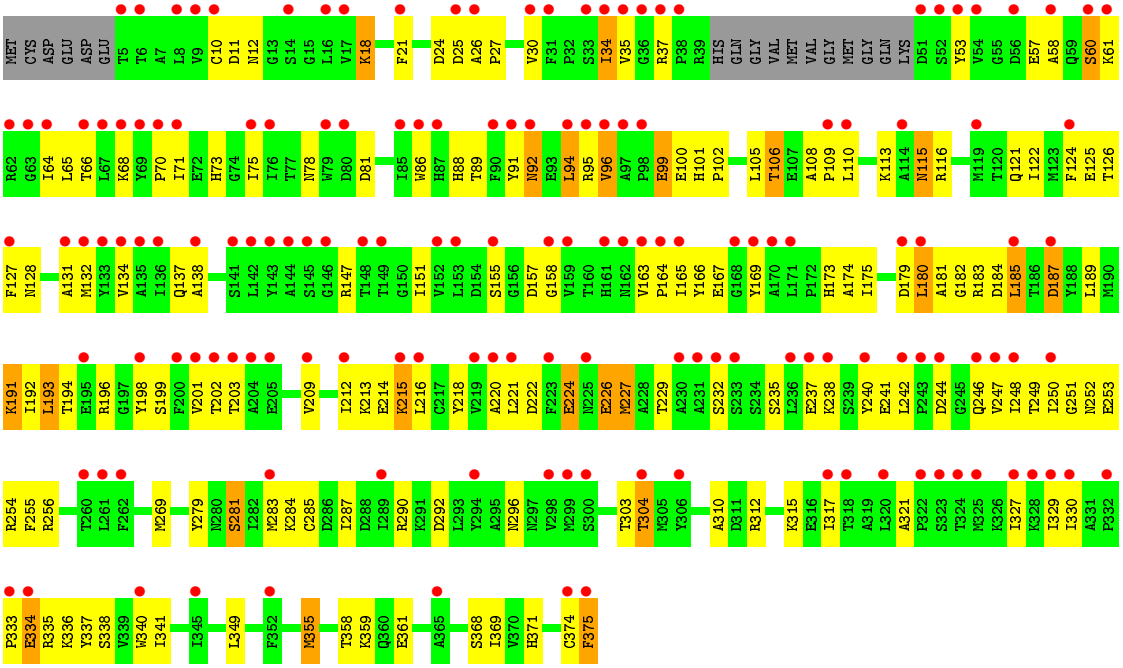
Chain F:



• Molecule 1: Actin, alpha skeletal muscle

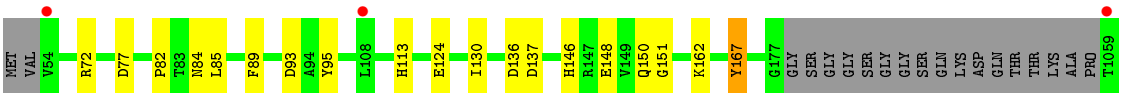
Chain I:

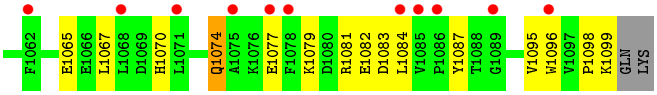




• Molecule 2: Gelsolin,Tropomodulin-1 chimera

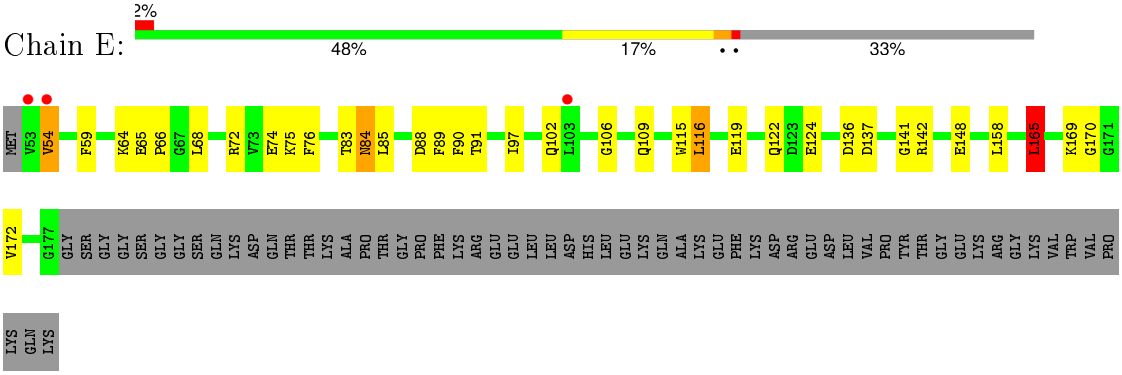
Chain B:





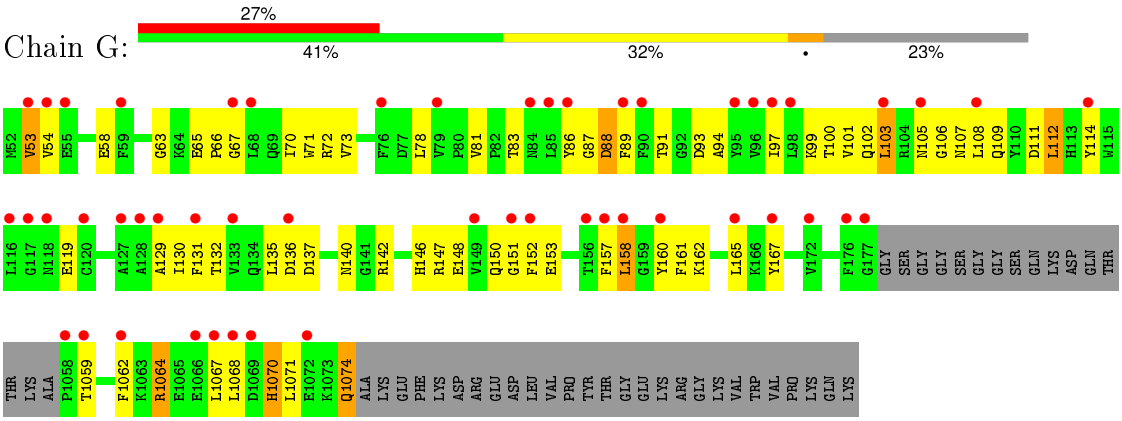
• Molecule 2: Gelsolin,Tropomodulin-1 chimera

Chain E:



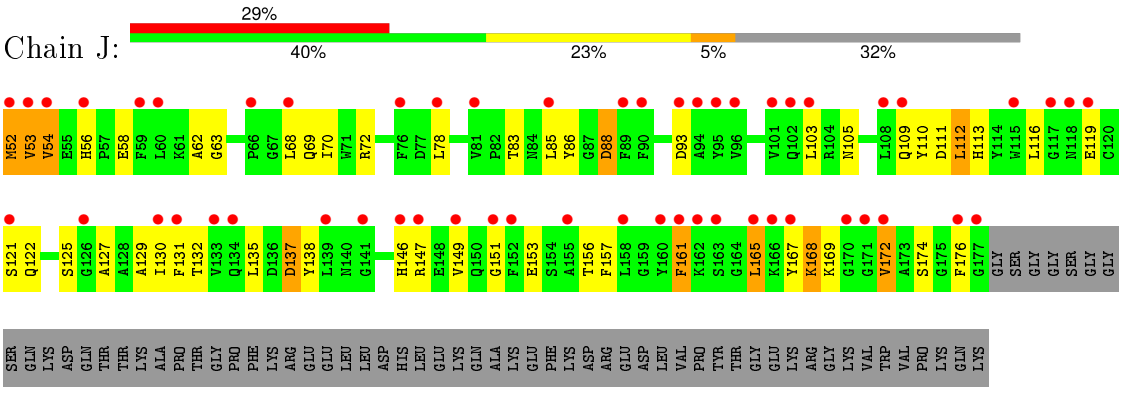
• Molecule 2: Gelsolin,Tropomodulin-1 chimera

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]	2.50 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.274 , 0.326 0.270 , 0.321	Depositor DCC
R_{free} test set	1875 reflections (1.47%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 138120 reflections	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 28.63 % 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 1.7819e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.95	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

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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:N	2:J:52:MET:SD	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

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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:F:364:GLU:O	5:F:521:HOH:O	1.95	0.83
1:A:169:TYR:OH	2:B:137:ASP:OD2	1.96	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:N	1:D:253:GLU:OE2	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:1070:HIS:O	2:G:1074:GLN:N	2.24	0.69
2:G:88:ASP:O	5:G:1311:HOH:O	2.09	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:N	1:I:115:ASN:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:GLU:OE1	5:J:1317:HOH:O	2.15	0.65
1:I:214:GLU:OE1	5:I:517: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
2:E:74:GLU:OE1	5:E:1355:HOH:O	2.14	0.64
1:A:186:THR:HG21	1:A:206:ARG:HE	1.63	0.64
1:F:147:ARG:NH1	2:G:147:ARG:HH12	1.96	0.64
1:A:117:GLU:OE2	1:A:371:HIS:HE1	1.81	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:372:ARG:NH1	5:A:554:HOH:O	2.23	0.61
1:A:285:CYS:O	1:A:290:ARG:NH2	2.33	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
2:G:63:GLY:HA2	2:G:100:THR:HG21	1.83	0.60
1:F:286:ASP:OD1	1:F:288:ASP:N	2.23	0.60
1:I:355:MET:SD	5:I:543:HOH:O	2.57	0.59
2:E:72:ARG:NH1	2:E:172:VAL:HG23	2.17	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
1:F:372:ARG:NH1	2:J:153[A]:GLU:OE2	2.36	0.59
2:E:68:LEU:HD11	2:E:97:ILE:HG23	1.84	0.59
1:F:214:GLU:OE2	3:F:401:ADP:C4	2.55	0.59
2:E:141:GLY:N	5:E:1303:HOH:O	2.34	0.59
1:D:95:ARG:HG3	1:D:95:ARG:HH21	1.68	0.59

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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
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
2:E:66:PRO:O	5:E:1349:HOH:O	2.17	0.58
1:I:253:GLU:HA	1:I:256:ARG:HB2	1.84	0.58
1:I:96:VAL:HG11	1:I:101:HIS:CE1	2.38	0.58
2:J:137:ASP:HB3	5:J:1301:HOH:O	2.03	0.58
2:E:89:PHE:CD2	2:E:165:LEU:HD13	2.38	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:D:113:LYS:HG3	1:D:371:HIS:CE1	2.40	0.56
1:A:117:GLU:OE2	1:A:371:HIS:CE1	2.58	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
2:E:64:LYS:N	5:E:1369:HOH:O	2.38	0.56
1:A:207:GLU:OE2	1:A:210:ARG:NH1	2.37	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: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
1:F:214:GLU:OE2	3:F:401:ADP:C5	2.59	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:180:LEU:HD11	1:I:185:LEU:HD11	1.88	0.55
1:I:73:HIS:HB3	1:I:179:ASP:OD1	2.06	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
2:G:103:LEU:HD23	2:G:105:ASN:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLU:N	1:F:224:GLU:OE1	2.41	0.54
1:D:28:ARG:CG	1:D:28:ARG:HH11	2.20	0.54
1:F:38:PRO:HA	1:F:65:LEU:HD23	1.90	0.54
1:A:200:PHE:HB3	1:A:205:GLU:HB3	1.89	0.54
1:F:7:ALA:HB3	1:F:22:ALA:HB3	1.90	0.54
1:I:349:LEU:HD11	2:J:130:ILE:HG21	1.90	0.54
2:E:89:PHE:HD2	2:E:165:LEU:HD13	1.71	0.54
1:D:51:ASP:N	1:D:51:ASP:OD1	2.40	0.54
1:I:180:LEU:HD12	1:I:181:ALA:N	2.22	0.54
1:A:198:TYR:CE1	1:A:248:ILE:HG23	2.43	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
2:E:54:VAL:HG11	2:E:59:PHE:CD2	2.43	0.53
1:D:216:LEU:HD12	1:D:250:ILE:HD12	1.91	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:F:372:ARG:CD	2:J:165:LEU:HD11	2.39	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:HD22	1:F:216:LEU:N	2.23	0.53
1:I:155:SER:OG	1:I:303:THR:HG23	2.09	0.53
1:I:218:TYR:HD1	1:I:254:ARG:NH1	2.05	0.53
2:E:102:GLN:HE22	2:E:106:GLY:C	2.11	0.53
1:I:355:MET:N	5:I:543:HOH:O	2.41	0.53
1:I:242:LEU:HD13	1:I:244:ASP:OD2	2.09	0.53
1:I:18:LYS:HG3	1:I:30:VAL:HG13	1.91	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:99:GLU:OE2	1:I:100:GLU:HG3	2.10	0.52
1:I:60:SER:O	1:I:60:SER:OG	2.25	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:F:372:ARG:NH1	2:J:153[B]:GLU:OE1	2.42	0.52
1:A:207:GLU:OE2	1:A:210:ARG:NE	2.42	0.52

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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
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:233:SER:OG	1:D:234:SER:N	2.44	0.51
1:I:37:ARG:O	1:I:66:THR:OG1	2.26	0.51
1:D:164:PRO:HG3	1:D:281:SER:OG	2.11	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:H	1:F:216:LEU:HD22	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:I:196:ARG:NH1	5:I:509:HOH:O	2.44	0.50
1:A:113:LYS:HB3	1:A:113:LYS:NZ	2.27	0.50
1:I:184:ASP:O	1:I:187:ASP:N	2.45	0.49
1:F:357:ILE:HG23	1:F:369:ILE:HD12	1.94	0.49
2:J:56:HIS:CE1	2:J:58:GLU:HB2	2.46	0.49
2:G:106:GLY:HA3	1:I:334:GLU:HG3	1.94	0.49
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: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:I:157:ASP:OD1	3:I:401:ADP:O3'	2.30	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
2:E:158:LEU:HD23	2:E:165:LEU:HD23	1.94	0.49
2:G:94:ALA:HB2	5:G:1327:HOH:O	2.12	0.49
1:F:116:ARG:NH2	1:F:371:HIS:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH1	1:A:204:ALA:HA	2.28	0.49
2:B:1081:ARG:NH2	2:B:1083:ASP:OD1	2.46	0.48
2:G:89:PHE:CD2	2:G:165:LEU:HD11	2.48	0.48
1:D:17:VAL:O	1:D:30:VAL:HA	2.13	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:F:183:ARG:NE	5:F:539:HOH:O	2.37	0.48
1:A:363:ASP:O	2:B:1096:TRP:HD1	1.96	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
1:I:99:GLU:OE2	1:I:100:GLU:CG	2.62	0.48
2:E:84:ASN:HD22	2:E:85:LEU:N	2.10	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:J:72:ARG:HH12	2:J:172:VAL:HB	1.79	0.47
2:B:113:HIS:CE1	2:B:146:HIS:CD2	3.02	0.47
1:F:335:ARG:HA	1:F:338:SER:OG	2.13	0.47
1:F:208:ILE:HG21	1:F:242:LEU:HD23	1.96	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: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:D:6:THR:O	1:D:101:HIS:ND1	2.33	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:I:121:GLN:HG3	1:I:125:GLU:OE2	2.14	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:A:242:LEU:HD21	1:A:248:ILE:HD12	1.97	0.47
1:D:70:PRO:HG3	1:D:85:ILE:HD12	1.95	0.47
1:A:252:ASN:ND2	1:A:256:ARG:HD2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:78:ASN:ND2	1:D:81:ASP:OD2	2.48	0.47
1:I:108:ALA:HB1	1:I:109:PRO:HD2	1.96	0.47
1:D:318:THR:HA	1:D:327:ILE:HD12	1.97	0.46
2:J:147:ARG:HH12	2:J:149:VAL:HG22	1.79	0.46
1:I:287:ILE:HA	1:I:290:ARG:CD	2.45	0.46
1:F:282:ILE:HD12	1:F:294:TYR:CE1	2.50	0.46
1:F:258:PRO:HG3	1:F:306:TYR:CE1	2.50	0.46
1:F:113:LYS:HG3	1:F:114:ALA:N	2.30	0.46
1:D:28:ARG:CG	1:D:28:ARG:NH1	2.77	0.46
2:G:88:ASP:N	2:G:88:ASP:OD1	2.47	0.46
1:I:58:ALA:HB1	1:I:61:LYS:CG	2.45	0.46
1:A:84:LYS:HG2	2:B:1087:TYR:CD2	2.50	0.46
1:A:10[A]:CYS:HB2	1:A:105:LEU:HD23	1.97	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:D:70:PRO:CG	1:D:85:ILE:CD1	2.94	0.46
1:A:330:ILE:HD12	1:A:330:ILE:N	2.31	0.46
1:F:166:TYR:N	1:F:169:TYR:O	2.45	0.46
2:B:82:PRO:HG2	2:B:85:LEU:HD12	1.98	0.46
1:A:87:HIS:CD2	2:B:1087:TYR:HB2	2.51	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:106:THR:HG21	1:I:137:GLN:HE21	1.80	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
1:F:214:GLU:HA	3:F:401:ADP:C6	2.51	0.45
1:D:64:ILE:CG1	1:D:65:LEU:N	2.80	0.45
2:J:111:ASP:HB3	2:J:113:HIS:NE2	2.30	0.45
2:B:1065:GLU:OE2	2:B:1065:GLU:HA	2.16	0.45
1:F:147:ARG:CZ	2:G:147:ARG:NH1	2.79	0.45
1:A:227:MET:O	1:A:230:ALA:HB3	2.17	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
1:I:78:ASN:CG	1:I:81:ASP:HB3	2.37	0.45
1:D:104:LEU:HD23	1:D:104:LEU:C	2.37	0.45
2:B:72:ARG:NH1	2:B:93:ASP:OD2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:253:GLU:CD	1:I:253:GLU:H	2.20	0.45
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:HD22	1:I:128:ASN:N	2.15	0.45
2:G:97:ILE:HG13	2:G:157:PHE:CE1	2.52	0.45
1:F:151:ILE:HD12	1:F:164:PRO:HD3	1.99	0.45
1:D:332:PRO:O	1:D:335:ARG:NE	2.42	0.45
1:I:192:ILE:CD1	1:I:253:GLU:HB3	2.47	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
2:E:54:VAL:HG11	2:E:59:PHE:CE2	2.52	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:D:28:ARG:HG3	1:D:28:ARG:NH1	2.32	0.44
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.53	0.44
1:F:188:TYR:HB2	1:F:267:ILE:HD11	2.00	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: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:C	1:I:222:ASP:OD1	2.55	0.44
2:J:129:ALA:O	2:J:132:THR:HB	2.18	0.44
1:D:156:GLY:O	1:D:181:ALA:HB1	2.17	0.44
1:A:100:GLU:CG	1:A:101:HIS:CD2	3.00	0.44
1:I:11:ASP:OD1	1:I:106:THR:HG21	2.17	0.44
1:F:107:GLU:OE2	1:F:134:VAL:HG22	2.18	0.44
1:F:372:ARG:HD3	2:J:165:LEU:HD11	1.99	0.44
2:E:65:GLU:N	5:E:1369:HOH:O	2.46	0.44
1:A:92:ASN:HD22	1:A:92:ASN:N	2.14	0.44
1:D:180:LEU:HA	1:D:184:ASP:OD2	2.18	0.44
1:I:251:GLY:C	1:I:253:GLU:OE2	2.56	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:F:257:CYS:HB3	1:F:258:PRO:HD3	1.99	0.44
1:A:164:PRO:O	1:A:171:LEU:HD12	2.18	0.44
1:F:136:ILE:CG2	1:F:139:VAL:HG23	2.48	0.44
1:A:99:GLU:OE2	1:A:99:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HD11	1:D:96:VAL:HG21	1.99	0.44
1:F:208:ILE:HG21	1:F:242:LEU:CD2	2.48	0.43
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:I:35:VAL:CG2	1:I:81:ASP:OD1	2.66	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: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
2:G:58:GLU:HB3	2:G:71:TRP:NE1	2.33	0.43
1:F:112:PRO:O	1:F:116:ARG:HG3	2.19	0.43
1:I:58:ALA:HB1	1:I:61:LYS:HG2	2.01	0.43
1:I:155:SER:O	1:I:303:THR:HG22	2.18	0.43
1:F:219:VAL:CG2	1:F:258:PRO:HB2	2.48	0.43
1:A:92:ASN:N	1:A:92:ASN:ND2	2.65	0.43
2:G:53:VAL:HG22	2:G:54:VAL:N	2.33	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:I:122:ILE:CG2	1:I:127:PHE:HE2	2.32	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:D:303:THR:CG2	1:D:303:THR:O	2.67	0.43
1:A:121:GLN:O	1:A:125:GLU:HG3	2.19	0.43
1:F:196:ARG:NE	1:F:196:ARG:HA	2.34	0.43
2:E:75:LYS:O	2:E:76:PHE:HB2	2.18	0.43
1:I:158:GLY:HA2	1:I:183:ARG:HH22	1.84	0.43
1:I:196:ARG:NH1	1:I:251:GLY:HA3	2.33	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
2:G:1068:LEU:HD12	2:G:1068:LEU:H	1.84	0.43
1:A:248:ILE:CG2	1:A:249:THR:N	2.81	0.43
1:F:302:GLY:HA2	1:F:336:LYS:HD2	2.01	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: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:A:238:LYS:HG3	1:A:239:SER:H	1.84	0.43
1:F:372:ARG:HH12	2:J:151:GLY:HA2	1.84	0.42
1:D:192:ILE:HD12	1:D:253:GLU:HG3	2.01	0.42
1:A:196:ARG:NH2	5:A:567:HOH:O	2.51	0.42

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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
1:I:349:LEU:HD21	2:J:127:ALA:HB2	2.00	0.42
2:E:84:ASN:N	2:E:84:ASN:HD22	2.18	0.42
1:F:164:PRO:HG3	1:F:174:ALA:CB	2.49	0.42
2:J:122:GLN:HA	2:J:125:SER:OG	2.19	0.42
2:G:87:GLY:HA2	2:G:161:PHE:CE1	2.55	0.42
1:I:371:HIS:O	1:I:375:PHE:HB3	2.18	0.42
1:D:37:ARG:NH2	1:D:81:ASP:OD1	2.46	0.42
1:F:157:ASP:N	3:F:401:ADP:H5'1	2.33	0.42
2:J:151:GLY:N	2:J:167:TYR:OH	2.52	0.42
1:I:21:PHE:N	1:I:21:PHE:CD1	2.88	0.42
1:F:349:LEU:HD11	2:G:130:ILE:HG21	2.01	0.42
2:B:151:GLY:N	2:B:167:TYR:OH	2.45	0.42
1:I:329:ILE:HD12	1:I:329:ILE:N	2.33	0.42
1:A:169:TYR:CD1	2:E:169:LYS:HE3	2.55	0.42
1:A:8:LEU:HG	1:A:101:HIS:HB3	2.02	0.42
1:F:37:ARG:NH1	1:F:68:LYS:HZ2	2.18	0.42
1:A:192:ILE:HD12	1:A:253:GLU:CB	2.48	0.42
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.02	0.42
1:F:203:THR:OG1	1:F:203:THR:O	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:J:147:ARG:HH11	2:J:147:ARG:HG3	1.84	0.42
2:G:112:LEU:HD21	2:G:135:LEU:HD13	2.01	0.42
1:F:147:ARG:NH1	5:F:525:HOH:O	2.38	0.42
2:E:54:VAL:O	2:E:54:VAL:HG12	2.20	0.42
1:F:212:ILE:HG23	1:F:216:LEU:HD23	2.02	0.42
2:E:84:ASN:HD22	2:E:85:LEU:H	1.66	0.42
1:A:107:GLU:OE1	1:A:116:ARG:HD2	2.20	0.42
1:I:193:LEU:HD23	1:I:198:TYR:CD2	2.55	0.42
1:I:240:TYR:HD2	1:I:248:ILE:HD11	1.85	0.42
2:G:53:VAL:HG22	2:G:54:VAL:H	1.85	0.42
1:I:341:ILE:HD11	5:I:532:HOH:O	2.18	0.42
1:F:171:LEU:HB3	1:F:173:HIS:CE1	2.55	0.42
1:I:252:ASN:CB	1:I:255:PHE:CZ	3.02	0.41
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.01	0.41
1:D:36:GLY:HA2	1:D:66:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:C	1:A:65:LEU:HD12	2.41	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:A:191:LYS:HA	1:A:191:LYS:HD2	1.95	0.41
1:A:143:TYR:CD2	2:B:130:ILE:HG12	2.56	0.41
1:F:372:ARG:HD3	2:J:165:LEU:CD1	2.50	0.41
1:F:223:PHE:CZ	1:F:256:ARG:HG3	2.55	0.41
1:I:336:LYS:CE	5:I:545:HOH:O	2.67	0.41
1:F:182:GLY:HA2	1:F:185:LEU:HD12	2.01	0.41
1:D:202:THR:HB	1:D:205:GLU:HG3	2.03	0.41
1:I:102:PRO:HA	1:I:131:ALA:O	2.21	0.41
1:F:202:THR:OG1	1:F:203:THR:N	2.51	0.41
2:B:1096:TRP:CH2	2:B:1098:PRO:HA	2.56	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:E:88:ASP:OD2	5:E:1354:HOH:O	2.22	0.41
1:A:233:SER:O	1:A:234:SER:CB	2.69	0.41
1:I:58:ALA:CB	1:I:61:LYS:HG3	2.51	0.41
2:G:70:ILE:HG22	2:G:81:VAL:HG21	2.03	0.41
1:A:124:PHE:O	1:A:128:ASN:HA	2.21	0.41
1:A:100:GLU:CG	1:A:101:HIS:NE2	2.84	0.41
1:I:53:TYR:CD2	1:I:65:LEU:HD11	2.56	0.41
1:A:10[B]:CYS:HB3	1:A:105:LEU:HD23	2.01	0.41
1:I:106:THR:HG23	1:I:137:GLN:CG	2.51	0.41
1:D:202:THR:OG1	1:D:205:GLU:OE1	2.17	0.41
1:D:97:ALA:HA	1:D:98:PRO:HD3	1.94	0.41
1:A:193:LEU:O	1:A:198:TYR:N	2.44	0.41
2:G:87:GLY:CA	2:G:161:PHE:CE1	3.04	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:A:72:GLU:HG2	1:A:77:THR:HG21	2.03	0.41
1:F:89:THR:O	1:F:94:LEU:HD13	2.21	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:F:354:GLN:HG3	2:G:53:VAL:O	2.21	0.41
1:A:309:ILE:HG23	1:A:310:ALA:N	2.36	0.41
1:A:218:TYR:OH	1:A:226:GLU:OE2	2.20	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
2:G:1064:ARG:O	2:G:1068:LEU:HD12	2.21	0.40
2:J:147:ARG:HG3	2:J:147:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:LEU:HA	1:F:184:ASP:OD2	2.22	0.40
1:I:304:THR:O	1:I:335:ARG:CZ	2.69	0.40
1:D:310:ALA:HA	1:D:329:ILE:HG21	2.03	0.40
1:I:194:THR:HA	1:I:198:TYR:O	2.21	0.40
1:A:316:GLU:HA	1:A:316:GLU:OE2	2.22	0.40
1:F:60:SER:HA	1:F:62:ARG:CZ	2.51	0.40
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.56	0.40
2:G:66:PRO:HA	2:G:100:THR:OG1	2.22	0.40
1:A:314:GLN:O	1:A:318:THR:N	2.48	0.40
2:J:68:LEU:CD2	2:J:70:ILE:HG13	2.51	0.40
1:A:110:LEU:HD23	1:A:110:LEU:N	2.36	0.40
2:G:153:GLU:HB2	2:G:158:LEU:HD23	2.03	0.40
1:A:62:ARG:HH21	1:A:62:ARG:HG2	1.87	0.40
1:I:279:TYR:CE1	1:I:283:MET:SD	3.14	0.40
1:F:198:TYR:CD2	1:F:248:ILE:HD12	2.56	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	361/377 (96%)	341 (94%)	19 (5%)	1 (0%)	46 42
1	I	357/377 (95%)	339 (95%)	17 (5%)	1 (0%)	46 42
2	B	161/186 (87%)	156 (97%)	5 (3%)	0	100 100
2	E	123/186 (66%)	118 (96%)	4 (3%)	1 (1%)	24 15
2	G	139/186 (75%)	135 (97%)	3 (2%)	1 (1%)	26 18
2	J	125/186 (67%)	122 (98%)	1 (1%)	2 (2%)	12 5
All	All	1980/2252 (88%)	1908 (96%)	66 (3%)	6 (0%)	46 42

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

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%)	17 10
1	D	307/320 (96%)	281 (92%)	26 (8%)	13 8
1	F	310/320 (97%)	260 (84%)	50 (16%)	3 1
1	I	307/320 (96%)	266 (87%)	41 (13%)	5 1
2	B	138/153 (90%)	129 (94%)	9 (6%)	21 15
2	E	102/153 (67%)	97 (95%)	5 (5%)	31 26
2	G	119/153 (78%)	104 (87%)	15 (13%)	5 2
2	J	104/153 (68%)	91 (88%)	13 (12%)	6 2
All	All	1694/1892 (90%)	1512 (89%)	182 (11%)	8 4

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

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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

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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

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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

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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

Some 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

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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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	401	4	22,29,29	1.34	4 (18%)	27,45,45	2.06	8 (29%)
3	ADP	D	401	4	22,29,29	1.13	2 (9%)	27,45,45	2.18	11 (40%)
3	ADP	F	401	-	22,29,29	1.13	3 (13%)	27,45,45	2.28	7 (25%)
3	ADP	I	401	4	22,29,29	1.12	2 (9%)	27,45,45	2.51	11 (40%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	PB-O3B	-2.52	1.45	1.54
3	F	401	ADP	C2-N3	2.00	1.35	1.32
3	I	401	ADP	C8-N7	2.07	1.38	1.34
3	D	401	ADP	O4'-C1'	2.38	1.44	1.41
3	A	401	ADP	C2-N3	2.53	1.36	1.32
3	F	401	ADP	O4'-C1'	2.63	1.44	1.41
3	A	401	ADP	C5-C4	2.68	1.46	1.40
3	F	401	ADP	C5-C4	2.92	1.47	1.40
3	D	401	ADP	C5-C4	2.93	1.47	1.40
3	I	401	ADP	C5-C4	2.99	1.47	1.40
3	A	401	ADP	O4'-C1'	3.10	1.45	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	401	ADP	N3-C2-N1	-6.69	123.77	128.89
3	F	401	ADP	N3-C2-N1	-6.48	123.93	128.89
3	A	401	ADP	C4-C5-N7	-5.44	104.47	109.48
3	D	401	ADP	N3-C2-N1	-4.83	125.19	128.89
3	I	401	ADP	C1'-N9-C4	-4.80	119.70	126.94
3	A	401	ADP	N3-C2-N1	-4.47	125.47	128.89
3	F	401	ADP	C2'-C1'-N9	-4.21	107.86	114.29
3	I	401	ADP	PA-O3A-PB	-4.11	118.90	132.67
3	I	401	ADP	C2'-C1'-N9	-4.04	108.12	114.29
3	I	401	ADP	O3'-C3'-C2'	-3.47	100.54	111.83
3	F	401	ADP	C4'-O4'-C1'	-3.30	106.09	109.72
3	F	401	ADP	C4-C5-N7	-3.22	106.52	109.48
3	A	401	ADP	O3B-PB-O3A	-3.07	91.17	105.09
3	D	401	ADP	C1'-N9-C4	-2.97	122.46	126.94
3	F	401	ADP	C1'-N9-C4	-2.90	122.56	126.94
3	I	401	ADP	C4-C5-N7	-2.84	106.86	109.48
3	D	401	ADP	C4-C5-N7	-2.70	107.00	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	401	ADP	C4'-O4'-C1'	-2.54	106.92	109.72
3	D	401	ADP	C2'-C1'-N9	-2.49	110.49	114.29
3	D	401	ADP	O3'-C3'-C4'	-2.44	103.74	111.05
3	D	401	ADP	C5'-C4'-C3'	-2.26	106.23	115.21
3	D	401	ADP	PA-O3A-PB	-2.22	125.23	132.67
3	D	401	ADP	O3A-PA-O5'	-2.21	97.08	102.94
3	D	401	ADP	O4'-C4'-C3'	2.14	109.45	105.15
3	A	401	ADP	O3B-PB-O2B	2.15	115.58	107.38
3	A	401	ADP	C2'-C3'-C4'	2.16	107.06	102.61
3	A	401	ADP	O4'-C1'-N9	2.22	112.74	108.10
3	F	401	ADP	O3B-PB-O1B	2.23	117.75	110.58
3	I	401	ADP	O4'-C4'-C3'	2.23	109.64	105.15
3	I	401	ADP	O3B-PB-O2B	2.57	117.16	107.38
3	I	401	ADP	C2-N1-C6	2.74	123.67	118.77
3	I	401	ADP	O3B-PB-O1B	2.84	119.73	110.58
3	A	401	ADP	C4'-O4'-C1'	3.28	113.32	109.72
3	A	401	ADP	O3B-PB-O1B	3.47	121.75	110.58
3	D	401	ADP	O3B-PB-O1B	3.50	121.84	110.58
3	F	401	ADP	O4'-C1'-N9	4.65	117.83	108.10
3	D	401	ADP	O4'-C1'-N9	5.13	118.83	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0
3	F	401	ADP	6	0
3	I	401	ADP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.36	11 (3%) 52 62	18, 46, 80, 120	1 (0%)
1	D	360/377 (95%)	0.25	9 (2%) 61 69	17, 38, 82, 116	0
1	F	365/377 (96%)	1.91	136 (37%) 0 1	56, 79, 127, 182	0
1	I	360/377 (95%)	2.09	153 (42%) 0 1	57, 81, 126, 166	0
2	B	165/186 (88%)	0.45	14 (8%) 13 19	18, 38, 101, 129	0
2	E	125/186 (67%)	0.07	3 (2%) 62 71	16, 29, 52, 95	0
2	G	143/186 (76%)	1.86	51 (35%) 0 1	57, 77, 110, 167	0
2	J	126/186 (67%)	1.99	54 (42%) 0 1	60, 80, 106, 142	0
All	All	2003/2252 (88%)	1.13	431 (21%) 1 2	16, 67, 111, 182	1 (0%)

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	327	ILE	14.7
1	F	209	VAL	10.8
2	G	55	GLU	9.4
1	I	54	VAL	8.6
2	J	53	VAL	8.5
1	I	91	TYR	8.4
1	I	203	THR	8.3
1	F	248	ILE	8.2
1	F	375	PHE	8.1
1	I	201	VAL	8.0
1	I	158	GLY	7.7
1	F	232	SER	7.7
2	J	108	LEU	7.5
1	F	58	ALA	7.4
1	F	178	LEU	7.2
1	F	53	TYR	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	276	GLU	6.9
2	G	54	VAL	6.7
1	F	152	VAL	6.5
1	I	202	THR	6.5
2	G	85	LEU	6.4
1	F	219	VAL	6.4
1	I	250	ILE	6.3
1	I	200	PHE	6.3
1	I	69	TYR	6.2
1	F	317	ILE	6.1
1	D	201	VAL	6.1
1	F	19	ALA	6.0
1	I	375	PHE	5.9
2	B	54	VAL	5.9
2	J	152	PHE	5.7
1	F	8	LEU	5.7
1	I	163	VAL	5.6
2	G	1062	PHE	5.6
2	J	103	LEU	5.5
1	I	317	ILE	5.5
1	I	58	ALA	5.5
2	B	1078	PHE	5.3
1	F	251	GLY	5.3
1	F	5	THR	5.3
1	F	306	TYR	5.3
1	F	236	LEU	5.2
1	I	64	ILE	5.2
1	I	79	TRP	5.2
1	I	324	THR	5.2
2	J	76	PHE	5.2
1	F	304	THR	5.1
2	J	171	GLY	5.0
2	J	96	VAL	5.0
1	F	200	PHE	5.0
1	I	60	SER	4.9
1	I	333	PRO	4.9
1	I	304	THR	4.9
1	I	63	GLY	4.8
1	I	138	ALA	4.7
1	I	127	PHE	4.7
2	J	59	PHE	4.6
1	I	165	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
2	J	155	ALA	4.5
1	F	233	SER	4.5
2	G	176	PHE	4.4
2	G	1067	LEU	4.4
1	I	215	LYS	4.4
1	I	36	GLY	4.4
2	J	54	VAL	4.3
1	I	26	ALA	4.3
1	F	88	HIS	4.3
1	F	20	GLY	4.2
1	F	238	LYS	4.2
1	I	365	ALA	4.2
2	J	149	VAL	4.1
1	F	242	LEU	4.1
1	D	64	ILE	4.1
2	G	103	LEU	4.1
1	F	230	ALA	4.1
2	J	90	PHE	4.1
2	G	98	LEU	4.1
1	A	240	TYR	4.1
1	F	17	VAL	4.1
1	F	289	ILE	4.1
1	F	282	ILE	4.0
2	G	152	PHE	4.0
1	I	329	ILE	4.0
1	I	164	PRO	4.0
1	D	203	THR	3.9
1	F	164	PRO	3.9
1	I	195	GLU	3.9
2	J	115	TRP	3.9
1	F	246	GLN	3.9
1	I	90	PHE	3.9
2	J	162	LYS	3.9
1	F	244	ASP	3.8
1	I	328	LYS	3.8
1	I	161	HIS	3.8
2	G	1069	ASP	3.8
1	F	247	VAL	3.8
2	B	1085	VAL	3.8
1	F	57	GLU	3.8
1	I	261	LEU	3.8
2	J	146	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	262	PHE	3.8
1	F	170	ALA	3.7
2	G	131	PHE	3.7
1	F	198	TYR	3.7
1	I	143	TYR	3.7
2	G	67	GLY	3.7
1	F	9	VAL	3.7
1	F	250	ILE	3.7
2	G	165	LEU	3.7
1	I	31	PHE	3.7
1	I	374	CYS	3.7
2	G	97	ILE	3.7
2	G	90	PHE	3.6
1	F	266	PHE	3.6
1	F	159	VAL	3.6
1	I	110	LEU	3.6
1	I	294	TYR	3.6
1	F	158	GLY	3.6
1	A	228	ALA	3.6
1	I	142	LEU	3.6
1	F	79	TRP	3.6
1	F	217	CYS	3.6
1	F	30	VAL	3.6
1	F	96	VAL	3.6
1	F	177	ARG	3.6
1	I	162	ASN	3.6
1	F	28	ARG	3.5
2	E	53	VAL	3.5
1	F	261	LEU	3.5
1	I	62	ARG	3.5
1	F	280	ASN	3.5
1	I	10[A]	CYS	3.5
1	I	171	LEU	3.5
1	I	131	ALA	3.5
2	G	177	GLY	3.5
2	G	95	TYR	3.4
1	A	65	LEU	3.4
1	I	153	LEU	3.4
1	F	340	TRP	3.4
2	B	1086	PRO	3.4
1	F	234	SER	3.4
1	I	240	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	68	LYS	3.4
1	F	188	TYR	3.4
2	G	167	TYR	3.4
1	D	58	ALA	3.3
2	G	1072	GLU	3.3
1	I	148	THR	3.3
1	I	170	ALA	3.3
2	B	1068	LEU	3.3
2	J	85	LEU	3.3
1	D	324	THR	3.3
2	J	167	TYR	3.3
1	F	86	TRP	3.3
1	F	174	ALA	3.3
2	E	54	VAL	3.3
1	I	185	LEU	3.3
2	J	170	GLY	3.3
2	J	109	GLN	3.3
2	J	119	GLU	3.3
1	I	180	LEU	3.3
1	I	232	SER	3.3
1	F	31	PHE	3.2
2	G	149	VAL	3.2
2	G	68	LEU	3.2
1	I	96	VAL	3.2
2	G	1068	LEU	3.2
2	G	1059	THR	3.2
1	A	277	THR	3.2
1	D	250	ILE	3.1
1	I	325	MET	3.1
1	I	5	THR	3.1
1	I	155	SER	3.1
1	A	250	ILE	3.1
1	F	64	ILE	3.1
1	I	71	ILE	3.1
2	G	96	VAL	3.1
2	G	116	LEU	3.1
1	F	292	ASP	3.1
1	F	185	LEU	3.1
1	I	6	THR	3.1
1	I	198	TYR	3.0
1	I	231	ALA	3.0
1	F	206	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	248	ILE	3.0
1	I	345	ILE	3.0
1	F	294	TYR	3.0
1	I	306	TYR	3.0
2	J	95	TYR	3.0
1	F	25	ASP	3.0
1	F	21	PHE	3.0
2	G	84	ASN	3.0
1	I	75	ILE	3.0
1	F	295	ALA	3.0
1	I	52	SER	3.0
1	I	98	PRO	3.0
1	F	309	ILE	3.0
1	F	171	LEU	3.0
1	F	7	ALA	3.0
1	F	231	ALA	3.0
1	I	87	HIS	3.0
1	I	37	ARG	2.9
2	G	117	GLY	2.9
1	I	8	LEU	2.9
2	G	105	ASN	2.9
1	F	202	THR	2.9
1	I	330	ILE	2.9
1	I	67	LEU	2.9
1	I	86	TRP	2.9
1	I	9	VAL	2.9
1	I	135	ALA	2.9
1	I	223	PHE	2.9
1	D	248	ILE	2.9
1	F	357	ILE	2.8
2	B	1084	LEU	2.8
2	G	128	ALA	2.8
1	F	179	ASP	2.8
1	F	265	SER	2.8
2	J	172	VAL	2.8
1	I	352	PHE	2.8
2	G	76	PHE	2.8
1	A	319	ALA	2.8
1	I	236	LEU	2.8
2	J	151	GLY	2.8
1	I	238	LYS	2.8
2	B	1077	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	305	MET	2.8
1	I	262	PHE	2.8
1	I	144	ALA	2.8
1	A	203	THR	2.8
1	F	71	ILE	2.8
1	I	298	VAL	2.8
1	F	56	ASP	2.7
1	I	38	PRO	2.7
1	F	223	PHE	2.7
2	J	161	PHE	2.7
1	F	260	THR	2.7
1	I	221	LEU	2.7
1	F	227	MET	2.7
1	F	203	THR	2.7
2	J	176	PHE	2.7
2	J	102	GLN	2.7
2	G	136	ASP	2.7
1	I	243	PRO	2.7
2	J	66	PRO	2.7
1	F	281	SER	2.7
1	I	300	SER	2.7
1	I	53	TYR	2.7
1	I	216	LEU	2.7
1	I	76	ILE	2.7
1	F	201	VAL	2.7
2	J	60	LEU	2.6
1	F	369	ILE	2.6
1	I	318	THR	2.6
2	B	1075	ALA	2.6
1	F	235	SER	2.6
2	J	131	PHE	2.6
2	J	78	LEU	2.6
1	F	349	LEU	2.6
1	I	244	ASP	2.6
1	I	30	VAL	2.6
2	G	1066	GLU	2.6
1	F	124	PHE	2.6
1	F	243	PRO	2.6
1	F	264	PRO	2.6
1	I	109	PRO	2.6
1	I	299	MET	2.6
2	G	118	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	45	VAL	2.6
1	I	169	TYR	2.5
1	A	236	LEU	2.5
1	F	110	LEU	2.5
1	F	189	LEU	2.5
1	I	242	LEU	2.5
1	F	240	TYR	2.5
1	F	221	LEU	2.5
1	I	320	LEU	2.5
1	F	127	PHE	2.5
1	I	230	ALA	2.5
2	J	94	ALA	2.5
1	I	187	ASP	2.5
2	G	86	TYR	2.5
2	G	158	LEU	2.5
1	F	274	ILE	2.5
1	I	152	VAL	2.5
1	I	209	VAL	2.5
2	J	133	VAL	2.5
1	F	229	THR	2.5
1	F	121	GLN	2.5
2	J	89	PHE	2.5
1	I	94	LEU	2.5
1	F	29	ALA	2.4
2	G	1058	PRO	2.4
1	I	80	ASP	2.4
1	I	119	MET	2.4
1	I	145	SER	2.4
1	F	130	PRO	2.4
1	F	356	TRP	2.4
1	I	340	TRP	2.4
1	F	69	TYR	2.4
1	I	21	PHE	2.4
2	B	108	LEU	2.4
2	G	160	TYR	2.4
1	I	260	THR	2.4
1	I	283	MET	2.4
1	F	195	GLU	2.4
1	F	293	LEU	2.4
2	J	139	LEU	2.4
1	F	220	ALA	2.4
1	F	370	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	208	ILE	2.4
1	I	212	ILE	2.4
2	J	93	ASP	2.4
1	F	142	LEU	2.4
1	F	216	LEU	2.4
1	I	168	GLY	2.4
2	G	156	THR	2.4
2	G	79	VAL	2.3
2	J	101	VAL	2.3
1	A	60	SER	2.3
1	F	52	SER	2.3
2	J	121	SER	2.3
1	F	157	ASP	2.3
2	G	89	PHE	2.3
1	F	162	ASN	2.3
1	D	244	ASP	2.3
1	F	81	ASP	2.3
1	I	133	TYR	2.3
1	F	253	GLU	2.3
1	F	365	ALA	2.3
1	I	204	ALA	2.3
2	J	166	LYS	2.3
1	I	334	GLU	2.3
1	I	289	ILE	2.3
1	I	149	THR	2.3
1	F	105	LEU	2.3
2	J	68	LEU	2.3
1	I	237	GLU	2.3
2	J	117	GLY	2.3
1	I	247	VAL	2.3
2	J	81	VAL	2.3
1	F	122	ILE	2.3
1	F	267	ILE	2.3
1	F	95	ARG	2.3
1	I	114	ALA	2.3
2	E	103	LEU	2.3
2	J	177	GLY	2.2
2	J	52	MET	2.2
1	I	34	ILE	2.2
1	I	51	ASP	2.2
1	I	220	ALA	2.2
2	G	151	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	65	LEU	2.2
1	F	258	PRO	2.2
1	F	126	THR	2.2
1	I	17	VAL	2.2
1	I	35	VAL	2.2
1	I	134	VAL	2.2
1	I	219	VAL	2.2
1	F	136	ILE	2.2
1	F	15	GLY	2.2
1	I	141	SER	2.2
2	J	141	GLY	2.2
1	F	44	MET	2.2
2	G	157	PHE	2.2
1	F	129	VAL	2.2
1	I	33	SER	2.2
1	I	136	ILE	2.2
1	F	193	LEU	2.2
2	J	134	GLN	2.2
2	G	172	VAL	2.2
1	I	25	ASP	2.2
1	I	322	PRO	2.2
1	I	16	LEU	2.2
2	J	147	ARG	2.2
1	F	352	PHE	2.2
1	I	233	SER	2.2
2	J	160	TYR	2.2
2	G	127	ALA	2.2
1	I	132	MET	2.1
1	F	125	GLU	2.1
1	I	14	SER	2.1
1	I	66	THR	2.1
1	I	61	LYS	2.1
1	I	97	ALA	2.1
1	D	190	MET	2.1
2	J	130	ILE	2.1
2	B	1089	GLY	2.1
2	J	126	GLY	2.1
2	B	1059	THR	2.1
2	J	158	LEU	2.1
1	I	95	ARG	2.1
1	F	204	ALA	2.1
1	I	159	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	146	GLY	2.1
2	G	120	CYS	2.1
1	I	179	ASP	2.1
2	B	1062	PHE	2.1
1	F	143	TYR	2.1
2	J	56	HIS	2.1
2	B	1096	TRP	2.1
2	G	53	VAL	2.1
2	G	133	VAL	2.1
1	I	92	ASN	2.1
1	F	249	THR	2.1
1	F	153	LEU	2.1
1	F	362	TYR	2.1
1	F	94	LEU	2.1
2	J	165	LEU	2.1
1	A	231	ALA	2.1
1	F	146	GLY	2.1
1	I	225	ASN	2.1
1	I	246	GLN	2.1
2	J	118	ASN	2.1
1	I	323	SER	2.1
2	G	59	PHE	2.1
1	F	358	THR	2.0
1	I	205	GLU	2.0
1	I	70	PRO	2.0
1	F	245	GLY	2.0
2	J	163	SER	2.0
1	I	56	ASP	2.0
1	I	124	PHE	2.0
2	G	114	TYR	2.0
1	I	85	ILE	2.0
2	B	1071	LEU	2.0
2	G	108	LEU	2.0
2	G	129	ALA	2.0
1	F	62	ARG	2.0
1	F	106	THR	2.0
1	I	332	PRO	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CA	F	403	1/1	0.96	0.24	0.96	55,55,55,55	0
3	ADP	A	401	27/27	0.96	0.13	0.02	18,41,55,57	0
3	ADP	D	401	27/27	0.97	0.11	-0.57	16,30,40,42	0
4	CA	D	402	1/1	0.91	0.10	-0.81	64,64,64,64	0
3	ADP	I	401	27/27	0.92	0.13	-1.05	35,48,59,62	0
3	ADP	F	401	27/27	0.94	0.12	-1.59	38,57,69,74	0
4	CA	J	1201	1/1	0.92	0.13	-1.74	60,60,60,60	0
4	CA	A	402	1/1	0.94	0.07	-1.82	63,63,63,63	0
4	CA	I	402	1/1	0.77	0.12	-1.99	81,81,81,81	0
4	CA	D	403	1/1	0.89	0.07	-2.04	63,63,63,63	0
4	CA	E	1201	1/1	0.99	0.06	-2.61	24,24,24,24	0
4	CA	B	1201	1/1	0.99	0.06	-2.91	26,26,26,26	0
4	CA	I	403	1/1	0.91	0.10	-4.18	67,67,67,67	0
4	CA	F	402	1/1	0.70	0.09	-4.36	91,91,91,91	0
4	CA	G	1201	1/1	0.99	0.13	-4.52	56,56,56,56	0
4	CA	A	403	1/1	0.98	0.05	-7.21	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.