



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:13 PM GMT

PDB ID : 4V0U
Title : The crystal structure of ternary PP1G-PPP1R15B and G-actin complex
Authors : Chen, R.; Yan, Y.; Casado, A.C.; Ron, D.; Read, R.J.
Deposited on : 2014-09-18
Resolution : 7.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

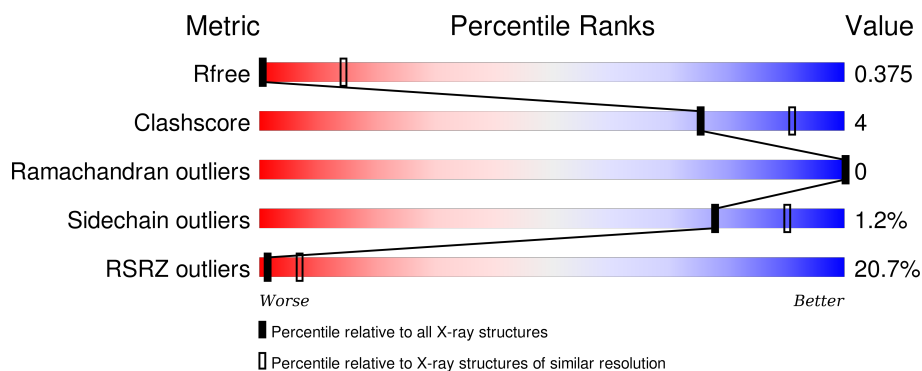
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.88 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	<div> <div>13%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	B	375	<div> <div>16%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	375	<div> <div>23%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	L	375	<div> <div>28%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	M	375	<div> <div>18%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	323	
2	F	323	
2	H	323	
2	J	323	
2	N	323	
3	E	84	
3	G	84	
3	I	84	
3	K	84	
3	O	84	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LAB	A	1376	-	-	-	X
4	LAB	B	1376	-	-	-	X
4	LAB	C	1376	-	-	-	X
4	LAB	L	1376	-	-	-	X
5	ATP	A	1377	-	-	-	X
5	ATP	B	1377	-	-	-	X
5	ATP	C	1377	-	-	-	X
5	ATP	L	1377	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27065 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	B	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	C	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	L	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	M	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	F	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	H	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	J	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	N	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			

- Molecule 3 is a protein called PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	0	0	0
			167	107	25	35			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	20	Total	C	N	O	0	0	0
			167	107	25	35			
3	I	20	Total	C	N	O	0	0	0
			167	107	25	35			
3	K	20	Total	C	N	O	0	0	0
			167	107	25	35			
3	O	20	Total	C	N	O	0	0	0
			167	107	25	35			

There are 65 discrepancies between the modelled and reference sequences:

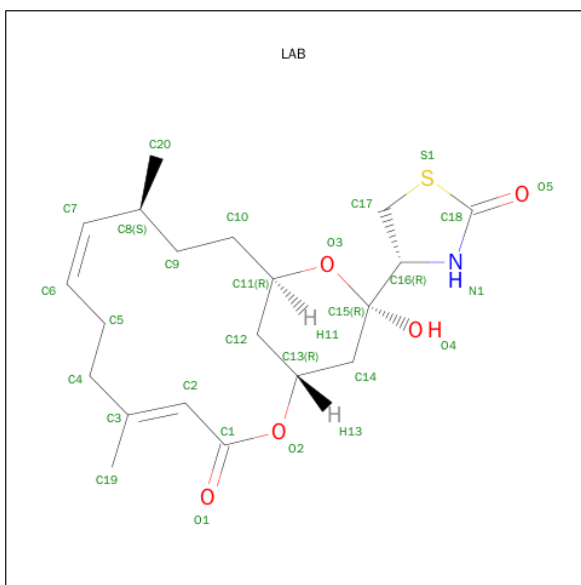
Chain	Residue	Modelled	Actual	Comment	Reference
E	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
E	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
E	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
E	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
E	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1
E	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
E	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
E	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
E	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
E	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
E	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
E	708	HIS	-	EXPRESSION TAG	UNP Q5SWA1
E	709	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
G	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
G	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
G	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
G	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1
G	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
G	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
G	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	708	HIS	-	EXPRESSION TAG	UNP Q5SWA1
G	709	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
I	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
I	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
I	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
I	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1

Continued on next page...

Continued from previous page...

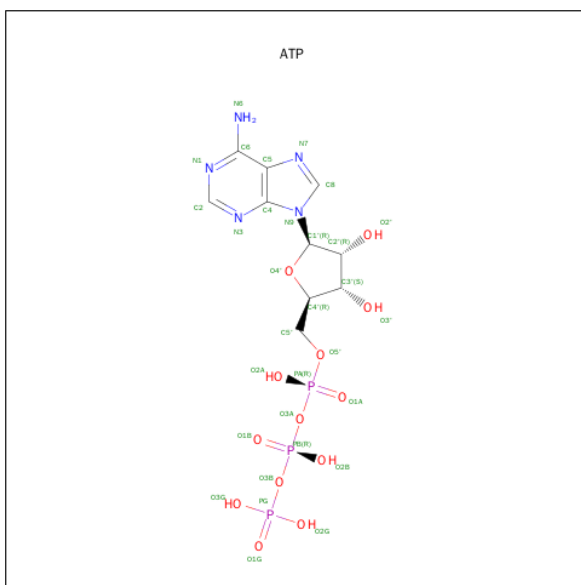
Chain	Residue	Modelled	Actual	Comment	Reference
I	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
I	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
I	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	708	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	709	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
K	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
K	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
K	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
K	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1
K	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
K	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
K	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	708	HIS	-	EXPRESSION TAG	UNP Q5SWA1
K	709	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
O	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
O	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
O	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
O	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1
O	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
O	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
O	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	708	HIS	-	EXPRESSION TAG	UNP Q5SWA1
O	709	HIS	-	EXPRESSION TAG	UNP Q5SWA1

- Molecule 4 is LATRUNCULIN B (three-letter code: LAB) (formula: C₂₀H₂₉NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	L	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	M	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	L	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	M	1	Total 31	C 10	N 5	O 13	P 3	0	0

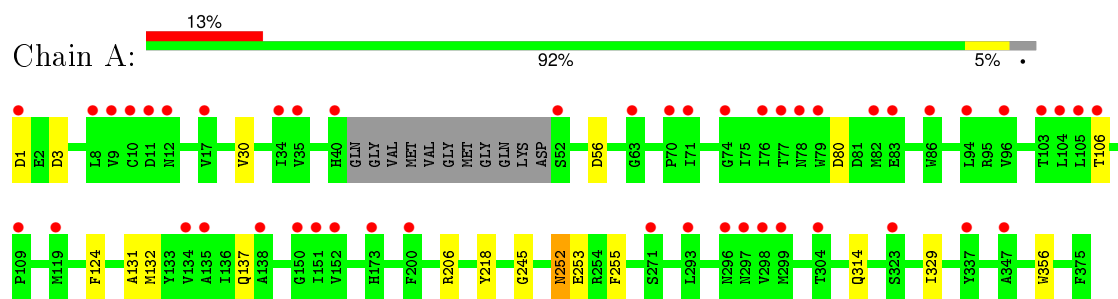
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	2	Total Mn 2 2	0	0
6	J	2	Total Mn 2 2	0	0
6	D	2	Total Mn 2 2	0	0
6	N	2	Total Mn 2 2	0	0
6	F	2	Total Mn 2 2	0	0

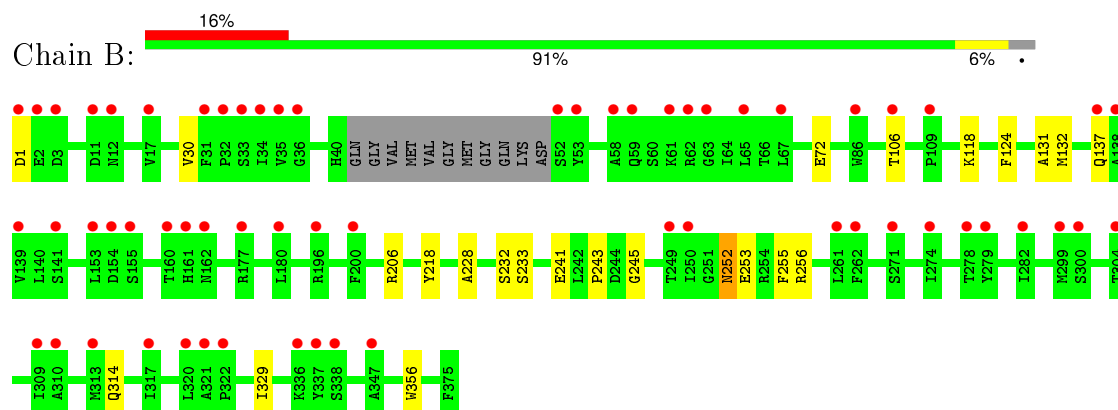
3 Residue-property plots [i](#)

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.

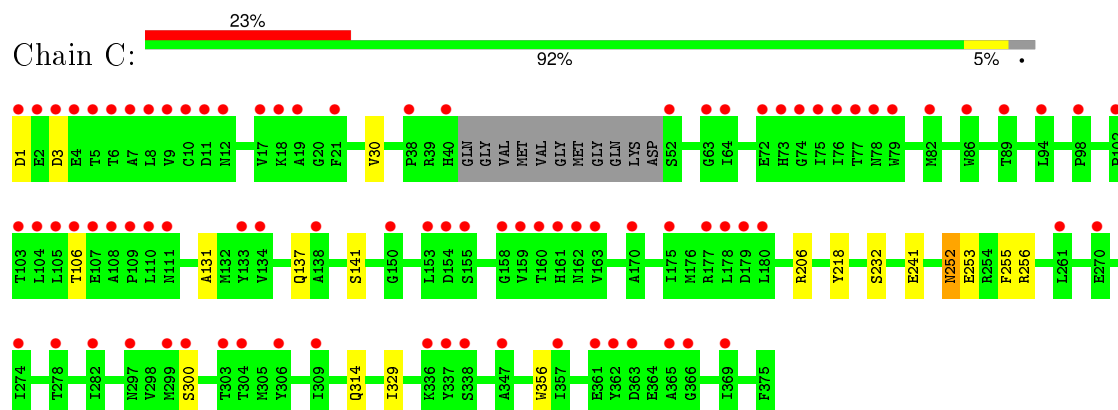
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



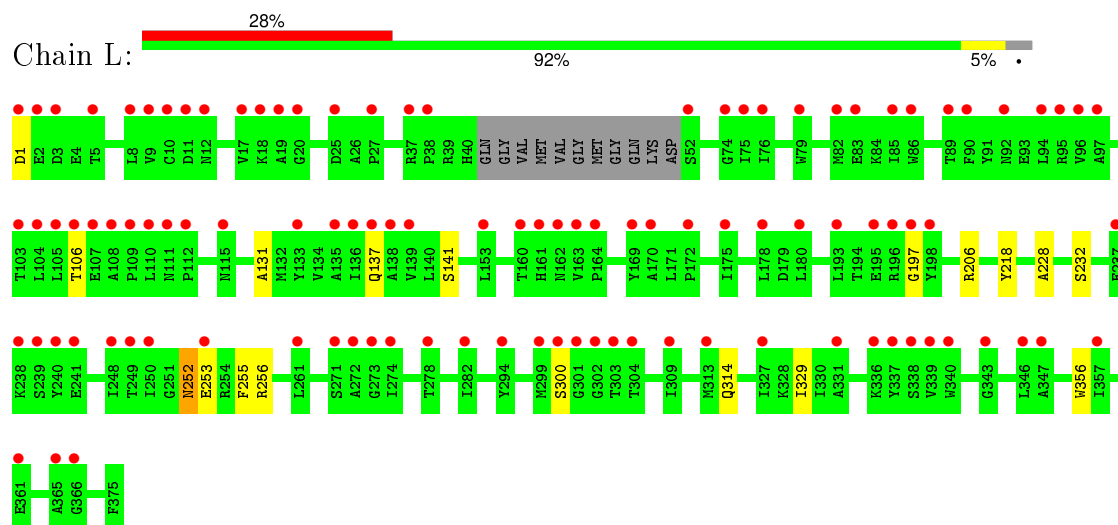
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



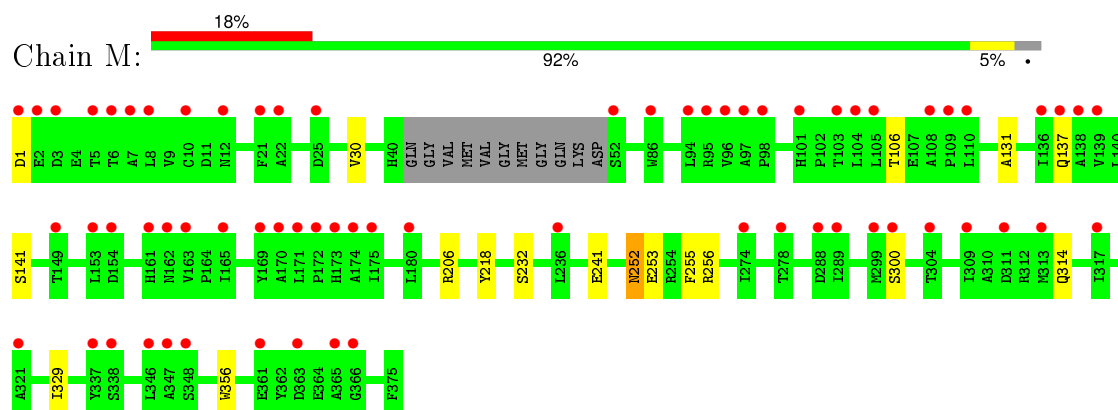
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



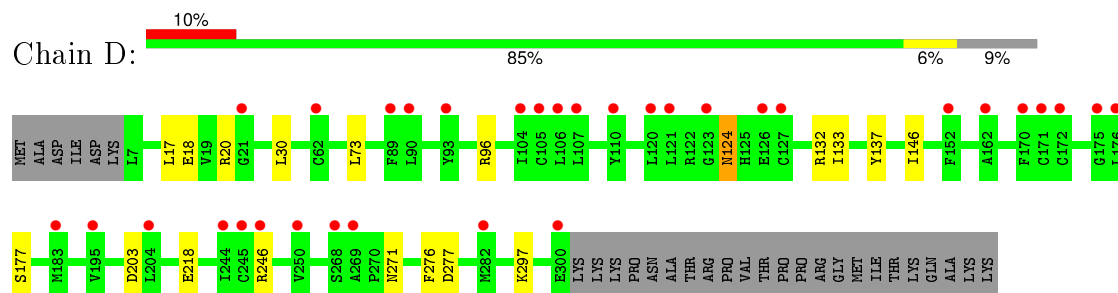
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



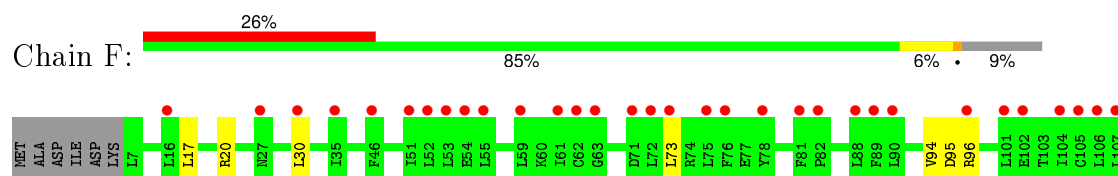
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

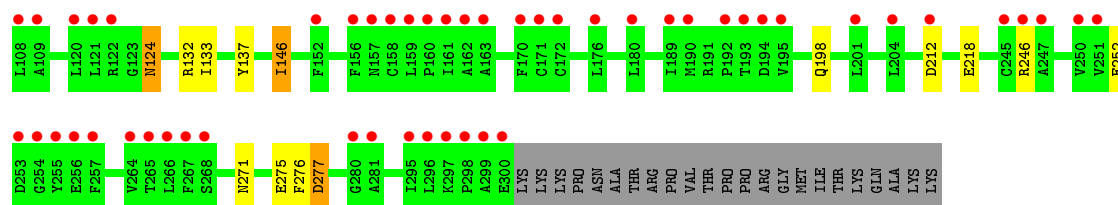


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

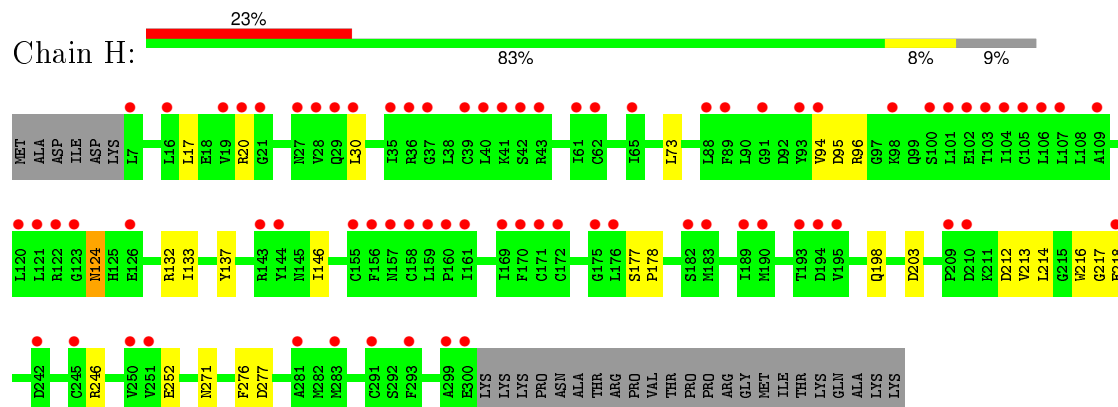


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

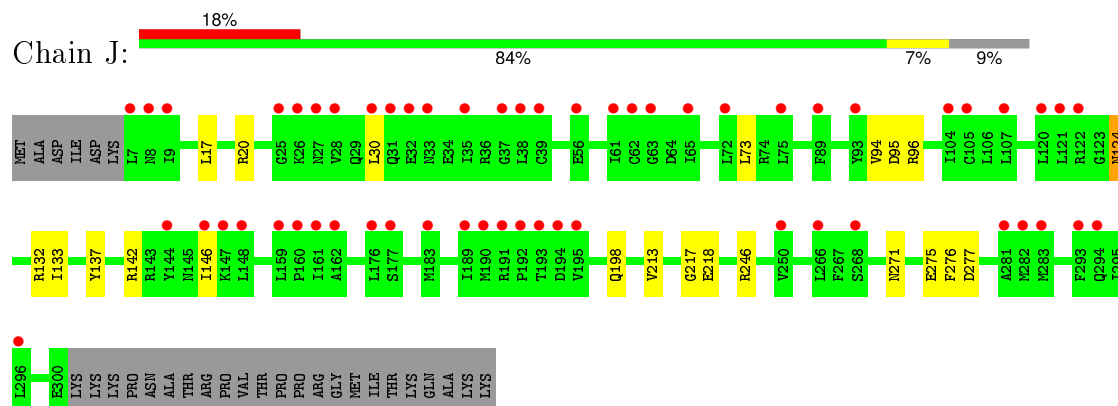




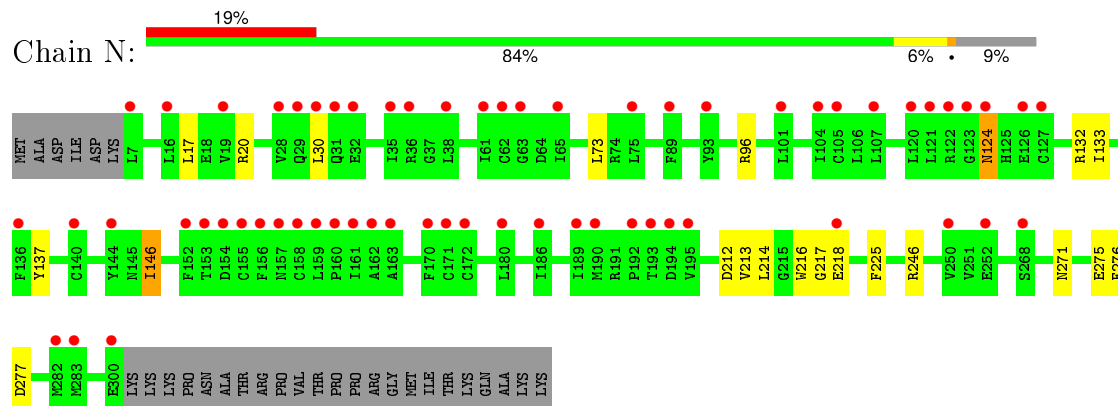
• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT



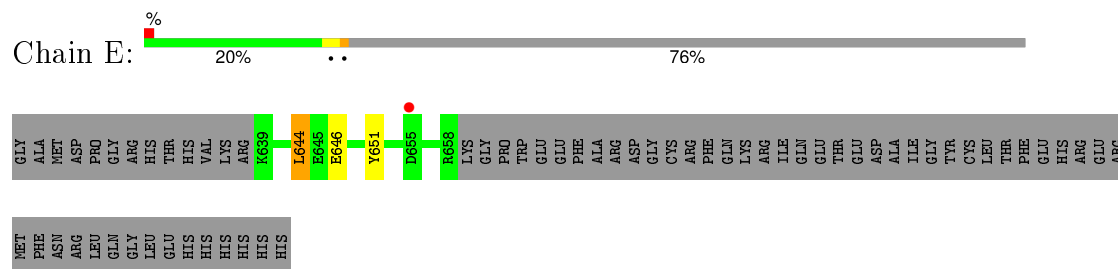
• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT



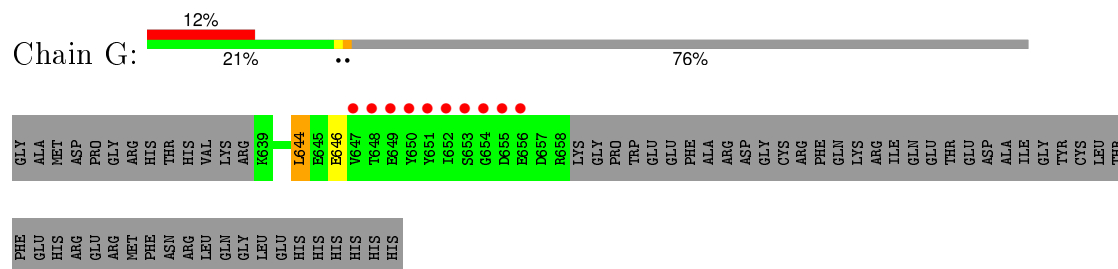
• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT



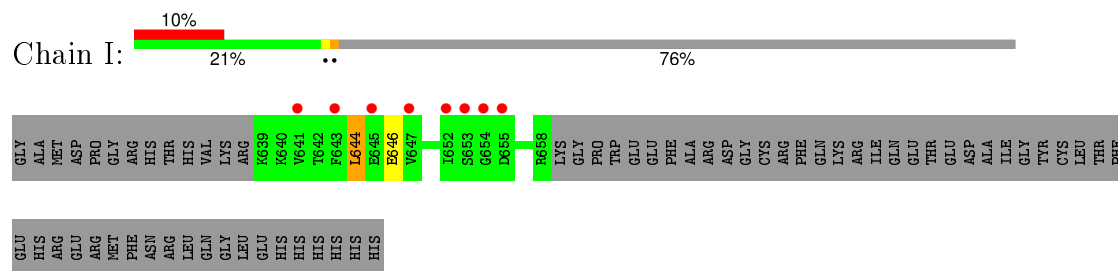
- Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



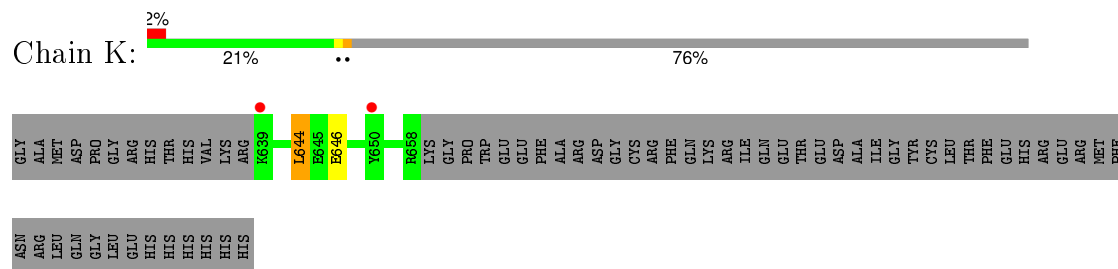
- Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



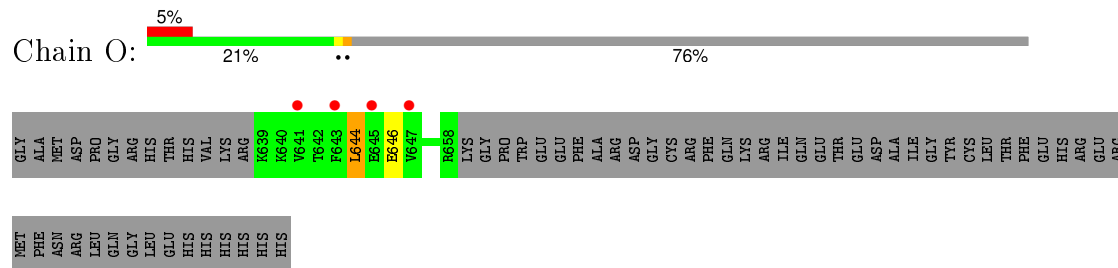
- Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



- Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



- Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 149.93Å 318.72Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	82.79 – 7.88 82.79 – 7.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (82.79-7.88) 97.8 (82.79-7.88)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.370 , 0.400 0.354 , 0.375	Depositor DCC
R_{free} test set	290 reflections (5.67%)	DCC
Wilson B-factor (Å ²)	356.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 456.6	EDS
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 5402 reflections (0.019%)	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	27065	wwPDB-VP
Average B, all atoms (Å ²)	394.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, LAB, ATP

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	0.47	0/2896	0.60	0/3927
1	B	0.47	0/2896	0.60	0/3927
1	C	0.46	0/2896	0.60	0/3927
1	L	0.47	0/2896	0.60	0/3927
1	M	0.47	0/2896	0.60	0/3927
2	D	0.29	0/2404	0.52	0/3250
2	F	0.30	0/2404	0.52	1/3250 (0.0%)
2	H	0.29	0/2404	0.52	0/3250
2	J	0.29	0/2404	0.52	0/3250
2	N	0.29	0/2404	0.52	1/3250 (0.0%)
3	E	0.37	0/169	0.59	0/226
3	G	0.31	0/169	0.56	0/226
3	I	0.32	0/169	0.56	0/226
3	K	0.31	0/169	0.55	0/226
3	O	0.31	0/169	0.56	0/226
All	All	0.39	0/27345	0.57	2/37015 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	146	ILE	CB-CA-C	-5.50	100.59	111.60
2	F	146	ILE	CB-CA-C	-5.34	100.93	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2835	0	2787	46	4
1	B	2835	0	2787	22	5
1	C	2835	0	2787	24	0
1	L	2835	0	2787	19	2
1	M	2835	0	2787	14	0
2	D	2351	0	2304	16	4
2	F	2351	0	2303	65	0
2	H	2351	0	2304	51	0
2	J	2351	0	2304	29	2
2	N	2351	0	2304	28	0
3	E	167	0	157	4	5
3	G	167	0	157	1	0
3	I	167	0	157	1	0
3	K	167	0	157	1	0
3	O	167	0	157	1	0
4	A	27	0	29	1	0
4	B	27	0	29	1	0
4	C	27	0	29	1	0
4	L	27	0	29	1	0
4	M	27	0	29	1	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
5	L	31	0	12	0	0
5	M	31	0	12	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	H	2	0	0	0	0
6	J	2	0	0	0	0
6	N	2	0	0	0	0
All	All	27065	0	26444	210	11

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 4.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:HB3	2:F:146:ILE:CG1	1.49	1.43
1:A:1:ASP:HB3	2:F:146:ILE:CD1	1.50	1.40
1:A:1:ASP:CB	2:F:146:ILE:CD1	2.02	1.35
1:A:1:ASP:CB	2:F:146:ILE:HD11	1.55	1.35
2:F:198:GLN:NE2	1:M:232:SER:O	1.61	1.33
2:J:142:ARG:NH1	1:L:197:GLY:HA2	1.47	1.28
1:C:232:SER:O	2:J:198:GLN:NE2	1.69	1.25
1:C:1:ASP:CG	2:H:137:TYR:OH	1.74	1.24
1:A:1:ASP:O	2:F:146:ILE:HG13	1.29	1.21
2:F:277:ASP:OD1	2:H:214:LEU:HB3	1.48	1.14
1:A:1:ASP:HB3	2:F:146:ILE:HG12	1.16	1.10
2:F:275:GLU:OE1	2:H:217:GLY:HA2	1.52	1.09
1:B:232:SER:O	2:H:198:GLN:NE2	1.87	1.08
1:C:1:ASP:HB3	2:H:146:ILE:HD11	1.37	1.06
1:A:1:ASP:HB2	2:F:146:ILE:HD11	1.32	1.05
1:A:1:ASP:O	2:F:146:ILE:CG1	2.05	1.04
1:M:1:ASP:OD2	2:N:137:TYR:OH	1.73	1.04
2:J:276:PHE:HA	2:N:212:ASP:O	1.60	1.00
2:J:142:ARG:CD	1:L:197:GLY:HA3	1.91	0.99
2:J:142:ARG:HD2	1:L:197:GLY:HA3	1.01	0.97
2:J:142:ARG:HH11	1:L:197:GLY:CA	1.80	0.95
2:J:142:ARG:HD2	1:L:197:GLY:CA	1.95	0.94
2:J:142:ARG:NH1	1:L:197:GLY:CA	2.32	0.93
1:A:1:ASP:C	2:F:146:ILE:HD11	1.89	0.92
1:A:1:ASP:CB	2:F:146:ILE:CG1	2.36	0.91
2:F:275:GLU:HB3	2:H:216:TRP:O	1.70	0.91
1:A:1:ASP:CA	2:F:146:ILE:HD11	2.02	0.90
1:A:1:ASP:CB	2:F:146:ILE:HG12	1.98	0.90
2:J:142:ARG:HH11	1:L:197:GLY:HA2	1.06	0.89
1:C:1:ASP:CG	2:H:137:TYR:HH	1.65	0.87
1:C:1:ASP:OD1	2:H:137:TYR:OH	1.95	0.84
2:J:271:ASN:ND2	2:J:276:PHE:O	2.12	0.82
1:A:3:ASP:CB	2:F:146:ILE:HD12	2.10	0.82
2:N:271:ASN:ND2	2:N:276:PHE:O	2.12	0.81
1:A:1:ASP:HB2	2:F:146:ILE:CD1	1.91	0.81
2:D:271:ASN:ND2	2:D:276:PHE:O	2.12	0.81
1:C:1:ASP:OD1	2:H:137:TYR:CE2	2.34	0.81
2:F:271:ASN:ND2	2:F:276:PHE:O	2.12	0.81
1:A:1:ASP:C	2:F:146:ILE:CD1	2.49	0.81
2:F:277:ASP:OD2	2:H:214:LEU:HD23	1.81	0.80
2:H:271:ASN:ND2	2:H:276:PHE:O	2.12	0.79
1:M:1:ASP:CG	2:N:137:TYR:OH	2.18	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:HB3	2:F:146:ILE:HD13	1.64	0.77
1:A:3:ASP:OD2	2:F:146:ILE:HD13	1.84	0.77
2:F:275:GLU:OE1	2:H:217:GLY:CA	2.31	0.76
2:J:275:GLU:OE1	2:N:217:GLY:HA2	1.86	0.76
1:C:1:ASP:OD1	2:H:137:TYR:CZ	2.41	0.73
2:J:275:GLU:CD	2:N:217:GLY:HA2	2.09	0.73
1:A:1:ASP:CB	2:F:146:ILE:HD13	2.15	0.72
1:A:3:ASP:HB3	2:F:146:ILE:HD12	1.72	0.72
1:A:1:ASP:O	2:F:146:ILE:CD1	2.38	0.70
2:F:252:GLU:HB3	2:H:212:ASP:OD1	1.94	0.67
2:F:275:GLU:CB	2:H:216:TRP:O	2.41	0.67
2:D:297:LYS:HE2	3:E:651:TYR:OH	1.93	0.67
2:F:277:ASP:OD1	2:H:214:LEU:CB	2.37	0.67
1:A:56:ASP:CG	1:B:243:PRO:O	2.33	0.67
1:A:3:ASP:OD2	2:F:146:ILE:HG21	1.96	0.66
1:A:1:ASP:C	2:F:146:ILE:CG1	2.65	0.65
1:A:3:ASP:N	2:F:146:ILE:HD12	2.13	0.64
1:A:3:ASP:CG	2:F:146:ILE:CD1	2.67	0.63
1:C:1:ASP:CB	2:H:146:ILE:HD11	2.22	0.63
2:F:17:LEU:O	2:F:20:ARG:NH1	2.32	0.63
2:N:17:LEU:O	2:N:20:ARG:NH1	2.32	0.63
2:D:297:LYS:HD3	3:E:651:TYR:CZ	2.32	0.63
2:J:275:GLU:OE1	2:N:217:GLY:CA	2.46	0.63
2:D:17:LEU:O	2:D:20:ARG:NH1	2.31	0.63
2:H:17:LEU:O	2:H:20:ARG:NH1	2.32	0.63
2:F:276:PHE:HA	2:H:213:VAL:HA	1.81	0.63
1:C:3:ASP:HB3	2:H:146:ILE:HD12	1.81	0.62
2:J:17:LEU:O	2:J:20:ARG:NH1	2.32	0.62
2:F:277:ASP:OD2	2:H:214:LEU:CD2	2.47	0.62
2:F:275:GLU:CD	2:H:217:GLY:HA2	2.19	0.62
1:M:1:ASP:OD1	2:N:137:TYR:OH	2.18	0.61
2:D:17:LEU:HB3	2:D:20:ARG:NH1	2.18	0.59
2:N:17:LEU:HB3	2:N:20:ARG:NH1	2.18	0.59
1:C:1:ASP:OD1	2:H:137:TYR:HE2	1.86	0.59
2:H:17:LEU:HB3	2:H:20:ARG:NH1	2.17	0.58
2:J:17:LEU:HB3	2:J:20:ARG:NH1	2.18	0.58
2:F:17:LEU:HB3	2:F:20:ARG:NH1	2.18	0.58
2:F:275:GLU:OE1	2:H:218:GLU:N	2.37	0.58
1:C:1:ASP:HB3	2:H:146:ILE:CD1	2.24	0.58
2:F:20:ARG:HG2	2:F:73:LEU:HD13	1.86	0.58
2:F:277:ASP:CG	2:H:214:LEU:HD23	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:ARG:HG2	2:N:73:LEU:HD13	1.86	0.58
2:J:20:ARG:HG2	2:J:73:LEU:HD13	1.86	0.57
2:D:20:ARG:HG2	2:D:73:LEU:HD13	1.86	0.57
1:C:30:VAL:O	1:M:241:GLU:OE2	2.23	0.57
2:J:218:GLU:N	2:N:275:GLU:OE1	2.36	0.57
1:A:1:ASP:CA	2:F:146:ILE:CG1	2.82	0.57
2:F:277:ASP:CG	2:H:214:LEU:HB3	2.23	0.56
1:B:1:ASP:OD2	2:D:146:ILE:HD11	2.05	0.56
2:H:20:ARG:HG2	2:H:73:LEU:HD13	1.86	0.56
1:C:241:GLU:OE2	1:M:30:VAL:O	2.24	0.55
1:A:3:ASP:CG	2:F:146:ILE:HD13	2.27	0.54
2:J:275:GLU:HB3	2:N:213:VAL:HG23	1.88	0.54
1:A:3:ASP:CG	2:F:146:ILE:HD12	2.28	0.54
1:A:30:VAL:O	1:B:241:GLU:OE2	2.26	0.53
2:N:218:GLU:OE1	2:N:218:GLU:HA	2.08	0.53
2:D:297:LYS:CE	3:E:651:TYR:OH	2.57	0.53
2:J:217:GLY:HA2	2:N:275:GLU:OE1	2.09	0.53
1:B:228:ALA:CB	2:H:178:PRO:HB2	2.39	0.53
2:N:17:LEU:HB3	2:N:20:ARG:HH12	1.74	0.53
2:D:17:LEU:HB3	2:D:20:ARG:HH12	1.74	0.53
2:H:124:ASN:HD22	2:H:124:ASN:H	1.57	0.53
2:F:124:ASN:H	2:F:124:ASN:HD22	1.57	0.52
1:C:3:ASP:OD2	2:H:146:ILE:CD1	2.57	0.52
2:D:124:ASN:HD22	2:D:124:ASN:H	1.57	0.52
2:F:17:LEU:HB3	2:F:20:ARG:HH12	1.74	0.52
2:J:218:GLU:OE1	2:J:218:GLU:HA	2.09	0.52
2:J:217:GLY:HA2	2:N:275:GLU:CD	2.30	0.52
1:L:232:SER:HB3	2:N:225:PHE:HZ	1.75	0.52
2:H:218:GLU:OE1	2:H:218:GLU:HA	2.10	0.52
2:N:124:ASN:HD22	2:N:124:ASN:H	1.57	0.51
2:H:17:LEU:HB3	2:H:20:ARG:HH12	1.74	0.51
2:F:275:GLU:HB3	2:H:217:GLY:HA2	1.91	0.51
2:J:124:ASN:HD22	2:J:124:ASN:H	1.57	0.51
2:F:277:ASP:CG	2:H:214:LEU:CD2	2.80	0.50
2:F:218:GLU:HA	2:F:218:GLU:OE1	2.10	0.50
2:J:17:LEU:HB3	2:J:20:ARG:HH12	1.74	0.50
1:L:232:SER:CB	2:N:225:PHE:HZ	2.24	0.50
1:B:228:ALA:HB3	2:H:178:PRO:HB2	1.92	0.50
2:D:218:GLU:OE1	2:D:218:GLU:HA	2.11	0.50
1:L:232:SER:HB3	2:N:225:PHE:CZ	2.48	0.48
1:A:56:ASP:HB3	1:B:243:PRO:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:CB	2:H:137:TYR:OH	2.59	0.47
2:F:277:ASP:CG	2:H:214:LEU:CB	2.82	0.47
2:F:275:GLU:O	2:H:214:LEU:O	2.33	0.47
2:J:275:GLU:O	2:N:213:VAL:HA	2.14	0.47
3:I:644:LEU:HD22	3:I:646:GLU:H	1.80	0.47
2:F:275:GLU:CB	2:H:217:GLY:HA2	2.45	0.47
1:A:56:ASP:CB	1:B:243:PRO:O	2.62	0.47
1:B:252:ASN:HD22	1:B:253:GLU:N	2.13	0.47
1:L:252:ASN:HD22	1:L:253:GLU:N	2.13	0.47
1:B:218:TYR:O	1:B:255:PHE:HA	2.15	0.47
1:M:218:TYR:O	1:M:255:PHE:HA	2.15	0.47
1:C:1:ASP:CG	2:H:137:TYR:CZ	2.77	0.46
1:A:252:ASN:HD22	1:A:253:GLU:N	2.13	0.46
1:C:252:ASN:HD22	1:C:253:GLU:N	2.13	0.46
1:L:218:TYR:O	1:L:255:PHE:HA	2.16	0.46
3:O:644:LEU:HD22	3:O:646:GLU:H	1.80	0.46
3:K:644:LEU:HD22	3:K:646:GLU:H	1.80	0.46
1:M:252:ASN:HD22	1:M:253:GLU:N	2.13	0.46
3:E:644:LEU:HD22	3:E:646:GLU:H	1.81	0.46
3:G:644:LEU:HD22	3:G:646:GLU:H	1.80	0.46
2:J:213:VAL:HG23	2:N:275:GLU:O	2.16	0.46
1:A:245:GLY:CA	1:B:30:VAL:O	2.64	0.46
1:C:218:TYR:O	1:C:255:PHE:HA	2.16	0.46
1:A:56:ASP:OD2	1:B:245:GLY:N	2.49	0.46
1:A:218:TYR:O	1:A:255:PHE:HA	2.15	0.45
2:F:275:GLU:CG	2:H:216:TRP:O	2.65	0.45
2:J:132:ARG:HA	2:J:137:TYR:HB2	1.99	0.45
2:N:146:ILE:HG21	2:N:146:ILE:HD13	1.74	0.45
1:A:245:GLY:HA2	1:B:30:VAL:O	2.17	0.45
1:L:206:ARG:HG2	4:L:1376:LAB:S1	2.57	0.44
2:N:132:ARG:HA	2:N:137:TYR:HB2	2.00	0.44
2:J:132:ARG:NH2	2:J:133:ILE:HD11	2.33	0.44
1:A:314:GLN:OE1	1:A:329:ILE:HG12	2.18	0.44
1:L:314:GLN:OE1	1:L:329:ILE:HG12	2.18	0.44
2:H:132:ARG:NH2	2:H:133:ILE:HD11	2.33	0.44
1:C:314:GLN:OE1	1:C:329:ILE:HG12	2.18	0.44
2:F:132:ARG:HA	2:F:137:TYR:HB2	1.99	0.44
1:A:3:ASP:OD2	2:F:146:ILE:CD1	2.62	0.44
1:B:233:SER:HB3	2:H:198:GLN:NE2	2.33	0.44
2:N:132:ARG:NH2	2:N:133:ILE:HD11	2.33	0.44
1:B:314:GLN:OE1	1:B:329:ILE:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:ARG:NH2	2:D:133:ILE:HD11	2.33	0.43
1:B:1:ASP:OD2	2:D:137:TYR:OH	2.36	0.43
2:F:146:ILE:HG21	2:F:146:ILE:HD13	1.74	0.43
2:H:132:ARG:HA	2:H:137:TYR:HB2	2.00	0.43
1:B:131:ALA:HB1	1:B:356:TRP:HB3	2.01	0.43
1:A:30:VAL:O	1:B:241:GLU:CD	2.57	0.43
1:M:314:GLN:OE1	1:M:329:ILE:HG12	2.18	0.43
2:F:212:ASP:OD1	2:H:252:GLU:HB3	2.19	0.43
2:J:275:GLU:O	2:N:214:LEU:N	2.41	0.43
2:F:132:ARG:NH2	2:F:133:ILE:HD11	2.33	0.43
1:B:206:ARG:HG2	4:B:1376:LAB:S1	2.59	0.43
1:C:206:ARG:HG2	4:C:1376:LAB:S1	2.59	0.43
2:H:146:ILE:HG21	2:H:146:ILE:HD13	1.76	0.42
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.42
1:L:131:ALA:HB1	1:L:356:TRP:HB3	2.01	0.42
2:F:252:GLU:CB	2:H:212:ASP:OD1	2.64	0.42
1:L:141:SER:HB3	1:L:300:SER:OG	2.20	0.42
1:C:131:ALA:HB1	1:C:356:TRP:HB3	2.00	0.42
1:A:3:ASP:CA	2:F:146:ILE:HD12	2.49	0.42
2:D:132:ARG:HA	2:D:137:TYR:HB2	2.00	0.42
2:D:146:ILE:HG21	2:D:146:ILE:HD13	1.76	0.42
1:M:206:ARG:HG2	4:M:1376:LAB:S1	2.59	0.42
1:C:106:THR:HB	1:C:137:GLN:HG3	2.02	0.42
1:M:141:SER:HB3	1:M:300:SER:OG	2.20	0.42
1:A:206:ARG:HG2	4:A:1376:LAB:S1	2.60	0.42
1:M:131:ALA:HB1	1:M:356:TRP:HB3	2.01	0.42
1:L:228:ALA:HB2	2:N:216:TRP:CD1	2.55	0.42
1:A:3:ASP:CB	2:F:146:ILE:CD1	2.90	0.41
1:L:252:ASN:ND2	1:L:256:ARG:HH11	2.19	0.41
2:H:94:VAL:O	2:H:95:ASP:HB2	2.21	0.41
1:B:106:THR:HB	1:B:137:GLN:HG3	2.02	0.41
1:C:252:ASN:ND2	1:C:256:ARG:HH11	2.19	0.41
1:A:3:ASP:HB3	2:F:146:ILE:CD1	2.47	0.41
1:B:252:ASN:ND2	1:B:256:ARG:HH11	2.19	0.41
2:J:94:VAL:O	2:J:95:ASP:HB2	2.21	0.41
2:D:177:SER:HB2	2:D:203:ASP:HB2	2.03	0.41
2:H:177:SER:HB2	2:H:203:ASP:HB2	2.03	0.41
1:M:252:ASN:ND2	1:M:256:ARG:HH11	2.19	0.41
1:M:106:THR:HB	1:M:137:GLN:HG3	2.02	0.41
1:A:106:THR:HB	1:A:137:GLN:HG3	2.02	0.41
2:F:94:VAL:O	2:F:95:ASP:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:THR:HB	1:L:137:GLN:HG3	2.02	0.41
1:C:141:SER:HB3	1:C:300:SER:OG	2.20	0.40
1:A:124:PHE:CZ	1:A:132:MET:HG3	2.57	0.40
1:B:124:PHE:CZ	1:B:132:MET:HG3	2.57	0.40

All (11) 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:80:ASP:OD1	2:D:18:GLU:OE2[2_756]	1.24	0.96
2:J:137:TYR:OH	1:L:1:ASP:OD1[2_655]	1.30	0.90
1:B:72:GLU:OE2	3:E:646:GLU:OE1[4_756]	1.33	0.87
1:A:80:ASP:CG	2:D:18:GLU:OE2[2_756]	1.50	0.70
1:B:72:GLU:OE2	3:E:646:GLU:CD[4_756]	1.65	0.55
1:A:80:ASP:OD2	2:D:18:GLU:OE2[2_756]	1.68	0.52
2:J:146:ILE:CD1	1:L:1:ASP:CB[2_655]	1.69	0.51
1:A:80:ASP:OD1	2:D:18:GLU:CD[2_756]	2.00	0.20
1:B:118:LYS:NZ	3:E:651:TYR:CE1[4_756]	2.01	0.19
1:B:72:GLU:OE2	3:E:646:GLU:OE2[4_756]	2.02	0.18
1:B:118:LYS:NZ	3:E:651:TYR:CZ[4_756]	2.17	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	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	B	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	C	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	L	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	M	360/375 (96%)	353 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	F	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	H	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	J	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	N	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
3	E	18/84 (21%)	18 (100%)	0	0	100	100
3	G	18/84 (21%)	18 (100%)	0	0	100	100
3	I	18/84 (21%)	18 (100%)	0	0	100	100
3	K	18/84 (21%)	18 (100%)	0	0	100	100
3	O	18/84 (21%)	18 (100%)	0	0	100	100
All	All	3350/3910 (86%)	3260 (97%)	90 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/318 (96%)	304 (100%)	1 (0%)	94	96
1	B	305/318 (96%)	304 (100%)	1 (0%)	94	96
1	C	305/318 (96%)	304 (100%)	1 (0%)	94	96
1	L	305/318 (96%)	304 (100%)	1 (0%)	94	96
1	M	305/318 (96%)	304 (100%)	1 (0%)	94	96
2	D	255/285 (90%)	250 (98%)	5 (2%)	63	85
2	F	255/285 (90%)	250 (98%)	5 (2%)	63	85
2	H	255/285 (90%)	250 (98%)	5 (2%)	63	85
2	J	255/285 (90%)	250 (98%)	5 (2%)	63	85
2	N	255/285 (90%)	250 (98%)	5 (2%)	63	85
3	E	18/74 (24%)	17 (94%)	1 (6%)	26	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	18/74 (24%)	17 (94%)	1 (6%)	26	62
3	I	18/74 (24%)	17 (94%)	1 (6%)	26	62
3	K	18/74 (24%)	17 (94%)	1 (6%)	26	62
3	O	18/74 (24%)	17 (94%)	1 (6%)	26	62
All	All	2890/3385 (85%)	2855 (99%)	35 (1%)	78	90

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	252	ASN
1	C	252	ASN
2	D	30	LEU
2	D	96	ARG
2	D	124	ASN
2	D	246	ARG
2	D	277	ASP
3	E	644	LEU
2	F	30	LEU
2	F	96	ARG
2	F	124	ASN
2	F	246	ARG
2	F	277	ASP
3	G	644	LEU
2	H	30	LEU
2	H	96	ARG
2	H	124	ASN
2	H	246	ARG
2	H	277	ASP
3	I	644	LEU
2	J	30	LEU
2	J	96	ARG
2	J	124	ASN
2	J	246	ARG
2	J	277	ASP
3	K	644	LEU
1	L	252	ASN
1	M	252	ASN
2	N	30	LEU
2	N	96	ARG
2	N	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	246	ARG
2	N	277	ASP
3	O	644	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	88	HIS
1	A	252	ASN
1	A	280	ASN
1	B	59	GLN
1	B	88	HIS
1	B	252	ASN
1	B	280	ASN
1	C	59	GLN
1	C	88	HIS
1	C	252	ASN
1	C	280	ASN
2	J	198	GLN
1	L	59	GLN
1	L	88	HIS
1	L	252	ASN
1	L	280	ASN
1	M	59	GLN
1	M	88	HIS
1	M	252	ASN
1	M	280	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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$
4	LAB	A	1376	-	27,29,29	4.26	7 (25%)	28,41,41	3.71	9 (32%)
5	ATP	A	1377	-	24,33,33	1.44	3 (12%)	31,52,52	1.84	2 (6%)
4	LAB	B	1376	-	27,29,29	4.25	7 (25%)	28,41,41	3.72	9 (32%)
5	ATP	B	1377	-	24,33,33	1.45	3 (12%)	31,52,52	1.85	2 (6%)
4	LAB	C	1376	-	27,29,29	4.26	7 (25%)	28,41,41	3.71	9 (32%)
5	ATP	C	1377	-	24,33,33	1.44	3 (12%)	31,52,52	1.85	2 (6%)
4	LAB	L	1376	-	27,29,29	4.26	7 (25%)	28,41,41	3.72	9 (32%)
5	ATP	L	1377	-	24,33,33	1.45	3 (12%)	31,52,52	1.84	2 (6%)
4	LAB	M	1376	-	27,29,29	4.26	7 (25%)	28,41,41	3.71	9 (32%)
5	ATP	M	1377	-	24,33,33	1.43	3 (12%)	31,52,52	1.85	2 (6%)

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
4	LAB	A	1376	-	-	0/21/49/49	0/1/3/3
5	ATP	A	1377	-	-	0/18/38/38	0/3/3/3
4	LAB	B	1376	-	-	0/21/49/49	0/1/3/3
5	ATP	B	1377	-	-	0/18/38/38	0/3/3/3
4	LAB	C	1376	-	-	0/21/49/49	0/1/3/3
5	ATP	C	1377	-	-	0/18/38/38	0/3/3/3
4	LAB	L	1376	-	-	0/21/49/49	0/1/3/3
5	ATP	L	1377	-	-	0/18/38/38	0/3/3/3
4	LAB	M	1376	-	-	0/21/49/49	0/1/3/3
5	ATP	M	1377	-	-	0/18/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1376	LAB	C17-S1	-9.02	1.64	1.81
4	C	1376	LAB	C17-S1	-8.99	1.64	1.81
4	M	1376	LAB	C17-S1	-8.95	1.64	1.81
4	A	1376	LAB	C17-S1	-8.95	1.64	1.81
4	L	1376	LAB	C17-S1	-8.92	1.64	1.81
4	B	1376	LAB	C14-C13	-5.70	1.40	1.51
4	A	1376	LAB	C14-C13	-5.68	1.40	1.51
4	L	1376	LAB	C14-C13	-5.67	1.40	1.51
4	C	1376	LAB	C14-C13	-5.64	1.40	1.51
4	M	1376	LAB	C14-C13	-5.61	1.40	1.51
5	B	1377	ATP	C2'-C3'	-4.18	1.42	1.53
5	C	1377	ATP	C2'-C3'	-4.18	1.42	1.53
5	L	1377	ATP	C2'-C3'	-4.18	1.42	1.53
5	A	1377	ATP	C2'-C3'	-4.16	1.42	1.53
5	M	1377	ATP	C2'-C3'	-4.15	1.42	1.53
5	M	1377	ATP	O4'-C4'	-2.06	1.40	1.45
5	B	1377	ATP	O4'-C4'	-2.04	1.40	1.45
5	C	1377	ATP	O4'-C4'	-2.03	1.40	1.45
5	L	1377	ATP	O4'-C4'	-2.03	1.40	1.45
5	A	1377	ATP	O4'-C4'	-2.01	1.40	1.45
4	L	1376	LAB	C17-C16	3.25	1.59	1.53
4	A	1376	LAB	C17-C16	3.26	1.59	1.53
4	B	1376	LAB	C17-C16	3.29	1.59	1.53
4	C	1376	LAB	C17-C16	3.29	1.59	1.53
4	M	1376	LAB	C17-C16	3.31	1.59	1.53
5	M	1377	ATP	C6-N6	3.76	1.46	1.34
5	B	1377	ATP	C6-N6	3.79	1.46	1.34
5	L	1377	ATP	C6-N6	3.80	1.46	1.34
5	A	1377	ATP	C6-N6	3.81	1.46	1.34
5	C	1377	ATP	C6-N6	3.81	1.46	1.34
4	M	1376	LAB	O5-C18	8.36	1.35	1.22
4	L	1376	LAB	O5-C18	8.37	1.35	1.22
4	A	1376	LAB	O5-C18	8.38	1.35	1.22
4	B	1376	LAB	O5-C18	8.40	1.35	1.22
4	C	1376	LAB	O5-C18	8.43	1.35	1.22
4	B	1376	LAB	C16-N1	8.96	1.56	1.46
4	A	1376	LAB	C16-N1	8.97	1.56	1.46
4	C	1376	LAB	C16-N1	8.97	1.56	1.46
4	M	1376	LAB	C16-N1	9.01	1.56	1.46
4	L	1376	LAB	C16-N1	9.02	1.56	1.46
4	A	1376	LAB	C2-C3	9.44	1.53	1.33
4	B	1376	LAB	C2-C3	9.46	1.54	1.33
4	L	1376	LAB	C2-C3	9.46	1.54	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1376	LAB	C2-C3	9.48	1.54	1.33
4	M	1376	LAB	C2-C3	9.49	1.54	1.33
4	B	1376	LAB	C18-N1	9.96	1.51	1.36
4	C	1376	LAB	C18-N1	10.10	1.51	1.36
4	A	1376	LAB	C18-N1	10.11	1.51	1.36
4	M	1376	LAB	C18-N1	10.12	1.51	1.36
4	L	1376	LAB	C18-N1	10.14	1.51	1.36

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1376	LAB	O5-C18-N1	-17.52	105.88	125.81
4	B	1376	LAB	O5-C18-N1	-17.49	105.91	125.81
4	A	1376	LAB	O5-C18-N1	-17.49	105.92	125.81
4	M	1376	LAB	O5-C18-N1	-17.48	105.93	125.81
4	C	1376	LAB	O5-C18-N1	-17.47	105.94	125.81
5	B	1377	ATP	N3-C2-N1	-8.60	122.31	128.89
5	M	1377	ATP	N3-C2-N1	-8.55	122.35	128.89
5	C	1377	ATP	N3-C2-N1	-8.53	122.36	128.89
5	A	1377	ATP	N3-C2-N1	-8.52	122.37	128.89
5	L	1377	ATP	N3-C2-N1	-8.52	122.37	128.89
4	M	1376	LAB	C19-C3-C2	-3.74	110.59	122.42
4	C	1376	LAB	C19-C3-C2	-3.74	110.59	122.42
4	L	1376	LAB	C19-C3-C2	-3.73	110.63	122.42
4	A	1376	LAB	C19-C3-C2	-3.72	110.65	122.42
4	B	1376	LAB	C19-C3-C2	-3.72	110.65	122.42
4	B	1376	LAB	C16-N1-C18	-3.34	108.66	113.04
4	L	1376	LAB	C16-N1-C18	-3.33	108.68	113.04
4	C	1376	LAB	C16-N1-C18	-3.32	108.69	113.04
4	M	1376	LAB	C16-N1-C18	-3.31	108.70	113.04
4	A	1376	LAB	C16-N1-C18	-3.30	108.71	113.04
4	B	1376	LAB	C19-C3-C4	-2.50	111.58	115.41
4	C	1376	LAB	C19-C3-C4	-2.50	111.59	115.41
4	L	1376	LAB	C19-C3-C4	-2.50	111.60	115.41
4	A	1376	LAB	C19-C3-C4	-2.49	111.61	115.41
4	M	1376	LAB	C19-C3-C4	-2.48	111.62	115.41
4	L	1376	LAB	O1-C1-C2	-2.23	120.32	126.20
4	M	1376	LAB	O1-C1-C2	-2.22	120.34	126.20
4	C	1376	LAB	O1-C1-C2	-2.22	120.37	126.20
4	A	1376	LAB	O1-C1-C2	-2.21	120.37	126.20
5	M	1377	ATP	C4-C5-N7	-2.21	107.44	109.48
4	B	1376	LAB	O1-C1-C2	-2.21	120.37	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1377	ATP	C4-C5-N7	-2.21	107.45	109.48
5	C	1377	ATP	C4-C5-N7	-2.20	107.46	109.48
5	A	1377	ATP	C4-C5-N7	-2.16	107.50	109.48
5	L	1377	ATP	C4-C5-N7	-2.16	107.50	109.48
4	M	1376	LAB	C3-C2-C1	-2.05	122.74	127.73
4	L	1376	LAB	C3-C2-C1	-2.04	122.74	127.73
4	B	1376	LAB	C3-C2-C1	-2.04	122.75	127.73
4	C	1376	LAB	C3-C2-C1	-2.04	122.76	127.73
4	A	1376	LAB	C3-C2-C1	-2.03	122.77	127.73
4	B	1376	LAB	C16-C17-S1	2.71	110.09	105.94
4	M	1376	LAB	C16-C17-S1	2.72	110.11	105.94
4	L	1376	LAB	C16-C17-S1	2.74	110.14	105.94
4	A	1376	LAB	C16-C17-S1	2.74	110.14	105.94
4	C	1376	LAB	C16-C17-S1	2.76	110.17	105.94
4	L	1376	LAB	C5-C4-C3	2.77	121.73	112.71
4	B	1376	LAB	C5-C4-C3	2.77	121.73	112.71
4	A	1376	LAB	C5-C4-C3	2.77	121.74	112.71
4	M	1376	LAB	C5-C4-C3	2.78	121.77	112.71
4	C	1376	LAB	C5-C4-C3	2.79	121.79	112.71
4	A	1376	LAB	O2-C1-C2	3.12	119.21	111.51
4	C	1376	LAB	O2-C1-C2	3.13	119.22	111.51
4	B	1376	LAB	O2-C1-C2	3.13	119.24	111.51
4	L	1376	LAB	O2-C1-C2	3.14	119.25	111.51
4	M	1376	LAB	O2-C1-C2	3.15	119.28	111.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1376	LAB	1	0
4	B	1376	LAB	1	0
4	C	1376	LAB	1	0
4	L	1376	LAB	1	0
4	M	1376	LAB	1	0

5.7 Other polymers [i](#)

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, 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	364/375 (97%)	0.95	48 (13%) 4 10	237, 303, 352, 385	0
1	B	364/375 (97%)	1.10	61 (16%) 2 8	252, 327, 380, 404	0
1	C	364/375 (97%)	1.37	86 (23%) 1 6	356, 410, 453, 502	0
1	L	364/375 (97%)	1.56	106 (29%) 1 5	403, 490, 565, 619	0
1	M	364/375 (97%)	1.09	67 (18%) 2 7	454, 521, 589, 621	0
2	D	294/323 (91%)	0.83	33 (11%) 7 12	232, 291, 334, 368	0
2	F	294/323 (91%)	1.39	83 (28%) 1 5	303, 364, 419, 450	0
2	H	294/323 (91%)	1.34	75 (25%) 1 6	311, 382, 436, 457	0
2	J	294/323 (91%)	1.02	57 (19%) 1 7	303, 367, 432, 478	0
2	N	294/323 (91%)	1.16	62 (21%) 1 6	285, 372, 419, 450	0
3	E	20/84 (23%)	0.81	1 (5%) 32 32	446, 573, 869, 969	0
3	G	20/84 (23%)	2.38	10 (50%) 0 4	497, 563, 717, 732	0
3	I	20/84 (23%)	2.01	8 (40%) 0 4	583, 761, 1000, 1000	0
3	K	20/84 (23%)	0.86	2 (10%) 9 14	471, 544, 652, 721	0
3	O	20/84 (23%)	0.85	4 (20%) 1 7	644, 682, 763, 789	0
All	All	3390/3910 (86%)	1.19	703 (20%) 1 7	232, 377, 559, 1000	0

All (703) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	PRO	14.7
1	L	108	ALA	12.9
2	N	194	ASP	11.2
1	C	10	CYS	9.7
2	D	172	CYS	9.3
2	F	265	THR	9.1
1	M	109	PRO	8.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	193	THR	8.1
1	C	12	ASN	7.9
2	F	172	CYS	7.6
2	H	28	VAL	7.3
2	J	194	ASP	7.3
1	M	2	GLU	7.3
1	L	137	GLN	6.8
2	F	266	LEU	6.7
1	L	110	LEU	6.7
1	L	136	ILE	6.6
1	C	11	ASP	6.6
1	C	74	GLY	6.4
1	L	96	VAL	6.4
1	M	6	THR	6.4
1	C	105	LEU	6.3
2	F	162	ALA	6.3
1	C	109	PRO	6.3
1	C	1	ASP	6.2
1	L	239	SER	6.1
2	F	62	CYS	6.0
2	F	105	CYS	6.0
2	F	63	GLY	6.0
1	M	7	ALA	6.0
2	F	161	ILE	6.0
2	F	163	ALA	5.9
1	L	10	CYS	5.9
1	C	2	GLU	5.9
1	L	86	TRP	5.7
2	N	157	ASN	5.7
2	H	93	TYR	5.7
2	H	194	ASP	5.6
2	F	171	CYS	5.6
1	L	111	ASN	5.6
1	M	108	ALA	5.6
1	L	107	GLU	5.6
1	L	12	ASN	5.5
1	M	138	ALA	5.5
2	H	104	ILE	5.4
2	F	250	VAL	5.4
3	G	649	GLU	5.4
2	F	90	LEU	5.4
2	N	161	ILE	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	94	LEU	5.3
3	I	643	PHE	5.3
2	H	250	VAL	5.3
1	L	82	MET	5.3
2	F	299	ALA	5.3
1	C	76	ILE	5.3
2	F	268	SER	5.3
1	B	138	ALA	5.3
3	G	650	TYR	5.2
1	M	96	VAL	5.2
1	L	271	SER	5.2
2	F	300	GLU	5.2
2	H	94	VAL	5.1
2	J	193	THR	5.1
2	F	245	CYS	5.1
2	J	250	VAL	5.1
1	C	179	ASP	5.1
2	H	120	LEU	5.1
2	H	105	CYS	5.0
1	C	7	ALA	5.0
1	A	150	GLY	5.0
2	F	61	ILE	5.0
2	H	101	LEU	4.9
2	H	29	GLN	4.8
2	H	172	CYS	4.8
2	N	122	ARG	4.8
1	C	75	ILE	4.8
2	H	195	VAL	4.8
1	L	90	PHE	4.8
2	F	160	PRO	4.8
1	L	197	GLY	4.8
2	F	255	TYR	4.8
1	L	170	ALA	4.7
1	L	337	TYR	4.7
2	F	297	LYS	4.7
1	M	103	THR	4.7
1	L	106	THR	4.7
1	B	12	ASN	4.7
1	B	36	GLY	4.7
1	L	248	ILE	4.7
2	N	28	VAL	4.7
2	F	104	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	105	CYS	4.6
3	G	651	TYR	4.6
2	J	35	ILE	4.6
2	H	100	SER	4.6
1	L	76	ILE	4.6
2	H	175	GLY	4.6
1	B	109	PRO	4.6
1	A	12	ASN	4.6
2	D	171	CYS	4.6
1	L	89	THR	4.6
1	L	8	LEU	4.5
1	C	161	HIS	4.5
2	N	62	CYS	4.5
2	N	162	ALA	4.5
1	M	8	LEU	4.5
1	C	178	LEU	4.5
1	M	172	PRO	4.5
3	G	654	GLY	4.5
2	N	126	GLU	4.5
2	N	195	VAL	4.5
2	F	193	THR	4.5
1	C	160	THR	4.4
1	C	177	ARG	4.4
1	L	196	ARG	4.4
2	D	245	CYS	4.4
2	N	156	PHE	4.4
1	C	8	LEU	4.4
2	H	122	ARG	4.4
2	H	193	THR	4.4
1	L	178	LEU	4.4
2	F	256	GLU	4.4
2	N	171	CYS	4.4
2	H	121	LEU	4.3
3	G	652	ILE	4.3
1	M	347	ALA	4.3
2	F	195	VAL	4.3
1	L	52	SER	4.3
1	B	161	HIS	4.3
1	M	299	MET	4.3
2	F	106	LEU	4.3
1	M	173	HIS	4.2
1	L	195	GLU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	11	ASP	4.2
1	B	1	ASP	4.2
1	L	365	ALA	4.2
1	C	77	THR	4.2
2	N	30	LEU	4.2
1	M	365	ALA	4.2
1	C	365	ALA	4.1
1	A	52	SER	4.1
1	M	170	ALA	4.1
2	H	27	ASN	4.1
3	G	653	SER	4.1
1	C	104	LEU	4.1
2	N	163	ALA	4.1
1	C	106	THR	4.1
1	M	153	LEU	4.0
2	N	29	GLN	4.0
1	M	337	TYR	4.0
2	N	192	PRO	4.0
1	A	76	ILE	4.0
1	B	52	SER	4.0
1	L	303	THR	4.0
1	L	304	THR	4.0
2	H	39	CYS	4.0
2	J	282	MET	4.0
1	C	52	SER	4.0
1	L	180	LEU	4.0
1	M	288	ASP	3.9
1	L	300	SER	3.9
1	L	104	LEU	3.9
2	F	296	LEU	3.9
1	M	304	THR	3.9
1	C	366	GLY	3.9
1	M	21	PHE	3.9
2	N	152	PHE	3.9
1	C	73	HIS	3.9
1	C	304	THR	3.8
1	M	10	CYS	3.8
2	J	268	SER	3.8
1	B	35	VAL	3.8
1	C	309	ILE	3.8
2	F	257	PHE	3.8
1	L	19	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	264	VAL	3.8
3	I	641	VAL	3.8
1	C	303	THR	3.8
1	C	103	THR	3.8
1	B	337	TYR	3.8
1	M	104	LEU	3.8
1	M	300	SER	3.8
2	H	7	LEU	3.8
1	L	17	VAL	3.8
2	J	161	ILE	3.8
2	F	89	PHE	3.8
2	F	281	ALA	3.7
1	L	274	ILE	3.7
1	L	250	ILE	3.7
2	N	268	SER	3.7
2	N	35	ILE	3.7
2	N	283	MET	3.7
1	A	106	THR	3.7
1	C	337	TYR	3.7
2	F	251	VAL	3.7
3	K	639	LYS	3.6
1	A	35	VAL	3.6
1	B	2	GLU	3.6
1	L	25	ASP	3.6
1	B	300	SER	3.6
1	M	1	ASP	3.6
2	J	65	ILE	3.6
2	H	103	THR	3.6
2	H	156	PHE	3.6
2	H	245	CYS	3.6
2	N	155	CYS	3.6
1	A	70	PRO	3.6
1	L	9	VAL	3.6
2	H	299	ALA	3.6
1	L	138	ALA	3.6
1	L	339	VAL	3.6
1	L	249	THR	3.6
2	N	189	ILE	3.5
1	B	154	ASP	3.5
1	L	95	ARG	3.5
1	M	171	LEU	3.5
3	G	655	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	3	ASP	3.5
2	F	120	LEU	3.5
2	H	89	PHE	3.5
2	N	16	LEU	3.5
2	H	102	GLU	3.5
2	F	194	ASP	3.5
1	L	193	LEU	3.5
1	M	169	TYR	3.5
1	B	53	TYR	3.4
1	B	153	LEU	3.4
1	L	240	TYR	3.4
2	F	158	CYS	3.4
2	N	144	TYR	3.4
1	M	346	LEU	3.4
2	N	7	LEU	3.4
1	C	6	THR	3.4
2	F	246	ARG	3.4
2	N	153	THR	3.4
2	F	295	ILE	3.4
2	N	61	ILE	3.4
1	A	40	HIS	3.4
1	L	163	VAL	3.4
1	A	105	LEU	3.4
2	H	88	LEU	3.4
2	N	159	LEU	3.4
1	M	274	ILE	3.4
3	G	656	GLU	3.4
1	L	1	ASP	3.4
1	L	272	ALA	3.4
1	M	110	LEU	3.4
2	N	190	MET	3.3
2	H	35	ILE	3.3
2	F	107	LEU	3.3
1	L	299	MET	3.3
2	D	175	GLY	3.3
1	C	347	ALA	3.3
3	G	647	VAL	3.3
2	N	282	MET	3.3
1	L	161	HIS	3.3
2	H	291	CYS	3.3
1	M	175	ILE	3.3
1	C	299	MET	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	105	CYS	3.3
1	A	10	CYS	3.3
2	J	195	VAL	3.3
1	C	108	ALA	3.3
2	F	27	ASN	3.3
1	C	278	THR	3.3
1	M	95	ARG	3.3
2	J	62	CYS	3.3
2	F	212	ASP	3.3
1	B	180	LEU	3.2
2	J	32	GLU	3.2
1	B	34	ILE	3.2
1	C	274	ILE	3.2
1	L	85	ILE	3.2
1	B	11	ASP	3.2
2	H	159	LEU	3.2
2	D	250	VAL	3.2
2	J	294	GLN	3.2
1	L	169	TYR	3.2
2	H	160	PRO	3.2
1	C	3	ASP	3.2
2	J	293	PHE	3.2
1	L	164	PRO	3.2
2	N	170	PHE	3.2
1	A	109	PRO	3.2
2	F	122	ARG	3.1
2	H	283	MET	3.1
2	F	88	LEU	3.1
2	J	148	LEU	3.1
2	F	108	LEU	3.1
1	L	336	LYS	3.1
1	C	110	LEU	3.1
2	F	192	PRO	3.1
1	A	297	ASN	3.1
2	J	160	PRO	3.1
1	A	104	LEU	3.1
2	F	16	LEU	3.1
2	N	120	LEU	3.1
2	H	161	ILE	3.1
1	B	309	ILE	3.1
3	E	655	ASP	3.1
1	B	32	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	83	GLU	3.1
2	D	176	LEU	3.1
2	H	20	ARG	3.1
2	D	204	LEU	3.0
1	L	135	ALA	3.0
1	A	11	ASP	3.0
2	H	155	CYS	3.0
2	J	122	ARG	3.0
2	F	204	LEU	3.0
2	H	190	MET	3.0
2	N	121	LEU	3.0
1	A	82	MET	3.0
1	A	86	TRP	3.0
1	B	58	ALA	3.0
2	J	120	LEU	3.0
3	I	645	GLU	3.0
2	J	25	GLY	3.0
2	H	16	LEU	3.0
1	L	75	ILE	3.0
2	J	281	ALA	3.0
1	B	347	ALA	3.0
1	C	336	LYS	3.0
2	D	89	PHE	3.0
3	O	641	VAL	2.9
1	B	321	ALA	2.9
1	L	160	THR	2.9
2	H	62	CYS	2.9
1	C	162	ASN	2.9
1	C	357	ILE	2.9
2	F	73	LEU	2.9
2	F	159	LEU	2.9
2	H	242	ASP	2.9
1	C	86	TRP	2.9
2	F	121	LEU	2.9
2	H	300	GLU	2.9
1	B	274	ILE	2.9
1	C	270	GLU	2.9
1	L	347	ALA	2.9
1	M	165	ILE	2.9
1	B	160	THR	2.9
2	F	254	GLY	2.9
2	N	160	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	134	VAL	2.9
2	N	154	ASP	2.9
2	N	65	ILE	2.9
2	D	269	ALA	2.9
2	H	182	SER	2.9
1	L	172	PRO	2.9
1	M	161	HIS	2.9
2	F	298	PRO	2.8
1	C	369	ILE	2.8
2	N	158	CYS	2.8
1	L	105	LEU	2.8
1	M	136	ILE	2.8
2	N	63	GLY	2.8
1	C	38	PRO	2.8
1	C	261	LEU	2.8
1	C	17	VAL	2.8
1	C	159	VAL	2.8
2	H	126	GLU	2.8
2	F	35	ILE	2.8
1	M	52	SER	2.8
2	H	19	VAL	2.8
1	L	338	SER	2.8
1	B	261	LEU	2.8
1	C	306	TYR	2.8
1	M	12	ASN	2.8
1	L	343	GLY	2.8
1	B	299	MET	2.8
2	F	176	LEU	2.8
2	J	33	ASN	2.8
2	D	62	CYS	2.8
1	M	25	ASP	2.8
1	B	106	THR	2.8
2	F	59	LEU	2.8
1	L	261	LEU	2.8
1	C	111	ASN	2.8
1	A	347	ALA	2.8
2	H	106	LEU	2.8
1	B	317	ILE	2.8
1	A	63	GLY	2.8
1	L	346	LEU	2.8
2	H	107	LEU	2.8
2	J	39	CYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	61	ILE	2.7
2	J	104	ILE	2.7
1	A	103	THR	2.7
2	J	8	ASN	2.7
2	J	146	ILE	2.7
2	D	246	ARG	2.7
1	L	2	GLU	2.7
2	F	72	LEU	2.7
2	H	40	LEU	2.7
1	A	152	VAL	2.7
2	N	136	PHE	2.7
2	N	104	ILE	2.7
2	D	268	SER	2.7
2	J	177	SER	2.7
2	D	120	LEU	2.7
2	H	91	GLY	2.7
2	J	162	ALA	2.7
1	B	17	VAL	2.7
1	B	200	PHE	2.7
1	M	22	ALA	2.7
2	H	42	SER	2.7
2	D	21	GLY	2.7
1	C	297	ASN	2.7
1	C	89	THR	2.7
1	L	162	ASN	2.7
1	C	9	VAL	2.7
1	B	278	THR	2.6
2	F	51	ILE	2.6
1	C	40	HIS	2.6
1	C	180	LEU	2.6
2	J	30	LEU	2.6
1	B	196	ARG	2.6
3	O	645	GLU	2.6
1	L	3	ASP	2.6
3	I	655	ASP	2.6
1	C	133	TYR	2.6
2	D	162	ALA	2.6
2	F	75	LEU	2.6
2	J	56	GLU	2.6
1	A	94	LEU	2.6
2	F	71	ASP	2.6
1	L	175	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	171	CYS	2.6
2	J	190	MET	2.6
2	N	101	LEU	2.6
2	J	61	ILE	2.6
1	M	174	ALA	2.6
2	J	75	LEU	2.6
2	F	189	ILE	2.6
1	A	74	GLY	2.6
2	F	102	GLU	2.6
2	J	72	LEU	2.6
2	J	89	PHE	2.6
1	C	338	SER	2.6
1	A	151	ILE	2.6
2	H	251	VAL	2.6
1	L	97	ALA	2.6
2	N	252	GLU	2.6
1	C	94	LEU	2.6
1	M	162	ASN	2.6
2	N	31	GLN	2.5
2	D	110	TYR	2.5
1	L	273	GLY	2.5
1	A	83	GLU	2.5
2	D	123	GLY	2.5
1	A	96	VAL	2.5
1	L	294	TYR	2.5
2	F	55	LEU	2.5
1	L	327	ILE	2.5
2	F	96	ARG	2.5
2	N	38	LEU	2.5
1	A	293	LEU	2.5
2	J	63	GLY	2.5
2	N	123	GLY	2.5
2	D	107	LEU	2.5
2	F	201	LEU	2.5
1	L	27	PRO	2.5
2	H	65	ILE	2.5
2	D	90	LEU	2.5
1	B	59	GLN	2.5
2	N	19	VAL	2.5
1	B	62	ARG	2.5
1	B	67	LEU	2.5
1	C	300	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	79	TRP	2.5
1	A	134	VAL	2.5
1	B	338	SER	2.5
1	L	5	THR	2.5
1	B	162	ASN	2.5
1	B	137	GLN	2.5
2	J	266	LEU	2.5
2	H	183	MET	2.5
2	J	159	LEU	2.5
1	C	107	GLU	2.5
1	M	105	LEU	2.5
2	N	89	PHE	2.5
1	L	331	ALA	2.5
1	A	77	THR	2.5
2	H	210	ASP	2.4
1	A	173	HIS	2.4
1	B	262	PHE	2.4
1	M	86	TRP	2.4
2	J	189	ILE	2.4
1	C	63	GLY	2.4
2	J	192	PRO	2.4
2	N	93	TYR	2.4
1	L	92	ASN	2.4
1	M	149	THR	2.4
1	M	278	THR	2.4
1	C	163	VAL	2.4
1	A	138	ALA	2.4
1	A	9	VAL	2.4
3	O	647	VAL	2.4
1	A	71	ILE	2.4
1	B	313	MET	2.4
1	C	153	LEU	2.4
1	M	163	VAL	2.4
2	F	190	MET	2.4
2	N	127	CYS	2.4
1	L	253	GLU	2.4
1	B	336	LYS	2.4
1	C	170	ALA	2.4
1	L	112	PRO	2.4
1	A	1	ASP	2.4
1	C	64	ILE	2.4
2	J	7	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	337	TYR	2.4
1	A	296	ASN	2.4
2	D	105	CYS	2.4
1	L	198	TYR	2.4
2	N	172	CYS	2.4
2	F	109	ALA	2.4
1	C	102	PRO	2.4
2	H	41	LYS	2.4
2	F	152	PHE	2.4
2	D	170	PHE	2.4
1	M	94	LEU	2.4
2	H	170	PHE	2.4
2	J	283	MET	2.4
3	O	643	PHE	2.4
1	M	101	HIS	2.4
1	L	309	ILE	2.4
2	F	180	LEU	2.4
2	J	9	ILE	2.3
1	B	320	LEU	2.3
1	L	238	LYS	2.3
2	J	144	TYR	2.3
1	B	155	SER	2.3
2	H	176	LEU	2.3
2	F	156	PHE	2.3
1	B	249	THR	2.3
2	D	244	ILE	2.3
2	D	183	MET	2.3
2	J	191	ARG	2.3
1	M	98	PRO	2.3
2	H	144	TYR	2.3
1	M	361	GLU	2.3
2	F	76	PHE	2.3
1	C	21	PHE	2.3
1	M	338	SER	2.3
1	C	4	GLU	2.3
1	A	79	TRP	2.3
1	A	304	THR	2.3
1	L	133	TYR	2.3
2	D	126	GLU	2.3
2	F	247	ALA	2.3
2	D	121	LEU	2.3
3	I	654	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	293	PHE	2.3
1	A	298	VAL	2.3
1	L	361	GLU	2.3
2	F	253	ASP	2.3
1	A	17	VAL	2.3
1	A	299	MET	2.3
1	L	340	TRP	2.3
2	H	30	LEU	2.3
1	C	282	ILE	2.3
1	C	82	MET	2.3
2	N	36	ARG	2.3
2	N	32	GLU	2.3
2	N	300	GLU	2.3
2	F	157	ASN	2.3
1	M	137	GLN	2.3
2	H	158	CYS	2.3
3	I	647	VAL	2.3
2	D	282	MET	2.3
2	H	43	ARG	2.3
2	J	37	GLY	2.3
1	L	278	THR	2.3
1	M	154	ASP	2.3
2	F	30	LEU	2.3
2	F	82	PRO	2.3
2	H	21	GLY	2.3
2	J	31	GLN	2.2
1	A	78	ASN	2.2
1	B	282	ILE	2.2
1	C	19	ALA	2.2
1	L	139	VAL	2.2
1	L	237	GLU	2.2
1	B	139	VAL	2.2
1	B	33	SER	2.2
1	M	348	SER	2.2
3	I	653	SER	2.2
2	F	170	PHE	2.2
1	C	150	GLY	2.2
2	D	300	GLU	2.2
2	N	250	VAL	2.2
1	A	200	PHE	2.2
1	C	362	TYR	2.2
1	L	37	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	236	LEU	2.2
2	N	186	ILE	2.2
1	C	361	GLU	2.2
2	F	78	TYR	2.2
1	M	313	MET	2.2
2	D	195	VAL	2.2
1	M	366	GLY	2.2
1	M	97	ALA	2.2
1	M	363	ASP	2.2
2	H	123	GLY	2.2
2	H	98	LYS	2.2
2	H	143	ARG	2.2
1	C	18	LYS	2.2
1	M	311	ASP	2.2
2	D	93	TYR	2.2
1	L	103	THR	2.2
1	L	282	ILE	2.2
2	J	38	LEU	2.2
3	G	648	THR	2.2
1	L	357	ILE	2.2
1	L	20	GLY	2.2
2	D	106	LEU	2.2
2	F	101	LEU	2.2
1	C	98	PRO	2.2
1	B	65	LEU	2.2
2	H	157	ASN	2.2
2	J	296	LEU	2.2
1	B	86	TRP	2.2
1	B	322	PRO	2.2
1	M	317	ILE	2.1
2	J	26	LYS	2.1
2	J	107	LEU	2.1
1	B	177	ARG	2.1
2	D	127	CYS	2.1
1	L	79	TRP	2.1
1	L	302	GLY	2.1
2	J	176	LEU	2.1
1	C	138	ALA	2.1
1	A	8	LEU	2.1
1	A	135	ALA	2.1
1	M	289	ILE	2.1
2	F	280	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	313	MET	2.1
2	F	54	GLU	2.1
3	I	652	ILE	2.1
1	C	175	ILE	2.1
2	H	281	ALA	2.1
2	J	183	MET	2.1
1	C	363	ASP	2.1
2	F	53	LEU	2.1
2	N	107	LEU	2.1
2	N	180	LEU	2.1
1	B	61	LYS	2.1
1	B	310	ALA	2.1
2	F	52	LEU	2.1
1	L	18	LYS	2.1
1	M	139	VAL	2.1
1	B	271	SER	2.1
1	L	115	ASN	2.1
2	H	169	ILE	2.1
2	H	189	ILE	2.1
1	A	34	ILE	2.1
1	C	5	THR	2.1
1	L	241	GLU	2.1
1	A	323	SER	2.1
1	L	301	GLY	2.1
1	M	321	ALA	2.1
2	J	93	TYR	2.1
1	A	119	MET	2.1
2	F	46	PHE	2.1
1	B	63	GLY	2.1
1	B	31	PHE	2.1
1	M	309	ILE	2.1
1	B	279	TYR	2.1
2	H	36	ARG	2.1
2	D	104	ILE	2.1
2	H	109	ALA	2.1
2	H	209	PRO	2.1
1	M	180	LEU	2.1
1	C	154	ASP	2.1
1	L	153	LEU	2.1
1	C	72	GLU	2.1
2	F	267	PHE	2.1
1	C	155	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	121	LEU	2.1
2	D	152	PHE	2.0
1	C	158	GLY	2.0
2	H	37	GLY	2.0
1	B	304	THR	2.0
1	M	5	THR	2.0
1	L	74	GLY	2.0
1	L	366	GLY	2.0
2	N	124	ASN	2.0
2	J	27	ASN	2.0
1	B	141	SER	2.0
2	F	81	PHE	2.0
1	C	78	ASN	2.0
2	N	75	LEU	2.0
2	N	140	CYS	2.0
2	J	28	VAL	2.0
1	B	3	ASP	2.0
2	J	147	LYS	2.0
1	A	271	SER	2.0
1	B	250	ILE	2.0
3	K	650	TYR	2.0
2	N	218	GLU	2.0
2	H	218	GLU	2.0
1	L	38	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	LAB	C	1376	27/27	0.69	0.66	2.07	253,258,268,271	0
4	LAB	A	1376	27/27	0.88	0.64	1.28	139,142,147,149	0
4	LAB	L	1376	27/27	0.81	0.57	1.17	303,322,330,334	0
4	LAB	B	1376	27/27	0.74	0.73	0.86	165,173,181,186	0
4	LAB	M	1376	27/27	0.83	0.37	0.77	321,332,340,340	0
5	ATP	A	1377	31/31	0.82	0.46	-0.14	135,137,142,143	0
5	ATP	C	1377	31/31	0.84	0.57	-0.34	242,246,249,250	0
5	ATP	B	1377	31/31	0.81	0.45	-0.38	155,160,163,164	0
5	ATP	L	1377	31/31	0.72	0.43	-0.57	290,306,327,332	0
5	ATP	M	1377	31/31	0.75	0.27	-0.72	334,341,360,361	0
6	MN	F	1302	1/1	0.71	0.24	-1.09	203,203,203,203	0
6	MN	J	1301	1/1	0.67	0.19	-1.17	200,200,200,200	0
6	MN	F	1301	1/1	0.77	0.21	-1.19	207,207,207,207	0
6	MN	J	1302	1/1	0.65	0.18	-1.38	197,197,197,197	0
6	MN	N	1302	1/1	0.74	0.17	-1.85	213,213,213,213	0
6	MN	D	1301	1/1	0.77	0.27	-1.89	166,166,166,166	0
6	MN	N	1301	1/1	0.73	0.15	-2.19	213,213,213,213	0
6	MN	H	1302	1/1	0.61	0.16	-2.71	230,230,230,230	0
6	MN	D	1302	1/1	0.68	0.19	-2.72	165,165,165,165	0
6	MN	H	1301	1/1	0.69	0.20	-2.93	234,234,234,234	0

6.5 Other polymers ⓘ

There are no such residues in this entry.