



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:41 am 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

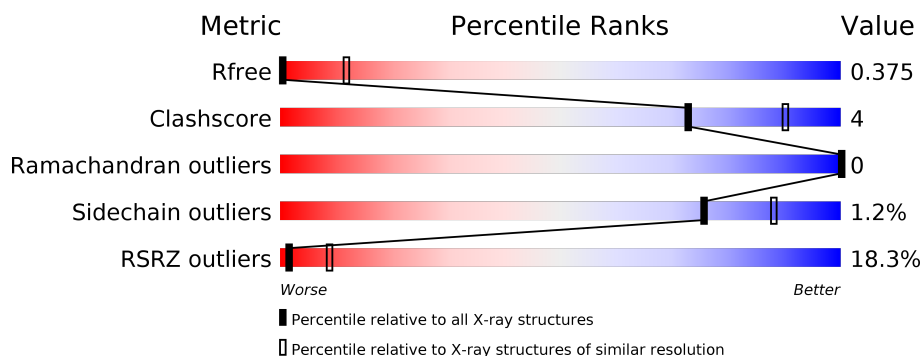
1 Overall quality at a glance

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}	100719	1100 (10.00-3.70)
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)
RSRZ outliers	101464	1004 (11.50-3.72)

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	
1	B	375	
1	C	375	
1	L	375	
1	M	375	
2	D	323	

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Mol	Chain	Length	Quality of chain
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			

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

There are 65 discrepancies between the modelled and reference sequences:

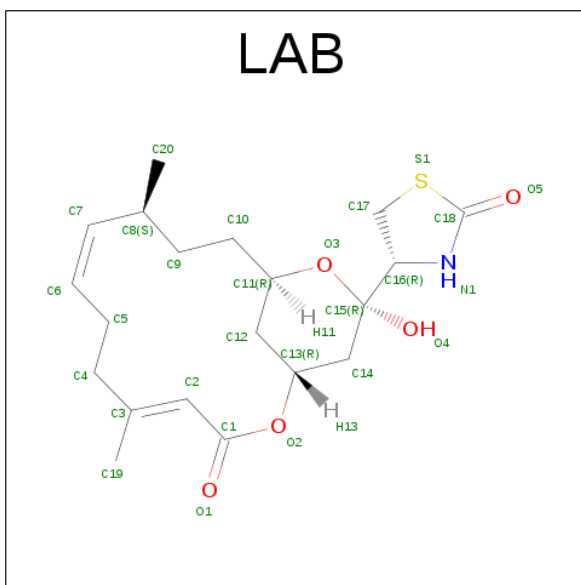
Chain	Residue	Modelled	Actual	Comment	Reference
E	626	GLY	-	EXPRESSION TAG	UNP Q5SWA1
E	627	ALA	-	EXPRESSION TAG	UNP Q5SWA1
E	628	MET	-	EXPRESSION TAG	UNP Q5SWA1
E	629	ASP	-	EXPRESSION TAG	UNP Q5SWA1
E	630	PRO	-	EXPRESSION TAG	UNP Q5SWA1
E	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
E	703	GLU	-	EXPRESSION TAG	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

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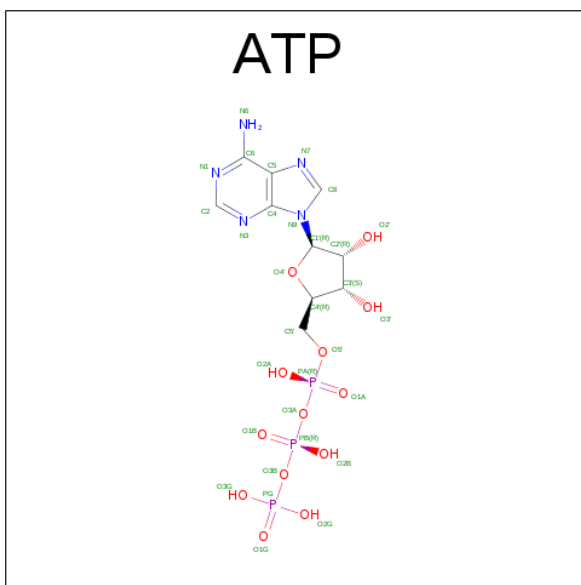
Chain	Residue	Modelled	Actual	Comment	Reference
I	702	LEU	-	EXPRESSION TAG	UNP Q5SWA1
I	703	GLU	-	EXPRESSION TAG	UNP Q5SWA1
I	704	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	705	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	706	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	707	HIS	-	EXPRESSION TAG	UNP Q5SWA1
I	708	HIS	-	EXPRESSION TAG	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	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

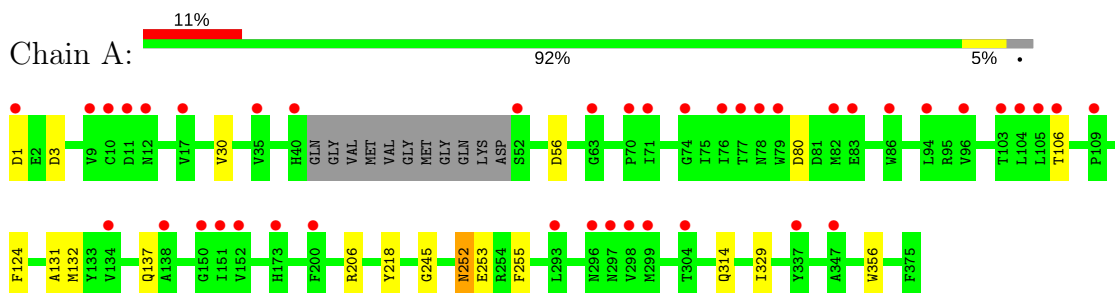
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

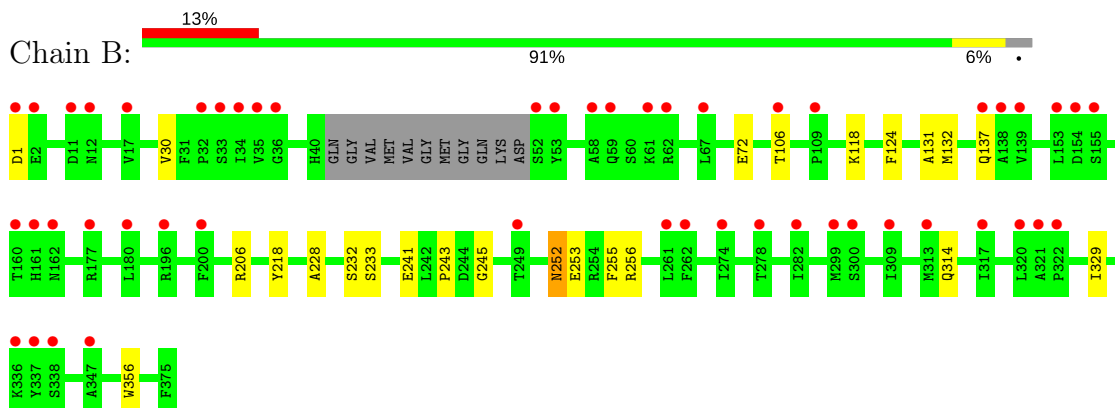
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

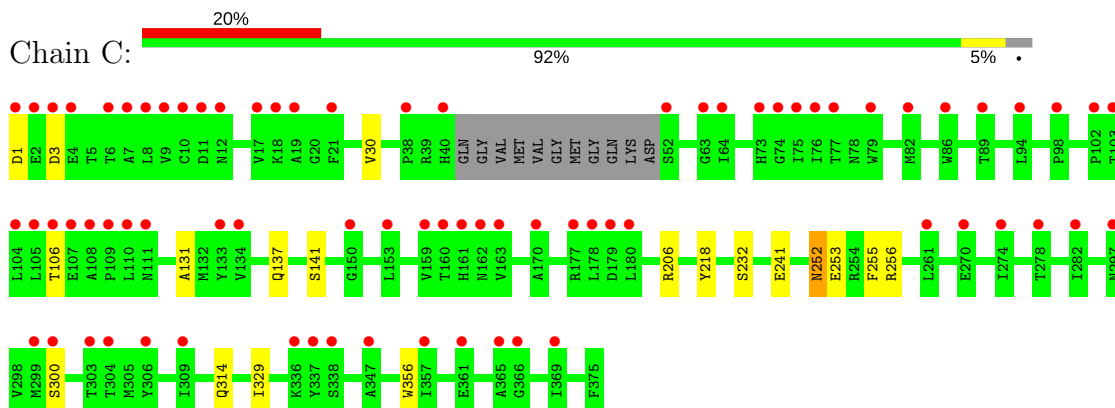
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



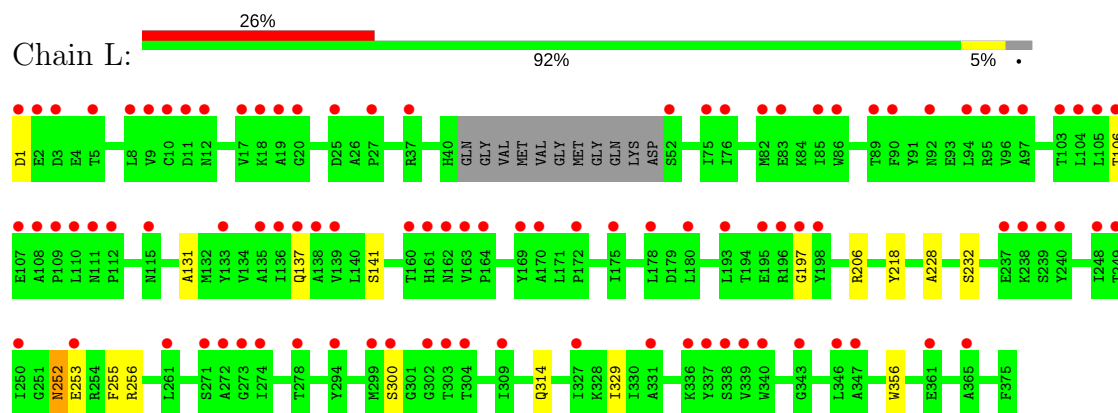
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



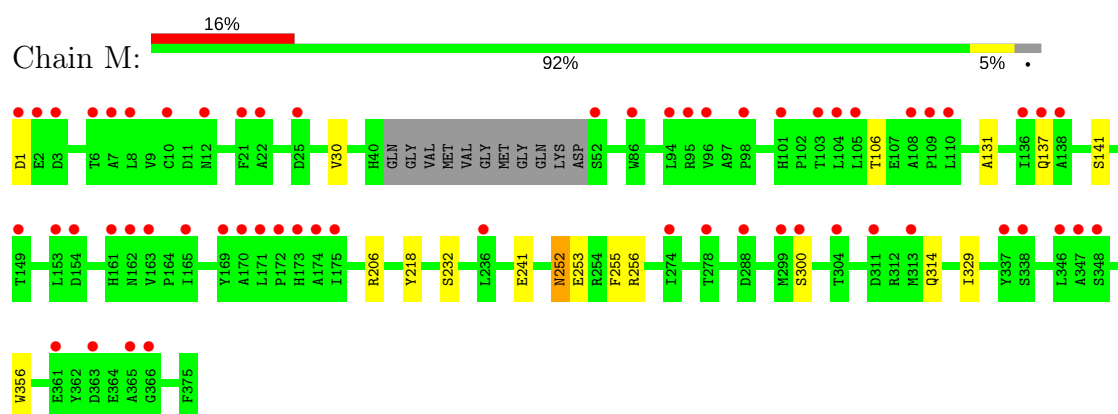
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



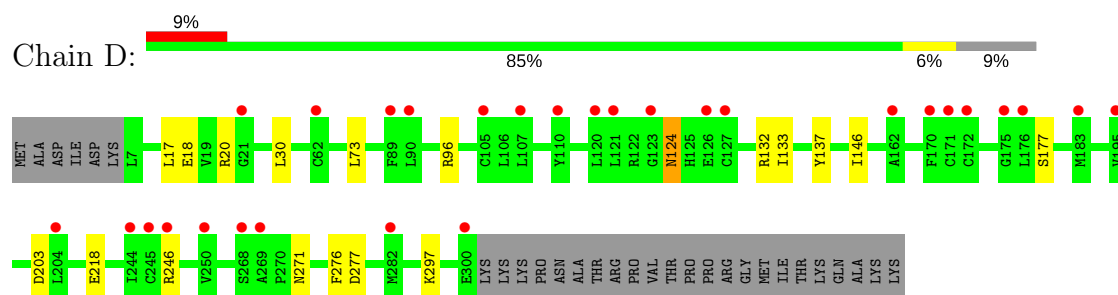
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



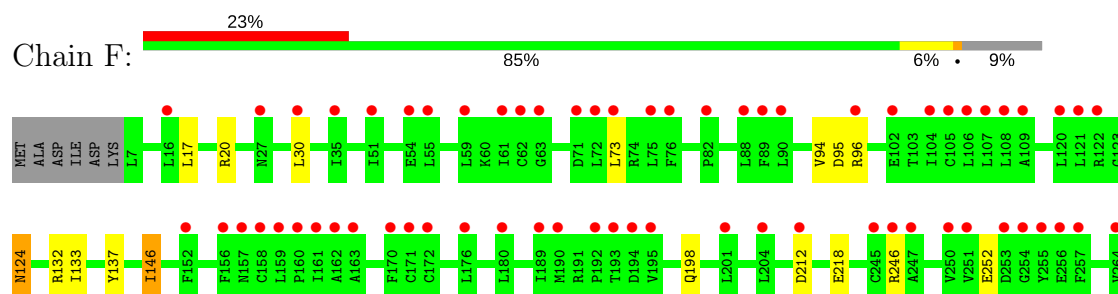
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

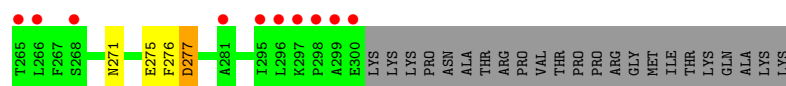


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

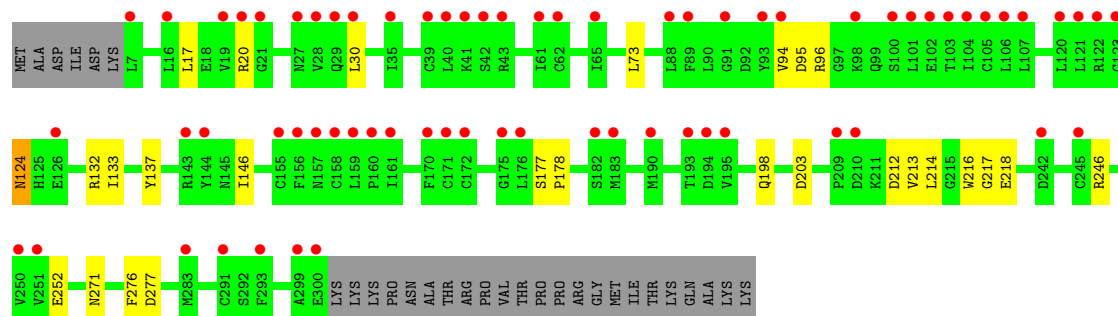
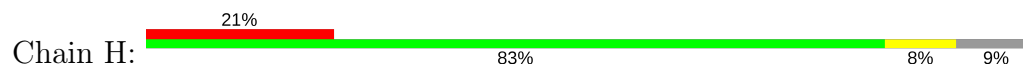


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

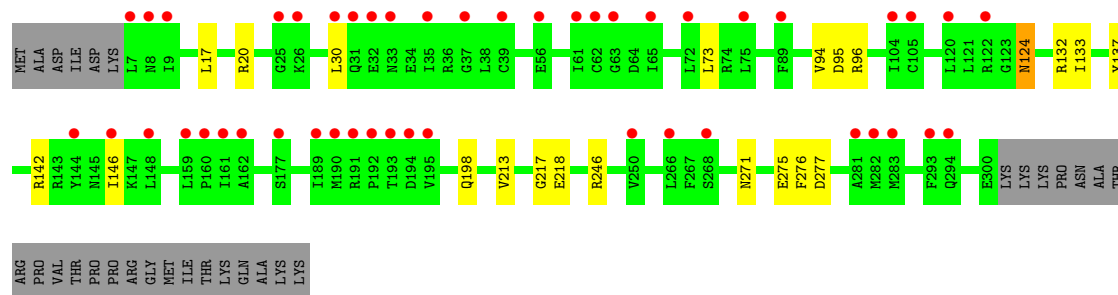
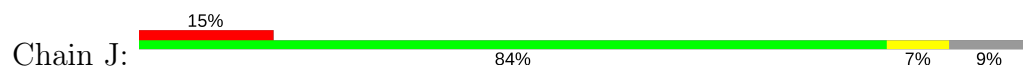




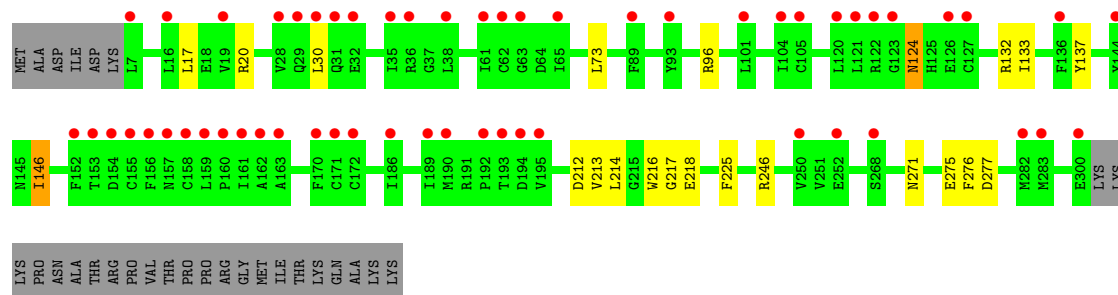
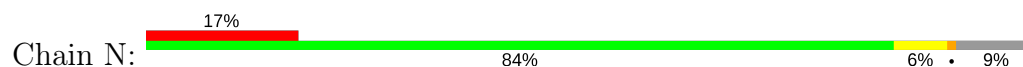
• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT



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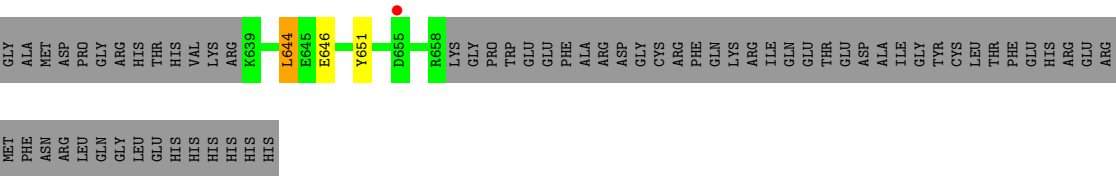


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

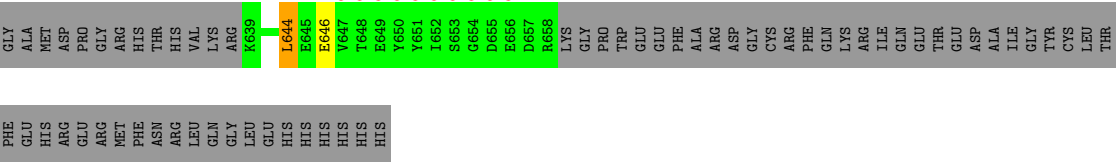


• Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B

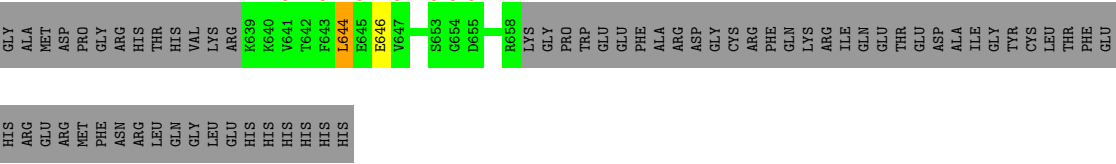




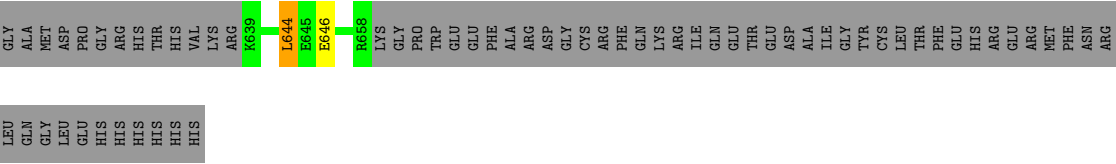
● Molecule 3: PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B



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● 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 , 456.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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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:D:297:LYS:HE2	3:E:651:TYR:OH	1.93	0.67
2:F:275:GLU:CB	2:H:216:TRP:O	2.41	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
2:F:17:LEU:O	2:F:20:ARG:NH1	2.32	0.63
1:C:1:ASP:CB	2:H:146:ILE:HD11	2.22	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:D:17:LEU:O	2:D:20:ARG:NH1	2.31	0.63
2:J:275:GLU:OE1	2:N:217:GLY:CA	2.46	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

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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
1:B:228:ALA:CB	2:H:178:PRO:HB2	2.39	0.53
2:J:217:GLY:HA2	2:N:275:GLU:OE1	2.09	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:HA	2:J:218:GLU:OE1	2.09	0.52
1:L:232:SER:HB3	2:N:225:PHE:HZ	1.75	0.52
2:J:217:GLY:HA2	2:N:275:GLU:CD	2.30	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:HA	2:D:218:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:277:ASP:CG	2:H:214:LEU:CB	2.82	0.47
1:C:1:ASP:CB	2:H:137:TYR:OH	2.59	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
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
2:F:275:GLU:CB	2:H:217:GLY:HA2	2.45	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
1:A:245:GLY:CA	1:B:30:VAL:O	2.64	0.46
2:J:213:VAL:HG23	2:N:275:GLU:O	2.16	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
1:A:314:GLN:OE1	1:A:329:ILE:HG12	2.18	0.44
2:J:132:ARG:NH2	2:J:133:ILE:HD11	2.33	0.44
1:L:314:GLN:OE1	1:L:329:ILE:HG12	2.18	0.44
2:N:132:ARG:HA	2:N:137:TYR:HB2	2.00	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
2:H:132:ARG:NH2	2:H:133:ILE:HD11	2.33	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:ASN:ND2	1:M:256:ARG:HH11	2.19	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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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%)	60	82
2	F	255/285 (90%)	250 (98%)	5 (2%)	60	82
2	H	255/285 (90%)	250 (98%)	5 (2%)	60	82
2	J	255/285 (90%)	250 (98%)	5 (2%)	60	82
2	N	255/285 (90%)	250 (98%)	5 (2%)	60	82
3	E	18/74 (24%)	17 (94%)	1 (6%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	18/74 (24%)	17 (94%)	1 (6%)	25	57
3	I	18/74 (24%)	17 (94%)	1 (6%)	25	57
3	K	18/74 (24%)	17 (94%)	1 (6%)	25	57
3	O	18/74 (24%)	17 (94%)	1 (6%)	25	57
All	All	2890/3385 (85%)	2855 (99%)	35 (1%)	75	88

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

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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	-	28,29,29	4.33	8 (28%)	35,41,41	3.97	10 (28%)
5	ATP	A	1377	-	27,33,33	1.41	4 (14%)	25,52,52	1.81	1 (4%)
4	LAB	B	1376	-	28,29,29	4.33	8 (28%)	35,41,41	3.97	10 (28%)
5	ATP	B	1377	-	27,33,33	1.43	4 (14%)	25,52,52	1.82	2 (8%)
4	LAB	C	1376	-	28,29,29	4.34	8 (28%)	35,41,41	3.96	10 (28%)
5	ATP	C	1377	-	27,33,33	1.42	4 (14%)	25,52,52	1.81	2 (8%)
4	LAB	L	1376	-	28,29,29	4.34	8 (28%)	35,41,41	3.98	10 (28%)
5	ATP	L	1377	-	27,33,33	1.42	4 (14%)	25,52,52	1.81	1 (4%)
4	LAB	M	1376	-	28,29,29	4.34	8 (28%)	35,41,41	3.97	10 (28%)
5	ATP	M	1377	-	27,33,33	1.41	4 (14%)	25,52,52	1.81	2 (8%)

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 (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1376	LAB	C17-S1	-8.24	1.64	1.80
4	C	1376	LAB	C17-S1	-8.21	1.64	1.80
4	M	1376	LAB	C17-S1	-8.17	1.64	1.80
4	A	1376	LAB	C17-S1	-8.17	1.64	1.80
4	L	1376	LAB	C17-S1	-8.15	1.64	1.80
4	B	1376	LAB	C14-C13	-5.90	1.40	1.51
4	A	1376	LAB	C14-C13	-5.88	1.40	1.51
4	L	1376	LAB	C14-C13	-5.86	1.40	1.51
4	C	1376	LAB	C14-C13	-5.84	1.40	1.51
4	M	1376	LAB	C14-C13	-5.80	1.40	1.51
5	B	1377	ATP	C2'-C3'	-4.31	1.42	1.53
5	C	1377	ATP	C2'-C3'	-4.31	1.42	1.53
5	L	1377	ATP	C2'-C3'	-4.31	1.42	1.53
5	A	1377	ATP	C2'-C3'	-4.29	1.42	1.53
5	M	1377	ATP	C2'-C3'	-4.28	1.42	1.53
4	A	1376	LAB	C18-S1	-3.94	1.68	1.78
4	B	1376	LAB	C18-S1	-3.92	1.68	1.78
4	M	1376	LAB	C18-S1	-3.91	1.69	1.78
4	L	1376	LAB	C18-S1	-3.91	1.69	1.78
4	C	1376	LAB	C18-S1	-3.89	1.69	1.78
5	M	1377	ATP	O4'-C4'	-2.09	1.40	1.45
5	B	1377	ATP	O4'-C4'	-2.07	1.40	1.45
5	C	1377	ATP	O4'-C4'	-2.07	1.40	1.45
5	L	1377	ATP	O4'-C4'	-2.06	1.40	1.45
5	A	1377	ATP	O4'-C4'	-2.05	1.40	1.45
5	M	1377	ATP	PG-O3B	2.14	1.63	1.60
5	A	1377	ATP	PG-O3B	2.17	1.63	1.60
5	C	1377	ATP	PG-O3B	2.17	1.63	1.60
5	L	1377	ATP	PG-O3B	2.20	1.63	1.60
5	B	1377	ATP	PG-O3B	2.20	1.63	1.60
5	M	1377	ATP	C6-N6	3.05	1.46	1.34
5	B	1377	ATP	C6-N6	3.06	1.46	1.34
5	L	1377	ATP	C6-N6	3.08	1.46	1.34
5	A	1377	ATP	C6-N6	3.08	1.46	1.34
5	C	1377	ATP	C6-N6	3.08	1.46	1.34
4	L	1376	LAB	C17-C16	3.45	1.59	1.53
4	A	1376	LAB	C17-C16	3.47	1.59	1.53
4	B	1376	LAB	C17-C16	3.49	1.59	1.53
4	C	1376	LAB	C17-C16	3.50	1.59	1.53
4	M	1376	LAB	C17-C16	3.52	1.59	1.53
4	M	1376	LAB	O5-C18	8.63	1.35	1.22
4	L	1376	LAB	O5-C18	8.64	1.35	1.22
4	A	1376	LAB	O5-C18	8.65	1.35	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1376	LAB	O5-C18	8.67	1.35	1.22
4	C	1376	LAB	O5-C18	8.70	1.35	1.22
4	B	1376	LAB	C16-N1	9.11	1.56	1.46
4	A	1376	LAB	C16-N1	9.12	1.56	1.46
4	C	1376	LAB	C16-N1	9.12	1.56	1.46
4	M	1376	LAB	C16-N1	9.16	1.56	1.46
4	L	1376	LAB	C16-N1	9.16	1.56	1.46
4	A	1376	LAB	C2-C3	10.04	1.53	1.33
4	B	1376	LAB	C2-C3	10.06	1.54	1.33
4	L	1376	LAB	C2-C3	10.06	1.54	1.33
4	C	1376	LAB	C2-C3	10.08	1.54	1.33
4	M	1376	LAB	C2-C3	10.09	1.54	1.33
4	B	1376	LAB	C18-N1	10.45	1.51	1.36
4	C	1376	LAB	C18-N1	10.61	1.51	1.36
4	A	1376	LAB	C18-N1	10.61	1.51	1.36
4	M	1376	LAB	C18-N1	10.62	1.51	1.36
4	L	1376	LAB	C18-N1	10.64	1.51	1.36

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1376	LAB	O5-C18-N1	-20.16	105.88	125.83
4	B	1376	LAB	O5-C18-N1	-20.13	105.91	125.83
4	A	1376	LAB	O5-C18-N1	-20.12	105.92	125.83
4	M	1376	LAB	O5-C18-N1	-20.11	105.93	125.83
4	C	1376	LAB	O5-C18-N1	-20.10	105.94	125.83
5	B	1377	ATP	N3-C2-N1	-7.52	122.31	128.86
5	M	1377	ATP	N3-C2-N1	-7.47	122.35	128.86
5	C	1377	ATP	N3-C2-N1	-7.46	122.36	128.86
5	A	1377	ATP	N3-C2-N1	-7.45	122.37	128.86
5	L	1377	ATP	N3-C2-N1	-7.45	122.37	128.86
4	M	1376	LAB	C19-C3-C2	-3.85	110.59	122.61
4	C	1376	LAB	C19-C3-C2	-3.85	110.59	122.61
4	L	1376	LAB	C19-C3-C2	-3.84	110.63	122.61
4	A	1376	LAB	C19-C3-C2	-3.83	110.65	122.61
4	B	1376	LAB	C19-C3-C2	-3.83	110.65	122.61
4	B	1376	LAB	C16-N1-C18	-3.14	108.66	113.28
4	L	1376	LAB	C16-N1-C18	-3.13	108.68	113.28
4	C	1376	LAB	C16-N1-C18	-3.12	108.69	113.28
4	M	1376	LAB	C16-N1-C18	-3.12	108.70	113.28
4	A	1376	LAB	C16-N1-C18	-3.11	108.71	113.28
4	L	1376	LAB	O1-C1-C2	-2.26	120.32	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1376	LAB	O1-C1-C2	-2.25	120.34	126.20
4	C	1376	LAB	O1-C1-C2	-2.24	120.37	126.20
4	A	1376	LAB	O1-C1-C2	-2.24	120.37	126.20
4	B	1376	LAB	O1-C1-C2	-2.24	120.37	126.20
4	B	1376	LAB	C19-C3-C4	-2.13	111.58	115.29
4	C	1376	LAB	C19-C3-C4	-2.13	111.59	115.29
4	L	1376	LAB	C19-C3-C4	-2.13	111.60	115.29
4	A	1376	LAB	C19-C3-C4	-2.12	111.61	115.29
4	M	1376	LAB	C19-C3-C4	-2.11	111.62	115.29
5	M	1377	ATP	C4-C5-N7	-2.04	107.44	109.41
5	B	1377	ATP	C4-C5-N7	-2.03	107.45	109.41
5	C	1377	ATP	C4-C5-N7	-2.02	107.46	109.41
4	L	1376	LAB	C5-C4-C3	2.60	121.73	112.93
4	B	1376	LAB	C5-C4-C3	2.60	121.73	112.93
4	A	1376	LAB	C5-C4-C3	2.60	121.74	112.93
4	M	1376	LAB	C5-C4-C3	2.61	121.77	112.93
4	C	1376	LAB	C5-C4-C3	2.62	121.79	112.93
4	B	1376	LAB	C16-C17-S1	2.76	110.09	105.97
4	M	1376	LAB	C16-C17-S1	2.77	110.11	105.97
4	L	1376	LAB	C16-C17-S1	2.79	110.14	105.97
4	A	1376	LAB	C16-C17-S1	2.79	110.14	105.97
4	C	1376	LAB	C16-C17-S1	2.81	110.17	105.97
4	C	1376	LAB	C10-C9-C8	2.90	118.80	113.90
4	M	1376	LAB	C10-C9-C8	2.93	118.84	113.90
4	B	1376	LAB	C10-C9-C8	2.93	118.85	113.90
4	L	1376	LAB	C10-C9-C8	2.94	118.85	113.90
4	A	1376	LAB	C10-C9-C8	2.95	118.87	113.90
4	A	1376	LAB	O2-C1-C2	3.23	119.21	111.43
4	C	1376	LAB	O2-C1-C2	3.23	119.22	111.43
4	B	1376	LAB	O2-C1-C2	3.24	119.24	111.43
4	L	1376	LAB	O2-C1-C2	3.24	119.25	111.43
4	M	1376	LAB	O2-C1-C2	3.25	119.28	111.43
4	C	1376	LAB	C17-S1-C18	7.18	95.83	92.00
4	L	1376	LAB	C17-S1-C18	7.21	95.85	92.00
4	B	1376	LAB	C17-S1-C18	7.22	95.86	92.00
4	A	1376	LAB	C17-S1-C18	7.25	95.87	92.00
4	M	1376	LAB	C17-S1-C18	7.32	95.91	92.00

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 [i](#)

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%)	0.86	42 (11%) 5 13	237, 303, 352, 385	0
1	B	364/375 (97%)	1.00	50 (13%) 3 11	252, 327, 380, 404	0
1	C	364/375 (97%)	1.26	76 (20%) 1 8	356, 410, 453, 502	0
1	L	364/375 (97%)	1.44	96 (26%) 1 7	403, 490, 565, 619	0
1	M	364/375 (97%)	0.99	59 (16%) 2 9	454, 521, 589, 621	0
2	D	294/323 (91%)	0.75	29 (9%) 8 15	232, 291, 334, 368	0
2	F	294/323 (91%)	1.28	75 (25%) 1 7	303, 364, 419, 450	0
2	H	294/323 (91%)	1.24	68 (23%) 1 7	311, 382, 436, 457	0
2	J	294/323 (91%)	0.93	47 (15%) 2 10	303, 367, 432, 478	0
2	N	294/323 (91%)	1.06	56 (19%) 1 8	285, 372, 419, 450	0
3	E	20/84 (23%)	0.74	1 (5%) 30 32	446, 573, 869, 969	0
3	G	20/84 (23%)	2.22	10 (50%) 0 4	497, 563, 717, 732	0
3	I	20/84 (23%)	1.88	7 (35%) 0 5	583, 761, 1000, 1000	0
3	K	20/84 (23%)	0.78	1 (5%) 30 32	471, 544, 652, 721	0
3	O	20/84 (23%)	0.77	4 (20%) 1 8	644, 682, 763, 789	0
All	All	3390/3910 (86%)	1.09	621 (18%) 1 9	232, 377, 559, 1000	0

All (621) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	PRO	14.4
1	L	108	ALA	11.8
2	N	194	ASP	10.8
1	C	10	CYS	9.5
2	D	172	CYS	9.2
1	M	109	PRO	8.7
2	F	265	THR	8.6

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Mol	Chain	Res	Type	RSRZ
1	C	12	ASN	7.7
2	N	193	THR	7.7
2	F	172	CYS	7.4
1	M	2	GLU	7.0
2	J	194	ASP	7.0
2	H	28	VAL	6.9
1	L	137	GLN	6.6
1	C	11	ASP	6.3
2	F	266	LEU	6.3
1	L	110	LEU	6.2
1	L	136	ILE	6.2
1	C	109	PRO	6.1
1	C	74	GLY	6.1
1	L	96	VAL	6.1
1	M	6	THR	6.0
2	F	62	CYS	6.0
1	C	1	ASP	6.0
2	F	105	CYS	5.9
1	C	105	LEU	5.9
1	L	239	SER	5.9
1	L	10	CYS	5.8
2	F	162	ALA	5.8
2	F	63	GLY	5.7
1	C	2	GLU	5.6
2	F	161	ILE	5.6
2	F	171	CYS	5.5
2	N	157	ASN	5.5
1	M	7	ALA	5.5
1	L	111	ASN	5.4
2	F	163	ALA	5.4
2	H	194	ASP	5.4
1	L	12	ASN	5.4
1	L	107	GLU	5.3
1	L	86	TRP	5.2
3	G	649	GLU	5.2
2	H	93	TYR	5.2
2	F	250	VAL	5.1
1	M	108	ALA	5.1
2	H	104	ILE	5.1
2	F	268	SER	5.1
1	M	138	ALA	5.0
1	L	82	MET	5.0

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Mol	Chain	Res	Type	RSRZ
2	F	245	CYS	5.0
2	F	90	LEU	5.0
3	I	643	PHE	5.0
2	H	250	VAL	5.0
2	N	161	ILE	5.0
1	L	94	LEU	5.0
1	L	271	SER	5.0
2	H	105	CYS	5.0
2	F	300	GLU	4.9
1	C	76	ILE	4.9
1	M	96	VAL	4.9
2	H	94	VAL	4.8
1	C	179	ASP	4.8
2	F	299	ALA	4.8
2	J	193	THR	4.8
2	J	250	VAL	4.8
1	B	138	ALA	4.8
2	H	172	CYS	4.8
3	G	650	TYR	4.8
1	A	150	GLY	4.8
2	H	120	LEU	4.7
2	N	122	ARG	4.7
2	F	61	ILE	4.7
2	F	160	PRO	4.7
2	H	29	GLN	4.7
2	F	297	LYS	4.7
1	C	7	ALA	4.6
2	N	105	CYS	4.6
1	B	12	ASN	4.6
2	H	195	VAL	4.6
1	L	197	GLY	4.5
1	L	90	PHE	4.5
2	H	101	LEU	4.5
1	C	75	ILE	4.5
2	D	171	CYS	4.5
1	B	109	PRO	4.5
2	H	100	SER	4.4
1	A	12	ASN	4.4
1	M	103	THR	4.4
1	B	36	GLY	4.4
2	N	62	CYS	4.4
1	L	106	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	N	28	VAL	4.4
1	M	172	PRO	4.4
1	L	248	ILE	4.3
2	F	104	ILE	4.3
2	H	175	GLY	4.3
1	L	170	ALA	4.3
2	F	255	TYR	4.3
1	L	337	TYR	4.3
2	D	245	CYS	4.3
2	J	35	ILE	4.3
1	L	76	ILE	4.3
2	N	171	CYS	4.3
1	C	161	HIS	4.3
1	L	89	THR	4.3
2	N	126	GLU	4.3
1	C	177	ARG	4.3
1	L	196	ARG	4.3
3	G	651	TYR	4.2
2	H	122	ARG	4.2
3	G	654	GLY	4.2
2	N	195	VAL	4.2
1	L	8	LEU	4.2
2	F	256	GLU	4.2
2	F	193	THR	4.2
1	C	160	THR	4.2
1	M	8	LEU	4.2
1	C	178	LEU	4.2
1	L	52	SER	4.1
2	N	156	PHE	4.1
2	H	193	THR	4.1
2	N	162	ALA	4.1
1	C	8	LEU	4.1
2	F	195	VAL	4.1
1	L	178	LEU	4.1
1	B	161	HIS	4.1
3	G	652	ILE	4.0
2	H	121	LEU	4.0
1	L	195	GLU	4.0
1	M	299	MET	4.0
1	L	11	ASP	4.0
1	B	1	ASP	4.0
1	M	173	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	27	ASN	4.0
1	A	52	SER	4.0
2	F	106	LEU	3.9
1	M	347	ALA	3.9
1	C	77	THR	3.9
3	G	653	SER	3.9
2	N	192	PRO	3.9
2	H	39	CYS	3.9
2	N	29	GLN	3.9
2	N	30	LEU	3.9
1	L	365	ALA	3.8
1	B	52	SER	3.8
1	C	106	THR	3.8
1	C	52	SER	3.8
1	C	104	LEU	3.8
1	M	10	CYS	3.8
1	M	365	ALA	3.8
1	C	365	ALA	3.8
1	M	153	LEU	3.8
1	L	300	SER	3.7
2	J	282	MET	3.7
1	M	170	ALA	3.7
1	L	303	THR	3.7
1	L	304	THR	3.7
1	M	288	ASP	3.7
1	A	76	ILE	3.7
2	N	163	ALA	3.7
2	J	268	SER	3.7
1	L	180	LEU	3.7
1	C	366	GLY	3.7
1	M	21	PHE	3.6
1	M	300	SER	3.6
2	N	152	PHE	3.6
1	C	73	HIS	3.6
1	M	337	TYR	3.6
1	M	304	THR	3.6
1	L	104	LEU	3.6
1	B	35	VAL	3.6
2	F	296	LEU	3.6
2	F	264	VAL	3.6
3	I	641	VAL	3.6
2	F	257	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	304	THR	3.6
2	N	268	SER	3.6
1	C	303	THR	3.6
1	C	103	THR	3.6
3	K	639	LYS	3.6
1	L	17	VAL	3.6
1	C	309	ILE	3.6
1	M	104	LEU	3.5
2	F	89	PHE	3.5
2	H	245	CYS	3.5
2	N	155	CYS	3.5
2	H	7	LEU	3.5
2	J	161	ILE	3.5
1	A	70	PRO	3.5
1	L	19	ALA	3.5
1	L	274	ILE	3.5
2	N	283	MET	3.5
1	L	250	ILE	3.5
1	B	2	GLU	3.5
1	B	337	TYR	3.5
1	B	300	SER	3.5
2	F	251	VAL	3.5
1	A	106	THR	3.4
2	N	35	ILE	3.4
1	L	25	ASP	3.4
1	M	1	ASP	3.4
1	A	35	VAL	3.4
1	L	95	ARG	3.4
2	F	281	ALA	3.4
2	H	156	PHE	3.4
1	L	9	VAL	3.4
2	F	158	CYS	3.4
2	H	103	THR	3.4
1	B	154	ASP	3.4
1	L	339	VAL	3.3
2	J	65	ILE	3.3
1	C	337	TYR	3.3
1	L	249	THR	3.3
3	G	655	ASP	3.3
1	M	3	ASP	3.3
2	H	102	GLU	3.3
2	F	194	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	246	ARG	3.3
2	N	189	ILE	3.3
2	H	89	PHE	3.3
1	M	171	LEU	3.3
2	H	291	CYS	3.2
2	H	299	ALA	3.2
1	L	138	ALA	3.2
2	F	120	LEU	3.2
2	J	105	CYS	3.2
1	A	10	CYS	3.2
2	N	16	LEU	3.2
1	A	40	HIS	3.2
3	G	656	GLU	3.2
1	C	6	THR	3.2
1	L	193	LEU	3.2
2	N	153	THR	3.2
1	L	163	VAL	3.2
2	J	62	CYS	3.2
1	B	153	LEU	3.2
1	L	1	ASP	3.2
1	M	346	LEU	3.2
2	N	7	LEU	3.2
2	F	27	ASN	3.2
2	N	61	ILE	3.2
2	F	295	ILE	3.2
2	N	190	MET	3.2
2	D	175	GLY	3.1
1	L	299	MET	3.1
1	M	95	ARG	3.1
1	A	105	LEU	3.1
2	H	88	LEU	3.1
1	M	169	TYR	3.1
1	M	274	ILE	3.1
1	B	53	TYR	3.1
2	N	159	LEU	3.1
3	G	647	VAL	3.1
2	N	282	MET	3.1
1	L	161	HIS	3.1
1	L	240	TYR	3.1
2	N	144	TYR	3.1
1	C	299	MET	3.1
1	M	110	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	35	ILE	3.1
2	H	160	PRO	3.1
2	F	107	LEU	3.1
1	L	164	PRO	3.1
2	F	212	ASP	3.1
2	J	195	VAL	3.1
2	J	32	GLU	3.1
1	A	109	PRO	3.1
1	B	11	ASP	3.1
1	L	336	LYS	3.1
1	M	175	ILE	3.1
2	J	294	GLN	3.0
1	L	272	ALA	3.0
1	C	278	THR	3.0
2	F	122	ARG	3.0
2	F	192	PRO	3.0
2	J	160	PRO	3.0
1	A	297	ASN	3.0
1	C	3	ASP	3.0
1	C	347	ALA	3.0
2	D	250	VAL	3.0
1	B	180	LEU	3.0
1	C	274	ILE	3.0
1	B	34	ILE	3.0
1	L	85	ILE	3.0
2	H	159	LEU	3.0
1	B	32	PRO	3.0
2	J	293	PHE	3.0
1	C	108	ALA	3.0
2	N	170	PHE	3.0
2	H	283	MET	3.0
2	H	155	CYS	2.9
2	H	20	ARG	2.9
1	L	83	GLU	2.9
2	F	88	LEU	2.9
3	E	655	ASP	2.9
2	J	148	LEU	2.9
2	J	122	ARG	2.9
2	F	108	LEU	2.9
1	C	336	LYS	2.9
1	C	110	LEU	2.9
1	A	104	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	16	LEU	2.9
1	L	169	TYR	2.9
1	A	11	ASP	2.9
2	N	120	LEU	2.9
2	H	62	CYS	2.9
2	H	161	ILE	2.9
1	B	309	ILE	2.8
3	I	645	GLU	2.8
2	H	190	MET	2.8
1	C	162	ASN	2.8
1	A	82	MET	2.8
2	D	176	LEU	2.8
2	N	160	PRO	2.8
2	D	204	LEU	2.8
2	J	25	GLY	2.8
1	L	172	PRO	2.8
2	F	204	LEU	2.8
2	N	158	CYS	2.8
2	N	121	LEU	2.8
2	F	298	PRO	2.8
2	J	120	LEU	2.8
3	O	641	VAL	2.8
2	H	300	GLU	2.8
2	D	89	PHE	2.8
1	C	270	GLU	2.8
2	H	242	ASP	2.8
1	C	38	PRO	2.7
1	L	135	ALA	2.7
2	H	16	LEU	2.7
1	L	75	ILE	2.7
1	A	86	TRP	2.7
2	H	182	SER	2.7
1	L	160	THR	2.7
2	N	154	ASP	2.7
2	D	62	CYS	2.7
2	F	254	GLY	2.7
1	B	58	ALA	2.7
1	C	134	VAL	2.7
1	M	12	ASN	2.7
1	C	357	ILE	2.7
2	F	73	LEU	2.7
2	J	33	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	160	THR	2.7
1	M	52	SER	2.7
2	F	159	LEU	2.7
2	J	39	CYS	2.7
1	L	338	SER	2.7
1	M	161	HIS	2.7
2	H	126	GLU	2.7
1	B	274	ILE	2.7
2	F	121	LEU	2.7
2	J	281	ALA	2.7
1	B	347	ALA	2.7
1	C	111	ASN	2.7
1	M	165	ILE	2.7
1	C	17	VAL	2.7
2	N	65	ILE	2.7
1	B	321	ALA	2.7
2	N	63	GLY	2.7
1	C	159	VAL	2.7
1	C	86	TRP	2.6
2	H	19	VAL	2.6
2	J	8	ASN	2.6
1	C	369	ILE	2.6
1	M	25	ASP	2.6
1	L	343	GLY	2.6
1	B	299	MET	2.6
1	L	105	LEU	2.6
1	L	347	ALA	2.6
1	M	136	ILE	2.6
2	D	246	ARG	2.6
1	C	261	LEU	2.6
2	F	35	ILE	2.6
1	B	261	LEU	2.6
1	L	2	GLU	2.6
1	B	106	THR	2.6
2	D	269	ALA	2.6
1	A	63	GLY	2.6
2	D	268	SER	2.6
2	J	177	SER	2.6
1	C	297	ASN	2.6
2	F	176	LEU	2.6
1	L	162	ASN	2.6
2	F	59	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	42	SER	2.6
1	L	261	LEU	2.6
1	B	317	ILE	2.6
1	A	103	THR	2.6
2	H	106	LEU	2.6
1	A	152	VAL	2.5
1	L	346	LEU	2.5
2	H	107	LEU	2.5
2	H	61	ILE	2.5
1	B	196	ARG	2.5
2	J	104	ILE	2.5
2	H	91	GLY	2.5
2	H	171	CYS	2.5
1	C	306	TYR	2.5
2	N	136	PHE	2.5
1	B	17	VAL	2.5
2	J	146	ILE	2.5
2	D	21	GLY	2.5
1	B	200	PHE	2.5
2	F	72	LEU	2.5
2	H	40	LEU	2.5
3	O	645	GLU	2.5
2	N	104	ILE	2.5
1	A	347	ALA	2.5
1	C	9	VAL	2.5
2	D	120	LEU	2.5
1	L	3	ASP	2.5
3	I	655	ASP	2.5
1	C	89	THR	2.5
1	C	40	HIS	2.5
2	J	56	GLU	2.5
1	B	278	THR	2.5
1	M	162	ASN	2.5
2	F	71	ASP	2.5
1	C	338	SER	2.4
1	L	27	PRO	2.4
2	F	102	GLU	2.4
2	N	31	GLN	2.4
2	F	51	ILE	2.4
2	J	162	ALA	2.4
2	N	252	GLU	2.4
2	J	190	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	180	LEU	2.4
2	J	30	LEU	2.4
1	M	22	ALA	2.4
2	F	96	ARG	2.4
1	A	74	GLY	2.4
1	A	83	GLU	2.4
2	H	251	VAL	2.4
1	B	62	ARG	2.4
1	A	94	LEU	2.4
2	F	75	LEU	2.4
1	B	162	ASN	2.4
1	B	59	GLN	2.4
1	L	175	ILE	2.4
2	J	89	PHE	2.4
2	N	101	LEU	2.4
1	L	273	GLY	2.4
2	J	61	ILE	2.4
1	A	96	VAL	2.4
1	C	300	SER	2.4
2	D	123	GLY	2.4
2	F	189	ILE	2.4
2	J	75	LEU	2.4
2	J	192	PRO	2.4
2	J	72	LEU	2.4
1	B	338	SER	2.4
1	A	151	ILE	2.4
2	J	63	GLY	2.4
2	N	123	GLY	2.4
1	B	137	GLN	2.4
2	N	127	CYS	2.4
1	B	336	LYS	2.3
1	C	94	LEU	2.3
1	L	92	ASN	2.3
1	C	133	TYR	2.3
1	L	112	PRO	2.3
2	D	162	ALA	2.3
2	N	19	VAL	2.3
1	C	107	GLU	2.3
2	F	55	LEU	2.3
2	D	105	CYS	2.3
1	L	327	ILE	2.3
2	N	172	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	2.3
1	M	174	ALA	2.3
1	A	293	LEU	2.3
2	H	210	ASP	2.3
2	N	38	LEU	2.3
2	H	65	ILE	2.3
2	D	107	LEU	2.3
2	F	201	LEU	2.3
2	H	41	LYS	2.3
1	A	296	ASN	2.3
2	H	183	MET	2.3
1	C	102	PRO	2.3
2	D	90	LEU	2.3
1	L	97	ALA	2.3
1	L	5	THR	2.3
1	B	67	LEU	2.3
1	A	173	HIS	2.3
1	L	238	LYS	2.3
1	L	253	GLU	2.3
1	C	63	GLY	2.3
2	D	110	TYR	2.3
2	N	89	PHE	2.3
1	B	262	PHE	2.3
1	C	163	VAL	2.3
1	A	9	VAL	2.3
1	A	77	THR	2.3
1	L	294	TYR	2.3
2	J	266	LEU	2.3
3	O	647	VAL	2.3
1	A	1	ASP	2.3
2	J	159	LEU	2.3
1	B	313	MET	2.3
1	M	98	PRO	2.3
1	M	163	VAL	2.3
1	C	79	TRP	2.3
1	M	105	LEU	2.3
1	M	149	THR	2.3
1	M	278	THR	2.3
2	F	190	MET	2.3
2	J	189	ILE	2.2
1	A	71	ILE	2.2
2	J	191	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	155	SER	2.2
1	M	86	TRP	2.2
1	C	153	LEU	2.2
1	M	361	GLU	2.2
1	C	64	ILE	2.2
1	L	331	ALA	2.2
1	M	338	SER	2.2
2	F	152	PHE	2.2
2	H	158	CYS	2.2
2	J	7	LEU	2.2
2	J	283	MET	2.2
1	M	101	HIS	2.2
2	D	170	PHE	2.2
1	C	4	GLU	2.2
2	H	170	PHE	2.2
3	O	643	PHE	2.2
1	A	138	ALA	2.2
2	D	126	GLU	2.2
2	F	82	PRO	2.2
2	F	157	ASN	2.2
2	N	93	TYR	2.2
2	D	183	MET	2.2
1	L	361	GLU	2.2
2	N	36	ARG	2.2
2	F	156	PHE	2.2
1	M	94	LEU	2.2
1	B	249	THR	2.2
1	L	309	ILE	2.2
2	F	253	ASP	2.2
1	C	170	ALA	2.2
2	F	180	LEU	2.2
2	H	43	ARG	2.2
2	J	9	ILE	2.2
1	M	137	GLN	2.2
1	A	78	ASN	2.2
2	F	76	PHE	2.2
1	B	320	LEU	2.2
1	C	21	PHE	2.2
2	N	32	GLU	2.2
2	N	300	GLU	2.2
1	A	17	VAL	2.1
1	A	298	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	654	GLY	2.1
2	H	176	LEU	2.1
2	D	244	ILE	2.1
1	A	299	MET	2.1
1	A	304	THR	2.1
1	A	337	TYR	2.1
2	F	109	ALA	2.1
2	J	31	GLN	2.1
2	H	293	PHE	2.1
1	L	198	TYR	2.1
2	H	98	LYS	2.1
1	C	82	MET	2.1
1	C	18	LYS	2.1
1	M	154	ASP	2.1
3	I	647	VAL	2.1
1	B	33	SER	2.1
1	M	348	SER	2.1
2	D	121	LEU	2.1
3	I	653	SER	2.1
1	L	237	GLU	2.1
2	D	282	MET	2.1
2	J	37	GLY	2.1
1	L	37	ARG	2.1
2	H	21	GLY	2.1
2	H	30	LEU	2.1
1	A	79	TRP	2.1
1	C	98	PRO	2.1
2	D	300	GLU	2.1
2	J	26	LYS	2.1
1	C	282	ILE	2.1
2	J	144	TYR	2.1
1	B	322	PRO	2.1
1	B	139	VAL	2.1
1	L	139	VAL	2.1
1	L	278	THR	2.1
2	D	127	CYS	2.1
2	H	143	ARG	2.1
1	C	361	GLU	2.1
2	H	144	TYR	2.1
2	H	157	ASN	2.1
1	L	340	TRP	2.1
2	F	247	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	250	VAL	2.1
1	C	150	GLY	2.1
2	F	30	LEU	2.1
1	L	133	TYR	2.1
1	M	363	ASP	2.1
2	F	170	PHE	2.1
1	B	61	LYS	2.1
1	B	282	ILE	2.1
1	L	18	LYS	2.1
2	D	195	VAL	2.1
1	M	366	GLY	2.1
1	B	177	ARG	2.0
1	M	311	ASP	2.0
1	M	313	MET	2.0
1	A	200	PHE	2.0
2	H	123	GLY	2.0
2	N	186	ILE	2.0
1	L	20	GLY	2.0
1	L	115	ASN	2.0
1	M	236	LEU	2.0
1	L	103	THR	2.0
2	F	54	GLU	2.0
3	G	648	THR	2.0
1	C	19	ALA	2.0
2	H	209	PRO	2.0
1	L	302	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	1.27	139,142,147,149	0
4	LAB	L	1376	27/27	0.81	0.57	1.18	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.