



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:44 am GMT

PDB ID : 3MX5
Title : Lassa fever virus nucleoprotein complexed with UTP
Authors : Qi, X.; Lan, S.; Wang, W.; Schelde, L.M.; Dong, H.; Wallat, G.; Liang, Y.;
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Deposited on : 2010-05-06
Resolution : 1.90 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

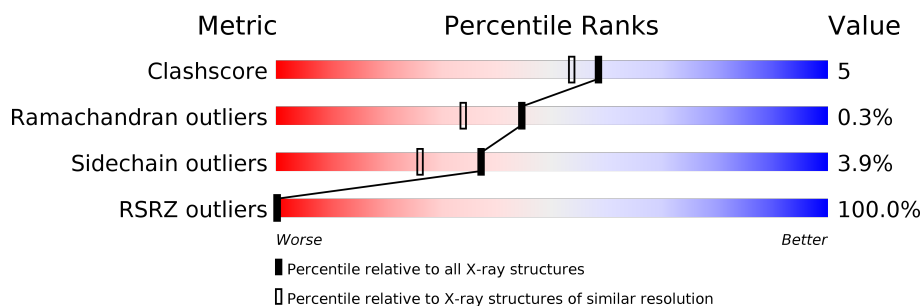
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	577	<div> <div>89%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	577	<div> <div>89%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	577	<div> <div>89%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>

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
2	UTP	A	993	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UTP	B	993	-	-	-	X
2	UTP	C	993	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12276 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4038	2536	702	773	27			
1	B	515	Total	C	N	O	S	0	0	0
			4027	2528	701	771	27			
1	C	512	Total	C	N	O	S	0	0	0
			4006	2517	697	765	27			

There are 24 discrepancies between the modelled and reference sequences:

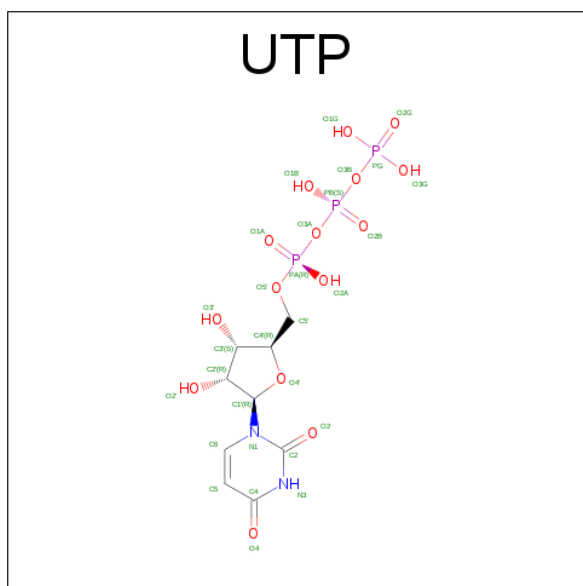
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13699
A	-6	ALA	-	EXPRESSION TAG	UNP P13699
A	-5	MET	-	EXPRESSION TAG	UNP P13699
A	-4	ASP	-	EXPRESSION TAG	UNP P13699
A	-3	HIS	-	EXPRESSION TAG	UNP P13699
A	-2	VAL	-	EXPRESSION TAG	UNP P13699
A	-1	GLU	-	EXPRESSION TAG	UNP P13699
A	0	PHE	-	EXPRESSION TAG	UNP P13699
B	-7	GLY	-	EXPRESSION TAG	UNP P13699
B	-6	ALA	-	EXPRESSION TAG	UNP P13699
B	-5	MET	-	EXPRESSION TAG	UNP P13699
B	-4	ASP	-	EXPRESSION TAG	UNP P13699
B	-3	HIS	-	EXPRESSION TAG	UNP P13699
B	-2	VAL	-	EXPRESSION TAG	UNP P13699
B	-1	GLU	-	EXPRESSION TAG	UNP P13699
B	0	PHE	-	EXPRESSION TAG	UNP P13699
C	-7	GLY	-	EXPRESSION TAG	UNP P13699
C	-6	ALA	-	EXPRESSION TAG	UNP P13699
C	-5	MET	-	EXPRESSION TAG	UNP P13699
C	-4	ASP	-	EXPRESSION TAG	UNP P13699
C	-3	HIS	-	EXPRESSION TAG	UNP P13699
C	-2	VAL	-	EXPRESSION TAG	UNP P13699
C	-1	GLU	-	EXPRESSION TAG	UNP P13699

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PHE	-	EXPRESSION TAG	UNP P13699

- Molecule 2 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

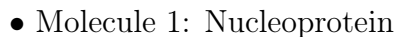
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

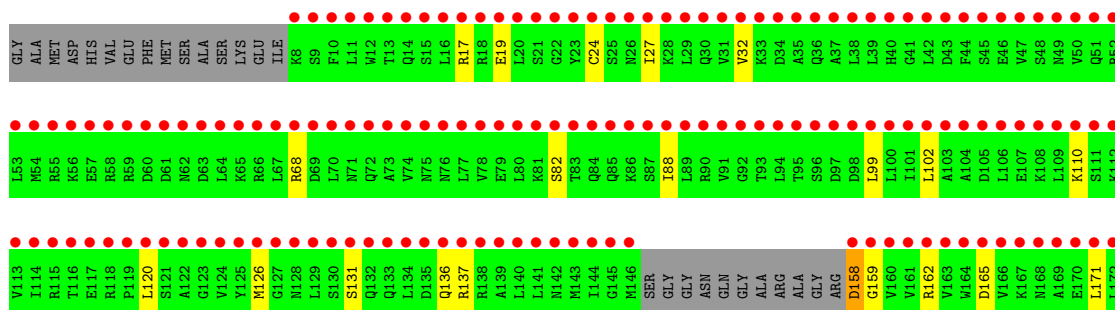
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	50	Total 50	O 50	0	0
4	C	29	Total 29	O 29	0	0

89% 77% 11% 11%



Category	Percentage
Very bad	89%
Bad	73%
Good	14%
Very good	11%



D533	C534	I535	M536	F537	D538	A539	A540	V541	S542	G543	G544	L545	ASN	THR	S548	V549	L550	R551	A552	V553	L554	P555	R556	D557	M558	V559	F560	R561	THR	SER	THR	PRO	ARG	VAL	VAL	LEU																											
S473	Q474	G475	R476	K477	D478	I479	K480	L481	I482	D483	I484	A485	L486	S487	K488	T489	D490	S491	R492	K493	V494	E495	N496	A497	V498	W499	D500	D501	Y502	K503	D504	L505	C506	H507	M508	H509	T510	G511	V512	V513	V514	E515	K516	K517	LYS	ARG	GLY	GLY	K522	E523	E524	I525	T526	P527	H528	C529	A530	L531	M532				
F413	F414	R415	E416	P417	T418	D419	L420	K421	Q422	F423	K424	Q425	D426	A427	K428	Y429	S430	H431	G432	L433	D434	V435	T436	D437	L438	F439	A440	T441	Q442	P443	G444	L445	T446	S447	A448	V449	T450	D451	A452	L453	P454	R455	M456	M457	V458	I459	T460	C461	Q462	G463	S464	D465	D466	I467	R468	K469	L470	L471	E472				
SER	LYS	SER	LEU	GLN	SER	ALA	GLY	PHE	THR	ALA	G364	L365	T366	Y367	S368	Q369	L370	H371	T372	L373	K374	D375	A376	K377	L378	Q379	L380	P381	P382	K383	A384	K385	T386	W387	K388	D389	I390	E391	G392	R393	P394	E395	D396	P397	V398	E399	L400	A401	L402	Y403	Q404	P405	S406	S407	G408	C409	Y410	I411	H412				
I293	S294	D295	T296	P297	Q298	E299	R300	N301	P302	Y303	E304	N305	I306	L307	Y308	K309	I310	C311	L312	S313	G314	D315	G255	A256	C257	P318	I319	L320	D260	G261	G262	W263	N264	L265	E266	T267	I268	K269	V270	S271	P272	Q273	T274	T275	D276	G277	L278	L279	K280	S281	T282	L283	K284	V285	L286	LYS	GLN	ALA	ASP	SER	ASN	M291	F292
N173	N174	Q175	F176	G177	T178	M179	P180	S181	L182	T183	L184	A185	C186	L187	T188	K189	Q190	G191	Q192	V193	D194	L195	N196	D197	A198	V199	Q200	A201	L202	T203	D204	L205	G206	L207	I208	Y209	T210	K211	K212	Y213	P214	N215	T216	S217	D218	L219	D220	R221	L222	T223	Q224	S225	H226	P227	I228	L229	N230	M231	I232				

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	177.11Å 177.11Å 56.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.70 – 1.90 76.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	51.1 (76.70-1.90) 99.9 (76.69-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.183 , 0.224 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 93.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l 0.049 for h,-h-k,-l 0.030 for -k,-h,-l	Xtriage
Reported twinning fraction	0.513 for H, K, L 0.487 for K, H, -L	Depositor
Outliers	0 of 155929 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12276	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/4095	0.74	1/5528 (0.0%)
1	B	0.65	0/4084	0.75	0/5513
1	C	0.53	0/4062	0.67	0/5481
All	All	0.61	0/12241	0.72	1/16522 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4038	0	4110	35	0
1	B	4027	0	4098	47	0
1	C	4006	0	4079	51	0
2	A	29	0	11	0	0
2	B	29	0	11	4	0
2	C	29	0	11	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	36	0	0	4	0
4	B	50	0	0	2	0
4	C	29	0	0	3	0
All	All	12276	0	12320	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (134) 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:C:233:ASP:HB2	1:C:236:LYS:HG3	1.37	1.05
1:C:24:CYS:SG	1:C:268:ILE:HG12	2.05	0.97
1:C:256:ALA:HA	4:C:588:HOH:O	1.66	0.96
1:B:216:THR:HG22	1:B:234:THR:OG1	1.74	0.88
1:C:262:GLY:O	1:C:263:ASN:HB2	1.72	0.87
1:A:295:ASP:HB3	4:A:602:HOH:O	1.73	0.87
2:B:993:UTP:H4'	4:B:612:HOH:O	1.75	0.85
1:A:306:ILE:HG12	1:A:310:ILE:HD12	1.62	0.82
1:C:209:TYR:CD2	1:C:264:MET:HE1	2.15	0.81
1:C:223:THR:HG21	1:C:230:ASN:HB3	1.63	0.79
1:B:370:LEU:O	1:B:374:LYS:HG2	1.82	0.78
1:B:502:TYR:CE1	1:B:550:LEU:HD13	2.19	0.77
1:B:394:PRO:HG2	1:B:469:LYS:HD3	1.68	0.76
1:B:53:LEU:HD22	1:B:63:ASP:OD1	1.86	0.75
1:A:7:ILE:CG2	1:A:10:PHE:H	2.05	0.69
1:C:209:TYR:CD2	1:C:264:MET:CE	2.76	0.68
1:C:110:LYS:HD2	1:C:331:TRP:CD1	2.28	0.67
1:A:115:ARG:NH2	1:A:295:ASP:O	2.27	0.67
1:B:286:LYS:HE2	1:B:291:MET:O	1.94	0.66
1:C:464:SER:HB2	1:C:483:ASP:HB2	1.77	0.65
1:B:502:TYR:CE1	1:B:550:LEU:CD1	2.79	0.65
1:B:21:SER:HB2	1:B:263:ASN:CG	2.17	0.64
1:B:370:LEU:O	1:B:374:LYS:CG	2.46	0.63
1:B:492:ARG:HH11	1:B:492:ARG:CG	2.11	0.63
1:B:195:LEU:O	1:B:199:VAL:HG12	1.98	0.63
1:B:269:LYS:HG3	1:B:317:TRP:NE1	2.14	0.62
1:C:256:ALA:HA	1:C:264:MET:HE2	1.81	0.62
1:A:117:GLU:OE1	1:A:329:ARG:NH2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLU:HG3	1:C:281:SER:HB3	1.80	0.62
1:A:397:PRO:HB2	1:A:400:ILE:HD11	1.81	0.61
1:A:7:ILE:HG23	1:A:10:PHE:H	1.67	0.60
1:B:223:THR:HG21	1:B:230:ASN:CG	2.23	0.59
1:B:216:THR:CG2	1:B:234:THR:OG1	2.47	0.59
1:B:180:PRO:HG3	1:B:320:ILE:HB	1.84	0.58
1:B:21:SER:HB2	1:B:263:ASN:OD1	2.04	0.58
1:C:209:TYR:HA	1:C:212:LYS:O	2.03	0.58
1:A:57:GLU:HB2	4:A:603:HOH:O	2.05	0.57
1:C:264:MET:HE2	4:C:588:HOH:O	2.06	0.55
1:A:320:ILE:HD12	1:A:320:ILE:C	2.26	0.55
1:A:329:ARG:HG3	1:A:331:TRP:CZ2	2.41	0.55
1:C:180:PRO:HB3	1:C:254:ALA:HA	1.91	0.52
1:A:180:PRO:HB3	1:A:254:ALA:HA	1.89	0.52
1:A:377:MET:CE	1:A:449:VAL:HG22	2.39	0.52
1:C:256:ALA:HB2	1:C:264:MET:HE3	1.90	0.52
1:C:110:LYS:HG3	1:C:331:TRP:CE2	2.44	0.52
1:A:165:ASP:OD1	1:A:551:ARG:NH2	2.42	0.52
1:C:265:LEU:O	1:C:268:ILE:HG13	2.08	0.52
1:B:492:ARG:HG2	1:B:492:ARG:HH11	1.75	0.52
1:A:468:ARG:NH2	4:A:597:HOH:O	2.42	0.52
1:C:208:ILE:HD12	1:C:222:LEU:HD11	1.91	0.52
1:C:88:ILE:HG22	1:C:337:ASP:HB2	1.92	0.52
1:A:464:SER:H	1:A:483:ASP:CG	2.14	0.51
1:C:386:THR:HB	1:C:459:ILE:HD13	1.91	0.51
1:A:17:ARG:HG2	1:A:263:ASN:O	2.10	0.51
1:A:91:VAL:CG2	1:A:338:LEU:HD13	2.41	0.51
1:B:394:PRO:CG	1:B:469:LYS:HD3	2.38	0.50
1:A:91:VAL:HG21	1:A:338:LEU:HD13	1.92	0.50
1:B:223:THR:HG21	1:B:230:ASN:OD1	2.09	0.50
1:A:53:LEU:HD22	1:A:63:ASP:OD1	2.11	0.50
1:C:388:MET:HG2	1:C:467:ILE:HD12	1.93	0.50
1:B:180:PRO:CG	1:B:320:ILE:HB	2.41	0.50
1:A:461:CYS:SG	1:A:464:SER:HA	2.51	0.50
1:B:323:ARG:NH2	2:B:993:UTP:O2B	2.39	0.49
1:C:165:ASP:OD1	1:C:551:ARG:NH2	2.40	0.49
1:A:387:TRP:O	1:A:402:LEU:HA	2.11	0.49
1:B:108:LYS:HE3	4:B:579:HOH:O	2.11	0.49
1:C:391:GLU:HB2	1:C:399:GLU:HB3	1.94	0.49
1:B:286:LYS:HG3	1:B:291:MET:HB2	1.94	0.48
1:C:209:TYR:CE2	1:C:264:MET:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:TYR:CZ	1:B:371:MET:SD	3.07	0.48
1:C:126:MET:SD	1:C:137:ARG:HB3	2.55	0.47
1:C:136:GLN:OE1	4:C:582:HOH:O	2.20	0.47
1:C:233:ASP:CB	1:C:236:LYS:HG3	2.25	0.47
1:C:68:ARG:NH1	1:C:171:LEU:O	2.48	0.47
1:B:377:MET:HE1	1:B:449:VAL:HG22	1.95	0.47
1:A:468:ARG:O	1:A:472:GLU:HG3	2.16	0.46
1:C:278:ILE:HG21	1:C:310:ILE:HD13	1.97	0.46
1:C:19:GLU:CG	1:C:281:SER:HB3	2.45	0.46
1:B:269:LYS:HG3	1:B:317:TRP:CD1	2.50	0.46
1:B:373:LEU:O	1:B:377:MET:HG2	2.16	0.46
1:C:99:LEU:HD22	1:C:336:VAL:HG13	1.98	0.45
1:C:373:LEU:O	1:C:377:MET:HG2	2.16	0.45
1:B:58:ARG:HH11	1:B:58:ARG:HG2	1.82	0.45
1:A:102:LEU:HG	1:A:283:LEU:HD11	1.99	0.45
1:A:126:MET:HG3	1:A:161:VAL:HG21	1.98	0.45
1:C:102:LEU:HG	1:C:283:LEU:HD11	1.98	0.45
1:C:17:ARG:HG2	1:C:263:ASN:O	2.17	0.45
1:A:121:SER:OG	4:A:582:HOH:O	2.20	0.45
1:B:463:GLY:O	1:B:466:ASP:OD1	2.33	0.45
1:B:373:LEU:HD11	1:B:377:MET:CE	2.47	0.45
1:A:105:ASP:OD2	1:A:303:TYR:OH	2.21	0.44
1:A:471:LEU:HD22	1:A:479:ILE:HD12	1.98	0.44
1:C:88:ILE:CG2	1:C:337:ASP:HB2	2.48	0.44
1:B:120:LEU:HD13	2:B:993:UTP:C4	2.53	0.44
1:B:110:LYS:O	1:B:114:ILE:HG13	2.18	0.44
1:B:216:THR:HG22	1:B:234:THR:HG1	1.77	0.44
1:B:141:LEU:HB3	1:B:146:MET:O	2.17	0.44
1:C:178:THR:HG21	1:C:250:ALA:HB2	1.99	0.44
1:A:293:ILE:HG23	1:A:304:GLU:HG2	1.99	0.44
1:C:229:LEU:O	1:C:232:ILE:HD12	2.18	0.43
1:C:32:VAL:HG13	1:C:195:LEU:HD21	2.00	0.43
1:C:476:ARG:HB3	1:C:479:ILE:HD12	2.00	0.43
1:C:410:TYR:CE2	1:C:550:LEU:HB3	2.52	0.43
1:A:188:THR:HG23	1:A:193:VAL:O	2.19	0.43
1:B:414:PHE:CE1	1:B:508:MET:HG2	2.54	0.43
1:B:441:THR:HG22	1:B:560:PHE:CE1	2.54	0.43
1:A:558:MET:HG3	1:A:558:MET:O	2.19	0.42
1:B:110:LYS:HG3	1:B:331:TRP:CE2	2.54	0.42
1:C:394:PRO:HB3	1:C:466:ASP:O	2.19	0.42
1:C:162:ARG:NH2	1:C:551:ARG:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LYS:HB2	1:C:477:LYS:HE3	1.78	0.42
1:C:380:LEU:HD11	1:C:411:ILE:HD11	2.01	0.42
1:B:240:ASN:HA	2:B:993:UTP:O2	2.20	0.42
1:C:386:THR:HG23	1:C:404:GLN:HG2	2.02	0.42
1:C:219:LEU:CD2	1:C:234:THR:HG22	2.50	0.42
1:A:442:GLN:NE2	1:A:443:PRO:HD2	2.35	0.42
1:A:124:VAL:HG13	1:A:378:LEU:HB3	2.02	0.42
1:B:102:LEU:HG	1:B:283:LEU:HD11	2.02	0.42
1:B:411:ILE:HG23	1:B:554:LEU:HD11	2.01	0.41
1:B:387:TRP:CH2	1:B:484:ILE:HG13	2.55	0.41
1:A:394:PRO:HG2	1:A:469:LYS:HE3	2.02	0.41
1:B:492:ARG:NH1	1:B:492:ARG:CG	2.72	0.41
1:A:309:LYS:HB3	1:A:318:PRO:HB2	2.01	0.41
1:B:213:TYR:HA	1:B:214:PRO:HD3	1.88	0.41
1:B:19:GLU:HG3	1:B:281:SER:HB3	2.02	0.41
1:B:117:GLU:OE1	1:B:329:ARG:NH2	2.52	0.41
1:A:414:PHE:HB2	1:A:441:THR:HG21	2.03	0.41
1:B:179:MET:HA	1:B:180:PRO:HD2	1.80	0.41
1:B:126:MET:SD	1:B:137:ARG:HB3	2.61	0.41
1:C:256:ALA:CB	1:C:264:MET:HE3	2.51	0.40
1:C:158:ASP:HB2	1:C:159:GLY:H	1.43	0.40
1:C:499:TRP:CZ2	1:C:532:MET:HG3	2.57	0.40
1:C:184:LEU:HD13	1:C:202:LEU:HD12	2.03	0.40
1:C:502:TYR:CE1	1:C:550:LEU:HD13	2.57	0.40

There are no symmetry-related clashes.

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	508/577 (88%)	493 (97%)	14 (3%)	1 (0%)	51 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	507/577 (88%)	498 (98%)	9 (2%)	0	100	100
1	C	502/577 (87%)	474 (94%)	25 (5%)	3 (1%)	28	16
All	All	1517/1731 (88%)	1465 (97%)	48 (3%)	4 (0%)	44	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	263	ASN
1	C	457	MET
1	A	260	ASP
1	C	260	ASP

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	453/498 (91%)	434 (96%)	19 (4%)	34	23
1	B	452/498 (91%)	436 (96%)	16 (4%)	41	30
1	C	449/498 (90%)	431 (96%)	18 (4%)	36	25
All	All	1354/1494 (91%)	1301 (96%)	53 (4%)	37	26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	75	ASN
1	A	83	THR
1	A	86	LYS
1	A	107	GLU
1	A	158	ASP
1	A	219	LEU
1	A	234	THR
1	A	273	GLN
1	A	287	LYS

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Mol	Chain	Res	Type
1	A	325	SER
1	A	329	ARG
1	A	339	GLU
1	A	365	LEU
1	A	370	LEU
1	A	424	LYS
1	A	469	LYS
1	A	484	ILE
1	A	557	ASP
1	B	29	LEU
1	B	66	ARG
1	B	143	MET
1	B	147	SER
1	B	158	ASP
1	B	199	VAL
1	B	234	THR
1	B	238	SER
1	B	241	ILE
1	B	269	LYS
1	B	374	LYS
1	B	416	GLU
1	B	420	LEU
1	B	464	SER
1	B	492	ARG
1	B	516	LYS
1	C	27	ILE
1	C	82	SER
1	C	120	LEU
1	C	131	SER
1	C	158	ASP
1	C	204	ASP
1	C	224	GLN
1	C	233	ASP
1	C	260	ASP
1	C	263	ASN
1	C	275	MET
1	C	294	SER
1	C	380	LEU
1	C	406	SER
1	C	455	ARG
1	C	473	SER
1	C	478	ASP

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Mol	Chain	Res	Type
1	C	549	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	442	GLN
1	C	442	GLN

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UTP	A	993	-	26,30,30	2.54	3 (11%)	29,47,47	2.41	5 (17%)
2	UTP	B	993	-	26,30,30	2.51	3 (11%)	29,47,47	2.49	5 (17%)
2	UTP	C	993	-	26,30,30	2.53	3 (11%)	29,47,47	2.44	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UTP	A	993	-	-	0/22/38/38	0/2/2/2
2	UTP	B	993	-	-	0/22/38/38	0/2/2/2
2	UTP	C	993	-	-	0/22/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	993	UTP	C6-C5	-9.45	1.35	1.52
2	C	993	UTP	C6-C5	-9.38	1.35	1.52
2	B	993	UTP	C6-C5	-9.15	1.35	1.52
2	B	993	UTP	C6-N1	-7.30	1.37	1.47
2	A	993	UTP	C6-N1	-7.16	1.38	1.47
2	C	993	UTP	C6-N1	-7.16	1.38	1.47
2	B	993	UTP	C5-C4	-3.58	1.41	1.50
2	C	993	UTP	C5-C4	-3.34	1.42	1.50
2	A	993	UTP	C5-C4	-3.33	1.42	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	993	UTP	C4-N3-C2	-5.99	120.68	125.81
2	A	993	UTP	C4-N3-C2	-5.71	120.92	125.81
2	B	993	UTP	C4-N3-C2	-5.60	121.01	125.81
2	A	993	UTP	O2-C2-N1	-2.57	119.90	123.12
2	C	993	UTP	O2-C2-N1	-2.44	120.06	123.12
2	B	993	UTP	O4'-C1'-C2'	-2.14	101.89	106.64
2	C	993	UTP	N3-C2-N1	2.76	119.48	116.73
2	B	993	UTP	C5-C4-N3	2.78	119.49	116.72
2	A	993	UTP	N3-C2-N1	2.81	119.53	116.73
2	A	993	UTP	C5-C4-N3	2.99	119.69	116.72
2	C	993	UTP	C5-C4-N3	3.52	120.22	116.72
2	B	993	UTP	N3-C2-N1	3.60	120.32	116.73
2	C	993	UTP	C5-C6-N1	9.93	121.02	110.70
2	A	993	UTP	C5-C6-N1	9.96	121.06	110.70
2	B	993	UTP	C5-C6-N1	10.15	121.25	110.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	993	UTP	4	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	516/577 (89%)	5.48	516 (100%) 0 0	44, 50, 63, 81	1 (0%)
1	B	515/577 (89%)	5.51	515 (100%) 0 0	43, 49, 63, 81	0
1	C	512/577 (88%)	5.63	512 (100%) 0 0	45, 56, 68, 83	0
All	All	1543/1731 (89%)	5.54	1543 (100%) 0 0	43, 52, 66, 83	1 (0%)

All (1543) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	THR	12.5
1	C	549	VAL	12.2
1	A	548	SER	10.9
1	C	475	GLY	10.8
1	C	317	TRP	10.8
1	A	259	LEU	10.1
1	A	380	LEU	9.9
1	C	23	TYR	9.9
1	A	241	ILE	9.8
1	A	338	LEU	9.8
1	C	29	LEU	9.6
1	B	529	CYS	9.6
1	C	24	CYS	9.5
1	C	161	VAL	9.5
1	C	308	TYR	9.4
1	C	367	TYR	9.4
1	C	106	LEU	9.1
1	C	463	GLY	9.1
1	A	211	ALA	9.1
1	C	327	THR	9.1
1	B	338	LEU	9.0
1	B	380	LEU	9.0
1	C	409	CYS	9.0

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Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	8.9
1	B	433	ILE	8.9
1	A	317	TRP	8.9
1	B	547	THR	8.9
1	C	199	VAL	8.8
1	C	486	LEU	8.8
1	A	499	TRP	8.7
1	B	147	SER	8.7
1	A	237	SER	8.7
1	B	265	LEU	8.7
1	C	550	LEU	8.6
1	C	499	TRP	8.6
1	B	193	VAL	8.6
1	A	7	ILE	8.6
1	C	414	PHE	8.6
1	B	11	LEU	8.5
1	B	486	LEU	8.5
1	B	549	VAL	8.5
1	A	471	LEU	8.5
1	B	541	VAL	8.5
1	C	164	TRP	8.5
1	B	471	LEU	8.5
1	C	88	ILE	8.4
1	B	307	LEU	8.4
1	C	39	LEU	8.4
1	B	237	SER	8.4
1	C	494	TYR	8.4
1	C	461	CYS	8.3
1	B	195	LEU	8.3
1	B	101	ILE	8.3
1	C	529	CYS	8.3
1	A	439	PHE	8.3
1	B	236	LYS	8.3
1	C	450	ILE	8.2
1	B	202	LEU	8.2
1	B	499	TRP	8.2
1	B	199	VAL	8.2
1	C	82	SER	8.2
1	B	327	THR	8.2
1	B	535	ILE	8.2
1	A	414	PHE	8.1
1	C	541	VAL	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	494	TYR	8.1
1	B	439	PHE	8.1
1	C	102	LEU	8.1
1	C	513	VAL	8.1
1	C	557	ASP	8.1
1	C	84	GLN	8.1
1	B	29	LEU	8.1
1	B	259	LEU	8.1
1	C	143	MET	8.1
1	B	241	ILE	8.1
1	C	559	VAL	8.0
1	C	454	PRO	8.0
1	A	80	LEU	8.0
1	B	365	LEU	8.0
1	C	418	THR	8.0
1	B	420	LEU	8.0
1	C	248	LEU	8.0
1	A	265	LEU	8.0
1	A	238	SER	8.0
1	C	458	VAL	8.0
1	C	444	GLY	7.9
1	A	506	CYS	7.9
1	A	12	TRP	7.9
1	A	427	ALA	7.9
1	C	545	LEU	7.9
1	A	186	CYS	7.9
1	C	91	VAL	7.9
1	B	12	TRP	7.9
1	B	494	TYR	7.9
1	C	543	GLY	7.9
1	C	485	ALA	7.9
1	A	268	ILE	7.9
1	B	317	TRP	7.9
1	C	435	VAL	7.9
1	B	461	CYS	7.8
1	C	331	TRP	7.8
1	A	485	ALA	7.8
1	A	202	LEU	7.8
1	B	293	ILE	7.8
1	C	187	LEU	7.8
1	C	283	LEU	7.8
1	C	50	VAL	7.8

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Mol	Chain	Res	Type	RSRZ
1	C	512	VAL	7.8
1	A	185	ALA	7.7
1	A	306	ILE	7.7
1	A	467	ILE	7.7
1	C	99	LEU	7.7
1	A	160	VAL	7.7
1	B	187	LEU	7.7
1	B	207	LEU	7.7
1	A	510	THR	7.7
1	B	31	VAL	7.7
1	C	234	THR	7.7
1	C	372	THR	7.6
1	B	506	CYS	7.6
1	C	134	LEU	7.6
1	C	184	LEU	7.6
1	A	113	VAL	7.6
1	C	122	ALA	7.6
1	B	83	THR	7.6
1	B	560	PHE	7.6
1	C	292	PHE	7.6
1	A	525	ILE	7.6
1	C	101	ILE	7.6
1	C	413	PHE	7.6
1	A	307	LEU	7.6
1	A	529	CYS	7.6
1	B	124	VAL	7.6
1	A	102	LEU	7.5
1	B	114	ILE	7.5
1	C	83	THR	7.5
1	B	164	TRP	7.5
1	B	234	THR	7.5
1	B	73	ALA	7.5
1	C	116	THR	7.4
1	A	484	ILE	7.4
1	B	74	VAL	7.4
1	A	403	TYR	7.4
1	A	13	THR	7.4
1	B	387	TRP	7.4
1	C	267	THR	7.4
1	C	11	LEU	7.4
1	B	106	LEU	7.4
1	B	331	TRP	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	414	PHE	7.4
1	C	560	PHE	7.4
1	A	320	ILE	7.4
1	A	479	ILE	7.4
1	A	275	MET	7.4
1	B	376	ALA	7.4
1	A	207	LEU	7.4
1	A	198	ALA	7.4
1	C	160	VAL	7.4
1	B	186	CYS	7.3
1	A	303	TYR	7.3
1	B	16	LEU	7.3
1	A	387	TRP	7.3
1	A	122	ALA	7.3
1	A	401	ALA	7.3
1	A	497	ALA	7.3
1	A	184	LEU	7.3
1	A	486	LEU	7.3
1	B	308	TYR	7.3
1	B	171	LEU	7.3
1	A	252	VAL	7.3
1	C	336	VAL	7.3
1	C	479	ILE	7.3
1	C	506	CYS	7.3
1	B	367	TYR	7.2
1	C	12	TRP	7.3
1	B	80	LEU	7.2
1	A	336	VAL	7.2
1	A	278	ILE	7.2
1	A	282	ILE	7.2
1	C	459	ILE	7.2
1	C	548	SER	7.2
1	C	10	PHE	7.2
1	B	409	CYS	7.2
1	A	527	PRO	7.2
1	B	129	LEU	7.2
1	A	458	VAL	7.2
1	B	525	ILE	7.2
1	B	10	PHE	7.2
1	A	402	LEU	7.2
1	C	259	LEU	7.2
1	C	282	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	LEU	7.2
1	A	435	VAL	7.2
1	A	535	ILE	7.2
1	B	27	ILE	7.2
1	B	229	LEU	7.2
1	C	471	LEU	7.2
1	C	74	VAL	7.2
1	B	325	SER	7.1
1	A	144	ILE	7.1
1	A	176	PHE	7.1
1	C	207	LEU	7.1
1	C	289	LEU	7.1
1	C	445	LEU	7.1
1	A	233	ASP	7.1
1	A	559	VAL	7.1
1	B	306	ILE	7.1
1	C	295	ASP	7.1
1	A	93	THR	7.1
1	B	95	THR	7.1
1	A	129	LEU	7.1
1	A	141	LEU	7.1
1	C	20	LEU	7.1
1	C	378	LEU	7.1
1	C	438	LEU	7.1
1	C	462	GLN	7.1
1	A	257	CYS	7.1
1	A	95	THR	7.1
1	B	303	TYR	7.1
1	A	283	LEU	7.1
1	B	370	LEU	7.1
1	C	103	ALA	7.1
1	C	120	LEU	7.1
1	A	166	VAL	7.1
1	B	534	CYS	7.1
1	C	238	SER	7.1
1	C	457	MET	7.1
1	C	227	PRO	7.1
1	A	470	LEU	7.1
1	A	541	VAL	7.1
1	C	186	CYS	7.1
1	B	413	PHE	7.1
1	C	256	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	53	LEU	7.0
1	C	338	LEU	7.0
1	A	285	VAL	7.0
1	A	177	GLY	7.0
1	B	311	CYS	7.0
1	B	373	LEU	7.0
1	A	449	VAL	7.0
1	C	482	ILE	7.0
1	A	545	LEU	7.0
1	B	94	LEU	7.0
1	C	223	THR	7.0
1	C	270	VAL	7.0
1	C	446	THR	7.0
1	A	232	ILE	7.0
1	A	423	PHE	7.0
1	A	534	CYS	7.0
1	B	441	THR	7.0
1	A	109	LEU	7.0
1	A	370	LEU	7.0
1	C	140	LEU	7.0
1	C	312	LEU	7.0
1	C	380	LEU	7.0
1	C	420	LEU	7.0
1	B	252	VAL	7.0
1	B	498	VAL	7.0
1	B	198	ALA	7.0
1	A	101	ILE	7.0
1	A	10	PHE	7.0
1	A	327	THR	7.0
1	A	164	TRP	6.9
1	B	366	THR	6.9
1	A	44	PHE	6.9
1	C	537	PHE	6.9
1	B	39	LEU	6.9
1	B	449	VAL	6.9
1	C	252	VAL	6.9
1	A	24	CYS	6.9
1	A	408	GLY	6.9
1	B	249	GLY	6.9
1	B	141	LEU	6.9
1	B	160	VAL	6.9
1	A	35	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	452	ALA	6.9
1	A	20	LEU	6.9
1	C	48	SER	6.9
1	B	228	ILE	6.9
1	C	208	ILE	6.9
1	B	423	PHE	6.9
1	A	205	LEU	6.9
1	C	198	ALA	6.9
1	C	552	ALA	6.9
1	B	435	VAL	6.9
1	C	124	VAL	6.9
1	B	188	THR	6.9
1	C	489	THR	6.9
1	C	272	PRO	6.8
1	A	254	ALA	6.8
1	A	413	PHE	6.8
1	B	37	ALA	6.8
1	B	93	THR	6.8
1	C	93	THR	6.8
1	A	16	LEU	6.8
1	A	29	LEU	6.8
1	A	229	LEU	6.8
1	B	282	ILE	6.8
1	B	103	ALA	6.8
1	A	99	LEU	6.8
1	A	187	LEU	6.8
1	C	402	LEU	6.8
1	A	27	ILE	6.8
1	A	210	THR	6.8
1	C	27	ILE	6.8
1	C	241	ILE	6.8
1	A	219	LEU	6.8
1	A	555	PRO	6.8
1	B	184	LEU	6.8
1	C	141	LEU	6.8
1	C	202	LEU	6.8
1	A	103	ALA	6.8
1	C	306	ILE	6.8
1	C	310	ILE	6.8
1	A	445	LEU	6.8
1	B	398	VAL	6.8
1	C	265	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	367	TYR	6.7
1	C	429	TYR	6.7
1	A	234	THR	6.7
1	A	251	ALA	6.7
1	B	251	ALA	6.7
1	A	208	ILE	6.7
1	C	302	PRO	6.7
1	C	165	ASP	6.7
1	B	270	VAL	6.7
1	B	312	LEU	6.7
1	B	553	VAL	6.7
1	C	16	LEU	6.7
1	A	246	PHE	6.7
1	A	213	TYR	6.7
1	C	271	SER	6.7
1	B	92	GLY	6.7
1	B	278	ILE	6.7
1	C	31	VAL	6.7
1	B	407	SER	6.7
1	C	497	ALA	6.7
1	C	527	PRO	6.7
1	B	390	ILE	6.7
1	B	482	ILE	6.7
1	C	144	ILE	6.7
1	A	513	VAL	6.7
1	B	545	LEU	6.7
1	C	195	LEU	6.7
1	A	539	ALA	6.7
1	A	311	CYS	6.7
1	B	548	SER	6.6
1	A	11	LEU	6.6
1	A	532	MET	6.6
1	B	403	TYR	6.6
1	C	125	TYR	6.6
1	A	454	PRO	6.6
1	B	314	GLY	6.6
1	B	326	ILE	6.6
1	C	484	ILE	6.6
1	B	122	ALA	6.6
1	A	228	ILE	6.6
1	A	550	LEU	6.6
1	C	481	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	297	PRO	6.6
1	A	372	THR	6.6
1	C	376	ALA	6.6
1	B	232	ILE	6.6
1	C	433	ILE	6.6
1	A	50	VAL	6.6
1	A	335	VAL	6.6
1	C	370	LEU	6.6
1	A	366	THR	6.6
1	A	436	THR	6.6
1	C	176	PHE	6.6
1	B	497	ALA	6.6
1	B	20	LEU	6.6
1	B	113	VAL	6.6
1	B	116	THR	6.5
1	B	126	MET	6.5
1	C	439	PHE	6.5
1	C	403	TYR	6.5
1	B	144	ILE	6.5
1	B	467	ILE	6.5
1	B	219	LEU	6.5
1	B	512	VAL	6.5
1	B	257	CYS	6.5
1	A	256	ALA	6.5
1	A	552	ALA	6.5
1	A	262	GLY	6.5
1	C	261	GLY	6.5
1	B	227	PRO	6.5
1	C	465	ASP	6.5
1	C	278	ILE	6.5
1	B	248	LEU	6.5
1	C	182	LEU	6.5
1	C	279	LEU	6.5
1	A	244	TYR	6.5
1	A	203	THR	6.5
1	C	166	VAL	6.5
1	A	94	LEU	6.5
1	B	70	LEU	6.5
1	B	179	MET	6.5
1	A	250	ALA	6.5
1	B	555	PRO	6.5
1	C	47	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	6.5
1	A	310	ILE	6.5
1	B	205	LEU	6.5
1	B	481	LEU	6.5
1	C	531	LEU	6.5
1	B	21	SER	6.4
1	C	131	SER	6.4
1	A	560	PHE	6.4
1	C	44	PHE	6.4
1	A	316	GLY	6.4
1	B	50	VAL	6.4
1	B	161	VAL	6.4
1	A	120	LEU	6.4
1	B	182	LEU	6.4
1	B	479	ILE	6.4
1	C	239	LEU	6.4
1	C	366	THR	6.4
1	C	303	TYR	6.4
1	C	387	TRP	6.4
1	A	47	VAL	6.4
1	A	302	PRO	6.4
1	A	390	ILE	6.4
1	A	433	ILE	6.4
1	B	448	ALA	6.4
1	A	116	THR	6.4
1	B	463	GLY	6.4
1	A	222	LEU	6.4
1	B	134	LEU	6.4
1	B	453	LEU	6.4
1	C	392	GLY	6.4
1	B	510	THR	6.4
1	B	429	TYR	6.4
1	C	15	SER	6.4
1	C	423	PHE	6.4
1	A	321	ALA	6.4
1	A	193	VAL	6.4
1	A	331	TRP	6.4
1	B	99	LEU	6.4
1	C	42	LEU	6.4
1	C	109	LEU	6.4
1	B	489	THR	6.4
1	C	535	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	406	SER	6.4
1	B	427	ALA	6.4
1	B	543	GLY	6.4
1	B	166	VAL	6.4
1	B	178	THR	6.4
1	A	182	LEU	6.3
1	A	247	SER	6.3
1	B	225	SER	6.3
1	B	406	SER	6.3
1	B	210	THR	6.3
1	A	124	VAL	6.3
1	A	199	VAL	6.3
1	A	420	LEU	6.3
1	A	531	LEU	6.3
1	C	464	SER	6.3
1	B	44	PHE	6.3
1	B	513	VAL	6.3
1	B	559	VAL	6.3
1	A	405	PRO	6.3
1	B	77	LEU	6.3
1	B	279	LEU	6.3
1	C	70	LEU	6.3
1	C	172	LEU	6.3
1	B	159	GLY	6.3
1	C	400	ILE	6.3
1	C	411	ILE	6.3
1	C	517	LYS	6.3
1	A	460	THR	6.3
1	C	13	THR	6.3
1	C	217	SER	6.3
1	A	308	TYR	6.3
1	A	512	VAL	6.3
1	C	449	VAL	6.3
1	A	482	ILE	6.3
1	B	372	THR	6.3
1	A	127	GLY	6.3
1	A	270	VAL	6.3
1	C	398	VAL	6.3
1	A	64	LEU	6.3
1	A	70	LEU	6.3
1	A	140	LEU	6.3
1	A	195	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	6.3
1	B	239	LEU	6.3
1	B	283	LEU	6.3
1	B	550	LEU	6.3
1	C	129	LEU	6.3
1	C	293	ILE	6.3
1	A	201	ALA	6.3
1	A	448	ALA	6.3
1	B	183	THR	6.3
1	A	417	PRO	6.2
1	C	206	GLY	6.2
1	C	314	GLY	6.2
1	A	125	TYR	6.2
1	B	23	TYR	6.2
1	C	193	VAL	6.2
1	C	514	VAL	6.2
1	B	531	LEU	6.2
1	C	222	LEU	6.2
1	A	459	ILE	6.2
1	C	440	ALA	6.2
1	C	452	ALA	6.2
1	A	498	VAL	6.2
1	A	373	LEU	6.2
1	B	532	MET	6.2
1	A	410	TYR	6.2
1	B	410	TYR	6.2
1	B	296	THR	6.2
1	B	42	LEU	6.2
1	B	176	PHE	6.2
1	B	185	ALA	6.2
1	B	402	LEU	6.2
1	B	440	ALA	6.2
1	B	88	ILE	6.2
1	C	237	SER	6.2
1	A	145	GLY	6.2
1	A	441	THR	6.2
1	C	417	PRO	6.2
1	C	534	CYS	6.2
1	C	211	ALA	6.2
1	A	400	ILE	6.2
1	C	225	SER	6.2
1	A	255	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	418	THR	6.2
1	A	104	ALA	6.2
1	B	32	VAL	6.2
1	A	38	LEU	6.1
1	B	67	LEU	6.1
1	A	298	GLY	6.1
1	B	336	VAL	6.1
1	A	378	LEU	6.1
1	A	558	MET	6.1
1	B	102	LEU	6.1
1	C	505	LEU	6.1
1	B	292	PHE	6.1
1	A	83	THR	6.1
1	B	526	THR	6.1
1	A	146	MET	6.1
1	A	171	LEU	6.1
1	C	80	LEU	6.1
1	C	95	THR	6.1
1	B	254	ALA	6.1
1	C	335	VAL	6.1
1	A	481	LEU	6.1
1	B	172	LEU	6.1
1	B	546	ASN	6.1
1	C	467	ILE	6.1
1	B	517	LYS	6.1
1	C	240	ASN	6.1
1	A	239	LEU	6.1
1	C	67	LEU	6.1
1	C	326	ILE	6.1
1	C	525	ILE	6.1
1	A	443	PRO	6.0
1	B	272	PRO	6.0
1	B	509	HIS	6.0
1	C	113	VAL	6.0
1	C	163	VAL	6.0
1	C	509	HIS	6.0
1	A	178	THR	6.0
1	B	13	THR	6.0
1	A	42	LEU	6.0
1	C	63	ASP	6.0
1	A	180	PRO	6.0
1	B	464	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	223	THR	6.0
1	A	267	THR	6.0
1	A	553	VAL	6.0
1	C	188	THR	6.0
1	C	216	THR	6.0
1	C	298	GLY	6.0
1	A	279	LEU	6.0
1	C	213	TYR	6.0
1	A	530	ALA	6.0
1	A	41	GLY	6.0
1	A	188	THR	6.0
1	B	267	THR	6.0
1	C	142	ASN	6.0
1	B	438	LEU	6.0
1	B	505	LEU	6.0
1	C	40	HIS	6.0
1	C	185	ALA	6.0
1	C	319	TYR	6.0
1	B	201	ALA	6.0
1	A	543	GLY	6.0
1	B	364	GLY	6.0
1	C	390	ILE	6.0
1	A	32	VAL	6.0
1	B	78	VAL	6.0
1	B	260	ASP	6.0
1	A	457	MET	5.9
1	B	136	GLN	5.9
1	C	480	LYS	5.9
1	A	293	ILE	5.9
1	A	326	ILE	5.9
1	B	268	ILE	5.9
1	B	82	SER	5.9
1	B	91	VAL	5.9
1	B	514	VAL	5.9
1	A	288	ALA	5.9
1	C	219	LEU	5.9
1	C	307	LEU	5.9
1	C	477	LYS	5.9
1	C	58	ARG	5.9
1	C	510	THR	5.9
1	C	232	ILE	5.9
1	B	121	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	316	GLY	5.9
1	B	104	ALA	5.9
1	A	100	LEU	5.9
1	A	312	LEU	5.9
1	B	109	LEU	5.9
1	C	470	LEU	5.9
1	A	409	CYS	5.9
1	B	125	TYR	5.9
1	A	82	SER	5.9
1	A	487	SER	5.9
1	B	411	ILE	5.9
1	C	249	GLY	5.9
1	C	126	MET	5.9
1	B	401	ALA	5.9
1	C	330	ALA	5.9
1	B	285	VAL	5.9
1	C	285	VAL	5.9
1	C	296	THR	5.9
1	A	53	LEU	5.9
1	C	473	SER	5.9
1	A	397	PRO	5.9
1	A	475	GLY	5.9
1	B	502	TYR	5.9
1	C	262	GLY	5.9
1	B	320	ILE	5.9
1	B	537	PHE	5.9
1	C	532	MET	5.9
1	B	321	ALA	5.9
1	C	250	ALA	5.9
1	A	183	THR	5.9
1	A	418	THR	5.9
1	C	436	THR	5.9
1	A	89	LEU	5.9
1	A	429	TYR	5.9
1	B	54	MET	5.8
1	B	485	ALA	5.8
1	B	203	THR	5.8
1	A	318	PRO	5.8
1	C	235	LYS	5.8
1	B	120	LEU	5.8
1	B	558	MET	5.8
1	C	321	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	5.8
1	B	223	THR	5.8
1	B	247	SER	5.8
1	B	163	VAL	5.8
1	C	498	VAL	5.8
1	A	546	ASN	5.8
1	A	23	TYR	5.8
1	B	48	SER	5.8
1	B	250	ALA	5.8
1	B	297	PRO	5.8
1	B	400	ILE	5.8
1	C	228	ILE	5.8
1	C	268	ILE	5.8
1	C	365	LEU	5.8
1	C	146	MET	5.8
1	C	200	GLN	5.8
1	C	427	ALA	5.8
1	C	226	HIS	5.8
1	A	292	PHE	5.8
1	C	434	ASP	5.8
1	A	133	GLN	5.8
1	B	238	SER	5.8
1	A	67	LEU	5.8
1	C	210	THR	5.8
1	B	180	PRO	5.8
1	A	319	TYR	5.8
1	B	158	ASP	5.8
1	C	244	TYR	5.8
1	A	514	VAL	5.8
1	B	130	SER	5.8
1	C	377	MET	5.7
1	A	39	LEU	5.7
1	B	38	LEU	5.7
1	C	53	LEU	5.7
1	A	526	THR	5.7
1	B	135	ASP	5.7
1	B	330	ALA	5.7
1	A	509	HIS	5.7
1	A	209	TYR	5.7
1	A	161	VAL	5.7
1	C	443	PRO	5.7
1	B	35	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	445	LEU	5.7
1	C	73	ALA	5.7
1	C	554	LEU	5.7
1	C	111	SER	5.7
1	C	313	SER	5.7
1	C	407	SER	5.7
1	A	502	TYR	5.7
1	B	527	PRO	5.7
1	C	474	GLN	5.7
1	C	139	ALA	5.7
1	A	438	LEU	5.7
1	A	8	LYS	5.7
1	B	302	PRO	5.7
1	A	139	ALA	5.7
1	B	487	SER	5.7
1	B	394	PRO	5.7
1	A	483	ASP	5.7
1	A	9	SER	5.7
1	A	37	ALA	5.7
1	A	540	ALA	5.7
1	B	288	ALA	5.7
1	B	491	SER	5.7
1	B	470	LEU	5.7
1	C	203	THR	5.6
1	C	181	SER	5.6
1	B	22	GLY	5.6
1	C	320	ILE	5.6
1	B	40	HIS	5.6
1	C	456	ASN	5.6
1	A	272	PRO	5.6
1	B	515	GLU	5.6
1	A	231	MET	5.6
1	A	296	THR	5.6
1	C	130	SER	5.6
1	C	368	SER	5.6
1	B	262	GLY	5.6
1	A	384	ALA	5.6
1	C	49	ASN	5.6
1	B	557	ASP	5.6
1	C	455	ARG	5.6
1	C	508	MET	5.6
1	B	45	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	368	SER	5.6
1	C	145	GLY	5.6
1	C	197	ASP	5.6
1	A	78	VAL	5.6
1	C	78	VAL	5.6
1	A	119	PRO	5.6
1	B	484	ILE	5.6
1	A	274	THR	5.6
1	A	444	GLY	5.6
1	C	229	LEU	5.6
1	B	220	ASP	5.6
1	C	397	PRO	5.6
1	A	31	VAL	5.6
1	B	258	MET	5.6
1	C	114	ILE	5.6
1	B	328	GLY	5.6
1	C	264	MET	5.6
1	B	333	ASN	5.6
1	A	289	LEU	5.6
1	B	64	LEU	5.6
1	C	171	LEU	5.6
1	A	330	ALA	5.6
1	A	281	SER	5.6
1	A	313	SER	5.6
1	B	233	ASP	5.6
1	B	273	GLN	5.6
1	B	24	CYS	5.5
1	A	77	LEU	5.5
1	B	289	LEU	5.5
1	B	211	ALA	5.5
1	B	530	ALA	5.5
1	B	111	SER	5.5
1	C	25	SER	5.5
1	A	377	MET	5.5
1	A	74	VAL	5.5
1	A	324	THR	5.5
1	A	549	VAL	5.5
1	C	516	LYS	5.5
1	B	222	LEU	5.5
1	A	557	ASP	5.5
1	C	448	ALA	5.5
1	C	466	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	444	GLY	5.5
1	C	277	GLY	5.5
1	A	126	MET	5.5
1	C	258	MET	5.5
1	A	216	THR	5.5
1	A	411	ILE	5.5
1	A	382	PRO	5.5
1	B	454	PRO	5.5
1	A	365	LEU	5.5
1	B	140	LEU	5.5
1	B	206	GLY	5.5
1	C	205	LEU	5.5
1	C	371	MET	5.5
1	C	441	THR	5.5
1	A	71	ASN	5.5
1	A	368	SER	5.5
1	A	191	GLY	5.5
1	A	206	GLY	5.5
1	B	310	ILE	5.5
1	C	544	GLY	5.5
1	B	275	MET	5.5
1	B	466	ASP	5.5
1	A	446	THR	5.5
1	A	111	SER	5.5
1	B	8	LYS	5.5
1	B	424	LYS	5.5
1	A	40	HIS	5.4
1	B	443	PRO	5.4
1	C	177	GLY	5.4
1	C	555	PRO	5.4
1	B	47	VAL	5.4
1	B	256	ALA	5.4
1	B	71	ASN	5.4
1	A	143	MET	5.4
1	A	179	MET	5.4
1	B	274	THR	5.4
1	C	487	SER	5.4
1	C	528	HIS	5.4
1	B	382	PRO	5.4
1	C	135	ASP	5.4
1	C	260	ASP	5.4
1	C	196	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	384	ALA	5.4
1	B	383	ASN	5.4
1	C	553	VAL	5.4
1	A	48	SER	5.4
1	C	45	SER	5.4
1	C	406	SER	5.4
1	A	398	VAL	5.4
1	B	335	VAL	5.4
1	B	460	THR	5.4
1	C	386	THR	5.4
1	A	227	PRO	5.4
1	C	119	PRO	5.4
1	C	502	TYR	5.4
1	C	490	ASP	5.4
1	C	281	SER	5.4
1	C	54	MET	5.4
1	B	119	PRO	5.4
1	B	405	PRO	5.4
1	B	319	TYR	5.3
1	A	197	ASP	5.3
1	B	100	LEU	5.3
1	A	130	SER	5.3
1	A	261	GLY	5.3
1	C	274	THR	5.3
1	C	180	PRO	5.3
1	B	458	VAL	5.3
1	A	15	SER	5.3
1	B	15	SER	5.3
1	C	178	THR	5.3
1	C	405	PRO	5.3
1	A	469	LYS	5.3
1	B	246	PHE	5.3
1	B	139	ALA	5.3
1	A	305	ASN	5.3
1	C	263	ASN	5.3
1	B	145	GLY	5.3
1	B	552	ALA	5.3
1	C	38	LEU	5.3
1	C	77	LEU	5.3
1	B	536	MET	5.3
1	C	333	ASN	5.3
1	C	32	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	460	THR	5.3
1	B	451	ASP	5.2
1	C	21	SER	5.2
1	C	478	ASP	5.2
1	C	491	SER	5.2
1	B	263	ASN	5.2
1	C	121	SER	5.2
1	A	537	PHE	5.2
1	B	271	SER	5.2
1	B	377	MET	5.2
1	B	508	MET	5.2
1	C	401	ALA	5.2
1	A	273	GLN	5.2
1	A	106	LEU	5.2
1	C	204	ASP	5.2
1	B	216	THR	5.2
1	A	192	GLN	5.2
1	A	364	GLY	5.2
1	A	392	GLY	5.2
1	B	217	SER	5.2
1	A	301	ASN	5.2
1	C	209	TYR	5.2
1	B	334	THR	5.2
1	A	54	MET	5.2
1	A	508	MET	5.2
1	B	291	MET	5.2
1	A	375	ASP	5.2
1	A	134	LEU	5.2
1	C	94	LEU	5.2
1	C	492	ARG	5.2
1	B	131	SER	5.2
1	B	243	GLY	5.2
1	B	277	GLY	5.2
1	C	159	GLY	5.2
1	A	263	ASN	5.2
1	B	49	ASN	5.2
1	B	215	ASN	5.2
1	A	452	ALA	5.2
1	B	412	HIS	5.1
1	B	318	PRO	5.1
1	C	22	GLY	5.1
1	C	100	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	THR	5.1
1	B	450	ILE	5.1
1	C	324	THR	5.1
1	B	169	ALA	5.1
1	C	251	ALA	5.1
1	C	468	ARG	5.1
1	A	271	SER	5.1
1	A	491	SER	5.1
1	C	257	CYS	5.1
1	B	209	TYR	5.1
1	C	85	GLN	5.1
1	C	388	MET	5.1
1	A	25	SER	5.1
1	B	181	SER	5.1
1	A	128	ASN	5.1
1	A	240	ASN	5.1
1	B	192	GLN	5.1
1	B	324	THR	5.1
1	A	226	HIS	5.1
1	C	311	CYS	5.1
1	C	201	ALA	5.1
1	C	530	ALA	5.1
1	B	315	ASP	5.1
1	B	221	ARG	5.1
1	B	386	THR	5.1
1	C	451	ASP	5.1
1	B	244	TYR	5.1
1	C	214	PRO	5.1
1	A	91	VAL	5.1
1	C	158	ASP	5.1
1	B	143	MET	5.1
1	C	231	MET	5.1
1	C	133	GLN	5.1
1	B	255	GLY	5.1
1	C	373	LEU	5.1
1	A	461	CYS	5.0
1	B	375	ASP	5.0
1	B	478	ASP	5.0
1	C	69	ASP	5.0
1	A	425	GLN	5.0
1	C	183	THR	5.0
1	C	26	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	258	MET	5.0
1	A	464	SER	5.0
1	B	408	GLY	5.0
1	C	255	GLY	5.0
1	A	172	LEU	5.0
1	B	89	LEU	5.0
1	C	453	LEU	5.0
1	A	114	ILE	5.0
1	B	556	ARG	5.0
1	C	488	LYS	5.0
1	A	290	GLY	5.0
1	A	325	SER	5.0
1	C	87	SER	5.0
1	B	496	ASN	5.0
1	A	450	ILE	5.0
1	C	254	ALA	5.0
1	A	230	ASN	5.0
1	C	174	ASN	5.0
1	C	305	ASN	5.0
1	C	337	ASP	5.0
1	C	221	ARG	5.0
1	B	84	GLN	5.0
1	B	379	GLN	5.0
1	C	334	THR	5.0
1	B	371	MET	5.0
1	B	457	MET	5.0
1	B	459	ILE	5.0
1	C	412	HIS	5.0
1	A	36	GLN	4.9
1	A	85	GLN	4.9
1	A	333	ASN	4.9
1	A	505	LEU	4.9
1	C	169	ALA	4.9
1	A	45	SER	4.9
1	B	322	SER	4.9
1	C	301	ASN	4.9
1	A	84	GLN	4.9
1	A	419	ASP	4.9
1	B	337	ASP	4.9
1	A	242	SER	4.9
1	A	249	GLY	4.9
1	C	41	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	ASN	4.9
1	B	226	HIS	4.9
1	C	72	GLN	4.9
1	A	22	GLY	4.9
1	C	280	LYS	4.9
1	A	297	PRO	4.9
1	B	446	THR	4.9
1	A	388	MET	4.9
1	A	536	MET	4.9
1	A	440	ALA	4.9
1	B	540	ALA	4.9
1	A	394	PRO	4.9
1	C	526	THR	4.9
1	B	516	LYS	4.9
1	B	9	SER	4.9
1	B	304	GLU	4.9
1	C	138	ARG	4.9
1	C	393	ARG	4.9
1	A	158	ASP	4.9
1	C	37	ALA	4.8
1	B	213	TYR	4.8
1	C	410	TYR	4.8
1	B	242	SER	4.8
1	C	132	GLN	4.8
1	B	384	ALA	4.8
1	A	26	ASN	4.8
1	C	230	ASN	4.8
1	C	422	GLN	4.8
1	A	105	ASP	4.8
1	C	325	SER	4.8
1	C	447	SER	4.8
1	B	388	MET	4.8
1	A	528	HIS	4.8
1	B	539	ALA	4.8
1	A	181	SER	4.8
1	A	314	GLY	4.8
1	C	243	GLY	4.8
1	B	128	ASN	4.8
1	B	30	GLN	4.8
1	B	240	ASN	4.8
1	A	218	ASP	4.8
1	B	197	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	386	THR	4.8
1	C	179	MET	4.8
1	C	168	ASN	4.8
1	B	381	ASP	4.8
1	C	288	ALA	4.7
1	A	269	LYS	4.7
1	B	175	GLN	4.7
1	A	456	ASN	4.7
1	C	245	ASN	4.7
1	C	275	MET	4.7
1	C	536	MET	4.7
1	C	558	MET	4.7
1	A	131	SER	4.7
1	A	243	GLY	4.7
1	A	224	GLN	4.7
1	A	422	GLN	4.7
1	A	434	ASP	4.7
1	C	504	ASP	4.7
1	A	488	LYS	4.7
1	B	469	LYS	4.7
1	B	107	GLU	4.7
1	B	224	GLN	4.7
1	C	273	GLN	4.7
1	C	318	PRO	4.7
1	A	260	ASP	4.7
1	B	43	ASP	4.7
1	B	490	ASP	4.7
1	C	136	GLN	4.7
1	C	64	LEU	4.7
1	B	276	ASP	4.7
1	B	305	ASN	4.7
1	B	421	LYS	4.7
1	A	73	ALA	4.7
1	A	432	GLY	4.7
1	B	123	GLY	4.7
1	B	214	PRO	4.7
1	C	408	GLY	4.7
1	A	34	ASP	4.7
1	A	276	ASP	4.7
1	A	136	GLN	4.7
1	C	191	GLY	4.7
1	A	407	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	284	LYS	4.7
1	B	329	ARG	4.7
1	C	18	ARG	4.7
1	C	127	GLY	4.6
1	B	96	SER	4.6
1	C	430	SER	4.6
1	C	192	GLN	4.6
1	B	436	THR	4.6
1	C	383	ASN	4.6
1	A	21	SER	4.6
1	A	473	SER	4.6
1	A	17	ARG	4.6
1	A	163	VAL	4.6
1	A	220	ASP	4.6
1	C	220	ASP	4.6
1	A	75	ASN	4.6
1	B	294	SER	4.6
1	C	284	LYS	4.6
1	A	315	ASP	4.6
1	B	295	ASP	4.6
1	B	170	GLU	4.6
1	A	56	LYS	4.6
1	B	554	LEU	4.6
1	C	107	GLU	4.6
1	A	421	LYS	4.6
1	C	246	PHE	4.6
1	C	19	GLU	4.6
1	C	290	GLY	4.6
1	A	322	SER	4.6
1	C	242	SER	4.6
1	B	397	PRO	4.5
1	A	556	ARG	4.5
1	B	456	ASN	4.5
1	A	225	SER	4.5
1	A	478	ASP	4.5
1	B	26	ASN	4.5
1	A	96	SER	4.5
1	A	554	LEU	4.5
1	B	538	ASP	4.5
1	C	391	GLU	4.5
1	B	281	SER	4.5
1	B	200	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	374	LYS	4.5
1	B	264	MET	4.5
1	A	123	GLY	4.5
1	C	247	SER	4.5
1	C	322	SER	4.5
1	B	369	GLN	4.5
1	A	383	ASN	4.5
1	B	168	ASN	4.5
1	B	173	ASN	4.5
1	A	517	LYS	4.5
1	B	86	LYS	4.5
1	B	17	ARG	4.5
1	C	30	GLN	4.5
1	B	425	GLN	4.4
1	B	468	ARG	4.4
1	B	177	GLY	4.4
1	A	430	SER	4.4
1	A	371	MET	4.4
1	C	539	ALA	4.4
1	A	522	LYS	4.4
1	B	85	GLN	4.4
1	B	462	GLN	4.4
1	C	369	GLN	4.4
1	C	382	PRO	4.4
1	B	127	GLY	4.4
1	B	528	HIS	4.4
1	B	231	MET	4.4
1	A	69	ASP	4.4
1	A	174	ASN	4.4
1	A	200	GLN	4.4
1	A	264	MET	4.4
1	C	89	LEU	4.4
1	C	35	ALA	4.4
1	A	167	LYS	4.4
1	C	76	ASN	4.4
1	A	277	GLY	4.4
1	B	313	SER	4.4
1	B	63	ASP	4.4
1	B	455	ARG	4.4
1	B	533	ASP	4.4
1	C	194	ASP	4.4
1	C	483	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	LYS	4.4
1	B	245	ASN	4.4
1	A	334	THR	4.4
1	B	61	ASP	4.4
1	C	224	GLN	4.4
1	B	477	LYS	4.4
1	A	496	ASN	4.4
1	C	173	ASN	4.4
1	B	417	PRO	4.4
1	A	474	GLN	4.4
1	C	511	GLY	4.4
1	A	87	SER	4.4
1	C	294	SER	4.4
1	A	190	GLN	4.3
1	B	204	ASP	4.3
1	C	162	ARG	4.3
1	C	112	LYS	4.3
1	B	25	SER	4.3
1	A	137	ARG	4.3
1	B	393	ARG	4.3
1	C	286	LYS	4.3
1	C	495	GLU	4.3
1	A	468	ARG	4.3
1	A	476	ARG	4.3
1	B	138	ARG	4.3
1	B	404	GLN	4.3
1	C	55	ARG	4.3
1	A	533	ASP	4.3
1	C	236	LYS	4.3
1	A	561	ARG	4.3
1	A	212	LYS	4.3
1	B	287	LYS	4.3
1	A	55	ARG	4.3
1	A	455	ARG	4.3
1	C	323	ARG	4.3
1	A	376	ALA	4.3
1	A	515	GLU	4.3
1	A	221	ARG	4.3
1	B	189	LYS	4.3
1	B	391	GLU	4.3
1	B	62	ASN	4.3
1	C	43	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	55	ARG	4.2
1	C	190	GLN	4.2
1	A	121	SER	4.2
1	B	542	SER	4.2
1	B	415	ARG	4.2
1	A	79	GLU	4.2
1	B	488	LYS	4.2
1	C	117	GLU	4.2
1	A	68	ARG	4.2
1	A	159	GLY	4.2
1	C	98	ASP	4.2
1	C	28	LYS	4.2
1	A	52	ARG	4.2
1	A	507	HIS	4.2
1	B	431	HIS	4.2
1	B	41	GLY	4.2
1	C	540	ALA	4.2
1	A	189	LYS	4.2
1	C	421	LYS	4.2
1	C	503	LYS	4.2
1	A	204	ASP	4.2
1	B	194	ASP	4.2
1	C	276	ASP	4.2
1	C	426	ASP	4.2
1	A	135	ASP	4.1
1	B	105	ASP	4.1
1	A	236	LYS	4.1
1	B	65	LYS	4.1
1	C	128	ASN	4.1
1	A	393	ARG	4.1
1	C	561	ARG	4.1
1	C	9	SER	4.1
1	A	381	ASP	4.1
1	A	504	ASP	4.1
1	B	110	LYS	4.1
1	C	60	ASP	4.1
1	C	61	ASP	4.1
1	C	424	LYS	4.1
1	A	245	ASN	4.1
1	A	412	HIS	4.1
1	B	301	ASN	4.1
1	C	62	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	472	GLU	4.1
1	B	434	ASP	4.1
1	B	52	ARG	4.1
1	A	92	GLY	4.1
1	C	493	LYS	4.1
1	A	60	ASP	4.1
1	A	49	ASN	4.1
1	A	168	ASN	4.1
1	A	235	LYS	4.1
1	B	212	LYS	4.1
1	C	328	GLY	4.1
1	A	415	ARG	4.1
1	B	561	ARG	4.1
1	B	501	GLN	4.1
1	C	167	LYS	4.1
1	C	432	GLY	4.1
1	A	337	ASP	4.1
1	A	217	SER	4.1
1	B	146	MET	4.1
1	A	304	GLU	4.1
1	A	524	GLU	4.1
1	B	474	GLN	4.1
1	C	75	ASN	4.1
1	C	329	ARG	4.1
1	A	51	GLN	4.1
1	B	72	GLN	4.1
1	C	218	ASP	4.1
1	B	66	ARG	4.0
1	A	215	ASN	4.0
1	B	422	GLN	4.0
1	C	374	LYS	4.0
1	A	490	ASP	4.0
1	C	315	ASP	4.0
1	B	290	GLY	4.0
1	B	316	GLY	4.0
1	C	92	GLY	4.0
1	C	123	GLY	4.0
1	A	108	LYS	4.0
1	B	87	SER	4.0
1	B	475	GLY	4.0
1	B	266	GLU	4.0
1	C	523	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	389	ASP	4.0
1	A	14	GLN	4.0
1	B	473	SER	4.0
1	C	542	SER	4.0
1	B	483	ASP	4.0
1	C	538	ASP	4.0
1	C	507	HIS	4.0
1	B	14	GLN	4.0
1	A	511	GLY	4.0
1	A	332	GLU	4.0
1	A	466	ASP	4.0
1	B	60	ASP	4.0
1	C	419	ASP	4.0
1	B	36	GLN	4.0
1	A	291	MET	4.0
1	A	214	PRO	4.0
1	B	399	GLU	4.0
1	B	298	GLY	4.0
1	B	90	ARG	4.0
1	B	115	ARG	4.0
1	C	556	ARG	4.0
1	B	51	GLN	4.0
1	A	495	GLU	4.0
1	B	392	GLY	3.9
1	A	447	SER	3.9
1	C	105	ASP	3.9
1	C	115	ARG	3.9
1	C	379	GLN	3.9
1	B	280	LYS	3.9
1	B	309	LYS	3.9
1	C	212	LYS	3.9
1	A	58	ARG	3.9
1	A	86	LYS	3.9
1	B	108	LYS	3.9
1	A	165	ASP	3.9
1	B	426	ASP	3.9
1	C	415	ARG	3.9
1	A	132	GLN	3.9
1	C	269	LYS	3.9
1	C	375	ASP	3.9
1	A	323	ARG	3.9
1	A	294	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	110	LYS	3.9
1	A	196	ASN	3.9
1	B	396	ASP	3.9
1	A	162	ARG	3.9
1	B	323	ARG	3.9
1	C	90	ARG	3.9
1	C	51	GLN	3.9
1	A	374	LYS	3.9
1	B	253	LYS	3.9
1	B	447	SER	3.9
1	A	117	GLU	3.9
1	A	295	ASP	3.9
1	B	137	ARG	3.9
1	C	404	GLN	3.9
1	A	65	LYS	3.9
1	A	424	LYS	3.9
1	C	395	GLU	3.9
1	B	174	ASN	3.8
1	A	501	GLN	3.8
1	B	286	LYS	3.8
1	C	385	LYS	3.8
1	B	430	SER	3.8
1	A	76	ASN	3.8
1	B	230	ASN	3.8
1	A	493	LYS	3.8
1	A	399	GLU	3.8
1	A	328	GLY	3.8
1	C	137	ARG	3.8
1	C	394	PRO	3.8
1	C	496	ASN	3.8
1	A	63	ASP	3.8
1	A	280	LYS	3.8
1	A	503	LYS	3.8
1	C	469	LYS	3.8
1	B	79	GLU	3.8
1	A	33	LYS	3.8
1	A	309	LYS	3.8
1	A	492	ARG	3.8
1	A	194	ASP	3.8
1	A	500	ASP	3.8
1	B	57	GLU	3.8
1	C	233	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	437	ASP	3.8
1	C	431	HIS	3.8
1	A	169	ALA	3.8
1	B	18	ARG	3.8
1	B	492	ARG	3.8
1	B	495	GLU	3.8
1	A	43	ASP	3.8
1	A	542	SER	3.8
1	C	476	ARG	3.8
1	A	465	ASP	3.7
1	B	269	LYS	3.7
1	A	451	ASP	3.7
1	B	500	ASP	3.7
1	C	500	ASP	3.7
1	B	432	GLY	3.7
1	C	96	SER	3.7
1	A	59	ARG	3.7
1	A	437	ASP	3.7
1	A	369	GLN	3.7
1	B	69	ASP	3.7
1	C	34	ASP	3.7
1	B	522	LYS	3.7
1	C	175	GLN	3.7
1	A	544	GLY	3.7
1	C	533	ASP	3.7
1	A	396	ASP	3.6
1	A	173	ASN	3.6
1	A	30	GLN	3.6
1	A	339	GLU	3.6
1	B	165	ASP	3.6
1	C	253	LYS	3.6
1	A	90	ARG	3.6
1	A	379	GLN	3.6
1	C	442	GLN	3.6
1	A	97	ASP	3.6
1	A	142	ASN	3.6
1	C	291	MET	3.6
1	B	544	GLY	3.6
1	A	329	ARG	3.6
1	C	52	ARG	3.6
1	C	118	ARG	3.6
1	C	215	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	57	GLU	3.6
1	C	399	GLU	3.6
1	C	472	GLU	3.6
1	A	57	GLU	3.6
1	B	117	GLU	3.6
1	C	304	GLU	3.6
1	B	112	LYS	3.6
1	A	389	ASP	3.5
1	B	504	ASP	3.5
1	A	523	GLU	3.5
1	A	18	ARG	3.5
1	A	551	ARG	3.5
1	B	68	ARG	3.5
1	C	86	LYS	3.5
1	B	511	GLY	3.5
1	C	79	GLU	3.5
1	C	522	LYS	3.5
1	C	551	ARG	3.5
1	C	14	GLN	3.5
1	B	507	HIS	3.5
1	C	71	ASN	3.5
1	B	97	ASP	3.5
1	B	118	ARG	3.5
1	B	75	ASN	3.5
1	C	97	ASP	3.5
1	B	503	LYS	3.5
1	C	332	GLU	3.5
1	C	396	ASP	3.5
1	B	190	GLN	3.5
1	B	142	ASN	3.5
1	B	34	ASP	3.4
1	B	419	ASP	3.4
1	B	191	GLY	3.4
1	A	19	GLU	3.4
1	A	266	GLU	3.4
1	A	404	GLN	3.4
1	B	480	LYS	3.4
1	B	162	ARG	3.4
1	C	59	ARG	3.4
1	B	19	GLU	3.4
1	B	551	ARG	3.4
1	C	17	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	132	GLN	3.4
1	B	33	LYS	3.4
1	A	300	ARG	3.4
1	C	300	ARG	3.4
1	A	175	GLN	3.4
1	C	110	LYS	3.4
1	B	218	ASP	3.4
1	B	437	ASP	3.4
1	B	133	GLN	3.4
1	B	76	ASN	3.3
1	A	81	LYS	3.3
1	C	287	LYS	3.3
1	B	332	GLU	3.3
1	A	66	ARG	3.3
1	B	472	GLU	3.3
1	C	66	ARG	3.3
1	A	462	GLN	3.3
1	C	309	LYS	3.3
1	A	391	GLU	3.3
1	B	299	GLU	3.3
1	A	170	GLU	3.3
1	A	426	ASP	3.3
1	A	115	ARG	3.3
1	A	538	ASP	3.3
1	B	196	ASN	3.3
1	C	33	LYS	3.3
1	B	58	ARG	3.3
1	C	501	GLN	3.3
1	A	46	GLU	3.2
1	A	107	GLU	3.2
1	B	493	LYS	3.2
1	C	515	GLU	3.2
1	A	516	LYS	3.2
1	B	59	ARG	3.2
1	B	442	GLN	3.2
1	A	287	LYS	3.2
1	C	104	ALA	3.2
1	A	72	GLN	3.2
1	C	425	GLN	3.2
1	C	170	GLU	3.2
1	A	138	ARG	3.2
1	A	299	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	LYS	3.2
1	A	98	ASP	3.1
1	A	118	ARG	3.1
1	B	465	ASP	3.1
1	B	524	GLU	3.1
1	C	46	GLU	3.1
1	C	524	GLU	3.1
1	A	61	ASP	3.1
1	A	442	GLN	3.1
1	B	300	ARG	3.1
1	B	428	LYS	3.1
1	C	189	LYS	3.1
1	A	480	LYS	3.1
1	B	284	LYS	3.1
1	A	395	GLU	3.0
1	B	261	GLY	3.0
1	A	112	LYS	3.0
1	B	523	GLU	3.0
1	A	463	GLY	3.0
1	A	253	LYS	3.0
1	C	81	LYS	3.0
1	B	476	ARG	3.0
1	B	395	GLU	3.0
1	C	36	GLN	3.0
1	B	56	LYS	3.0
1	B	167	LYS	2.9
1	C	266	GLU	2.9
1	B	385	LYS	2.9
1	C	428	LYS	2.9
1	A	28	LYS	2.9
1	B	28	LYS	2.9
1	B	98	ASP	2.9
1	A	428	LYS	2.9
1	C	56	LYS	2.9
1	A	385	LYS	2.8
1	C	108	LYS	2.8
1	C	68	ARG	2.8
1	C	381	ASP	2.8
1	C	8	LYS	2.7
1	A	431	HIS	2.7
1	B	416	GLU	2.7
1	C	389	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	477	LYS	2.6
1	C	364	GLY	2.6
1	C	299	GLU	2.6
1	B	81	LYS	2.6
1	C	65	LYS	2.5
1	A	416	GLU	2.5
1	B	46	GLU	2.5
1	C	416	GLU	2.4

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(Å ²)	Q<0.9
2	UTP	C	993	29/29	0.38	0.61	4.47	62,72,77,78	5
2	UTP	B	993	29/29	0.37	0.54	3.69	50,65,75,86	2
2	UTP	A	993	29/29	0.49	0.49	1.42	59,69,77,82	2
3	ZN	B	570	1/1	0.99	0.35	-1.77	46,46,46,46	0
3	ZN	A	570	1/1	0.98	0.34	-1.91	47,47,47,47	0
3	ZN	C	570	1/1	0.98	0.28	-3.44	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.