wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 11:44 PM GMT

PDB ID	:	1YAJ
Title	:	Crystal Structure of Human Liver Carboxylesterase in complex with benzil
Authors	:	Fleming, C.D.; Bencharit, S.; Edwards, C.C.; Hyatt, J.L.; Morton, C.M.; Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.
Deposited on	:	2004-12-17
Resolution	:	3.20 Å(reported)

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

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

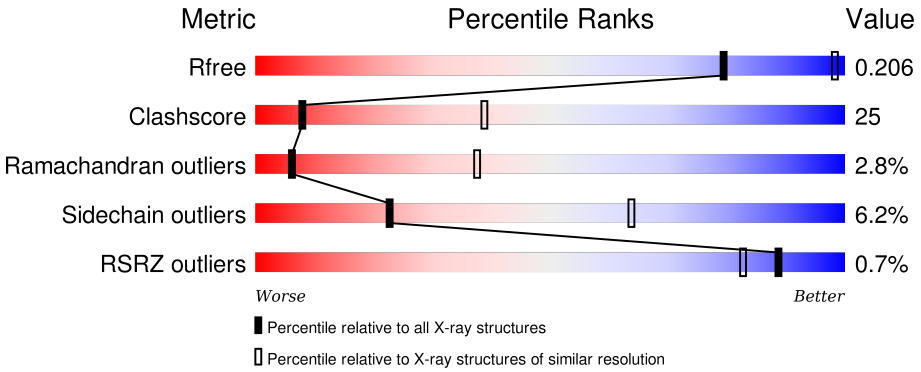
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	532	52% 44% .
1	B	532	% 56% 40% .
1	C	532	% 56% 40% .
1	D	532	% 52% 42% 5%
1	E	532	% 54% 42% .

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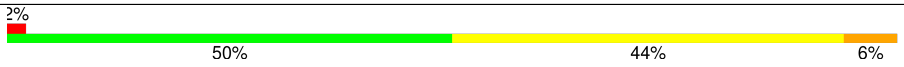
Mol	Chain	Length	Quality of chain
1	F	532	
1	G	532	
1	H	532	
1	I	532	
1	J	532	
1	K	532	
1	L	532	

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	NAG	B	1279	X	-	-	-
2	NAG	F	2379	X	-	-	-
2	NAG	G	3179	X	-	-	-
2	NAG	J	4179	X	-	-	-
2	NAG	K	4279	X	-	-	-
3	SIA	A	1181	-	-	X	-
3	SIA	J	1082	-	-	-	X
4	SO4	A	1184	-	-	-	X
4	SO4	A	1384	-	-	-	X
4	SO4	D	2184	-	-	-	X
4	SO4	D	2384	-	-	-	X
4	SO4	G	3184	-	-	-	X
4	SO4	I	3185	-	-	-	X
4	SO4	K	4385	-	-	-	X
4	SO4	L	4285	-	-	-	X
5	BEZ	A	11	-	-	-	X
5	BEZ	B	12	-	-	X	X
5	BEZ	D	2385	-	X	-	X
5	BEZ	K	4386	-	-	-	X
5	BEZ	L	4380	-	-	-	X

2 Entry composition (i)

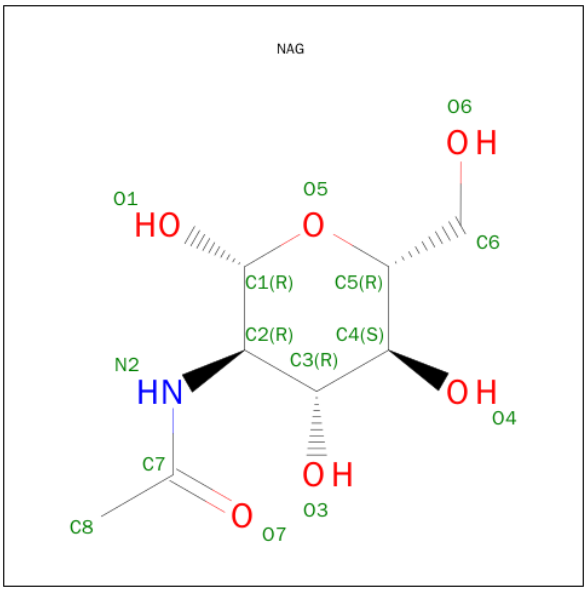
There are 6 unique types of molecules in this entry. The entry contains 50793 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CES1 protein.

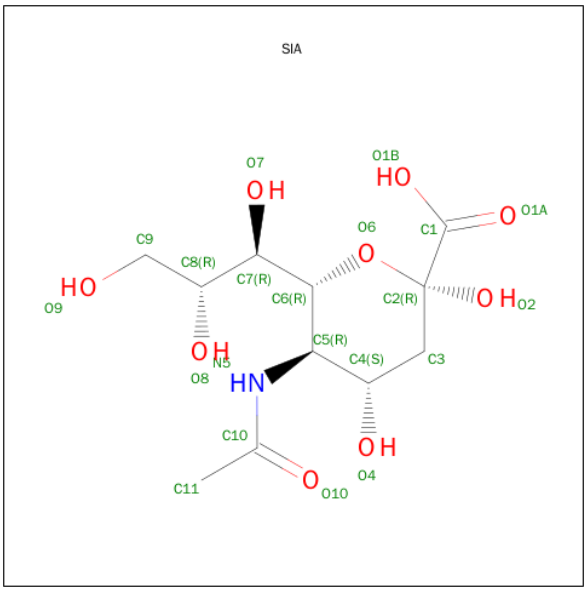
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	C	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	F	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	532	Total	C	N	O	S	0	0	0
			4129	2662	685	762	20			
1	I	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	J	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	K	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	L	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



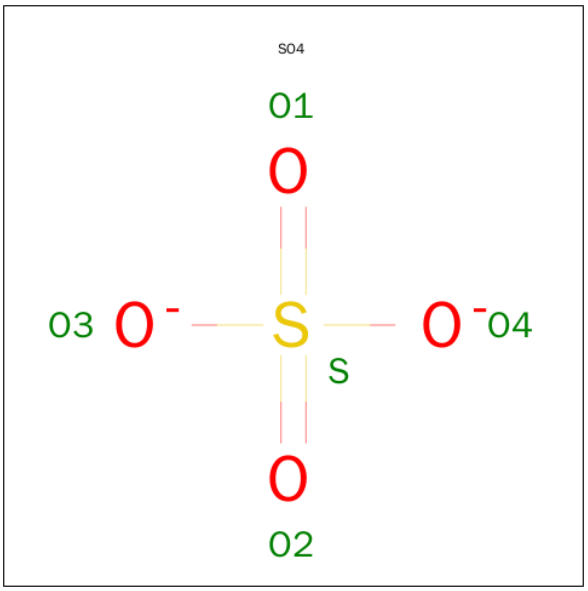
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	D	1	Total	C	N	O	0	0
			21	11	1	9		
3	E	1	Total	C	N	O	0	0
			21	11	1	9		
3	F	1	Total	C	N	O	0	0
			21	11	1	9		
3	G	1	Total	C	N	O	0	0
			21	11	1	9		
3	H	1	Total	C	N	O	0	0
			21	11	1	9		
3	I	1	Total	C	N	O	0	0
			21	11	1	9		
3	J	1	Total	C	N	O	0	0
			21	11	1	9		
3	K	1	Total	C	N	O	0	0
			21	11	1	9		
3	L	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

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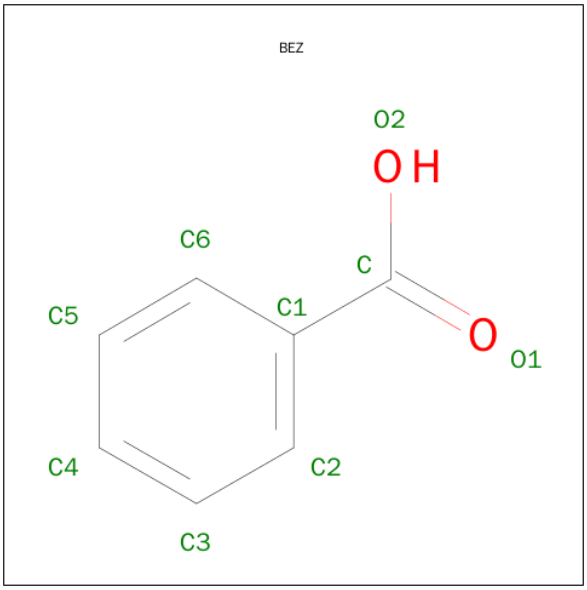
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

- Molecule 5 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 8 7 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 8 7 1	0	0
5	J	1	Total C O 8 7 1	0	0
5	A	1	Total C O 9 7 2	0	0
5	D	1	Total C O 9 7 2	0	0
5	G	1	Total C O 9 7 2	0	0
5	H	1	Total C O 9 7 2	0	0
5	I	1	Total C O 9 7 2	0	0
5	K	1	Total C O 9 7 2	0	0
5	L	1	Total C O 9 7 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	B	1	Total C O 9 7 2	0	0
5	D	1	Total C O 9 7 2	0	0
5	E	1	Total C O 9 7 2	0	0
5	F	1	Total C O 9 7 2	0	0
5	G	1	Total C O 9 7 2	0	0
5	H	1	Total C O 9 7 2	0	0
5	I	1	Total C O 9 7 2	0	0
5	J	1	Total C O 9 7 2	0	0
5	K	1	Total C O 9 7 2	0	0
5	L	1	Total C O 9 7 2	0	0
5	B	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 9 7 2	0	0
5	C	1	Total C O 9 7 2	0	0

- Molecule 6 is water.

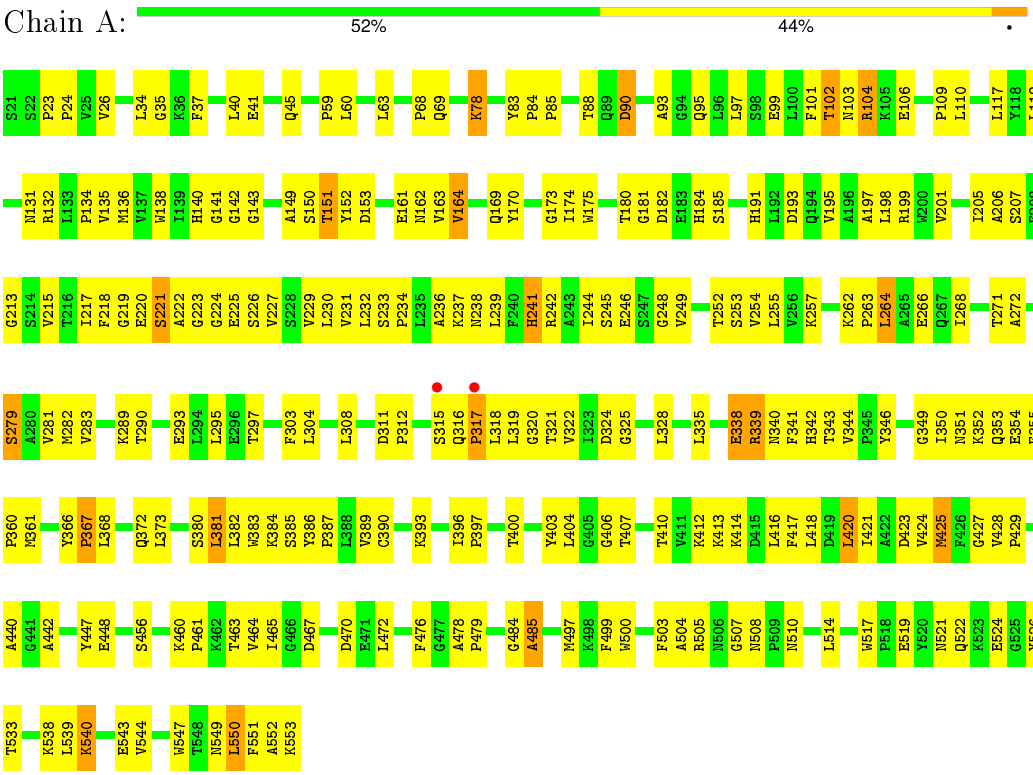
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	30	Total O 30 30	0	0
6	C	33	Total O 33 33	0	0
6	D	49	Total O 49 49	0	0
6	E	38	Total O 38 38	0	0
6	F	42	Total O 42 42	0	0
6	G	41	Total O 41 41	0	0
6	H	37	Total O 37 37	0	0
6	I	34	Total O 34 34	0	0
6	J	38	Total O 38 38	0	0
6	K	50	Total O 50 50	0	0
6	L	39	Total O 39 39	0	0

3 Residue-property plots (i)

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

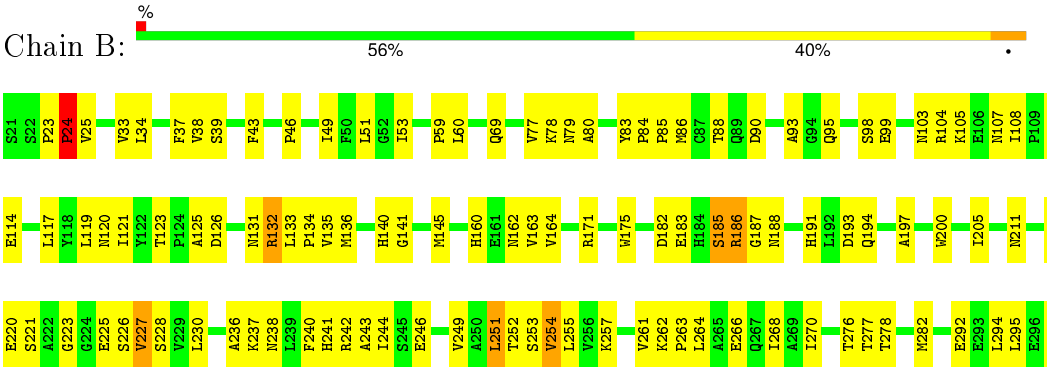
- Molecule 1: CES1 protein

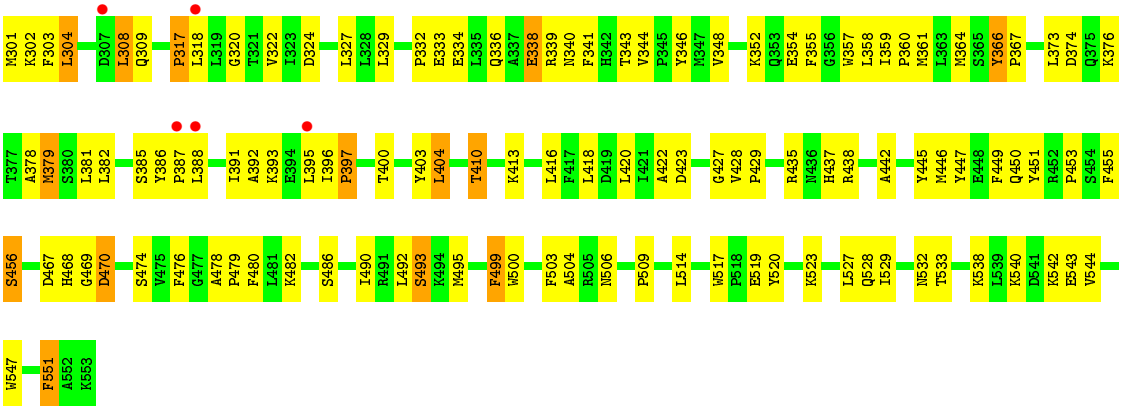
Chain A:



- Molecule 1: CES1 protein

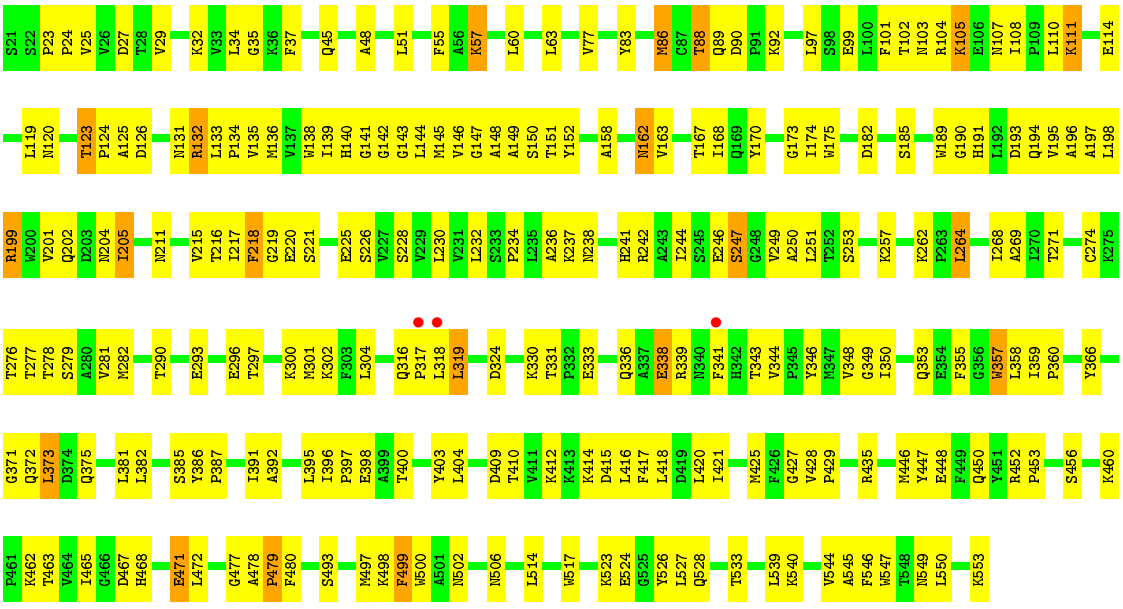
Chain B:





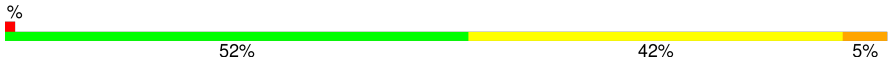
• Molecule 1: CES1 protein

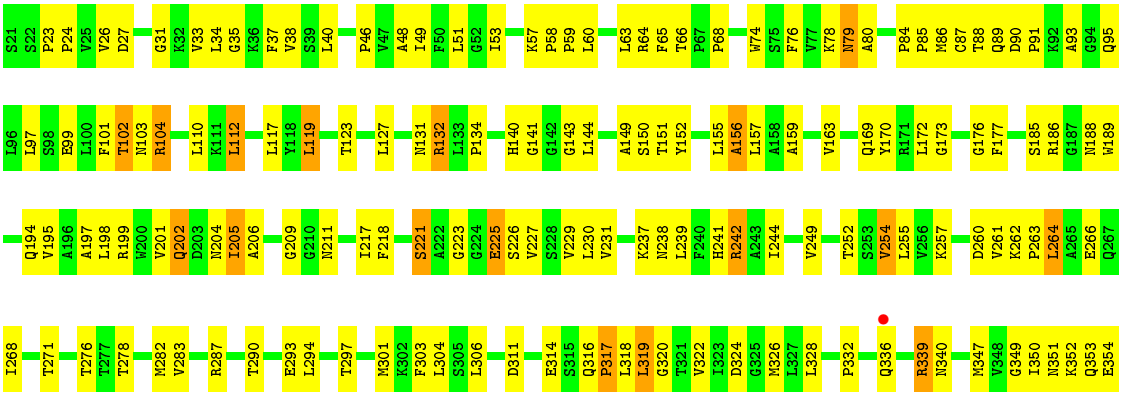
Chain C:

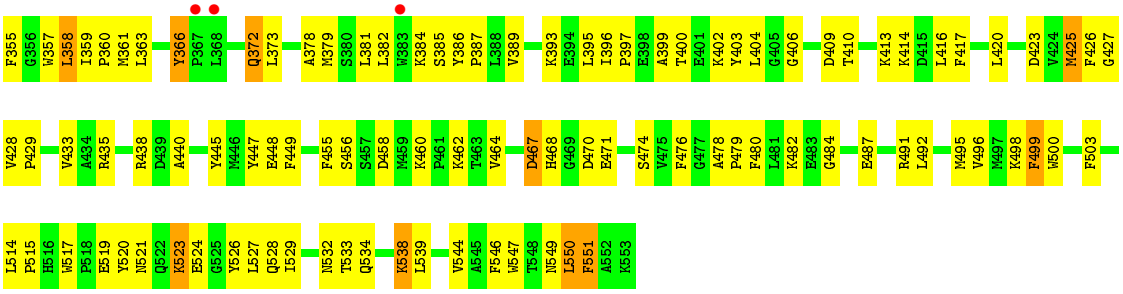


• Molecule 1: CES1 protein

Chain D:

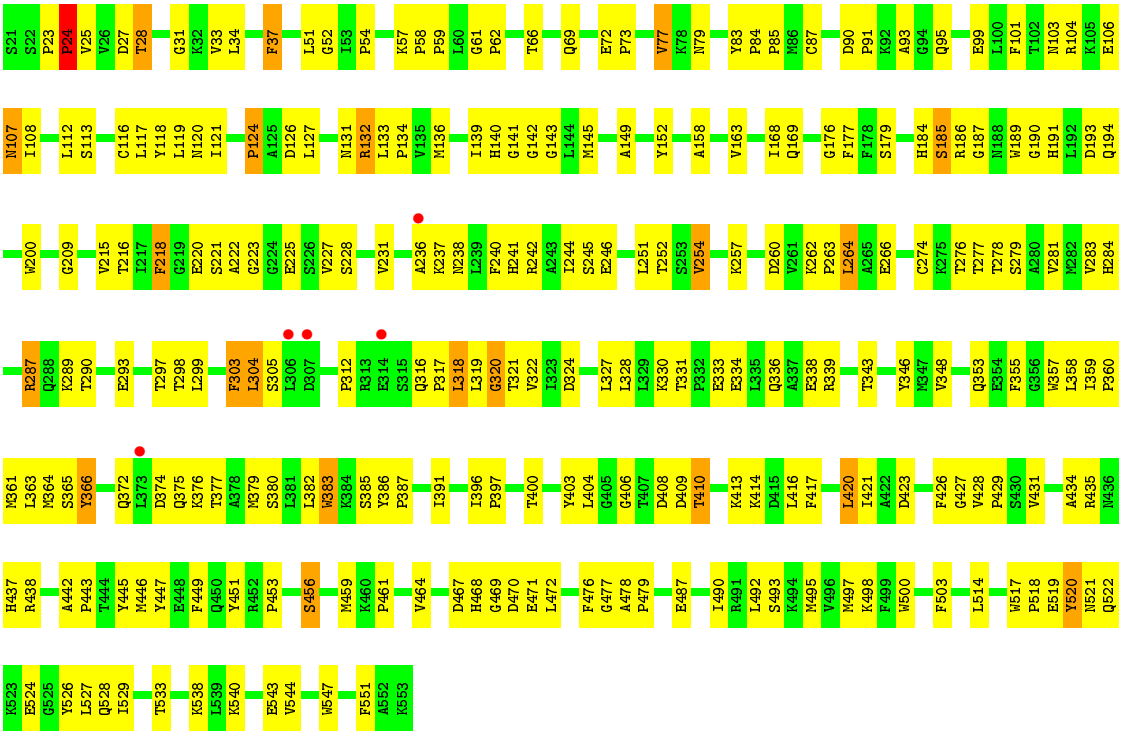






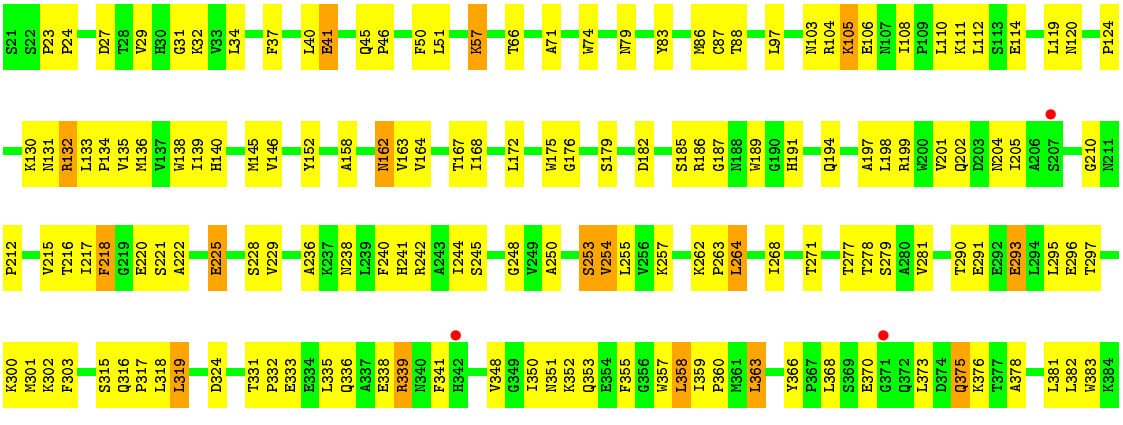
• Molecule 1: CES1 protein

Chain E:



• Molecule 1: CES1 protein

Chain F:



S385 Y386 P387 I391 L395 I396 P397 Y403 L404 G405 G406 T407 D408 D409 K413 K414 D415 L416 F417 L418 D419 L420 D423 F426 G427 V428 P429 S430 V431 D439 A440 G441 Y445 M446 Y447 E448 F449 Q450 Y451 R452 S456 S457 D458 M459 K460 P461 K462 T463 V464 D467

L472 F476 G477 A478 P479 K482 A485 S486 E487 E488 E489 I490 R491 L492 S493 K494 M495 V496 M497 K498 F499 F503 N508 P509 N510 L514 P515 H516 W517 Y520 K523 Y526 L527 Q528 A531 N532 T533 Q534 A535 A536 L539 K540 V544 A545 F546 W547 T548

N549 L550 K553

- Molecule 1: CES1 protein

Chain G: 55% 41%

S21 S22 P23 P24 V29 L34 F37 A48 L51 G52 A56 K57 R64 F65 Q69 P70 A71 E72 F76 V77 K78 N79 Y83 M86 C87 T88 Q89 L97 R104 K105 E106 N107 I108 P109 L110 K111 L112 S113 E114 Y118 L119 N120 I121 Y122 T123 P124

L127 N131 R132 L133 P134 V135 M136 V137 W138 I139 H140 G143 L144 M145 V146 G147 A148 A149 S150 T151 Y152 A156 L157 A158 N162 V163 V164 V165 V166 T167 I168 L172 G176 F177 G181 D182 E183 H184 S185 R186 W189 G190 H191 L192 D193 Q194 A197 L198 R199 W200

V201 Q202 D203 N204 I205 G209 G210 N211 V215 T216 I217 F218 G219 E220 S221 A222 E225 S226 V227 L230 V231 A236 L239 F240 H241 R242 A243 I244 G248 V249 A250 L251 T252 S253 V261 K262 P263 L264 A265 E266 Q267 I268 A269 I270 T271 T278 S279 Q288 K289 T290

E291 E292 E293 L294 L295 E296 T297 M301 K302 F303 L306 D307 L308 P312 Q316 P317 L318 L319 G320 T321 D324 P332 E333 E334 L335 Q336 A337 E338 R339 N340 T343 V348 G349 I350 N351 F355 G356 W357 L358 I359 P360 M361 L363 Y366 P367 L368 S369 E370 G371 Q372

L373 D374 Q375 M379 S380 L381 L382 W383 K384 S385 Y386 P387 L388 K393 E394 L395 I396 T400 Y403 L404 G405 G406 T410 K413 L416 L420 D423 V424 M425 F426 G427 V428 P429 S430 V431 I432 V433 R438 M446 Y447 E448 F449 Q450 Y451 R452 P453 S456 S457

D458 M459 K460 P461 V464 D467 H468 G469 D470 E471 L472 A478 P479 S486 I490 R491 L492 V496 M497 K498 F499 W500 A504 L514 W517 P518 K523 E524 G525 Y526 L527 Q528 I529 T533 Q534 K538 L539 K540 D541 V544 W547 L550 F551 A552 K553

- Molecule 1: CES1 protein

Chain H: % 54% 43%

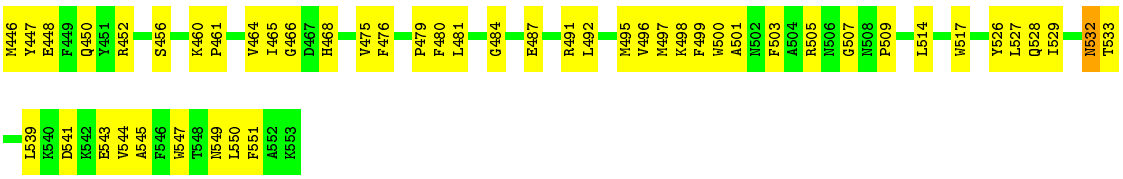
S21 S22 P23 P24 V25 V26 H30 L34 G35 V38 S39 Q45 P46 I49 A56 K57 P58 P59 L60 L63 R64 F65 T66 Q69 V77 K78 N79 Y83 P84 P85 M86 C87 T88 Q95 L96 L97 S98 E99 L100 F101 T102 N103 R104 K105 E106 N107 I108 D115

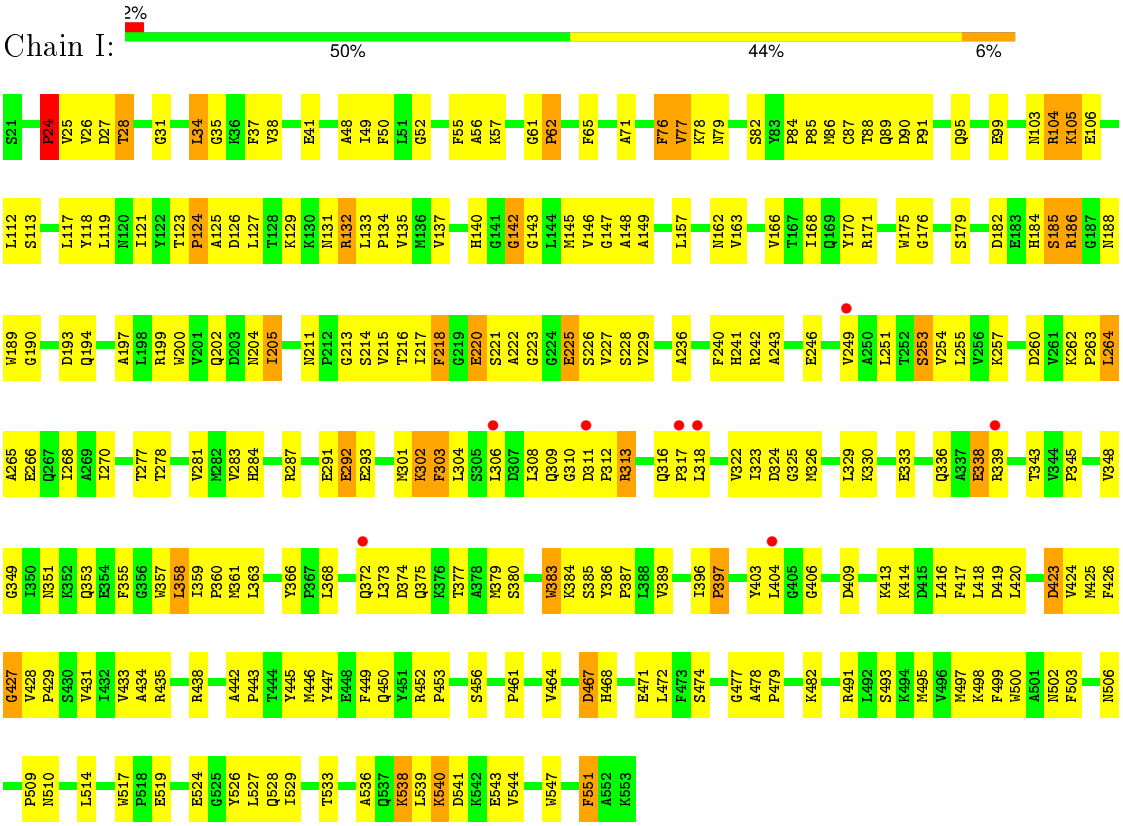
C116 L117 Y118 L119 N120 I121 Y122 K129 K130 N131 R132 L133 P134 V135 H140 G143 L144 S150 T151 Y152 A156 E161 N162 V163 V164 V165 V166 T167 I168 R171 L172 G173 I174 W175 G176 T180 H184 S185 R186 H191 L192 D193 Q194 V195 A196 A197 L198 R199 W200 V201

N204 I205 A206 S207 F208 G209 V215 T216 I217 F218 G219 E220 S221 A222 G223 G224 E225 S226 V227 S228 V229 L230 V231 A236 L239 F240 H241 R242 A243 I244 S245 E246 S247 G248 V249 T252 S253 V254 L255 V256 K257 K262 P263 L264 A265 E266 Q267 I268 A269 I270 T276 T277 T278

S279 M282 V283 R287 T290 E291 E292 E293 E296 K300 F303 L304 S305 L306 D307 P312 R313 Q316 P317 L318 L319 G320 T321 V322 I323 D324 K330 T331 P332 E333 E334 L335 E338 R339 N340 T343 M347 V348 G349 I350 N351 K352 Q353 E354 F355 G356 W357 L358

I359 P360 M361 L363 M364 S365 Y366 E370 G371 Q372 L381 L382 W383 K384 S385 Y386 P387 K393 E394 L395 I396 P397 E398 A399 T400 Y403 L404 K413 K414 D415 L416 F417 L418 D419 L420 I421 A422 D423 V424 M425 F426 G427 V428 P429 S430 V431 I432 V433 H437 R438 D439 T444 Y445



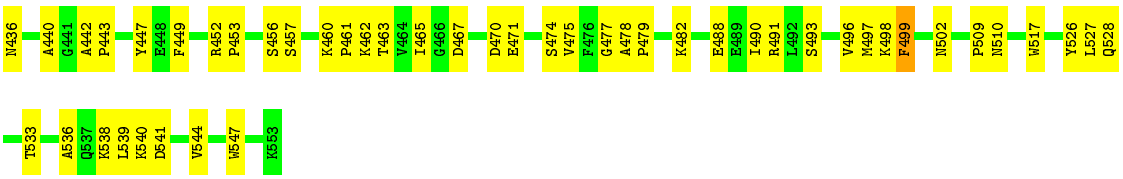


• Molecule 1: CES1 protein

Chain I:

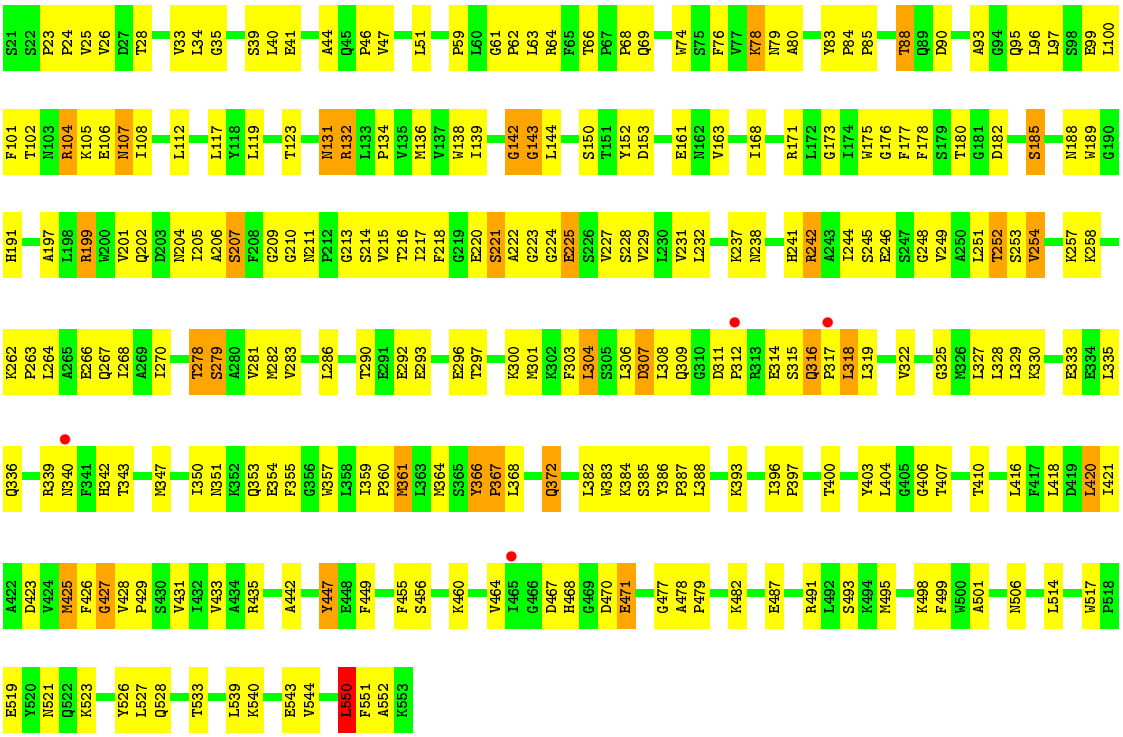
• Molecule 1: CES1 protein

Chain J:



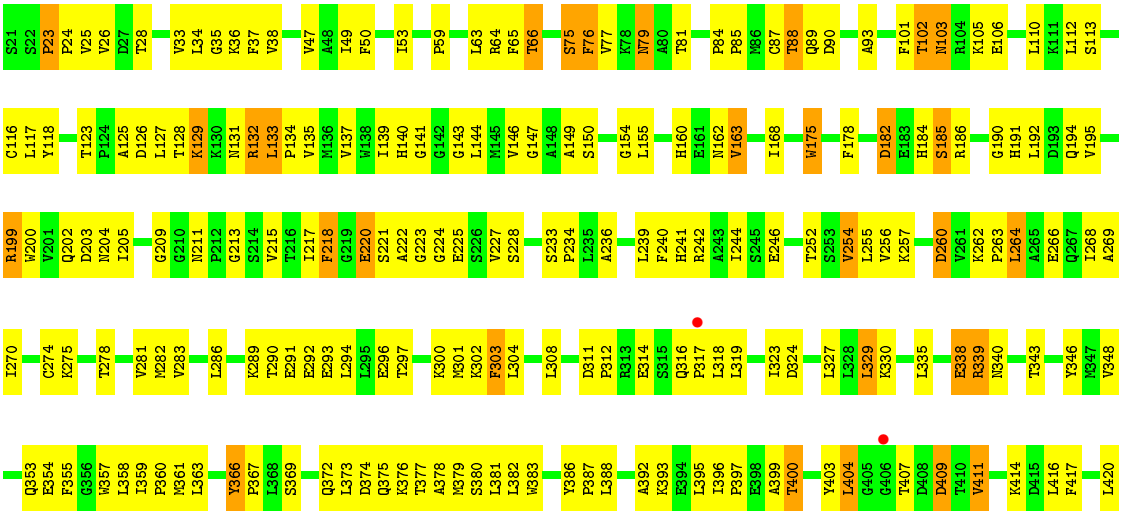
• Molecule 1: CES1 protein

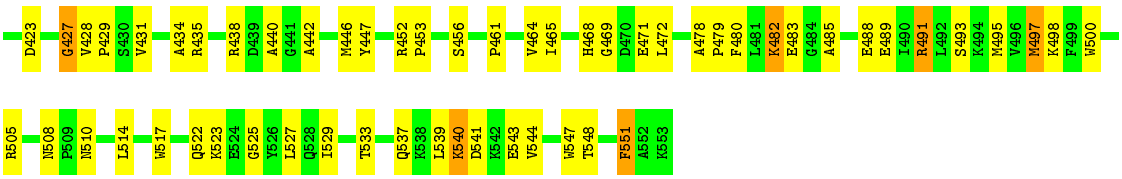
Chain K:



• Molecule 1: CES1 protein

Chain L:




D423
G427
V428
P429
S430
V431
A434
R435
R438
D439
A440
G441
A442
M446
Y447
R452
P453
S456
P461
V464
I465
H468
G469
D470
E471
L472
A478
P479
F480
L481
K482
E483
G484
A485
E488
E489
T490
R491
L492
S493
K494
M495
V496
M497
K498
P499
W500
R505
N508
P509
N510
L514
W517
Q522
K523
E524
G525
Y526
L527
Q528
I529
T533
Q537
K538
L539
K540
D541
K542
E543
V544
W547
T548
F551
A552
K553

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.56Å 181.49Å 202.71Å 90.12° 89.93° 89.72°	Depositor
Resolution (Å)	54.56 – 3.20 54.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.56-3.20) 95.8 (54.56-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.287 0.203 , 0.206	Depositor DCC
R_{free} test set	6249 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 28.0	EDS
Estimated twinning fraction	0.388 for h,-k,-l 0.377 for -h,k,-l 0.389 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 124758 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50793	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ, SIA, NAG, SO4

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	0.64	4/4236 (0.1%)	0.70	2/5754 (0.0%)
1	B	0.62	3/4237 (0.1%)	0.66	3/5754 (0.1%)
1	C	0.62	3/4237 (0.1%)	0.66	0/5754
1	D	0.60	0/4236	0.67	1/5754 (0.0%)
1	E	0.71	6/4237 (0.1%)	0.69	4/5754 (0.1%)
1	F	0.63	3/4237 (0.1%)	0.67	2/5754 (0.0%)
1	G	0.73	10/4236 (0.2%)	0.78	9/5754 (0.2%)
1	H	0.70	2/4235 (0.0%)	0.70	1/5752 (0.0%)
1	I	0.92	12/4237 (0.3%)	0.76	13/5754 (0.2%)
1	J	0.61	3/4237 (0.1%)	0.68	2/5754 (0.0%)
1	K	0.60	4/4236 (0.1%)	0.68	1/5754 (0.0%)
1	L	0.64	4/4237 (0.1%)	0.68	3/5754 (0.1%)
All	All	0.67	54/50838 (0.1%)	0.69	41/69046 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	2
1	K	0	1
All	All	0	4

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CD2-CE2	21.55	1.67	1.41
1	I	383	TRP	CE3-CZ3	20.67	1.73	1.38
1	H	77	VAL	CB-CG1	19.61	1.94	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CE2-CZ2	17.00	1.68	1.39
1	E	77	VAL	CB-CG1	15.91	1.86	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	550	LEU	O-C-N	13.71	144.63	122.70
1	G	550	LEU	CA-C-O	-12.66	93.51	120.10
1	G	182	ASP	CB-CG-OD1	11.15	128.34	118.30
1	A	550	LEU	O-C-N	8.86	136.88	122.70
1	I	186	ARG	NE-CZ-NH1	8.76	124.68	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	550	LEU	Mainchain
1	G	550	LEU	Mainchain
1	G	57	LYS	Mainchain
1	K	550	LEU	Mainchain

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	4130	0	4131	221	0
1	B	4131	0	4130	180	0
1	C	4131	0	4130	199	0
1	D	4130	0	4130	199	0
1	E	4131	0	4131	202	0
1	F	4131	0	4130	184	0
1	G	4130	0	4129	192	0
1	H	4129	0	4131	206	0
1	I	4131	0	4131	212	0
1	J	4131	0	4129	214	0
1	K	4130	0	4130	219	0
1	L	4131	0	4131	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	3	0
2	G	14	0	13	1	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	1	0
2	K	14	0	13	2	0
2	L	14	0	13	0	0
3	A	42	0	36	13	0
3	B	21	0	18	5	0
3	D	21	0	18	8	0
3	E	21	0	18	2	0
3	F	21	0	18	1	0
3	G	21	0	18	6	0
3	H	21	0	18	1	0
3	I	21	0	18	5	0
3	J	21	0	18	5	0
3	K	21	0	18	7	0
3	L	21	0	18	7	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	1	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
5	A	18	0	10	2	0
5	B	18	0	11	6	0
5	C	17	0	10	4	0
5	D	18	0	11	3	0
5	E	18	0	10	0	0
5	F	17	0	10	0	0
5	G	18	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	18	0	10	1	0
5	I	18	0	10	1	0
5	J	17	0	10	1	0
5	K	18	0	10	0	0
5	L	18	0	10	1	0
6	A	43	0	0	11	0
6	B	30	0	0	5	0
6	C	33	0	0	5	0
6	D	49	0	0	8	0
6	E	38	0	0	16	0
6	F	42	0	0	4	0
6	G	41	0	0	8	0
6	H	37	0	0	8	0
6	I	34	0	0	9	0
6	J	38	0	0	9	0
6	K	50	0	0	11	0
6	L	39	0	0	12	0
All	All	50793	0	50057	2486	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 25.

The worst 5 of 2486 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)
5:B:12:BEZ:C3	5:B:12:BEZ:C2	1.76	1.62
5:B:12:BEZ:C1	5:B:12:BEZ:C2	1.78	1.59
5:B:12:BEZ:C5	5:B:12:BEZ:C6	1.74	1.58
5:B:12:BEZ:C1	5:B:12:BEZ:C6	1.78	1.57
1:B:24:PRO:C	1:B:24:PRO:CA	1.76	1.54

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	530/532 (100%)	451 (85%)	67 (13%)	12 (2%)	8 44
1	B	530/532 (100%)	448 (84%)	65 (12%)	17 (3%)	5 33
1	C	530/532 (100%)	467 (88%)	54 (10%)	9 (2%)	11 52
1	D	530/532 (100%)	454 (86%)	60 (11%)	16 (3%)	5 35
1	E	530/532 (100%)	438 (83%)	80 (15%)	12 (2%)	8 44
1	F	530/532 (100%)	464 (88%)	51 (10%)	15 (3%)	6 37
1	G	530/532 (100%)	445 (84%)	62 (12%)	23 (4%)	3 25
1	H	530/532 (100%)	449 (85%)	71 (13%)	10 (2%)	10 50
1	I	530/532 (100%)	451 (85%)	60 (11%)	19 (4%)	4 30
1	J	530/532 (100%)	444 (84%)	74 (14%)	12 (2%)	8 44
1	K	530/532 (100%)	451 (85%)	64 (12%)	15 (3%)	6 37
1	L	530/532 (100%)	434 (82%)	80 (15%)	16 (3%)	5 35
All	All	6360/6384 (100%)	5396 (85%)	788 (12%)	176 (3%)	6 37

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	SER
1	B	358	LEU
1	E	185	SER
1	E	358	LEU
1	E	456	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/448 (100%)	423 (94%)	25 (6%)	26 68
1	B	448/448 (100%)	419 (94%)	29 (6%)	21 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	448/448 (100%)	419 (94%)	29 (6%)	21 61
1	D	448/448 (100%)	418 (93%)	30 (7%)	20 60
1	E	448/448 (100%)	417 (93%)	31 (7%)	19 59
1	F	448/448 (100%)	430 (96%)	18 (4%)	38 77
1	G	448/448 (100%)	423 (94%)	25 (6%)	26 68
1	H	448/448 (100%)	423 (94%)	25 (6%)	26 68
1	I	448/448 (100%)	418 (93%)	30 (7%)	20 60
1	J	448/448 (100%)	424 (95%)	24 (5%)	27 68
1	K	448/448 (100%)	417 (93%)	31 (7%)	19 59
1	L	448/448 (100%)	413 (92%)	35 (8%)	16 53
All	All	5376/5376 (100%)	5044 (94%)	332 (6%)	23 64

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	225	GLU
1	G	523	LYS
1	L	162	ASN
1	F	339	ARG
1	G	172	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	353	GLN
1	G	528	GLN
1	L	131	ASN
1	F	375	GLN
1	G	107	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

72 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	BEZ	A	11	-	6,9,9	3.31	4 (66%)	8,11,11	1.39	1 (12%)
2	NAG	A	1179	1	14,14,15	0.68	0	15,19,21	0.76	1 (6%)
3	SIA	A	1180	-	17,21,21	0.81	0	19,31,31	0.96	1 (5%)
3	SIA	A	1181	-	17,21,21	1.01	1 (5%)	19,31,31	0.70	0
4	SO4	A	1184	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	A	1384	-	4,4,4	0.27	0	6,6,6	0.14	0
5	BEZ	A	1385	-	6,9,9	3.64	2 (33%)	8,11,11	1.66	2 (25%)
5	BEZ	B	12	-	6,9,9	18.18	6 (100%)	8,11,11	1.38	1 (12%)
2	NAG	B	1279	1	14,14,15	0.66	0	15,19,21	0.96	1 (6%)
3	SIA	B	1280	-	17,21,21	0.83	0	19,31,31	1.13	2 (10%)
4	SO4	B	1284	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	B	1385	-	4,4,4	0.24	0	6,6,6	0.09	0
5	BEZ	B	1386	-	6,9,9	2.04	2 (33%)	8,11,11	0.39	0
4	SO4	C	1185	-	4,4,4	0.30	0	6,6,6	0.22	0
4	SO4	C	1285	-	4,4,4	0.38	0	6,6,6	0.18	0
2	NAG	C	1379	1	14,14,15	0.66	0	15,19,21	0.90	1 (6%)
5	BEZ	C	5013	1	8,8,9	2.19	3 (37%)	9,9,11	0.72	0
5	BEZ	C	5014	-	6,9,9	1.19	0	8,11,11	0.74	0
2	NAG	D	2179	1	14,14,15	0.70	0	15,19,21	0.73	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SIA	D	2180	-	17,21,21	0.95	1 (5%)	19,31,31	0.77	0
4	SO4	D	2184	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	D	2384	-	4,4,4	0.33	0	6,6,6	0.13	0
5	BEZ	D	2385	-	6,9,9	14.11	6 (100%)	8,11,11	2.23	5 (62%)
5	BEZ	D	2386	-	6,9,9	3.34	5 (83%)	8,11,11	0.92	0
2	NAG	E	2279	1	14,14,15	0.52	0	15,19,21	1.11	1 (6%)
4	SO4	E	2284	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	E	2385	-	4,4,4	0.26	0	6,6,6	0.15	0
5	BEZ	E	2386	-	6,9,9	0.82	0	8,11,11	0.70	0
5	BEZ	E	2387	-	6,9,9	0.93	0	8,11,11	0.93	0
3	SIA	E	582	-	17,21,21	0.79	0	19,31,31	0.96	0
4	SO4	F	2185	-	4,4,4	0.33	0	6,6,6	0.22	0
4	SO4	F	2285	-	4,4,4	0.33	0	6,6,6	0.09	0
2	NAG	F	2379	1	14,14,15	1.19	2 (14%)	15,19,21	1.21	2 (13%)
5	BEZ	F	5023	1	8,8,9	2.16	4 (50%)	9,9,11	0.61	0
5	BEZ	F	5024	-	6,9,9	1.58	0	8,11,11	0.49	0
3	SIA	F	682	-	17,21,21	1.14	2 (11%)	19,31,31	1.11	2 (10%)
2	NAG	G	3179	1	14,14,15	0.83	0	15,19,21	0.85	1 (6%)
4	SO4	G	3184	-	4,4,4	0.19	0	6,6,6	0.19	0
4	SO4	G	3384	-	4,4,4	0.33	0	6,6,6	0.20	0
5	BEZ	G	3385	-	6,9,9	0.86	0	8,11,11	1.01	0
5	BEZ	G	3386	-	6,9,9	3.89	5 (83%)	8,11,11	3.46	4 (50%)
3	SIA	G	782	-	17,21,21	0.88	0	19,31,31	0.86	0
2	NAG	H	3279	1	14,14,15	0.73	0	15,19,21	0.85	0
4	SO4	H	3284	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	H	3385	-	4,4,4	0.32	0	6,6,6	0.14	0
5	BEZ	H	3386	-	6,9,9	0.76	0	8,11,11	0.85	0
5	BEZ	H	3387	-	6,9,9	2.80	4 (66%)	8,11,11	1.76	3 (37%)
3	SIA	H	882	-	17,21,21	1.08	2 (11%)	19,31,31	0.83	0
4	SO4	I	3185	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	I	3285	-	4,4,4	0.35	0	6,6,6	0.09	0
2	NAG	I	3379	1	14,14,15	0.62	0	15,19,21	1.03	1 (6%)
5	BEZ	I	3380	-	6,9,9	0.83	0	8,11,11	1.01	0
5	BEZ	I	3381	-	6,9,9	1.88	2 (33%)	8,11,11	0.32	0
3	SIA	I	982	-	17,21,21	0.78	1 (5%)	19,31,31	0.96	2 (10%)
3	SIA	J	1082	-	17,21,21	1.01	1 (5%)	19,31,31	0.93	1 (5%)
2	NAG	J	4179	1	14,14,15	0.78	0	15,19,21	1.06	2 (13%)
4	SO4	J	4184	-	4,4,4	0.27	0	6,6,6	0.14	0
4	SO4	J	4185	-	4,4,4	0.32	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	J	4384	-	4,4,4	0.34	0	6,6,6	0.12	0
5	BEZ	J	5041	1	8,8,9	2.23	3 (37%)	9,9,11	0.60	0
5	BEZ	J	5042	-	6,9,9	4.24	2 (33%)	8,11,11	2.41	3 (37%)
3	SIA	K	1182	-	17,21,21	0.74	0	19,31,31	0.82	0
2	NAG	K	4279	1	14,14,15	0.81	0	15,19,21	0.75	0
4	SO4	K	4284	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	K	4385	-	4,4,4	0.27	0	6,6,6	0.11	0
5	BEZ	K	4386	-	6,9,9	1.00	0	8,11,11	0.79	0
5	BEZ	K	4387	-	6,9,9	3.21	4 (66%)	8,11,11	1.01	0
3	SIA	L	1282	-	17,21,21	0.69	0	19,31,31	1.21	1 (5%)
4	SO4	L	4285	-	4,4,4	0.34	0	6,6,6	0.11	0
2	NAG	L	4379	1	14,14,15	0.57	0	15,19,21	0.85	1 (6%)
5	BEZ	L	4380	-	6,9,9	1.28	0	8,11,11	0.65	0
5	BEZ	L	4381	-	6,9,9	0.85	0	8,11,11	0.84	0

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
5	BEZ	A	11	-	-	0/0/4/4	0/1/1/1
2	NAG	A	1179	1	-	0/6/23/26	0/1/1/1
3	SIA	A	1180	-	-	1/14/38/38	0/1/1/1
3	SIA	A	1181	-	-	1/14/38/38	0/1/1/1
4	SO4	A	1184	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1384	-	-	0/0/0/0	0/0/0/0
5	BEZ	A	1385	-	-	0/0/4/4	0/1/1/1
5	BEZ	B	12	-	-	0/0/4/4	0/1/1/1
2	NAG	B	1279	1	1/1/5/7	0/6/23/26	0/1/1/1
3	SIA	B	1280	-	-	0/14/38/38	0/1/1/1
4	SO4	B	1284	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
5	BEZ	B	1386	-	-	0/0/4/4	0/1/1/1
4	SO4	C	1185	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1285	-	-	0/0/0/0	0/0/0/0
2	NAG	C	1379	1	-	0/6/23/26	0/1/1/1
5	BEZ	C	5013	1	-	0/2/2/4	0/1/1/1
5	BEZ	C	5014	-	-	0/0/4/4	0/1/1/1
2	NAG	D	2179	1	-	0/6/23/26	0/1/1/1
3	SIA	D	2180	-	-	0/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	D	2184	-	-	0/0/0/0	0/0/0/0
4	SO4	D	2384	-	-	0/0/0/0	0/0/0/0
5	BEZ	D	2385	-	-	0/0/4/4	0/1/1/1
5	BEZ	D	2386	-	-	0/0/4/4	0/1/1/1
2	NAG	E	2279	1	-	0/6/23/26	0/1/1/1
4	SO4	E	2284	-	-	0/0/0/0	0/0/0/0
4	SO4	E	2385	-	-	0/0/0/0	0/0/0/0
5	BEZ	E	2386	-	-	0/0/4/4	0/1/1/1
5	BEZ	E	2387	-	-	0/0/4/4	0/1/1/1
3	SIA	E	582	-	-	0/14/38/38	0/1/1/1
4	SO4	F	2185	-	-	0/0/0/0	0/0/0/0
4	SO4	F	2285	-	-	0/0/0/0	0/0/0/0
2	NAG	F	2379	1	1/1/5/7	0/6/23/26	0/1/1/1
5	BEZ	F	5023	1	-	0/2/2/4	0/1/1/1
5	BEZ	F	5024	-	-	0/0/4/4	0/1/1/1
3	SIA	F	682	-	-	0/14/38/38	0/1/1/1
2	NAG	G	3179	1	1/1/5/7	0/6/23/26	0/1/1/1
4	SO4	G	3184	-	-	0/0/0/0	0/0/0/0
4	SO4	G	3384	-	-	0/0/0/0	0/0/0/0
5	BEZ	G	3385	-	-	0/0/4/4	0/1/1/1
5	BEZ	G	3386	-	-	0/0/4/4	0/1/1/1
3	SIA	G	782	-	-	0/14/38/38	0/1/1/1
2	NAG	H	3279	1	-	2/6/23/26	0/1/1/1
4	SO4	H	3284	-	-	0/0/0/0	0/0/0/0
4	SO4	H	3385	-	-	0/0/0/0	0/0/0/0
5	BEZ	H	3386	-	-	0/0/4/4	0/1/1/1
5	BEZ	H	3387	-	-	0/0/4/4	0/1/1/1
3	SIA	H	882	-	-	0/14/38/38	0/1/1/1
4	SO4	I	3185	-	-	0/0/0/0	0/0/0/0
4	SO4	I	3285	-	-	0/0/0/0	0/0/0/0
2	NAG	I	3379	1	-	0/6/23/26	0/1/1/1
5	BEZ	I	3380	-	-	0/0/4/4	0/1/1/1
5	BEZ	I	3381	-	-	0/0/4/4	0/1/1/1
3	SIA	I	982	-	-	0/14/38/38	0/1/1/1
3	SIA	J	1082	-	-	0/14/38/38	0/1/1/1
2	NAG	J	4179	1	1/1/5/7	0/6/23/26	0/1/1/1
4	SO4	J	4184	-	-	0/0/0/0	0/0/0/0
4	SO4	J	4185	-	-	0/0/0/0	0/0/0/0
4	SO4	J	4384	-	-	0/0/0/0	0/0/0/0
5	BEZ	J	5041	1	-	0/2/2/4	0/1/1/1
5	BEZ	J	5042	-	-	0/0/4/4	0/1/1/1
3	SIA	K	1182	-	-	0/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	4279	1	1/1/5/7	0/6/23/26	0/1/1/1
4	SO4	K	4284	-	-	0/0/0/0	0/0/0/0
4	SO4	K	4385	-	-	0/0/0/0	0/0/0/0
5	BEZ	K	4386	-	-	0/0/4/4	0/1/1/1
5	BEZ	K	4387	-	-	0/0/4/4	0/1/1/1
3	SIA	L	1282	-	-	2/14/38/38	0/1/1/1
4	SO4	L	4285	-	-	0/0/0/0	0/0/0/0
2	NAG	L	4379	1	-	0/6/23/26	0/1/1/1
5	BEZ	L	4380	-	-	0/0/4/4	0/1/1/1
5	BEZ	L	4381	-	-	0/0/4/4	0/1/1/1

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3386	BEZ	C2-C1	-5.76	1.26	1.39
5	G	3386	BEZ	C6-C1	-5.62	1.27	1.39
5	H	3387	BEZ	C4-C3	-4.43	1.26	1.38
5	C	5013	BEZ	O2-C	-3.97	1.24	1.41
5	J	5041	BEZ	O2-C	-3.82	1.25	1.41

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3386	BEZ	C5-C4-C3	-5.95	109.49	119.93
5	J	5042	BEZ	C6-C1-C2	-4.94	108.20	117.55
5	A	1385	BEZ	C6-C1-C2	-3.62	110.70	117.55
2	E	2279	NAG	C2-N2-C7	-3.54	118.49	123.04
2	I	3379	NAG	C2-N2-C7	-3.53	118.50	123.04

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1279	NAG	C1
2	J	4179	NAG	C1
2	F	2379	NAG	C1
2	G	3179	NAG	C1
2	K	4279	NAG	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1181	SIA	O10-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
3	L	1282	SIA	C11-C10-N5-C5
3	A	1180	SIA	O10-C10-N5-C5
2	H	3279	NAG	C8-C7-N2-C2
2	H	3279	NAG	O7-C7-N2-C2

There are no ring outliers.

28 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1180	SIA	3	0
3	A	1181	SIA	10	0
5	A	1385	BEZ	2	0
5	B	12	BEZ	6	0
2	B	1279	NAG	1	0
3	B	1280	SIA	5	0
5	C	5013	BEZ	3	0
5	C	5014	BEZ	1	0
3	D	2180	SIA	8	0
5	D	2385	BEZ	3	0
3	E	582	SIA	2	0
2	F	2379	NAG	3	0
3	F	682	SIA	1	0
2	G	3179	NAG	1	0
5	G	3385	BEZ	1	0
3	G	782	SIA	6	0
5	H	3386	BEZ	1	0
3	H	882	SIA	1	0
4	I	3285	SO4	1	0
5	I	3380	BEZ	1	0
3	I	982	SIA	5	0
3	J	1082	SIA	5	0
2	J	4179	NAG	1	0
5	J	5042	BEZ	1	0
3	K	1182	SIA	7	0
2	K	4279	NAG	2	0
3	L	1282	SIA	7	0
5	L	4380	BEZ	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	532/532 (100%)	-0.03	2 (0%)	93	90	2, 25, 69, 83	0
1	B	532/532 (100%)	0.04	5 (0%)	85	78	4, 29, 74, 86	0
1	C	532/532 (100%)	-0.00	3 (0%)	90	84	2, 26, 64, 85	0
1	D	532/532 (100%)	-0.03	4 (0%)	87	80	2, 25, 70, 84	0
1	E	532/532 (100%)	0.03	5 (0%)	85	78	4, 30, 73, 86	0
1	F	532/532 (100%)	-0.03	5 (0%)	85	78	3, 26, 65, 81	0
1	G	532/532 (100%)	-0.05	0	100	100	3, 26, 67, 85	0
1	H	532/532 (100%)	0.00	3 (0%)	90	84	3, 27, 71, 84	0
1	I	532/532 (100%)	0.07	8 (1%)	76	63	3, 31, 74, 85	0
1	J	532/532 (100%)	-0.02	2 (0%)	93	90	2, 26, 64, 83	0
1	K	532/532 (100%)	0.02	4 (0%)	87	80	3, 27, 71, 85	0
1	L	532/532 (100%)	0.04	2 (0%)	93	90	2, 31, 73, 83	0
All	All	6384/6384 (100%)	0.00	43 (0%)	89	83	2, 27, 70, 86	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	306	LEU	4.6
1	E	307	ASP	4.1
1	H	400	THR	3.8
1	A	315	SER	3.5
1	I	318	LEU	3.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	D	2384	5/5	0.92	0.34	6.85	76,77,77,77	0
5	BEZ	K	4386	9/9	0.87	0.54	5.88	48,49,50,50	0
4	SO4	D	2184	5/5	0.87	0.38	5.80	100,100,101,101	0
4	SO4	A	1384	5/5	0.84	0.38	5.03	76,76,77,77	0
4	SO4	L	4285	5/5	0.96	0.25	4.47	74,74,75,75	0
5	BEZ	L	4380	9/9	0.85	0.56	3.71	59,59,60,60	0
5	BEZ	A	11	9/9	0.94	0.43	3.35	49,51,52,52	0
4	SO4	I	3185	5/5	0.89	0.27	3.07	95,95,96,96	0
4	SO4	K	4385	5/5	0.85	0.44	2.48	97,98,98,99	0
3	SIA	J	1082	21/21	0.88	0.28	2.20	59,71,76,77	0
4	SO4	G	3184	5/5	0.96	0.27	2.08	86,86,87,88	0
4	SO4	A	1184	5/5	0.96	0.28	2.05	94,94,94,95	0
4	SO4	K	4284	5/5	0.95	0.29	1.89	85,85,86,86	0
4	SO4	H	3284	5/5	0.94	0.33	1.85	84,84,85,85	0
5	BEZ	D	2385	9/9	0.90	0.44	1.74	51,51,53,53	0
5	BEZ	G	3385	9/9	0.89	0.32	1.73	58,59,60,60	0
5	BEZ	J	5041	8/9	0.96	0.35	1.65	41,45,45,46	0
4	SO4	G	3384	5/5	0.95	0.33	1.62	81,81,81,81	0
3	SIA	F	682	21/21	0.92	0.25	1.60	52,56,62,62	0
3	SIA	G	782	21/21	0.90	0.27	1.52	61,69,73,74	0
3	SIA	I	982	21/21	0.89	0.29	1.44	51,60,64,65	0
5	BEZ	B	12	9/9	0.88	0.41	1.37	52,53,54,55	0
4	SO4	B	1284	5/5	0.93	0.23	1.36	80,80,81,81	0
4	SO4	C	1185	5/5	0.85	0.28	1.04	100,100,101,101	0
4	SO4	J	4184	5/5	0.95	0.22	1.01	94,94,95,95	0
3	SIA	B	1280	21/21	0.86	0.28	0.99	45,61,66,67	0
3	SIA	D	2180	21/21	0.90	0.27	0.93	57,69,72,73	0
3	SIA	A	1180	21/21	0.88	0.25	0.90	64,71,74,75	0
4	SO4	F	2185	5/5	0.86	0.28	0.79	106,106,106,106	0
4	SO4	H	3385	5/5	0.86	0.28	0.75	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	J	4185	5/5	0.87	0.25	0.60	96,96,97,97	0
3	SIA	L	1282	21/21	0.92	0.24	0.50	50,55,63,65	0
5	BEZ	I	3380	9/9	0.91	0.33	0.48	53,53,54,55	0
5	BEZ	H	3386	9/9	0.94	0.26	0.47	49,51,51,51	0
3	SIA	H	882	21/21	0.89	0.23	0.43	52,66,69,70	0
5	BEZ	F	5023	8/9	0.96	0.24	0.38	46,49,50,51	0
3	SIA	E	582	21/21	0.89	0.24	0.29	42,60,70,70	0
4	SO4	F	2285	5/5	0.93	0.24	0.27	80,80,81,81	0
4	SO4	I	3285	5/5	0.95	0.23	0.25	79,79,79,80	0
3	SIA	K	1182	21/21	0.93	0.23	0.22	60,63,67,69	0
5	BEZ	E	2387	9/9	0.92	0.22	-0.04	42,43,43,44	0
5	BEZ	F	5024	9/9	0.91	0.23	-0.06	42,44,46,46	0
5	BEZ	C	5013	8/9	0.97	0.20	-0.09	40,44,46,46	0
5	BEZ	K	4387	9/9	0.90	0.26	-0.13	36,39,40,41	0
4	SO4	C	1285	5/5	0.96	0.19	-0.27	76,76,77,77	0
3	SIA	A	1181	21/21	0.90	0.20	-0.34	44,57,67,68	0
5	BEZ	H	3387	9/9	0.84	0.21	-0.44	41,43,45,46	0
5	BEZ	A	1385	9/9	0.89	0.19	-0.47	49,50,52,52	0
5	BEZ	D	2386	9/9	0.93	0.16	-0.56	44,45,46,46	0
5	BEZ	C	5014	9/9	0.89	0.20	-0.65	36,40,40,41	0
5	BEZ	J	5042	9/9	0.95	0.16	-0.71	44,45,46,46	0
4	SO4	J	4384	5/5	0.94	0.19	-0.76	84,85,85,86	0
5	BEZ	E	2386	9/9	0.92	0.15	-0.79	47,47,49,50	0
4	SO4	E	2385	5/5	0.94	0.17	-0.82	94,94,94,95	0
5	BEZ	G	3386	9/9	0.90	0.20	-0.82	45,47,48,49	0
4	SO4	E	2284	5/5	0.94	0.17	-1.10	85,86,86,86	0
4	SO4	B	1385	5/5	0.93	0.16	-1.24	96,97,97,98	0
2	NAG	D	2179	14/15	0.86	0.45	-	70,76,78,79	0
2	NAG	K	4279	14/15	0.85	0.23	-	63,67,71,71	0
2	NAG	B	1279	14/15	0.93	0.30	-	59,64,68,70	0
2	NAG	L	4379	14/15	0.91	0.23	-	56,59,62,63	0
2	NAG	G	3179	14/15	0.86	0.24	-	67,72,75,75	0
2	NAG	C	1379	14/15	0.89	0.23	-	59,64,68,68	0
2	NAG	E	2279	14/15	0.94	0.29	-	57,60,62,63	0
2	NAG	J	4179	14/15	0.87	0.36	-	69,75,78,78	0
5	BEZ	B	1386	9/9	0.85	0.22	-	54,55,56,56	0
5	BEZ	I	3381	9/9	0.89	0.19	-	52,52,53,54	0
2	NAG	F	2379	14/15	0.90	0.16	-	59,64,66,66	0
2	NAG	H	3279	14/15	0.83	0.28	-	63,66,69,69	0
5	BEZ	L	4381	9/9	0.88	0.20	-	54,55,55,55	0
2	NAG	A	1179	14/15	0.76	0.53	-	70,76,78,78	0
2	NAG	I	3379	14/15	0.91	0.32	-	57,61,62,63	0

6.5 Other polymers (i)

There are no such residues in this entry.