



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:06 PM UTC

PDB ID : 1IWA / pdb_00001iwa
Title : RUBISCO FROM GALDIERIA PARTITA
Authors : Okano, Y.; Mizohata, E.; Xie, Y.; Matsumura, H.; Sugawara, H.; Inoue, T.;
Yokota, A.; Kai, Y.
Deposited on : 2002-04-30
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

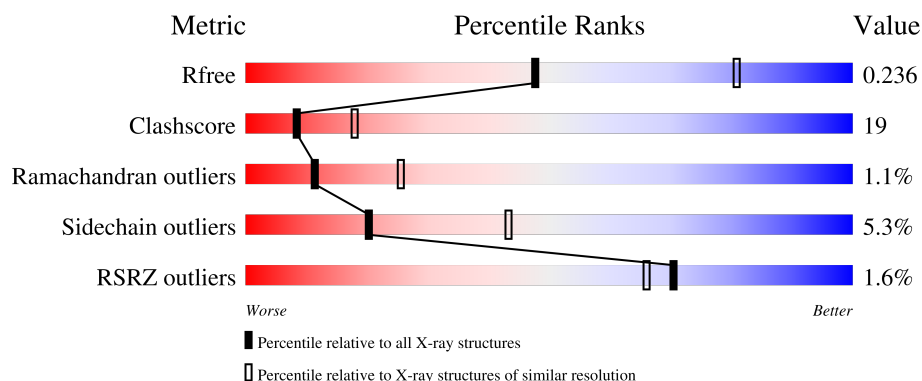
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	493	% 56% 35% • •
1	C	493	% 65% 26% 5% •
1	E	493	% 60% 31% • • •
1	G	493	5% 55% 36% 5% •
1	I	493	% 58% 34% • •

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Mol	Chain	Length	Quality of chain
1	K	493	4%54%39%
1	M	493	2%61%30%
1	O	493	%57%35%
2	B	138	67%30%
2	D	138	63%33%
2	F	138	65%33%
2	H	138	65%33%
2	J	138	71%28%
2	L	138	69%28%
2	N	138	63%35%
2	P	138	%62%33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42000 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 ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	C	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	E	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	G	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	I	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	K	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	M	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	O	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			

- Molecule 2 is a protein called ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit.

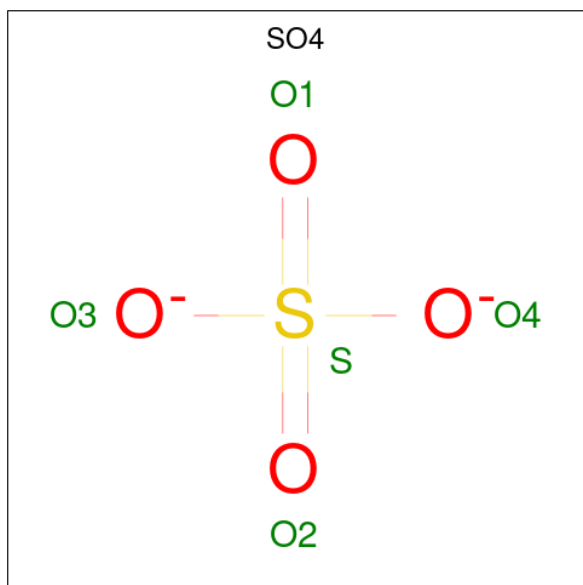
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	D	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	F	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	H	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	J	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	N	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	P	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

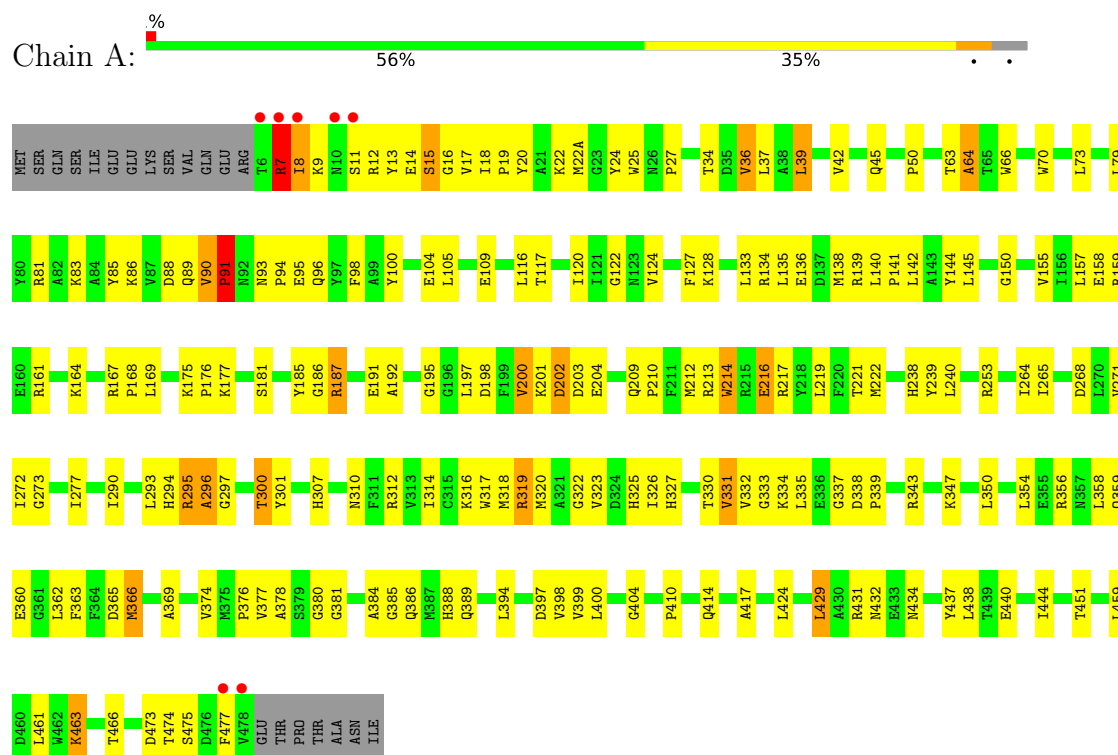
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	282	Total 282	O 282	0	0
4	B	102	Total 102	O 102	0	0
4	C	313	Total 313	O 313	0	0
4	D	117	Total 117	O 117	0	0
4	E	281	Total 281	O 281	0	0
4	F	113	Total 113	O 113	0	0
4	G	191	Total 191	O 191	0	0
4	H	120	Total 120	O 120	0	0
4	I	275	Total 275	O 275	0	0
4	J	145	Total 145	O 145	0	0
4	K	196	Total 196	O 196	0	0
4	L	143	Total 143	O 143	0	0
4	M	284	Total 284	O 284	0	0
4	N	134	Total 134	O 134	0	0
4	O	283	Total 283	O 283	0	0
4	P	133	Total 133	O 133	0	0

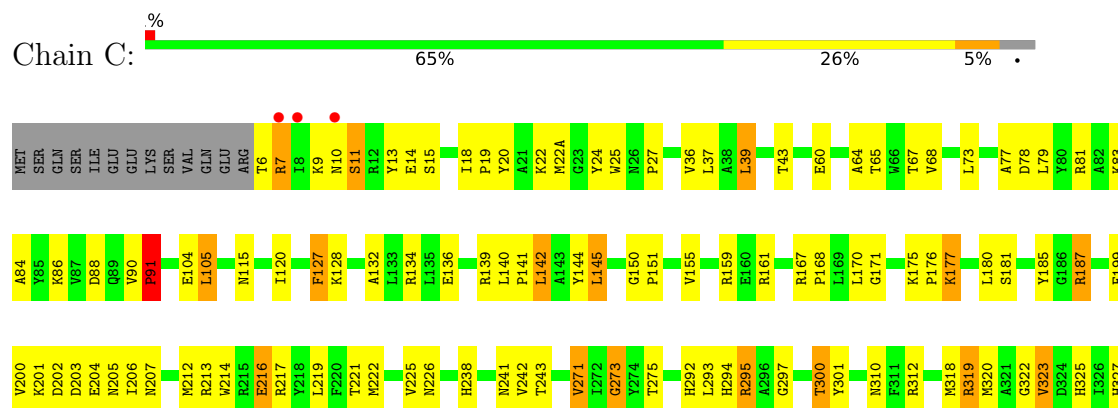
3 Residue-property plots [i](#)

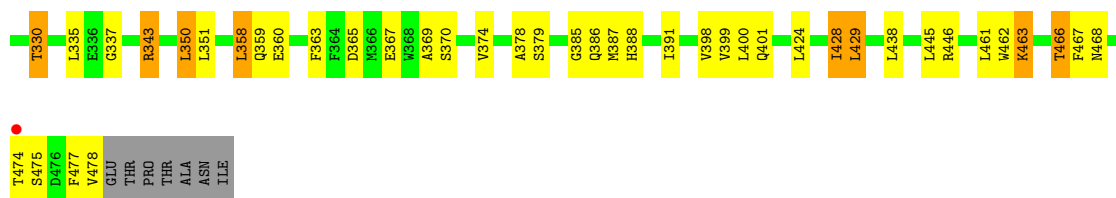
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

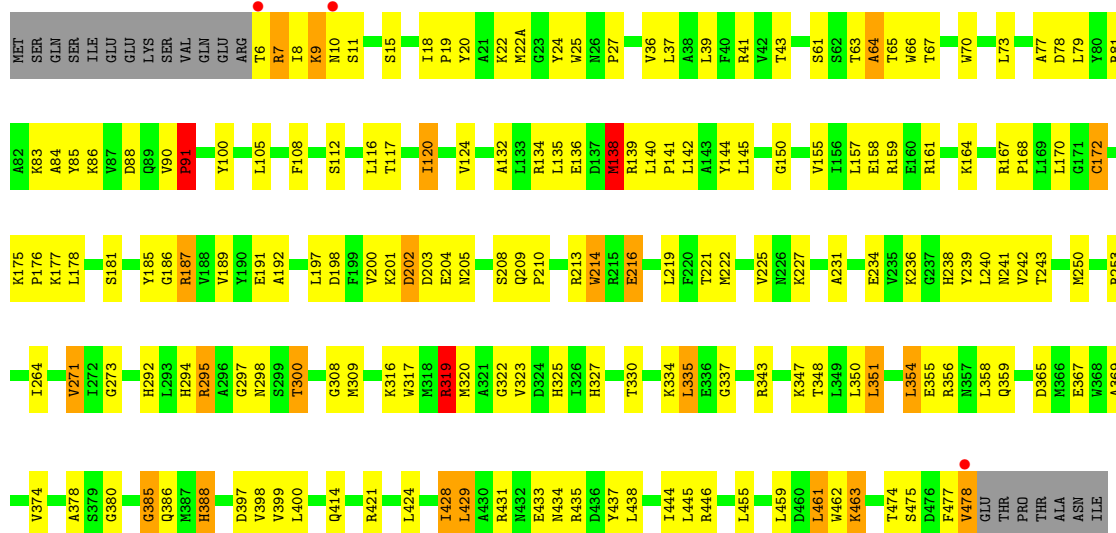


- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

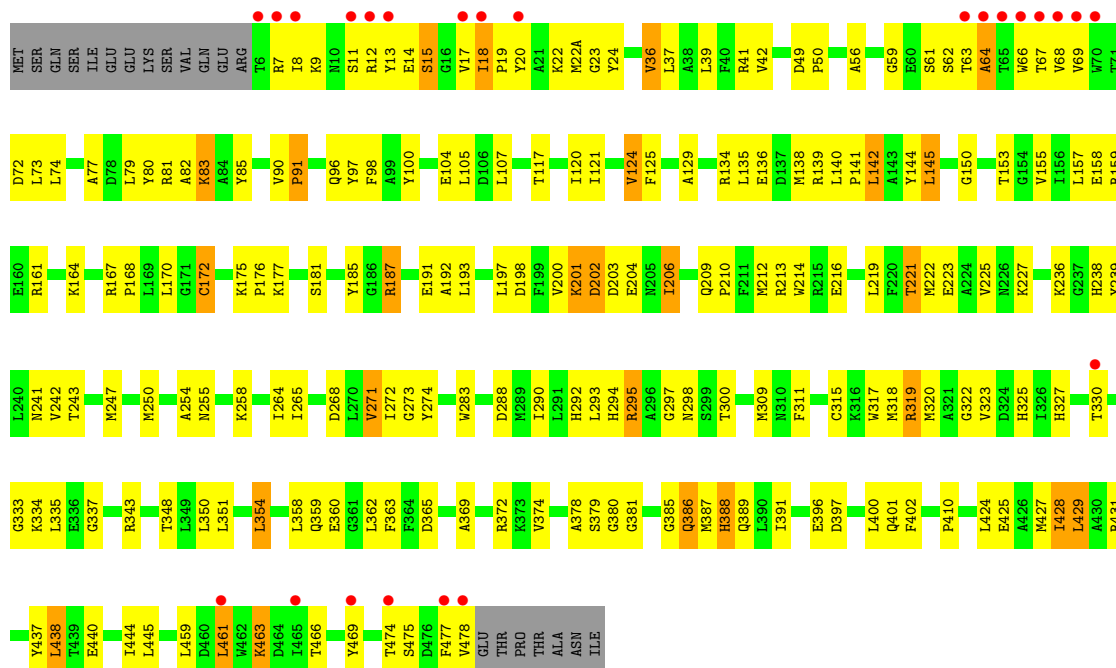




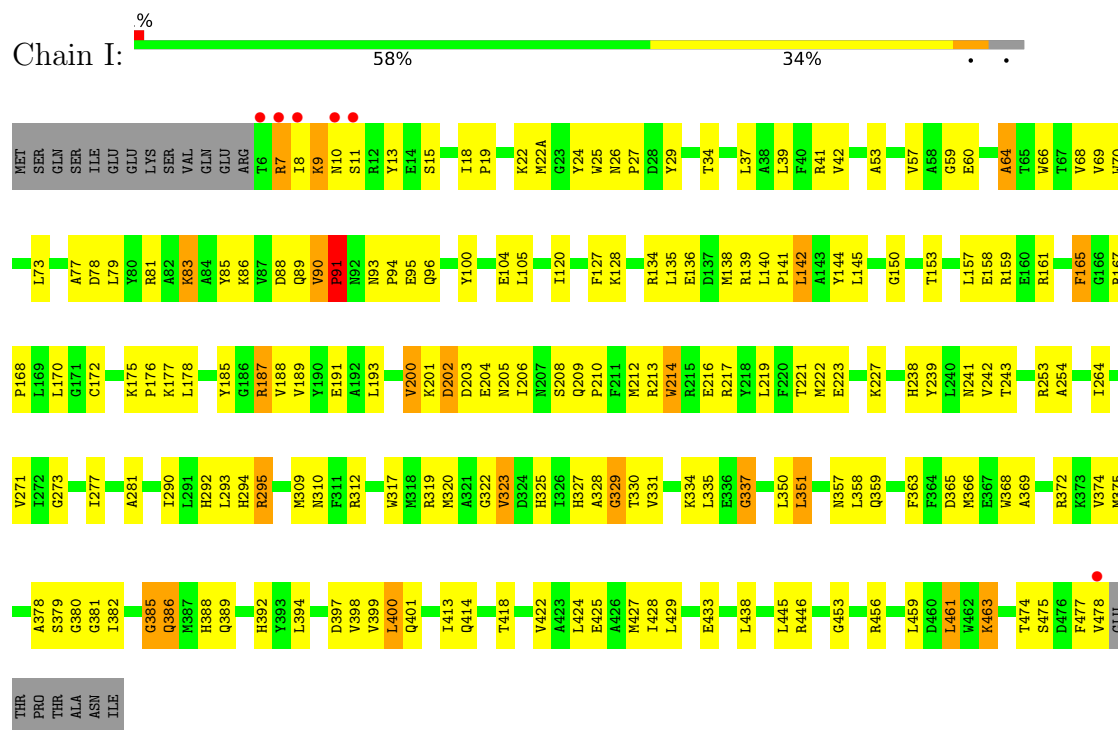
- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit



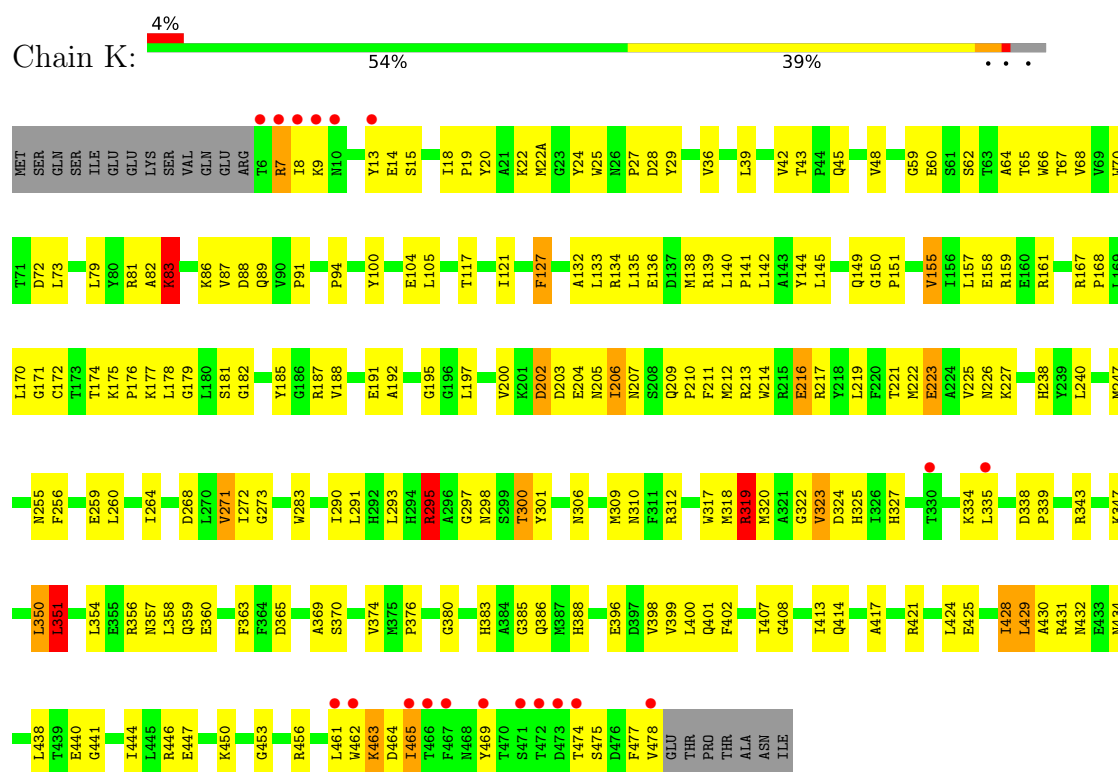
- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit



• Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

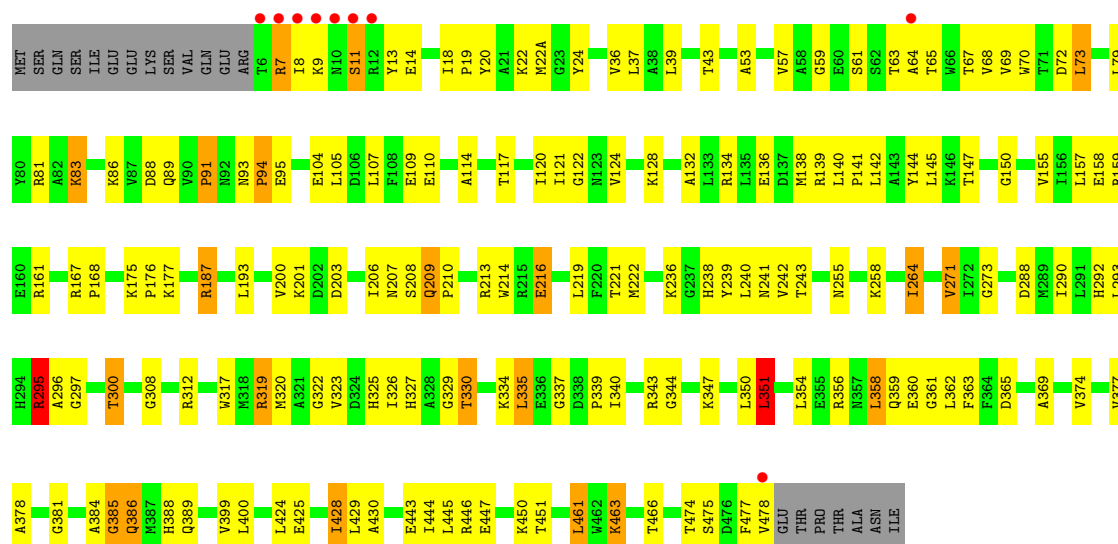


• Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

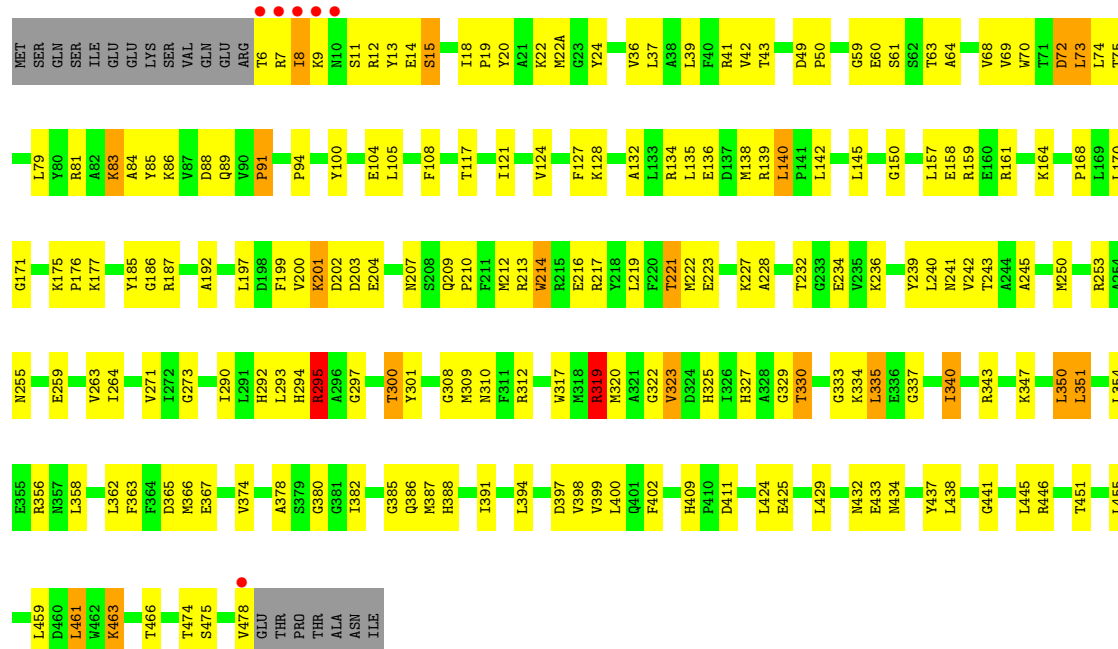


• Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

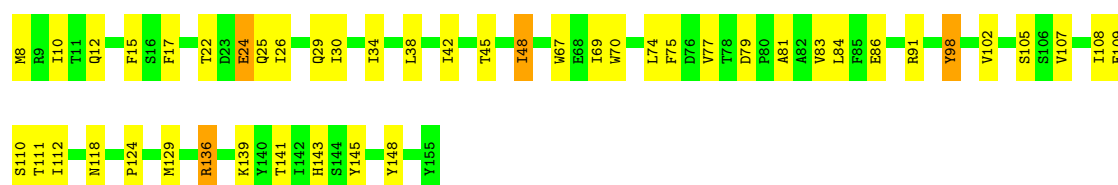




• Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

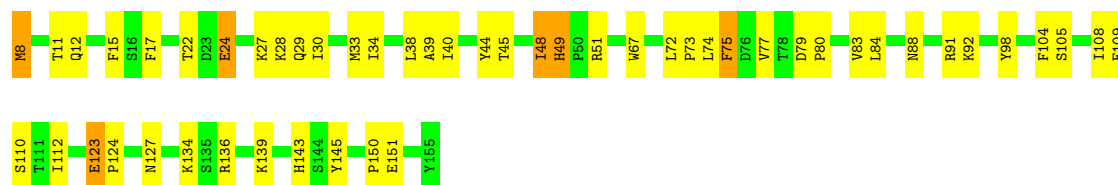


• Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit



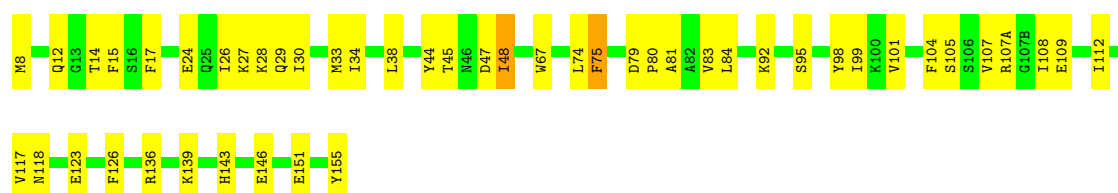
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain D:  63% 33%



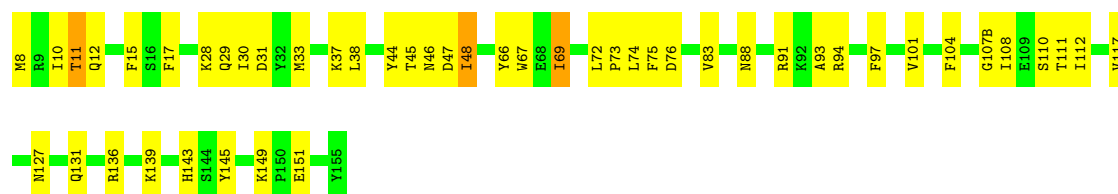
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain F:  65% 33%



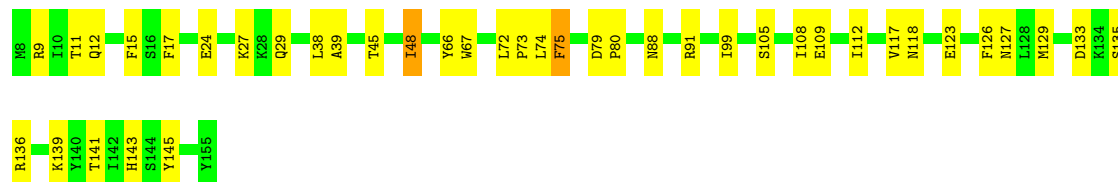
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain H:  65% 33%



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

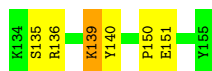
Chain J:  71% 28%



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain L:  69% 28%





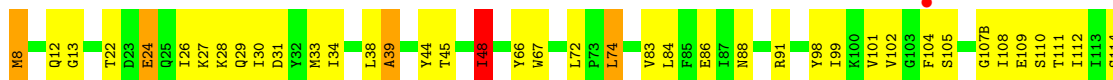
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain N: 63% 35% ..



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain P: % 62% 33% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.33Å 146.99Å 197.23Å 90.00° 99.79° 90.00°	Depositor
Resolution (Å)	25.65 – 2.60 25.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.65-2.60) 98.9 (25.65-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.172 , 0.235 0.172 , 0.236	Depositor DCC
R_{free} test set	8610 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42000	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/3793	0.96	18/5138 (0.4%)
1	C	0.41	0/3793	0.97	14/5138 (0.3%)
1	E	0.43	1/3793 (0.0%)	0.96	14/5138 (0.3%)
1	G	0.39	0/3793	0.93	14/5138 (0.3%)
1	I	0.38	0/3793	0.95	17/5138 (0.3%)
1	K	0.38	0/3793	0.91	13/5138 (0.3%)
1	M	0.41	0/3793	0.96	14/5138 (0.3%)
1	O	0.40	0/3793	0.94	20/5138 (0.4%)
2	B	0.37	0/1173	0.94	3/1583 (0.2%)
2	D	0.36	0/1173	0.99	7/1583 (0.4%)
2	F	0.37	0/1173	0.99	7/1583 (0.4%)
2	H	0.40	0/1173	0.94	2/1583 (0.1%)
2	J	0.39	0/1173	1.00	6/1583 (0.4%)
2	L	0.40	0/1173	1.05	7/1583 (0.4%)
2	N	0.38	0/1173	0.95	2/1583 (0.1%)
2	P	0.37	0/1173	1.00	5/1583 (0.3%)
All	All	0.39	1/39728 (0.0%)	0.96	163/53768 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	138	MET	SD-CE	-9.94	1.54	1.79

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	12	GLN	N-CA-C	-9.44	98.35	110.53
1	E	214	TRP	N-CA-C	9.06	121.16	111.28
1	C	214	TRP	N-CA-C	8.72	120.87	111.36
2	F	12	GLN	N-CA-C	-8.63	98.89	110.55
1	E	365	ASP	N-CA-C	-8.57	97.79	110.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3712	0	3694	161	0
1	C	3712	0	3694	129	0
1	E	3712	0	3694	144	0
1	G	3712	0	3694	187	0
1	I	3712	0	3694	152	0
1	K	3712	0	3694	211	0
1	M	3712	0	3694	136	0
1	O	3712	0	3694	159	0
2	B	1144	0	1131	37	0
2	D	1144	0	1131	46	0
2	F	1144	0	1131	44	0
2	H	1144	0	1131	46	0
2	J	1144	0	1131	38	0
2	L	1144	0	1131	39	0
2	N	1144	0	1131	48	0
2	P	1144	0	1131	49	0
3	A	5	0	0	0	0
3	C	5	0	0	1	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	1	0
3	K	5	0	0	0	0
3	M	5	0	0	0	0
3	O	5	0	0	0	0
4	A	282	0	0	11	0
4	B	102	0	0	2	0
4	C	313	0	0	10	0
4	D	117	0	0	3	0
4	E	281	0	0	8	0
4	F	113	0	0	5	0
4	G	191	0	0	9	0
4	H	120	0	0	5	0
4	I	275	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	145	0	0	1	0
4	K	196	0	0	10	0
4	L	143	0	0	3	0
4	M	284	0	0	10	0
4	N	134	0	0	5	0
4	O	283	0	0	13	0
4	P	133	0	0	5	0
All	All	42000	0	38600	1480	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 19.

The worst 5 of 1480 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:LEU:H	1:M:7:ARG:HG2	1.20	1.05
2:B:8:MET:HE1	2:B:10:ILE:HD13	1.35	1.05
1:G:273:GLY:HA3	1:K:273:GLY:HA3	1.42	1.01
2:L:139:LYS:HE2	2:L:139:LYS:HA	1.42	1.01
1:O:159:ARG:HD3	1:O:164:LYS:O	1.62	0.99

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	471/493 (96%)	436 (93%)	26 (6%)	9 (2%)	6	13
1	C	471/493 (96%)	440 (93%)	27 (6%)	4 (1%)	16	34
1	E	471/493 (96%)	441 (94%)	27 (6%)	3 (1%)	21	42
1	G	471/493 (96%)	425 (90%)	39 (8%)	7 (2%)	8	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	471/493 (96%)	443 (94%)	24 (5%)	4 (1%)	16	34
1	K	471/493 (96%)	423 (90%)	45 (10%)	3 (1%)	21	42
1	M	471/493 (96%)	438 (93%)	27 (6%)	6 (1%)	9	21
1	O	471/493 (96%)	438 (93%)	27 (6%)	6 (1%)	9	21
2	B	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	18
2	D	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	38
2	F	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	38
2	H	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	38
2	J	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	18
2	L	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	38
2	N	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	18
2	P	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	18
All	All	4856/5048 (96%)	4474 (92%)	328 (7%)	54 (1%)	11	25

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	VAL
1	C	91	PRO
1	K	465	ILE
1	O	11	SER
1	A	295	ARG

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	384/403 (95%)	367 (96%)	17 (4%)	25	50
1	C	384/403 (95%)	359 (94%)	25 (6%)	15	35
1	E	384/403 (95%)	351 (91%)	33 (9%)	10	22
1	G	384/403 (95%)	363 (94%)	21 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	384/403 (95%)	363 (94%)	21 (6%)	19	41
1	K	384/403 (95%)	362 (94%)	22 (6%)	18	40
1	M	384/403 (95%)	360 (94%)	24 (6%)	16	36
1	O	384/403 (95%)	363 (94%)	21 (6%)	19	41
2	B	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	D	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	F	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	H	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	J	126/126 (100%)	124 (98%)	2 (2%)	55	79
2	L	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	N	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	P	126/126 (100%)	121 (96%)	5 (4%)	28	55
All	All	4080/4232 (96%)	3862 (95%)	218 (5%)	20	43

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	9	LYS
1	K	206	ILE
1	O	221	THR
1	I	142	LEU
1	I	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	255	ASN
2	P	12	GLN
1	K	255	ASN
1	O	401	GLN
2	N	143	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	SO4	C	4002	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	K	4008	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	O	4007	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	I	4005	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	E	4003	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	M	4006	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	G	4004	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	4001	-	4,4,4	0.38	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4002	SO4	1	0
3	I	4005	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	473/493 (95%)	-0.42	7 (1%) 72 68	9, 27, 56, 77	0
1	C	473/493 (95%)	-0.54	4 (0%) 82 80	7, 21, 48, 70	0
1	E	473/493 (95%)	-0.55	3 (0%) 85 83	8, 21, 48, 75	0
1	G	473/493 (95%)	-0.09	24 (5%) 33 28	8, 31, 83, 101	0
1	I	473/493 (95%)	-0.44	6 (1%) 75 71	8, 25, 54, 87	0
1	K	473/493 (95%)	-0.11	19 (4%) 42 37	7, 29, 83, 98	0
1	M	473/493 (95%)	-0.61	9 (1%) 66 61	7, 19, 47, 95	0
1	O	473/493 (95%)	-0.51	6 (1%) 75 71	6, 22, 53, 96	0
2	B	138/138 (100%)	-0.29	0 100 100	14, 30, 46, 51	0
2	D	138/138 (100%)	-0.39	0 100 100	11, 28, 46, 54	0
2	F	138/138 (100%)	-0.47	0 100 100	15, 27, 42, 49	0
2	H	138/138 (100%)	-0.57	0 100 100	10, 22, 39, 48	0
2	J	138/138 (100%)	-0.62	0 100 100	9, 21, 37, 41	0
2	L	138/138 (100%)	-0.64	0 100 100	11, 22, 36, 44	0
2	N	138/138 (100%)	-0.54	0 100 100	9, 24, 41, 54	0
2	P	138/138 (100%)	-0.54	1 (0%) 84 82	10, 23, 41, 48	0
All	All	4888/5048 (96%)	-0.43	79 (1%) 70 66	6, 24, 56, 101	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	8	ILE	5.5
1	I	6	THR	5.0
1	O	7	ARG	4.8
1	M	6	THR	4.8
1	O	6	THR	4.7

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	G	4004	5/5	0.81	0.18	91,91,91,92	0
3	SO4	K	4008	5/5	0.83	0.16	100,100,101,101	0
3	SO4	A	4001	5/5	0.93	0.10	51,52,53,53	0
3	SO4	C	4002	5/5	0.95	0.10	60,61,61,61	0
3	SO4	E	4003	5/5	0.95	0.09	59,60,60,60	0
3	SO4	I	4005	5/5	0.97	0.07	40,41,42,43	0
3	SO4	O	4007	5/5	0.98	0.06	41,41,41,43	0
3	SO4	M	4006	5/5	1.00	0.03	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.