



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:21 PM GMT

PDB ID : 2V6A  
Title : CRYSTAL STRUCTURE OF CHLAMYDOMONAS REINHARDTII RUBISCO WITH LARGE-SUBUNIT MUTATIONS V331A, G344S  
Authors : Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.  
Deposited on : 2007-07-14  
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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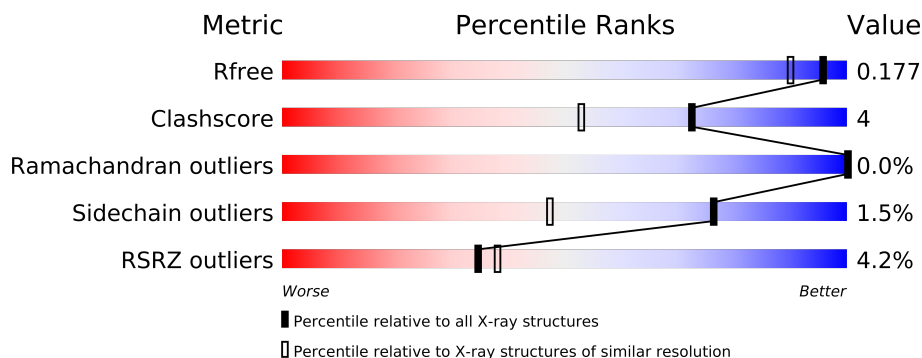
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.50 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))
$R_{free}$	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	
1	C	475	
1	D	475	
1	E	475	
1	F	475	
1	G	475	
1	H	475	
2	I	140	
2	J	140	
2	K	140	
2	L	140	
2	M	140	
2	N	140	

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Mol	Chain	Length	Quality of chain
2	O	140	
2	P	140	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	1479	-	X
5	EDO	A	1480	-	X
5	EDO	A	1482	-	X
5	EDO	A	1484	-	X
5	EDO	B	1480	-	X
5	EDO	B	1482	-	X
5	EDO	C	1478	-	X
5	EDO	C	1479	-	X
5	EDO	C	1480	-	X
5	EDO	C	1482	-	X
5	EDO	D	1478	-	X
5	EDO	D	1479	-	X
5	EDO	D	1480	-	X
5	EDO	D	1482	-	X
5	EDO	E	1478	-	X
5	EDO	E	1480	-	X
5	EDO	F	1479	-	X
5	EDO	F	1481	-	X
5	EDO	F	1483	-	X
5	EDO	G	1479	-	X
5	EDO	G	1480	-	X
5	EDO	H	1481	-	X
5	EDO	I	1141	-	X
5	EDO	J	1141	-	X
5	EDO	K	1141	-	X
5	EDO	L	1141	-	X
5	EDO	M	1141	-	X
5	EDO	O	1141	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42413 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	9	0
			3658	2309	640	680	29			
1	B	467	Total	C	N	O	S	0	9	0
			3658	2309	640	680	29			
1	C	467	Total	C	N	O	S	0	8	0
			3655	2306	640	680	29			
1	D	466	Total	C	N	O	S	0	10	0
			3656	2307	639	681	29			
1	E	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	F	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	G	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	H	467	Total	C	N	O	S	0	11	0
			3664	2313	640	682	29			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	CONFLICT	UNP P00877
A	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
A	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
B	46	PRO	LEU	CONFLICT	UNP P00877
B	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
B	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
C	46	PRO	LEU	CONFLICT	UNP P00877
C	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
C	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
D	46	PRO	LEU	CONFLICT	UNP P00877
D	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
D	344	SER	GLY	ENGINEERED MUTATION	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
E	46	PRO	LEU	CONFLICT	UNP P00877
E	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
E	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
F	46	PRO	LEU	CONFLICT	UNP P00877
F	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
F	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
G	46	PRO	LEU	CONFLICT	UNP P00877
G	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
G	344	SER	GLY	ENGINEERED MUTATION	UNP P00877
H	46	PRO	LEU	CONFLICT	UNP P00877
H	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
H	344	SER	GLY	ENGINEERED MUTATION	UNP P00877

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	3	0
			1147	740	190	205	12			
2	J	140	Total	C	N	O	S	0	4	0
			1155	747	190	206	12			
2	K	140	Total	C	N	O	S	0	5	0
			1162	753	190	207	12			
2	L	140	Total	C	N	O	S	0	6	0
			1163	754	190	206	13			
2	M	140	Total	C	N	O	S	0	6	0
			1164	754	190	207	13			
2	N	140	Total	C	N	O	S	0	5	0
			1163	754	190	206	13			
2	O	140	Total	C	N	O	S	0	6	0
			1158	748	190	206	14			
2	P	140	Total	C	N	O	S	0	5	0
			1162	753	190	207	12			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

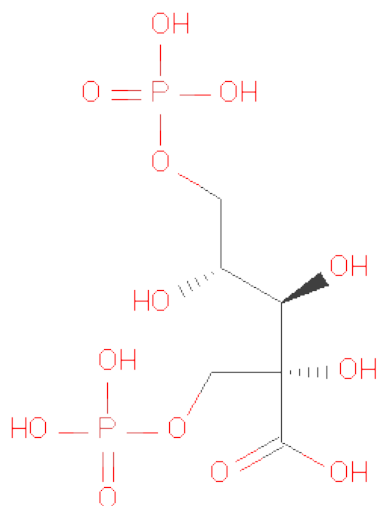
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



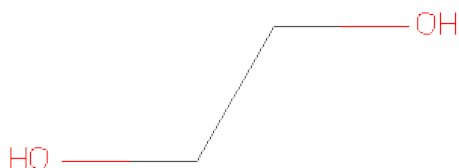
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			4	2	2			
5	A	1	Total	C	O		0	0
			4	2	2			
5	A	1	Total	C	O		0	0
			4	2	2			
5	A	1	Total	C	O		0	0
			4	2	2			
5	A	1	Total	C	O		0	0
			4	2	2			
5	B	1	Total	C	O		0	0
			4	2	2			
5	B	1	Total	C	O		0	0
			4	2	2			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 4 2 2	0	0
5	M	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	327	Total O 327 327	0	0
6	B	334	Total O 334 334	0	0
6	C	320	Total O 320 320	0	0
6	D	332	Total O 332 332	0	0
6	E	344	Total O 344 344	0	0
6	F	330	Total O 330 330	0	0
6	G	324	Total O 324 324	0	0
6	H	330	Total O 330 330	0	0
6	I	97	Total O 97 97	0	0
6	J	106	Total O 106 106	0	0
6	K	100	Total O 100 100	0	0

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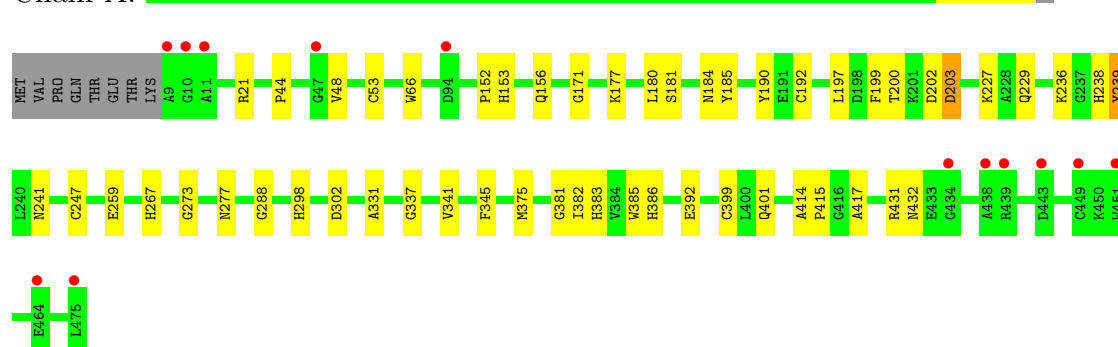
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	111	Total 111	O 111	0	0
6	M	112	Total 112	O 112	0	0
6	N	111	Total 111	O 111	0	0
6	O	114	Total 114	O 114	0	0
6	P	100	Total 100	O 100	0	0

### 3 Residue-property plots

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.

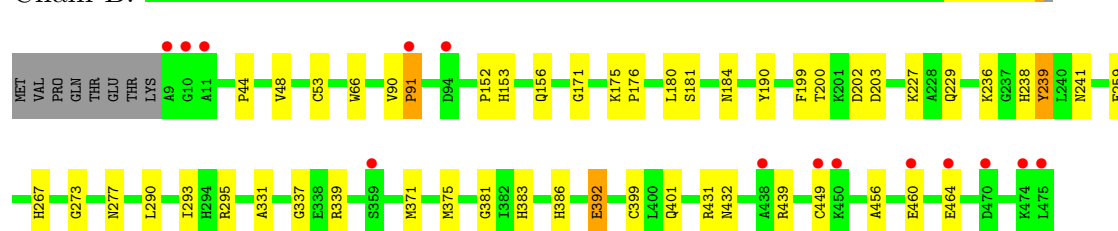
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:



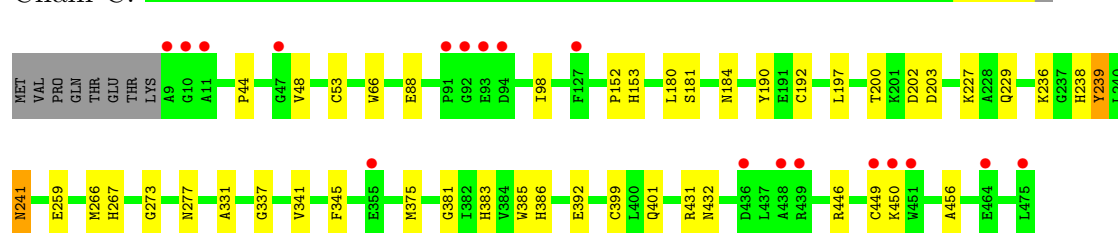
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



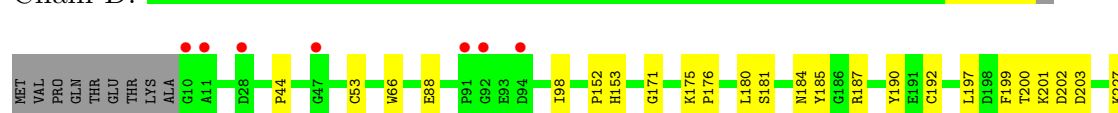
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain C:



#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

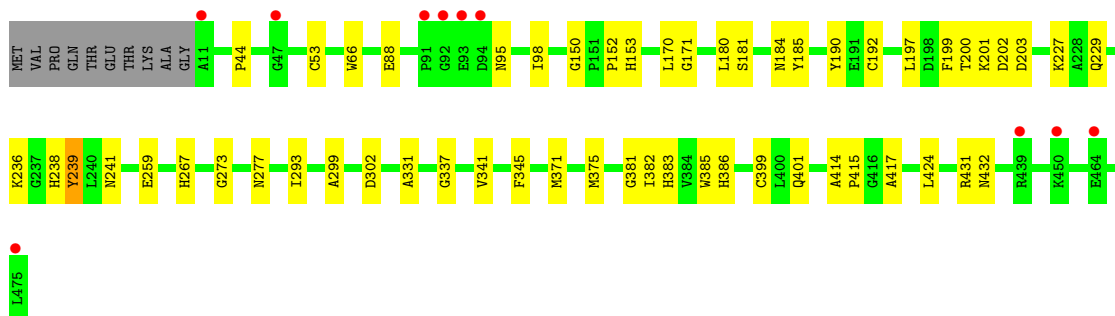
Chain D:





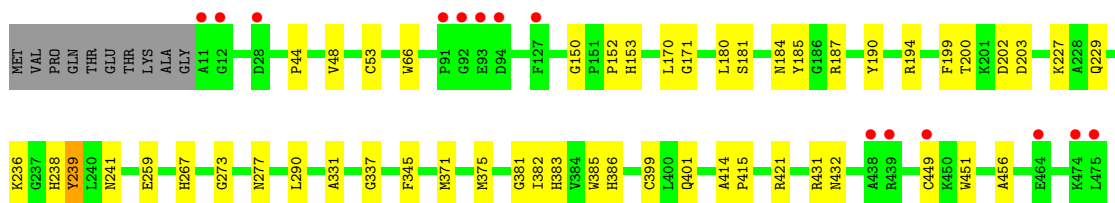
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E:



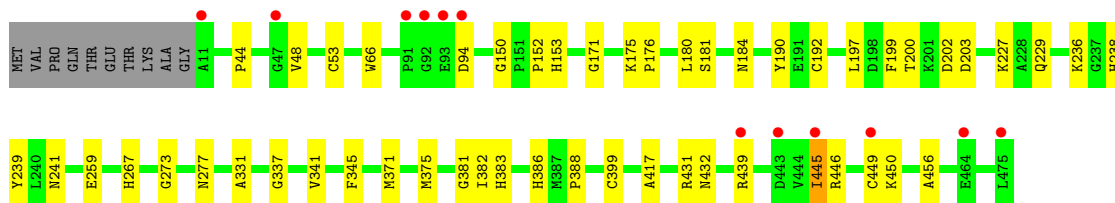
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain F:



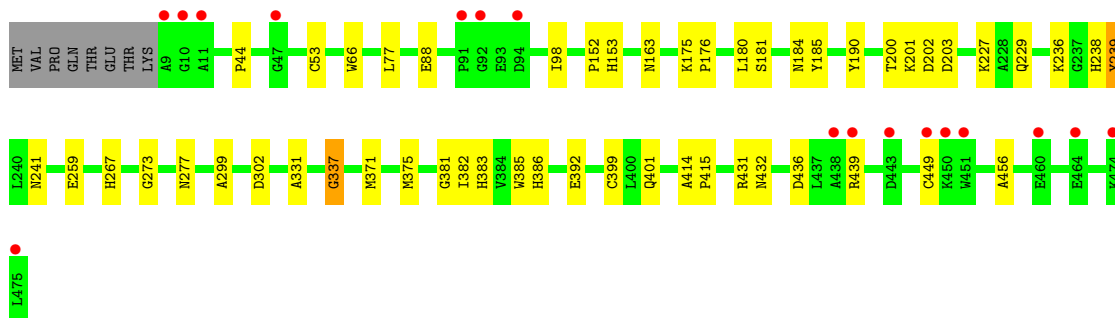
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain H:



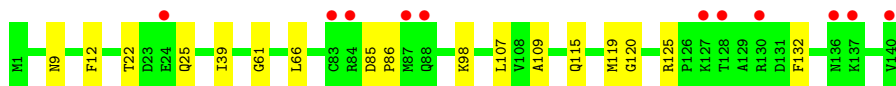
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain I: 



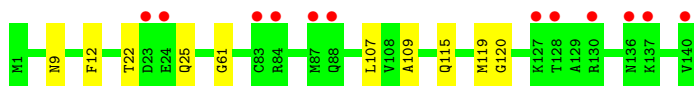
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain J: 



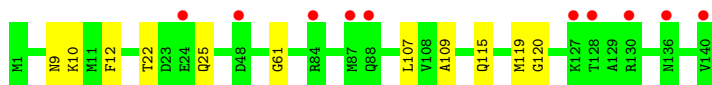
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain K: 



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain L: 



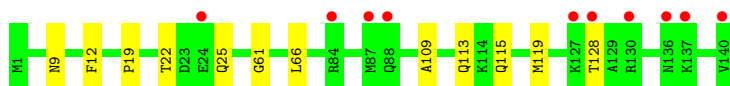
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain M: 



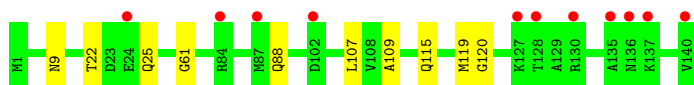
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain N: 



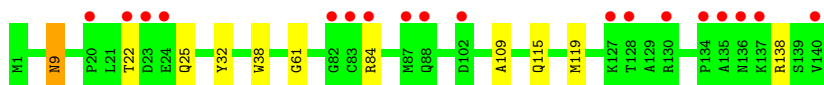
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain O: 



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.91Å 196.63Å 201.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 14.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-1.50) 95.9 (14.99-1.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.192 0.176 , 0.177	Depositor DCC
$R_{free}$ test set	39010 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 42.0	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 779980 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	42413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, EDO, HYP, MME, SMC, KCX

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	0.50	0/3743	0.65	0/5059
1	B	0.49	0/3743	0.64	0/5059
1	C	0.50	0/3735	0.64	0/5048
1	D	0.51	0/3747	0.65	2/5064 (0.0%)
1	E	0.50	0/3734	0.65	0/5047
1	F	0.51	0/3734	0.65	1/5047 (0.0%)
1	G	0.51	0/3734	0.66	0/5047
1	H	0.52	0/3758	0.65	0/5080
2	I	0.47	0/1184	0.60	0/1608
2	J	0.48	0/1197	0.62	0/1626
2	K	0.48	0/1210	0.62	0/1644
2	L	0.48	0/1217	0.62	0/1654
2	M	0.46	0/1218	0.62	0/1654
2	N	0.47	0/1212	0.60	0/1646
2	O	0.47	0/1213	0.62	0/1646
2	P	0.49	0/1210	0.61	0/1644
All	All	0.50	0/39589	0.64	3/53573 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	D	187	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	D	449	CYS	CA-CB-SG	5.05	123.08	114.00

There are no chirality outliers.

There are no planarity outliers.



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3658	0	3556	43	0
1	B	3658	0	3556	36	0
1	C	3655	0	3551	34	0
1	D	3656	0	3551	34	0
1	E	3648	0	3548	41	0
1	F	3648	0	3546	39	0
1	G	3648	0	3546	35	0
1	H	3664	0	3563	38	0
2	I	1147	0	1125	9	0
2	J	1155	0	1130	12	0
2	K	1162	0	1135	8	0
2	L	1163	0	1136	8	0
2	M	1164	0	1136	9	0
2	N	1163	0	1135	11	0
2	O	1158	0	1132	8	0
2	P	1162	0	1135	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	C	21	0	7	0	0
4	D	21	0	7	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	7	0	0
4	H	21	0	7	0	0
5	A	28	0	42	0	0
5	B	20	0	30	1	0
5	C	24	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	20	0	30	0	0
5	E	16	0	24	0	0
5	F	24	0	36	1	0
5	G	20	0	30	0	0
5	H	20	0	30	0	0
5	I	8	0	12	0	0
5	J	8	0	12	0	0
5	K	8	0	12	0	0
5	L	8	0	12	0	0
5	M	8	0	12	0	0
5	N	8	0	12	0	0
5	O	8	0	12	0	0
5	P	8	0	12	0	0
6	A	327	0	0	3	0
6	B	334	0	0	3	0
6	C	320	0	0	1	0
6	D	332	0	0	3	0
6	E	344	0	0	3	0
6	F	330	0	0	3	0
6	G	324	0	0	3	0
6	H	330	0	0	3	0
6	I	97	0	0	0	0
6	J	106	0	0	0	0
6	K	100	0	0	0	0
6	L	111	0	0	0	0
6	M	112	0	0	2	0
6	N	111	0	0	2	0
6	O	114	0	0	0	0
6	P	100	0	0	0	0
All	All	42413	0	37891	325	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (325) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.01	0.99
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.01	0.99
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.02	0.99
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.05	0.98
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.02	0.97
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.02	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:375[B]:MET:SD	1:G:399[B]:CYS:SG	2.63	0.96
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.03	0.95
1:D:184:ASN:HD22	2:N:115:GLN:HE21	1.14	0.95
1:G:184:ASN:HD22	2:M:115:GLN:HE21	1.14	0.94
1:H:371[B]:MET:SD	6:H:1127:HOH:O	2.25	0.94
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.06	0.93
1:H:184:ASN:HD22	2:J:115:GLN:HE21	1.16	0.92
1:C:184:ASN:HD22	2:I:115:GLN:HE21	1.18	0.90
1:F:184:ASN:HD22	2:P:115:GLN:HE21	1.19	0.89
1:E:184:ASN:HD22	2:K:115:GLN:HE21	1.18	0.88
1:A:184:ASN:HD22	2:O:115:GLN:HE21	1.16	0.88
1:F:371[B]:MET:SD	6:F:1122:HOH:O	2.32	0.87
1:C:375[B]:MET:SD	1:C:399[B]:CYS:SG	2.74	0.86
1:F:267:HIS:CD2	1:F:277:ASN:HD22	1.92	0.86
1:A:375[B]:MET:SD	1:A:399[B]:CYS:SG	2.73	0.85
1:B:184:ASN:HD22	2:L:115:GLN:HE21	1.21	0.85
1:D:267:HIS:CD2	1:D:277:ASN:HD22	1.94	0.84
1:G:267:HIS:CD2	1:G:277:ASN:HD22	1.93	0.84
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.96	0.83
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.94	0.83
1:D:375[B]:MET:SD	1:D:399[B]:CYS:SG	2.76	0.83
1:E:375[B]:MET:SD	1:E:399[B]:CYS:SG	2.77	0.82
1:D:383:HIS:H	1:D:386:HIS:HD2	1.27	0.82
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.94	0.81
1:F:375[B]:MET:SD	1:F:399[B]:CYS:SG	2.79	0.81
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.28	0.80
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.94	0.79
1:H:383:HIS:H	1:H:386:HIS:HD2	1.29	0.79
1:E:383:HIS:H	1:E:386:HIS:HD2	1.28	0.79
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.30	0.79
1:B:383:HIS:H	1:B:386:HIS:HD2	1.30	0.79
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.29	0.78
1:D:431:ARG:HH21	1:D:432:ASN:HD21	1.28	0.78
1:C:383:HIS:H	1:C:386:HIS:HD2	1.32	0.77
1:C:267:HIS:CD2	1:C:277:ASN:HD22	1.97	0.77
1:F:44:PRO:HB3	1:F:53[B]:CYS:SG	2.25	0.76
1:F:431:ARG:HH21	1:F:432:ASN:HD21	1.33	0.76
1:H:44:PRO:HB3	1:H:53[B]:CYS:SG	2.26	0.75
1:B:375[B]:MET:SD	1:B:399[B]:CYS:SG	2.83	0.75
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.33	0.75
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.34	0.75
1:G:44:PRO:HB3	1:G:53[B]:CYS:SG	2.28	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:22:THR:H	2:J:25:GLN:HE21	1.36	0.73
2:O:22:THR:H	2:O:25:GLN:HE21	1.34	0.72
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.37	0.72
1:D:44:PRO:HB3	1:D:53[B]:CYS:SG	2.29	0.72
1:F:383:HIS:H	1:F:386:HIS:HD2	1.38	0.72
1:A:383:HIS:H	1:A:386:HIS:HD2	1.34	0.72
1:E:44:PRO:HB3	1:E:53[B]:CYS:SG	2.30	0.71
2:N:22:THR:H	2:N:25:GLN:HE21	1.38	0.71
1:C:44:PRO:HB3	1:C:53[B]:CYS:SG	2.30	0.70
1:A:44:PRO:HB3	1:A:53[B]:CYS:SG	2.31	0.70
1:H:375[B]:MET:SD	1:H:399[B]:CYS:SG	2.90	0.70
1:G:383:HIS:H	1:G:386:HIS:HD2	1.40	0.70
2:I:22:THR:H	2:I:25:GLN:HE21	1.37	0.70
1:E:371[B]:MET:SD	6:E:1120:HOH:O	2.51	0.69
2:M:22:THR:H	2:M:25:GLN:HE21	1.41	0.68
2:L:22:THR:H	2:L:25:GLN:HE21	1.40	0.68
1:B:44:PRO:HB3	1:B:53[B]:CYS:SG	2.34	0.68
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.77	0.67
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.77	0.67
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.78	0.67
1:E:383:HIS:H	1:E:386:HIS:CD2	2.13	0.66
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.80	0.65
2:P:22:THR:H	2:P:25:GLN:HE21	1.44	0.65
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.79	0.64
2:K:22:THR:H	2:K:25:GLN:HE21	1.43	0.64
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.81	0.64
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.81	0.64
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.79	0.64
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.82	0.63
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.82	0.61
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.82	0.61
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.83	0.61
2:P:9:ASN:HD21	2:P:138:ARG:HG2	1.65	0.61
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.82	0.61
1:H:383:HIS:H	1:H:386:HIS:CD2	2.16	0.61
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.84	0.61
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.49	0.61
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.84	0.61
1:G:331:ALA:HA	1:G:337:GLY:O	2.01	0.61
1:E:331:ALA:HA	1:E:337:GLY:O	2.00	0.60
1:C:331:ALA:HA	1:C:337:GLY:O	2.00	0.60
2:J:109:ALA:HB3	2:J:119:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:439:ARG:NH1	6:G:1285:HOH:O	2.35	0.60
1:D:331:ALA:HA	1:D:337:GLY:O	2.02	0.59
2:O:109:ALA:HB3	2:O:119:MET:HG3	1.85	0.59
1:A:383:HIS:H	1:A:386:HIS:CD2	2.19	0.59
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.86	0.59
1:B:331:ALA:HA	1:B:337:GLY:O	2.03	0.59
1:A:331:ALA:HA	1:A:337:GLY:O	2.03	0.58
1:C:383:HIS:H	1:C:386:HIS:CD2	2.17	0.58
1:F:331:ALA:HA	1:F:337:GLY:O	2.04	0.58
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.52	0.58
1:G:383:HIS:H	1:G:386:HIS:CD2	2.21	0.58
1:C:88:GLU:HG3	1:C:98:ILE:HB	1.86	0.58
1:H:88:GLU:HG2	1:H:98:ILE:HB	1.84	0.58
1:E:88:GLU:HG3	1:E:98:ILE:HB	1.86	0.57
1:D:181:SER:H	2:N:115:GLN:NE2	2.03	0.57
1:B:383:HIS:H	1:B:386:HIS:CD2	2.18	0.56
1:H:331:ALA:HA	1:H:337:GLY:O	2.06	0.56
1:D:383:HIS:H	1:D:386:HIS:CD2	2.16	0.56
2:M:109:ALA:HB3	2:M:119:MET:HG3	1.87	0.56
1:G:192:CYS:HB3	1:G:197:LEU:HD12	1.88	0.56
1:E:229:GLN:HE21	1:E:236:LYS:H	1.54	0.56
1:F:383:HIS:H	1:F:386:HIS:CD2	2.22	0.55
1:C:181:SER:H	2:I:115:GLN:NE2	2.05	0.55
1:F:180:LEU:HA	2:P:115:GLN:HE22	1.72	0.54
2:O:22:THR:H	2:O:25:GLN:NE2	2.04	0.54
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.54	0.54
1:G:446:ARG:O	1:G:450:LYS:HG3	2.06	0.54
1:H:431:ARG:HE	1:H:432:ASN:HD22	1.55	0.54
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.55	0.54
2:M:125:ARG:HD2	6:M:1097:HOH:O	2.06	0.54
2:L:109:ALA:HB3	2:L:119:MET:HG3	1.90	0.53
2:I:109:ALA:HB3	2:I:119:MET:HG3	1.90	0.53
1:C:48:VAL:CG1	1:C:53[B]:CYS:SG	2.96	0.53
1:H:181:SER:H	2:J:115:GLN:NE2	2.07	0.53
1:D:259[B]:GLU:OE1	2:N:61:GLY:HA3	2.08	0.53
6:E:1204:HOH:O	1:F:267:HIS:HE1	1.90	0.53
1:B:181:SER:H	2:L:115:GLN:NE2	2.07	0.53
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.86	0.53
1:C:267:HIS:HE1	6:D:1198:HOH:O	1.92	0.53
1:A:229:GLN:HE21	1:A:236:LYS:H	1.57	0.53
1:G:181:SER:H	2:M:115:GLN:NE2	2.06	0.53
1:D:88:GLU:HG2	1:D:98:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.57	0.53
1:A:181:SER:H	2:O:115:GLN:NE2	2.06	0.52
1:C:229:GLN:HE21	1:C:236:LYS:H	1.57	0.52
1:F:181:SER:H	2:P:115:GLN:NE2	2.08	0.52
6:C:1192:HOH:O	1:D:267:HIS:HE1	1.93	0.52
1:E:181:SER:H	2:K:115:GLN:NE2	2.07	0.52
1:E:180:LEU:HA	2:K:115:GLN:HE22	1.74	0.51
1:H:229:GLN:HE21	1:H:236:LYS:H	1.59	0.51
1:B:180:LEU:HA	2:L:115:GLN:HE22	1.76	0.51
6:G:1190:HOH:O	1:H:267:HIS:HE1	1.93	0.50
1:H:180:LEU:HA	2:J:115:GLN:HE22	1.76	0.50
1:A:288:GLY:O	2:I:65[B]:CYS:SG	2.64	0.50
1:A:180:LEU:HA	2:O:115:GLN:HE22	1.77	0.50
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.47	0.50
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.09	0.50
1:A:48:VAL:CG1	1:A:53[B]:CYS:SG	3.00	0.50
1:D:229:GLN:HE21	1:D:236:LYS:H	1.60	0.50
1:C:48:VAL:HG12	1:C:53[B]:CYS:SG	2.51	0.50
1:G:180:LEU:HA	2:M:115:GLN:HE22	1.75	0.49
1:E:201:KCX:HB2	1:E:239:TYR:CD2	2.46	0.49
1:B:290:LEU:HG	2:J:66:LEU:HD11	1.95	0.49
1:C:180:LEU:HA	2:I:115:GLN:HE22	1.77	0.49
2:K:22:THR:H	2:K:25:GLN:NE2	2.09	0.49
1:F:259[B]:GLU:OE1	2:P:61:GLY:HA3	2.12	0.49
1:G:267:HIS:HE1	6:H:1208:HOH:O	1.95	0.49
1:A:259[B]:GLU:OE1	2:O:61:GLY:HA3	2.12	0.49
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.93	0.49
6:A:1195:HOH:O	1:B:267:HIS:HE1	1.94	0.49
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.94	0.49
1:C:381:GLY:HA2	1:D:66:TRP:CD1	2.48	0.49
2:K:109:ALA:HB3	2:K:119:MET:HG3	1.95	0.49
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.60	0.48
2:J:22:THR:H	2:J:25:GLN:NE2	2.09	0.48
1:E:267:HIS:HE1	6:F:1200:HOH:O	1.97	0.48
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.48	0.48
1:G:259[B]:GLU:OE1	2:M:61:GLY:HA3	2.13	0.48
2:N:22:THR:H	2:N:25:GLN:NE2	2.09	0.47
1:E:171:GLY:HA2	1:E:199:PHE:O	2.15	0.47
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.95	0.47
1:D:383:HIS:N	1:D:386:HIS:HD2	2.04	0.47
1:G:171:GLY:HA2	1:G:199:PHE:O	2.15	0.47
2:N:109:ALA:HB3	2:N:119:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.50	0.47
1:B:229:GLN:HE21	1:B:236:LYS:H	1.63	0.47
1:C:383:HIS:N	1:C:386:HIS:HD2	2.08	0.47
2:J:125:ARG:HD2	2:J:132:PHE:CE2	2.50	0.47
1:A:267:HIS:HE1	6:B:1207:HOH:O	1.98	0.46
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.50	0.46
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.97	0.46
1:D:239:TYR:HE2	1:D:401:GLN:NE2	2.14	0.46
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.96	0.46
1:G:153:HIS:HE1	6:G:1192:HOH:O	1.97	0.46
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.50	0.46
1:E:239:TYR:HE2	1:E:401:GLN:NE2	2.14	0.46
1:B:339:ARG:NH1	1:B:392:GLU:OE2	2.49	0.46
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.51	0.46
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.51	0.46
1:D:449:CYS:O	1:D:456:ALA:HB2	2.16	0.45
1:F:152:PRO:HB2	1:F:153:HIS:CD2	2.52	0.45
1:D:180:LEU:HA	2:N:115:GLN:HE22	1.81	0.45
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.63	0.45
1:F:150:GLY:HA3	1:F:371[B]:MET:SD	2.56	0.45
1:B:383:HIS:N	1:B:386:HIS:HD2	2.07	0.45
1:G:200:THR:OG1	1:G:238:HIS:CD2	2.65	0.45
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.51	0.45
1:E:259[B]:GLU:OE1	2:K:61:GLY:HA3	2.16	0.45
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.99	0.45
1:B:259[B]:GLU:OE1	2:L:61:GLY:HA3	2.16	0.45
2:P:109:ALA:HB3	2:P:119:MET:HG3	1.98	0.45
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.82	0.45
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.52	0.45
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.52	0.45
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.52	0.45
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.51	0.45
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.53	0.44
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.88	0.44
1:B:153:HIS:HE1	6:B:1211:HOH:O	2.00	0.44
1:A:171:GLY:HA2	1:A:199:PHE:O	2.17	0.44
1:E:44:PRO:O	1:E:95:ASN:ND2	2.50	0.44
1:G:381:GLY:HA2	1:H:66:TRP:CD1	2.52	0.44
1:H:77:LEU:HA	1:H:77:LEU:HD12	1.90	0.44
1:G:382:ILE:HA	1:G:386:HIS:CD2	2.53	0.44
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.98	0.44
1:G:66:TRP:CD1	1:H:381:GLY:HA2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.53	0.44
1:F:229:GLN:HE21	1:F:236:LYS:H	1.66	0.44
1:H:299:ALA:HA	1:H:302:ASP:OD1	2.18	0.44
1:E:192:CYS:HB3	1:E:197:LEU:HD12	1.99	0.44
1:E:190:TYR:CZ	1:E:227:LYS:HE3	2.53	0.43
1:D:449:CYS:HB3	1:D:456:ALA:HA	1.99	0.43
1:H:449:CYS:O	1:H:456:ALA:HB2	2.18	0.43
1:A:383:HIS:N	1:A:386:HIS:HD2	2.09	0.43
2:K:107:LEU:O	2:K:120:GLY:HA2	2.19	0.43
1:F:345:PHE:HE1	5:F:1483:EDO:H21	1.83	0.43
1:H:153:HIS:HE1	6:H:1213:HOH:O	2.02	0.43
2:M:107:LEU:O	2:M:120:GLY:HA2	2.18	0.43
1:A:153:HIS:HE1	6:A:1200:HOH:O	2.01	0.43
1:E:383:HIS:N	1:E:386:HIS:HD2	2.05	0.43
1:G:48:VAL:CG1	1:G:53[B]:CYS:SG	3.07	0.43
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.68	0.43
1:H:175:LYS:HA	1:H:176:PRO:C	2.39	0.43
1:A:273:GLY:HA3	1:B:273:GLY:HA3	2.01	0.43
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.54	0.43
1:D:192:CYS:HB3	1:D:197:LEU:HD12	2.00	0.43
1:D:341:VAL:HG12	1:D:345:PHE:CZ	2.54	0.43
1:C:200:THR:OG1	1:C:238:HIS:CD2	2.69	0.43
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.01	0.43
1:C:239:TYR:HE2	1:C:401:GLN:NE2	2.15	0.43
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.52	0.43
1:H:436:ASP:OD2	1:H:439:ARG:HD3	2.18	0.43
1:E:341:VAL:HG12	1:E:345:PHE:CZ	2.53	0.43
1:E:299:ALA:HA	1:E:302:ASP:OD1	2.18	0.43
2:O:107:LEU:O	2:O:120:GLY:HA2	2.19	0.43
1:D:171:GLY:HA2	1:D:199:PHE:O	2.19	0.43
1:G:341:VAL:HG12	1:G:345:PHE:CZ	2.54	0.43
1:G:388:PRO:HD3	1:G:445:ILE:HG13	2.01	0.42
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.55	0.42
1:H:259[B]:GLU:OE1	2:J:61:GLY:HA3	2.19	0.42
1:F:449:CYS:O	1:F:456:ALA:HB2	2.19	0.42
1:F:382:ILE:HA	1:F:386:HIS:CD2	2.54	0.42
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.55	0.42
2:I:22:THR:H	2:I:25:GLN:NE2	2.12	0.42
1:D:153:HIS:HE1	6:D:1201:HOH:O	2.02	0.42
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.42
1:G:229:GLN:HE21	1:G:236:LYS:H	1.65	0.42
1:H:200:THR:OG1	1:H:238:HIS:CD2	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:171:GLY:HA2	1:F:199:PHE:O	2.19	0.42
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.55	0.42
1:G:150:GLY:HA3	1:G:371[B]:MET:SD	2.60	0.42
1:C:341:VAL:HG12	1:C:345:PHE:CZ	2.54	0.42
1:B:295:ARG:HH12	5:B:1482:EDO:C1	2.32	0.42
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.54	0.42
1:E:200:THR:OG1	1:E:238:HIS:CD2	2.69	0.42
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.02	0.42
1:C:446:ARG:O	1:C:450:LYS:HG2	2.20	0.42
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.55	0.42
2:M:113:GLN:NE2	6:M:1083:HOH:O	2.52	0.42
1:D:382:ILE:HA	1:D:386:HIS:CD2	2.55	0.42
1:F:200:THR:OG1	1:F:238:HIS:CD2	2.71	0.42
1:G:175:LYS:HA	1:G:176:PRO:C	2.40	0.42
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.55	0.42
1:A:48:VAL:HG11	1:A:53[B]:CYS:SG	2.60	0.42
1:B:48:VAL:CG1	1:B:53[B]:CYS:SG	3.08	0.41
1:C:449:CYS:O	1:C:456:ALA:HB2	2.20	0.41
1:A:341:VAL:HG12	1:A:345:PHE:CZ	2.54	0.41
1:F:383:HIS:HE1	1:F:385:TRP:HB2	1.84	0.41
1:H:201:KCX:HB2	1:H:239:TYR:CD2	2.55	0.41
1:G:273:GLY:HA3	1:H:273:GLY:HA3	2.02	0.41
1:F:153:HIS:HE1	6:F:1206:HOH:O	2.03	0.41
2:J:107:LEU:O	2:J:120:GLY:HA2	2.20	0.41
1:F:451:TRP:CE2	2:N:19:PRO:HG3	2.55	0.41
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.55	0.41
1:C:273:GLY:HA3	1:D:273:GLY:HA3	2.02	0.41
1:A:197:LEU:HG	1:A:417:ALA:HB1	2.03	0.41
2:L:107:LEU:O	2:L:120:GLY:HA2	2.20	0.41
1:F:383:HIS:N	1:F:386:HIS:HD2	2.12	0.41
1:F:290:LEU:HG	2:N:66:LEU:HD11	2.01	0.41
1:E:277:ASN:HD21	1:E:293:ILE:HD12	1.85	0.41
1:F:48:VAL:CG1	1:F:53[B]:CYS:SG	3.09	0.41
1:E:150:GLY:HA3	1:E:371[B]:MET:SD	2.60	0.41
6:D:1174:HOH:O	2:L:10:LYS:HE3	2.21	0.41
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.56	0.41
1:A:177:LYS:HG2	1:A:203:ASP:OD2	2.21	0.41
1:B:90:VAL:HA	1:B:91:PRO:HD2	1.63	0.41
1:C:241:ASN:HA	1:C:266:MET:HG3	2.03	0.41
1:B:175:LYS:HA	1:B:176:PRO:C	2.40	0.41
1:C:259[B]:GLU:OE1	2:I:61:GLY:HA3	2.21	0.41
1:A:21:ARG:NH1	6:A:1016:HOH:O	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:113:GLN:NE2	6:N:1088:HOH:O	2.53	0.41
1:E:153:HIS:HE1	6:E:1209:HOH:O	2.03	0.41
1:B:371[B]:MET:SD	6:B:1127:HOH:O	2.63	0.41
1:E:170:LEU:HG	1:E:424:LEU:HD22	2.02	0.41
2:N:128:THR:HG23	6:N:1102:HOH:O	2.20	0.41
2:J:39:ILE:O	2:J:109:ALA:HA	2.20	0.40
1:D:201:KCX:HB2	1:D:239:TYR:CD2	2.57	0.40
1:F:190:TYR:CZ	1:F:227:LYS:HE3	2.56	0.40
2:P:32[A]:TYR:CE2	2:P:38:TRP:HZ3	2.39	0.40
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.55	0.40
1:F:190:TYR:CZ	1:F:194:ARG:HD3	2.56	0.40
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.56	0.40
1:G:449:CYS:O	1:G:456:ALA:HB2	2.21	0.40
2:J:85:ASP:HA	2:J:86:PRO:HD2	1.95	0.40
2:I:107:LEU:O	2:I:120:GLY:HA2	2.20	0.40
1:D:175:LYS:HA	1:D:176:PRO:C	2.42	0.40
1:A:48:VAL:HG12	1:A:53[B]:CYS:SG	2.61	0.40
1:A:298:HIS:ND1	1:A:302:ASP:OD2	2.35	0.40
1:B:449:CYS:HB3	1:B:456:ALA:HA	2.03	0.40
1:F:170:LEU:HD11	1:F:421:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/475 (99%)	456 (97%)	13 (3%)	0	100	100
1	B	469/475 (99%)	454 (97%)	14 (3%)	1 (0%)	56	26
1	C	468/475 (98%)	454 (97%)	14 (3%)	0	100	100
1	D	469/475 (99%)	456 (97%)	13 (3%)	0	100	100
1	E	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	F	467/475 (98%)	454 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	467/475 (98%)	453 (97%)	14 (3%)	0	100	100
1	H	471/475 (99%)	458 (97%)	12 (2%)	1 (0%)	56	26
2	I	141/140 (101%)	136 (96%)	5 (4%)	0	100	100
2	J	142/140 (101%)	138 (97%)	4 (3%)	0	100	100
2	K	143/140 (102%)	138 (96%)	5 (4%)	0	100	100
2	L	144/140 (103%)	139 (96%)	5 (4%)	0	100	100
2	M	144/140 (103%)	137 (95%)	7 (5%)	0	100	100
2	N	143/140 (102%)	138 (96%)	5 (4%)	0	100	100
2	O	144/140 (103%)	139 (96%)	5 (4%)	0	100	100
2	P	143/140 (102%)	137 (96%)	6 (4%)	0	100	100
All	All	4891/4920 (99%)	4741 (97%)	148 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	PRO
1	H	337	GLY

### 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	377/376 (100%)	372 (99%)	5 (1%)	80	53
1	B	377/376 (100%)	370 (98%)	7 (2%)	69	35
1	C	376/376 (100%)	372 (99%)	4 (1%)	84	61
1	D	378/376 (100%)	374 (99%)	4 (1%)	84	61
1	E	377/376 (100%)	373 (99%)	4 (1%)	84	61
1	F	377/376 (100%)	373 (99%)	4 (1%)	84	61
1	G	377/376 (100%)	371 (98%)	6 (2%)	75	44
1	H	379/376 (101%)	373 (98%)	6 (2%)	75	44
2	I	125/122 (102%)	122 (98%)	3 (2%)	61	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	126/122 (103%)	123 (98%)	3 (2%)	61	25
2	K	127/122 (104%)	125 (98%)	2 (2%)	75	44
2	L	128/122 (105%)	126 (98%)	2 (2%)	75	44
2	M	128/122 (105%)	125 (98%)	3 (2%)	63	26
2	N	127/122 (104%)	125 (98%)	2 (2%)	75	44
2	O	128/122 (105%)	126 (98%)	2 (2%)	75	44
2	P	127/122 (104%)	125 (98%)	2 (2%)	75	44
All	All	4034/3984 (101%)	3975 (98%)	59 (2%)	76	47

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	TYR
1	A	203	ASP
1	A	239	TYR
1	A	241	ASN
1	A	392	GLU
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	392	GLU
1	B	439	ARG
1	B	460	GLU
1	B	464	GLU
1	C	203	ASP
1	C	239	TYR
1	C	241	ASN
1	C	392	GLU
1	D	185	TYR
1	D	203	ASP
1	D	241	ASN
1	D	392	GLU
1	E	185	TYR
1	E	203	ASP
1	E	239	TYR
1	E	241	ASN
1	F	185	TYR
1	F	203	ASP
1	F	239	TYR
1	F	241	ASN

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Mol	Chain	Res	Type
1	G	94[A]	ASP
1	G	94[B]	ASP
1	G	203	ASP
1	G	239	TYR
1	G	241	ASN
1	G	445	ILE
1	H	163	ASN
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	392	GLU
2	I	9	ASN
2	I	12	PHE
2	I	137	LYS
2	J	9	ASN
2	J	12	PHE
2	J	98	LYS
2	K	9	ASN
2	K	12	PHE
2	L	9	ASN
2	L	12	PHE
2	M	9	ASN
2	M	12	PHE
2	M	125	ARG
2	N	9	ASN
2	N	12	PHE
2	O	9	ASN
2	O	88	GLN
2	P	9	ASN
2	P	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN

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Mol	Chain	Res	Type
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	432	ASN
1	C	153	HIS
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	386	HIS
1	C	401	GLN
1	C	432	ASN
1	D	153	HIS
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	267	HIS
1	D	277	ASN
1	D	304	GLN
1	D	386	HIS
1	D	401	GLN
1	D	420	ASN
1	D	432	ASN
1	E	153	HIS
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS

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Mol	Chain	Res	Type
1	E	401	GLN
1	E	432	ASN
1	F	153	HIS
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	304	GLN
1	F	386	HIS
1	F	401	GLN
1	F	432	ASN
1	G	153	HIS
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	386	HIS
1	G	401	GLN
1	G	432	ASN
1	H	153	HIS
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	432	ASN
2	I	8	ASN
2	I	9	ASN
2	I	25	GLN
2	I	29	GLN
2	I	115	GLN
2	I	133	GLN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	113	GLN

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Mol	Chain	Res	Type
2	J	115	GLN
2	J	133	GLN
2	K	9	ASN
2	K	25	GLN
2	K	29	GLN
2	K	115	GLN
2	K	133	GLN
2	L	9	ASN
2	L	25	GLN
2	L	29	GLN
2	L	115	GLN
2	M	8	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	113	GLN
2	M	115	GLN
2	M	133	GLN
2	N	8	ASN
2	N	9	ASN
2	N	25	GLN
2	N	29	GLN
2	N	113	GLN
2	N	115	GLN
2	N	133	GLN
2	O	8	ASN
2	O	9	ASN
2	O	25	GLN
2	O	29	GLN
2	O	115	GLN
2	O	133	GLN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	115	GLN
2	P	133	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.



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

48 non-standard protein/DNA/RNA residues 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$
1	HYP	A	104	1	8,8,9	6.36	2 (25%)	8,10,12	0.86	0
1	HYP	A	151	1	8,8,9	6.23	1 (12%)	8,10,12	1.63	1 (12%)
1	KCX	A	201	1,3	11,11,12	5.46	1 (9%)	10,12,14	2.13	2 (20%)
1	SMC	A	256	1	6,6,7	8.03	2 (33%)	4,6,8	1.39	1 (25%)
1	SMC	A	369	1	6,6,7	7.43	2 (33%)	4,6,8	1.61	2 (50%)
1	HYP	B	104	1	8,8,9	6.36	1 (12%)	8,10,12	0.84	0
1	HYP	B	151	1	8,8,9	5.92	1 (12%)	8,10,12	1.39	0
1	KCX	B	201	1,3	11,11,12	6.01	1 (9%)	10,12,14	2.01	2 (20%)
1	SMC	B	256	1	6,6,7	8.29	1 (16%)	4,6,8	1.71	1 (25%)
1	SMC	B	369	1	6,6,7	8.38	2 (33%)	4,6,8	1.82	1 (25%)
1	HYP	C	104	1	8,8,9	5.81	2 (25%)	8,10,12	0.76	0
1	HYP	C	151	1	8,8,9	6.37	2 (25%)	8,10,12	1.26	1 (12%)
1	KCX	C	201	1,3	11,11,12	5.76	2 (18%)	10,12,14	1.57	2 (20%)
1	SMC	C	256	1	6,6,7	8.29	2 (33%)	4,6,8	1.78	1 (25%)
1	SMC	C	369	1	6,6,7	7.73	2 (33%)	4,6,8	1.26	0
1	HYP	D	104	1	8,8,9	6.37	2 (25%)	8,10,12	0.81	0
1	HYP	D	151	1	8,8,9	6.61	1 (12%)	8,10,12	1.23	0
1	KCX	D	201	1,3	11,11,12	5.82	2 (18%)	10,12,14	1.77	2 (20%)
1	SMC	D	256	1	6,6,7	7.38	1 (16%)	4,6,8	2.05	1 (25%)
1	SMC	D	369	1	6,6,7	7.82	2 (33%)	4,6,8	1.65	2 (50%)
1	HYP	E	104	1	8,8,9	6.27	2 (25%)	8,10,12	0.69	0
1	HYP	E	151	1	8,8,9	6.72	1 (12%)	8,10,12	1.66	2 (25%)
1	KCX	E	201	1,3	11,11,12	5.49	1 (9%)	10,12,14	1.88	2 (20%)
1	SMC	E	256	1	6,6,7	7.15	1 (16%)	4,6,8	1.46	1 (25%)
1	SMC	E	369	1	6,6,7	7.82	2 (33%)	4,6,8	1.08	0
1	HYP	F	104	1	8,8,9	6.77	1 (12%)	8,10,12	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	F	151	1	8,8,9	6.41	1 (12%)	8,10,12	1.37	1 (12%)
1	KCX	F	201	1,3	11,11,12	5.69	2 (18%)	10,12,14	1.63	2 (20%)
1	SMC	F	256	1	6,6,7	7.62	2 (33%)	4,6,8	2.15	1 (25%)
1	SMC	F	369	1	6,6,7	7.63	1 (16%)	4,6,8	1.85	1 (25%)
1	HYP	G	104	1	8,8,9	6.23	2 (25%)	8,10,12	0.70	0
1	HYP	G	151	1	8,8,9	6.17	1 (12%)	8,10,12	1.29	1 (12%)
1	KCX	G	201	1,3	11,11,12	5.20	2 (18%)	10,12,14	1.62	2 (20%)
1	SMC	G	256	1	6,6,7	8.06	1 (16%)	4,6,8	1.64	1 (25%)
1	SMC	G	369	1	6,6,7	7.08	2 (33%)	4,6,8	1.61	1 (25%)
1	HYP	H	104	1	8,8,9	6.93	2 (25%)	8,10,12	0.98	0
1	HYP	H	151	1	8,8,9	6.24	1 (12%)	8,10,12	1.34	0
1	KCX	H	201	1,3	11,11,12	5.40	1 (9%)	10,12,14	1.56	2 (20%)
1	SMC	H	256	1	6,6,7	7.83	2 (33%)	4,6,8	1.95	1 (25%)
1	SMC	H	369	1	6,6,7	7.61	2 (33%)	4,6,8	1.35	1 (25%)
2	MME	I	1	2	8,8,9	6.97	3 (37%)	5,8,10	1.01	0
2	MME	J	1	2	8,8,9	7.10	3 (37%)	5,8,10	1.20	1 (20%)
2	MME	K	1	2	8,8,9	6.86	3 (37%)	5,8,10	1.09	0
2	MME	L	1	2	8,8,9	6.96	3 (37%)	5,8,10	1.20	1 (20%)
2	MME	M	1	2	8,8,9	6.85	3 (37%)	5,8,10	1.25	1 (20%)
2	MME	N	1	2	8,8,9	6.74	3 (37%)	5,8,10	1.23	1 (20%)
2	MME	O	1	2	8,8,9	7.00	3 (37%)	5,8,10	1.05	0
2	MME	P	1	2	8,8,9	7.14	3 (37%)	5,8,10	1.10	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
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	A	256	1	-	0/3/5/7	0/0/0/0
1	SMC	A	369	1	-	0/3/5/7	0/0/0/0
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/8/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	B	256	1	-	0/3/5/7	0/0/0/0
1	SMC	B	369	1	-	0/3/5/7	0/0/0/0
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	KCX	C	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	C	256	1	-	0/3/5/7	0/0/0/0
1	SMC	C	369	1	-	0/3/5/7	0/0/0/0
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	KCX	D	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	D	256	1	-	0/3/5/7	0/0/0/0
1	SMC	D	369	1	-	0/3/5/7	0/0/0/0
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	E	256	1	-	0/3/5/7	0/0/0/0
1	SMC	E	369	1	-	0/3/5/7	0/0/0/0
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	F	256	1	-	0/3/5/7	0/0/0/0
1	SMC	F	369	1	-	0/3/5/7	0/0/0/0
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	G	256	1	-	0/3/5/7	0/0/0/0
1	SMC	G	369	1	-	0/3/5/7	0/0/0/0
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	H	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	H	256	1	-	0/3/5/7	0/0/0/0
1	SMC	H	369	1	-	0/3/5/7	0/0/0/0
2	MME	I	1	2	-	0/6/8/10	0/0/0/0
2	MME	J	1	2	-	0/6/8/10	0/0/0/0
2	MME	K	1	2	-	0/6/8/10	0/0/0/0
2	MME	L	1	2	-	0/6/8/10	0/0/0/0
2	MME	M	1	2	-	0/6/8/10	0/0/0/0
2	MME	N	1	2	-	0/6/8/10	0/0/0/0
2	MME	O	1	2	-	0/6/8/10	0/0/0/0
2	MME	P	1	2	-	0/6/8/10	0/0/0/0

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	SMC	O-C	20.27	1.25	1.11
1	B	256	SMC	O-C	20.14	1.25	1.11
1	C	256	SMC	O-C	20.12	1.25	1.11
1	B	201	KCX	O-C	19.75	1.25	1.11
1	G	256	SMC	O-C	19.64	1.24	1.11
1	A	256	SMC	O-C	19.49	1.24	1.11
1	H	104	HYP	O-C	19.43	1.24	1.11
1	F	104	HYP	O-C	19.03	1.24	1.11
1	H	256	SMC	O-C	19.03	1.24	1.11
1	D	201	KCX	O-C	19.00	1.24	1.11
2	P	1	MME	O-C	18.98	1.24	1.11
1	E	369	SMC	O-C	18.95	1.24	1.11
1	D	369	SMC	O-C	18.94	1.24	1.11
1	E	151	HYP	O-C	18.88	1.24	1.11
2	J	1	MME	O-C	18.79	1.24	1.11
1	C	369	SMC	O-C	18.69	1.24	1.11
1	C	201	KCX	O-C	18.63	1.24	1.11
1	D	151	HYP	O-C	18.58	1.24	1.11
1	F	369	SMC	O-C	18.53	1.24	1.11
2	O	1	MME	O-C	18.52	1.24	1.11
1	F	201	KCX	O-C	18.46	1.24	1.11
1	F	256	SMC	O-C	18.45	1.24	1.11
1	H	369	SMC	O-C	18.43	1.24	1.11
2	I	1	MME	O-C	18.39	1.24	1.11
2	L	1	MME	O-C	18.35	1.24	1.11
2	M	1	MME	O-C	18.07	1.23	1.11
1	A	369	SMC	O-C	18.04	1.23	1.11
1	D	256	SMC	O-C	18.03	1.23	1.11
1	F	151	HYP	O-C	18.03	1.23	1.11
2	K	1	MME	O-C	18.01	1.23	1.11
1	E	201	KCX	O-C	17.94	1.23	1.11
1	B	104	HYP	O-C	17.87	1.23	1.11
1	C	151	HYP	O-C	17.85	1.23	1.11
1	D	104	HYP	O-C	17.81	1.23	1.11
1	A	201	KCX	O-C	17.80	1.23	1.11
1	A	104	HYP	O-C	17.79	1.23	1.11
2	N	1	MME	O-C	17.69	1.23	1.11
1	H	201	KCX	O-C	17.65	1.23	1.11
1	H	151	HYP	O-C	17.54	1.23	1.11
1	E	104	HYP	O-C	17.52	1.23	1.11
1	A	151	HYP	O-C	17.47	1.23	1.11
1	G	104	HYP	O-C	17.43	1.23	1.11
1	E	256	SMC	O-C	17.32	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	151	HYP	O-C	17.32	1.23	1.11
1	G	369	SMC	O-C	17.12	1.23	1.11
1	G	201	KCX	O-C	16.89	1.23	1.11
1	B	151	HYP	O-C	16.64	1.22	1.11
1	C	104	HYP	O-C	16.25	1.22	1.11
2	K	1	MME	CM-N	-6.31	1.27	1.46
2	P	1	MME	CM-N	-6.28	1.27	1.46
2	L	1	MME	CM-N	-6.27	1.27	1.46
2	J	1	MME	CM-N	-6.22	1.27	1.46
2	O	1	MME	CM-N	-6.21	1.27	1.46
2	I	1	MME	CM-N	-6.19	1.27	1.46
2	N	1	MME	CM-N	-6.15	1.27	1.46
2	M	1	MME	CM-N	-6.12	1.27	1.46
2	N	1	MME	CA-N	3.12	1.50	1.46
2	M	1	MME	CA-N	2.92	1.50	1.46
2	K	1	MME	CA-N	2.91	1.50	1.46
2	I	1	MME	CA-N	2.90	1.50	1.46
2	L	1	MME	CA-N	2.74	1.50	1.46
2	J	1	MME	CA-N	2.70	1.49	1.46
1	E	104	HYP	CA-C	2.64	1.53	1.48
1	H	369	SMC	CA-C	2.52	1.53	1.48
1	B	369	SMC	CA-C	2.48	1.52	1.48
1	H	104	HYP	CA-C	2.44	1.52	1.48
2	O	1	MME	CA-N	2.44	1.49	1.46
1	F	256	SMC	CA-C	2.42	1.52	1.48
1	D	104	HYP	CA-C	2.40	1.52	1.48
1	G	104	HYP	CA-C	2.40	1.52	1.48
1	A	104	HYP	CA-C	2.38	1.52	1.48
1	C	104	HYP	CA-C	2.34	1.52	1.48
2	P	1	MME	CA-N	2.33	1.49	1.46
1	F	201	KCX	OQ1-CX	2.30	1.26	1.21
1	A	256	SMC	CA-C	2.29	1.52	1.48
1	C	201	KCX	CB-CA	2.22	1.55	1.53
1	E	369	SMC	CA-C	2.17	1.52	1.48
1	D	369	SMC	CA-C	2.17	1.52	1.48
1	H	256	SMC	CA-C	2.15	1.52	1.48
1	C	151	HYP	CA-C	2.10	1.52	1.48
1	C	369	SMC	CA-C	2.09	1.52	1.48
1	G	369	SMC	CA-C	2.06	1.52	1.48
1	G	201	KCX	CA-C	2.05	1.52	1.48
1	A	369	SMC	CA-C	2.05	1.52	1.48
1	D	201	KCX	CX-NZ	2.03	1.34	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	SMC	CB-SG	2.02	1.83	1.80

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	KCX	OQ1-CX-NZ	-4.73	117.06	124.94
1	A	201	KCX	OQ2-CX-NZ	4.62	122.08	116.33
1	A	201	KCX	OQ1-CX-NZ	-4.21	117.93	124.94
1	E	201	KCX	OQ1-CX-NZ	-4.14	118.06	124.94
1	B	201	KCX	OQ2-CX-NZ	4.03	121.35	116.33
1	E	201	KCX	OQ2-CX-NZ	3.77	121.02	116.33
1	D	201	KCX	OQ2-CX-NZ	3.73	120.97	116.33
1	C	201	KCX	OQ1-CX-NZ	-3.68	118.81	124.94
1	D	201	KCX	OQ1-CX-NZ	-3.57	119.00	124.94
1	H	256	SMC	C-CA-N	-3.57	110.27	113.83
1	F	256	SMC	C-CA-N	-3.55	110.29	113.83
1	G	201	KCX	OQ1-CX-NZ	-3.53	119.06	124.94
1	D	256	SMC	C-CA-N	-3.44	110.39	113.83
1	F	201	KCX	OQ1-CX-NZ	-3.27	119.51	124.94
1	G	201	KCX	OQ2-CX-NZ	3.26	120.39	116.33
1	F	201	KCX	OQ2-CX-NZ	3.15	120.25	116.33
1	A	151	HYP	CG-CD-N	-3.12	100.45	105.47
1	H	201	KCX	OQ1-CX-NZ	-3.10	119.79	124.94
1	C	256	SMC	C-CA-N	-3.08	110.75	113.83
1	C	201	KCX	OQ2-CX-NZ	2.99	120.05	116.33
1	H	201	KCX	OQ2-CX-NZ	2.98	120.04	116.33
1	B	369	SMC	CA-CB-SG	-2.92	110.12	113.86
1	E	151	HYP	CB-CG-CD	-2.88	99.36	103.46
1	G	256	SMC	C-CA-N	-2.85	110.99	113.83
1	B	256	SMC	C-CA-N	-2.74	111.09	113.83
1	G	369	SMC	CB-CA-N	-2.58	105.90	110.27
1	F	369	SMC	CB-CA-N	-2.46	106.09	110.27
2	J	1	MME	CM-N-CA	2.38	120.37	113.11
2	M	1	MME	CM-N-CA	2.34	120.25	113.11
1	F	151	HYP	C-CA-N	2.32	115.16	110.86
1	A	369	SMC	CA-CB-SG	-2.31	110.90	113.86
1	A	256	SMC	C-CA-N	-2.28	111.55	113.83
2	L	1	MME	CM-N-CA	2.27	120.05	113.11
1	H	369	SMC	CB-CA-N	-2.27	106.42	110.27
1	G	151	HYP	CG-CD-N	-2.24	101.86	105.47
2	N	1	MME	CM-N-CA	2.21	119.85	113.11
1	E	256	SMC	C-CA-N	-2.20	111.63	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	HYP	CG-CD-N	-2.19	101.95	105.47
1	A	369	SMC	CB-CA-N	-2.19	106.56	110.27
1	D	369	SMC	CB-CA-N	-2.13	106.66	110.27
1	D	369	SMC	CA-CB-SG	-2.06	111.22	113.86
1	C	151	HYP	CG-CD-N	-2.01	102.23	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	CAP	A	1477	3	20,20,20	0.78	0	31,31,31	0.92	2 (6%)
5	EDO	A	1478	-	3,3,3	0.59	0	2,2,2	0.22	0
5	EDO	A	1479	-	3,3,3	0.48	0	2,2,2	0.42	0
5	EDO	A	1480	-	3,3,3	0.60	0	2,2,2	0.33	0
5	EDO	A	1481	-	3,3,3	0.53	0	2,2,2	0.47	0
5	EDO	A	1482	-	3,3,3	0.57	0	2,2,2	0.20	0
5	EDO	A	1483	-	3,3,3	0.63	0	2,2,2	0.09	0
5	EDO	A	1484	-	3,3,3	0.56	0	2,2,2	0.32	0
4	CAP	B	1477	3	20,20,20	0.80	0	31,31,31	0.93	0
5	EDO	B	1478	-	3,3,3	0.59	0	2,2,2	0.35	0
5	EDO	B	1479	-	3,3,3	0.57	0	2,2,2	0.17	0
5	EDO	B	1480	-	3,3,3	0.62	0	2,2,2	0.35	0
5	EDO	B	1481	-	3,3,3	0.59	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	1482	-	3,3,3	0.57	0	2,2,2	0.39	0
4	CAP	C	1477	3	20,20,20	0.83	0	31,31,31	0.97	0
5	EDO	C	1478	-	3,3,3	0.75	0	2,2,2	0.15	0
5	EDO	C	1479	-	3,3,3	0.58	0	2,2,2	0.17	0
5	EDO	C	1480	-	3,3,3	0.60	0	2,2,2	0.34	0
5	EDO	C	1481	-	3,3,3	0.53	0	2,2,2	0.46	0
5	EDO	C	1482	-	3,3,3	0.55	0	2,2,2	0.34	0
5	EDO	C	1483	-	3,3,3	0.58	0	2,2,2	0.14	0
4	CAP	D	1477	3	20,20,20	0.84	0	31,31,31	0.97	1 (3%)
5	EDO	D	1478	-	3,3,3	0.68	0	2,2,2	0.28	0
5	EDO	D	1479	-	3,3,3	0.53	0	2,2,2	0.19	0
5	EDO	D	1480	-	3,3,3	0.59	0	2,2,2	0.35	0
5	EDO	D	1481	-	3,3,3	0.60	0	2,2,2	0.23	0
5	EDO	D	1482	-	3,3,3	0.55	0	2,2,2	0.31	0
4	CAP	E	1477	3	20,20,20	0.76	0	31,31,31	1.04	3 (9%)
5	EDO	E	1478	-	3,3,3	0.75	0	2,2,2	0.09	0
5	EDO	E	1479	-	3,3,3	0.64	0	2,2,2	0.18	0
5	EDO	E	1480	-	3,3,3	0.69	0	2,2,2	0.15	0
5	EDO	E	1481	-	3,3,3	0.55	0	2,2,2	0.33	0
4	CAP	F	1477	3	20,20,20	0.69	0	31,31,31	0.95	1 (3%)
5	EDO	F	1478	-	3,3,3	0.62	0	2,2,2	0.19	0
5	EDO	F	1479	-	3,3,3	0.68	0	2,2,2	0.12	0
5	EDO	F	1480	-	3,3,3	0.59	0	2,2,2	0.09	0
5	EDO	F	1481	-	3,3,3	0.63	0	2,2,2	0.32	0
5	EDO	F	1482	-	3,3,3	0.51	0	2,2,2	0.50	0
5	EDO	F	1483	-	3,3,3	0.52	0	2,2,2	0.32	0
4	CAP	G	1477	3	20,20,20	0.86	0	31,31,31	0.95	1 (3%)
5	EDO	G	1478	-	3,3,3	0.72	0	2,2,2	0.20	0
5	EDO	G	1479	-	3,3,3	0.64	0	2,2,2	0.18	0
5	EDO	G	1480	-	3,3,3	0.66	0	2,2,2	0.21	0
5	EDO	G	1481	-	3,3,3	0.55	0	2,2,2	0.44	0
5	EDO	G	1482	-	3,3,3	0.56	0	2,2,2	0.35	0
4	CAP	H	1477	3	20,20,20	0.87	0	31,31,31	1.16	3 (9%)
5	EDO	H	1478	-	3,3,3	0.54	0	2,2,2	0.13	0
5	EDO	H	1479	-	3,3,3	0.75	0	2,2,2	0.11	0
5	EDO	H	1480	-	3,3,3	0.54	0	2,2,2	0.32	0
5	EDO	H	1481	-	3,3,3	0.60	0	2,2,2	0.31	0
5	EDO	H	1482	-	3,3,3	0.63	0	2,2,2	0.24	0
5	EDO	I	1141	-	3,3,3	0.59	0	2,2,2	0.27	0
5	EDO	I	1142	-	3,3,3	0.54	0	2,2,2	0.42	0
5	EDO	J	1141	-	3,3,3	0.58	0	2,2,2	0.23	0
5	EDO	J	1142	-	3,3,3	0.50	0	2,2,2	0.55	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	K	1141	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	K	1142	-	3,3,3	0.55	0	2,2,2	0.40	0
5	EDO	L	1141	-	3,3,3	0.60	0	2,2,2	0.17	0
5	EDO	L	1142	-	3,3,3	0.55	0	2,2,2	0.45	0
5	EDO	M	1141	-	3,3,3	0.57	0	2,2,2	0.34	0
5	EDO	M	1142	-	3,3,3	0.52	0	2,2,2	0.56	0
5	EDO	N	1141	-	3,3,3	0.54	0	2,2,2	0.39	0
5	EDO	N	1142	-	3,3,3	0.55	0	2,2,2	0.41	0
5	EDO	O	1141	-	3,3,3	0.56	0	2,2,2	0.37	0
5	EDO	O	1142	-	3,3,3	0.54	0	2,2,2	0.46	0
5	EDO	P	1141	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	P	1142	-	3,3,3	0.51	0	2,2,2	0.55	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
4	CAP	A	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	A	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1483	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1484	-	-	0/1/1/1	0/0/0/0
4	CAP	B	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	B	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1482	-	-	0/1/1/1	0/0/0/0
4	CAP	C	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	C	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1483	-	-	0/1/1/1	0/0/0/0
4	CAP	D	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	D	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1479	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1482	-	-	0/1/1/1	0/0/0/0
4	CAP	E	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	E	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1481	-	-	0/1/1/1	0/0/0/0
4	CAP	F	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	F	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1483	-	-	0/1/1/1	0/0/0/0
4	CAP	G	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	G	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1482	-	-	0/1/1/1	0/0/0/0
4	CAP	H	1477	3	-	0/29/29/29	0/0/0/0
5	EDO	H	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	I	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	I	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	J	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	J	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	L	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	L	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	M	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	M	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	N	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	N	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1141	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	P	1142	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1477	CAP	O4-C4-C5	-2.77	104.44	110.12
4	H	1477	CAP	O7-C-C2	2.73	119.53	113.58
4	E	1477	CAP	O2-C2-C	-2.64	103.83	108.77
4	F	1477	CAP	O1-C1-C2	2.64	111.42	108.34
4	D	1477	CAP	C1-C2-C	2.47	113.69	109.17
4	A	1477	CAP	O7-C-C2	2.45	118.93	113.58
4	E	1477	CAP	O7-C-C2	2.45	118.92	113.58
4	G	1477	CAP	O7-C-C2	2.39	118.79	113.58
4	A	1477	CAP	O1-C1-C2	2.24	110.96	108.34
4	E	1477	CAP	C1-C2-C	2.19	113.17	109.17
4	H	1477	CAP	O7-C-O6	-2.03	117.38	123.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	467/475 (98%)	-0.10	13 (2%)	50	56	10, 15, 28, 40	0
1	B	467/475 (98%)	-0.10	14 (2%)	48	53	10, 15, 28, 40	0
1	C	467/475 (98%)	-0.11	18 (3%)	37	41	10, 16, 28, 41	0
1	D	466/475 (98%)	-0.11	14 (3%)	48	53	11, 16, 27, 40	0
1	E	465/475 (97%)	-0.17	10 (2%)	59	66	10, 15, 28, 41	0
1	F	465/475 (97%)	-0.16	14 (3%)	48	53	11, 16, 28, 39	0
1	G	465/475 (97%)	-0.11	12 (2%)	53	59	10, 15, 28, 41	0
1	H	467/475 (98%)	-0.07	17 (3%)	41	44	10, 16, 28, 40	0
2	I	140/140 (100%)	0.35	14 (10%)	8	8	14, 21, 32, 36	0
2	J	140/140 (100%)	0.25	11 (7%)	13	14	14, 20, 33, 36	0
2	K	140/140 (100%)	0.27	12 (8%)	11	11	14, 21, 33, 37	0
2	L	140/140 (100%)	0.19	10 (7%)	16	17	14, 21, 32, 35	0
2	M	140/140 (100%)	0.17	10 (7%)	16	17	13, 20, 33, 35	0
2	N	140/140 (100%)	0.25	10 (7%)	16	17	14, 21, 33, 36	0
2	O	140/140 (100%)	0.21	11 (7%)	13	14	14, 21, 33, 36	0
2	P	140/140 (100%)	0.50	18 (12%)	4	4	14, 21, 33, 37	0
All	All	4849/4920 (98%)	-0.03	208 (4%)	35	37	10, 17, 30, 41	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	LEU	10.7
1	D	10	GLY	9.2
1	H	9	ALA	8.0
1	C	475	LEU	7.8
2	P	136	ASN	7.6

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Mol	Chain	Res	Type	RSRZ
1	E	475	LEU	7.6
1	D	475	LEU	7.2
1	G	475	LEU	7.0
1	A	10	GLY	6.8
1	G	94[A]	ASP	6.6
1	B	10	GLY	6.5
1	A	9	ALA	6.5
2	P	140	VAL	6.4
1	H	475	LEU	6.4
1	C	11	ALA	6.3
1	F	475	LEU	6.1
1	C	9	ALA	6.0
1	C	10	GLY	5.9
1	E	94[A]	ASP	5.9
1	D	11	ALA	5.8
2	P	135	ALA	5.7
1	F	11	ALA	5.7
1	H	11	ALA	5.7
1	G	92	GLY	5.6
1	D	94[A]	ASP	5.5
1	G	11	ALA	5.5
1	H	94[A]	ASP	5.5
1	H	10	GLY	5.5
1	F	94[A]	ASP	5.5
1	A	94[A]	ASP	5.4
1	A	475	LEU	5.2
1	E	11	ALA	5.2
1	C	439	ARG	5.1
1	D	92	GLY	5.1
1	B	9	ALA	4.9
1	H	91	PRO	4.9
2	P	137	LYS	4.9
2	K	84	ARG	4.8
1	B	91	PRO	4.7
1	A	439	ARG	4.7
2	P	134	PRO	4.6
1	C	92	GLY	4.4
1	G	439	ARG	4.3
1	E	92	GLY	4.3
1	D	439	ARG	4.2
1	E	439	ARG	4.1
2	P	23	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	92	GLY	4.0
1	B	449	CYS	4.0
1	H	439	ARG	4.0
1	C	94[A]	ASP	4.0
1	A	11	ALA	4.0
1	B	11	ALA	3.9
1	B	94[A]	ASP	3.8
1	G	91	PRO	3.8
2	I	130	ARG	3.7
2	O	136	ASN	3.7
1	F	464	GLU	3.7
1	C	91	PRO	3.7
1	F	439	ARG	3.6
1	D	449	CYS	3.5
2	P	127	LYS	3.5
1	B	464	GLU	3.4
2	K	128	THR	3.4
1	H	451	TRP	3.4
1	C	464	GLU	3.4
2	K	136	ASN	3.4
2	O	130	ARG	3.3
2	P	84	ARG	3.3
1	G	445	ILE	3.3
1	H	449	CYS	3.3
1	B	359	SER	3.3
2	J	83	CYS	3.2
2	P	22	THR	3.2
1	F	449	CYS	3.2
2	I	87	MET	3.2
2	I	84	ARG	3.2
2	N	87	MET	3.2
2	J	87	MET	3.2
2	K	87	MET	3.1
1	H	450	LYS	3.1
2	N	140	VAL	3.1
1	A	464	GLU	3.1
2	I	20	PRO	3.1
2	K	130	ARG	3.1
1	H	438	ALA	3.1
2	J	127	LYS	3.0
2	K	137	LYS	3.0
1	D	451	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	136	ASN	3.0
2	P	87	MET	3.0
1	A	47	GLY	3.0
1	E	47	GLY	3.0
2	I	140	VAL	3.0
2	J	128	THR	3.0
2	P	88	GLN	2.9
2	M	130	ARG	2.9
2	O	84	ARG	2.9
1	E	91	PRO	2.9
1	G	47	GLY	2.9
2	K	127	LYS	2.9
2	L	127	LYS	2.9
2	N	84	ARG	2.9
1	D	91	PRO	2.9
1	H	92	GLY	2.9
1	B	438	ALA	2.9
2	L	140	VAL	2.9
1	B	474	LYS	2.9
2	N	128	THR	2.8
2	P	24	GLU	2.8
2	I	88	GLN	2.8
2	J	130	ARG	2.8
2	O	87[A]	MET	2.8
2	L	87	MET	2.8
1	F	28	ASP	2.8
2	O	135	ALA	2.7
2	P	130	ARG	2.7
2	N	136	ASN	2.7
2	L	128	THR	2.7
2	O	128	THR	2.7
1	D	464	GLU	2.7
1	D	47	GLY	2.7
2	I	136	ASN	2.7
2	M	136	ASN	2.7
2	I	127	LYS	2.7
2	O	137	LYS	2.7
1	G	464	GLU	2.7
1	C	449	CYS	2.6
1	D	28	ASP	2.6
2	L	136	ASN	2.6
1	A	449	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	464	GLU	2.6
2	I	24	GLU	2.6
2	K	24	GLU	2.6
2	N	88	GLN	2.6
2	N	127	LYS	2.6
2	I	137	LYS	2.6
2	J	137	LYS	2.6
2	K	140	VAL	2.6
1	A	451	TRP	2.6
1	H	464	GLU	2.5
2	I	23	ASP	2.5
1	C	355	GLU	2.5
2	N	24	GLU	2.5
1	G	449	CYS	2.5
1	B	450	LYS	2.5
1	C	450	LYS	2.5
2	M	127	LYS	2.5
2	L	84	ARG	2.5
1	G	93	GLU	2.5
2	L	88	GLN	2.5
2	O	127	LYS	2.4
1	D	355	GLU	2.4
1	C	438	ALA	2.4
2	J	84	ARG	2.4
2	J	24	GLU	2.4
1	H	474	LYS	2.4
2	M	24	GLU	2.4
2	K	88	GLN	2.4
2	J	140	VAL	2.4
2	N	137	LYS	2.4
2	P	20	PRO	2.4
2	I	32	TYR	2.4
1	F	93	GLU	2.4
1	B	470	ASP	2.3
1	C	451	TRP	2.3
2	L	24	GLU	2.3
1	E	93	GLU	2.3
1	C	127	PHE	2.3
2	O	24	GLU	2.3
2	M	88	GLN	2.3
2	N	130	ARG	2.2
1	B	460	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	93	GLU	2.2
1	H	47	GLY	2.2
1	A	438	ALA	2.2
1	F	91	PRO	2.2
2	K	83	CYS	2.2
2	P	128	THR	2.2
2	M	23	ASP	2.2
1	D	460	GLU	2.2
2	M	84	ARG	2.2
2	O	102	ASP	2.2
2	O	140	VAL	2.2
2	P	83	CYS	2.2
1	F	12	GLY	2.1
2	L	130	ARG	2.1
2	L	48	ASP	2.1
1	A	443	ASP	2.1
1	H	443	ASP	2.1
2	I	48	ASP	2.1
1	C	47	GLY	2.1
1	F	438	ALA	2.1
2	M	137	LYS	2.1
2	K	23	ASP	2.1
2	I	128	THR	2.1
1	A	434	GLY	2.1
1	H	460	GLU	2.1
2	P	82	GLY	2.1
2	M	87	MET	2.0
2	J	88	GLN	2.0
1	G	443	ASP	2.0
1	F	127	PHE	2.0
1	F	474	LYS	2.0
2	M	140	VAL	2.0
1	C	436	ASP	2.0
2	P	102	ASP	2.0
1	E	450	LYS	2.0

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

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MME	J	1	9/10	0.21	3.75	27,29,37,38	0
2	MME	O	1	9/10	0.19	3.46	27,29,37,37	0
2	MME	L	1	9/10	0.15	2.63	26,28,35,35	0
2	MME	N	1	9/10	0.20	2.17	27,28,36,37	0
2	MME	M	1	9/10	0.14	1.32	26,28,36,36	0
2	MME	I	1	9/10	0.15	1.17	27,28,36,36	0
1	HYP	B	151	8/9	0.08	1.09	12,12,12,13	0
2	MME	P	1	9/10	0.18	0.83	27,28,35,36	0
1	KCX	G	201	12/13	0.07	0.73	12,12,13,13	0
1	KCX	A	201	12/13	0.07	0.67	12,13,14,14	0
1	KCX	D	201	12/13	0.07	0.66	12,13,14,15	0
1	KCX	H	201	12/13	0.07	0.65	12,12,14,16	0
1	KCX	B	201	12/13	0.07	0.60	12,13,13,15	0
1	KCX	C	201	12/13	0.07	0.46	13,13,15,15	0
1	HYP	F	151	8/9	0.07	0.39	12,13,13,13	0
1	KCX	E	201	12/13	0.07	0.29	12,14,15,15	0
2	MME	K	1	9/10	0.14	0.28	27,28,36,37	0
1	SMC	A	369	7/8	0.08	0.21	15,16,20,21	0
1	HYP	H	151	8/9	0.07	0.19	12,12,12,12	0
1	KCX	F	201	12/13	0.07	0.15	12,13,14,15	0
1	HYP	F	104	8/9	0.08	0.15	13,13,15,16	0
1	SMC	F	369	7/8	0.07	0.12	15,16,20,22	0
1	HYP	A	151	8/9	0.07	0.00	12,12,12,12	0
1	SMC	D	369	7/8	0.06	-0.24	15,16,20,22	0
1	HYP	H	104	8/9	0.07	-0.31	13,13,14,15	0
1	HYP	C	151	8/9	0.06	-0.38	12,12,13,14	0
1	SMC	C	369	7/8	0.06	-0.42	15,16,20,21	0
1	SMC	E	256	7/8	0.07	-0.55	11,11,12,13	0
1	SMC	B	369	7/8	0.06	-0.57	15,16,20,23	0
1	HYP	E	104	8/9	0.06	-0.59	12,12,13,15	0
1	HYP	D	104	8/9	0.06	-0.64	13,13,14,16	0
1	SMC	H	256	7/8	0.06	-0.69	10,11,12,13	0
1	SMC	D	256	7/8	0.06	-0.73	11,11,12,13	0
1	HYP	G	104	8/9	0.06	-0.73	13,13,14,16	0
1	HYP	C	104	8/9	0.05	-0.73	13,14,14,15	0
1	SMC	H	369	7/8	0.06	-0.74	15,16,20,20	0
1	SMC	B	256	7/8	0.06	-0.76	10,11,12,13	0
1	HYP	B	104	8/9	0.06	-0.78	12,13,13,15	0
1	SMC	C	256	7/8	0.06	-0.78	10,11,13,13	0
1	HYP	A	104	8/9	0.05	-0.81	13,13,14,15	0
1	SMC	A	256	7/8	0.05	-1.23	11,11,12,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SMC	E	369	7/8	0.05	-1.26	15,15,20,21	0
1	HYP	E	151	8/9	0.05	-1.26	11,12,12,12	0
1	HYP	D	151	8/9	0.05	-1.27	12,12,12,13	0
1	SMC	G	369	7/8	0.06	-1.27	14,15,19,22	0
1	SMC	F	256	7/8	0.04	-1.45	10,11,12,15	0
1	SMC	G	256	7/8	0.04	-1.70	10,11,12,13	0
1	HYP	G	151	8/9	0.04	-2.07	12,12,12,13	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	G	1480	4/4	0.20	9.15	37,38,38,39	0
5	EDO	A	1482	4/4	0.26	7.37	34,38,38,40	0
5	EDO	C	1480	4/4	0.16	6.26	34,34,35,35	0
5	EDO	B	1480	4/4	0.15	5.00	37,37,37,37	0
5	EDO	G	1479	4/4	0.13	4.88	27,27,28,29	0
5	EDO	B	1482	4/4	0.26	4.29	40,42,43,44	0
5	EDO	A	1479	4/4	0.11	3.85	23,23,23,24	0
5	EDO	F	1483	4/4	0.18	3.80	35,38,38,40	0
5	EDO	F	1481	4/4	0.15	3.76	37,38,38,38	0
5	EDO	K	1141	4/4	0.19	3.75	32,32,34,34	0
5	EDO	M	1141	4/4	0.21	3.68	31,31,32,32	0
5	EDO	C	1479	4/4	0.11	3.27	24,25,25,28	0
5	EDO	C	1478	4/4	0.11	3.17	20,21,22,22	0
5	EDO	E	1480	4/4	0.16	3.15	33,34,34,34	0
5	EDO	D	1480	4/4	0.15	2.85	43,43,43,43	0
5	EDO	A	1480	4/4	0.17	2.81	40,40,41,41	0
5	EDO	D	1478	4/4	0.11	2.71	21,21,22,23	0
5	EDO	E	1478	4/4	0.11	2.71	19,20,22,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	L	1141	4/4	0.16	2.70	30,31,31,32	0
5	EDO	J	1141	4/4	0.15	2.65	32,32,33,33	0
5	EDO	C	1482	4/4	0.20	2.44	50,51,51,51	0
5	EDO	D	1479	4/4	0.11	2.44	25,27,27,27	0
5	EDO	A	1484	4/4	0.25	2.33	53,53,54,54	0
5	EDO	O	1141	4/4	0.15	2.23	32,32,33,34	0
5	EDO	D	1482	4/4	0.15	2.16	57,58,58,58	0
5	EDO	H	1481	4/4	0.13	2.13	35,36,36,37	0
5	EDO	I	1141	4/4	0.16	2.08	31,31,33,33	0
5	EDO	F	1479	4/4	0.10	2.01	20,20,22,23	0
5	EDO	B	1479	4/4	0.10	1.87	24,24,25,25	0
5	EDO	B	1478	4/4	0.10	1.86	18,19,20,22	0
5	EDO	H	1480	4/4	0.11	1.76	25,25,26,27	0
5	EDO	H	1479	4/4	0.09	1.59	18,18,20,21	0
5	EDO	G	1478	4/4	0.10	1.45	20,20,22,23	0
5	EDO	N	1141	4/4	0.14	1.27	32,33,33,34	0
5	EDO	G	1482	4/4	0.14	1.16	43,43,43,43	0
5	EDO	M	1142	4/4	0.15	0.99	29,31,32,35	0
5	EDO	P	1141	4/4	0.11	0.97	34,34,35,36	0
5	EDO	N	1142	4/4	0.23	0.97	34,36,37,40	0
5	EDO	E	1479	4/4	0.09	0.93	22,23,23,23	0
5	EDO	A	1483	4/4	0.08	0.65	19,19,19,20	0
5	EDO	F	1480	4/4	0.08	0.62	25,26,26,26	0
5	EDO	H	1482	4/4	0.20	0.55	33,33,34,34	0
5	EDO	J	1142	4/4	0.17	0.44	35,37,38,39	0
5	EDO	P	1142	4/4	0.18	0.38	29,31,33,36	0
5	EDO	L	1142	4/4	0.15	0.33	31,33,35,37	0
5	EDO	I	1142	4/4	0.18	0.20	39,40,41,43	0
5	EDO	A	1478	4/4	0.08	0.09	18,20,21,21	0
5	EDO	K	1142	4/4	0.16	0.09	33,34,35,35	0
5	EDO	F	1478	4/4	0.06	-0.02	19,21,21,21	0
5	EDO	C	1483	4/4	0.06	-0.06	20,21,22,23	0
5	EDO	F	1482	4/4	0.12	-0.07	26,26,26,27	0
5	EDO	G	1481	4/4	0.15	-0.13	24,25,26,27	0
5	EDO	O	1142	4/4	0.13	-0.15	33,35,36,38	0
5	EDO	B	1481	4/4	0.14	-0.36	28,29,29,29	0
5	EDO	E	1481	4/4	0.11	-0.42	25,26,27,28	0
5	EDO	D	1481	4/4	0.10	-0.50	25,25,25,26	0
4	CAP	E	1477	21/21	0.06	-0.80	13,14,15,20	0
5	EDO	A	1481	4/4	0.10	-0.88	25,25,25,25	0
4	CAP	D	1477	21/21	0.06	-0.90	13,14,15,19	0
5	EDO	H	1478	4/4	0.05	-1.11	20,20,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CAP	F	1477	21/21	0.06	-1.13	13,15,17,21	0
5	EDO	C	1481	4/4	0.09	-1.15	30,31,31,31	0
4	CAP	H	1477	21/21	0.06	-1.17	14,14,16,19	0
4	CAP	C	1477	21/21	0.06	-1.31	14,15,17,20	0
4	CAP	A	1477	21/21	0.05	-1.43	13,14,15,19	0
4	CAP	G	1477	21/21	0.05	-1.67	12,14,16,19	0
4	CAP	B	1477	21/21	0.05	-2.04	14,14,16,20	0
3	MG	B	1476	1/1	0.04	-2.41	13,13,13,13	0
3	MG	A	1476	1/1	0.03	-3.05	13,13,13,13	0
3	MG	G	1476	1/1	0.03	-3.17	12,12,12,12	0
3	MG	D	1476	1/1	0.03	-3.18	13,13,13,13	0
3	MG	F	1476	1/1	0.04	-3.66	13,13,13,13	0
3	MG	H	1476	1/1	0.03	-5.53	13,13,13,13	0
3	MG	E	1476	1/1	0.02	-5.61	13,13,13,13	0
3	MG	C	1476	1/1	0.03	-6.17	13,13,13,13	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.