Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:47 PM GMT

PDB ID	:	1UZH
Title	:	A CHIMERIC CHLAMYDOMONAS, SYNECHOCOCCUS RUBISCO ENZYME
Authors	:	Karkehabadi, S.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2004-03-12
Resolution	:	2.20 Å(reported)

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

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

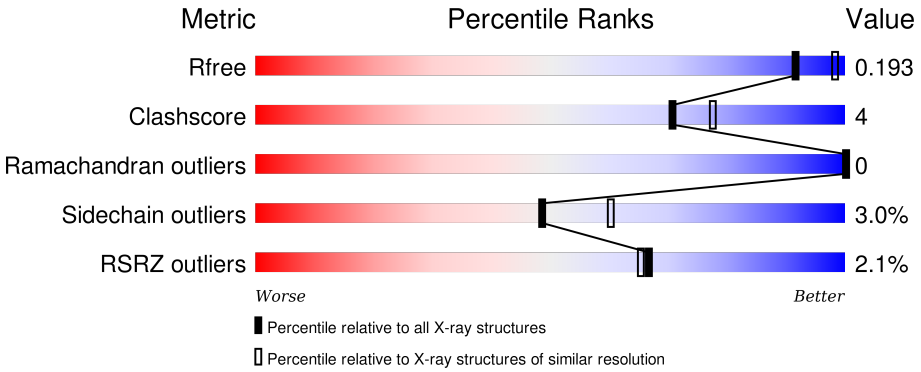
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	475	88% 9%
1	B	475	% 89% 9%
1	E	475	% 89% 9%
1	H	475	% 88% 10%
1	K	475	% 89% 8%

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Mol	Chain	Length	Quality of chain
1	O	475	91% 8%
1	R	475	88% 9%
1	V	475	88% 10%
2	C	122	82% 16%
2	F	122	6% 84% 14%
2	I	122	3% 82% 16%
2	J	122	9% 84% 14%
2	M	122	6% 87% 11%
2	P	122	4% 81% 17%
2	T	122	7% 83% 16%
2	W	122	9% 85% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1480	-	-	-	X
5	EDO	B	1476	-	-	-	X
5	EDO	H	1476	-	-	-	X
5	EDO	H	1478	-	-	-	X
5	EDO	H	1481	-	-	-	X
5	EDO	O	1477	-	-	-	X
5	EDO	O	1478	-	-	-	X
5	EDO	O	1480	-	-	-	X
5	EDO	R	1480	-	-	-	X
5	EDO	V	1476	-	-	-	X
5	EDO	V	1481	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40557 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 BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	3	0
			3640	2300	641	675	24			
1	B	467	Total	C	N	O	S	0	3	0
			3647	2305	642	676	24			
1	E	469	Total	C	N	O	S	0	3	0
			3665	2315	646	680	24			
1	H	469	Total	C	N	O	S	0	3	0
			3665	2315	646	680	24			
1	K	469	Total	C	N	O	S	0	5	0
			3673	2321	646	682	24			
1	O	469	Total	C	N	O	S	0	2	0
			3661	2313	646	678	24			
1	R	469	Total	C	N	O	S	0	2	0
			3662	2314	646	678	24			
1	V	469	Total	C	N	O	S	0	3	0
			3664	2316	645	679	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	CONFLICT	UNP P00877
B	46	PRO	LEU	CONFLICT	UNP P00877
E	46	PRO	LEU	CONFLICT	UNP P00877
H	46	PRO	LEU	CONFLICT	UNP P00877
K	46	PRO	LEU	CONFLICT	UNP P00877
O	46	PRO	LEU	CONFLICT	UNP P00877
R	46	PRO	LEU	CONFLICT	UNP P00877
V	46	PRO	LEU	CONFLICT	UNP P00877

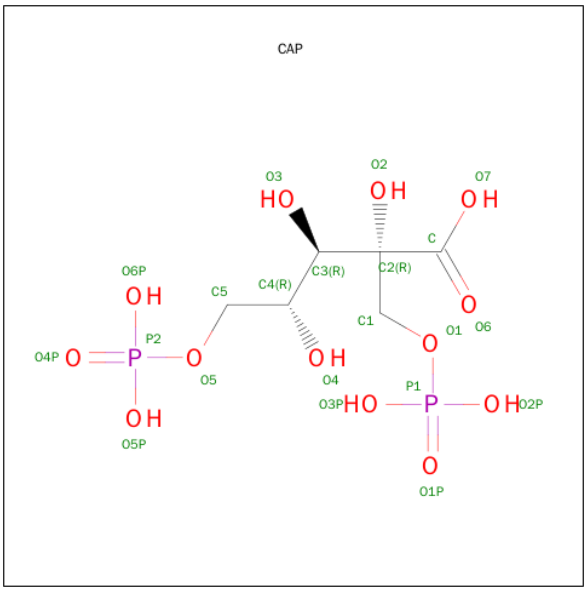
- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	2	0
			1009	654	167	178	10			
2	F	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	I	122	Total	C	N	O	S	0	1	0
			1006	653	166	177	10			
2	J	122	Total	C	N	O	S	0	1	0
			1006	653	166	176	11			
2	M	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	11			
2	P	122	Total	C	N	O	S	0	3	0
			1010	654	167	178	11			
2	T	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	W	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	11			

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

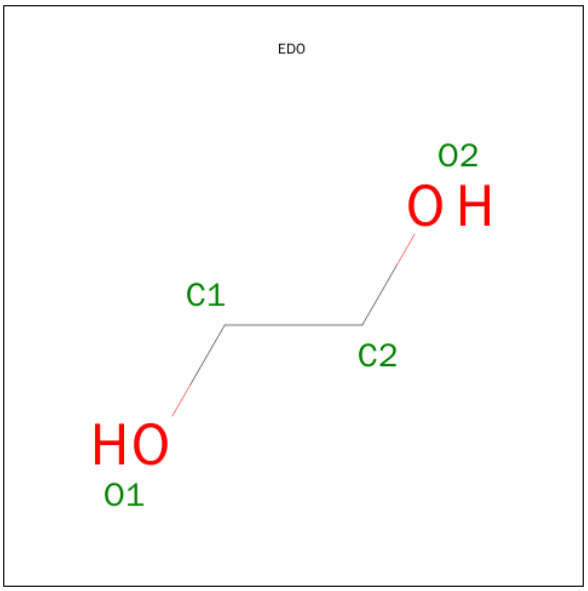
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	V	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	R	1	Total	Mg	0	0
			1	1		

- 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 21 6 13 2	0	0
4	B	1	Total C O P 21 6 13 2	0	0
4	E	1	Total C O P 21 6 13 2	0	0
4	H	1	Total C O P 21 6 13 2	0	0
4	K	1	Total C O P 21 6 13 2	0	0
4	O	1	Total C O P 21 6 13 2	0	0
4	R	1	Total C O P 21 6 13 2	0	0
4	V	1	Total C O P 21 6 13 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	W	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	294	Total O 294 294	0	0
6	B	317	Total O 317 317	0	0
6	C	61	Total O 61 61	0	0
6	E	292	Total O 292 292	0	0

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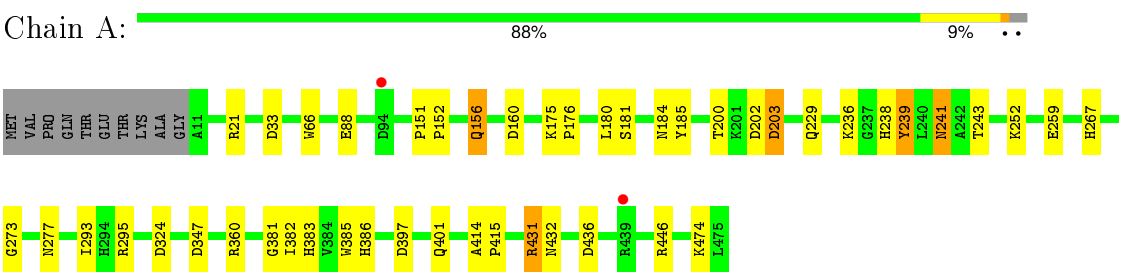
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	70	Total O 70 70	0	0
6	H	288	Total O 288 288	0	0
6	I	66	Total O 66 66	0	0
6	J	57	Total O 57 57	0	0
6	K	279	Total O 279 279	0	0
6	M	56	Total O 56 56	0	0
6	O	286	Total O 286 286	0	0
6	P	55	Total O 55 55	0	0
6	R	307	Total O 307 307	0	0
6	T	73	Total O 73 73	0	0
6	V	281	Total O 281 281	0	0
6	W	49	Total O 49 49	0	0

3 Residue-property plots (i)

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

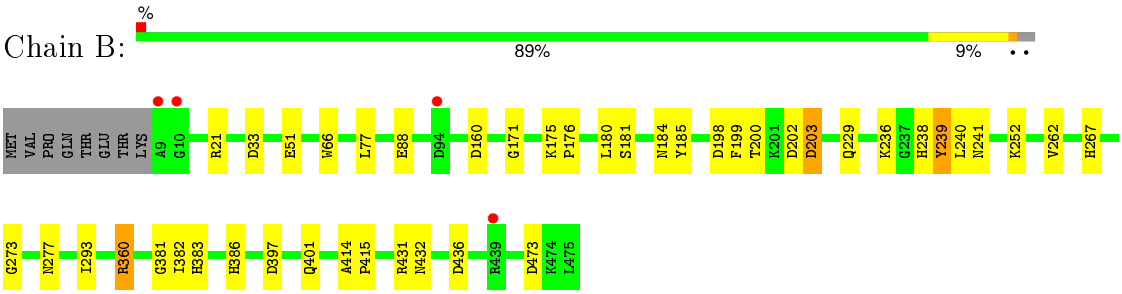
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:



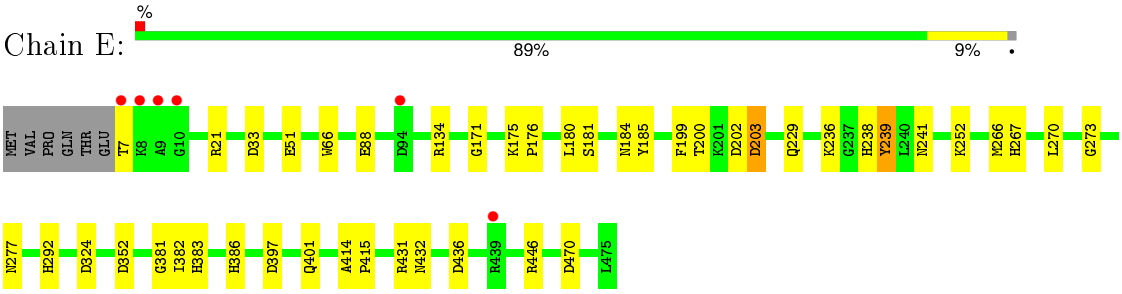
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



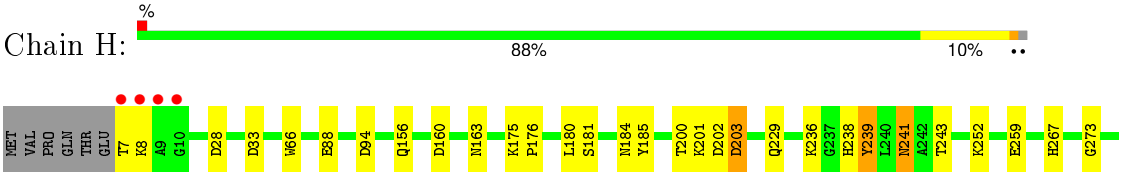
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

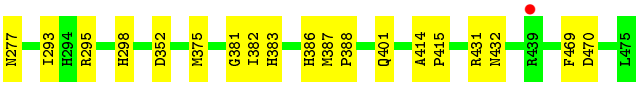
Chain E:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

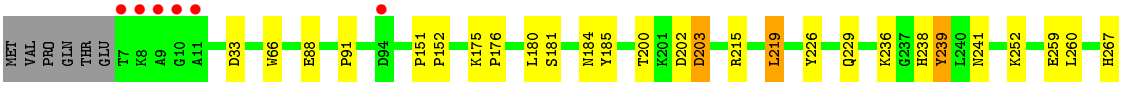
Chain H:

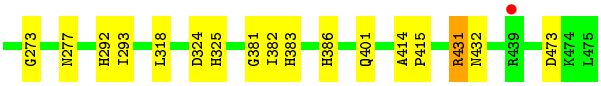




• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

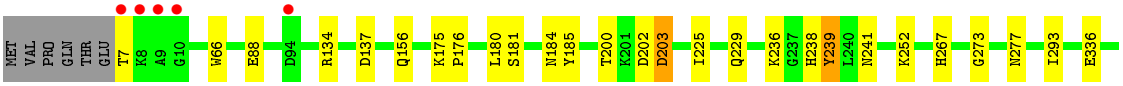
Chain K:





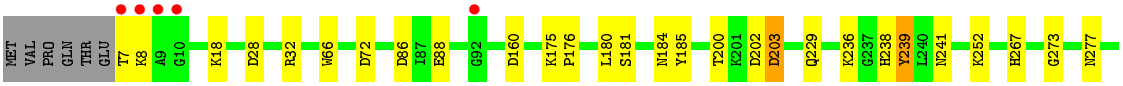
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain O:



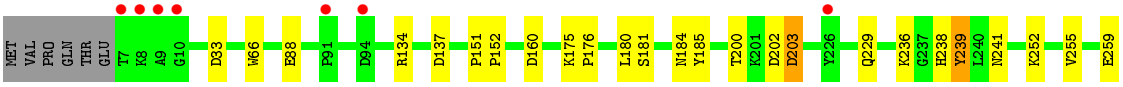
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

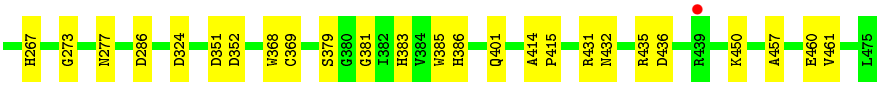
Chain R:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

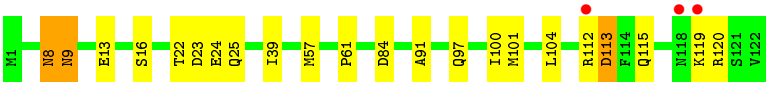
Chain V:





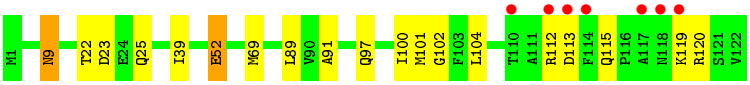
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain C:



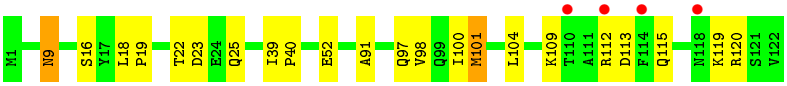
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain F:



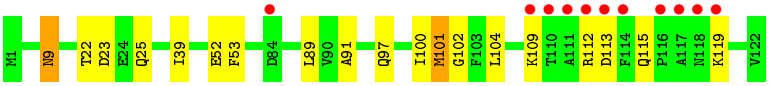
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain I:



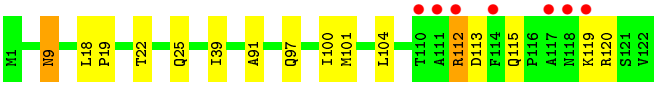
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain J:



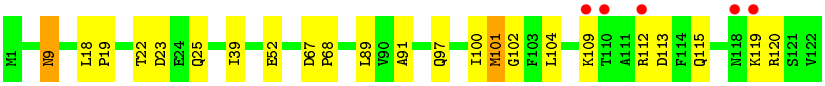
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain M:



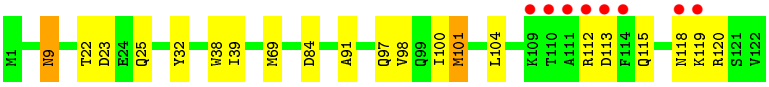
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain P:

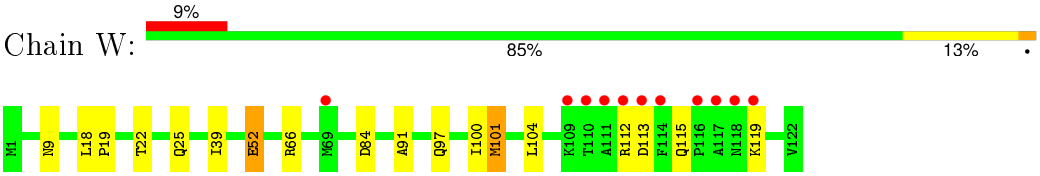


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain T:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	220.82Å 223.97Å 111.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.88 – 2.19	Depositor EDS
% Data completeness (in resolution range)	89.3 (30.00-2.20) 88.6 (29.88-2.19)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.160 , 0.193 0.162 , 0.193	Depositor DCC
R_{free} test set	12558 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.7	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 250002 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40557	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, EDO, HYP, 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	0.61	0/3695	0.75	6/4993 (0.1%)
1	B	0.62	0/3704	0.80	13/5005 (0.3%)
1	E	0.61	0/3720	0.76	7/5026 (0.1%)
1	H	0.60	0/3720	0.76	7/5026 (0.1%)
1	K	0.62	0/3736	0.75	5/5048 (0.1%)
1	O	0.60	0/3711	0.76	3/5014 (0.1%)
1	R	0.60	0/3711	0.76	10/5014 (0.2%)
1	V	0.61	0/3718	0.75	9/5024 (0.2%)
2	C	0.61	0/1049	0.71	3/1426 (0.2%)
2	F	0.59	0/1056	0.69	2/1435 (0.1%)
2	I	0.60	0/1041	0.69	2/1415 (0.1%)
2	J	0.61	0/1043	0.70	2/1417 (0.1%)
2	M	0.61	0/1049	0.72	1/1425 (0.1%)
2	P	0.60	0/1057	0.72	2/1436 (0.1%)
2	T	0.61	0/1056	0.70	3/1435 (0.2%)
2	W	0.60	0/1049	0.70	2/1425 (0.1%)
All	All	0.61	0/38115	0.75	77/51564 (0.1%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360[A]	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	360[B]	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	P	113	ASP	CB-CG-OD2	7.29	124.86	118.30
2	M	113	ASP	CB-CG-OD2	7.11	124.70	118.30
2	C	113	ASP	CB-CG-OD2	6.93	124.53	118.30
1	B	360[A]	ARG	CD-NE-CZ	6.91	133.27	123.60
1	B	360[B]	ARG	CD-NE-CZ	6.91	133.27	123.60
2	W	113	ASP	CB-CG-OD2	6.85	124.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	113	ASP	CB-CG-OD2	6.82	124.44	118.30
2	T	113	ASP	CB-CG-OD2	6.81	124.43	118.30
1	H	203	ASP	CB-CG-OD2	6.52	124.17	118.30
2	J	113	ASP	CB-CG-OD2	6.52	124.17	118.30
1	O	203	ASP	CB-CG-OD2	6.45	124.11	118.30
1	V	203	ASP	CB-CG-OD2	6.41	124.07	118.30
2	I	113	ASP	CB-CG-OD2	6.41	124.07	118.30
1	V	33	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	160	ASP	CB-CG-OD2	6.21	123.89	118.30
2	P	23	ASP	CB-CG-OD2	6.12	123.81	118.30
1	V	352	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	203	ASP	CB-CG-OD2	6.01	123.70	118.30
1	R	324	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	436	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	324	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	160	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	324	ASP	CB-CG-OD2	5.73	123.45	118.30
2	J	23	ASP	CB-CG-OD2	5.70	123.43	118.30
1	H	352	ASP	CB-CG-OD2	5.65	123.38	118.30
1	V	436	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	33	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	397	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	203	ASP	CB-CG-OD2	5.54	123.29	118.30
1	H	33	ASP	CB-CG-OD2	5.52	123.27	118.30
1	R	473	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	470	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	160	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	33[A]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	33[B]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	28	ASP	CB-CG-OD2	5.46	123.22	118.30
2	I	23	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	397	ASP	CB-CG-OD2	5.43	123.19	118.30
1	V	324	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	360[A]	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	360[B]	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	F	23	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	352	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	33	ASP	CB-CG-OD2	5.38	123.14	118.30
1	R	397	ASP	CB-CG-OD2	5.37	123.13	118.30
1	R	72	ASP	CB-CG-OD2	5.36	123.13	118.30
1	K	203	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	198	ASP	CB-CG-OD2	5.32	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	352	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	473	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	473	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	28	ASP	CB-CG-OD2	5.29	123.06	118.30
2	C	84	ASP	CB-CG-OD2	5.28	123.05	118.30
2	T	84	ASP	CB-CG-OD2	5.26	123.03	118.30
1	V	160	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	436	ASP	CB-CG-OD2	5.19	122.97	118.30
1	R	470	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	160	ASP	CB-CG-OD2	5.17	122.95	118.30
2	T	23	ASP	CB-CG-OD2	5.14	122.93	118.30
2	W	84	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	470	ASP	CB-CG-OD2	5.11	122.90	118.30
1	R	203	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	33	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	397	ASP	CB-CG-OD2	5.09	122.88	118.30
1	V	351	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	436	ASP	CB-CG-OD2	5.08	122.87	118.30
1	R	86	ASP	CB-CG-OD2	5.07	122.86	118.30
1	K	324	ASP	CB-CG-OD2	5.07	122.86	118.30
1	V	137	ASP	CB-CG-OD2	5.06	122.86	118.30
1	O	397	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	203	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	94	ASP	CB-CG-OD2	5.04	122.84	118.30
1	V	286	ASP	CB-CG-OD2	5.04	122.83	118.30
2	C	23	ASP	CB-CG-OD2	5.01	122.81	118.30
1	O	137	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3542	34	0
1	B	3647	0	3550	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3665	0	3570	30	0
1	H	3665	0	3570	37	0
1	K	3673	0	3581	33	0
1	O	3661	0	3568	30	0
1	R	3662	0	3572	32	0
1	V	3664	0	3575	32	0
2	C	1009	0	986	13	0
2	F	1014	0	989	13	0
2	I	1006	0	984	13	0
2	J	1006	0	984	15	0
2	M	1007	0	985	11	0
2	P	1010	0	987	13	0
2	T	1014	0	989	14	0
2	W	1007	0	985	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	7	0	0
4	E	21	0	8	0	0
4	H	21	0	8	1	0
4	K	21	0	8	0	0
4	O	21	0	8	0	0
4	R	21	0	9	0	0
4	V	21	0	7	0	0
5	A	20	0	30	0	0
5	B	24	0	36	2	0
5	C	4	0	6	0	0
5	E	20	0	30	2	0
5	F	4	0	6	0	0
5	H	24	0	36	3	0
5	J	4	0	6	1	0
5	K	20	0	30	0	0
5	M	4	0	6	0	0
5	O	20	0	30	1	0
5	P	4	0	6	0	0
5	R	20	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	4	0	6	0	0
5	V	24	0	36	0	0
5	W	4	0	6	0	0
6	A	294	0	0	7	0
6	B	317	0	0	5	0
6	C	61	0	0	1	0
6	E	292	0	0	1	0
6	F	70	0	0	2	0
6	H	288	0	0	11	0
6	I	66	0	0	1	0
6	J	57	0	0	4	0
6	K	279	0	0	6	0
6	M	56	0	0	1	0
6	O	286	0	0	2	0
6	P	55	0	0	1	0
6	R	307	0	0	7	0
6	T	73	0	0	2	0
6	V	281	0	0	5	0
6	W	49	0	0	3	0
All	All	40557	0	36780	326	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 4.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:375:MET:HG2	6:H:2185:HOH:O	1.31	1.28
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.04	0.99
1:V:255:VAL:O	1:V:259[B]:GLU:HG2	1.63	0.97
2:P:97:GLN:HE21	1:R:184:ASN:HD22	1.10	0.97
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.03	0.96
1:B:184:ASN:HD22	2:F:97:GLN:HE21	1.08	0.95
1:K:267:HIS:HD2	1:K:277:ASN:HD22	0.97	0.94
1:A:267:HIS:HD2	1:A:277:ASN:HD22	0.97	0.94
1:R:267:HIS:HD2	1:R:277:ASN:HD22	0.97	0.93
1:H:375:MET:CG	6:H:2185:HOH:O	2.00	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	0.96	0.93
1:O:267:HIS:HD2	1:O:277:ASN:HD22	0.98	0.93
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.01	0.91
1:H:184:ASN:HD22	2:W:97:GLN:HE21	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ASN:HD22	2:J:97:GLN:HE21	1.15	0.89
1:V:460:GLU:HB3	6:V:2259:HOH:O	1.71	0.89
1:R:435:ARG:HG3	6:R:2266:HOH:O	1.72	0.89
1:K:259[B]:GLU:CG	6:K:2157:HOH:O	2.19	0.89
1:R:267:HIS:CD2	1:R:277:ASN:HD22	1.90	0.88
2:F:52:GLU:HG3	6:F:2035:HOH:O	1.72	0.88
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.88	0.88
2:M:97:GLN:HE21	1:O:184:ASN:HD22	1.20	0.87
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.89	0.87
1:O:267:HIS:CD2	1:O:277:ASN:HD22	1.91	0.87
2:C:97:GLN:HE21	1:V:184:ASN:HD22	1.20	0.86
1:A:184:ASN:HD22	2:T:97:GLN:HE21	1.19	0.86
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.24	0.85
1:O:431:ARG:HH21	1:O:432:ASN:HD21	1.23	0.85
1:E:270:LEU:O	5:E:1480:EDO:H22	1.75	0.85
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.93	0.84
1:K:267:HIS:CD2	1:K:277:ASN:HD22	1.90	0.84
1:V:431:ARG:HH21	1:V:432:ASN:HD21	1.21	0.84
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.22	0.83
1:R:431:ARG:HH21	1:R:432:ASN:HD21	1.25	0.83
1:A:21:ARG:NH1	6:A:2015:HOH:O	1.89	0.83
1:V:383:HIS:H	1:V:386:HIS:HD2	1.27	0.82
1:E:383:HIS:H	1:E:386:HIS:HD2	1.27	0.82
1:H:375:MET:SD	6:H:2185:HOH:O	2.38	0.81
2:I:97:GLN:HE21	1:K:184:ASN:HD22	1.26	0.81
1:E:21:ARG:CZ	1:E:51[B]:GLU:HG3	2.10	0.81
1:O:383:HIS:H	1:O:386:HIS:HD2	1.30	0.80
1:A:383:HIS:H	1:A:386:HIS:HD2	1.30	0.79
1:K:431:ARG:HH21	1:K:432:ASN:HD21	1.28	0.79
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.27	0.79
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.95	0.79
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.30	0.78
1:K:383:HIS:H	1:K:386:HIS:HD2	1.29	0.77
1:V:267:HIS:CD2	1:V:277:ASN:HD22	1.97	0.77
1:R:383:HIS:H	1:R:386:HIS:HD2	1.30	0.76
1:E:21:ARG:NH2	1:E:51[A]:GLU:OE1	2.19	0.76
1:B:383:HIS:H	1:B:386:HIS:HD2	1.32	0.75
2:W:52:GLU:HG3	6:W:2023:HOH:O	1.85	0.75
1:E:267:HIS:HD2	1:E:277:ASN:ND2	1.80	0.74
1:O:267:HIS:HD2	1:O:277:ASN:ND2	1.82	0.74
1:K:259[B]:GLU:HG2	6:K:2157:HOH:O	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259[B]:GLU:HG3	6:K:2157:HOH:O	1.83	0.73
2:C:22:THR:H	2:C:25:GLN:HE21	1.35	0.73
1:H:383:HIS:H	1:H:386:HIS:HD2	1.38	0.72
1:B:21:ARG:NH2	1:B:51:GLU:OE1	2.23	0.71
1:E:21:ARG:NH1	1:E:51[B]:GLU:HG3	2.07	0.70
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.82	0.70
2:W:22:THR:H	2:W:25:GLN:HE21	1.40	0.70
2:M:22:THR:H	2:M:25:GLN:HE21	1.40	0.68
5:R:1480:EDO:H11	6:R:2195:HOH:O	1.95	0.67
1:K:267:HIS:HD2	1:K:277:ASN:ND2	1.83	0.67
1:H:375:MET:CE	6:H:2185:HOH:O	2.42	0.67
2:F:22:THR:H	2:F:25:GLN:HE21	1.41	0.67
1:O:202:ASP:OD1	1:O:238:HIS:HE1	1.78	0.67
2:I:22:THR:H	2:I:25:GLN:HE21	1.44	0.66
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.87	0.65
2:T:22:THR:H	2:T:25:GLN:HE21	1.43	0.64
2:J:22:THR:H	2:J:25:GLN:HE21	1.44	0.64
1:K:202:ASP:OD1	1:K:238:HIS:HE1	1.81	0.64
2:P:22:THR:H	2:P:25:GLN:HE21	1.45	0.64
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.81	0.64
1:K:200:THR:OG1	1:K:238:HIS:HD2	1.80	0.63
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.82	0.63
2:F:115:GLN:HE21	2:F:119:LYS:HB3	1.64	0.62
2:T:115:GLN:HE21	2:T:119:LYS:HB3	1.65	0.62
2:W:66:ARG:HD2	6:W:2030:HOH:O	2.00	0.62
2:J:115:GLN:HE21	2:J:119:LYS:HB3	1.65	0.62
1:R:202:ASP:OD1	1:R:238:HIS:HE1	1.83	0.62
2:C:97:GLN:NE2	1:V:181:SER:H	1.98	0.61
1:R:267:HIS:HD2	1:R:277:ASN:ND2	1.82	0.61
1:H:469:PHE:CZ	5:H:1480:EDO:H22	2.35	0.61
2:I:115:GLN:HE21	2:I:119:LYS:HB3	1.66	0.61
2:M:115:GLN:HE21	2:M:119:LYS:HB3	1.65	0.61
1:B:184:ASN:HD22	2:F:97:GLN:NE2	1.91	0.61
1:K:383:HIS:H	1:K:386:HIS:CD2	2.16	0.60
2:P:115:GLN:HE21	2:P:119:LYS:HB3	1.66	0.60
2:C:97:GLN:HE22	1:V:180:LEU:HA	1.66	0.60
2:M:97:GLN:HE22	1:O:180:LEU:HA	1.66	0.59
2:W:115:GLN:HE21	2:W:119:LYS:HB3	1.66	0.59
2:C:115:GLN:HE21	2:C:119:LYS:HB3	1.67	0.59
1:B:181:SER:H	2:F:97:GLN:NE2	2.01	0.59
1:O:200:THR:OG1	1:O:238:HIS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:200:THR:OG1	1:R:238:HIS:HD2	1.84	0.59
1:K:91:PRO:HA	6:K:2053:HOH:O	2.02	0.58
2:I:97:GLN:HE22	1:K:180:LEU:HA	1.67	0.58
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.86	0.58
1:H:66:TRP:CD1	1:R:381:GLY:HA2	2.38	0.58
6:H:2110:HOH:O	2:J:53:PHE:HD1	1.86	0.58
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.85	0.58
1:E:383:HIS:H	1:E:386:HIS:CD2	2.16	0.57
1:H:181:SER:H	2:W:97:GLN:NE2	2.03	0.57
1:V:200:THR:OG1	1:V:238:HIS:HD2	1.87	0.57
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.87	0.57
2:C:24:GLU:HB2	6:C:2020:HOH:O	2.04	0.57
1:A:383:HIS:H	1:A:386:HIS:CD2	2.17	0.57
2:W:66:ARG:HD3	6:W:2031:HOH:O	2.04	0.57
1:O:383:HIS:H	1:O:386:HIS:CD2	2.17	0.56
1:V:202:ASP:OD1	1:V:238:HIS:HE1	1.89	0.56
1:O:239:TYR:HE2	1:O:401:GLN:HE22	1.52	0.56
1:A:180:LEU:HA	2:T:97:GLN:HE22	1.70	0.56
1:A:181:SER:H	2:T:97:GLN:NE2	2.03	0.56
1:R:229:GLN:HE21	1:R:236:LYS:H	1.51	0.56
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.88	0.56
1:O:66:TRP:CD1	1:V:381:GLY:HA2	2.41	0.56
1:H:469:PHE:HZ	5:H:1480:EDO:H22	1.71	0.56
1:R:383:HIS:H	1:R:386:HIS:CD2	2.19	0.56
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.54	0.56
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.87	0.55
1:V:239:TYR:HE2	1:V:401:GLN:HE22	1.54	0.55
1:B:383:HIS:H	1:B:386:HIS:CD2	2.19	0.55
2:C:22:THR:H	2:C:25:GLN:NE2	2.04	0.55
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.55	0.55
2:T:118:ASN:HA	6:T:2067:HOH:O	2.06	0.55
2:P:97:GLN:NE2	1:R:181:SER:H	2.04	0.54
1:H:180:LEU:HA	2:W:97:GLN:HE22	1.72	0.54
1:E:180:LEU:HA	2:J:97:GLN:HE22	1.72	0.54
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.90	0.54
1:R:239:TYR:HE2	1:R:401:GLN:HE22	1.54	0.54
1:K:229:GLN:HE21	1:K:236:LYS:H	1.55	0.54
2:M:22:THR:H	2:M:25:GLN:NE2	2.05	0.54
1:K:226:TYR:HB2	6:K:2137:HOH:O	2.08	0.54
2:M:97:GLN:NE2	1:O:181:SER:H	2.06	0.54
2:J:109:LYS:CG	6:J:2041:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:450:LYS:HE3	6:V:2253:HOH:O	2.08	0.54
1:H:229:GLN:HE21	1:H:236:LYS:H	1.54	0.54
1:H:267:HIS:HE1	6:R:2181:HOH:O	1.90	0.53
1:H:163:ASN:HB3	6:H:2109:HOH:O	2.07	0.53
2:W:22:THR:H	2:W:25:GLN:NE2	2.06	0.53
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.42	0.53
1:E:181:SER:H	2:J:97:GLN:NE2	2.07	0.53
1:E:66:TRP:CD1	1:K:381:GLY:HA2	2.44	0.53
1:O:229:GLN:HE21	1:O:236:LYS:H	1.57	0.52
1:R:435:ARG:NE	6:R:2266:HOH:O	2.33	0.52
1:R:435:ARG:CG	6:R:2266:HOH:O	2.43	0.52
1:K:383:HIS:N	1:K:386:HIS:HD2	2.05	0.52
1:K:239:TYR:HE2	1:K:401:GLN:HE22	1.57	0.52
1:B:229:GLN:HE21	1:B:236:LYS:H	1.55	0.52
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.57	0.52
1:V:383:HIS:H	1:V:386:HIS:CD2	2.18	0.52
2:J:22:THR:H	2:J:25:GLN:NE2	2.07	0.52
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.45	0.52
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.58	0.51
1:O:336:GLU:O	5:O:1480:EDO:H12	2.10	0.51
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.93	0.51
2:I:22:THR:H	2:I:25:GLN:NE2	2.06	0.51
1:E:229:GLN:HE21	1:E:236:LYS:H	1.57	0.51
1:O:435:ARG:HG3	6:O:2254:HOH:O	2.10	0.51
2:P:22:THR:H	2:P:25:GLN:NE2	2.09	0.51
2:J:91:ALA:HB3	2:J:101:MET:HG2	1.93	0.50
2:T:22:THR:H	2:T:25:GLN:NE2	2.08	0.50
1:E:381:GLY:HA2	1:K:66:TRP:CD1	2.47	0.50
1:H:163:ASN:ND2	6:H:2110:HOH:O	2.44	0.50
2:P:97:GLN:HE22	1:R:180:LEU:HA	1.76	0.50
1:B:180:LEU:HA	2:F:97:GLN:HE22	1.76	0.50
6:A:2176:HOH:O	1:B:267:HIS:HE1	1.94	0.50
1:E:383:HIS:N	1:E:386:HIS:HD2	2.04	0.50
1:A:474:LYS:HE3	6:A:2282:HOH:O	2.11	0.50
1:V:229:GLN:HE21	1:V:236:LYS:H	1.59	0.49
2:P:109:LYS:HG2	6:P:2037:HOH:O	2.12	0.49
2:I:97:GLN:NE2	1:K:181:SER:H	2.10	0.49
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.47	0.49
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.94	0.49
1:B:360[B]:ARG:NH2	6:B:2233:HOH:O	2.45	0.49
1:O:414:ALA:HB3	1:O:415:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:ARG:HH21	1:H:432:ASN:ND2	2.03	0.49
1:A:383:HIS:N	1:A:386:HIS:HD2	2.05	0.49
5:B:1481:EDO:H11	6:B:2316:HOH:O	2.12	0.49
1:A:229:GLN:HE21	1:A:236:LYS:H	1.59	0.49
2:J:39:ILE:O	2:J:91:ALA:HA	2.13	0.49
2:T:32[A]:TYR:HD2	2:T:101:MET:CE	2.26	0.48
2:J:109:LYS:HG2	6:J:2041:HOH:O	2.13	0.48
1:O:381:GLY:HA2	1:V:66:TRP:CD1	2.47	0.48
1:E:431:ARG:HH21	1:E:432:ASN:ND2	2.00	0.48
1:B:383:HIS:N	1:B:386:HIS:HD2	2.06	0.48
2:C:13:GLU:O	2:C:16[A]:SER:OG	2.22	0.48
1:V:457:ALA:O	1:V:461[A]:VAL:HG23	2.14	0.48
1:O:277:ASN:HD21	1:O:293:ILE:HD12	1.79	0.48
2:F:22:THR:H	2:F:25:GLN:NE2	2.11	0.48
1:O:273:GLY:HA3	1:V:273:GLY:HA3	1.96	0.48
1:O:156[A]:GLN:HG3	2:T:98:VAL:HB	1.96	0.48
2:I:109:LYS:HE2	6:I:2048:HOH:O	2.14	0.47
2:F:39:ILE:O	2:F:91:ALA:HA	2.13	0.47
1:V:414:ALA:HB3	1:V:415:PRO:HD3	1.96	0.47
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.96	0.47
1:A:175:LYS:HA	1:A:176:PRO:C	2.35	0.47
6:O:2165:HOH:O	1:V:267:HIS:HE1	1.97	0.47
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.95	0.47
2:J:39:ILE:HG12	5:J:1123:EDO:H11	1.97	0.47
1:K:414:ALA:HB3	1:K:415:PRO:HD3	1.97	0.47
1:V:431:ARG:HH21	1:V:432:ASN:ND2	2.02	0.46
1:R:414:ALA:HB3	1:R:415:PRO:HD3	1.97	0.46
1:A:156[A]:GLN:HG3	2:I:98:VAL:HB	1.97	0.46
1:E:270:LEU:O	5:E:1480:EDO:C2	2.56	0.46
1:K:219[A]:LEU:HD12	1:K:260:LEU:HD21	1.97	0.46
1:H:383:HIS:H	1:H:386:HIS:CD2	2.24	0.46
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.80	0.46
2:I:39:ILE:O	2:I:91:ALA:HA	2.16	0.46
1:O:383:HIS:N	1:O:386:HIS:HD2	2.05	0.46
1:A:474:LYS:CE	6:A:2282:HOH:O	2.64	0.46
1:H:273:GLY:HA3	1:R:273:GLY:HA3	1.98	0.46
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.51	0.45
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.96	0.45
1:E:446:ARG:HD3	6:E:2258:HOH:O	2.17	0.45
1:H:295:ARG:HG3	1:H:298:HIS:CD2	2.52	0.45
2:C:9:ASN:HD21	2:C:120:ARG:HG2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:LYS:HA	1:E:176:PRO:C	2.37	0.45
6:H:2165:HOH:O	1:R:267:HIS:HE1	1.99	0.45
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.52	0.45
1:R:386:HIS:HE1	6:R:2210:HOH:O	1.98	0.45
1:R:18:LYS:O	5:R:1477:EDO:H21	2.16	0.45
1:K:382:ILE:HA	1:K:386:HIS:CD2	2.52	0.45
5:H:1481:EDO:H11	6:H:2173:HOH:O	2.16	0.45
2:T:39:ILE:O	2:T:91:ALA:HA	2.16	0.44
1:V:175:LYS:HA	1:V:176:PRO:C	2.37	0.44
1:E:267:HIS:HE1	6:K:2161:HOH:O	2.00	0.44
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.52	0.44
2:F:9:ASN:HD21	2:F:120:ARG:HG2	1.83	0.44
1:H:383:HIS:N	1:H:386:HIS:HD2	2.10	0.44
1:A:446:ARG:HD3	6:A:2265:HOH:O	2.17	0.44
1:B:184:ASN:ND2	2:F:97:GLN:HE21	1.93	0.44
2:I:91:ALA:HB3	2:I:101:MET:HG2	2.00	0.44
1:V:435:ARG:HD3	6:V:2246:HOH:O	2.17	0.44
2:M:9:ASN:HD21	2:M:120:ARG:HG2	1.83	0.44
1:K:175:LYS:HA	1:K:176:PRO:C	2.38	0.44
1:R:347:ASP:OD2	1:R:360[B]:ARG:NH2	2.37	0.44
1:A:295:ARG:HG2	6:A:2287:HOH:O	2.18	0.44
2:T:9:ASN:HD21	2:T:120:ARG:HG2	1.83	0.43
2:J:109:LYS:HD3	6:J:2054:HOH:O	2.17	0.43
1:E:273:GLY:HA3	1:K:273:GLY:HA3	1.98	0.43
1:A:347:ASP:OD2	1:A:360[B]:ARG:NH2	2.38	0.43
1:H:277:ASN:HD21	1:H:293:ILE:HD12	1.83	0.43
1:R:431:ARG:HH21	1:R:432:ASN:ND2	2.05	0.43
1:H:163:ASN:CG	6:H:2110:HOH:O	2.56	0.43
2:T:91:ALA:HB3	2:T:101:MET:HG2	2.00	0.43
1:H:175:LYS:HA	1:H:176:PRO:C	2.39	0.43
1:A:267:HIS:HE1	6:A:2160:HOH:O	2.02	0.43
1:K:200:THR:OG1	1:K:238:HIS:CD2	2.68	0.43
1:K:151:HYP:HA	1:K:152:PRO:HD3	1.94	0.43
2:C:13:GLU:O	2:C:16[B]:SER:HB2	2.19	0.43
1:H:241:ASN:ND2	1:H:243:THR:H	2.16	0.43
2:P:18:LEU:HB3	2:P:19:PRO:HD2	2.00	0.43
1:H:381:GLY:HA2	1:R:66:TRP:CD1	2.54	0.43
1:R:32:ARG:HD2	6:R:2033:HOH:O	2.17	0.43
1:V:383:HIS:CE1	1:V:385:TRP:HB2	2.54	0.43
2:C:39:ILE:O	2:C:91:ALA:HA	2.19	0.43
1:O:431:ARG:HE	1:O:432:ASN:HD22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:91:ALA:HB3	2:P:101:MET:HG2	2.01	0.42
1:O:175:LYS:HA	1:O:176:PRO:C	2.39	0.42
1:K:215:ARG:O	1:K:219[B]:LEU:HG	2.19	0.42
1:B:240:LEU:HD12	1:B:262:VAL:HG21	2.01	0.42
1:A:151:HYP:HA	1:A:152:PRO:HD3	1.95	0.42
1:B:200:THR:O	1:B:238:HIS:HA	2.18	0.42
1:V:450:LYS:CE	6:V:2253:HOH:O	2.65	0.42
1:K:293:ILE:HG13	1:K:318:LEU:HD21	2.00	0.42
1:B:51:GLU:HG3	6:B:2044:HOH:O	2.18	0.42
1:K:200:THR:O	1:K:238:HIS:HA	2.20	0.42
2:C:8[B]:ASN:HD22	2:C:113:ASP:HA	1.83	0.42
1:H:201:KCX:OQ1	4:H:477:CAP:O3	2.38	0.42
2:J:9:ASN:ND2	6:J:2004:HOH:O	2.53	0.42
2:T:69:MET:HE3	6:T:2045:HOH:O	2.19	0.42
2:P:39:ILE:O	2:P:91:ALA:HA	2.19	0.42
1:B:175:LYS:HA	1:B:176:PRO:C	2.40	0.42
2:I:9:ASN:HD21	2:I:120:ARG:HG2	1.85	0.42
2:T:32[A]:TYR:CE2	2:T:38:TRP:HZ3	2.38	0.42
1:R:331:VAL:HA	1:R:337:GLY:O	2.20	0.42
1:O:431:ARG:HE	1:O:432:ASN:ND2	2.18	0.41
1:K:292:HIS:HA	1:K:325:HIS:HB2	2.02	0.41
2:P:89:LEU:O	2:P:102:GLY:HA2	2.19	0.41
2:W:39:ILE:O	2:W:91:ALA:HA	2.20	0.41
1:A:241:ASN:HD22	1:A:243:THR:H	1.68	0.41
2:M:18:LEU:HB3	2:M:19:PRO:HD2	2.02	0.41
1:V:368:TRP:O	1:V:369:SMC:C	2.68	0.41
2:F:89:LEU:O	2:F:102:GLY:HA2	2.20	0.41
1:B:77:LEU:HA	1:B:77:LEU:HD12	1.94	0.41
2:P:67:ASP:HA	2:P:68:PRO:HD2	1.91	0.41
1:B:386:HIS:HE1	6:B:2204:HOH:O	2.03	0.41
2:P:9:ASN:HD21	2:P:120:ARG:HG2	1.85	0.41
1:A:277:ASN:HD21	1:A:293:ILE:HD12	1.85	0.41
1:R:383:HIS:N	1:R:386:HIS:HD2	2.07	0.41
2:I:39:ILE:HA	2:I:40:PRO:HD3	1.95	0.41
1:V:151:HYP:HA	1:V:152:PRO:HD3	1.94	0.41
2:W:18:LEU:HB3	2:W:19:PRO:HD2	2.01	0.41
2:M:97:GLN:NE2	1:O:184:ASN:HD22	2.01	0.41
1:K:431:ARG:HH21	1:K:432:ASN:ND2	2.07	0.41
2:F:69:MET:HE3	6:F:2048:HOH:O	2.21	0.41
2:I:18:LEU:HB3	2:I:19:PRO:HD2	2.02	0.41
1:R:175:LYS:HA	1:R:176:PRO:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:382:ILE:HA	1:O:386:HIS:CD2	2.56	0.41
1:R:200:THR:OG1	1:R:238:HIS:CD2	2.69	0.41
2:M:39:ILE:O	2:M:91:ALA:HA	2.20	0.41
2:J:89:LEU:O	2:J:102:GLY:HA2	2.20	0.41
1:O:200:THR:O	1:O:238:HIS:HA	2.21	0.41
2:W:91:ALA:HB3	2:W:101:MET:HG2	2.03	0.41
2:C:57:MET:SD	2:C:61:PRO:HD3	2.61	0.41
1:R:383:HIS:CE1	1:R:385:TRP:HB2	2.56	0.41
1:H:386:HIS:HE1	6:H:2264:HOH:O	2.04	0.41
1:B:171:GLY:HA2	1:B:199:PHE:O	2.22	0.40
1:H:387:MET:HB3	1:H:388:PRO:HD3	2.03	0.40
1:R:457:ALA:O	1:R:461:VAL:HG22	2.21	0.40
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.55	0.40
1:V:379:SER:HB2	1:V:401:GLN:HB2	2.03	0.40
1:V:267:HIS:HD2	1:V:277:ASN:ND2	1.89	0.40
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.68	0.40
1:O:379:SER:HB2	1:O:401:GLN:HB2	2.02	0.40
1:A:241:ASN:ND2	1:A:243:THR:H	2.20	0.40
1:V:386:HIS:HE1	6:V:2190:HOH:O	2.03	0.40
5:B:1481:EDO:H22	6:B:2192:HOH:O	2.21	0.40
2:M:112:ARG:HB3	6:M:2054:HOH:O	2.22	0.40
1:E:266:MET:HA	1:E:292:HIS:O	2.21	0.40
1:E:171:GLY:HA2	1:E:199:PHE:O	2.21	0.40
1:O:225:ILE:HD11	1:O:238:HIS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/475 (97%)	448 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	463/475 (98%)	449 (97%)	14 (3%)	0	100	100
1	E	465/475 (98%)	451 (97%)	14 (3%)	0	100	100
1	H	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	K	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	O	464/475 (98%)	451 (97%)	13 (3%)	0	100	100
1	R	464/475 (98%)	450 (97%)	14 (3%)	0	100	100
1	V	465/475 (98%)	453 (97%)	12 (3%)	0	100	100
2	C	122/122 (100%)	115 (94%)	7 (6%)	0	100	100
2	F	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	I	121/122 (99%)	117 (97%)	4 (3%)	0	100	100
2	J	121/122 (99%)	116 (96%)	5 (4%)	0	100	100
2	M	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	P	123/122 (101%)	117 (95%)	6 (5%)	0	100	100
2	T	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	W	122/122 (100%)	116 (95%)	6 (5%)	0	100	100
All	All	4689/4776 (98%)	4540 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/376 (99%)	360 (97%)	11 (3%)	48	60
1	B	371/376 (99%)	365 (98%)	6 (2%)	70	82
1	E	373/376 (99%)	365 (98%)	8 (2%)	61	74
1	H	373/376 (99%)	361 (97%)	12 (3%)	46	57
1	K	375/376 (100%)	366 (98%)	9 (2%)	57	69
1	O	372/376 (99%)	363 (98%)	9 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	372/376 (99%)	362 (97%)	10 (3%)	52 64
1	V	373/376 (99%)	366 (98%)	7 (2%)	65 77
2	C	111/109 (102%)	104 (94%)	7 (6%)	22 24
2	F	111/109 (102%)	105 (95%)	6 (5%)	27 31
2	I	110/109 (101%)	102 (93%)	8 (7%)	17 18
2	J	110/109 (101%)	104 (94%)	6 (6%)	27 30
2	M	111/109 (102%)	106 (96%)	5 (4%)	34 41
2	P	112/109 (103%)	106 (95%)	6 (5%)	27 31
2	T	111/109 (102%)	106 (96%)	5 (4%)	34 41
2	W	111/109 (102%)	105 (95%)	6 (5%)	27 31
All	All	3867/3880 (100%)	3746 (97%)	121 (3%)	48 59

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	156[A]	GLN
1	A	156[B]	GLN
1	A	185	TYR
1	A	203	ASP
1	A	239	TYR
1	A	241	ASN
1	A	252	LYS
1	A	259[A]	GLU
1	A	259[B]	GLU
1	A	431	ARG
1	B	88	GLU
1	B	185	TYR
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	252	LYS
2	C	8[A]	ASN
2	C	8[B]	ASN
2	C	9	ASN
2	C	100	ILE
2	C	101	MET
2	C	104	LEU

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Mol	Chain	Res	Type
2	C	112	ARG
1	E	7	THR
1	E	88	GLU
1	E	134	ARG
1	E	185	TYR
1	E	203	ASP
1	E	239	TYR
1	E	241	ASN
1	E	252	LYS
2	F	9	ASN
2	F	52	GLU
2	F	100	ILE
2	F	101	MET
2	F	104	LEU
2	F	112	ARG
1	H	7	THR
1	H	8	LYS
1	H	88	GLU
1	H	156[A]	GLN
1	H	156[B]	GLN
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	252	LYS
1	H	259[A]	GLU
1	H	259[B]	GLU
2	I	9	ASN
2	I	16[A]	SER
2	I	16[B]	SER
2	I	52	GLU
2	I	100	ILE
2	I	101	MET
2	I	104	LEU
2	I	112	ARG
2	J	9	ASN
2	J	52	GLU
2	J	100	ILE
2	J	101	MET
2	J	104	LEU
2	J	112	ARG
1	K	88	GLU

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Mol	Chain	Res	Type
1	K	185	TYR
1	K	203	ASP
1	K	219[A]	LEU
1	K	219[B]	LEU
1	K	239	TYR
1	K	241	ASN
1	K	252	LYS
1	K	431	ARG
2	M	9	ASN
2	M	100	ILE
2	M	101	MET
2	M	104	LEU
2	M	112	ARG
1	O	7	THR
1	O	88	GLU
1	O	134	ARG
1	O	185	TYR
1	O	203	ASP
1	O	239	TYR
1	O	241	ASN
1	O	252	LYS
1	O	431	ARG
2	P	9	ASN
2	P	52	GLU
2	P	100	ILE
2	P	101	MET
2	P	104	LEU
2	P	112	ARG
1	R	7	THR
1	R	8	LYS
1	R	88	GLU
1	R	185	TYR
1	R	203	ASP
1	R	239	TYR
1	R	241	ASN
1	R	252	LYS
1	R	431	ARG
1	R	461	VAL
2	T	9	ASN
2	T	100	ILE
2	T	101	MET
2	T	104	LEU

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Mol	Chain	Res	Type
2	T	112	ARG
1	V	88	GLU
1	V	134	ARG
1	V	185	TYR
1	V	203	ASP
1	V	239	TYR
1	V	241	ASN
1	V	252	LYS
2	W	9	ASN
2	W	52	GLU
2	W	100	ILE
2	W	101	MET
2	W	104	LEU
2	W	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	163	ASN
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
2	C	9	ASN
2	C	25	GLN

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Mol	Chain	Res	Type
2	C	29	GLN
2	C	97	GLN
2	C	115	GLN
1	E	153	HIS
1	E	163	ASN
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
1	E	401	GLN
1	E	432	ASN
2	F	9	ASN
2	F	25	GLN
2	F	29	GLN
2	F	97	GLN
2	F	115	GLN
1	H	153	HIS
1	H	163	ASN
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	97	GLN
2	I	115	GLN
2	J	8	ASN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	97	GLN
2	J	115	GLN

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Mol	Chain	Res	Type
1	K	153	HIS
1	K	229	GLN
1	K	238	HIS
1	K	241	ASN
1	K	267	HIS
1	K	277	ASN
1	K	304	GLN
1	K	386	HIS
1	K	401	GLN
1	K	432	ASN
2	M	8	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	97	GLN
2	M	115	GLN
1	O	153	HIS
1	O	163	ASN
1	O	229	GLN
1	O	238	HIS
1	O	241	ASN
1	O	267	HIS
1	O	277	ASN
1	O	304	GLN
1	O	386	HIS
1	O	401	GLN
1	O	432	ASN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	97	GLN
2	P	115	GLN
1	R	153	HIS
1	R	163	ASN
1	R	229	GLN
1	R	238	HIS
1	R	241	ASN
1	R	267	HIS
1	R	277	ASN
1	R	304	GLN
1	R	386	HIS
1	R	401	GLN

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Mol	Chain	Res	Type
1	R	432	ASN
2	T	9	ASN
2	T	25	GLN
2	T	29	GLN
2	T	97	GLN
2	T	115	GLN
1	V	153	HIS
1	V	163	ASN
1	V	229	GLN
1	V	238	HIS
1	V	241	ASN
1	V	267	HIS
1	V	277	ASN
1	V	304	GLN
1	V	386	HIS
1	V	401	GLN
1	V	432	ASN
2	W	9	ASN
2	W	25	GLN
2	W	29	GLN
2	W	97	GLN
2	W	115	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

40 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	7,8,9	0.68	0	5,10,12	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	A	151	1	7,8,9	0.96	1 (14%)	5,10,12	1.40	1 (20%)
1	KCX	A	201	1,3	7,11,12	0.93	0	7,12,14	0.84	0
1	SMC	A	256	1	5,6,7	0.89	0	2,6,8	1.56	0
1	SMC	A	369	1	5,6,7	1.70	1 (20%)	2,6,8	1.75	1 (50%)
1	HYP	B	104	1	7,8,9	0.51	0	5,10,12	0.86	0
1	HYP	B	151	1	7,8,9	0.68	0	5,10,12	1.17	0
1	KCX	B	201	1,3	7,11,12	1.03	0	7,12,14	1.02	0
1	SMC	B	256	1	5,6,7	0.55	0	2,6,8	1.68	1 (50%)
1	SMC	B	369	1	5,6,7	0.96	0	2,6,8	1.67	0
1	HYP	E	104	1	7,8,9	0.53	0	5,10,12	1.81	2 (40%)
1	HYP	E	151	1	7,8,9	1.40	1 (14%)	5,10,12	1.28	1 (20%)
1	KCX	E	201	1,3	7,11,12	0.97	0	7,12,14	0.88	0
1	SMC	E	256	1	5,6,7	1.07	1 (20%)	2,6,8	1.34	0
1	SMC	E	369	1	5,6,7	0.63	0	2,6,8	1.35	0
1	HYP	H	104	1	7,8,9	0.61	0	5,10,12	1.14	1 (20%)
1	HYP	H	151	1	7,8,9	0.71	0	5,10,12	1.37	1 (20%)
1	KCX	H	201	1,3	7,11,12	0.93	0	7,12,14	0.78	0
1	SMC	H	256	1	5,6,7	0.59	0	2,6,8	1.72	1 (50%)
1	SMC	H	369	1	5,6,7	1.43	1 (20%)	2,6,8	1.70	0
1	HYP	K	104	1	7,8,9	0.70	0	5,10,12	1.11	1 (20%)
1	HYP	K	151	1	7,8,9	0.89	0	5,10,12	1.40	1 (20%)
1	KCX	K	201	1,3	7,11,12	0.93	1 (14%)	7,12,14	0.84	0
1	SMC	K	256	1	5,6,7	0.97	0	2,6,8	1.57	1 (50%)
1	SMC	K	369	1	5,6,7	0.54	0	2,6,8	0.86	0
1	HYP	O	104	1	7,8,9	0.63	0	5,10,12	0.96	0
1	HYP	O	151	1	7,8,9	1.25	1 (14%)	5,10,12	1.36	0
1	KCX	O	201	1,3	7,11,12	0.81	0	7,12,14	0.87	0
1	SMC	O	256	1	5,6,7	1.02	1 (20%)	2,6,8	1.63	1 (50%)
1	SMC	O	369	1	5,6,7	0.92	0	2,6,8	0.95	0
1	HYP	R	104	1	7,8,9	0.38	0	5,10,12	1.31	1 (20%)
1	HYP	R	151	1	7,8,9	0.83	0	5,10,12	1.28	1 (20%)
1	KCX	R	201	1,3	7,11,12	0.98	0	7,12,14	1.06	0
1	SMC	R	256	1	5,6,7	1.19	1 (20%)	2,6,8	1.56	1 (50%)
1	SMC	R	369	1	5,6,7	1.64	1 (20%)	2,6,8	1.36	0
1	HYP	V	104	1	7,8,9	0.38	0	5,10,12	1.48	1 (20%)
1	HYP	V	151	1	7,8,9	0.94	1 (14%)	5,10,12	1.48	1 (20%)
1	KCX	V	201	1,3	7,11,12	0.76	0	7,12,14	0.90	0
1	SMC	V	256	1	5,6,7	1.52	1 (20%)	2,6,8	1.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SMC	V	369	1	5,6,7	1.38	1 (20%)	2,6,8	1.26	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	-	0/6/10/12	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	-	0/6/10/12	0/0/0/0
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	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	-	0/6/10/12	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	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	-	0/6/10/12	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
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	K	256	1	-	0/3/5/7	0/0/0/0
1	SMC	K	369	1	-	0/3/5/7	0/0/0/0
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	KCX	O	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	O	256	1	-	0/3/5/7	0/0/0/0
1	SMC	O	369	1	-	0/3/5/7	0/0/0/0
1	HYP	R	104	1	-	0/0/11/13	0/1/1/1
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	KCX	R	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	R	256	1	-	0/3/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	R	369	1	-	0/3/5/7	0/0/0/0
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	V	256	1	-	0/3/5/7	0/0/0/0
1	SMC	V	369	1	-	0/3/5/7	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	151	HYP	CA-N	-3.54	1.43	1.47
1	O	151	HYP	CA-N	-2.71	1.44	1.47
1	V	151	HYP	CA-N	-2.37	1.44	1.47
1	A	151	HYP	CA-N	-2.15	1.44	1.47
1	O	256	SMC	CB-SG	2.10	1.83	1.80
1	K	201	KCX	CE-NZ	2.11	1.51	1.46
1	E	256	SMC	CB-SG	2.12	1.83	1.80
1	R	256	SMC	CB-SG	2.50	1.83	1.80
1	V	369	SMC	CB-SG	2.72	1.83	1.80
1	H	369	SMC	CB-SG	2.93	1.83	1.80
1	V	256	SMC	CB-SG	3.22	1.84	1.80
1	R	369	SMC	CB-SG	3.45	1.84	1.80
1	A	369	SMC	CB-SG	3.57	1.84	1.80

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	104	HYP	OD1-CG-CD	-2.81	104.36	110.47
1	V	104	HYP	O-C-CA	-2.65	118.45	125.44
1	B	256	SMC	O-C-CA	-2.38	119.30	125.49
1	A	369	SMC	CS-SG-CB	-2.29	97.48	101.21
1	O	256	SMC	O-C-CA	-2.29	119.52	125.49
1	V	151	HYP	O-C-CA	-2.29	119.39	125.44
1	K	256	SMC	O-C-CA	-2.22	119.70	125.49
1	R	256	SMC	O-C-CA	-2.19	119.79	125.49
1	H	104	HYP	O-C-CA	-2.15	119.75	125.44
1	K	151	HYP	OD1-CG-CD	-2.10	105.91	110.47
1	K	104	HYP	O-C-CA	-2.09	119.93	125.44
1	R	104	HYP	O-C-CA	-2.06	120.01	125.44
1	A	151	HYP	O-C-CA	-2.03	120.07	125.44
1	R	151	HYP	O-C-CA	-2.02	120.09	125.44
1	H	256	SMC	O-C-CA	-2.02	120.22	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	151	HYP	O-C-CA	-2.02	120.10	125.44
1	H	151	HYP	O-C-CA	-2.02	120.11	125.44
1	E	104	HYP	CB-CG-CD	2.56	106.30	103.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	151	HYP	1	0
1	H	201	KCX	1	0
1	K	151	HYP	1	0
1	V	151	HYP	1	0
1	V	369	SMC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 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	$\#\|Z\| > 2$
5	EDO	A	1476	-	3,3,3	0.32	0	2,2,2	0.36	0
5	EDO	A	1477	-	3,3,3	0.29	0	2,2,2	0.18	0
5	EDO	A	1478	-	3,3,3	0.33	0	2,2,2	0.29	0
5	EDO	A	1479	-	3,3,3	0.39	0	2,2,2	0.24	0
5	EDO	A	1480	-	3,3,3	0.34	0	2,2,2	0.75	0
4	CAP	A	477	3	14,20,20	0.89	1 (7%)	15,31,31	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	1476	-	3,3,3	0.36	0	2,2,2	0.55	0
5	EDO	B	1477	-	3,3,3	0.38	0	2,2,2	0.22	0
5	EDO	B	1478	-	3,3,3	0.29	0	2,2,2	0.46	0
5	EDO	B	1479	-	3,3,3	0.35	0	2,2,2	0.37	0
5	EDO	B	1480	-	3,3,3	0.40	0	2,2,2	0.08	0
5	EDO	B	1481	-	3,3,3	0.34	0	2,2,2	0.21	0
4	CAP	B	477	3	14,20,20	0.60	0	15,31,31	0.99	1 (6%)
5	EDO	C	1123	-	3,3,3	0.29	0	2,2,2	0.66	0
5	EDO	E	1476	-	3,3,3	0.34	0	2,2,2	0.17	0
5	EDO	E	1477	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	E	1478	-	3,3,3	0.28	0	2,2,2	0.51	0
5	EDO	E	1479	-	3,3,3	0.38	0	2,2,2	0.30	0
5	EDO	E	1480	-	3,3,3	0.36	0	2,2,2	0.26	0
4	CAP	E	477	3	14,20,20	0.89	0	15,31,31	1.20	2 (13%)
5	EDO	F	1123	-	3,3,3	0.33	0	2,2,2	0.88	0
5	EDO	H	1476	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	H	1477	-	3,3,3	0.38	0	2,2,2	0.19	0
5	EDO	H	1478	-	3,3,3	0.26	0	2,2,2	0.13	0
5	EDO	H	1479	-	3,3,3	0.30	0	2,2,2	0.41	0
5	EDO	H	1480	-	3,3,3	0.36	0	2,2,2	0.36	0
5	EDO	H	1481	-	3,3,3	0.37	0	2,2,2	0.28	0
4	CAP	H	477	3	14,20,20	0.72	0	15,31,31	0.78	0
5	EDO	J	1123	-	3,3,3	0.27	0	2,2,2	0.66	0
5	EDO	K	1476	-	3,3,3	0.48	0	2,2,2	0.22	0
5	EDO	K	1477	-	3,3,3	0.33	0	2,2,2	0.28	0
5	EDO	K	1478	-	3,3,3	0.28	0	2,2,2	0.68	0
5	EDO	K	1479	-	3,3,3	0.37	0	2,2,2	0.19	0
5	EDO	K	1480	-	3,3,3	0.32	0	2,2,2	0.34	0
4	CAP	K	477	3	14,20,20	0.68	0	15,31,31	1.08	1 (6%)
5	EDO	M	1123	-	3,3,3	0.30	0	2,2,2	0.46	0
5	EDO	O	1476	-	3,3,3	0.36	0	2,2,2	0.25	0
5	EDO	O	1477	-	3,3,3	0.29	0	2,2,2	0.39	0
5	EDO	O	1478	-	3,3,3	0.28	0	2,2,2	0.41	0
5	EDO	O	1479	-	3,3,3	0.39	0	2,2,2	0.33	0
5	EDO	O	1480	-	3,3,3	0.44	0	2,2,2	0.42	0
4	CAP	O	477	3	14,20,20	0.60	0	15,31,31	1.01	1 (6%)
5	EDO	P	1123	-	3,3,3	0.32	0	2,2,2	0.31	0
5	EDO	R	1476	-	3,3,3	0.41	0	2,2,2	0.27	0
5	EDO	R	1477	-	3,3,3	0.34	0	2,2,2	0.07	0
5	EDO	R	1478	-	3,3,3	0.33	0	2,2,2	0.29	0
5	EDO	R	1479	-	3,3,3	0.35	0	2,2,2	0.27	0
5	EDO	R	1480	-	3,3,3	0.36	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAP	R	477	3	14,20,20	0.62	0	15,31,31	0.97	0
5	EDO	T	1123	-	3,3,3	0.29	0	2,2,2	0.68	0
5	EDO	V	1476	-	3,3,3	0.43	0	2,2,2	0.08	0
5	EDO	V	1477	-	3,3,3	0.37	0	2,2,2	0.27	0
5	EDO	V	1478	-	3,3,3	0.29	0	2,2,2	0.25	0
5	EDO	V	1479	-	3,3,3	0.37	0	2,2,2	0.18	0
5	EDO	V	1480	-	3,3,3	0.31	0	2,2,2	0.17	0
5	EDO	V	1481	-	3,3,3	0.38	0	2,2,2	0.23	0
4	CAP	V	477	3	14,20,20	0.86	0	15,31,31	0.85	0
5	EDO	W	1123	-	3,3,3	0.29	0	2,2,2	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1477	-	-	0/1/1/1	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
4	CAP	A	477	3	-	0/23/29/29	0/0/0/0
5	EDO	B	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1477	-	-	0/1/1/1	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
4	CAP	B	477	3	-	0/23/29/29	0/0/0/0
5	EDO	C	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1477	-	-	0/1/1/1	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
4	CAP	E	477	3	-	0/23/29/29	0/0/0/0
5	EDO	F	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1477	-	-	0/1/1/1	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	H	1481	-	-	0/1/1/1	0/0/0/0
4	CAP	H	477	3	-	0/23/29/29	0/0/0/0
5	EDO	J	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1480	-	-	0/1/1/1	0/0/0/0
4	CAP	K	477	3	-	0/23/29/29	0/0/0/0
5	EDO	M	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1480	-	-	0/1/1/1	0/0/0/0
4	CAP	O	477	3	-	0/23/29/29	0/0/0/0
5	EDO	P	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1480	-	-	0/1/1/1	0/0/0/0
4	CAP	R	477	3	-	0/23/29/29	0/0/0/0
5	EDO	T	1123	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1481	-	-	0/1/1/1	0/0/0/0
4	CAP	V	477	3	-	0/23/29/29	0/0/0/0
5	EDO	W	1123	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	477	CAP	O2-C2	2.18	1.46	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	477	CAP	O4-C4-C5	-2.30	105.17	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	477	CAP	O6P-P2-O4P	-2.29	103.22	110.58
4	K	477	CAP	O3-C3-C4	2.02	113.22	108.91
4	O	477	CAP	O3-C3-C4	2.22	113.67	108.91
4	E	477	CAP	O6P-P2-O5	2.55	113.91	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1481	EDO	2	0
5	E	1480	EDO	2	0
5	H	1480	EDO	2	0
5	H	1481	EDO	1	0
4	H	477	CAP	1	0
5	J	1123	EDO	1	0
5	O	1480	EDO	1	0
5	R	1477	EDO	1	0
5	R	1480	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	460/475 (96%)	-0.77	2 (0%)	93	93	13, 19, 34, 49	0
1	B	462/475 (97%)	-0.73	4 (0%)	85	85	12, 19, 34, 66	0
1	E	464/475 (97%)	-0.76	6 (1%)	79	78	13, 19, 35, 76	0
1	H	464/475 (97%)	-0.77	5 (1%)	82	82	13, 19, 35, 72	0
1	K	464/475 (97%)	-0.71	7 (1%)	76	75	13, 19, 35, 81	0
1	O	464/475 (97%)	-0.76	5 (1%)	82	82	13, 19, 35, 80	0
1	R	464/475 (97%)	-0.76	6 (1%)	79	78	12, 19, 35, 84	0
1	V	464/475 (97%)	-0.73	8 (1%)	73	72	13, 19, 35, 80	0
2	C	122/122 (100%)	-0.29	3 (2%)	61	60	18, 27, 58, 69	0
2	F	122/122 (100%)	-0.23	7 (5%)	27	27	18, 27, 58, 69	1 (0%)
2	I	122/122 (100%)	-0.33	4 (3%)	50	49	18, 27, 58, 69	1 (0%)
2	J	122/122 (100%)	-0.15	11 (9%)	12	11	18, 27, 58, 69	1 (0%)
2	M	122/122 (100%)	-0.18	7 (5%)	27	27	18, 27, 58, 69	1 (0%)
2	P	122/122 (100%)	-0.29	5 (4%)	41	39	18, 27, 58, 69	0
2	T	122/122 (100%)	-0.24	8 (6%)	22	21	18, 27, 58, 69	0
2	W	122/122 (100%)	-0.01	11 (9%)	12	11	18, 27, 58, 69	1 (0%)
All	All	4682/4776 (98%)	-0.64	99 (2%)	67	65	12, 20, 41, 84	5 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	112	ARG	8.7
1	E	9	ALA	6.9
2	W	111	ALA	6.6
2	T	112	ARG	6.2
2	J	112	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
2	W	112	ARG	5.3
2	M	111	ALA	5.2
1	B	10	GLY	5.1
1	O	10	GLY	5.1
1	B	9	ALA	5.1
1	O	8	LYS	4.9
2	W	110	THR	4.6
1	K	8	LYS	4.5
2	F	112	ARG	4.5
2	P	112	ARG	4.3
1	V	9	ALA	4.3
2	C	118	ASN	4.2
2	J	118	ASN	4.2
2	F	110	THR	4.2
2	C	112	ARG	4.1
2	T	110	THR	4.0
2	I	112	ARG	4.0
2	J	114	PHE	4.0
2	T	118	ASN	4.0
1	O	7	THR	4.0
2	I	118	ASN	3.9
2	T	113	ASP	3.8
2	W	118	ASN	3.8
1	V	7	THR	3.7
2	J	116	PRO	3.7
1	H	8	LYS	3.6
1	H	7	THR	3.6
2	J	117	ALA	3.5
2	M	118	ASN	3.5
1	O	9	ALA	3.5
1	E	8	LYS	3.4
1	V	10	GLY	3.4
1	H	9	ALA	3.4
2	W	117	ALA	3.3
2	J	119	LYS	3.3
1	K	9	ALA	3.3
2	I	114	PHE	3.2
1	K	10	GLY	3.2
1	R	8	LYS	3.1
2	J	110	THR	3.1
1	V	8	LYS	3.1
1	E	10	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	111	ALA	3.1
2	T	119	LYS	3.1
1	B	94	ASP	3.1
2	P	119	LYS	3.1
2	W	109	LYS	3.0
1	R	92	GLY	3.0
2	P	118	ASN	2.9
1	R	10	GLY	2.9
1	B	439	ARG	2.8
1	R	9	ALA	2.8
2	T	111	ALA	2.7
1	K	439	ARG	2.7
1	R	7	THR	2.7
2	F	119	LYS	2.7
2	W	114	PHE	2.6
1	V	439	ARG	2.6
2	M	110	THR	2.6
2	F	114	PHE	2.6
2	M	119	LYS	2.6
2	J	113	ASP	2.6
2	W	116	PRO	2.5
1	V	226	TYR	2.5
1	K	94	ASP	2.5
1	E	94	ASP	2.5
1	O	94	ASP	2.5
1	H	439	ARG	2.5
2	P	110	THR	2.5
2	J	109	LYS	2.5
1	K	7	THR	2.4
2	M	114	PHE	2.4
1	K	11	ALA	2.4
2	C	119	LYS	2.4
2	I	110	THR	2.3
2	W	113	ASP	2.3
1	A	94	ASP	2.3
2	M	117	ALA	2.3
2	T	114	PHE	2.3
1	V	94	ASP	2.3
2	W	119	LYS	2.3
2	F	118	ASN	2.3
1	E	7	THR	2.2
1	A	439	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	439	ARG	2.2
2	F	113	ASP	2.2
2	W	69	MET	2.2
2	T	109	LYS	2.1
1	H	10	GLY	2.1
1	V	91	PRO	2.1
1	E	439	ARG	2.1
2	F	117	ALA	2.1
2	P	109	LYS	2.0
2	J	84	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	K	104	8/9	0.98	0.06	-	14,16,17,18	0
1	SMC	E	369	7/8	0.98	0.06	-	17,17,19,21	0
1	HYP	A	151	8/9	0.97	0.07	-	13,15,16,16	0
1	SMC	B	256	7/8	0.98	0.08	-	14,14,16,19	0
1	HYP	H	151	8/9	0.99	0.07	-	14,15,16,16	0
1	KCX	O	201	12/13	0.98	0.08	-	13,15,16,16	0
1	SMC	R	256	7/8	0.99	0.06	-	14,15,16,18	0
1	KCX	H	201	12/13	0.98	0.08	-	13,15,16,17	0
1	HYP	O	151	8/9	0.99	0.06	-	14,15,16,16	0
1	HYP	E	104	8/9	0.98	0.07	-	14,16,17,18	0
1	SMC	V	369	7/8	0.99	0.05	-	17,17,19,21	0
1	SMC	A	256	7/8	0.97	0.07	-	14,14,16,18	0
1	KCX	V	201	12/13	0.97	0.08	-	13,14,16,17	0
1	HYP	R	151	8/9	0.98	0.07	-	14,14,16,16	0
1	HYP	B	151	8/9	0.95	0.09	-	13,15,16,16	0
1	KCX	R	201	12/13	0.97	0.11	-	13,15,16,16	0
1	SMC	K	369	7/8	0.99	0.06	-	16,17,19,21	0
1	HYP	H	104	8/9	0.97	0.07	-	14,16,17,18	0
1	SMC	H	369	7/8	0.97	0.07	-	17,17,19,21	0
1	HYP	A	104	8/9	0.96	0.12	-	14,16,18,18	0
1	HYP	K	151	8/9	0.98	0.06	-	14,15,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	V	151	8/9	0.98	0.07	-	14,15,15,16	0
1	KCX	K	201	12/13	0.97	0.10	-	13,15,16,16	0
1	KCX	E	201	12/13	0.97	0.09	-	13,15,16,17	0
1	SMC	K	256	7/8	0.99	0.07	-	14,14,16,18	0
1	KCX	B	201	12/13	0.98	0.10	-	13,15,16,17	0
1	SMC	R	369	7/8	0.97	0.06	-	17,17,19,21	0
1	SMC	O	369	7/8	0.99	0.07	-	17,17,18,20	0
1	SMC	B	369	7/8	0.98	0.08	-	17,17,18,20	0
1	SMC	A	369	7/8	0.98	0.07	-	17,17,18,21	0
1	SMC	H	256	7/8	0.98	0.08	-	14,14,16,18	0
1	HYP	E	151	8/9	0.97	0.06	-	14,15,16,16	0
1	KCX	A	201	12/13	0.98	0.10	-	13,15,16,16	0
1	SMC	O	256	7/8	0.98	0.07	-	14,14,16,19	0
1	HYP	O	104	8/9	0.98	0.05	-	14,16,17,18	0
1	HYP	R	104	8/9	0.97	0.07	-	14,16,18,18	0
1	HYP	V	104	8/9	0.97	0.07	-	14,16,17,18	0
1	SMC	E	256	7/8	0.99	0.07	-	14,14,16,19	0
1	SMC	V	256	7/8	0.99	0.07	-	14,15,16,18	0
1	HYP	B	104	8/9	0.98	0.07	-	14,15,17,17	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	O	1480	4/4	0.83	0.22	17.61	29,36,41,46	0
5	EDO	H	1476	4/4	0.98	0.33	12.92	2,5,5,10	4
5	EDO	V	1481	4/4	0.77	0.25	9.61	34,40,43,48	0
5	EDO	B	1476	4/4	0.98	0.30	8.08	2,3,3,6	4
5	EDO	H	1481	4/4	0.86	0.15	6.27	42,45,46,49	0
5	EDO	A	1480	4/4	0.91	0.16	4.46	38,40,41,44	0
5	EDO	V	1476	4/4	0.95	0.16	3.63	21,21,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	R	1480	4/4	0.95	0.11	3.36	31,33,33,37	0
5	EDO	H	1478	4/4	0.98	0.11	2.99	24,26,28,29	0
5	EDO	O	1478	4/4	0.92	0.11	2.75	33,35,37,39	0
5	EDO	O	1477	4/4	0.97	0.11	2.68	22,25,26,27	0
5	EDO	R	1478	4/4	0.92	0.10	1.93	32,32,33,34	0
5	EDO	V	1478	4/4	0.98	0.11	1.83	23,27,30,31	0
5	EDO	E	1480	4/4	0.96	0.11	1.72	29,31,32,32	0
5	EDO	A	1477	4/4	0.98	0.10	1.65	18,18,23,24	0
5	EDO	K	1476	4/4	0.95	0.11	1.55	21,22,23,27	0
5	EDO	P	1123	4/4	0.93	0.17	1.30	29,31,36,37	0
5	EDO	B	1478	4/4	0.97	0.09	1.25	21,23,27,29	0
5	EDO	B	1479	4/4	0.93	0.09	1.05	26,32,33,35	0
5	EDO	R	1477	4/4	0.98	0.09	0.96	23,26,28,30	0
5	EDO	H	1479	4/4	0.94	0.10	0.95	28,28,32,37	0
5	EDO	R	1476	4/4	0.97	0.09	0.84	19,21,23,23	0
5	EDO	A	1478	4/4	0.91	0.12	0.82	27,34,34,38	0
5	EDO	H	1477	4/4	0.97	0.09	0.81	16,23,23,25	0
5	EDO	J	1123	4/4	0.96	0.18	0.73	35,39,43,46	0
5	EDO	M	1123	4/4	0.93	0.16	0.65	30,38,38,43	0
5	EDO	K	1478	4/4	0.96	0.10	0.57	31,31,32,34	0
5	EDO	C	1123	4/4	0.94	0.15	0.48	25,29,34,38	0
5	EDO	B	1481	4/4	0.97	0.09	0.44	30,35,37,38	0
5	EDO	F	1123	4/4	0.96	0.13	0.37	29,32,35,36	0
5	EDO	K	1480	4/4	0.96	0.09	0.24	33,33,36,41	0
5	EDO	V	1479	4/4	0.95	0.10	0.10	27,29,31,33	0
5	EDO	T	1123	4/4	0.96	0.11	0.06	27,27,30,35	0
5	EDO	W	1123	4/4	0.90	0.14	0.02	33,38,38,45	0
5	EDO	E	1476	4/4	0.97	0.08	-0.06	21,22,24,28	0
5	EDO	K	1477	4/4	0.96	0.07	-0.26	26,31,32,33	0
5	EDO	B	1477	4/4	0.97	0.07	-0.29	16,19,22,25	0
5	EDO	E	1478	4/4	0.96	0.07	-0.61	34,34,35,37	0
4	CAP	E	477	21/21	0.99	0.07	-0.87	15,19,22,24	0
4	CAP	H	477	21/21	0.99	0.07	-0.89	16,20,23,28	0
5	EDO	O	1476	4/4	0.98	0.06	-0.94	22,26,26,29	0
4	CAP	K	477	21/21	0.99	0.07	-0.95	13,16,21,24	0
4	CAP	B	477	21/21	0.99	0.08	-1.07	14,18,20,22	0
4	CAP	R	477	21/21	0.99	0.07	-1.13	11,16,20,26	0
5	EDO	V	1477	4/4	0.98	0.07	-1.16	21,21,24,26	0
4	CAP	V	477	21/21	0.99	0.07	-1.17	16,18,22,23	0
5	EDO	A	1476	4/4	0.98	0.06	-1.28	22,22,24,27	0
5	EDO	E	1477	4/4	0.99	0.06	-1.61	19,21,21,22	0
4	CAP	O	477	21/21	0.99	0.06	-1.69	12,17,20,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	V	476	1/1	0.98	0.05	-1.71	16,16,16,16	0
3	MG	K	476	1/1	0.98	0.04	-1.71	19,19,19,19	0
4	CAP	A	477	21/21	0.99	0.07	-1.87	12,17,22,24	0
3	MG	E	476	1/1	0.99	0.04	-2.37	13,13,13,13	0
3	MG	R	476	1/1	0.99	0.04	-2.56	11,11,11,11	0
3	MG	H	476	1/1	0.99	0.03	-2.93	16,16,16,16	0
3	MG	B	476	1/1	0.98	0.04	-3.02	12,12,12,12	0
3	MG	A	476	1/1	1.00	0.04	-3.31	17,17,17,17	0
3	MG	O	476	1/1	0.98	0.03	-3.52	15,15,15,15	0
5	EDO	O	1479	4/4	0.95	0.15	-	24,26,32,33	0
5	EDO	H	1480	4/4	0.87	0.24	-	39,51,53,53	0
5	EDO	E	1479	4/4	0.94	0.12	-	38,38,38,40	0
5	EDO	B	1480	4/4	0.97	0.14	-	22,33,34,35	0
5	EDO	A	1479	4/4	0.98	0.12	-	15,25,26,27	0
5	EDO	V	1480	4/4	0.98	0.12	-	24,27,29,30	0
5	EDO	K	1479	4/4	0.93	0.17	-	28,29,34,34	0
5	EDO	R	1479	4/4	0.98	0.10	-	29,31,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.