Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:55 AM GMT

PDB ID	:	2V63
Title	:	Crystal structure of Rubisco from Chlamydomonas reinhardtii with a large-subunit V331A mutation
Authors	:	Karkehabadi, S.; Satagopagan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2007-07-13
Resolution	:	1.80 Å(reported)

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

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

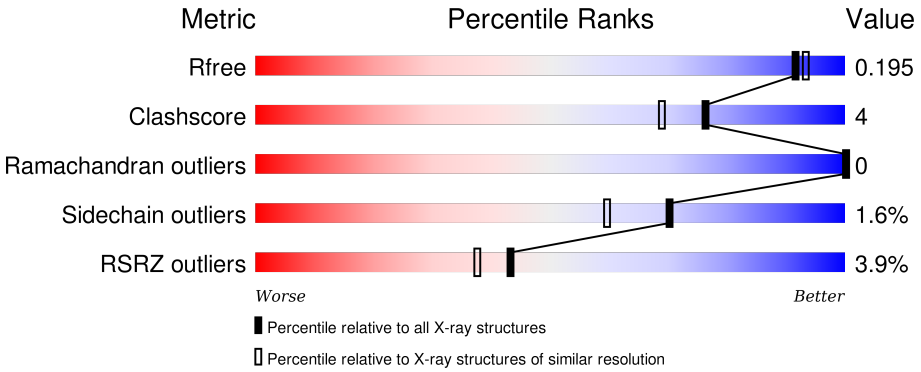
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	2% 89% 9%
1	B	475	3% 87% 11%
1	C	475	3% 88% 10%
1	D	475	3% 88% 9%
1	E	475	5% 89% 8%

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Mol	Chain	Length	Quality of chain
1	F	475	5% 89% 9%
1	G	475	2% 89% 9%
1	H	475	2% 90% 8%
2	I	140	9% 89% 11%
2	J	140	8% 91% 8%
2	K	140	3% 92% 8%
2	L	140	4% 88% 12%
2	M	140	4% 90% 10%
2	N	140	6% 91% 9%
2	O	140	7% 92% 8%
2	P	140	7% 88% 11%

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	1478	-	-	-	X
5	EDO	B	1475	-	-	-	X
5	EDO	B	1477	-	-	-	X
5	EDO	C	1476	-	-	-	X
5	EDO	C	1477	-	-	-	X
5	EDO	C	1479	-	-	-	X
5	EDO	D	1477	-	-	-	X
5	EDO	D	1478	-	-	-	X
5	EDO	E	1475	-	-	-	X
5	EDO	F	1476	-	-	-	X
5	EDO	G	1475	-	-	-	X
5	EDO	G	1478	-	-	-	X
5	EDO	G	1479	-	-	-	X
5	EDO	G	1480	-	-	-	X
5	EDO	H	1476	-	-	-	X
5	EDO	H	1478	-	-	-	X
5	EDO	I	1141	-	-	-	X
5	EDO	J	1141	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	K	1142	-	-	-	X
5	EDO	L	1141	-	-	-	X
5	EDO	L	1142	-	-	X	X
5	EDO	M	1141	-	-	-	X
5	EDO	M	1142	-	-	-	X
5	EDO	O	1141	-	-	-	X
5	EDO	P	1141	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 41473 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	466	Total	C	N	O	S	0	4	0
			3643	2302	642	675	24			
1	B	466	Total	C	N	O	S	0	4	0
			3638	2296	642	675	25			
1	C	466	Total	C	N	O	S	0	3	0
			3639	2298	642	675	24			
1	D	464	Total	C	N	O	S	0	2	0
			3626	2291	640	671	24			
1	E	464	Total	C	N	O	S	0	2	0
			3626	2291	640	671	24			
1	F	466	Total	C	N	O	S	0	1	0
			3630	2294	639	673	24			
1	G	466	Total	C	N	O	S	0	2	0
			3634	2295	642	673	24			
1	H	466	Total	C	N	O	S	0	1	0
			3631	2294	641	672	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	VARIANT	UNP P00877
A	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
B	46	PRO	LEU	VARIANT	UNP P00877
B	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
C	46	PRO	LEU	VARIANT	UNP P00877
C	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
D	46	PRO	LEU	VARIANT	UNP P00877
D	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
E	46	PRO	LEU	VARIANT	UNP P00877
E	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
F	46	PRO	LEU	VARIANT	UNP P00877
F	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877

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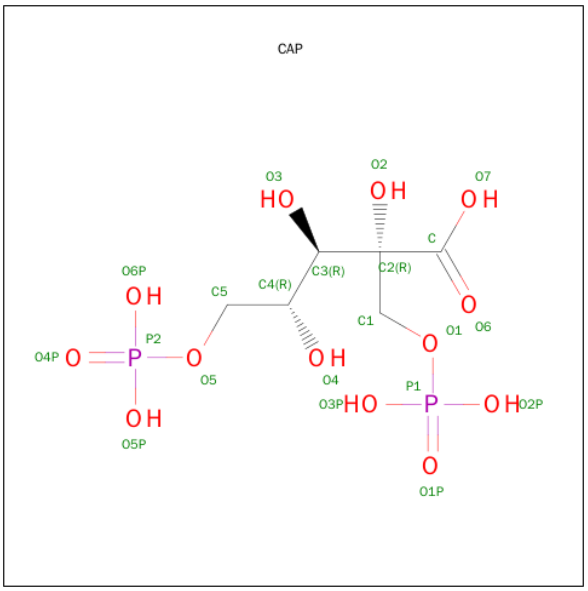
Chain	Residue	Modelled	Actual	Comment	Reference
G	46	PRO	LEU	VARIANT	UNP P00877
G	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877
H	46	PRO	LEU	VARIANT	UNP P00877
H	331	ALA	VAL	ENGINEERED MUTATION	UNP P00877

- 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	0	0
			1143	739	190	203	11			
2	J	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	K	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	L	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	M	140	Total	C	N	O	S	0	2	0
			1146	740	190	204	12			
2	N	140	Total	C	N	O	S	0	1	0
			1144	739	190	204	11			
2	O	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	P	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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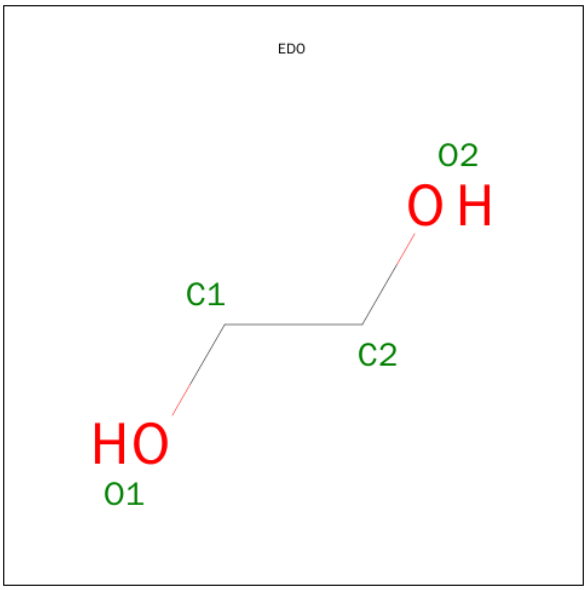
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- 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	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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	296	Total O 296 296	0	0

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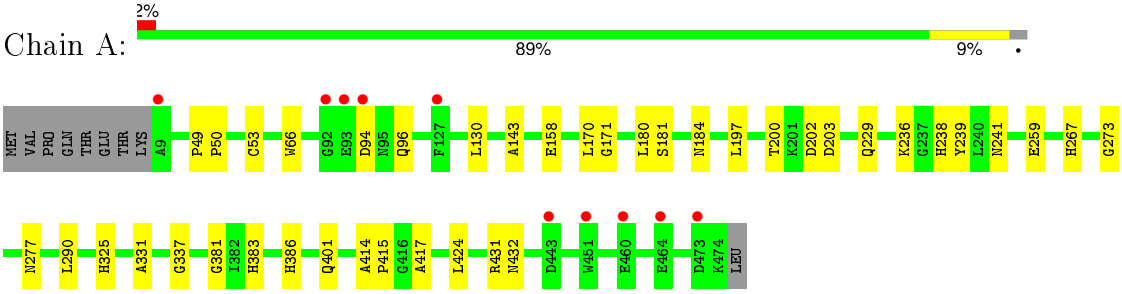
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	287	Total O 287 287	0	0
6	C	282	Total O 282 282	0	0
6	D	262	Total O 262 262	0	0
6	E	262	Total O 262 262	0	0
6	F	253	Total O 253 253	0	0
6	G	287	Total O 287 287	0	0
6	H	281	Total O 281 281	0	0
6	I	75	Total O 75 75	0	0
6	J	84	Total O 84 84	0	0
6	K	91	Total O 91 91	0	0
6	L	96	Total O 96 96	0	0
6	M	106	Total O 106 106	0	0
6	N	72	Total O 72 72	0	0
6	O	81	Total O 81 81	0	0
6	P	77	Total O 77 77	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.

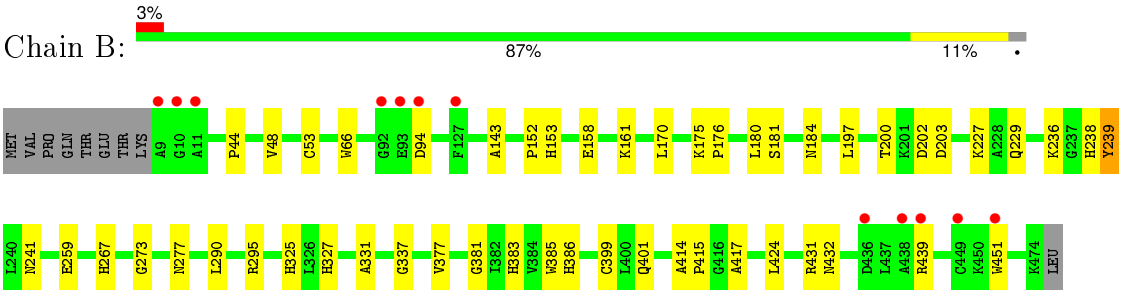
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:



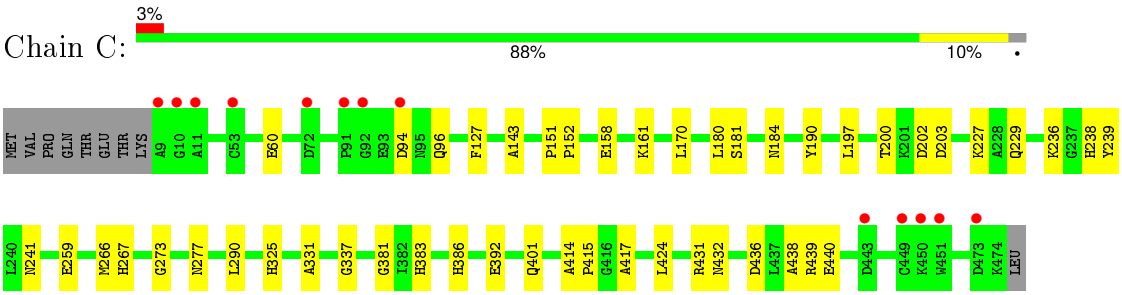
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



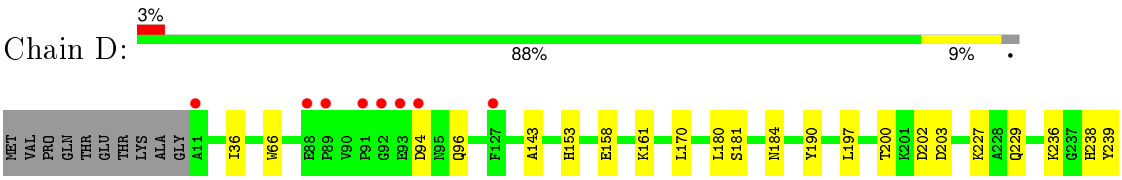
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

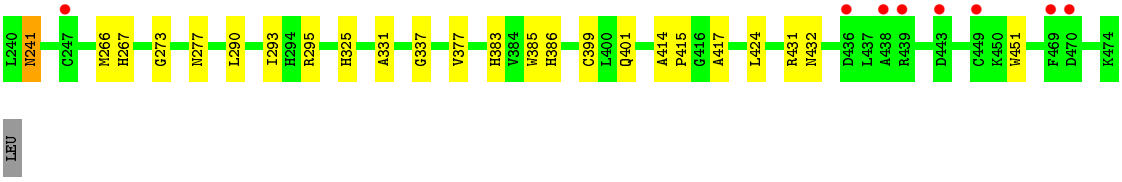
Chain C:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

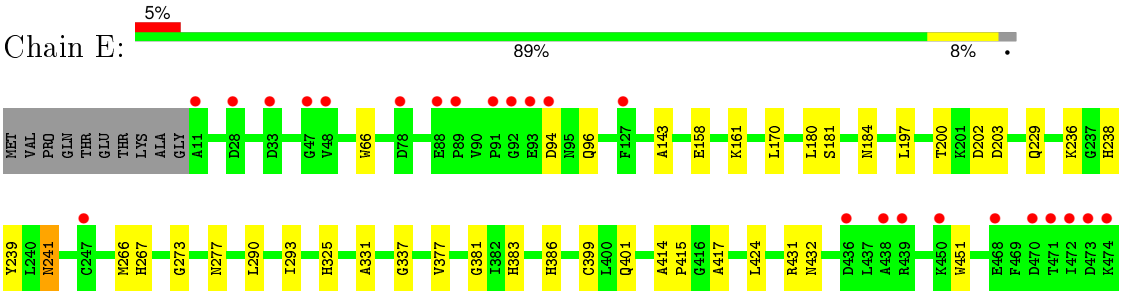
Chain D:





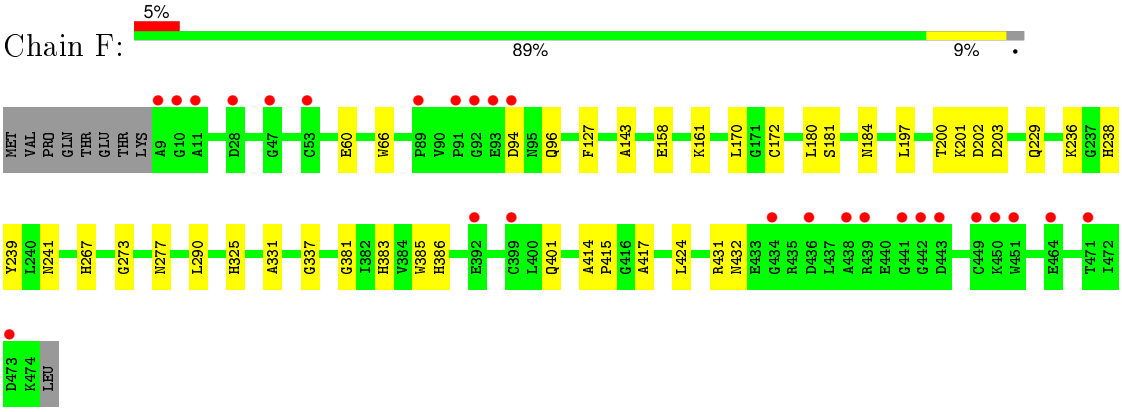
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E:



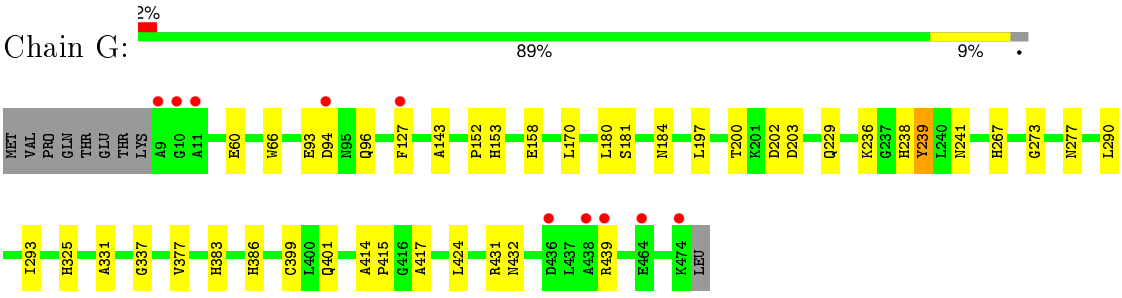
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain F:



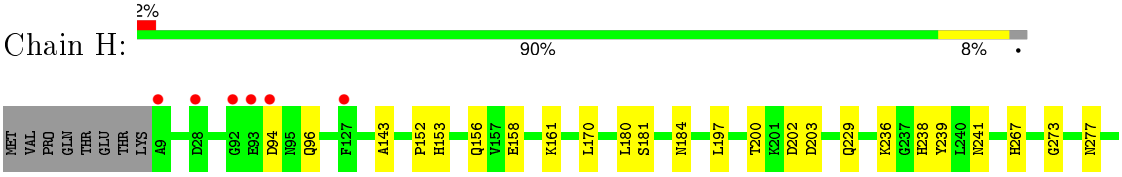
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G:



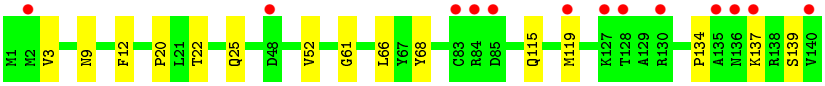
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain H:



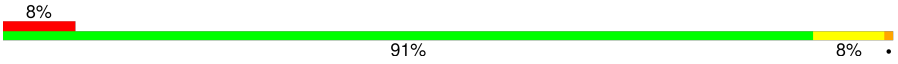
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

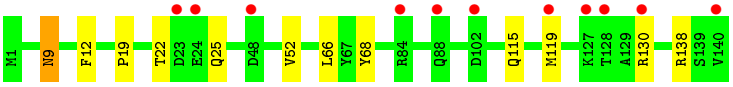
Chain I:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

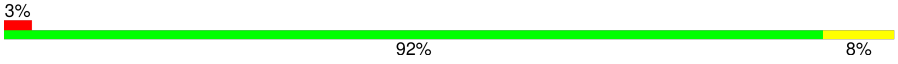
Chain J:

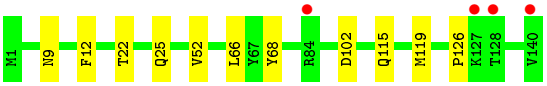




• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

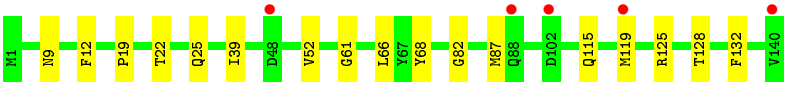
Chain K:





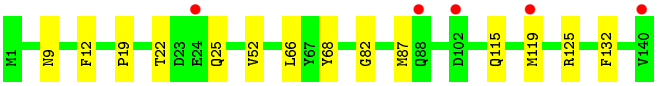
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain L:



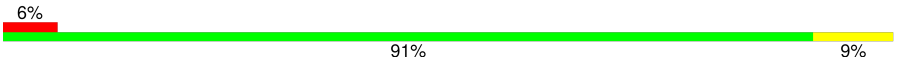
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

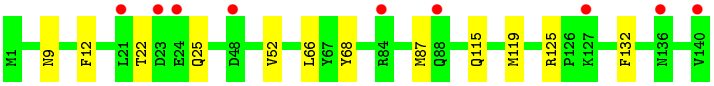
Chain M:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

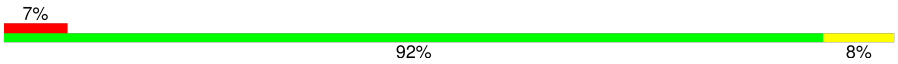
Chain N:





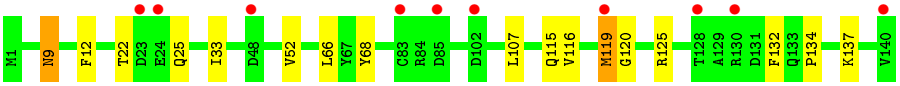
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain O:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.38Å 177.45Å 122.57Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-1.80) 92.1 (29.98-1.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.214 0.193 , 0.195	Depositor DCC
R_{free} test set	19570 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.6	EDS
Estimated twinning fraction	0.005 for -h-l,k,h 0.005 for l,k,-h-l 0.016 for h,-k,-h-l 0.014 for -h-l,-k,l 0.196 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 389563 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41473	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 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	0.41	0/3701	0.53	0/5002
1	B	0.43	0/3699	0.55	0/4999
1	C	0.42	0/3693	0.54	0/4991
1	D	0.42	0/3675	0.55	0/4967
1	E	0.43	0/3675	0.54	0/4967
1	F	0.44	0/3673	0.55	0/4965
1	G	0.43	0/3684	0.54	0/4979
1	H	0.43	0/3675	0.54	0/4967
2	I	0.39	0/1166	0.50	0/1584
2	J	0.39	0/1174	0.51	0/1594
2	K	0.41	0/1174	0.51	0/1594
2	L	0.40	0/1166	0.52	0/1584
2	M	0.40	0/1180	0.53	0/1602
2	N	0.40	0/1172	0.51	0/1592
2	O	0.40	0/1174	0.52	0/1594
2	P	0.41	0/1166	0.53	0/1584
All	All	0.42	0/38847	0.54	0/52565

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3643	0	3548	32	0
1	B	3638	0	3534	39	0
1	C	3639	0	3541	33	0
1	D	3626	0	3531	34	0
1	E	3626	0	3531	31	0
1	F	3630	0	3534	31	0
1	G	3634	0	3535	28	0
1	H	3631	0	3535	29	0
2	I	1143	0	1122	10	0
2	J	1145	0	1123	10	0
2	K	1145	0	1123	8	0
2	L	1143	0	1122	18	0
2	M	1146	0	1124	13	0
2	N	1144	0	1123	8	0
2	O	1145	0	1123	7	0
2	P	1143	0	1122	13	0
3	A	21	0	7	0	0
3	B	21	0	7	0	0
3	C	21	0	8	0	0
3	D	21	0	7	0	0
3	E	21	0	7	0	0
3	F	21	0	7	0	0
3	G	21	0	7	0	0
3	H	21	0	7	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	16	0	24	0	0
5	B	16	0	24	0	0
5	C	20	0	30	0	0
5	D	16	0	24	1	0
5	E	12	0	18	0	0
5	F	8	0	12	0	0
5	G	24	0	36	0	0
5	H	16	0	24	0	0
5	I	4	0	6	0	0
5	J	8	0	12	0	0
5	K	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	8	0	12	6	0
5	M	8	0	12	3	0
5	N	8	0	12	0	0
5	O	8	0	12	0	0
5	P	4	0	6	0	0
6	A	296	0	0	2	0
6	B	287	0	0	2	0
6	C	282	0	0	0	0
6	D	262	0	0	3	0
6	E	262	0	0	2	0
6	F	253	0	0	2	0
6	G	287	0	0	2	0
6	H	281	0	0	2	0
6	I	75	0	0	1	0
6	J	84	0	0	0	0
6	K	91	0	0	0	0
6	L	96	0	0	4	0
6	M	106	0	0	1	0
6	N	72	0	0	1	0
6	O	81	0	0	0	0
6	P	77	0	0	1	0
All	All	41473	0	37604	285	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 (285) 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:A:53:CYS:SG	1:A:130[B]:LEU:HD21	1.30	1.66
1:A:53:CYS:SG	1:A:130[B]:LEU:CD2	2.12	1.38
2:L:82:GLY:H	5:L:1142:EDO:H12	1.13	1.10
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.08	1.02
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.06	1.01
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.12	0.97
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.09	0.95
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.14	0.95
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.14	0.94
2:M:82:GLY:H	5:M:1142:EDO:H12	1.31	0.94
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.12	0.93
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.13	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:HD22	2:L:115:GLN:HE21	1.19	0.91
1:H:184:ASN:HD22	2:J:115:GLN:HE21	1.17	0.91
1:C:184:ASN:HD22	2:I:115:GLN:HE21	1.19	0.86
1:A:184:ASN:HD22	2:O:115:GLN:HE21	1.22	0.86
1:D:184:ASN:HD22	2:N:115:GLN:HE21	1.25	0.84
1:A:53:CYS:HG	1:A:130[B]:LEU:CD2	1.87	0.84
1:G:184:ASN:HD22	2:M:115:GLN:HE21	1.21	0.83
1:E:184:ASN:HD22	2:K:115:GLN:HE21	1.23	0.83
1:F:184:ASN:HD22	2:P:115:GLN:HE21	1.27	0.82
1:G:267:HIS:CD2	1:G:277:ASN:HD22	1.97	0.80
1:F:267:HIS:CD2	1:F:277:ASN:HD22	2.01	0.79
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.99	0.79
1:D:267:HIS:CD2	1:D:277:ASN:HD22	1.98	0.78
2:M:82:GLY:H	5:M:1142:EDO:C1	1.96	0.78
1:H:267:HIS:CD2	1:H:277:ASN:HD22	2.02	0.77
1:D:431:ARG:HH21	1:D:432:ASN:HD21	1.32	0.76
1:F:431:ARG:HH21	1:F:432:ASN:HD21	1.34	0.76
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.34	0.76
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.32	0.75
1:C:267:HIS:CD2	1:C:277:ASN:HD22	2.02	0.74
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.35	0.74
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.35	0.74
1:A:383:HIS:H	1:A:386:HIS:HD2	1.35	0.73
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.37	0.72
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.72	0.72
1:H:383:HIS:H	1:H:386:HIS:HD2	1.35	0.72
1:D:383:HIS:H	1:D:386:HIS:HD2	1.37	0.71
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.73	0.71
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.74	0.70
1:G:383:HIS:H	1:G:386:HIS:HD2	1.37	0.70
1:B:383:HIS:H	1:B:386:HIS:HD2	1.40	0.70
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.03	0.69
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.40	0.69
1:E:383:HIS:H	1:E:386:HIS:HD2	1.41	0.69
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.75	0.69
1:F:383:HIS:H	1:F:386:HIS:HD2	1.36	0.69
1:B:267:HIS:CD2	1:B:277:ASN:HD22	2.03	0.69
1:C:383:HIS:H	1:C:386:HIS:HD2	1.38	0.69
1:C:436:ASP:O	1:C:440:GLU:HB2	1.93	0.68
2:P:134:PRO:HG2	2:P:137:LYS:HB2	1.76	0.68
2:L:22:THR:H	2:L:25:GLN:HE21	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:GLY:N	5:L:1142:EDO:H12	1.97	0.68
1:D:290:LEU:HG	2:L:66:LEU:HD11	1.74	0.68
2:L:82:GLY:H	5:L:1142:EDO:C1	2.00	0.67
1:B:44:PRO:HB3	1:B:53[B]:CYS:SG	2.35	0.67
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.77	0.66
2:N:22:THR:H	2:N:25:GLN:HE21	1.43	0.66
1:C:290:LEU:HG	2:K:66:LEU:HD11	1.79	0.65
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.79	0.65
2:M:22:THR:H	2:M:25:GLN:HE21	1.43	0.64
2:I:22:THR:H	2:I:25:GLN:HE21	1.45	0.64
2:P:22:THR:H	2:P:25:GLN:HE21	1.43	0.64
1:A:290:LEU:HG	2:I:66:LEU:HD11	1.80	0.64
1:H:290:LEU:HG	2:P:66:LEU:HD11	1.79	0.64
1:E:290:LEU:HG	2:M:66:LEU:HD11	1.80	0.64
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.78	0.64
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.81	0.63
1:G:93:GLU:O	6:G:2058:HOH:O	2.15	0.63
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.82	0.62
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.81	0.62
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.83	0.62
1:B:290:LEU:HG	2:J:66:LEU:HD11	1.80	0.62
1:F:181:SER:H	2:P:115:GLN:NE2	1.97	0.61
1:G:290:LEU:HG	2:O:66:LEU:HD11	1.80	0.61
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.83	0.61
1:F:290:LEU:HG	2:N:66:LEU:HD11	1.82	0.61
2:I:20:PRO:O	6:I:2010:HOH:O	2.16	0.60
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.85	0.60
2:K:22:THR:H	2:K:25:GLN:HE21	1.50	0.59
2:K:52:VAL:HG13	2:K:68:TYR:HB3	1.84	0.59
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.86	0.59
2:I:134:PRO:HG2	2:I:137:LYS:HB2	1.84	0.59
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.85	0.59
1:F:180:LEU:HA	2:P:115:GLN:HE22	1.68	0.58
1:A:53:CYS:SG	1:A:130[B]:LEU:HD23	2.31	0.58
2:J:22:THR:H	2:J:25:GLN:HE21	1.51	0.58
1:A:171:GLY:HA3	6:A:2164:HOH:O	2.04	0.58
1:C:180:LEU:HA	2:I:115:GLN:HE22	1.67	0.58
2:O:22:THR:H	2:O:25:GLN:HE21	1.50	0.58
1:D:158:GLU:CD	1:D:325:HIS:HE2	2.08	0.57
1:B:48:VAL:CG1	1:B:53[B]:CYS:SG	2.93	0.57
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:SER:H	2:L:115:GLN:NE2	2.03	0.56
1:H:181:SER:H	2:J:115:GLN:NE2	2.03	0.56
1:B:158:GLU:CD	1:B:325:HIS:HE2	2.08	0.56
1:B:180:LEU:HA	2:L:115:GLN:HE22	1.70	0.56
1:G:181:SER:H	2:M:115:GLN:NE2	2.04	0.56
2:M:87:MET:HG2	6:M:2066:HOH:O	2.05	0.56
1:C:392:GLU:HG3	1:C:438:ALA:HB2	1.87	0.56
1:G:158:GLU:CD	1:G:325:HIS:HE2	2.09	0.56
1:D:181:SER:H	2:N:115:GLN:NE2	2.04	0.56
1:D:180:LEU:HA	2:N:115:GLN:HE22	1.71	0.55
1:G:180:LEU:HA	2:M:115:GLN:HE22	1.71	0.55
1:H:229:GLN:HE21	1:H:236:LYS:H	1.54	0.55
1:C:181:SER:H	2:I:115:GLN:NE2	2.03	0.55
1:E:180:LEU:HA	2:K:115:GLN:HE22	1.72	0.55
2:L:87:MET:HG2	6:L:2063:HOH:O	2.07	0.55
1:A:259[B]:GLU:OE1	2:O:61:GLY:HA3	2.06	0.55
2:M:52:VAL:HG13	2:M:68:TYR:HB3	1.88	0.55
2:M:82:GLY:N	5:M:1142:EDO:H12	2.13	0.54
2:P:9:ASN:HB3	6:P:2005:HOH:O	2.07	0.54
2:L:128:THR:HG23	6:L:2090:HOH:O	2.07	0.54
1:B:229:GLN:HE21	1:B:236:LYS:H	1.55	0.54
1:E:181:SER:H	2:K:115:GLN:NE2	2.06	0.54
1:A:229:GLN:HE21	1:A:236:LYS:H	1.56	0.54
2:J:52:VAL:HG13	2:J:68:TYR:HB3	1.90	0.54
1:C:436:ASP:OD2	1:C:439:ARG:HD2	2.07	0.54
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.10	0.54
1:H:158:GLU:CD	1:H:325:HIS:HE2	2.10	0.53
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.11	0.53
1:B:227:LYS:HA	5:L:1141:EDO:H12	1.89	0.53
1:F:229:GLN:HE21	1:F:236:LYS:H	1.56	0.53
1:C:267:HIS:HE1	6:D:2168:HOH:O	1.92	0.53
1:C:161:LYS:HE2	6:E:2122:HOH:O	2.08	0.53
1:F:158:GLU:CD	1:F:325:HIS:HE2	2.12	0.53
1:H:180:LEU:HA	2:J:115:GLN:HE22	1.75	0.52
1:B:48:VAL:HG12	1:B:53[B]:CYS:SG	2.49	0.52
2:I:52:VAL:HG13	2:I:68:TYR:HB3	1.92	0.52
2:O:52:VAL:HG13	2:O:68:TYR:HB3	1.92	0.52
1:A:180:LEU:HA	2:O:115:GLN:HE22	1.74	0.52
1:A:181:SER:H	2:O:115:GLN:NE2	2.08	0.52
1:G:197:LEU:HG	1:G:417:ALA:HB1	1.92	0.52
1:D:295:ARG:HH12	5:D:1478:EDO:H12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HG	1:D:417:ALA:HB1	1.92	0.51
1:E:158:GLU:CD	1:E:325:HIS:HE2	2.12	0.51
6:G:2173:HOH:O	1:H:267:HIS:HE1	1.93	0.51
1:G:229:GLN:HE21	1:G:236:LYS:H	1.58	0.51
1:H:156:GLN:HG3	2:P:116:VAL:HB	1.92	0.51
2:I:3:VAL:O	2:I:139:SER:HA	2.11	0.51
1:C:197:LEU:HG	1:C:417:ALA:HB1	1.93	0.51
1:F:239:TYR:HE2	1:F:401:GLN:NE2	2.08	0.50
1:B:227:LYS:HA	5:L:1141:EDO:C1	2.42	0.50
1:C:273:GLY:HA3	1:D:273:GLY:HA3	1.94	0.50
1:H:200:THR:OG1	1:H:238:HIS:CD2	2.63	0.49
2:L:39:ILE:HG12	5:L:1142:EDO:H11	1.94	0.49
1:H:197:LEU:HG	1:H:417:ALA:HB1	1.94	0.49
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.59	0.49
2:L:52:VAL:HG13	2:L:68:TYR:HB3	1.94	0.49
1:D:200:THR:OG1	1:D:238:HIS:CD2	2.59	0.49
1:C:259[B]:GLU:OE1	2:I:61:GLY:HA3	2.13	0.49
1:B:259[B]:GLU:OE1	2:L:61:GLY:HA3	2.11	0.49
2:P:125:ARG:HD2	2:P:132:PHE:CE2	2.47	0.49
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.61	0.49
1:F:197:LEU:HG	1:F:417:ALA:HB1	1.96	0.48
1:E:200:THR:OG1	1:E:238:HIS:CD2	2.64	0.48
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.61	0.48
1:E:331:ALA:HA	1:E:337:GLY:O	2.13	0.48
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.95	0.48
1:D:161:LYS:HD3	2:L:66:LEU:HD13	1.96	0.48
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.60	0.48
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.61	0.48
1:G:267:HIS:HE1	6:H:2175:HOH:O	1.97	0.48
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.49	0.48
2:L:22:THR:HG22	6:L:2013:HOH:O	2.15	0.47
1:E:239:TYR:HE2	1:E:401:GLN:NE2	2.12	0.47
6:E:2153:HOH:O	1:F:267:HIS:HE1	1.96	0.47
1:E:229:GLN:HE21	1:E:236:LYS:H	1.61	0.47
1:F:200:THR:OG1	1:F:238:HIS:CD2	2.61	0.47
1:F:331:ALA:HA	1:F:337:GLY:O	2.15	0.47
1:C:229:GLN:HE21	1:C:236:LYS:H	1.63	0.47
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.64	0.47
2:N:125:ARG:HD2	2:N:132:PHE:CE2	2.50	0.47
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.61	0.47
1:B:48:VAL:HG11	1:B:53[B]:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:TYR:HE2	1:D:401:GLN:NE2	2.13	0.47
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.96	0.46
1:C:331:ALA:HA	1:C:337:GLY:O	2.15	0.46
1:A:267:HIS:HE1	6:B:2171:HOH:O	1.97	0.46
1:F:181:SER:H	2:P:115:GLN:HE22	1.61	0.46
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.50	0.46
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.97	0.46
1:H:331:ALA:HA	1:H:337:GLY:O	2.15	0.46
1:A:239:TYR:HE2	1:A:401:GLN:NE2	2.12	0.46
1:C:239:TYR:HE2	1:C:401:GLN:NE2	2.13	0.46
1:G:239:TYR:HE2	1:G:401:GLN:NE2	2.13	0.46
1:D:229:GLN:HE21	1:D:236:LYS:H	1.62	0.46
1:E:267:HIS:HE1	6:F:2157:HOH:O	1.97	0.45
2:L:87:MET:HE3	6:L:2065:HOH:O	2.17	0.45
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.62	0.45
1:G:273:GLY:HA3	1:H:273:GLY:HA3	1.98	0.45
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.99	0.45
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.99	0.45
1:A:331:ALA:HA	1:A:337:GLY:O	2.17	0.45
1:B:153:HIS:HE1	6:B:2176:HOH:O	1.99	0.45
2:N:52:VAL:HG13	2:N:68:TYR:HB3	1.97	0.45
1:E:143:ALA:HA	1:H:143:ALA:HA	1.99	0.45
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.98	0.45
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.99	0.45
1:G:331:ALA:HA	1:G:337:GLY:O	2.17	0.45
1:D:331:ALA:HA	1:D:337:GLY:O	2.17	0.45
2:P:107:LEU:O	2:P:120:GLY:HA2	2.17	0.45
2:P:52:VAL:HG13	2:P:68:TYR:HB3	1.98	0.45
1:C:143:ALA:HA	1:F:143:ALA:HA	1.98	0.44
1:H:383:HIS:H	1:H:386:HIS:CD2	2.24	0.44
1:G:66:TRP:CD1	1:H:381:GLY:HA2	2.53	0.44
1:E:161:LYS:HD3	2:M:66:LEU:HD13	1.99	0.44
1:H:239:TYR:HE2	1:H:401:GLN:NE2	2.15	0.44
1:H:293:ILE:HG13	1:H:318:LEU:HD21	1.98	0.44
6:D:2142:HOH:O	1:F:161:LYS:HE2	2.18	0.44
1:H:170:LEU:HG	1:H:424:LEU:HD22	1.99	0.44
1:B:197:LEU:HG	1:B:417:ALA:HB1	2.00	0.44
1:C:381:GLY:HA2	1:D:66:TRP:CD1	2.53	0.44
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.53	0.44
1:A:273:GLY:HA3	1:B:273:GLY:HA3	2.00	0.43
1:F:60:GLU:HG3	1:F:127:PHE:CZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:CYS:HB2	1:F:197:LEU:HD13	1.99	0.43
1:E:383:HIS:H	1:E:386:HIS:CD2	2.29	0.43
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.53	0.43
1:G:277:ASN:HD21	1:G:293:ILE:HD12	1.84	0.43
1:B:170:LEU:HG	1:B:424:LEU:HD22	1.99	0.43
2:L:125:ARG:HD2	2:L:132:PHE:CE2	2.54	0.43
1:G:414:ALA:HB3	1:G:415:PRO:HD3	2.00	0.43
1:C:383:HIS:N	1:C:386:HIS:HD2	2.12	0.43
1:G:170:LEU:HG	1:G:424:LEU:HD22	2.00	0.43
2:K:102:ASP:O	2:K:126:PRO:HB3	2.19	0.43
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.66	0.43
1:D:383:HIS:CE1	1:D:385:TRP:HB2	2.53	0.43
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.53	0.43
1:A:170:LEU:HG	1:A:424:LEU:HD22	2.00	0.43
1:B:239:TYR:HE2	1:B:401:GLN:NE2	2.17	0.43
1:E:277:ASN:HD21	1:E:293:ILE:HD12	1.82	0.43
1:B:451:TRP:CE2	2:J:19:PRO:HG3	2.54	0.43
1:D:277:ASN:HD21	1:D:293:ILE:HD12	1.83	0.42
6:A:2179:HOH:O	1:B:267:HIS:HE1	2.02	0.42
2:M:125:ARG:HD2	2:M:132:PHE:CE2	2.55	0.42
1:G:377:VAL:HG22	1:G:399:CYS:HB3	2.01	0.42
2:P:33:ILE:HD11	2:P:119:MET:SD	2.60	0.42
1:E:241:ASN:HA	1:E:266:MET:HG2	2.01	0.42
1:E:451:TRP:CE2	2:M:19:PRO:HG3	2.55	0.42
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.55	0.42
1:C:239:TYR:HB3	1:C:266:MET:HB3	2.02	0.42
1:D:158:GLU:OE2	1:D:325:HIS:NE2	2.34	0.42
1:C:290:LEU:HG	2:K:66:LEU:CD1	2.49	0.42
1:E:377:VAL:HG22	1:E:399:CYS:HB3	2.02	0.42
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.55	0.42
1:D:241:ASN:HA	1:D:266:MET:HG2	2.02	0.42
1:C:170:LEU:HG	1:C:424:LEU:HD22	2.01	0.42
1:B:200:THR:OG1	1:B:238:HIS:CD2	2.72	0.42
1:G:200:THR:OG1	1:G:238:HIS:CD2	2.71	0.42
1:H:181:SER:H	2:J:115:GLN:HE22	1.67	0.42
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.54	0.42
1:B:377:VAL:HG22	1:B:399:CYS:HB3	2.00	0.42
1:B:295:ARG:HG2	1:B:327:HIS:HB2	2.01	0.42
1:F:383:HIS:N	1:F:386:HIS:HD2	2.12	0.41
1:E:239:TYR:HB3	1:E:266:MET:HB3	2.01	0.41
1:F:170:LEU:HG	1:F:424:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ALA:HA	1:D:143:ALA:HA	2.02	0.41
1:E:170:LEU:HG	1:E:424:LEU:HD22	2.03	0.41
1:D:36:ILE:N	1:D:36:ILE:HD12	2.36	0.41
1:A:49:PRO:HA	1:A:50:PRO:HD3	1.98	0.41
2:N:87:MET:HE3	6:N:2046:HOH:O	2.19	0.41
1:D:451:TRP:CE2	2:L:19:PRO:HG3	2.56	0.41
2:J:9:ASN:HD21	2:J:138:ARG:HG2	1.86	0.41
1:H:153:HIS:HE1	6:H:2179:HOH:O	2.02	0.41
1:F:201:KCX:HB2	1:F:239:TYR:CD2	2.56	0.41
1:D:170:LEU:HG	1:D:424:LEU:HD22	2.03	0.41
1:B:161:LYS:HB3	2:J:66:LEU:HD22	2.03	0.41
1:B:414:ALA:HB3	1:B:415:PRO:HD3	2.03	0.41
1:C:151:HYP:HA	1:C:152:PRO:HD3	1.94	0.41
1:B:143:ALA:HA	1:G:143:ALA:HA	2.02	0.41
1:A:383:HIS:H	1:A:386:HIS:CD2	2.24	0.41
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.56	0.41
1:D:153:HIS:HE1	6:D:2172:HOH:O	2.02	0.41
1:E:414:ALA:HB3	1:E:415:PRO:HD3	2.03	0.41
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.56	0.40
1:D:377:VAL:HG22	1:D:399:CYS:HB3	2.04	0.40
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.56	0.40
1:B:331:ALA:HA	1:B:337:GLY:O	2.21	0.40
6:F:2131:HOH:O	1:H:161:LYS:HE2	2.20	0.40
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.57	0.40
1:G:60:GLU:HG3	1:G:127:PHE:CZ	2.57	0.40
1:D:383:HIS:N	1:D:386:HIS:HD2	2.11	0.40
1:B:175:LYS:HA	1:B:176:PRO:C	2.42	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	463/475 (98%)	453 (98%)	10 (2%)	0	100	100
1	B	463/475 (98%)	454 (98%)	9 (2%)	0	100	100
1	C	462/475 (97%)	450 (97%)	12 (3%)	0	100	100
1	D	459/475 (97%)	448 (98%)	11 (2%)	0	100	100
1	E	459/475 (97%)	447 (97%)	12 (3%)	0	100	100
1	F	460/475 (97%)	450 (98%)	10 (2%)	0	100	100
1	G	461/475 (97%)	450 (98%)	11 (2%)	0	100	100
1	H	460/475 (97%)	449 (98%)	11 (2%)	0	100	100
2	I	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
2	J	139/140 (99%)	135 (97%)	4 (3%)	0	100	100
2	K	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	L	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
2	M	140/140 (100%)	135 (96%)	5 (4%)	0	100	100
2	N	139/140 (99%)	131 (94%)	8 (6%)	0	100	100
2	O	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	P	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
All	All	4797/4920 (98%)	4666 (97%)	131 (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	370/375 (99%)	366 (99%)	4 (1%)	80	74
1	B	370/375 (99%)	365 (99%)	5 (1%)	74	65
1	C	369/375 (98%)	365 (99%)	4 (1%)	80	74
1	D	368/375 (98%)	364 (99%)	4 (1%)	80	74
1	E	368/375 (98%)	364 (99%)	4 (1%)	80	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	367/375 (98%)	363 (99%)	4 (1%)	80 74
1	G	368/375 (98%)	362 (98%)	6 (2%)	70 59
1	H	367/375 (98%)	362 (99%)	5 (1%)	74 65
2	I	122/122 (100%)	119 (98%)	3 (2%)	55 39
2	J	123/122 (101%)	119 (97%)	4 (3%)	45 27
2	K	123/122 (101%)	120 (98%)	3 (2%)	57 41
2	L	122/122 (100%)	119 (98%)	3 (2%)	55 39
2	M	124/122 (102%)	121 (98%)	3 (2%)	57 41
2	N	123/122 (101%)	120 (98%)	3 (2%)	57 41
2	O	123/122 (101%)	119 (97%)	4 (3%)	45 27
2	P	122/122 (100%)	119 (98%)	3 (2%)	55 39
All	All	3929/3976 (99%)	3867 (98%)	62 (2%)	70 59

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	96	GLN
1	A	203	ASP
1	A	241	ASN
1	B	94	ASP
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	439	ARG
1	C	94	ASP
1	C	96	GLN
1	C	203	ASP
1	C	241	ASN
1	D	94	ASP
1	D	96	GLN
1	D	203	ASP
1	D	241	ASN
1	E	94	ASP
1	E	96	GLN
1	E	203	ASP
1	E	241	ASN
1	F	94	ASP

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Mol	Chain	Res	Type
1	F	96	GLN
1	F	203	ASP
1	F	241	ASN
1	G	94	ASP
1	G	96	GLN
1	G	203	ASP
1	G	239	TYR
1	G	241	ASN
1	G	439	ARG
1	H	94	ASP
1	H	96	GLN
1	H	203	ASP
1	H	241	ASN
1	H	335	LEU
2	I	9	ASN
2	I	12	PHE
2	I	119	MET
2	J	9	ASN
2	J	12	PHE
2	J	119	MET
2	J	130	ARG
2	K	9	ASN
2	K	12	PHE
2	K	119	MET
2	L	9	ASN
2	L	12	PHE
2	L	119	MET
2	M	9	ASN
2	M	12	PHE
2	M	119	MET
2	N	9	ASN
2	N	12	PHE
2	N	119	MET
2	O	9	ASN
2	O	12	PHE
2	O	119	MET
2	O	130	ARG
2	P	9	ASN
2	P	12	PHE
2	P	119	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) 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
1	A	386	HIS
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	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	432	ASN
1	D	153	HIS
1	D	163	ASN
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	432	ASN
1	E	153	HIS
1	E	163	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN

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Mol	Chain	Res	Type
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
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	432	ASN
1	H	153	HIS
1	H	207	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	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

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Mol	Chain	Res	Type
2	J	29	GLN
2	J	115	GLN
2	K	8	ASN
2	K	9	ASN
2	K	25	GLN
2	K	29	GLN
2	K	115	GLN
2	L	8	ASN
2	L	9	ASN
2	L	25	GLN
2	L	29	GLN
2	L	88	GLN
2	L	115	GLN
2	L	133	GLN
2	M	8	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	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	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	P	8	ASN
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 molecules in this entry.

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

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	7,8,9	0.63	0	5,10,12	1.06	0
1	HYP	A	151	1	7,8,9	0.67	0	5,10,12	1.51	1 (20%)
1	KCX	A	201	1,4	7,11,12	0.88	1 (14%)	7,12,14	0.79	0
1	SMC	A	256	1	5,6,7	0.79	0	2,6,8	1.45	0
1	SMC	A	369	1	5,6,7	0.81	0	2,6,8	1.12	0
1	HYP	B	104	1	7,8,9	0.66	0	5,10,12	1.01	0
1	HYP	B	151	1	7,8,9	0.89	0	5,10,12	1.53	1 (20%)
1	KCX	B	201	1,4	7,11,12	0.70	0	7,12,14	0.87	0
1	SMC	B	256	1	5,6,7	0.96	0	2,6,8	1.53	1 (50%)
1	SMC	B	369	1	5,6,7	0.75	0	2,6,8	1.21	0
1	HYP	C	104	1	7,8,9	0.65	0	5,10,12	1.07	0
1	HYP	C	151	1	7,8,9	0.67	0	5,10,12	1.58	1 (20%)
1	KCX	C	201	1,4	7,11,12	0.98	1 (14%)	7,12,14	0.77	0
1	SMC	C	256	1	5,6,7	0.47	0	2,6,8	1.57	1 (50%)
1	SMC	C	369	1	5,6,7	0.54	0	2,6,8	1.09	0
1	HYP	D	104	1	7,8,9	0.53	0	5,10,12	1.25	1 (20%)
1	HYP	D	151	1	7,8,9	0.66	0	5,10,12	1.28	0
1	KCX	D	201	1,4	7,11,12	0.95	0	7,12,14	0.75	0
1	SMC	D	256	1	5,6,7	0.65	0	2,6,8	1.94	1 (50%)
1	SMC	D	369	1	5,6,7	0.66	0	2,6,8	1.19	0
1	HYP	E	104	1	7,8,9	0.67	0	5,10,12	1.20	0
1	HYP	E	151	1	7,8,9	0.72	0	5,10,12	1.53	0
1	KCX	E	201	1,4	7,11,12	0.71	0	7,12,14	1.15	1 (14%)
1	SMC	E	256	1	5,6,7	0.77	0	2,6,8	1.42	0
1	SMC	E	369	1	5,6,7	0.66	0	2,6,8	0.98	0
1	HYP	F	104	1	7,8,9	0.73	0	5,10,12	0.97	0
1	HYP	F	151	1	7,8,9	0.57	0	5,10,12	1.55	1 (20%)
1	KCX	F	201	1,4	7,11,12	0.82	0	7,12,14	0.90	0
1	SMC	F	256	1	5,6,7	0.43	0	2,6,8	1.92	0
1	SMC	F	369	1	5,6,7	0.57	0	2,6,8	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	G	104	1	7,8,9	0.68	0	5,10,12	1.17	0
1	HYP	G	151	1	7,8,9	0.56	0	5,10,12	1.48	1 (20%)
1	KCX	G	201	1,4	7,11,12	0.89	0	7,12,14	0.78	0
1	SMC	G	256	1	5,6,7	0.81	0	2,6,8	1.56	1 (50%)
1	SMC	G	369	1	5,6,7	0.83	0	2,6,8	1.16	0
1	HYP	H	104	1	7,8,9	0.58	0	5,10,12	1.15	0
1	HYP	H	151	1	7,8,9	0.72	0	5,10,12	1.51	1 (20%)
1	KCX	H	201	1,4	7,11,12	0.78	0	7,12,14	0.67	0
1	SMC	H	256	1	5,6,7	0.81	0	2,6,8	1.37	0
1	SMC	H	369	1	5,6,7	0.75	0	2,6,8	1.28	0
2	MME	I	1	2	7,8,9	2.73	1 (14%)	4,8,10	1.08	0
2	MME	J	1	2	7,8,9	2.73	1 (14%)	4,8,10	0.98	0
2	MME	K	1	2	7,8,9	2.74	1 (14%)	4,8,10	0.99	0
2	MME	L	1	2	7,8,9	2.73	1 (14%)	4,8,10	1.04	0
2	MME	M	1	2	7,8,9	2.76	1 (14%)	4,8,10	0.94	0
2	MME	N	1	2	7,8,9	2.73	1 (14%)	4,8,10	1.00	0
2	MME	O	1	2	7,8,9	2.74	1 (14%)	4,8,10	1.04	0
2	MME	P	1	2	7,8,9	2.73	1 (14%)	4,8,10	1.06	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	1,4	-	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	1,4	-	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	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	1,4	-	0/6/10/12	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	0/6/10/12	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	1,4	-	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	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	1,4	-	0/6/10/12	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	1,4	-	0/6/10/12	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	1,4	-	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
2	MME	I	1	2	-	0/4/8/10	0/0/0/0
2	MME	J	1	2	-	0/4/8/10	0/0/0/0
2	MME	K	1	2	-	0/4/8/10	0/0/0/0
2	MME	L	1	2	-	0/4/8/10	0/0/0/0
2	MME	M	1	2	-	0/4/8/10	0/0/0/0
2	MME	N	1	2	-	0/4/8/10	0/0/0/0
2	MME	O	1	2	-	0/4/8/10	0/0/0/0
2	MME	P	1	2	-	0/4/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	MME	CM-N	-7.08	1.27	1.46
2	O	1	MME	CM-N	-7.04	1.27	1.46
2	L	1	MME	CM-N	-7.03	1.27	1.46
2	I	1	MME	CM-N	-7.02	1.27	1.46
2	P	1	MME	CM-N	-7.01	1.27	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	MME	CM-N	-7.00	1.27	1.46
2	K	1	MME	CM-N	-6.99	1.27	1.46
2	N	1	MME	CM-N	-6.96	1.27	1.46
1	A	201	KCX	CE-NZ	2.01	1.50	1.46
1	C	201	KCX	CE-NZ	2.22	1.51	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	201	KCX	CE-NZ-CX	-2.40	120.77	123.49
1	F	151	HYP	O-C-CA	-2.22	119.58	125.44
1	A	151	HYP	O-C-CA	-2.22	119.59	125.44
1	G	151	HYP	O-C-CA	-2.19	119.65	125.44
1	H	151	HYP	O-C-CA	-2.19	119.65	125.44
1	C	256	SMC	O-C-CA	-2.18	119.81	125.49
1	G	256	SMC	O-C-CA	-2.13	119.94	125.49
1	D	256	SMC	O-C-CA	-2.09	120.05	125.49
1	B	256	SMC	O-C-CA	-2.07	120.10	125.49
1	C	151	HYP	O-C-CA	-2.04	120.05	125.44
1	B	151	HYP	O-C-CA	-2.02	120.10	125.44
1	D	104	HYP	O-C-CA	-2.01	120.13	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	151	HYP	1	0
1	F	201	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 8 are monoatomic - leaving 54 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	1477	-	3,3,3	0.47	0	2,2,2	0.38	0
5	EDO	A	1478	-	3,3,3	0.53	0	2,2,2	0.37	0
5	EDO	A	1479	-	3,3,3	0.47	0	2,2,2	0.38	0
5	EDO	A	1480	-	3,3,3	0.53	0	2,2,2	0.37	0
3	CAP	A	476	4	14,20,20	0.96	1 (7%)	15,31,31	0.62	0
5	EDO	B	1475	-	3,3,3	0.61	0	2,2,2	0.12	0
5	EDO	B	1476	-	3,3,3	0.49	0	2,2,2	0.34	0
5	EDO	B	1477	-	3,3,3	0.47	0	2,2,2	0.43	0
5	EDO	B	1478	-	3,3,3	0.49	0	2,2,2	0.31	0
3	CAP	B	477	4	14,20,20	0.83	0	15,31,31	0.65	0
5	EDO	C	1475	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	C	1476	-	3,3,3	0.53	0	2,2,2	0.20	0
5	EDO	C	1477	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	C	1478	-	3,3,3	0.55	0	2,2,2	0.31	0
5	EDO	C	1479	-	3,3,3	0.48	0	2,2,2	0.39	0
3	CAP	C	477	4	14,20,20	0.95	1 (7%)	15,31,31	0.69	0
5	EDO	D	1475	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	D	1476	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	D	1477	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	D	1478	-	3,3,3	0.47	0	2,2,2	0.47	0
3	CAP	D	477	4	14,20,20	0.78	0	15,31,31	0.66	0
5	EDO	E	1475	-	3,3,3	0.54	0	2,2,2	0.31	0
5	EDO	E	1476	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	E	1477	-	3,3,3	0.45	0	2,2,2	0.48	0
3	CAP	E	477	4	14,20,20	0.77	0	15,31,31	0.71	0
5	EDO	F	1475	-	3,3,3	0.49	0	2,2,2	0.34	0
5	EDO	F	1476	-	3,3,3	0.51	0	2,2,2	0.37	0
3	CAP	F	477	4	14,20,20	0.87	1 (7%)	15,31,31	0.68	0
5	EDO	G	1475	-	3,3,3	0.56	0	2,2,2	0.26	0
5	EDO	G	1476	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	G	1477	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	G	1478	-	3,3,3	0.52	0	2,2,2	0.36	0
5	EDO	G	1479	-	3,3,3	0.52	0	2,2,2	0.20	0
5	EDO	G	1480	-	3,3,3	0.51	0	2,2,2	0.38	0
3	CAP	G	477	4	14,20,20	0.93	1 (7%)	15,31,31	0.59	0
5	EDO	H	1475	-	3,3,3	0.45	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	H	1476	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	H	1477	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	H	1478	-	3,3,3	0.47	0	2,2,2	0.43	0
3	CAP	H	477	4	14,20,20	0.89	0	15,31,31	0.77	0
5	EDO	I	1141	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	J	1141	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	J	1142	-	3,3,3	0.42	0	2,2,2	0.53	0
5	EDO	K	1141	-	3,3,3	0.47	0	2,2,2	0.41	0
5	EDO	K	1142	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	L	1141	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	L	1142	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	M	1141	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	M	1142	-	3,3,3	0.50	0	2,2,2	0.22	0
5	EDO	N	1141	-	3,3,3	0.47	0	2,2,2	0.40	0
5	EDO	N	1142	-	3,3,3	0.49	0	2,2,2	0.42	0
5	EDO	O	1141	-	3,3,3	0.49	0	2,2,2	0.37	0
5	EDO	O	1142	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	P	1141	-	3,3,3	0.46	0	2,2,2	0.43	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	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
3	CAP	A	476	4	-	0/23/29/29	0/0/0/0
5	EDO	B	1475	-	-	0/1/1/1	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
3	CAP	B	477	4	-	0/23/29/29	0/0/0/0
5	EDO	C	1475	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1477	-	-	0/1/1/1	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
3	CAP	C	477	4	-	0/23/29/29	0/0/0/0
5	EDO	D	1475	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1476	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1478	-	-	0/1/1/1	0/0/0/0
3	CAP	D	477	4	-	0/23/29/29	0/0/0/0
5	EDO	E	1475	-	-	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
3	CAP	E	477	4	-	0/23/29/29	0/0/0/0
5	EDO	F	1475	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1476	-	-	0/1/1/1	0/0/0/0
3	CAP	F	477	4	-	0/23/29/29	0/0/0/0
5	EDO	G	1475	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1476	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1477	-	-	0/1/1/1	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
3	CAP	G	477	4	-	0/23/29/29	0/0/0/0
5	EDO	H	1475	-	-	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
3	CAP	H	477	4	-	0/23/29/29	0/0/0/0
5	EDO	I	1141	-	-	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	477	CAP	O2-C2	2.01	1.45	1.43
3	G	477	CAP	O2-C2	2.31	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	476	CAP	O2-C2	2.37	1.46	1.43
3	C	477	CAP	O2-C2	2.38	1.46	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1478	EDO	1	0
5	L	1141	EDO	2	0
5	L	1142	EDO	4	0
5	M	1142	EDO	3	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	461/475 (97%)	0.05	10 (2%)	65	60	5, 12, 25, 37	0
1	B	461/475 (97%)	-0.01	12 (2%)	59	54	5, 12, 25, 37	0
1	C	461/475 (97%)	0.03	13 (2%)	56	51	5, 12, 25, 37	0
1	D	459/475 (96%)	0.07	16 (3%)	48	42	5, 12, 25, 37	0
1	E	459/475 (96%)	0.11	24 (5%)	31	25	5, 12, 25, 37	0
1	F	461/475 (97%)	0.10	26 (5%)	28	22	5, 12, 26, 37	0
1	G	461/475 (97%)	-0.01	10 (2%)	65	60	5, 11, 25, 37	0
1	H	461/475 (97%)	0.00	11 (2%)	62	57	5, 12, 25, 37	1 (0%)
2	I	139/140 (99%)	0.42	13 (9%)	11	8	9, 16, 28, 31	0
2	J	139/140 (99%)	0.34	11 (7%)	15	12	9, 17, 28, 31	0
2	K	139/140 (99%)	0.21	4 (2%)	55	49	9, 16, 27, 31	0
2	L	139/140 (99%)	0.17	5 (3%)	46	40	9, 16, 27, 31	0
2	M	139/140 (99%)	0.25	5 (3%)	46	40	9, 16, 26, 31	0
2	N	139/140 (99%)	0.36	9 (6%)	22	18	10, 17, 30, 32	0
2	O	139/140 (99%)	0.28	10 (7%)	18	14	9, 16, 28, 31	0
2	P	139/140 (99%)	0.36	10 (7%)	18	14	10, 17, 27, 31	0
All	All	4796/4920 (97%)	0.10	189 (3%)	43	37	5, 13, 26, 37	1 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	92	GLY	6.9
1	E	94	ASP	6.8
1	E	93	GLU	6.0
1	D	92	GLY	5.3
1	F	94	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	94	ASP	5.2
1	C	11	ALA	5.2
2	I	83	CYS	4.7
2	P	83	CYS	4.6
2	I	140	VAL	4.6
2	I	128	THR	4.6
1	D	436	ASP	4.5
1	F	91	PRO	4.5
1	D	94	ASP	4.4
1	A	94	ASP	4.4
1	H	94	ASP	4.4
1	C	10	GLY	4.4
1	G	11	ALA	4.3
1	F	438	ALA	4.3
1	B	94	ASP	4.2
1	F	11	ALA	4.1
2	N	140	VAL	4.1
1	D	11	ALA	4.1
1	H	9	ALA	4.0
2	P	128	THR	4.0
1	E	11	ALA	4.0
1	F	473	ASP	4.0
2	N	48	ASP	3.9
1	A	92	GLY	3.9
2	O	130	ARG	3.8
2	J	128	THR	3.8
1	D	93	GLU	3.8
2	L	140	VAL	3.8
1	E	127	PHE	3.7
1	F	10	GLY	3.6
1	H	92	GLY	3.6
1	G	10	GLY	3.6
1	D	438	ALA	3.5
1	D	91	PRO	3.5
1	F	451	TRP	3.5
1	E	91	PRO	3.5
2	I	48	ASP	3.5
1	B	9	ALA	3.4
1	C	9	ALA	3.4
1	D	469	PHE	3.4
1	E	438	ALA	3.3
2	J	140	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	436	ASP	3.3
2	K	140	VAL	3.3
1	B	10	GLY	3.3
1	F	434	GLY	3.3
2	N	23	ASP	3.3
1	E	48	VAL	3.2
1	A	9	ALA	3.2
1	D	439	ARG	3.2
1	E	470	ASP	3.1
1	C	91	PRO	3.1
1	F	89	PRO	3.1
2	J	130	ARG	3.1
1	F	392	GLU	3.1
1	F	443	ASP	3.1
1	F	464	GLU	3.0
1	F	9	ALA	3.0
2	O	140	VAL	3.0
2	P	48	ASP	3.0
1	G	439	ARG	3.0
1	G	9	ALA	2.9
1	F	439	ARG	2.9
2	M	119	MET	2.9
1	G	94	ASP	2.9
1	B	127	PHE	2.9
1	A	464	GLU	2.9
2	O	84	ARG	2.9
1	E	78	ASP	2.9
2	J	23	ASP	2.9
1	B	93	GLU	2.9
2	J	119	MET	2.8
2	J	24	GLU	2.8
2	M	140	VAL	2.8
1	D	449	CYS	2.8
2	J	102	ASP	2.8
2	L	48	ASP	2.8
1	G	127	PHE	2.8
2	I	136	ASN	2.7
1	A	473	ASP	2.7
1	D	127	PHE	2.7
1	F	450	LYS	2.7
1	F	53	CYS	2.6
1	F	442	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	436	ASP	2.6
2	L	88	GLN	2.6
2	K	128	THR	2.6
1	B	439	ARG	2.6
1	E	439	ARG	2.6
2	I	137	LYS	2.6
2	N	136	ASN	2.6
1	C	92	GLY	2.5
2	I	135	ALA	2.5
2	I	119	MET	2.5
2	P	119	MET	2.5
1	A	460	GLU	2.5
1	C	449	CYS	2.5
1	H	449	CYS	2.5
2	O	128	THR	2.5
1	D	89	PRO	2.5
1	F	436	ASP	2.5
2	O	48	ASP	2.5
1	B	11	ALA	2.5
1	D	443	ASP	2.5
2	N	21	LEU	2.5
1	E	474	LYS	2.4
1	G	474	LYS	2.4
2	O	127	LYS	2.4
1	E	247	CYS	2.4
2	J	48	ASP	2.4
2	I	2	MET	2.4
1	C	473	ASP	2.4
2	P	85	ASP	2.4
1	F	441	GLY	2.4
1	H	93	GLU	2.3
2	O	113	GLN	2.3
2	O	119	MET	2.3
1	D	470	ASP	2.3
1	F	93	GLU	2.3
1	E	472	ILE	2.3
2	O	23	ASP	2.3
2	O	102	ASP	2.3
1	B	451	TRP	2.3
1	H	127	PHE	2.3
1	C	450	LYS	2.3
1	H	438	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	460	GLU	2.2
2	N	84	ARG	2.2
1	A	451	TRP	2.2
1	C	451	TRP	2.2
1	B	449	CYS	2.2
1	F	449	CYS	2.2
1	H	28	ASP	2.2
1	F	471	THR	2.2
1	E	88	GLU	2.2
1	G	438	ALA	2.2
2	I	84	ARG	2.2
1	F	92	GLY	2.2
2	N	24	GLU	2.2
1	E	89	PRO	2.2
1	E	450	LYS	2.2
1	H	443	ASP	2.2
2	I	127	LYS	2.2
2	K	127	LYS	2.2
2	P	23	ASP	2.2
2	P	24	GLU	2.2
1	E	28	ASP	2.2
1	F	47	GLY	2.1
2	L	102	ASP	2.1
1	B	438	ALA	2.1
1	C	443	ASP	2.1
1	G	436	ASP	2.1
1	A	93	GLU	2.1
1	F	399	CYS	2.1
1	E	33	ASP	2.1
1	G	464	GLU	2.1
1	B	92	GLY	2.1
1	E	47	GLY	2.1
1	A	127	PHE	2.1
1	E	473	ASP	2.1
2	J	88	GLN	2.1
1	H	464	GLU	2.1
2	M	24	GLU	2.1
1	F	28	ASP	2.1
2	M	102	ASP	2.1
2	N	88	GLN	2.1
1	E	468	GLU	2.0
2	I	130	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	471	THR	2.0
1	D	88	GLU	2.0
2	I	85	ASP	2.0
2	M	88	GLN	2.0
2	K	84	ARG	2.0
2	J	127	LYS	2.0
1	A	443	ASP	2.0
2	P	102	ASP	2.0
1	C	53	CYS	2.0
1	D	247	CYS	2.0
2	J	84	ARG	2.0
2	P	130	ARG	2.0
2	P	140	VAL	2.0
2	L	119	MET	2.0
2	N	127	LYS	2.0
1	C	72	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	KCX	G	201	12/13	0.96	0.12	-	7,9,10,11	0
1	HYP	F	104	8/9	0.95	0.10	-	8,8,9,10	0
1	SMC	H	369	7/8	0.94	0.09	-	11,12,16,17	0
1	SMC	B	369	7/8	0.92	0.12	-	11,12,16,16	0
2	MME	K	1	9/10	0.80	0.19	-	23,24,32,32	0
2	MME	J	1	9/10	0.87	0.20	-	23,24,32,33	0
1	HYP	E	151	8/9	0.96	0.10	-	8,9,9,9	0
1	SMC	D	369	7/8	0.94	0.09	-	11,12,16,17	0
1	SMC	A	369	7/8	0.93	0.11	-	11,12,16,17	0
1	KCX	B	201	12/13	0.96	0.11	-	7,9,10,11	0
1	KCX	E	201	12/13	0.95	0.11	-	7,9,10,10	0
1	SMC	C	369	7/8	0.93	0.10	-	11,12,17,17	0
1	HYP	B	151	8/9	0.96	0.10	-	8,9,9,9	0
1	HYP	D	151	8/9	0.95	0.09	-	9,9,9,9	0
1	SMC	G	256	7/8	0.98	0.06	-	5,6,7,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	H	104	8/9	0.97	0.07	-	8,8,8,9	0
2	MME	P	1	9/10	0.90	0.16	-	23,24,32,33	0
1	HYP	A	151	8/9	0.94	0.10	-	8,9,9,9	0
1	HYP	C	151	8/9	0.97	0.07	-	8,9,9,9	0
1	SMC	F	369	7/8	0.95	0.10	-	11,12,16,17	0
2	MME	L	1	9/10	0.88	0.20	-	23,24,32,32	0
1	SMC	D	256	7/8	0.98	0.06	-	6,6,7,8	0
1	SMC	E	369	7/8	0.95	0.10	-	11,12,16,17	0
1	SMC	A	256	7/8	0.98	0.07	-	5,5,7,8	0
1	SMC	G	369	7/8	0.91	0.12	-	11,12,16,17	0
1	HYP	F	151	8/9	0.95	0.08	-	9,9,9,9	0
1	HYP	E	104	8/9	0.94	0.07	-	8,9,9,9	0
1	HYP	D	104	8/9	0.94	0.10	-	8,8,9,10	0
1	KCX	F	201	12/13	0.97	0.08	-	8,9,10,11	0
1	KCX	H	201	12/13	0.96	0.10	-	8,9,10,11	0
1	SMC	F	256	7/8	0.98	0.06	-	6,6,7,9	0
2	MME	M	1	9/10	0.89	0.17	-	23,23,32,32	0
2	MME	O	1	9/10	0.88	0.17	-	23,24,32,33	0
2	MME	N	1	9/10	0.89	0.15	-	23,24,32,32	0
1	SMC	C	256	7/8	0.98	0.06	-	5,5,7,9	0
1	KCX	A	201	12/13	0.96	0.10	-	8,9,10,11	0
1	SMC	E	256	7/8	0.98	0.07	-	6,6,7,8	0
1	KCX	C	201	12/13	0.96	0.10	-	7,9,10,10	0
1	HYP	G	104	8/9	0.96	0.08	-	8,8,8,9	0
1	HYP	H	151	8/9	0.95	0.09	-	8,9,9,9	0
1	SMC	B	256	7/8	0.96	0.09	-	6,6,7,8	0
1	HYP	C	104	8/9	0.96	0.08	-	8,8,9,10	0
1	HYP	B	104	8/9	0.98	0.08	-	8,8,9,9	0
1	HYP	A	104	8/9	0.97	0.07	-	8,8,9,9	0
2	MME	I	1	9/10	0.91	0.16	-	23,24,32,33	0
1	KCX	D	201	12/13	0.96	0.10	-	8,9,10,11	0
1	HYP	G	151	8/9	0.96	0.08	-	8,9,9,9	0
1	SMC	H	256	7/8	0.98	0.06	-	5,5,7,8	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	L	1142	4/4	0.66	0.33	12.88	25,25,26,26	4
5	EDO	G	1479	4/4	0.87	0.30	11.42	8,11,11,13	4
5	EDO	J	1141	4/4	0.62	0.30	6.96	43,43,43,44	0
5	EDO	G	1478	4/4	0.60	0.33	6.16	41,43,43,45	0
5	EDO	I	1141	4/4	0.71	0.30	5.91	19,20,20,20	4
5	EDO	B	1477	4/4	0.80	0.20	5.81	51,51,52,52	0
5	EDO	M	1142	4/4	0.72	0.27	5.70	18,18,18,19	4
5	EDO	C	1477	4/4	0.70	0.45	5.53	29,29,29,29	4
5	EDO	G	1480	4/4	0.75	0.22	4.98	41,42,42,42	0
5	EDO	D	1478	4/4	0.75	0.38	4.96	22,22,23,24	4
5	EDO	O	1141	4/4	0.67	0.29	4.75	33,33,33,34	0
5	EDO	C	1476	4/4	0.89	0.23	4.40	12,13,15,15	4
5	EDO	M	1141	4/4	0.75	0.31	4.22	22,23,23,24	4
5	EDO	F	1476	4/4	0.74	0.32	3.99	17,17,17,18	4
5	EDO	H	1478	4/4	0.73	0.31	3.88	49,50,51,51	0
5	EDO	L	1141	4/4	0.70	0.28	3.85	38,38,39,39	1
5	EDO	C	1479	4/4	0.76	0.34	3.56	46,47,47,47	0
5	EDO	H	1476	4/4	0.56	0.21	3.10	36,37,38,38	0
5	EDO	P	1141	4/4	0.78	0.23	2.84	36,37,37,37	0
5	EDO	K	1142	4/4	0.70	0.22	2.57	36,37,37,38	0
5	EDO	D	1477	4/4	0.87	0.17	2.51	21,22,23,24	0
5	EDO	G	1475	4/4	0.85	0.18	2.49	19,20,22,22	0
5	EDO	B	1475	4/4	0.82	0.18	2.23	17,19,21,21	0
5	EDO	A	1478	4/4	0.56	0.19	2.08	35,36,36,36	0
5	EDO	E	1475	4/4	0.78	0.21	2.07	31,31,32,32	0
5	EDO	N	1142	4/4	0.74	0.28	1.36	28,29,31,32	0
5	EDO	A	1479	4/4	0.83	0.18	0.95	37,38,38,39	0
5	EDO	K	1141	4/4	0.84	0.21	0.93	33,33,33,34	0
5	EDO	N	1141	4/4	0.77	0.15	0.84	40,40,40,40	0
5	EDO	D	1475	4/4	0.90	0.11	0.67	21,21,21,22	0
5	EDO	O	1142	4/4	0.95	0.18	0.59	24,24,25,25	0
5	EDO	F	1475	4/4	0.87	0.12	0.52	23,24,25,25	0
5	EDO	E	1476	4/4	0.90	0.13	0.14	25,26,27,27	0
5	EDO	A	1477	4/4	0.94	0.11	0.07	19,19,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	J	1142	4/4	0.96	0.13	-0.04	23,24,25,26	0
5	EDO	B	1476	4/4	0.94	0.10	-0.12	18,19,20,20	0
5	EDO	C	1475	4/4	0.94	0.10	-0.20	19,19,20,21	0
5	EDO	G	1476	4/4	0.95	0.09	-0.39	20,20,21,22	0
3	CAP	E	477	21/21	0.96	0.09	-0.47	10,13,15,17	0
3	CAP	F	477	21/21	0.97	0.09	-0.49	11,13,15,17	0
3	CAP	H	477	21/21	0.96	0.09	-0.55	9,13,14,17	0
3	CAP	A	476	21/21	0.96	0.10	-0.85	10,13,14,17	0
3	CAP	C	477	21/21	0.97	0.08	-1.05	10,13,14,16	0
3	CAP	B	477	21/21	0.97	0.08	-1.31	10,13,14,17	0
5	EDO	H	1475	4/4	0.95	0.07	-1.40	19,19,20,20	0
3	CAP	G	477	21/21	0.97	0.08	-1.41	10,13,14,16	0
3	CAP	D	477	21/21	0.97	0.08	-1.47	10,13,15,17	0
4	MG	G	476	1/1	0.99	0.08	-2.00	8,8,8,8	0
4	MG	C	476	1/1	0.99	0.06	-2.08	9,9,9,9	0
4	MG	F	476	1/1	0.98	0.05	-2.61	10,10,10,10	0
4	MG	H	476	1/1	0.99	0.04	-3.36	9,9,9,9	0
4	MG	E	476	1/1	0.98	0.05	-3.70	10,10,10,10	0
4	MG	D	476	1/1	0.99	0.04	-4.19	9,9,9,9	0
4	MG	A	477	1/1	0.99	0.04	-4.53	9,9,9,9	0
4	MG	B	476	1/1	0.99	0.04	-5.16	9,9,9,9	0
5	EDO	B	1478	4/4	0.86	0.19	-	30,32,32,32	0
5	EDO	C	1478	4/4	0.83	0.29	-	26,27,27,27	0
5	EDO	H	1477	4/4	0.96	0.09	-	21,23,23,23	0
5	EDO	D	1476	4/4	0.86	0.17	-	38,38,39,39	0
5	EDO	A	1480	4/4	0.91	0.14	-	26,26,27,27	0
5	EDO	E	1477	4/4	0.75	0.27	-	50,51,51,52	0
5	EDO	G	1477	4/4	0.94	0.09	-	25,25,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.