



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2V69
Title : CRYSTAL STRUCTURE OF CHLAMYDOMONAS REINHARDTII RUBISCO WITH A LARGE-SUBUNIT MUTATION D473E
Authors : Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on : 2007-07-14
Resolution : 2.80 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 ⓘ](#)) 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

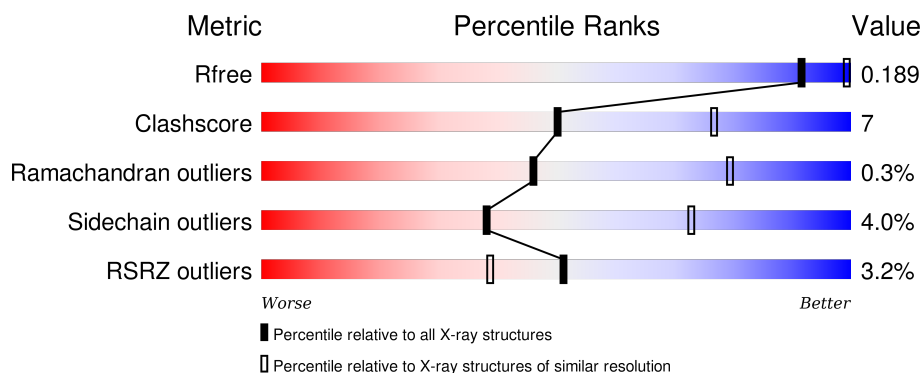
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	475	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	C	475	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	D	475	<div> <div>%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	E	475	<div> <div>%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	475	
1	G	475	
1	H	475	
2	I	140	
2	J	140	
2	K	140	
2	L	140	
2	M	140	
2	N	140	
2	O	140	
2	P	140	

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	1472	-	-	-	X
5	EDO	B	1472	-	-	-	X
5	EDO	B	1473	-	-	-	X
5	EDO	C	1475	-	-	-	X
5	EDO	D	1477	-	-	-	X
5	EDO	D	1479	-	-	-	X
5	EDO	F	1472	-	-	-	X
5	EDO	G	1472	-	-	-	X
5	EDO	G	1474	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38504 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	459	Total	C	N	O	S	0	0	0
			3579	2265	630	660	24			
1	B	460	Total	C	N	O	S	0	0	0
			3583	2267	631	661	24			
1	C	459	Total	C	N	O	S	0	0	0
			3582	2266	630	662	24			
1	D	464	Total	C	N	O	S	0	0	0
			3620	2290	636	670	24			
1	E	459	Total	C	N	O	S	0	0	0
			3579	2265	630	660	24			
1	F	461	Total	C	N	O	S	0	0	0
			3588	2270	632	662	24			
1	G	461	Total	C	N	O	S	0	0	0
			3588	2270	632	662	24			
1	H	458	Total	C	N	O	S	0	0	0
			3574	2262	629	659	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	CONFLICT	UNP P00877
A	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
B	46	PRO	LEU	CONFLICT	UNP P00877
B	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
C	46	PRO	LEU	CONFLICT	UNP P00877
C	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
D	46	PRO	LEU	CONFLICT	UNP P00877
D	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
E	46	PRO	LEU	CONFLICT	UNP P00877
E	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
F	46	PRO	LEU	CONFLICT	UNP P00877
F	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	46	PRO	LEU	CONFLICT	UNP P00877
G	473	GLU	ASP	ENGINEERED MUTATION	UNP P00877
H	46	PRO	LEU	CONFLICT	UNP P00877
H	473	GLU	ASP	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	0	0
			1143	739	190	203	11			
2	K	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
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	0	0
			1143	739	190	203	11			
2	N	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	O	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	P	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			

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

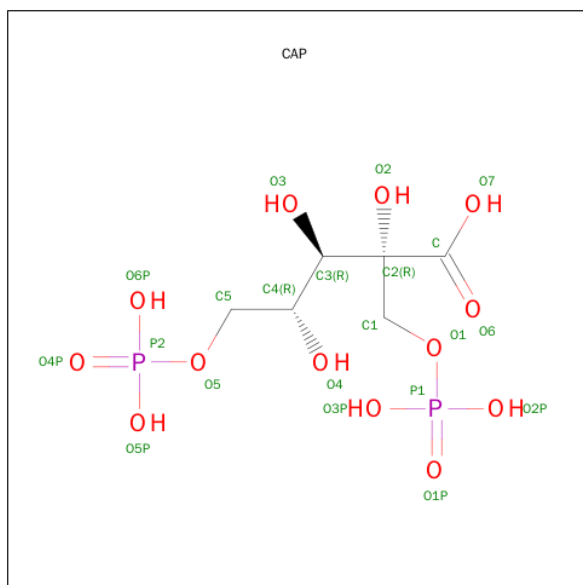
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $\text{C}_6\text{H}_{14}\text{O}_{13}\text{P}_2$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	52	Total O 52 52	0	0
6	B	29	Total O 29 29	0	0
6	C	57	Total O 57 57	0	0
6	D	39	Total O 39 39	0	0
6	E	54	Total O 54 54	0	0
6	F	41	Total O 41 41	0	0
6	G	45	Total O 45 45	0	0
6	H	43	Total O 43 43	0	0
6	I	6	Total O 6 6	0	0

Continued on next page...

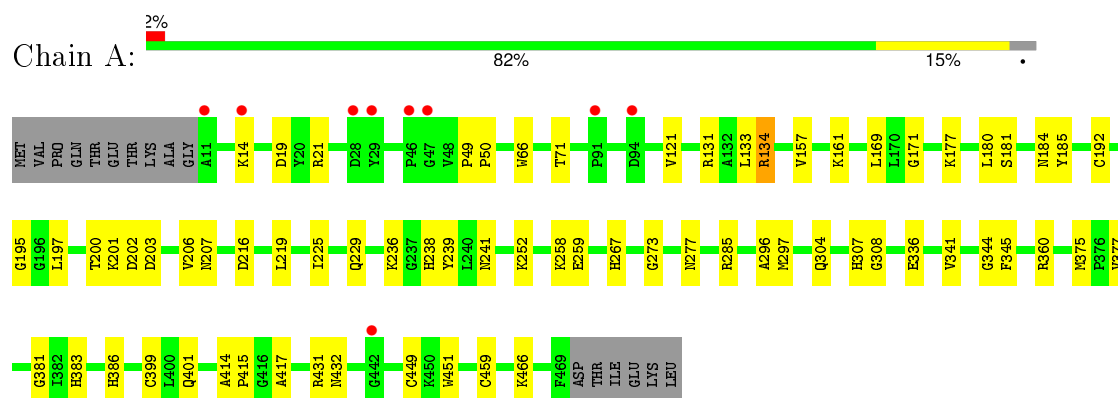
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	3	Total 3	O 3	0	0
6	K	6	Total 6	O 6	0	0
6	L	2	Total 2	O 2	0	0
6	M	4	Total 4	O 4	0	0
6	N	4	Total 4	O 4	0	0
6	O	5	Total 5	O 5	0	0
6	P	5	Total 5	O 5	0	0

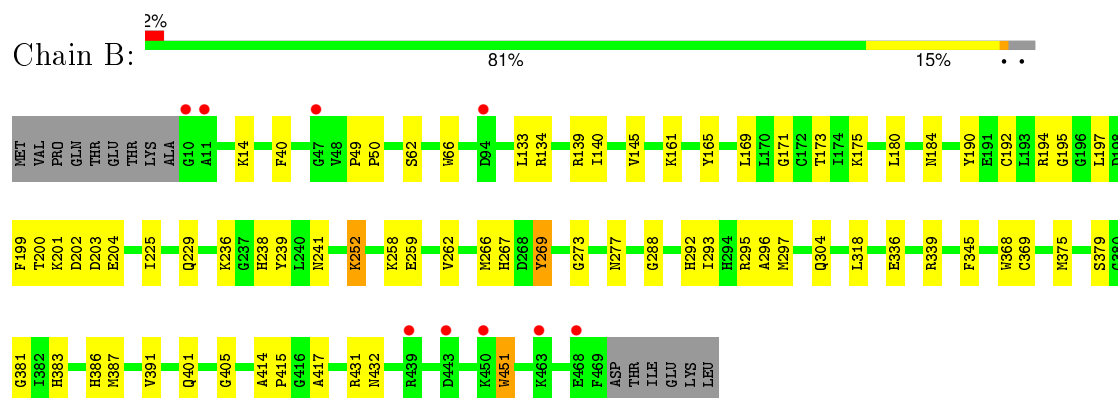
3 Residue-property plots [i](#)

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.

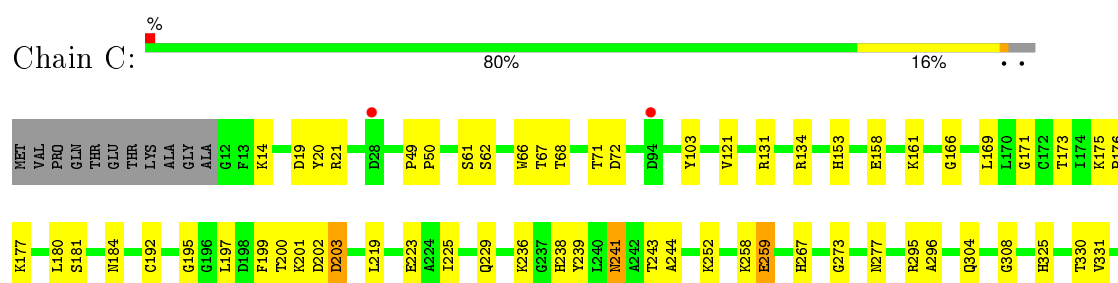
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

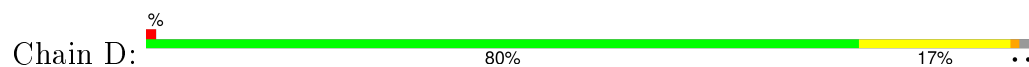


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

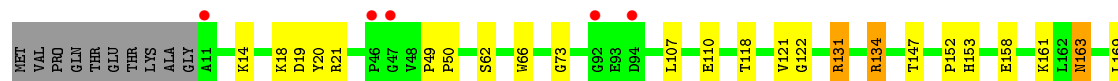
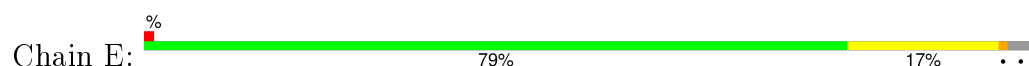




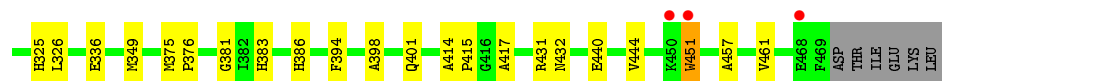
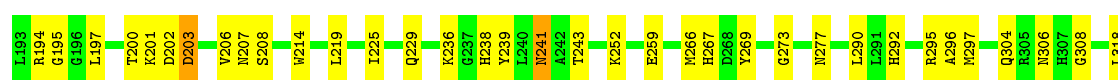
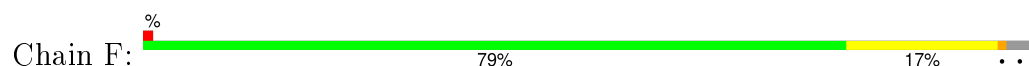
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



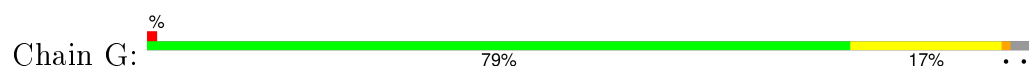
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

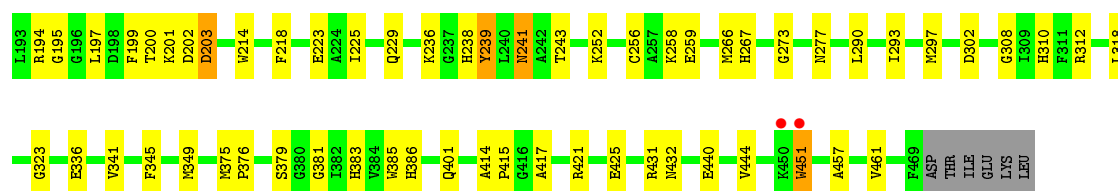


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

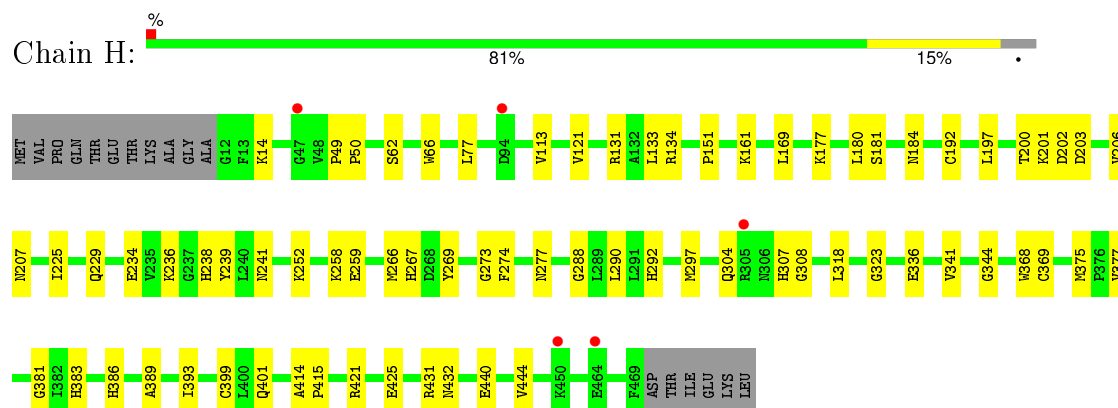


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

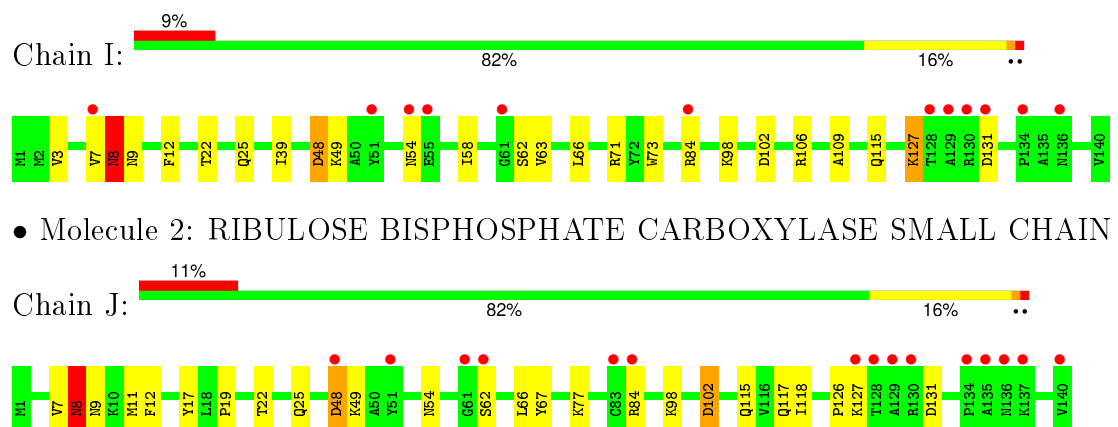




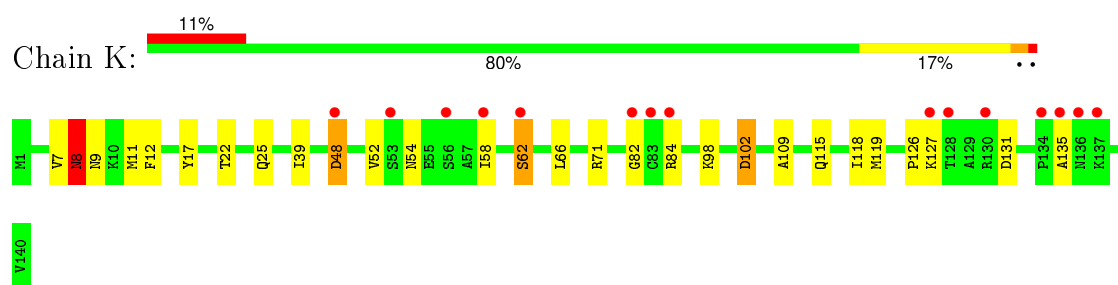
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



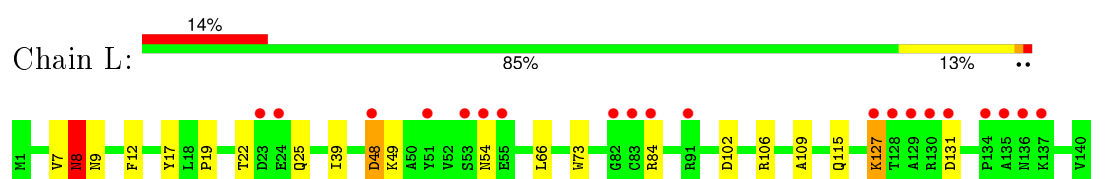
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1




• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain M:  4% 84% 14% ..




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain N:  6% 79% 19% ..




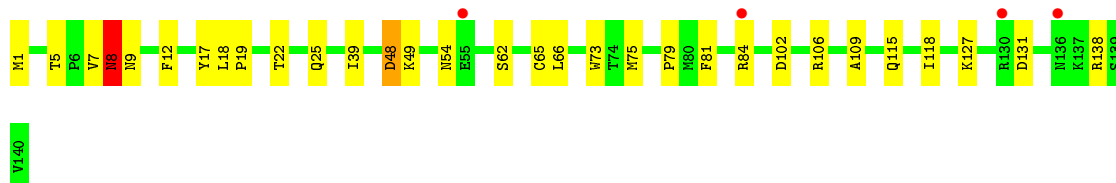
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain O:  9% 82% 16% ..



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P:  3% 78% 21% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.24Å 169.14Å 137.18Å 90.00° 96.24° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-2.80) 98.0 (19.97-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.228 0.192 , 0.189	Depositor DCC
R_{free} test set	6262 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 125029 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38504	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.59	0/3617	0.61	0/4890
1	B	0.68	0/3621	0.67	0/4895
1	C	0.62	0/3620	0.66	0/4894
1	D	0.64	0/3658	0.68	0/4945
1	E	0.63	0/3617	0.66	0/4890
1	F	0.64	0/3626	0.68	0/4902
1	G	0.66	1/3626 (0.0%)	0.68	0/4902
1	H	0.63	0/3612	0.66	0/4883
2	I	0.56	0/1166	0.62	1/1584 (0.1%)
2	J	0.64	0/1166	0.64	1/1584 (0.1%)
2	K	0.61	0/1166	0.66	1/1584 (0.1%)
2	L	0.69	0/1166	0.69	1/1584 (0.1%)
2	M	0.61	0/1166	0.66	1/1584 (0.1%)
2	N	0.58	0/1166	0.67	1/1584 (0.1%)
2	O	0.61	0/1166	0.66	1/1584 (0.1%)
2	P	0.60	0/1166	0.66	1/1584 (0.1%)
All	All	0.63	1/38325 (0.0%)	0.66	8/51873 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
2	M	0	1
2	N	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
2	P	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	53	CYS	CB-SG	-5.17	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	8	ASN	N-CA-C	-6.65	93.04	111.00
2	M	8	ASN	N-CA-C	-6.31	93.96	111.00
2	O	8	ASN	N-CA-C	-6.16	94.37	111.00
2	I	8	ASN	N-CA-C	-6.16	94.38	111.00
2	P	8	ASN	N-CA-C	-5.98	94.85	111.00
2	K	8	ASN	N-CA-C	-5.59	95.91	111.00
2	J	8	ASN	N-CA-C	-5.29	96.71	111.00
2	N	8	ASN	N-CA-C	-5.29	96.72	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	469	PHE	Peptide
1	D	470	ASP	Peptide
2	I	7	VAL	Peptide
2	J	7	VAL	Peptide
2	K	7	VAL	Peptide
2	L	7	VAL	Peptide
2	M	7	VAL	Peptide
2	N	7	VAL	Peptide
2	O	7	VAL	Peptide
2	P	7	VAL	Peptide

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	3579	0	3487	51	0
1	B	3583	0	3490	61	0
1	C	3582	0	3486	61	0
1	D	3620	0	3528	59	0
1	E	3579	0	3487	63	0
1	F	3588	0	3495	63	0
1	G	3588	0	3495	63	0
1	H	3574	0	3482	61	0
2	I	1143	0	1122	16	0
2	J	1143	0	1122	18	0
2	K	1143	0	1122	17	0
2	L	1143	0	1122	13	0
2	M	1143	0	1122	17	0
2	N	1143	0	1122	16	0
2	O	1143	0	1122	17	0
2	P	1143	0	1122	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	8	0	0
4	C	21	0	7	0	0
4	D	21	0	9	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	8	0	0
4	H	21	0	8	0	0
5	A	12	0	18	1	0
5	B	8	0	12	0	0
5	C	12	0	18	5	0
5	D	12	0	18	0	0
5	E	16	0	24	1	0
5	F	8	0	12	0	0
5	G	12	0	18	3	0
5	H	16	0	24	0	0
6	A	52	0	0	6	0
6	B	29	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	57	0	0	5	0
6	D	39	0	0	4	0
6	E	54	0	0	4	0
6	F	41	0	0	2	0
6	G	45	0	0	3	0
6	H	43	0	0	2	0
6	I	6	0	0	0	0
6	J	3	0	0	0	0
6	K	6	0	0	0	0
6	L	2	0	0	0	0
6	M	4	0	0	0	0
6	N	4	0	0	0	0
6	O	5	0	0	1	0
6	P	5	0	0	0	0
All	All	38504	0	37131	523	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 7.

All (523) 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:F:267:HIS:CD2	1:F:277:ASN:HD22	1.77	1.01
1:F:184:ASN:HD22	2:P:115:GLN:HE21	1.08	1.00
1:G:267:HIS:CD2	1:G:277:ASN:HD22	1.80	0.98
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.02	0.98
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.00	0.97
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.10	0.97
1:G:267:HIS:HD2	1:G:277:ASN:HD22	0.99	0.97
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.08	0.96
1:G:184:ASN:HD22	2:M:115:GLN:HE21	1.03	0.95
1:C:184:ASN:HD22	2:I:115:GLN:HE21	1.13	0.95
1:F:267:HIS:HD2	1:F:277:ASN:HD22	0.94	0.94
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.85	0.93
1:A:184:ASN:HD22	2:O:115:GLN:HE21	1.05	0.93
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.05	0.93
1:H:184:ASN:HD22	2:J:115:GLN:HE21	1.16	0.92
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.88	0.92
1:H:267:HIS:HD2	1:H:277:ASN:HD22	0.96	0.91
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.91	0.88
1:C:72:ASP:OD2	5:C:1473:EDO:H11	1.72	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:CYS:HG	1:A:459:CYS:HG	1.06	0.87
1:E:449:CYS:HG	1:E:459:CYS:HG	1.18	0.87
1:C:267:HIS:CD2	1:C:277:ASN:HD22	1.91	0.86
1:D:267:HIS:CD2	1:D:277:ASN:HD22	1.94	0.84
1:C:383:HIS:H	1:C:386:HIS:HD2	1.27	0.82
1:G:383:HIS:H	1:G:386:HIS:HD2	1.26	0.82
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.99	0.80
1:D:184:ASN:HD22	2:N:115:GLN:HE21	1.29	0.80
1:E:184:ASN:HD22	2:K:115:GLN:HE21	1.28	0.79
1:C:449:CYS:HG	1:C:459:CYS:HG	1.01	0.79
1:A:383:HIS:H	1:A:386:HIS:HD2	1.31	0.78
1:F:267:HIS:HD2	1:F:277:ASN:ND2	1.77	0.77
1:G:267:HIS:HD2	1:G:277:ASN:ND2	1.80	0.77
1:B:184:ASN:HD22	2:L:115:GLN:HE21	1.31	0.77
1:F:383:HIS:H	1:F:386:HIS:HD2	1.33	0.76
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.67	0.76
1:H:383:HIS:H	1:H:386:HIS:HD2	1.32	0.75
1:H:229:GLN:HE21	1:H:236:LYS:H	1.36	0.74
1:G:184:ASN:ND2	2:M:115:GLN:HE21	1.84	0.74
2:K:22:THR:H	2:K:25:GLN:HE21	1.33	0.73
2:J:22:THR:H	2:J:25:GLN:HE21	1.34	0.72
1:G:229:GLN:HE21	1:G:236:LYS:H	1.37	0.72
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.72	0.71
1:B:195:GLY:HA3	1:B:417:ALA:HB3	1.71	0.71
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.73	0.71
1:C:295:ARG:HH12	5:C:1475:EDO:H12	1.56	0.71
2:L:22:THR:H	2:L:25:GLN:HE21	1.38	0.70
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.74	0.70
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.80	0.70
1:G:161:LYS:HD3	2:O:66:LEU:HD13	1.73	0.70
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.73	0.69
1:A:466:LYS:O	5:A:1473:EDO:H12	1.93	0.69
1:D:383:HIS:H	1:D:386:HIS:HD2	1.41	0.69
1:E:169:LEU:HD12	1:E:375:MET:HE3	1.75	0.69
1:D:449:CYS:HG	1:D:459:CYS:HG	0.70	0.69
2:O:22:THR:H	2:O:25:GLN:HE21	1.40	0.69
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.75	0.68
1:B:252:LYS:HE3	6:B:1018:HOH:O	1.93	0.68
1:B:383:HIS:H	1:B:386:HIS:HD2	1.41	0.68
1:E:383:HIS:H	1:E:386:HIS:HD2	1.42	0.67
1:D:158:GLU:OE2	1:D:325:HIS:NE2	2.17	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:22:THR:H	2:P:25:GLN:HE21	1.40	0.67
1:E:169:LEU:HD12	1:E:375:MET:CE	2.25	0.67
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.78	0.67
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.74	0.67
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.86	0.66
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.78	0.66
1:F:184:ASN:ND2	2:P:115:GLN:HE21	1.88	0.65
1:E:131:ARG:HD2	6:E:1006:HOH:O	1.96	0.65
1:H:234:GLU:OE1	6:H:1017:HOH:O	2.13	0.65
1:A:229:GLN:HE21	1:A:236:LYS:H	1.44	0.65
2:N:22:THR:H	2:N:25:GLN:HE21	1.43	0.65
2:M:22:THR:H	2:M:25:GLN:HE21	1.44	0.65
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.80	0.64
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.79	0.64
1:C:180:LEU:HA	2:I:115:GLN:HE22	1.63	0.64
2:I:22:THR:H	2:I:25:GLN:HE21	1.43	0.64
1:C:68:THR:HG23	5:C:1473:EDO:H12	1.80	0.62
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.82	0.62
1:F:229:GLN:HE21	1:F:236:LYS:H	1.47	0.62
1:F:181:SER:H	2:P:115:GLN:NE2	1.98	0.62
6:A:1026:HOH:O	1:G:161:LYS:HE2	1.98	0.61
1:F:158:GLU:OE2	1:F:325:HIS:NE2	2.26	0.61
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.84	0.61
1:G:181:SER:H	2:M:115:GLN:NE2	1.99	0.61
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.83	0.60
1:H:200:THR:OG1	1:H:238:HIS:CD2	2.51	0.60
1:A:360:ARG:HD3	6:A:1043:HOH:O	2.02	0.59
2:M:73:TRP:CZ3	2:M:106:ARG:HG2	2.36	0.59
1:A:219:LEU:HB3	6:O:1003:HOH:O	2.02	0.59
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.84	0.59
1:G:169:LEU:HD12	1:G:375:MET:CE	2.33	0.59
1:G:66:TRP:CD1	1:H:381:GLY:HA2	2.38	0.58
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.86	0.58
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.86	0.58
1:F:304:GLN:HA	1:F:304:GLN:HE21	1.68	0.58
1:A:169:LEU:HD12	1:A:375:MET:HE3	1.86	0.58
6:C:1040:HOH:O	1:E:252:LYS:HE3	2.03	0.58
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.87	0.58
1:H:169:LEU:HD12	1:H:375:MET:CE	2.34	0.58
1:D:377:VAL:HG22	1:D:399:CYS:HB3	1.84	0.57
1:G:200:THR:OG1	1:G:238:HIS:CD2	2.57	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.85	0.57
1:D:195:GLY:HA3	1:D:417:ALA:HB3	1.84	0.57
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.51	0.57
1:C:381:GLY:HA2	1:D:66:TRP:CD1	2.39	0.57
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.53	0.57
1:D:180:LEU:HA	2:N:115:GLN:HE22	1.69	0.57
1:E:200:THR:O	1:E:238:HIS:HA	2.05	0.57
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.86	0.57
1:H:290:LEU:HG	2:P:66:LEU:HD11	1.87	0.57
1:D:267:HIS:HE1	6:D:1022:HOH:O	1.88	0.57
1:B:180:LEU:HA	2:L:115:GLN:HE22	1.70	0.57
1:C:295:ARG:NH1	5:C:1475:EDO:H12	2.19	0.57
1:A:184:ASN:ND2	2:O:115:GLN:HE21	1.89	0.56
1:B:258:LYS:HE3	2:J:62:SER:HB3	1.87	0.56
1:A:169:LEU:HD12	1:A:375:MET:CE	2.35	0.56
1:E:121:VAL:HG23	1:F:297:MET:HG3	1.86	0.56
1:F:180:LEU:HA	2:P:115:GLN:HE22	1.69	0.56
1:F:304:GLN:NE2	1:F:304:GLN:HA	2.20	0.56
1:D:329:GLY:HA2	6:D:1036:HOH:O	2.05	0.56
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.88	0.56
1:B:169:LEU:HD12	1:B:375:MET:CE	2.36	0.56
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.40	0.56
1:G:161:LYS:HB3	2:O:66:LEU:HD22	1.88	0.56
1:C:258:LYS:HE3	2:K:62:SER:HB3	1.86	0.56
6:G:1017:HOH:O	2:M:71:ARG:HD2	2.06	0.56
1:B:169:LEU:HD12	1:B:375:MET:HE3	1.88	0.55
1:D:229:GLN:HE21	1:D:236:LYS:H	1.54	0.55
1:G:169:LEU:HD12	1:G:375:MET:HE3	1.86	0.55
1:A:180:LEU:HA	2:O:115:GLN:HE22	1.70	0.55
1:G:383:HIS:H	1:G:386:HIS:CD2	2.17	0.55
1:E:158:GLU:OE2	1:E:325:HIS:NE2	2.29	0.55
1:H:180:LEU:HA	2:J:115:GLN:HE22	1.71	0.55
1:G:192:CYS:HB3	1:G:197:LEU:HD12	1.87	0.55
1:G:273:GLY:HA3	1:H:273:GLY:HA3	1.89	0.55
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.88	0.55
1:A:181:SER:H	2:O:115:GLN:NE2	2.05	0.55
1:F:292:HIS:HA	1:F:325:HIS:HB2	1.88	0.55
1:C:431:ARG:HE	1:C:432:ASN:ND2	2.04	0.55
1:C:304:GLN:NE2	1:C:304:GLN:HA	2.22	0.55
1:B:318:LEU:C	1:B:318:LEU:HD13	2.26	0.55
1:G:379:SER:HB2	1:G:401:GLN:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ASN:HD22	2:P:115:GLN:NE2	1.91	0.54
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.55	0.54
1:G:121:VAL:HG23	1:H:297:MET:HG3	1.88	0.54
1:F:192:CYS:HB3	1:F:197:LEU:HD12	1.90	0.54
1:H:161:LYS:HB3	2:P:66:LEU:HD22	1.89	0.54
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.89	0.54
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.91	0.54
1:A:216:ASP:HA	6:A:1026:HOH:O	2.07	0.54
1:G:421:ARG:O	1:G:425:GLU:HG3	2.07	0.54
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.42	0.54
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.90	0.54
1:G:151:HYP:HB2	1:G:323:GLY:O	2.09	0.53
1:D:383:HIS:H	1:D:386:HIS:CD2	2.25	0.53
1:E:161:LYS:HD3	2:M:66:LEU:HD13	1.90	0.53
1:F:241:ASN:ND2	1:F:243:THR:H	2.07	0.53
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.91	0.53
1:E:229:GLN:HE21	1:E:236:LYS:H	1.55	0.53
1:H:200:THR:O	1:H:238:HIS:HA	2.09	0.53
1:F:225:ILE:HD11	1:F:238:HIS:HB3	1.91	0.53
1:E:304:GLN:HA	1:E:304:GLN:NE2	2.24	0.53
1:B:225:ILE:HD11	1:B:238:HIS:HB3	1.91	0.52
1:F:161:LYS:HB3	2:N:66:LEU:HD22	1.91	0.52
2:N:102:ASP:O	2:N:126:PRO:HB3	2.08	0.52
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.91	0.52
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.54	0.52
1:E:241:ASN:HD22	1:E:242:ALA:N	2.06	0.52
1:C:377:VAL:HG22	1:C:399:CYS:HB3	1.90	0.52
1:C:273:GLY:HA3	1:D:273:GLY:HA3	1.90	0.52
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.62	0.52
1:B:318:LEU:O	1:B:318:LEU:HD13	2.10	0.52
1:H:161:LYS:HD3	2:P:66:LEU:HD13	1.92	0.52
2:N:32:TYR:HD2	2:N:119:MET:HE3	1.74	0.52
1:A:161:LYS:HD3	2:I:66:LEU:HD13	1.91	0.52
1:C:62:SER:O	1:D:177:LYS:HB2	2.11	0.51
1:G:457:ALA:O	1:G:461:VAL:HG23	2.10	0.51
1:E:318:LEU:HD12	1:E:326:LEU:HD22	1.92	0.51
1:D:473:GLU:HG3	1:D:474:LYS:H	1.76	0.51
1:G:223:GLU:OE2	2:M:71:ARG:HB2	2.10	0.51
1:G:239:TYR:HB3	1:G:266:MET:HB3	1.92	0.51
1:C:386:HIS:HE1	6:C:1055:HOH:O	1.94	0.51
1:B:267:HIS:HD2	1:B:277:ASN:ND2	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HD3	2:J:66:LEU:HD13	1.93	0.51
2:O:11:MET:HG3	2:O:17:TYR:CE1	2.46	0.51
1:B:201:KCX:HB2	1:B:239:TYR:CD2	2.46	0.50
1:C:200:THR:OG1	1:C:238:HIS:CD2	2.62	0.50
1:G:381:GLY:HA2	1:H:66:TRP:CD1	2.46	0.50
1:D:202:ASP:OD1	1:D:238:HIS:CE1	2.61	0.50
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.46	0.50
1:F:457:ALA:O	1:F:461:VAL:HG23	2.11	0.50
1:D:161:LYS:HD3	2:L:66:LEU:HD13	1.91	0.50
1:E:195:GLY:HA3	1:E:417:ALA:HB3	1.94	0.50
1:F:200:THR:OG1	1:F:238:HIS:CD2	2.64	0.50
1:H:169:LEU:HD12	1:H:375:MET:HE1	1.92	0.50
1:F:171:GLY:HA3	1:F:401:GLN:HG2	1.94	0.50
1:B:229:GLN:HE21	1:B:236:LYS:H	1.58	0.50
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.93	0.50
1:G:180:LEU:HA	2:M:115:GLN:HE22	1.76	0.50
1:F:239:TYR:HB3	1:F:266:MET:HB3	1.93	0.50
1:G:451:TRP:CZ2	2:O:19:PRO:HG3	2.47	0.50
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.93	0.50
1:B:304:GLN:HA	1:B:304:GLN:NE2	2.25	0.50
1:B:171:GLY:HA3	1:B:401:GLN:HG2	1.93	0.50
1:D:170:LEU:HB3	1:D:197:LEU:HD23	1.94	0.50
1:D:292:HIS:HA	1:D:325:HIS:HB2	1.94	0.49
1:A:344:GLY:HA2	6:A:1043:HOH:O	2.11	0.49
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.60	0.49
1:E:73:GLY:HA3	2:P:81:PHE:CE1	2.47	0.49
2:L:48:ASP:N	2:L:48:ASP:OD1	2.44	0.49
1:F:161:LYS:HD3	2:N:66:LEU:HD13	1.94	0.49
1:D:134:ARG:HA	1:D:308:GLY:O	2.12	0.49
2:J:8:ASN:HB2	2:J:131:ASP:HA	1.94	0.49
1:H:269:TYR:CE2	1:H:318:LEU:HB2	2.47	0.49
1:A:383:HIS:H	1:A:386:HIS:CD2	2.20	0.49
1:E:290:LEU:HG	2:M:66:LEU:HD11	1.94	0.49
1:E:241:ASN:ND2	1:E:243:THR:H	2.11	0.49
1:C:195:GLY:HA3	1:C:417:ALA:HB3	1.94	0.49
1:G:177:LYS:HG2	1:G:203:ASP:OD2	2.13	0.49
1:A:206:VAL:C	1:A:207:ASN:HD22	2.16	0.49
1:B:269:TYR:CD2	1:B:318:LEU:HD23	2.48	0.49
1:F:201:KCX:HB2	1:F:239:TYR:CD2	2.48	0.49
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.48	0.49
1:H:304:GLN:HA	1:H:304:GLN:NE2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:HIS:HE1	1:G:385:TRP:HB2	1.76	0.49
1:A:201:KCX:HB2	1:A:239:TYR:CD2	2.48	0.49
1:G:195:GLY:HA3	1:G:417:ALA:HB3	1.94	0.49
1:F:9:ALA:HA	2:K:82:GLY:O	2.13	0.49
1:C:267:HIS:HD2	1:C:277:ASN:ND2	1.85	0.49
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.60	0.49
2:J:11:MET:HG3	2:J:17:TYR:CE1	2.48	0.48
1:G:139:ARG:HD2	1:G:139:ARG:C	2.33	0.48
1:H:134:ARG:HA	1:H:308:GLY:O	2.13	0.48
1:H:421:ARG:O	1:H:425:GLU:HG3	2.13	0.48
1:E:206:VAL:C	1:E:207:ASN:HD22	2.16	0.48
1:E:258:LYS:HG3	6:E:1040:HOH:O	2.12	0.48
1:E:304:GLN:HA	1:E:304:GLN:HE21	1.79	0.48
1:H:258:LYS:HE3	2:P:62:SER:HB3	1.94	0.48
2:O:8:ASN:HB2	2:O:131:ASP:HA	1.95	0.48
1:H:225:ILE:HD11	1:H:238:HIS:HB3	1.95	0.48
1:G:201:KCX:HB2	1:G:239:TYR:CD2	2.47	0.48
1:C:20:TYR:CD1	5:C:1474:EDO:H22	2.48	0.48
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.96	0.48
1:F:169:LEU:HD12	1:F:375:MET:CE	2.44	0.48
1:F:267:HIS:CD2	1:F:277:ASN:ND2	2.62	0.48
1:B:266:MET:HA	1:B:292:HIS:O	2.13	0.48
1:F:269:TYR:CD2	1:F:318:LEU:HD23	2.48	0.48
1:C:201:KCX:HB2	1:C:239:TYR:CD2	2.48	0.48
1:E:251:MET:O	1:E:255:VAL:HG23	2.13	0.48
1:E:190:TYR:CZ	1:E:194:ARG:HD3	2.49	0.47
1:C:169:LEU:HD12	1:C:375:MET:HE3	1.96	0.47
2:K:39:ILE:O	2:K:109:ALA:HA	2.14	0.47
1:F:306:ASN:HB3	6:F:1003:HOH:O	2.14	0.47
1:D:473:GLU:HG3	1:D:474:LYS:N	2.29	0.47
1:B:304:GLN:HA	1:B:304:GLN:HE21	1.79	0.47
1:B:190:TYR:CZ	1:B:194:ARG:HD3	2.49	0.47
1:D:267:HIS:HD2	1:D:277:ASN:ND2	1.92	0.47
1:H:383:HIS:H	1:H:386:HIS:CD2	2.22	0.47
1:A:161:LYS:HB3	2:I:66:LEU:HD22	1.97	0.47
1:G:177:LYS:HB2	1:H:62:SER:O	2.13	0.47
1:F:440:GLU:O	1:F:444:VAL:HG23	2.14	0.47
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.61	0.47
1:H:177:LYS:HG2	1:H:203:ASP:OD2	2.13	0.47
1:A:304:GLN:NE2	1:A:304:GLN:HA	2.28	0.47
1:C:121:VAL:HG23	1:D:297:MET:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:HA	1:D:176:PRO:C	2.35	0.47
1:E:225:ILE:HD11	1:E:238:HIS:HB3	1.97	0.47
2:O:107:LEU:O	2:O:120:GLY:HA2	2.15	0.47
1:E:171:GLY:HA2	1:E:199:PHE:O	2.13	0.47
1:H:201:KCX:HB2	1:H:239:TYR:CD2	2.50	0.47
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.63	0.47
1:D:206:VAL:C	1:D:207:ASN:HD22	2.18	0.47
1:F:19:ASP:HB3	1:F:21:ARG:HG2	1.97	0.47
1:B:202:ASP:OD1	1:B:238:HIS:CE1	2.62	0.47
2:L:73:TRP:CZ3	2:L:106:ARG:HG2	2.49	0.47
1:D:151:HYP:HB2	1:D:323:GLY:O	2.15	0.47
1:D:451:TRP:CZ2	2:L:19:PRO:HG3	2.50	0.47
1:D:19:ASP:HB3	1:D:21:ARG:HG2	1.96	0.47
1:E:303:ARG:NE	1:E:336:GLU:HG2	2.30	0.47
1:E:19:ASP:HB3	1:E:21:ARG:HG2	1.97	0.47
1:E:293:ILE:HG13	1:E:318:LEU:HD21	1.96	0.46
1:G:225:ILE:HD11	1:G:238:HIS:HB3	1.97	0.46
1:A:258:LYS:HE3	2:I:62:SER:HB3	1.96	0.46
1:D:474:LYS:HE3	1:D:474:LYS:HB3	1.74	0.46
1:G:49:PRO:HA	1:G:50:PRO:HD2	1.76	0.46
2:O:48:ASP:N	2:O:48:ASP:OD1	2.48	0.46
2:P:39:ILE:O	2:P:109:ALA:HA	2.16	0.46
1:G:153:HIS:CE1	1:G:161:LYS:HE3	2.51	0.46
1:C:345:PHE:O	1:C:349:MET:HG3	2.15	0.46
1:H:192:CYS:HB3	1:H:197:LEU:HD12	1.98	0.46
2:P:48:ASP:N	2:P:48:ASP:OD1	2.49	0.46
1:D:169:LEU:HD12	1:D:375:MET:CE	2.45	0.46
1:G:290:LEU:HG	2:O:66:LEU:HD11	1.97	0.46
2:J:102:ASP:O	2:J:126:PRO:HB3	2.15	0.46
2:J:67:TYR:CD2	2:J:67:TYR:C	2.89	0.46
2:M:48:ASP:OD1	2:M:48:ASP:N	2.49	0.46
1:B:239:TYR:HB3	1:B:266:MET:HB3	1.98	0.46
1:D:387:MET:O	1:D:391:VAL:HG23	2.16	0.46
1:A:377:VAL:HG22	1:A:399:CYS:HB3	1.98	0.46
1:E:200:THR:OG1	1:E:238:HIS:CD2	2.68	0.46
1:H:169:LEU:HD12	1:H:375:MET:HE3	1.98	0.46
1:E:192:CYS:HB3	1:E:197:LEU:HD12	1.98	0.46
1:C:181:SER:H	2:I:115:GLN:NE2	2.14	0.45
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.64	0.45
1:H:288:GLY:O	2:P:66:LEU:HD12	2.16	0.45
2:L:39:ILE:O	2:L:109:ALA:HA	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:ARG:O	1:D:425:GLU:HG3	2.17	0.45
2:P:18:LEU:HB3	2:P:19:PRO:CD	2.47	0.45
2:I:48:ASP:OD1	2:I:48:ASP:N	2.49	0.45
2:I:58:ILE:HD11	2:K:58:ILE:HB	1.98	0.45
1:B:200:THR:OG1	1:B:238:HIS:CD2	2.68	0.45
1:C:169:LEU:HD12	1:C:375:MET:CE	2.46	0.45
1:B:368:TRP:O	1:B:369:SMC:C	2.64	0.45
1:F:137:ASP:OD1	1:F:138:LEU:N	2.47	0.45
2:I:73:TRP:CZ3	2:I:106:ARG:HG2	2.51	0.45
1:H:344:GLY:HA2	6:H:1027:HOH:O	2.16	0.45
1:E:118:THR:O	1:E:122:GLY:HA3	2.16	0.45
2:I:8:ASN:HB2	2:I:131:ASP:HA	1.97	0.45
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.50	0.45
1:B:184:ASN:HD22	2:L:115:GLN:NE2	2.07	0.45
1:B:184:ASN:ND2	2:L:115:GLN:HE21	2.07	0.45
1:C:295:ARG:O	1:C:296:ALA:C	2.54	0.45
1:D:140:ILE:HG22	1:D:145:VAL:HG23	1.99	0.45
1:C:173:THR:HB	1:C:175:LYS:HE2	1.99	0.45
1:D:201:KCX:HB2	1:D:239:TYR:CD2	2.52	0.45
1:C:431:ARG:HE	1:C:432:ASN:HD22	1.65	0.45
1:C:158:GLU:OE2	1:C:325:HIS:NE2	2.26	0.45
2:N:48:ASP:OD1	2:N:48:ASP:N	2.50	0.45
1:G:170:LEU:HB3	1:G:197:LEU:HD23	1.98	0.45
2:N:8:ASN:HB2	2:N:131:ASP:HA	1.98	0.45
1:H:184:ASN:ND2	2:J:115:GLN:HE21	1.98	0.45
1:C:200:THR:O	1:C:238:HIS:HA	2.17	0.45
1:E:107:LEU:HD13	1:F:178:LEU:HD12	1.99	0.45
1:E:177:LYS:HB2	1:F:62:SER:O	2.17	0.45
1:D:203:ASP:HB2	6:D:1014:HOH:O	2.17	0.45
2:I:3:VAL:HG22	2:O:77:LYS:H	1.82	0.45
1:C:451:TRP:HH2	2:K:135:ALA:HB1	1.82	0.45
1:B:40:PHE:HB3	1:B:133:LEU:HD11	1.99	0.45
1:E:169:LEU:HD12	1:E:375:MET:HE1	1.98	0.44
1:D:302:ASP:HB2	6:D:1031:HOH:O	2.17	0.44
1:B:288:GLY:O	2:J:66:LEU:HD12	2.17	0.44
2:P:73:TRP:CZ3	2:P:106:ARG:HG2	2.52	0.44
2:L:8:ASN:HB2	2:L:131:ASP:HA	1.98	0.44
1:C:244:ALA:HA	6:C:1029:HOH:O	2.17	0.44
1:D:269:TYR:CD2	1:D:318:LEU:HD23	2.52	0.44
2:J:77:LYS:HE2	2:P:1:MME:O	2.17	0.44
2:M:127:LYS:HA	2:M:127:LYS:HD2	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:O	1:B:238:HIS:HA	2.16	0.44
1:E:161:LYS:HB3	2:M:66:LEU:HD22	1.99	0.44
1:C:175:LYS:HA	1:C:176:PRO:C	2.37	0.44
1:B:165:TYR:CD1	2:J:117:GLN:HB3	2.52	0.44
6:E:1021:HOH:O	2:K:71:ARG:HD2	2.17	0.44
2:P:118:ILE:HG13	2:P:118:ILE:O	2.18	0.44
1:H:181:SER:H	2:J:115:GLN:NE2	2.16	0.44
1:H:202:ASP:OD1	1:H:238:HIS:CE1	2.64	0.44
1:B:293:ILE:HG13	1:B:318:LEU:HD21	2.00	0.44
1:F:318:LEU:HG	1:F:326:LEU:HD13	1.99	0.44
1:C:177:LYS:HB2	1:D:62:SER:O	2.18	0.44
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.64	0.44
1:F:394:PHE:HB3	1:F:398:ALA:HB2	2.00	0.44
1:B:296:ALA:O	1:B:297:MET:CB	2.65	0.44
1:B:139:ARG:C	1:B:139:ARG:HD2	2.38	0.44
1:C:49:PRO:HA	1:C:50:PRO:HD2	1.79	0.44
1:C:61:SER:HG	1:C:103:TYR:HE1	1.65	0.44
1:G:214:TRP:O	1:G:218:PHE:CD1	2.71	0.44
1:B:161:LYS:HB3	2:J:66:LEU:HD22	1.99	0.44
1:F:195:GLY:HA3	1:F:417:ALA:HB3	2.00	0.44
2:K:8:ASN:HB2	2:K:131:ASP:HA	1.98	0.44
1:E:134:ARG:HA	1:E:308:GLY:O	2.18	0.44
1:B:49:PRO:HA	1:B:50:PRO:HD2	1.76	0.44
2:P:22:THR:H	2:P:25:GLN:NE2	2.13	0.43
2:M:73:TRP:CE3	2:M:106:ARG:HG2	2.53	0.43
1:B:171:GLY:HA2	1:B:199:PHE:O	2.18	0.43
1:F:241:ASN:ND2	1:F:243:THR:OG1	2.47	0.43
1:D:169:LEU:HD12	1:D:375:MET:HE1	2.00	0.43
1:A:19:ASP:HB3	1:A:21:ARG:HG2	1.99	0.43
1:F:140:ILE:HG22	1:F:145:VAL:HG23	1.99	0.43
1:A:225:ILE:HD11	1:A:238:HIS:HB3	2.01	0.43
1:F:206:VAL:C	1:F:207:ASN:HD22	2.22	0.43
1:D:177:LYS:HG2	1:D:203:ASP:OD2	2.19	0.43
1:A:121:VAL:HG23	1:B:297:MET:HG3	2.00	0.43
1:G:241:ASN:ND2	1:G:243:THR:H	2.17	0.43
1:C:229:GLN:HE21	1:C:236:LYS:H	1.65	0.43
1:G:171:GLY:HA2	1:G:199:PHE:O	2.18	0.43
1:C:19:ASP:HB3	1:C:21:ARG:HG2	2.00	0.43
2:N:73:TRP:CZ3	2:N:106:ARG:HG2	2.54	0.43
1:A:177:LYS:HG2	1:A:203:ASP:OD2	2.18	0.43
2:K:102:ASP:O	2:K:126:PRO:HB3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:SER:O	1:F:177:LYS:HB2	2.18	0.43
1:D:457:ALA:O	1:D:461:VAL:HG23	2.18	0.43
1:F:169:LEU:HD12	1:F:375:MET:HE3	2.00	0.43
2:N:118:ILE:HG13	2:N:118:ILE:O	2.18	0.43
1:G:293:ILE:HG13	1:G:318:LEU:HD21	2.00	0.43
1:G:258:LYS:HE3	2:O:62:SER:HB3	2.01	0.43
1:H:389:ALA:O	1:H:393:ILE:HG13	2.19	0.43
1:C:259:GLU:HB3	2:I:63:VAL:HG21	2.01	0.43
1:C:225:ILE:HD11	1:C:238:HIS:HB3	2.01	0.42
2:P:18:LEU:HB3	2:P:19:PRO:HD2	2.00	0.42
1:E:295:ARG:O	1:E:296:ALA:C	2.56	0.42
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.54	0.42
1:A:49:PRO:HA	1:A:50:PRO:HD2	1.74	0.42
1:D:49:PRO:HA	1:D:50:PRO:HD2	1.70	0.42
1:G:134:ARG:HA	1:G:308:GLY:O	2.19	0.42
1:E:185:TYR:OH	1:E:202:ASP:HA	2.19	0.42
1:H:425:GLU:OE1	2:P:17:TYR:HB2	2.18	0.42
1:G:20:TYR:CD1	5:G:1473:EDO:H21	2.54	0.42
1:E:110:GLU:HB3	1:E:147:THR:HB	2.01	0.42
1:G:451:TRP:HH2	2:O:135:ALA:HB1	1.84	0.42
1:E:394:PHE:HB3	1:E:398:ALA:HB2	2.01	0.42
1:F:295:ARG:O	1:F:296:ALA:C	2.55	0.42
1:H:49:PRO:HA	1:H:50:PRO:HD2	1.71	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.20	0.42
1:C:134:ARG:HA	1:C:308:GLY:O	2.19	0.42
1:G:175:LYS:HA	1:G:176:PRO:C	2.40	0.42
1:C:241:ASN:ND2	1:C:243:THR:H	2.18	0.42
1:G:190:TYR:CZ	1:G:194:ARG:HD3	2.55	0.42
1:H:206:VAL:C	1:H:207:ASN:HD22	2.22	0.42
1:F:197:LEU:HG	1:F:417:ALA:HB1	2.01	0.42
1:H:304:GLN:HA	1:H:304:GLN:HE21	1.84	0.42
1:A:134:ARG:HA	1:A:308:GLY:O	2.19	0.42
2:J:118:ILE:O	2:J:118:ILE:HG13	2.19	0.42
1:E:435:ARG:HD2	1:E:440:GLU:OE1	2.19	0.42
1:F:431:ARG:HH21	1:F:432:ASN:HD21	1.68	0.42
1:D:158:GLU:CD	1:D:325:HIS:HE2	2.14	0.42
1:G:185:TYR:OH	1:G:202:ASP:HA	2.19	0.42
1:C:304:GLN:HE21	1:C:304:GLN:HA	1.81	0.42
1:C:330:THR:O	1:C:331:VAL:HB	2.20	0.42
1:G:297:MET:HG3	1:H:121:VAL:HG23	2.01	0.42
1:H:292:HIS:HE1	1:H:377:VAL:HG21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:377:VAL:HG22	1:H:399:CYS:HB3	2.01	0.42
1:D:200:THR:OG1	1:D:238:HIS:CD2	2.69	0.42
1:A:185:TYR:OH	1:A:202:ASP:HA	2.20	0.42
1:F:290:LEU:HG	2:N:66:LEU:HD11	2.02	0.42
1:C:66:TRP:CE2	1:C:67:THR:HG22	2.55	0.42
1:D:168:GLY:HA2	1:D:396:ASP:O	2.20	0.42
1:F:134:ARG:HA	1:F:308:GLY:O	2.20	0.42
1:E:241:ASN:HA	1:E:266:MET:HG3	2.01	0.42
1:B:140:ILE:HG22	1:B:145:VAL:HG23	2.01	0.42
1:F:190:TYR:CZ	1:F:194:ARG:HD3	2.54	0.42
1:C:153:HIS:HE1	6:C:1038:HOH:O	2.01	0.42
1:A:285:ARG:HD2	6:A:1034:HOH:O	2.20	0.42
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.67	0.42
1:E:180:LEU:HA	2:K:115:GLN:HE22	1.84	0.41
1:H:161:LYS:CD	2:P:66:LEU:HD13	2.50	0.41
1:D:110:GLU:HB3	1:D:147:THR:HB	2.02	0.41
1:B:173:THR:HB	1:B:175:LYS:HE2	2.01	0.41
1:B:451:TRP:CZ2	2:J:19:PRO:HG3	2.55	0.41
2:L:127:LYS:HD2	2:L:127:LYS:HA	1.69	0.41
2:P:5:THR:HG22	2:P:138:ARG:O	2.20	0.41
1:G:50:PRO:HG3	1:G:97:TYR:CZ	2.55	0.41
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.69	0.41
1:G:310:HIS:CE1	1:G:312:ARG:NH2	2.88	0.41
1:D:153:HIS:CD2	1:D:290:LEU:HD23	2.55	0.41
1:F:181:SER:H	2:P:115:GLN:HE22	1.68	0.41
1:D:266:MET:HA	1:D:292:HIS:O	2.20	0.41
1:B:269:TYR:CE2	1:B:318:LEU:HB2	2.55	0.41
5:G:1472:EDO:H21	5:G:1473:EDO:H22	2.01	0.41
1:F:349:MET:HE1	1:F:376:PRO:HA	2.02	0.41
2:M:8:ASN:HB2	2:M:131:ASP:HA	2.02	0.41
2:N:107:LEU:O	2:N:120:GLY:HA2	2.20	0.41
2:I:127:LYS:HA	2:I:127:LYS:HD2	1.78	0.41
1:D:181:SER:H	2:N:115:GLN:NE2	2.18	0.41
1:D:239:TYR:HB3	1:D:266:MET:HB3	2.03	0.41
1:H:77:LEU:HA	1:H:77:LEU:HD12	1.80	0.41
1:C:203:ASP:HB2	6:C:1025:HOH:O	2.18	0.41
1:D:425:GLU:OE1	2:L:17:TYR:HB2	2.21	0.41
1:F:49:PRO:HA	1:F:50:PRO:HD2	1.75	0.41
1:F:208:SER:HB2	1:F:214:TRP:HB3	2.02	0.41
1:E:18:LYS:HD3	6:E:1001:HOH:O	2.19	0.41
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:48:ASP:N	2:K:48:ASP:OD1	2.54	0.41
1:E:20:TYR:CD1	5:E:1473:EDO:H22	2.55	0.41
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.69	0.41
2:K:11:MET:HG3	2:K:17:TYR:CE1	2.56	0.41
1:G:302:ASP:HB2	6:G:1036:HOH:O	2.21	0.41
1:E:258:LYS:HA	2:M:65:CYS:SG	2.61	0.41
1:B:295:ARG:O	1:B:296:ALA:C	2.59	0.41
1:C:223:GLU:OE2	2:I:71:ARG:HB2	2.21	0.41
2:P:75:MET:SD	2:P:79:PRO:HD3	2.61	0.41
1:B:383:HIS:H	1:B:386:HIS:CD2	2.29	0.41
1:B:379:SER:HB2	1:B:401:GLN:HB2	2.03	0.41
1:H:290:LEU:HG	2:P:66:LEU:CD1	2.50	0.41
1:H:151:HYP:HB2	1:H:323:GLY:O	2.20	0.41
1:A:133:LEU:O	1:A:307:HIS:HA	2.21	0.41
1:F:151:HYP:HA	1:F:152:PRO:HD3	1.99	0.41
1:H:239:TYR:HB3	1:H:266:MET:HB3	2.02	0.41
1:H:258:LYS:HA	2:P:65:CYS:SG	2.60	0.41
1:A:177:LYS:HB2	1:B:62:SER:O	2.20	0.41
2:N:11:MET:HG3	2:N:17:TYR:CE1	2.56	0.41
2:I:39:ILE:O	2:I:109:ALA:HA	2.20	0.41
1:H:368:TRP:O	1:H:369:SMC:C	2.68	0.41
1:C:166:GLY:HA2	2:K:118:ILE:O	2.20	0.41
1:C:171:GLY:HA2	1:C:199:PHE:O	2.21	0.41
1:A:202:ASP:OD1	1:A:238:HIS:CE1	2.64	0.41
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.19	0.41
1:B:262:VAL:HB	6:B:1019:HOH:O	2.21	0.41
1:A:171:GLY:HA3	1:A:401:GLN:HG2	2.02	0.40
1:A:304:GLN:HE21	1:A:304:GLN:HA	1.86	0.40
1:H:440:GLU:O	1:H:444:VAL:HG23	2.21	0.40
1:A:296:ALA:O	1:A:297:MET:CB	2.69	0.40
6:G:1044:HOH:O	2:O:114:LYS:HE2	2.21	0.40
1:H:292:HIS:CE1	1:H:377:VAL:HG21	2.56	0.40
1:F:451:TRP:HH2	2:N:135:ALA:HB1	1.87	0.40
1:G:349:MET:HE1	1:G:376:PRO:HA	2.02	0.40
1:C:161:LYS:HB3	2:K:66:LEU:HD22	2.02	0.40
2:K:22:THR:H	2:K:25:GLN:NE2	2.09	0.40
1:D:185:TYR:OH	1:D:202:ASP:HA	2.21	0.40
1:E:177:LYS:HG2	1:E:203:ASP:OD2	2.21	0.40
2:M:13:GLU:HB3	2:M:14:THR:H	1.70	0.40
1:E:49:PRO:HA	1:E:50:PRO:HD2	1.79	0.40
1:G:440:GLU:O	1:G:444:VAL:HG23	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:VAL:HG11	1:H:274:PHE:CE1	2.56	0.40
1:F:203:ASP:HB2	6:F:1016:HOH:O	2.21	0.40
1:G:256:SMC:HB3	5:G:1474:EDO:H21	2.04	0.40
2:J:48:ASP:N	2:J:48:ASP:OD1	2.54	0.40
2:P:8:ASN:HB2	2:P:131:ASP:HA	2.02	0.40
1:C:166:GLY:HA3	2:K:119:MET:HA	2.03	0.40
1:A:157:VAL:HG23	6:A:1014:HOH:O	2.21	0.40
1:B:339:ARG:HD2	6:B:1024:HOH:O	2.21	0.40
1:E:163:ASN:HD22	1:E:163:ASN:HA	1.74	0.40
1:B:203:ASP:HB2	6:B:1009:HOH:O	2.20	0.40
1:E:269:TYR:CE2	1:E:318:LEU:HB2	2.57	0.40
1:B:387:MET:O	1:B:391:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/475 (95%)	432 (96%)	20 (4%)	0	100	100
1	B	453/475 (95%)	430 (95%)	22 (5%)	1 (0%)	52	84
1	C	452/475 (95%)	433 (96%)	19 (4%)	0	100	100
1	D	457/475 (96%)	430 (94%)	25 (6%)	2 (0%)	39	74
1	E	452/475 (95%)	431 (95%)	21 (5%)	0	100	100
1	F	454/475 (96%)	434 (96%)	19 (4%)	1 (0%)	52	84
1	G	454/475 (96%)	429 (94%)	25 (6%)	0	100	100
1	H	451/475 (95%)	431 (96%)	20 (4%)	0	100	100
2	I	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	26	62
2	J	138/140 (99%)	123 (89%)	14 (10%)	1 (1%)	26	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
2	L	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	26	62
2	M	138/140 (99%)	119 (86%)	18 (13%)	1 (1%)	26	62
2	N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	14	42
2	O	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	26	62
2	P	138/140 (99%)	123 (89%)	14 (10%)	1 (1%)	26	62
All	All	4729/4920 (96%)	4443 (94%)	274 (6%)	12 (0%)	46	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	10	GLY
2	M	49	LYS
1	D	470	ASP
2	J	49	LYS
2	N	83	CYS
2	O	49	LYS
2	P	49	LYS
2	I	49	LYS
2	L	49	LYS
1	B	405	GLY
1	D	471	THR
2	N	49	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/376 (96%)	351 (97%)	11 (3%)	48	82
1	B	362/376 (96%)	352 (97%)	10 (3%)	51	84
1	C	363/376 (96%)	350 (96%)	13 (4%)	42	76
1	D	367/376 (98%)	357 (97%)	10 (3%)	52	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	362/376 (96%)	352 (97%)	10 (3%)	51	84
1	F	362/376 (96%)	353 (98%)	9 (2%)	55	86
1	G	362/376 (96%)	349 (96%)	13 (4%)	42	76
1	H	362/376 (96%)	355 (98%)	7 (2%)	65	91
2	I	122/122 (100%)	113 (93%)	9 (7%)	17	43
2	J	122/122 (100%)	113 (93%)	9 (7%)	17	43
2	K	122/122 (100%)	111 (91%)	11 (9%)	12	34
2	L	122/122 (100%)	114 (93%)	8 (7%)	21	51
2	M	122/122 (100%)	113 (93%)	9 (7%)	17	43
2	N	122/122 (100%)	111 (91%)	11 (9%)	12	34
2	O	122/122 (100%)	113 (93%)	9 (7%)	17	43
2	P	122/122 (100%)	114 (93%)	8 (7%)	21	51
All	All	3878/3984 (97%)	3721 (96%)	157 (4%)	38	73

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	71	THR
1	A	131	ARG
1	A	134	ARG
1	A	241	ASN
1	A	252	LYS
1	A	259	GLU
1	A	336	GLU
1	A	341	VAL
1	A	345	PHE
1	A	451	TRP
1	B	14	LYS
1	B	134	ARG
1	B	204	GLU
1	B	241	ASN
1	B	252	LYS
1	B	259	GLU
1	B	269	TYR
1	B	336	GLU
1	B	345	PHE
1	B	451	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	14	LYS
1	C	71	THR
1	C	131	ARG
1	C	203	ASP
1	C	219	LEU
1	C	241	ASN
1	C	252	LYS
1	C	259	GLU
1	C	336	GLU
1	C	341	VAL
1	C	345	PHE
1	C	451	TRP
1	C	470	ASP
1	D	14	LYS
1	D	134	ARG
1	D	203	ASP
1	D	241	ASN
1	D	252	LYS
1	D	259	GLU
1	D	336	GLU
1	D	341	VAL
1	D	345	PHE
1	D	474	LYS
1	E	14	LYS
1	E	131	ARG
1	E	134	ARG
1	E	163	ASN
1	E	239	TYR
1	E	241	ASN
1	E	252	LYS
1	E	259	GLU
1	E	336	GLU
1	E	341	VAL
1	F	14	LYS
1	F	131	ARG
1	F	203	ASP
1	F	219	LEU
1	F	241	ASN
1	F	252	LYS
1	F	259	GLU
1	F	336	GLU
1	F	451	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	14	LYS
1	G	131	ARG
1	G	134	ARG
1	G	163	ASN
1	G	203	ASP
1	G	239	TYR
1	G	241	ASN
1	G	252	LYS
1	G	259	GLU
1	G	336	GLU
1	G	341	VAL
1	G	345	PHE
1	G	451	TRP
1	H	14	LYS
1	H	131	ARG
1	H	241	ASN
1	H	252	LYS
1	H	259	GLU
1	H	336	GLU
1	H	341	VAL
2	I	8	ASN
2	I	9	ASN
2	I	12	PHE
2	I	48	ASP
2	I	54	ASN
2	I	84	ARG
2	I	98	LYS
2	I	102	ASP
2	I	127	LYS
2	J	8	ASN
2	J	9	ASN
2	J	12	PHE
2	J	48	ASP
2	J	54	ASN
2	J	84	ARG
2	J	98	LYS
2	J	102	ASP
2	J	127	LYS
2	K	8	ASN
2	K	9	ASN
2	K	12	PHE
2	K	48	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	52	VAL
2	K	54	ASN
2	K	62	SER
2	K	84	ARG
2	K	98	LYS
2	K	102	ASP
2	K	127	LYS
2	L	8	ASN
2	L	9	ASN
2	L	12	PHE
2	L	48	ASP
2	L	54	ASN
2	L	84	ARG
2	L	102	ASP
2	L	127	LYS
2	M	8	ASN
2	M	9	ASN
2	M	48	ASP
2	M	52	VAL
2	M	54	ASN
2	M	84	ARG
2	M	98	LYS
2	M	102	ASP
2	M	127	LYS
2	N	8	ASN
2	N	9	ASN
2	N	12	PHE
2	N	46	GLU
2	N	48	ASP
2	N	52	VAL
2	N	54	ASN
2	N	84	ARG
2	N	98	LYS
2	N	102	ASP
2	N	127	LYS
2	O	8	ASN
2	O	9	ASN
2	O	12	PHE
2	O	48	ASP
2	O	52	VAL
2	O	54	ASN
2	O	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	102	ASP
2	O	127	LYS
2	P	8	ASN
2	P	9	ASN
2	P	12	PHE
2	P	48	ASP
2	P	54	ASN
2	P	84	ARG
2	P	102	ASP
2	P	127	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	207	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	207	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	420	ASN
1	B	432	ASN
1	C	153	HIS
1	C	163	ASN
1	C	229	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	386	HIS
1	C	401	GLN
1	C	432	ASN
1	D	153	HIS
1	D	163	ASN
1	D	207	ASN
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	267	HIS
1	D	304	GLN
1	D	386	HIS
1	D	432	ASN
1	E	153	HIS
1	E	163	ASN
1	E	207	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	432	ASN
1	F	153	HIS
1	F	163	ASN
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	287	ASN
1	F	304	GLN
1	F	386	HIS
1	F	401	GLN
1	F	432	ASN
1	G	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	163	ASN
1	G	207	ASN
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	386	HIS
1	G	401	GLN
1	G	432	ASN
1	H	153	HIS
1	H	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	420	ASN
1	H	432	ASN
2	I	9	ASN
2	I	25	GLN
2	I	29	GLN
2	I	115	GLN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	115	GLN
2	K	9	ASN
2	K	25	GLN
2	K	29	GLN
2	K	115	GLN
2	L	9	ASN
2	L	25	GLN
2	L	29	GLN
2	L	115	GLN
2	L	133	GLN
2	M	9	ASN
2	M	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	29	GLN
2	M	115	GLN
2	M	133	GLN
2	N	9	ASN
2	N	25	GLN
2	N	29	GLN
2	N	115	GLN
2	O	9	ASN
2	O	25	GLN
2	O	29	GLN
2	O	115	GLN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	115	GLN
2	P	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	HYP	A	104	1	7,8,9	0.72	0	5,10,12	1.60	2 (40%)
1	HYP	A	151	1	7,8,9	0.72	0	5,10,12	1.44	1 (20%)
1	KCX	A	201	1,3	7,11,12	0.75	0	7,12,14	0.95	0
1	SMC	A	256	1	5,6,7	0.52	0	2,6,8	1.84	0
1	SMC	A	369	1	5,6,7	0.47	0	2,6,8	1.23	0
1	HYP	B	104	1	7,8,9	0.59	0	5,10,12	1.75	2 (40%)
1	HYP	B	151	1	7,8,9	0.71	0	5,10,12	1.73	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	201	1,3	7,11,12	0.82	0	7,12,14	1.04	0
1	SMC	B	256	1	5,6,7	0.71	0	2,6,8	1.47	0
1	SMC	B	369	1	5,6,7	0.60	0	2,6,8	1.41	0
1	HYP	C	104	1	7,8,9	0.73	0	5,10,12	1.79	2 (40%)
1	HYP	C	151	1	7,8,9	0.95	1 (14%)	5,10,12	1.89	2 (40%)
1	KCX	C	201	1,3	7,11,12	1.46	1 (14%)	7,12,14	1.15	0
1	SMC	C	256	1	5,6,7	0.53	0	2,6,8	1.78	0
1	SMC	C	369	1	5,6,7	0.51	0	2,6,8	1.46	0
1	HYP	D	104	1	7,8,9	0.53	0	5,10,12	1.68	2 (40%)
1	HYP	D	151	1	7,8,9	0.99	0	5,10,12	1.37	0
1	KCX	D	201	1,3	7,11,12	0.77	0	7,12,14	0.77	0
1	SMC	D	256	1	5,6,7	1.06	1 (20%)	2,6,8	1.27	0
1	SMC	D	369	1	5,6,7	0.83	0	2,6,8	1.62	1 (50%)
1	HYP	E	104	1	7,8,9	0.72	0	5,10,12	1.57	1 (20%)
1	HYP	E	151	1	7,8,9	1.22	1 (14%)	5,10,12	1.56	2 (40%)
1	KCX	E	201	1,3	7,11,12	0.65	0	7,12,14	0.72	0
1	SMC	E	256	1	5,6,7	0.56	0	2,6,8	2.98	2 (100%)
1	SMC	E	369	1	5,6,7	0.89	0	2,6,8	2.91	1 (50%)
1	HYP	F	104	1	7,8,9	0.74	0	5,10,12	1.46	0
1	HYP	F	151	1	7,8,9	0.84	0	5,10,12	1.22	0
1	KCX	F	201	1,3	7,11,12	0.75	0	7,12,14	1.10	0
1	SMC	F	256	1	5,6,7	0.64	0	2,6,8	1.46	0
1	SMC	F	369	1	5,6,7	0.86	0	2,6,8	1.69	1 (50%)
1	HYP	G	104	1	7,8,9	0.95	0	5,10,12	1.13	1 (20%)
1	HYP	G	151	1	7,8,9	0.78	0	5,10,12	1.29	1 (20%)
1	KCX	G	201	1,3	7,11,12	0.67	0	7,12,14	1.42	1 (14%)
1	SMC	G	256	1	5,6,7	0.76	0	2,6,8	1.60	0
1	SMC	G	369	1	5,6,7	0.97	0	2,6,8	1.79	1 (50%)
1	HYP	H	104	1	7,8,9	0.65	0	5,10,12	1.53	2 (40%)
1	HYP	H	151	1	7,8,9	0.72	0	5,10,12	1.42	1 (20%)
1	KCX	H	201	1,3	7,11,12	0.89	0	7,12,14	1.51	1 (14%)
1	SMC	H	256	1	5,6,7	0.55	0	2,6,8	1.63	0
1	SMC	H	369	1	5,6,7	0.62	0	2,6,8	1.42	0
2	MME	I	1	2	7,8,9	2.83	2 (28%)	4,8,10	1.14	0
2	MME	J	1	2	7,8,9	2.77	2 (28%)	4,8,10	1.10	0
2	MME	K	1	2	7,8,9	2.77	1 (14%)	4,8,10	1.12	0
2	MME	L	1	2	7,8,9	2.85	2 (28%)	4,8,10	1.23	0
2	MME	M	1	2	7,8,9	2.82	2 (28%)	4,8,10	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MME	N	1	2	7,8,9	2.76	2 (28%)	4,8,10	1.25	1 (25%)
2	MME	O	1	2	7,8,9	2.80	2 (28%)	4,8,10	1.44	0
2	MME	P	1	2	7,8,9	2.76	2 (28%)	4,8,10	1.23	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	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	KCX	C	201	1,3	-	0/6/10/12	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
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	KCX	D	201	1,3	-	0/6/10/12	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	1,3	-	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	F	104	1	-	0/0/11/13	0/1/1/1
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	1,3	-	0/6/10/12	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	201	1,3	-	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	1,3	-	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
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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	MME	CM-N	-7.03	1.27	1.46
2	M	1	MME	CM-N	-7.01	1.27	1.46
2	K	1	MME	CM-N	-6.96	1.27	1.46
2	I	1	MME	CM-N	-6.96	1.27	1.46
2	O	1	MME	CM-N	-6.94	1.27	1.46
2	J	1	MME	CM-N	-6.93	1.27	1.46
2	P	1	MME	CM-N	-6.78	1.27	1.46
2	N	1	MME	CM-N	-6.72	1.28	1.46
1	C	201	KCX	CB-CA	-3.15	1.50	1.53
1	E	151	HYP	CA-N	-2.10	1.44	1.47
1	C	151	HYP	CA-N	-2.07	1.44	1.47
2	J	1	MME	CA-N	2.02	1.51	1.47
1	D	256	SMC	CB-SG	2.13	1.83	1.80
2	M	1	MME	CA-N	2.18	1.51	1.47
2	O	1	MME	CA-N	2.24	1.51	1.47
2	L	1	MME	CA-N	2.35	1.51	1.47
2	P	1	MME	CA-N	2.40	1.51	1.47
2	I	1	MME	CA-N	2.41	1.51	1.47
2	N	1	MME	CA-N	2.62	1.52	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	369	SMC	CS-SG-CB	-3.83	94.98	101.21
1	H	201	KCX	CE-NZ-CX	-3.56	119.46	123.49
1	C	104	HYP	OD1-CG-CB	-3.24	101.31	110.00
1	G	201	KCX	CE-NZ-CX	-3.21	119.85	123.49
1	C	151	HYP	CB-CG-CD	-2.83	99.63	103.14
1	H	104	HYP	OD1-CG-CB	-2.69	102.79	110.00
1	A	104	HYP	OD1-CG-CB	-2.48	103.35	110.00
1	F	369	SMC	O-C-CA	-2.29	119.53	125.49
1	D	369	SMC	O-C-CA	-2.28	119.55	125.49
1	G	151	HYP	O-C-CA	-2.25	119.51	125.44
1	E	256	SMC	O-C-CA	-2.24	119.64	125.49
1	B	151	HYP	OD1-CG-CB	-2.24	104.00	110.00
1	A	151	HYP	O-C-CA	-2.23	119.54	125.44
1	D	104	HYP	O-C-CA	-2.23	119.55	125.44
1	B	151	HYP	O-C-CA	-2.21	119.60	125.44
1	H	151	HYP	O-C-CA	-2.19	119.66	125.44
1	A	104	HYP	O-C-CA	-2.10	119.90	125.44
1	E	151	HYP	CB-CG-CD	-2.09	100.55	103.14
1	G	104	HYP	O-C-CA	-2.05	120.02	125.44
1	C	151	HYP	O-C-CA	-2.05	120.02	125.44
1	E	151	HYP	O-C-CA	-2.04	120.06	125.44
1	B	104	HYP	OD1-CG-CB	-2.02	104.58	110.00
1	C	104	HYP	O-C-CA	-2.02	120.11	125.44
2	N	1	MME	O-C-CA	-2.02	120.11	125.44
1	G	369	SMC	O-C-CA	-2.02	120.24	125.49
1	H	104	HYP	O-C-CA	-2.02	120.12	125.44
1	D	104	HYP	CB-CG-CD	2.14	105.79	103.14
1	E	104	HYP	CB-CG-CD	2.17	105.82	103.14
1	B	104	HYP	CB-CG-CD	2.72	106.50	103.14
1	E	256	SMC	CS-SG-CB	3.57	107.02	101.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	KCX	1	0
1	B	201	KCX	1	0
1	B	369	SMC	1	0
1	C	201	KCX	1	0
1	D	151	HYP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	201	KCX	1	0
1	F	151	HYP	1	0
1	F	201	KCX	1	0
1	G	151	HYP	1	0
1	G	201	KCX	1	0
1	G	256	SMC	1	0
1	H	151	HYP	1	0
1	H	201	KCX	1	0
1	H	369	SMC	1	0
2	P	1	MME	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CAP	A	1471	3	14,20,20	0.95	1 (7%)	15,31,31	1.14	1 (6%)
5	EDO	A	1472	-	3,3,3	0.52	0	2,2,2	0.40	0
5	EDO	A	1473	-	3,3,3	0.60	0	2,2,2	0.16	0
5	EDO	A	1474	-	3,3,3	0.53	0	2,2,2	0.43	0
4	CAP	B	1471	3	14,20,20	1.07	2 (14%)	15,31,31	1.17	1 (6%)
5	EDO	B	1472	-	3,3,3	0.64	0	2,2,2	0.13	0
5	EDO	B	1473	-	3,3,3	0.57	0	2,2,2	0.35	0
4	CAP	C	1472	3	14,20,20	0.82	0	15,31,31	1.23	1 (6%)
5	EDO	C	1473	-	3,3,3	0.65	0	2,2,2	0.10	0
5	EDO	C	1474	-	3,3,3	0.49	0	2,2,2	0.28	0
5	EDO	C	1475	-	3,3,3	0.54	0	2,2,2	0.31	0
4	CAP	D	1476	3	14,20,20	0.96	1 (7%)	15,31,31	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	1477	-	3,3,3	0.60	0	2,2,2	0.28	0
5	EDO	D	1478	-	3,3,3	0.53	0	2,2,2	0.68	0
5	EDO	D	1479	-	3,3,3	0.66	0	2,2,2	0.56	0
4	CAP	E	1471	3	14,20,20	0.84	0	15,31,31	1.49	3 (20%)
5	EDO	E	1472	-	3,3,3	0.68	0	2,2,2	0.06	0
5	EDO	E	1473	-	3,3,3	0.55	0	2,2,2	0.04	0
5	EDO	E	1474	-	3,3,3	0.42	0	2,2,2	0.77	0
5	EDO	E	1475	-	3,3,3	0.43	0	2,2,2	0.75	0
4	CAP	F	1471	3	14,20,20	0.88	1 (7%)	15,31,31	1.02	0
5	EDO	F	1472	-	3,3,3	0.54	0	2,2,2	0.39	0
5	EDO	F	1473	-	3,3,3	0.60	0	2,2,2	0.08	0
4	CAP	G	1471	3	14,20,20	0.84	1 (7%)	15,31,31	1.34	2 (13%)
5	EDO	G	1472	-	3,3,3	0.49	0	2,2,2	0.59	0
5	EDO	G	1473	-	3,3,3	0.50	0	2,2,2	0.27	0
5	EDO	G	1474	-	3,3,3	0.73	0	2,2,2	0.11	0
4	CAP	H	1471	3	14,20,20	0.92	1 (7%)	15,31,31	0.97	0
5	EDO	H	1472	-	3,3,3	0.53	0	2,2,2	0.25	0
5	EDO	H	1473	-	3,3,3	0.55	0	2,2,2	0.37	0
5	EDO	H	1474	-	3,3,3	0.36	0	2,2,2	0.88	0
5	EDO	H	1475	-	3,3,3	0.56	0	2,2,2	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	A	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	A	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1473	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1474	-	-	0/1/1/1	0/0/0/0
4	CAP	B	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	B	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1473	-	-	0/1/1/1	0/0/0/0
4	CAP	C	1472	3	-	0/23/29/29	0/0/0/0
5	EDO	C	1473	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1474	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1475	-	-	0/1/1/1	0/0/0/0
4	CAP	D	1476	3	-	0/23/29/29	0/0/0/0
5	EDO	D	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1479	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	E	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	E	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1473	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1474	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1475	-	-	0/1/1/1	0/0/0/0
4	CAP	F	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	F	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	F	1473	-	-	0/1/1/1	0/0/0/0
4	CAP	G	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	G	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1473	-	-	0/1/1/1	0/0/0/0
5	EDO	G	1474	-	-	0/1/1/1	0/0/0/0
4	CAP	H	1471	3	-	0/23/29/29	0/0/0/0
5	EDO	H	1472	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1473	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1474	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1475	-	-	0/1/1/1	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1471	CAP	O2-C2	2.04	1.45	1.43
4	H	1471	CAP	O2-C2	2.05	1.45	1.43
4	F	1471	CAP	O2-C2	2.16	1.46	1.43
4	B	1471	CAP	C5-C4	2.21	1.55	1.51
4	A	1471	CAP	O2-C2	2.27	1.46	1.43
4	D	1476	CAP	O2-C2	2.52	1.46	1.43
4	B	1471	CAP	O2-C2	2.78	1.46	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1472	CAP	O6P-P2-O4P	-2.50	102.52	110.58
4	E	1471	CAP	O6P-P2-O4P	-2.27	103.26	110.58
4	A	1471	CAP	O6P-P2-O4P	-2.27	103.28	110.58
4	D	1476	CAP	O4-C4-C5	-2.11	105.59	110.19
4	E	1471	CAP	O4-C4-C5	-2.08	105.67	110.19
4	B	1471	CAP	O6P-P2-O4P	-2.01	104.10	110.58
4	G	1471	CAP	O3P-P1-O1	2.22	112.97	106.56
4	G	1471	CAP	O3-C3-C4	2.63	114.55	108.91
4	E	1471	CAP	O3P-P1-O1	2.79	114.59	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1473	EDO	1	0
5	C	1473	EDO	2	0
5	C	1474	EDO	1	0
5	C	1475	EDO	2	0
5	E	1473	EDO	1	0
5	G	1472	EDO	1	0
5	G	1473	EDO	2	0
5	G	1474	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/475 (95%)	-0.42	9 (1%) 68 58	31, 52, 82, 90	0
1	B	455/475 (95%)	-0.47	9 (1%) 68 58	32, 52, 82, 90	0
1	C	454/475 (95%)	-0.49	7 (1%) 76 68	31, 52, 82, 91	0
1	D	459/475 (96%)	-0.53	7 (1%) 76 68	31, 52, 83, 98	0
1	E	454/475 (95%)	-0.52	7 (1%) 76 68	31, 52, 82, 90	0
1	F	456/475 (96%)	-0.44	7 (1%) 76 68	31, 52, 82, 90	0
1	G	456/475 (96%)	-0.42	6 (1%) 79 71	31, 52, 82, 90	0
1	H	453/475 (95%)	-0.51	5 (1%) 82 74	31, 52, 82, 90	0
2	I	139/140 (99%)	0.34	12 (8%) 13 6	57, 74, 99, 101	0
2	J	139/140 (99%)	0.43	15 (10%) 8 3	57, 74, 99, 101	0
2	K	139/140 (99%)	0.24	15 (10%) 8 3	56, 74, 99, 101	0
2	L	139/140 (99%)	0.48	20 (14%) 3 2	57, 74, 99, 101	0
2	M	139/140 (99%)	0.17	6 (4%) 39 27	57, 74, 99, 101	0
2	N	139/140 (99%)	0.09	8 (5%) 26 16	57, 74, 99, 101	0
2	O	139/140 (99%)	0.19	13 (9%) 11 5	57, 74, 99, 101	0
2	P	139/140 (99%)	0.12	4 (2%) 55 43	57, 74, 99, 101	0
All	All	4753/4920 (96%)	-0.30	150 (3%) 51 39	31, 57, 93, 101	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	10	GLY	6.2
2	L	128	THR	5.9
2	K	128	THR	5.3
1	B	10	GLY	5.3
2	I	130	ARG	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	128	THR	5.2
1	G	9	ALA	5.2
2	J	61	GLY	5.1
2	J	130	ARG	4.9
1	D	94	ASP	4.9
1	G	10	GLY	4.9
1	A	11	ALA	4.8
2	I	128	THR	4.8
2	J	135	ALA	4.7
2	J	136	ASN	4.6
1	C	94	ASP	4.5
2	L	130	ARG	4.5
2	M	130	ARG	4.2
2	J	137	LYS	4.2
1	F	9	ALA	4.2
2	J	84	ARG	4.1
2	K	136	ASN	4.0
1	D	11	ALA	4.0
2	K	130	ARG	4.0
2	K	84	ARG	4.0
1	F	11	ALA	4.0
1	C	470	ASP	3.8
2	P	130	ARG	3.8
2	J	127	LYS	3.7
2	O	134	PRO	3.7
2	L	84	ARG	3.6
1	G	94	ASP	3.6
1	H	94	ASP	3.4
2	K	134	PRO	3.4
2	N	53	SER	3.4
1	C	464	GLU	3.3
2	K	127	LYS	3.3
1	B	94	ASP	3.3
2	N	130	ARG	3.3
2	L	83	CYS	3.3
1	D	450	LYS	3.3
2	M	55	GLU	3.2
1	B	450	LYS	3.2
2	I	84	ARG	3.2
2	L	134	PRO	3.2
2	J	129	ALA	3.2
2	I	136	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	83	CYS	3.1
2	M	84	ARG	3.0
1	A	46	PRO	3.0
2	O	52	VAL	3.0
2	L	53	SER	3.0
1	A	14	LYS	3.0
1	E	11	ALA	2.9
2	L	54	ASN	2.9
1	H	450	LYS	2.9
2	L	135	ALA	2.9
1	A	94	ASP	2.9
2	L	137	LYS	2.9
1	E	47	GLY	2.9
2	J	62	SER	2.9
2	L	129	ALA	2.9
1	D	439	ARG	2.8
2	N	84	ARG	2.8
2	I	51	TYR	2.8
2	J	83	CYS	2.8
1	C	450	LYS	2.8
1	B	443	ASP	2.8
2	I	55	GLU	2.8
2	I	131	ASP	2.8
2	M	83	CYS	2.7
2	I	54	ASN	2.7
1	D	464	GLU	2.7
1	B	439	ARG	2.7
2	L	127	LYS	2.7
1	G	451	TRP	2.7
2	O	53	SER	2.7
2	P	55	GLU	2.6
2	P	84	ARG	2.6
1	G	450	LYS	2.6
1	D	443	ASP	2.6
1	G	11	ALA	2.6
2	I	134	PRO	2.6
2	J	134	PRO	2.6
1	A	28	ASP	2.6
1	F	451	TRP	2.6
2	L	136	ASN	2.6
1	E	94	ASP	2.6
2	L	51	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	7	VAL	2.6
1	B	468	GLU	2.5
1	F	468	GLU	2.5
1	B	11	ALA	2.5
2	J	51	TYR	2.5
1	C	28	ASP	2.5
1	F	94	ASP	2.5
1	H	464	GLU	2.5
2	K	135	ALA	2.5
2	N	98	LYS	2.5
1	A	29	TYR	2.5
1	B	47	GLY	2.4
2	K	137	LYS	2.4
2	K	62	SER	2.4
2	O	58	ILE	2.4
2	O	51	TYR	2.4
2	N	140	VAL	2.4
2	M	87	MET	2.4
2	O	130	ARG	2.4
2	K	56	SER	2.4
2	L	55	GLU	2.4
2	L	48	ASP	2.4
1	A	91	PRO	2.3
2	J	140	VAL	2.3
1	E	439	ARG	2.3
1	C	443	ASP	2.3
2	K	53	SER	2.3
2	O	84	ARG	2.3
2	M	48	ASP	2.3
1	E	46	PRO	2.3
1	E	92	GLY	2.3
1	H	47	GLY	2.3
2	I	129	ALA	2.2
2	L	131	ASP	2.2
1	A	442	GLY	2.2
2	K	58	ILE	2.2
2	J	48	ASP	2.2
2	O	136	ASN	2.2
2	O	65	CYS	2.2
2	O	55	GLU	2.2
1	C	451	TRP	2.2
1	A	47	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	450	LYS	2.1
2	K	82	GLY	2.1
2	I	61	GLY	2.1
1	H	305	ARG	2.1
2	O	137	LYS	2.1
2	L	82	GLY	2.1
2	K	48	ASP	2.1
2	L	23	ASP	2.1
1	E	468	GLU	2.1
2	L	91	ARG	2.1
2	O	83	CYS	2.0
2	N	56	SER	2.0
2	O	140	VAL	2.0
1	D	355	GLU	2.0
2	N	54	ASN	2.0
2	P	136	ASN	2.0
2	N	136	ASN	2.0
2	L	24	GLU	2.0
1	B	463	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SMC	A	369	7/8	0.98	0.09	-	48,49,51,52	0
1	SMC	A	256	7/8	0.98	0.09	-	34,36,37,37	0
1	SMC	G	256	7/8	0.99	0.10	-	34,36,37,37	0
1	SMC	H	369	7/8	0.98	0.08	-	48,49,51,52	0
1	HYP	A	104	8/9	0.97	0.09	-	45,45,46,47	0
1	HYP	C	104	8/9	0.98	0.14	-	45,45,45,46	0
2	MME	K	1	9/10	0.88	0.26	-	75,76,78,78	0
1	SMC	D	369	7/8	0.97	0.14	-	49,49,52,53	0
1	KCX	B	201	12/13	0.98	0.11	-	46,47,53,54	0
1	KCX	A	201	12/13	0.96	0.14	-	46,46,53,53	0
1	SMC	G	369	7/8	0.97	0.12	-	48,49,51,52	0
1	SMC	B	256	7/8	0.98	0.07	-	34,36,37,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SMC	E	369	7/8	0.97	0.10	-	48,49,52,52	0
1	HYP	D	104	8/9	0.96	0.11	-	45,46,46,47	0
1	KCX	D	201	12/13	0.97	0.13	-	46,46,52,53	0
1	HYP	B	104	8/9	0.97	0.10	-	45,45,46,47	0
2	MME	J	1	9/10	0.87	0.33	-	75,76,78,79	0
2	MME	I	1	9/10	0.88	0.35	-	75,76,78,78	0
1	SMC	H	256	7/8	0.99	0.10	-	33,36,37,37	0
1	HYP	G	151	8/9	0.95	0.10	-	37,38,39,39	0
1	SMC	F	369	7/8	0.98	0.14	-	48,49,51,52	0
1	HYP	B	151	8/9	0.97	0.10	-	37,38,38,38	0
1	KCX	C	201	12/13	0.97	0.14	-	45,46,53,53	0
1	HYP	F	151	8/9	0.98	0.08	-	37,38,38,39	0
1	SMC	E	256	7/8	0.98	0.09	-	33,36,37,37	0
1	HYP	E	104	8/9	0.97	0.09	-	45,46,46,47	0
1	HYP	H	151	8/9	0.98	0.10	-	36,38,38,38	0
1	HYP	C	151	8/9	0.98	0.09	-	37,38,38,38	0
1	HYP	A	151	8/9	0.99	0.09	-	37,38,38,38	0
1	SMC	F	256	7/8	0.98	0.09	-	34,36,37,37	0
1	HYP	H	104	8/9	0.97	0.10	-	46,46,46,46	0
1	SMC	C	256	7/8	0.99	0.10	-	33,36,37,37	0
1	KCX	E	201	12/13	0.98	0.13	-	46,46,52,52	0
1	HYP	D	151	8/9	0.97	0.10	-	38,38,38,38	0
2	MME	L	1	9/10	0.87	0.38	-	75,76,78,78	0
1	KCX	F	201	12/13	0.98	0.14	-	46,46,52,53	0
1	HYP	G	104	8/9	0.97	0.13	-	45,45,46,47	0
1	HYP	F	104	8/9	0.98	0.10	-	45,45,45,46	0
1	KCX	H	201	12/13	0.96	0.13	-	46,46,53,53	0
1	SMC	D	256	7/8	0.99	0.09	-	34,36,37,37	0
1	SMC	B	369	7/8	0.98	0.12	-	48,49,50,52	0
2	MME	O	1	9/10	0.87	0.23	-	75,76,78,78	0
2	MME	M	1	9/10	0.91	0.26	-	75,76,77,78	0
2	MME	N	1	9/10	0.88	0.22	-	75,76,78,78	0
1	SMC	C	369	7/8	0.98	0.10	-	48,49,50,51	0
2	MME	P	1	9/10	0.88	0.26	-	75,76,78,78	0
1	KCX	G	201	12/13	0.98	0.12	-	46,46,52,53	0
1	HYP	E	151	8/9	0.98	0.11	-	37,38,38,38	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	1473	4/4	0.85	0.26	5.10	68,68,68,69	0
5	EDO	G	1472	4/4	0.83	0.27	4.34	80,82,83,83	0
5	EDO	D	1479	4/4	0.90	0.23	4.25	44,45,47,48	0
5	EDO	C	1475	4/4	0.91	0.26	3.74	57,57,57,59	0
5	EDO	B	1472	4/4	0.93	0.18	3.69	67,68,68,69	0
5	EDO	D	1477	4/4	0.90	0.23	3.69	59,60,60,61	0
5	EDO	F	1472	4/4	0.96	0.23	3.23	51,53,53,55	0
5	EDO	A	1472	4/4	0.76	0.35	2.57	79,81,82,83	0
5	EDO	G	1474	4/4	0.79	0.27	2.31	49,50,51,51	0
5	EDO	C	1473	4/4	0.93	0.18	1.99	58,60,60,60	0
5	EDO	E	1474	4/4	0.81	0.30	1.62	73,74,76,77	0
5	EDO	H	1473	4/4	0.92	0.20	1.28	54,54,55,57	0
5	EDO	F	1473	4/4	0.92	0.19	1.21	70,71,72,74	0
5	EDO	C	1474	4/4	0.94	0.19	0.97	55,55,57,59	0
5	EDO	E	1472	4/4	0.93	0.17	0.89	59,60,60,61	0
5	EDO	G	1473	4/4	0.95	0.17	0.86	50,51,53,55	0
5	EDO	D	1478	4/4	0.94	0.15	0.44	46,48,54,59	0
4	CAP	G	1471	21/21	0.96	0.14	0.27	48,54,56,56	0
5	EDO	E	1475	4/4	0.97	0.13	0.13	45,47,48,50	0
5	EDO	H	1474	4/4	0.95	0.16	0.13	47,48,49,49	0
3	MG	G	1470	1/1	0.96	0.13	-0.08	46,46,46,46	0
5	EDO	H	1472	4/4	0.95	0.12	-0.42	40,40,41,42	0
4	CAP	D	1476	21/21	0.97	0.12	-0.51	48,54,56,56	0
4	CAP	B	1471	21/21	0.96	0.12	-0.54	50,55,56,57	0
4	CAP	A	1471	21/21	0.97	0.12	-0.54	49,54,56,56	0
5	EDO	E	1473	4/4	0.97	0.12	-0.97	51,52,52,53	0
4	CAP	F	1471	21/21	0.97	0.11	-1.22	49,54,56,56	0
5	EDO	A	1474	4/4	0.97	0.09	-1.22	42,44,45,45	0
4	CAP	C	1472	21/21	0.98	0.11	-1.34	49,54,56,56	0
4	CAP	E	1471	21/21	0.98	0.10	-1.40	48,54,56,57	0
4	CAP	H	1471	21/21	0.98	0.10	-1.53	48,54,56,57	0
3	MG	A	1470	1/1	0.93	0.06	-1.88	47,47,47,47	0
3	MG	F	1470	1/1	0.99	0.07	-2.17	47,47,47,47	0
3	MG	B	1470	1/1	0.97	0.07	-2.21	47,47,47,47	0
3	MG	D	1475	1/1	0.99	0.04	-2.60	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	C	1471	1/1	0.99	0.06	-3.41	46,46,46,46	0
3	MG	E	1470	1/1	0.97	0.06	-3.67	46,46,46,46	0
3	MG	H	1470	1/1	0.97	0.05	-5.09	47,47,47,47	0
5	EDO	H	1475	4/4	0.76	0.39	-	71,74,77,77	0
5	EDO	A	1473	4/4	0.75	0.41	-	75,75,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.