Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:46 PM GMT

PDB ID	:	1UW9
Title	:	L290F-A222T CHLAMYDOMONAS RUBISCO MUTANT
Authors	:	Karkehabadi, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2004-02-03
Resolution	:	2.05 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:

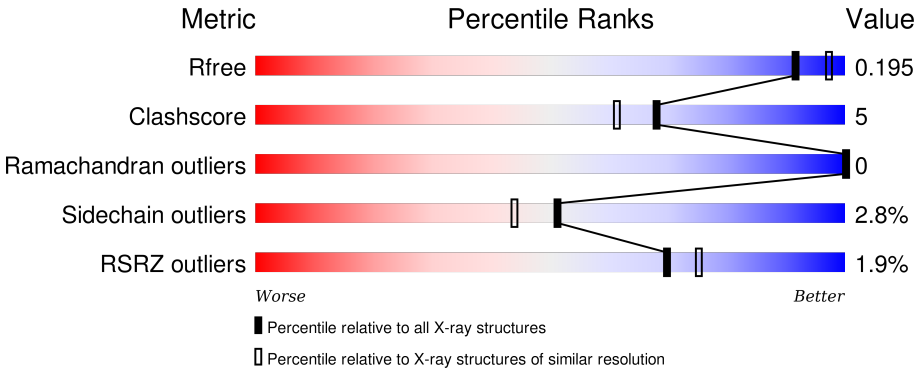
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	87% 11%
1	B	475	86% 11%
1	E	475	87% 10%
1	H	475	89% 9%
1	K	475	87% 11%

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Mol	Chain	Length	Quality of chain
1	O	475	2% 88% 10%
1	R	475	% 87% 10%
1	V	475	% 85% 12%
2	C	140	4% 86% 11%
2	F	140	3% 86% 11%
2	I	140	2% 86% 11%
2	J	140	4% 88% 10%
2	M	140	% 86% 11%
2	P	140	3% 89% 9%
2	T	140	4% 88% 10%
2	W	140	% 86% 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	1480	-	-	-	X
5	EDO	A	1482	-	-	-	X
5	EDO	A	1483	-	-	X	X
5	EDO	B	1482	-	-	-	X
5	EDO	E	1479	-	-	-	X
5	EDO	E	1482	-	-	-	X
5	EDO	H	1479	-	-	-	X
5	EDO	H	1480	-	-	-	X
5	EDO	H	1482	-	-	-	X
5	EDO	I	1141	-	-	-	X
5	EDO	K	1477	-	-	-	X
5	EDO	K	1479	-	-	-	X
5	EDO	K	1481	-	-	-	X
5	EDO	M	1141	-	-	-	X
5	EDO	O	1483	-	-	-	X
5	EDO	O	1484	-	-	-	X
5	EDO	R	1481	-	-	-	X
5	EDO	T	1141	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	V	1480	-	-	-	X
5	EDO	W	1141	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 41674 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	4	0
			3646	2304	641	676	25			
1	B	467	Total	C	N	O	S	0	4	0
			3654	2309	642	677	26			
1	E	465	Total	C	N	O	S	0	4	0
			3646	2304	641	676	25			
1	H	469	Total	C	N	O	S	0	4	0
			3671	2319	646	681	25			
1	K	469	Total	C	N	O	S	0	6	0
			3679	2325	646	683	25			
1	O	469	Total	C	N	O	S	0	2	0
			3663	2315	645	678	25			
1	R	465	Total	C	N	O	S	0	3	0
			3643	2303	641	674	25			
1	V	466	Total	C	N	O	S	0	5	0
			3653	2309	642	677	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	CONFLICT	UNP P00877
B	46	PRO	LEU	CONFLICT	UNP P00877
E	46	PRO	LEU	CONFLICT	UNP P00877
H	46	PRO	LEU	CONFLICT	UNP P00877
K	46	PRO	LEU	CONFLICT	UNP P00877
O	46	PRO	LEU	CONFLICT	UNP P00877
R	46	PRO	LEU	CONFLICT	UNP P00877
V	46	PRO	LEU	CONFLICT	UNP P00877
A	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
A	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
B	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
B	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
E	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
E	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
H	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
H	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
K	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
K	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
O	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
O	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
R	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
R	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
V	222	THR	ALA	ENGINEERED MUTATION	UNP P00877
V	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	2	0
			1149	741	192	205	11			
2	F	140	Total	C	N	O	S	0	2	0
			1154	747	191	204	12			
2	I	140	Total	C	N	O	S	0	1	0
			1146	740	191	204	11			
2	J	140	Total	C	N	O	S	0	2	0
			1154	747	191	204	12			
2	M	140	Total	C	N	O	S	0	2	0
			1147	740	191	204	12			
2	P	140	Total	C	N	O	S	0	3	0
			1150	741	192	205	12			
2	T	140	Total	C	N	O	S	0	3	0
			1157	748	192	205	12			
2	W	140	Total	C	N	O	S	0	2	0
			1147	740	191	204	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	128	SER	THR	CONFLICT	UNP P00873
I	132	TRP	PHE	CONFLICT	UNP P00873
C	128	SER	THR	CONFLICT	UNP P00873
C	132	TRP	PHE	CONFLICT	UNP P00873
F	128	SER	THR	CONFLICT	UNP P00873
F	132	TRP	PHE	CONFLICT	UNP P00873

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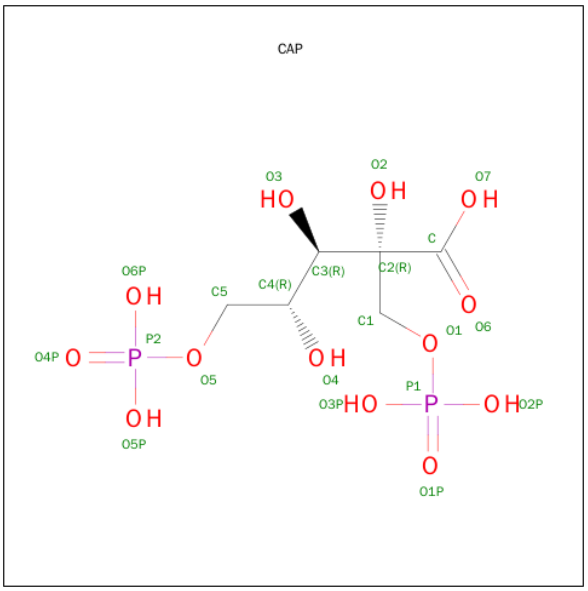
Chain	Residue	Modelled	Actual	Comment	Reference
J	128	SER	THR	CONFLICT	UNP P00873
J	132	TRP	PHE	CONFLICT	UNP P00873
P	128	SER	THR	CONFLICT	UNP P00873
P	132	TRP	PHE	CONFLICT	UNP P00873
T	128	SER	THR	CONFLICT	UNP P00873
T	132	TRP	PHE	CONFLICT	UNP P00873
M	128	SER	THR	CONFLICT	UNP P00873
M	132	TRP	PHE	CONFLICT	UNP P00873
W	128	SER	THR	CONFLICT	UNP P00873
W	132	TRP	PHE	CONFLICT	UNP P00873

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

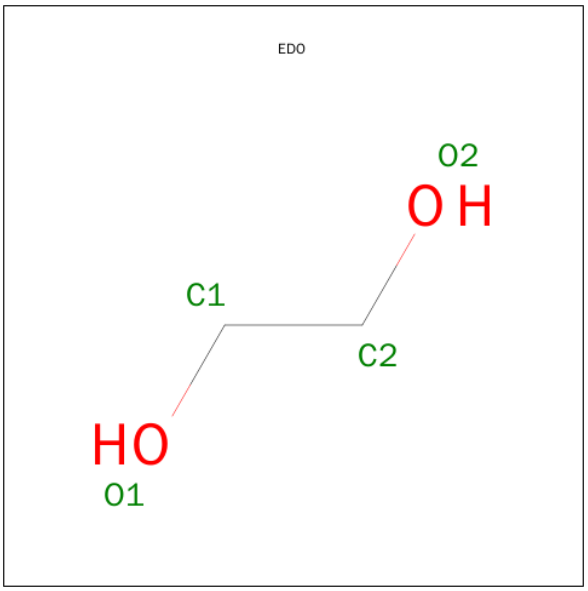
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	R	1	Total Mg 1 1	0	0

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



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

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



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

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

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

- Molecule 6 is water.

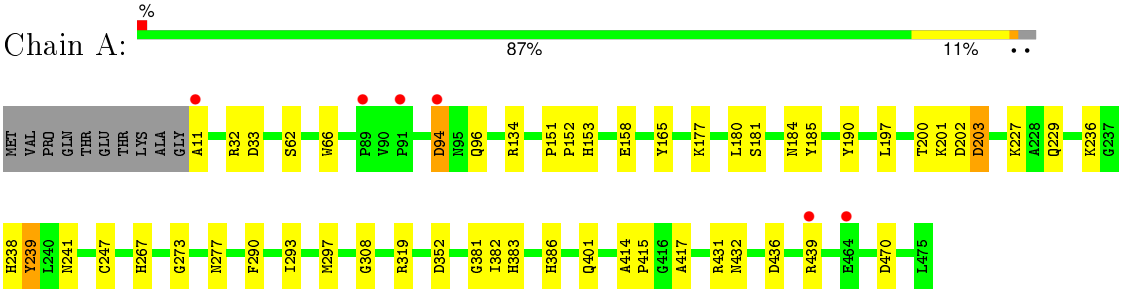
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	283	Total O 283 283	0	0
6	B	276	Total O 276 276	0	0
6	C	80	Total O 80 80	0	0
6	E	285	Total O 285 285	0	0
6	F	96	Total O 96 96	0	0
6	H	271	Total O 271 271	0	0
6	I	67	Total O 67 67	0	0
6	J	74	Total O 74 74	0	0
6	K	253	Total O 253 253	0	0
6	M	87	Total O 87 87	0	0
6	O	281	Total O 281 281	0	0
6	P	60	Total O 60 60	0	0
6	R	261	Total O 261 261	0	0
6	T	76	Total O 76 76	0	0
6	V	289	Total O 289 289	0	0
6	W	80	Total O 80 80	0	0

3 Residue-property plots (i)

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

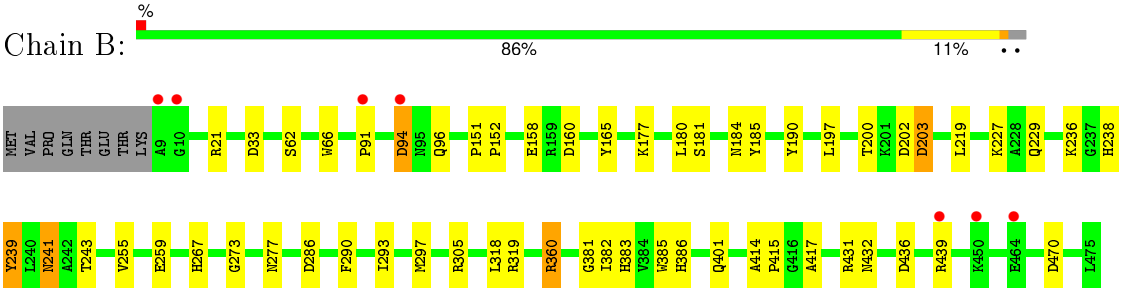
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:



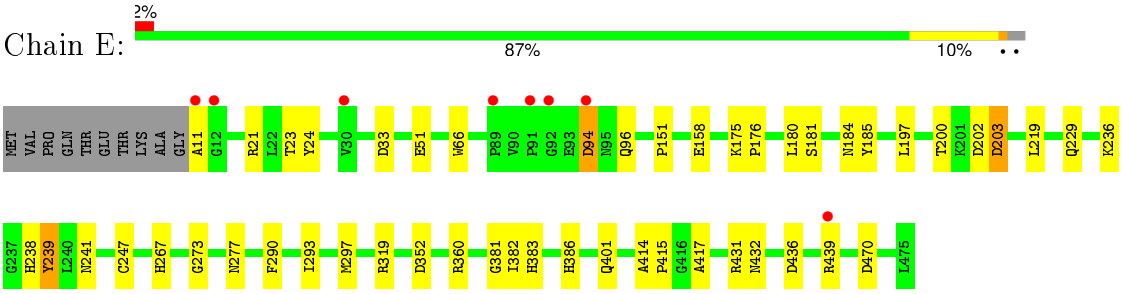
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



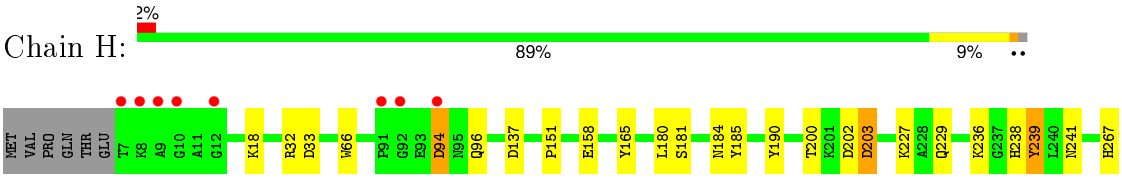
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

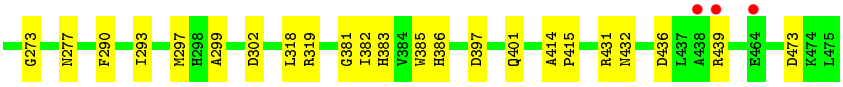
Chain E:



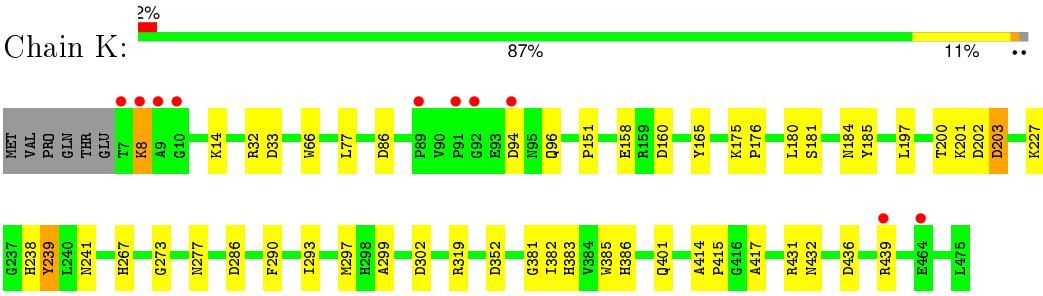
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain H:

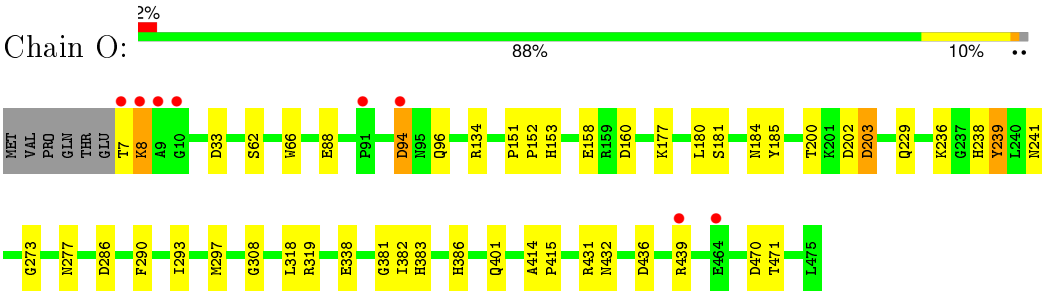




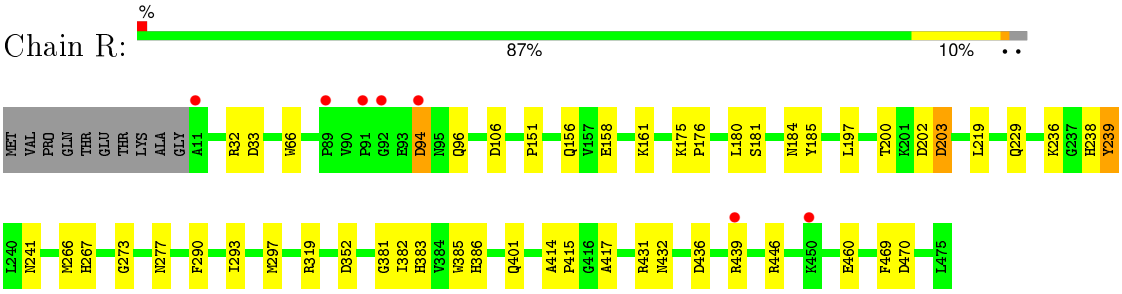
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



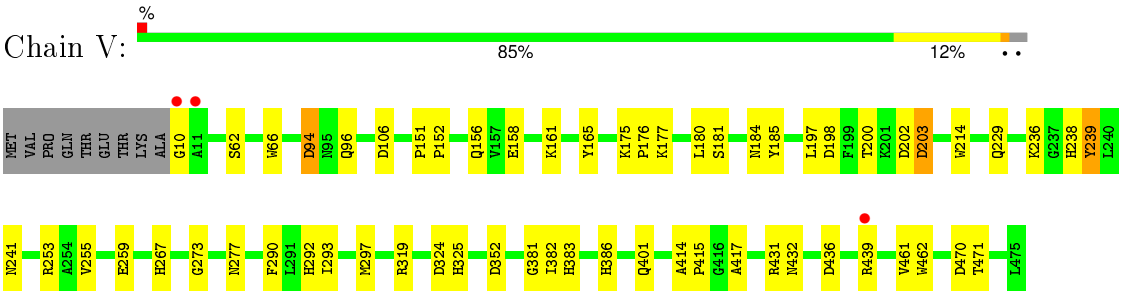
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



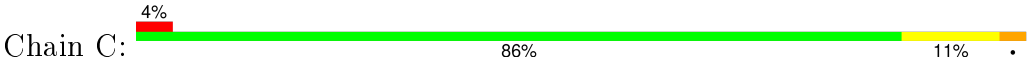
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

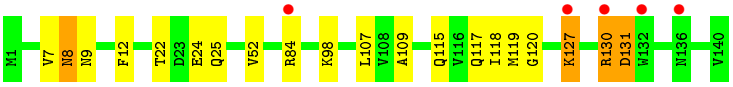


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



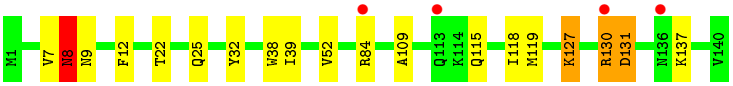
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1





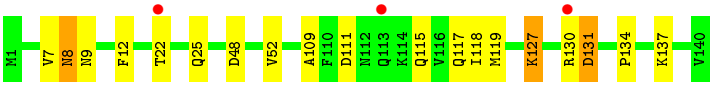
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain F:



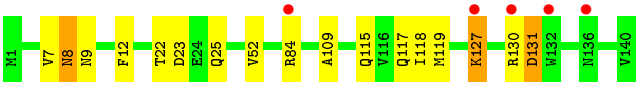
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain I:



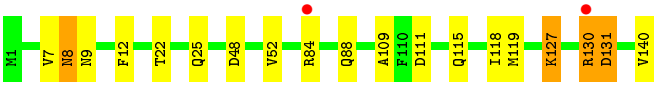
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain J:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain M:

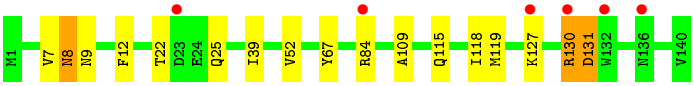


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P:

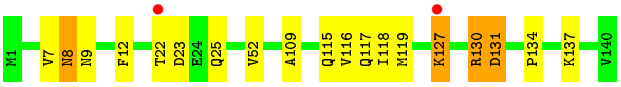
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain T:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain W:


M1
V7
N8
N9
F12
T22
D23
E24
Q25
V52
A109
Q115
V116
Q117
I118
M119
K127
R130
D131
P134
K137
V140

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.07Å 178.20Å 120.46Å 90.00° 120.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05 19.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.05) 89.6 (19.82-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.194 0.166 , 0.195	Depositor DCC
R_{free} test set	11867 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.3	EDS
Estimated twinning fraction	0.086 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 238513 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41674	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/3707	0.71	5/5009 (0.1%)
1	B	0.50	0/3722	0.76	12/5029 (0.2%)
1	E	0.46	0/3707	0.70	5/5009 (0.1%)
1	H	0.48	0/3732	0.70	6/5042 (0.1%)
1	K	0.46	0/3748	0.71	7/5064 (0.1%)
1	O	0.47	0/3714	0.71	6/5018 (0.1%)
1	R	0.47	0/3698	0.71	6/4997 (0.1%)
1	V	0.47	0/3718	0.71	7/5024 (0.1%)
2	C	0.50	0/1191	0.75	3/1618 (0.2%)
2	F	0.50	0/1198	0.73	2/1627 (0.1%)
2	I	0.50	0/1183	0.74	4/1607 (0.2%)
2	J	0.47	0/1198	0.73	3/1627 (0.2%)
2	M	0.48	0/1191	0.73	4/1617 (0.2%)
2	P	0.49	0/1199	0.74	4/1628 (0.2%)
2	T	0.48	0/1206	0.76	3/1638 (0.2%)
2	W	0.48	0/1191	0.73	3/1617 (0.2%)
All	All	0.48	0/39303	0.72	80/53171 (0.2%)

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
2	C	0	1
2	F	0	1
2	I	0	1
2	J	0	1
2	M	0	1
2	P	0	1
2	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	W	0	1
All	All	0	8

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360[A]	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	B	360[B]	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	B	360[A]	ARG	CD-NE-CZ	7.75	134.45	123.60
1	B	360[B]	ARG	CD-NE-CZ	7.75	134.45	123.60
2	F	8	ASN	N-CA-C	-7.01	92.06	111.00
2	W	8	ASN	N-CA-C	-6.71	92.88	111.00
2	C	8[A]	ASN	N-CA-C	-6.68	92.95	111.00
2	C	8[B]	ASN	N-CA-C	-6.68	92.95	111.00
2	I	8	ASN	N-CA-C	-6.63	93.10	111.00
2	J	8	ASN	N-CA-C	-6.57	93.25	111.00
1	K	203	ASP	CB-CG-OD2	6.57	124.21	118.30
1	H	203	ASP	CB-CG-OD2	6.41	124.07	118.30
2	P	8[A]	ASN	N-CA-C	-6.34	93.88	111.00
2	P	8[B]	ASN	N-CA-C	-6.34	93.88	111.00
2	M	8	ASN	N-CA-C	-6.34	93.89	111.00
1	V	203	ASP	CB-CG-OD2	6.33	124.00	118.30
2	T	8[A]	ASN	N-CA-C	-6.21	94.24	111.00
2	T	8[B]	ASN	N-CA-C	-6.21	94.24	111.00
1	O	203	ASP	CB-CG-OD2	6.20	123.88	118.30
2	T	131	ASP	CB-CG-OD2	6.11	123.80	118.30
1	R	203	ASP	CB-CG-OD2	6.06	123.76	118.30
1	O	160	ASP	CB-CG-OD2	6.03	123.73	118.30
2	M	131	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	352	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	360[A]	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	360[B]	ARG	NE-CZ-NH1	-5.96	117.32	120.30
2	J	131	ASP	CB-CG-OD2	5.88	123.59	118.30
2	F	131	ASP	CB-CG-OD2	5.83	123.55	118.30
2	P	131	ASP	CB-CG-OD2	5.81	123.53	118.30
2	C	131	ASP	CB-CG-OD2	5.79	123.51	118.30
1	O	33	ASP	CB-CG-OD2	5.74	123.47	118.30
1	V	94	ASP	CB-CG-OD2	5.69	123.42	118.30
2	I	131	ASP	CB-CG-OD2	5.67	123.41	118.30
1	R	33	ASP	CB-CG-OD2	5.65	123.39	118.30
1	V	352	ASP	CB-CG-OD2	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	470	ASP	CB-CG-OD2	5.62	123.36	118.30
1	H	473	ASP	CB-CG-OD2	5.62	123.36	118.30
1	K	86	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	33	ASP	CB-CG-OD2	5.59	123.33	118.30
1	R	352	ASP	CB-CG-OD2	5.55	123.30	118.30
2	I	48	ASP	CB-CG-OD2	5.54	123.29	118.30
1	O	286	ASP	CB-CG-OD2	5.53	123.28	118.30
1	K	160	ASP	CB-CG-OD2	5.50	123.25	118.30
2	W	131	ASP	CB-CG-OD2	5.49	123.24	118.30
1	R	94	ASP	CB-CG-OD2	5.47	123.22	118.30
1	O	94	ASP	CB-CG-OD2	5.44	123.20	118.30
1	H	94	ASP	CB-CG-OD2	5.43	123.19	118.30
1	V	470	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	94	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	470	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	33	ASP	CB-CG-OD2	5.39	123.15	118.30
2	W	23	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	33	ASP	CB-CG-OD2	5.34	123.10	118.30
1	E	94	ASP	CB-CG-OD2	5.32	123.09	118.30
1	H	33	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	203	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	470	ASP	CB-CG-OD2	5.30	123.07	118.30
1	R	106	ASP	CB-CG-OD2	5.28	123.06	118.30
1	K	33[A]	ASP	CB-CG-OD2	5.27	123.04	118.30
1	K	33[B]	ASP	CB-CG-OD2	5.27	123.04	118.30
1	H	397	ASP	CB-CG-OD2	5.26	123.04	118.30
2	M	111	ASP	CB-CG-OD2	5.25	123.02	118.30
2	M	48	ASP	CB-CG-OD2	5.25	123.02	118.30
1	K	286	ASP	CB-CG-OD2	5.24	123.02	118.30
2	I	111	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	286	ASP	CB-CG-OD2	5.21	122.99	118.30
1	V	198	ASP	CB-CG-OD2	5.21	122.99	118.30
2	P	111	ASP	CB-CG-OD2	5.18	122.97	118.30
1	R	470	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	203	ASP	CB-CG-OD2	5.16	122.95	118.30
1	V	324	ASP	CB-CG-OD2	5.16	122.95	118.30
1	H	137	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	352	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	94	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	203	ASP	CB-CG-OD2	5.12	122.91	118.30
1	K	352	ASP	CB-CG-OD2	5.10	122.89	118.30
2	J	23	ASP	CB-CG-OD2	5.09	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	470	ASP	CB-CG-OD2	5.07	122.87	118.30
1	B	160	ASP	CB-CG-OD2	5.05	122.85	118.30
1	V	106	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	7	VAL	Peptide
2	F	7	VAL	Peptide
2	I	7	VAL	Peptide
2	J	7	VAL	Peptide
2	M	7	VAL	Peptide
2	P	7	VAL	Peptide
2	T	7	VAL	Peptide
2	W	7	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3646	0	3544	38	0
1	B	3654	0	3555	39	0
1	E	3646	0	3544	33	0
1	H	3671	0	3572	31	0
1	K	3679	0	3583	34	3
1	O	3663	0	3566	34	1
1	R	3643	0	3546	33	2
1	V	3653	0	3556	44	0
2	C	1149	0	1123	18	0
2	F	1154	0	1126	20	0
2	I	1146	0	1121	12	0
2	J	1154	0	1126	12	0
2	M	1147	0	1122	19	0
2	P	1150	0	1124	12	0
2	T	1157	0	1128	13	0
2	W	1147	0	1122	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	E	21	0	7	0	0
4	O	42	0	15	0	0
4	R	42	0	15	0	0
4	V	21	0	7	0	0
5	A	24	0	36	4	0
5	B	20	0	30	0	0
5	C	8	0	12	0	0
5	E	20	0	30	3	0
5	H	24	0	36	2	0
5	I	4	0	6	1	0
5	J	8	0	12	1	0
5	K	20	0	30	1	0
5	M	8	0	12	0	0
5	O	24	0	36	0	0
5	P	8	0	12	0	0
5	R	16	0	24	1	0
5	T	8	0	12	1	0
5	V	20	0	30	0	0
5	W	8	0	12	0	0
6	A	283	0	0	7	0
6	B	276	0	0	5	0
6	C	80	0	0	3	0
6	E	285	0	0	7	0
6	F	96	0	0	9	0
6	H	271	0	0	3	0
6	I	67	0	0	0	0
6	J	74	0	0	2	0
6	K	253	0	0	2	0
6	M	87	0	0	4	0
6	O	281	0	0	4	0
6	P	60	0	0	0	0
6	R	261	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	76	0	0	4	0
6	V	289	0	0	2	0
6	W	80	0	0	0	0
All	All	41674	0	37846	363	3

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 5.

All (363) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:ARG:NH1	6:C:2073:HOH:O	1.79	1.12
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.05	1.02
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.04	1.00
1:A:267:HIS:HD2	1:A:277:ASN:HD22	0.99	0.97
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.02	0.94
1:O:267:HIS:HD2	1:O:277:ASN:HD22	1.07	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.02	0.93
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.08	0.93
1:R:267:HIS:HD2	1:R:277:ASN:HD22	0.98	0.92
1:R:267:HIS:CD2	1:R:277:ASN:HD22	1.88	0.92
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.89	0.90
2:F:8:ASN:CG	6:F:2005:HOH:O	2.11	0.87
1:B:184:ASN:HD22	2:F:115:GLN:HE21	1.18	0.86
2:W:8:ASN:HB3	2:W:131:ASP:HA	1.57	0.86
1:E:184:ASN:HD22	2:J:115:GLN:HE21	1.22	0.86
2:C:8[A]:ASN:HB3	2:C:131:ASP:HA	1.56	0.86
2:M:8:ASN:HB3	2:M:131:ASP:HA	1.58	0.85
2:T:8[B]:ASN:HB3	2:T:131:ASP:HA	1.57	0.85
2:T:130:ARG:NH1	6:T:2071:HOH:O	2.07	0.85
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.92	0.85
1:V:267:HIS:CD2	1:V:277:ASN:HD22	1.93	0.84
2:I:22:THR:H	2:I:25:GLN:HE21	1.26	0.84
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.95	0.83
2:I:8:ASN:HB3	2:I:131:ASP:HA	1.58	0.83
1:B:21:ARG:NH1	6:B:2016:HOH:O	2.10	0.82
2:F:8:ASN:HB3	2:F:131:ASP:HA	1.61	0.82
1:O:267:HIS:CD2	1:O:277:ASN:HD22	1.95	0.82
2:M:115:GLN:HE21	1:O:184:ASN:HD22	1.25	0.82
2:T:8[A]:ASN:HB3	2:T:131:ASP:HA	1.61	0.82
2:F:84:ARG:HD2	6:F:2060:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:267:HIS:CD2	1:K:277:ASN:HD22	1.96	0.81
2:C:8[B]:ASN:HB3	2:C:131:ASP:HA	1.60	0.81
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.96	0.81
2:F:22:THR:H	2:F:25:GLN:HE21	1.30	0.80
1:E:21:ARG:CZ	1:E:51[B]:GLU:HG3	2.11	0.80
2:I:115:GLN:HE21	1:K:184:ASN:HD22	1.29	0.80
2:C:115:GLN:HE21	1:V:184:ASN:HD22	1.28	0.80
1:B:383:HIS:H	1:B:386:HIS:HD2	1.29	0.80
2:W:22:THR:H	2:W:25:GLN:HE21	1.26	0.80
1:H:383:HIS:H	1:H:386:HIS:HD2	1.30	0.80
2:M:22:THR:H	2:M:25:GLN:HE21	1.28	0.80
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.29	0.80
1:O:383:HIS:H	1:O:386:HIS:HD2	1.30	0.79
1:K:431:ARG:HH21	1:K:432:ASN:HD21	1.28	0.79
1:A:383:HIS:H	1:A:386:HIS:HD2	1.29	0.79
1:K:383:HIS:H	1:K:386:HIS:HD2	1.28	0.79
2:C:22:THR:H	2:C:25:GLN:HE21	1.28	0.79
2:J:8:ASN:HB3	2:J:131:ASP:HA	1.62	0.79
1:A:184:ASN:HD22	2:T:115:GLN:HE21	1.30	0.79
2:P:8[A]:ASN:HB3	2:P:131:ASP:HA	1.65	0.78
1:V:383:HIS:H	1:V:386:HIS:HD2	1.27	0.78
2:P:22:THR:H	2:P:25:GLN:HE21	1.31	0.78
1:R:446:ARG:HD3	6:R:2229:HOH:O	1.85	0.78
2:P:115:GLN:HE21	1:R:184:ASN:HD22	1.29	0.77
1:E:383:HIS:H	1:E:386:HIS:HD2	1.31	0.76
1:H:184:ASN:HD22	2:W:115:GLN:HE21	1.32	0.76
1:R:383:HIS:H	1:R:386:HIS:HD2	1.31	0.76
2:J:22:THR:H	2:J:25:GLN:HE21	1.31	0.75
1:R:431:ARG:HH21	1:R:432:ASN:HD21	1.32	0.75
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.31	0.75
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.31	0.75
1:V:431:ARG:HH21	1:V:432:ASN:HD21	1.33	0.74
2:M:84:ARG:HD2	1:V:10:GLY:N	2.02	0.74
2:M:84:ARG:HH11	1:V:10:GLY:N	1.85	0.74
2:C:98:LYS:HE2	6:C:2055:HOH:O	1.88	0.74
2:T:22:THR:H	2:T:25:GLN:HE21	1.33	0.73
2:P:8[B]:ASN:HB3	2:P:131:ASP:HA	1.69	0.73
1:O:431:ARG:HH21	1:O:432:ASN:HD21	1.37	0.73
2:F:130:ARG:HD3	6:F:2087:HOH:O	1.88	0.73
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.34	0.72
2:M:88:GLN:HG3	6:M:2061:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:436:ASP:OD2	1:K:439:ARG:HD3	1.92	0.69
1:E:229:GLN:HE21	1:E:236:LYS:H	1.42	0.68
1:V:229:GLN:HE21	1:V:236:LYS:H	1.42	0.67
1:E:21:ARG:NH2	1:E:51[B]:GLU:HG3	2.10	0.67
1:B:229:GLN:HE21	1:B:236:LYS:H	1.41	0.66
1:R:156[B]:GLN:CD	6:R:2092:HOH:O	2.34	0.66
1:E:247[B]:CYS:SG	6:E:2034:HOH:O	2.55	0.65
2:T:84:ARG:HD3	6:T:2054:HOH:O	1.96	0.65
1:A:11:ALA:N	6:A:2002:HOH:O	2.29	0.64
5:A:1483:EDO:H21	6:A:2283:HOH:O	1.98	0.64
1:O:229:GLN:HE21	1:O:236:LYS:H	1.44	0.64
1:O:259:GLU:HG2	6:T:2036:HOH:O	1.98	0.63
1:A:229:GLN:HE21	1:A:236:LYS:H	1.44	0.63
2:F:84:ARG:NH1	6:F:2060:HOH:O	2.28	0.63
1:K:229:GLN:HE21	1:K:236:LYS:H	1.47	0.62
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.82	0.62
1:R:200:THR:OG1	1:R:238:HIS:HD2	1.82	0.62
1:K:200:THR:OG1	1:K:238:HIS:HD2	1.83	0.62
1:K:202:ASP:OD1	1:K:238:HIS:HE1	1.82	0.62
1:R:229:GLN:HE21	1:R:236:LYS:H	1.47	0.61
1:O:200:THR:OG1	1:O:238:HIS:HD2	1.84	0.61
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.83	0.61
1:H:229:GLN:HE21	1:H:236:LYS:H	1.48	0.61
2:M:84:ARG:NH1	1:V:10:GLY:HA2	2.15	0.60
2:T:8[B]:ASN:HB3	2:T:131:ASP:CA	2.31	0.60
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.84	0.60
2:M:115:GLN:HE22	1:O:180:LEU:HA	1.67	0.60
1:H:180:LEU:HA	2:W:115:GLN:HE22	1.66	0.59
1:B:255:VAL:O	1:B:259[A]:GLU:HG3	2.02	0.59
1:K:239:TYR:HE2	1:K:401:GLN:HE22	1.51	0.59
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.85	0.59
1:O:239:TYR:HE2	1:O:401:GLN:HE22	1.51	0.59
2:I:115:GLN:HE22	1:K:180:LEU:HA	1.68	0.58
2:M:84:ARG:NH1	1:V:10:GLY:N	2.50	0.58
1:R:202:ASP:OD1	1:R:238:HIS:HE1	1.87	0.58
2:W:22:THR:H	2:W:25:GLN:NE2	2.00	0.58
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.86	0.58
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.86	0.58
2:T:22:THR:H	2:T:25:GLN:NE2	2.02	0.58
1:V:200:THR:OG1	1:V:238:HIS:HD2	1.87	0.58
1:O:202:ASP:OD1	1:O:238:HIS:HE1	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1482:EDO:C2	6:E:2284:HOH:O	2.50	0.58
5:A:1483:EDO:C2	6:A:2283:HOH:O	2.50	0.58
1:R:239:TYR:HE2	1:R:401:GLN:HE22	1.51	0.57
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.52	0.57
1:H:181:SER:H	2:W:115:GLN:NE2	2.02	0.57
1:B:91:PRO:HD3	6:B:2059:HOH:O	2.04	0.57
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.51	0.57
6:O:2127:HOH:O	1:R:161:LYS:HE2	2.03	0.57
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.53	0.57
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.88	0.56
1:A:383:HIS:H	1:A:386:HIS:CD2	2.18	0.56
6:O:2150:HOH:O	1:V:267:HIS:HE1	1.87	0.56
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.89	0.56
1:V:239:TYR:HE2	1:V:401:GLN:HE22	1.53	0.56
2:M:22:THR:H	2:M:25:GLN:NE2	2.03	0.56
1:A:32:ARG:HD2	6:A:2032:HOH:O	2.06	0.56
2:W:8:ASN:HB3	2:W:131:ASP:CA	2.33	0.55
1:K:383:HIS:H	1:K:386:HIS:CD2	2.18	0.55
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.89	0.55
2:P:8[A]:ASN:HB3	2:P:131:ASP:CA	2.36	0.55
1:V:202:ASP:OD1	1:V:238:HIS:HE1	1.90	0.55
2:I:109:ALA:HB3	2:I:119:MET:HG3	1.87	0.55
2:P:115:GLN:HE22	1:R:180:LEU:HA	1.72	0.55
2:C:115:GLN:NE2	1:V:181:SER:H	2.04	0.55
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.88	0.55
2:I:8:ASN:HB3	2:I:131:ASP:CA	2.35	0.54
2:C:115:GLN:HE22	1:V:180:LEU:HA	1.72	0.54
1:V:414:ALA:HB3	1:V:415:PRO:HD3	1.89	0.54
2:P:22:THR:H	2:P:25:GLN:NE2	2.01	0.54
2:I:22:THR:H	2:I:25:GLN:NE2	2.00	0.54
1:E:383:HIS:H	1:E:386:HIS:CD2	2.19	0.54
1:A:180:LEU:HA	2:T:115:GLN:HE22	1.72	0.54
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.55	0.54
2:C:8[A]:ASN:HB3	2:C:131:ASP:CA	2.36	0.54
2:C:8[B]:ASN:HB3	2:C:131:ASP:CA	2.35	0.53
1:B:383:HIS:H	1:B:386:HIS:CD2	2.19	0.53
2:M:130:ARG:HD3	6:M:2082:HOH:O	2.07	0.53
1:E:180:LEU:HA	2:J:115:GLN:HE22	1.74	0.53
2:I:115:GLN:NE2	1:K:181:SER:H	2.07	0.53
1:A:181:SER:H	2:T:115:GLN:NE2	2.07	0.53
2:F:22:THR:H	2:F:25:GLN:NE2	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.91	0.52
2:P:115:GLN:NE2	1:R:181:SER:H	2.07	0.52
2:M:84:ARG:NH1	1:V:10:GLY:CA	2.72	0.52
1:O:383:HIS:H	1:O:386:HIS:CD2	2.19	0.52
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.93	0.51
5:I:1141:EDO:C2	1:K:227:LYS:HA	2.41	0.51
2:F:8:ASN:ND2	6:F:2004:HOH:O	2.43	0.51
2:M:115:GLN:NE2	1:O:181:SER:H	2.09	0.51
1:B:360[B]:ARG:HG3	1:B:360[B]:ARG:HH21	1.76	0.51
1:B:383:HIS:N	1:B:386:HIS:HD2	2.05	0.50
1:O:386:HIS:HE1	6:O:2178:HOH:O	1.93	0.50
1:B:180:LEU:HA	2:F:115:GLN:HE22	1.75	0.50
2:J:22:THR:H	2:J:25:GLN:NE2	2.02	0.50
2:W:109:ALA:HB3	2:W:119:MET:HG3	1.92	0.50
1:B:181:SER:H	2:F:115:GLN:NE2	2.09	0.50
1:O:414:ALA:HB3	1:O:415:PRO:HD3	1.93	0.50
1:R:383:HIS:H	1:R:386:HIS:CD2	2.20	0.50
5:A:1483:EDO:C1	6:A:2282:HOH:O	2.60	0.50
1:V:436:ASP:OD2	1:V:439:ARG:HD3	2.12	0.50
1:E:383:HIS:N	1:E:386:HIS:HD2	2.05	0.49
1:O:381:GLY:HA2	1:V:66:TRP:CD1	2.47	0.49
2:F:8:ASN:HB3	2:F:131:ASP:CA	2.37	0.49
2:F:8:ASN:ND2	6:F:2005:HOH:O	2.41	0.49
2:C:22:THR:H	2:C:25:GLN:NE2	2.03	0.49
1:V:383:HIS:H	1:V:386:HIS:CD2	2.17	0.49
5:E:1482:EDO:H22	6:E:2284:HOH:O	2.11	0.49
1:O:383:HIS:N	1:O:386:HIS:HD2	2.06	0.49
1:R:277:ASN:HD21	1:R:293:ILE:HD12	1.78	0.49
1:H:383:HIS:H	1:H:386:HIS:CD2	2.19	0.49
1:K:414:ALA:HB3	1:K:415:PRO:HD3	1.94	0.48
1:E:11:ALA:N	6:E:2001:HOH:O	2.45	0.48
1:R:267:HIS:HD2	1:R:277:ASN:ND2	1.83	0.48
5:J:1141:EDO:H21	6:J:2038:HOH:O	2.14	0.48
1:A:383:HIS:N	1:A:386:HIS:HD2	2.05	0.48
1:R:414:ALA:HB3	1:R:415:PRO:HD3	1.96	0.48
2:J:109:ALA:HB3	2:J:119:MET:HG3	1.96	0.48
2:F:109:ALA:HB3	2:F:119:MET:HG3	1.95	0.48
1:H:381:GLY:HA2	1:R:66:TRP:CD1	2.49	0.48
2:M:127:LYS:HG2	6:M:2069:HOH:O	2.13	0.48
2:M:8:ASN:HB3	2:M:131:ASP:CA	2.36	0.47
1:E:181:SER:H	2:J:115:GLN:NE2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:TRP:CD1	1:R:381:GLY:HA2	2.49	0.47
1:H:32:ARG:HD2	6:H:2034:HOH:O	2.15	0.47
1:O:273:GLY:HA3	1:V:273:GLY:HA3	1.96	0.47
1:A:158:GLU:HA	1:A:290:PHE:CZ	2.50	0.47
1:B:305:ARG:NH1	6:B:2062:HOH:O	2.46	0.47
1:O:267:HIS:HE1	6:V:2162:HOH:O	1.97	0.47
1:O:382:ILE:HA	1:O:386:HIS:CD2	2.50	0.47
1:O:66:TRP:CD1	1:V:381:GLY:HA2	2.49	0.47
5:H:1477:EDO:C2	6:H:2264:HOH:O	2.63	0.47
2:C:84:ARG:HD3	1:O:8:LYS:O	2.15	0.47
2:M:140:VAL:HB	6:M:2087:HOH:O	2.14	0.47
2:C:24:GLU:HB2	6:C:2018:HOH:O	2.13	0.47
2:C:109:ALA:HB3	2:C:119:MET:HG3	1.97	0.47
1:E:21:ARG:NH1	1:E:51[B]:GLU:HG3	2.30	0.47
1:H:383:HIS:N	1:H:386:HIS:HD2	2.06	0.47
2:M:109:ALA:HB3	2:M:119:MET:HG3	1.97	0.47
1:V:158:GLU:HA	1:V:290:PHE:CZ	2.50	0.46
1:O:293:ILE:HG13	1:O:318:LEU:HD21	1.97	0.46
2:P:130:ARG:HB3	2:P:130:ARG:HE	1.49	0.46
1:E:158:GLU:HA	1:E:290:PHE:CZ	2.49	0.46
1:K:277:ASN:HD21	1:K:293:ILE:HD12	1.80	0.46
2:J:8:ASN:HB3	2:J:131:ASP:CA	2.40	0.46
1:E:360[B]:ARG:NH2	6:E:2203:HOH:O	2.46	0.46
2:F:127:LYS:HG2	2:F:127:LYS:H	1.62	0.46
1:R:158:GLU:HA	1:R:290:PHE:CZ	2.50	0.46
1:K:32:ARG:HD2	6:K:2021:HOH:O	2.16	0.46
1:A:151:HYP:HD23	1:A:319:ARG:O	2.15	0.46
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.97	0.46
1:R:200:THR:OG1	1:R:238:HIS:CD2	2.65	0.46
1:R:469:PHE:CE2	5:R:1482:EDO:H21	2.51	0.46
1:V:461[B]:VAL:HG23	1:V:462:TRP:CD2	2.51	0.46
5:A:1483:EDO:H12	6:A:2282:HOH:O	2.16	0.46
1:A:151:HYP:HA	1:A:152:PRO:HD3	1.90	0.45
1:B:436:ASP:OD2	1:B:439:ARG:HD3	2.16	0.45
1:O:151:HYP:HD23	1:O:319:ARG:O	2.17	0.45
2:F:8:ASN:CB	6:F:2005:HOH:O	2.59	0.45
1:H:273:GLY:HA3	1:R:273:GLY:HA3	1.99	0.45
1:V:277:ASN:HD21	1:V:293:ILE:HD12	1.82	0.45
2:J:127:LYS:HG2	6:J:2056:HOH:O	2.16	0.45
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.51	0.45
2:C:130:ARG:HE	2:C:130:ARG:HB3	1.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:HYP:HD23	1:H:319:ARG:O	2.16	0.45
1:O:158:GLU:HA	1:O:290:PHE:CZ	2.51	0.45
1:K:151:HYP:HD23	1:K:319:ARG:O	2.16	0.45
1:K:158:GLU:HA	1:K:290:PHE:CZ	2.52	0.45
1:B:151:HYP:HD23	1:B:319:ARG:O	2.17	0.45
1:B:386:HIS:HE1	6:B:2188:HOH:O	2.00	0.45
1:H:158:GLU:HA	1:H:290:PHE:CZ	2.52	0.45
1:V:471:THR:CB	6:V:2273:HOH:O	2.59	0.45
2:P:109:ALA:HB3	2:P:119:MET:HG3	1.99	0.45
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.51	0.45
1:E:151:HYP:HD23	1:E:319:ARG:O	2.17	0.45
1:E:277:ASN:HD21	1:E:293:ILE:HD12	1.82	0.44
1:V:175:LYS:HA	1:V:176:PRO:C	2.38	0.44
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.52	0.44
1:R:32:ARG:HD2	6:R:2028:HOH:O	2.17	0.44
1:R:436:ASP:OD2	1:R:439:ARG:HD3	2.18	0.44
2:C:127:LYS:HG2	2:C:127:LYS:H	1.66	0.44
1:B:360[B]:ARG:HG3	1:B:360[B]:ARG:NH2	2.31	0.44
1:E:66:TRP:CD1	1:K:381:GLY:HA2	2.52	0.44
2:T:109:ALA:HB3	2:T:119:MET:HG3	2.00	0.44
2:P:127:LYS:HG2	2:P:127:LYS:H	1.61	0.44
5:E:1482:EDO:C1	6:E:2282:HOH:O	2.65	0.44
1:V:156[B]:GLN:HG3	2:W:116:VAL:HB	2.00	0.44
1:E:267:HIS:HE1	6:K:2148:HOH:O	2.00	0.44
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.52	0.44
1:B:158:GLU:HA	1:B:290:PHE:CZ	2.53	0.44
1:V:151:HYP:HA	1:V:152:PRO:HD3	1.90	0.44
2:W:134:PRO:HG2	2:W:137:LYS:HB2	2.00	0.44
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.53	0.44
1:H:165:TYR:CD1	2:J:117:GLN:HB3	2.53	0.43
1:B:151:HYP:HA	1:B:152:PRO:HD3	1.92	0.43
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.99	0.43
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.53	0.43
1:V:214:TRP:CD2	1:V:253:ARG:HG2	2.53	0.43
1:E:273:GLY:HA3	1:K:273:GLY:HA3	2.00	0.43
1:H:267:HIS:HE1	6:R:2152:HOH:O	2.00	0.43
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.54	0.43
1:R:383:HIS:N	1:R:386:HIS:HD2	2.06	0.43
1:V:277:ASN:HD21	1:V:293:ILE:CD1	2.31	0.43
1:V:229:GLN:NE2	1:V:236:LYS:H	2.13	0.43
1:O:277:ASN:HD21	1:O:293:ILE:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HG13	1:B:318:LEU:HD21	2.00	0.43
1:K:382:ILE:HA	1:K:386:HIS:CD2	2.53	0.43
1:E:381:GLY:HA2	1:K:66:TRP:CD1	2.53	0.43
1:E:436:ASP:OD2	1:E:439:ARG:HD3	2.17	0.43
1:B:165:TYR:CD1	2:C:117:GLN:HB3	2.54	0.43
1:R:197:LEU:HG	1:R:417:ALA:HB1	2.01	0.43
1:A:267:HIS:HE1	6:B:2163:HOH:O	2.01	0.43
1:K:77:LEU:HD21	5:K:1477:EDO:H12	2.01	0.43
1:O:200:THR:OG1	1:O:238:HIS:CD2	2.69	0.43
2:J:84:ARG:HD3	1:K:8:LYS:O	2.19	0.43
1:B:229:GLN:NE2	1:B:236:LYS:H	2.14	0.42
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.55	0.42
1:R:239:TYR:HB3	1:R:266:MET:HB3	2.01	0.42
2:I:134:PRO:HG2	2:I:137:LYS:HB2	2.01	0.42
1:H:18:LYS:O	5:H:1479:EDO:H12	2.20	0.42
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.54	0.42
1:V:151:HYP:HD23	1:V:319:ARG:O	2.19	0.42
5:T:1141:EDO:H21	6:T:2042:HOH:O	2.19	0.42
6:E:2153:HOH:O	1:K:267:HIS:HE1	2.01	0.42
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.84	0.42
2:J:127:LYS:HG2	2:J:127:LYS:H	1.63	0.42
2:F:137:LYS:HE3	6:F:2092:HOH:O	2.18	0.42
2:M:130:ARG:HB3	2:M:130:ARG:HE	1.45	0.42
1:R:151:HYP:HD23	1:R:319:ARG:O	2.20	0.42
1:R:383:HIS:CE1	1:R:385:TRP:HB2	2.54	0.42
1:K:201:KCX:HB2	1:K:239:TYR:CD2	2.55	0.42
1:A:197:LEU:HG	1:A:417:ALA:HB1	2.00	0.42
1:H:436:ASP:OD2	1:H:439:ARG:HD3	2.20	0.42
1:A:165:TYR:CD1	2:I:117:GLN:HB3	2.55	0.42
1:R:175:LYS:HA	1:R:176:PRO:C	2.40	0.42
6:H:2128:HOH:O	1:V:161:LYS:HE2	2.19	0.42
2:W:8:ASN:CB	2:W:131:ASP:HA	2.40	0.42
1:K:165:TYR:CD1	2:P:117:GLN:HB3	2.54	0.42
1:O:134:ARG:HA	1:O:308:GLY:O	2.20	0.42
1:E:277:ASN:HD21	1:E:293:ILE:CD1	2.33	0.41
2:T:67:TYR:C	2:T:67:TYR:CD2	2.93	0.41
1:A:134:ARG:HA	1:A:308:GLY:O	2.20	0.41
2:I:8:ASN:CB	2:I:131:ASP:HA	2.41	0.41
1:B:197:LEU:HG	1:B:417:ALA:HB1	2.01	0.41
2:I:127:LYS:H	2:I:127:LYS:HG2	1.61	0.41
1:A:436:ASP:OD2	1:A:439:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:382:ILE:HA	1:R:386:HIS:CD2	2.56	0.41
1:H:200:THR:OG1	1:H:238:HIS:CD2	2.72	0.41
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.70	0.41
2:M:8:ASN:CB	2:M:131:ASP:HA	2.40	0.41
1:V:382:ILE:HA	1:V:386:HIS:CD2	2.55	0.41
1:H:299:ALA:HA	1:H:302:ASP:OD1	2.21	0.41
2:C:107:LEU:O	2:C:120:GLY:HA2	2.19	0.41
1:O:177:LYS:HB2	1:V:62:SER:O	2.21	0.41
1:V:255:VAL:O	1:V:259[B]:GLU:HG2	2.21	0.41
1:E:175:LYS:HA	1:E:176:PRO:C	2.41	0.41
1:V:200:THR:OG1	1:V:238:HIS:CD2	2.71	0.41
1:H:277:ASN:HD21	1:H:293:ILE:HD12	1.85	0.41
1:H:293:ILE:HG13	1:H:318:LEU:HD21	2.02	0.41
1:K:383:HIS:CE1	1:K:385:TRP:HB2	2.55	0.41
1:V:383:HIS:N	1:V:386:HIS:HD2	2.05	0.41
2:T:39:ILE:O	2:T:109:ALA:HA	2.21	0.41
2:F:32[A]:TYR:CE2	2:F:38:TRP:HZ3	2.39	0.41
1:V:165:TYR:CD1	2:W:117:GLN:HB3	2.55	0.41
1:O:62:SER:O	1:V:177:LYS:HB2	2.21	0.41
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.56	0.41
1:A:277:ASN:HD21	1:A:293:ILE:HD12	1.85	0.41
1:A:386:HIS:HE1	6:A:2179:HOH:O	2.04	0.41
1:A:177:LYS:HB2	1:B:62:SER:O	2.21	0.41
1:B:241:ASN:ND2	1:B:243:THR:H	2.19	0.41
1:A:201:KCX:HB2	1:A:239:TYR:CD2	2.56	0.41
2:W:130:ARG:HE	2:W:130:ARG:HB3	1.51	0.41
1:K:200:THR:OG1	1:K:238:HIS:CD2	2.69	0.40
1:K:299:ALA:HA	1:K:302:ASP:OD1	2.21	0.40
1:O:152:PRO:HB2	1:O:153:HIS:CD2	2.56	0.40
1:V:292:HIS:HA	1:V:325:HIS:HB2	2.02	0.40
2:W:127:LYS:HG2	2:W:127:LYS:H	1.63	0.40
1:K:439:ARG:HH11	1:K:439:ARG:HG2	1.87	0.40
1:O:7:THR:N	6:O:2001:HOH:O	2.54	0.40
1:K:197:LEU:HG	1:K:417:ALA:HB1	2.03	0.40
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.57	0.40
2:F:39:ILE:O	2:F:109:ALA:HA	2.21	0.40
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.57	0.40
1:O:338:GLU:HB2	1:O:471:THR:HG21	2.03	0.40
1:A:62:SER:O	1:B:177:LYS:HB2	2.21	0.40
1:V:197:LEU:HG	1:V:417:ALA:HB1	2.04	0.40
1:K:175:LYS:HA	1:K:176:PRO:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.01	0.40
2:F:8:ASN:HB2	6:F:2005:HOH:O	2.20	0.40
1:O:436:ASP:OD2	1:O:439:ARG:HD3	2.19	0.40
1:E:23:THR:HB	1:E:24:TYR:CD2	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:LYS:CE	1:R:460:GLU:OE2[2_646]	1.53	0.67
1:K:439:ARG:NH1	1:O:88:GLU:CG[1_556]	2.08	0.12
1:K:14:LYS:NZ	1:R:460:GLU:OE2[2_646]	2.09	0.11

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	462/475 (97%)	451 (98%)	11 (2%)	0	100	100
1	B	465/475 (98%)	454 (98%)	11 (2%)	0	100	100
1	E	462/475 (97%)	448 (97%)	14 (3%)	0	100	100
1	H	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	K	468/475 (98%)	454 (97%)	14 (3%)	0	100	100
1	O	464/475 (98%)	453 (98%)	11 (2%)	0	100	100
1	R	461/475 (97%)	450 (98%)	11 (2%)	0	100	100
1	V	464/475 (98%)	452 (97%)	12 (3%)	0	100	100
2	C	140/140 (100%)	132 (94%)	8 (6%)	0	100	100
2	F	140/140 (100%)	134 (96%)	6 (4%)	0	100	100
2	I	139/140 (99%)	134 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	140/140 (100%)	134 (96%)	6 (4%)	0	100	100
2	M	140/140 (100%)	135 (96%)	5 (4%)	0	100	100
2	P	141/140 (101%)	135 (96%)	6 (4%)	0	100	100
2	T	141/140 (101%)	137 (97%)	4 (3%)	0	100	100
2	W	140/140 (100%)	133 (95%)	7 (5%)	0	100	100
All	All	4833/4920 (98%)	4688 (97%)	145 (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	373/377 (99%)	366 (98%)	7 (2%)	65	60
1	B	374/377 (99%)	366 (98%)	8 (2%)	61	56
1	E	373/377 (99%)	365 (98%)	8 (2%)	61	56
1	H	375/377 (100%)	368 (98%)	7 (2%)	65	60
1	K	377/377 (100%)	369 (98%)	8 (2%)	61	56
1	O	373/377 (99%)	365 (98%)	8 (2%)	61	56
1	R	372/377 (99%)	364 (98%)	8 (2%)	60	53
1	V	374/377 (99%)	367 (98%)	7 (2%)	65	60
2	C	125/123 (102%)	119 (95%)	6 (5%)	31	22
2	F	125/123 (102%)	118 (94%)	7 (6%)	26	16
2	I	124/123 (101%)	118 (95%)	6 (5%)	31	22
2	J	125/123 (102%)	119 (95%)	6 (5%)	31	22
2	M	125/123 (102%)	119 (95%)	6 (5%)	31	22
2	P	126/123 (102%)	120 (95%)	6 (5%)	31	22
2	T	126/123 (102%)	120 (95%)	6 (5%)	31	22
2	W	125/123 (102%)	119 (95%)	6 (5%)	31	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3992/4000 (100%)	3882 (97%)	110 (3%)	51 44

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	96	GLN
1	A	185	TYR
1	A	203	ASP
1	A	239	TYR
1	A	241	ASN
1	A	297	MET
1	B	94	ASP
1	B	96	GLN
1	B	185	TYR
1	B	203	ASP
1	B	219	LEU
1	B	239	TYR
1	B	241	ASN
1	B	297	MET
2	C	9	ASN
2	C	12	PHE
2	C	52	VAL
2	C	118	ILE
2	C	127	LYS
2	C	130	ARG
1	E	94	ASP
1	E	96	GLN
1	E	185	TYR
1	E	203	ASP
1	E	219	LEU
1	E	239	TYR
1	E	241	ASN
1	E	297	MET
2	F	8	ASN
2	F	9	ASN
2	F	12	PHE
2	F	52	VAL
2	F	118	ILE
2	F	127	LYS
2	F	130	ARG
1	H	94	ASP

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Mol	Chain	Res	Type
1	H	96	GLN
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	297	MET
2	I	9	ASN
2	I	12	PHE
2	I	52	VAL
2	I	118	ILE
2	I	127	LYS
2	I	130	ARG
2	J	9	ASN
2	J	12	PHE
2	J	52	VAL
2	J	118	ILE
2	J	127	LYS
2	J	130	ARG
1	K	8	LYS
1	K	94	ASP
1	K	96	GLN
1	K	185	TYR
1	K	203	ASP
1	K	239	TYR
1	K	241	ASN
1	K	297	MET
2	M	9	ASN
2	M	12	PHE
2	M	52	VAL
2	M	118	ILE
2	M	127	LYS
2	M	130	ARG
1	O	8	LYS
1	O	94	ASP
1	O	96	GLN
1	O	185	TYR
1	O	203	ASP
1	O	239	TYR
1	O	241	ASN
1	O	297	MET
2	P	9	ASN
2	P	12	PHE

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Mol	Chain	Res	Type
2	P	52	VAL
2	P	118	ILE
2	P	127	LYS
2	P	130	ARG
1	R	94	ASP
1	R	96	GLN
1	R	185	TYR
1	R	203	ASP
1	R	219	LEU
1	R	239	TYR
1	R	241	ASN
1	R	297	MET
2	T	9	ASN
2	T	12	PHE
2	T	52	VAL
2	T	118	ILE
2	T	127	LYS
2	T	130	ARG
1	V	94	ASP
1	V	96	GLN
1	V	185	TYR
1	V	203	ASP
1	V	239	TYR
1	V	241	ASN
1	V	297	MET
2	W	9	ASN
2	W	12	PHE
2	W	52	VAL
2	W	118	ILE
2	W	127	LYS
2	W	130	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN

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Mol	Chain	Res	Type
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	163	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	432	ASN
2	C	9	ASN
2	C	25	GLN
2	C	29	GLN
2	C	115	GLN
1	E	153	HIS
1	E	163	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	432	ASN
2	F	8	ASN
2	F	9	ASN
2	F	25	GLN
2	F	29	GLN
2	F	88	GLN
2	F	115	GLN
1	H	153	HIS
1	H	163	ASN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS

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Mol	Chain	Res	Type
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	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	115	GLN
1	K	153	HIS
1	K	163	ASN
1	K	229	GLN
1	K	238	HIS
1	K	241	ASN
1	K	267	HIS
1	K	277	ASN
1	K	304	GLN
1	K	386	HIS
1	K	401	GLN
1	K	432	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	115	GLN
1	O	153	HIS
1	O	156	GLN
1	O	163	ASN
1	O	229	GLN
1	O	238	HIS
1	O	241	ASN
1	O	267	HIS
1	O	277	ASN
1	O	304	GLN
1	O	386	HIS
1	O	401	GLN
1	O	432	ASN
2	P	9	ASN
2	P	25	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	104	1	7,8,9	0.79	0	5,10,12	3.08	4 (80%)
1	HYP	A	151	1	7,8,9	0.97	1 (14%)	5,10,12	4.05	4 (80%)
1	KCX	A	201	1,3	7,11,12	0.80	0	7,12,14	0.75	0
1	SMC	A	256	1	5,6,7	1.34	1 (20%)	2,6,8	1.76	1 (50%)
1	SMC	A	369	1	5,6,7	0.75	0	2,6,8	1.50	0
1	HYP	B	104	1	7,8,9	0.71	0	5,10,12	2.90	3 (60%)
1	HYP	B	151	1	7,8,9	1.19	1 (14%)	5,10,12	3.55	4 (80%)
1	KCX	B	201	1,3	7,11,12	1.00	1 (14%)	7,12,14	0.87	0
1	SMC	B	256	1	5,6,7	1.28	1 (20%)	2,6,8	1.32	0
1	SMC	B	369	1	5,6,7	0.78	0	2,6,8	1.21	0
1	HYP	E	104	1	7,8,9	0.85	0	5,10,12	3.21	4 (80%)
1	HYP	E	151	1	7,8,9	1.04	0	5,10,12	3.66	4 (80%)
1	KCX	E	201	1,3	7,11,12	0.89	0	7,12,14	1.31	1 (14%)
1	SMC	E	256	1	5,6,7	0.82	0	2,6,8	1.73	1 (50%)
1	SMC	E	369	1	5,6,7	1.66	1 (20%)	2,6,8	1.01	0
1	HYP	H	104	1	7,8,9	0.94	1 (14%)	5,10,12	3.18	4 (80%)
1	HYP	H	151	1	7,8,9	0.99	0	5,10,12	3.70	4 (80%)
1	KCX	H	201	1,3	7,11,12	0.86	0	7,12,14	1.05	1 (14%)
1	SMC	H	256	1	5,6,7	1.09	1 (20%)	2,6,8	1.55	1 (50%)
1	SMC	H	369	1	5,6,7	0.97	0	2,6,8	1.30	0
1	HYP	K	104	1	7,8,9	0.78	0	5,10,12	3.14	4 (80%)
1	HYP	K	151	1	7,8,9	1.05	1 (14%)	5,10,12	3.80	4 (80%)
1	KCX	K	201	1,3	7,11,12	0.82	0	7,12,14	0.95	0
1	SMC	K	256	1	5,6,7	1.71	1 (20%)	2,6,8	1.39	0
1	SMC	K	369	1	5,6,7	1.25	1 (20%)	2,6,8	1.36	0
1	HYP	O	104	1	7,8,9	0.82	0	5,10,12	3.00	4 (80%)
1	HYP	O	151	1	7,8,9	1.16	1 (14%)	5,10,12	3.69	4 (80%)
1	KCX	O	201	1,3	7,11,12	0.81	0	7,12,14	1.09	1 (14%)
1	SMC	O	256	1	5,6,7	1.01	1 (20%)	2,6,8	1.85	1 (50%)
1	SMC	O	369	1	5,6,7	0.79	0	2,6,8	1.31	0
1	HYP	R	104	1	7,8,9	0.73	0	5,10,12	3.29	4 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	R	151	1	7,8,9	1.17	1 (14%)	5,10,12	3.66	4 (80%)
1	KCX	R	201	1,3	7,11,12	0.66	0	7,12,14	1.07	0
1	SMC	R	256	1	5,6,7	1.03	1 (20%)	2,6,8	1.45	1 (50%)
1	SMC	R	369	1	5,6,7	1.12	1 (20%)	2,6,8	1.21	0
1	HYP	V	104	1	7,8,9	0.83	0	5,10,12	2.99	3 (60%)
1	HYP	V	151	1	7,8,9	1.08	1 (14%)	5,10,12	3.65	4 (80%)
1	KCX	V	201	1,3	7,11,12	0.91	0	7,12,14	1.08	0
1	SMC	V	256	1	5,6,7	1.31	1 (20%)	2,6,8	1.80	1 (50%)
1	SMC	V	369	1	5,6,7	1.21	1 (20%)	2,6,8	1.27	0

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

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

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	256	SMC	CB-SG	-3.71	1.76	1.80
1	E	369	SMC	CB-SG	-3.61	1.76	1.80
1	A	256	SMC	CB-SG	-2.88	1.77	1.80
1	V	256	SMC	CB-SG	-2.75	1.77	1.80
1	B	256	SMC	CB-SG	-2.72	1.77	1.80
1	V	369	SMC	CB-SG	-2.57	1.77	1.80
1	K	369	SMC	CB-SG	-2.53	1.78	1.80
1	V	151	HYP	CA-N	-2.48	1.44	1.47
1	R	151	HYP	CA-N	-2.40	1.44	1.47
1	O	151	HYP	CA-N	-2.38	1.44	1.47
1	B	151	HYP	CA-N	-2.31	1.44	1.47
1	R	369	SMC	CB-SG	-2.31	1.78	1.80
1	H	256	SMC	CB-SG	-2.28	1.78	1.80
1	H	104	HYP	CA-N	-2.19	1.44	1.47
1	R	256	SMC	CB-SG	-2.17	1.78	1.80
1	K	151	HYP	CA-N	-2.14	1.44	1.47
1	A	151	HYP	CA-N	-2.01	1.45	1.47
1	O	256	SMC	CB-SG	-2.00	1.78	1.80
1	B	201	KCX	CE-NZ	2.18	1.51	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	HYP	OD1-CG-CD	-5.83	97.81	110.47
1	K	151	HYP	OD1-CG-CD	-4.93	99.77	110.47
1	V	151	HYP	OD1-CG-CD	-4.91	99.80	110.47
1	H	151	HYP	OD1-CG-CD	-4.66	100.36	110.47
1	B	151	HYP	OD1-CG-CB	-4.49	97.98	110.00
1	O	151	HYP	OD1-CG-CD	-4.47	100.77	110.47
1	E	151	HYP	OD1-CG-CD	-4.44	100.83	110.47
1	R	151	HYP	OD1-CG-CB	-4.43	98.15	110.00
1	R	151	HYP	OD1-CG-CD	-4.27	101.20	110.47
1	K	151	HYP	OD1-CG-CB	-4.08	99.06	110.00
1	O	151	HYP	OD1-CG-CB	-4.01	99.27	110.00
1	E	151	HYP	OD1-CG-CB	-3.98	99.35	110.00
1	H	151	HYP	OD1-CG-CB	-3.94	99.45	110.00
1	R	104	HYP	OD1-CG-CD	-3.91	101.98	110.47
1	E	104	HYP	OD1-CG-CD	-3.87	102.07	110.47
1	K	104	HYP	OD1-CG-CD	-3.77	102.28	110.47
1	A	151	HYP	OD1-CG-CB	-3.76	99.93	110.00
1	B	151	HYP	OD1-CG-CD	-3.74	102.36	110.47
1	V	151	HYP	OD1-CG-CB	-3.74	99.99	110.00
1	R	104	HYP	OD1-CG-CB	-3.57	100.43	110.00
1	H	104	HYP	OD1-CG-CB	-3.56	100.46	110.00
1	V	104	HYP	OD1-CG-CB	-3.52	100.56	110.00
1	B	104	HYP	OD1-CG-CB	-3.51	100.61	110.00
1	O	104	HYP	OD1-CG-CB	-3.48	100.67	110.00
1	H	104	HYP	OD1-CG-CD	-3.31	103.29	110.47
1	O	104	HYP	OD1-CG-CD	-3.24	103.42	110.47
1	A	104	HYP	OD1-CG-CD	-3.23	103.46	110.47
1	A	104	HYP	OD1-CG-CB	-3.10	101.70	110.00
1	K	104	HYP	OD1-CG-CB	-2.99	101.99	110.00
1	E	201	KCX	CE-NZ-CX	-2.83	120.29	123.49
1	E	104	HYP	OD1-CG-CB	-2.81	102.46	110.00
1	H	151	HYP	O-C-CA	-2.53	118.76	125.44
1	V	151	HYP	O-C-CA	-2.38	119.15	125.44
1	A	151	HYP	O-C-CA	-2.35	119.23	125.44
1	B	104	HYP	OD1-CG-CD	-2.34	105.39	110.47
1	O	256	SMC	O-C-CA	-2.34	119.41	125.49
1	E	256	SMC	O-C-CA	-2.33	119.43	125.49
1	V	104	HYP	OD1-CG-CD	-2.31	105.45	110.47
1	O	151	HYP	O-C-CA	-2.29	119.38	125.44
1	R	151	HYP	O-C-CA	-2.29	119.39	125.44
1	K	151	HYP	O-C-CA	-2.28	119.43	125.44
1	E	151	HYP	O-C-CA	-2.27	119.44	125.44
1	H	256	SMC	O-C-CA	-2.18	119.81	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	104	HYP	O-C-CA	-2.18	119.68	125.44
1	A	256	SMC	O-C-CA	-2.12	119.96	125.49
1	A	104	HYP	O-C-CA	-2.12	119.84	125.44
1	H	104	HYP	O-C-CA	-2.12	119.85	125.44
1	V	256	SMC	O-C-CA	-2.11	119.98	125.49
1	O	201	KCX	CE-NZ-CX	-2.09	121.12	123.49
1	E	104	HYP	O-C-CA	-2.09	119.93	125.44
1	H	201	KCX	CE-NZ-CX	-2.08	121.14	123.49
1	B	151	HYP	O-C-CA	-2.01	120.13	125.44
1	K	104	HYP	O-C-CA	-2.01	120.14	125.44
1	O	104	HYP	O-C-CA	-2.00	120.15	125.44
1	R	256	SMC	O-C-CA	-2.00	120.28	125.49
1	O	104	HYP	CB-CG-CD	4.19	108.32	103.14
1	B	104	HYP	CB-CG-CD	4.50	108.70	103.14
1	R	104	HYP	CB-CG-CD	4.55	108.76	103.14
1	K	104	HYP	CB-CG-CD	4.59	108.81	103.14
1	H	104	HYP	CB-CG-CD	4.66	108.90	103.14
1	V	104	HYP	CB-CG-CD	4.69	108.94	103.14
1	A	104	HYP	CB-CG-CD	4.71	108.97	103.14
1	V	151	HYP	CB-CG-CD	4.76	109.03	103.14
1	E	104	HYP	CB-CG-CD	4.88	109.17	103.14
1	R	151	HYP	CB-CG-CD	4.90	109.20	103.14
1	B	151	HYP	CB-CG-CD	4.90	109.20	103.14
1	H	151	HYP	CB-CG-CD	4.96	109.27	103.14
1	K	151	HYP	CB-CG-CD	5.08	109.43	103.14
1	E	151	HYP	CB-CG-CD	5.12	109.47	103.14
1	O	151	HYP	CB-CG-CD	5.14	109.49	103.14
1	A	151	HYP	CB-CG-CD	5.28	109.67	103.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	151	HYP	2	0
1	A	201	KCX	1	0
1	B	151	HYP	2	0
1	E	151	HYP	1	0
1	H	151	HYP	1	0
1	K	151	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	201	KCX	1	0
1	O	151	HYP	1	0
1	R	151	HYP	1	0
1	V	151	HYP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 71 ligands modelled in this entry, 8 are monoatomic - leaving 63 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CAP	A	1477	3	14,20,20	0.68	0	15,31,31	0.86	0
5	EDO	A	1478	-	3,3,3	0.45	0	2,2,2	0.19	0
5	EDO	A	1479	-	3,3,3	0.30	0	2,2,2	0.40	0
5	EDO	A	1480	-	3,3,3	0.31	0	2,2,2	0.44	0
5	EDO	A	1481	-	3,3,3	0.35	0	2,2,2	0.28	0
5	EDO	A	1482	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	A	1483	-	3,3,3	0.35	0	2,2,2	0.22	0
4	CAP	B	1477	3	14,20,20	0.83	1 (7%)	15,31,31	0.66	0
5	EDO	B	1478	-	3,3,3	0.44	0	2,2,2	0.16	0
5	EDO	B	1479	-	3,3,3	0.33	0	2,2,2	0.49	0
5	EDO	B	1480	-	3,3,3	0.35	0	2,2,2	0.27	0
5	EDO	B	1481	-	3,3,3	0.32	0	2,2,2	0.37	0
5	EDO	B	1482	-	3,3,3	0.32	0	2,2,2	0.44	0
5	EDO	C	1141	-	3,3,3	0.32	0	2,2,2	0.16	0
5	EDO	C	1142	-	3,3,3	0.33	0	2,2,2	0.54	0
4	CAP	E	1477	3	14,20,20	0.59	0	15,31,31	0.96	2 (13%)
5	EDO	E	1478	-	3,3,3	0.35	0	2,2,2	0.09	0
5	EDO	E	1479	-	3,3,3	0.30	0	2,2,2	0.34	0
5	EDO	E	1480	-	3,3,3	0.35	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	E	1481	-	3,3,3	0.38	0	2,2,2	0.17	0
5	EDO	E	1482	-	3,3,3	0.28	0	2,2,2	0.23	0
5	EDO	H	1477	-	3,3,3	0.36	0	2,2,2	0.46	0
5	EDO	H	1478	-	3,3,3	0.39	0	2,2,2	0.44	0
5	EDO	H	1479	-	3,3,3	0.35	0	2,2,2	0.10	0
5	EDO	H	1480	-	3,3,3	0.36	0	2,2,2	0.25	0
5	EDO	H	1481	-	3,3,3	0.33	0	2,2,2	0.31	0
5	EDO	H	1482	-	3,3,3	0.32	0	2,2,2	0.25	0
5	EDO	I	1141	-	3,3,3	0.29	0	2,2,2	0.32	0
5	EDO	J	1141	-	3,3,3	0.33	0	2,2,2	0.26	0
5	EDO	J	1142	-	3,3,3	0.29	0	2,2,2	0.45	0
5	EDO	K	1477	-	3,3,3	0.45	0	2,2,2	0.07	0
5	EDO	K	1478	-	3,3,3	0.32	0	2,2,2	0.40	0
5	EDO	K	1479	-	3,3,3	0.30	0	2,2,2	0.43	0
5	EDO	K	1480	-	3,3,3	0.38	0	2,2,2	0.10	0
5	EDO	K	1481	-	3,3,3	0.36	0	2,2,2	0.15	0
5	EDO	M	1141	-	3,3,3	0.30	0	2,2,2	0.26	0
5	EDO	M	1142	-	3,3,3	0.33	0	2,2,2	0.29	0
4	CAP	O	1476	3	14,20,20	0.68	0	15,31,31	0.74	0
4	CAP	O	1478	3	14,20,20	0.80	0	15,31,31	0.75	0
5	EDO	O	1479	-	3,3,3	0.43	0	2,2,2	0.24	0
5	EDO	O	1480	-	3,3,3	0.32	0	2,2,2	0.32	0
5	EDO	O	1481	-	3,3,3	0.36	0	2,2,2	0.29	0
5	EDO	O	1482	-	3,3,3	0.39	0	2,2,2	0.35	0
5	EDO	O	1483	-	3,3,3	0.33	0	2,2,2	0.52	0
5	EDO	O	1484	-	3,3,3	0.35	0	2,2,2	0.31	0
5	EDO	P	1141	-	3,3,3	0.32	0	2,2,2	0.31	0
5	EDO	P	1142	-	3,3,3	0.31	0	2,2,2	0.33	0
4	CAP	R	1476	3	14,20,20	0.72	0	15,31,31	0.76	0
4	CAP	R	1478	3	14,20,20	0.69	0	15,31,31	0.77	0
5	EDO	R	1479	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	R	1480	-	3,3,3	0.33	0	2,2,2	0.32	0
5	EDO	R	1481	-	3,3,3	0.36	0	2,2,2	0.42	0
5	EDO	R	1482	-	3,3,3	0.37	0	2,2,2	0.07	0
5	EDO	T	1141	-	3,3,3	0.32	0	2,2,2	0.26	0
5	EDO	T	1142	-	3,3,3	0.29	0	2,2,2	0.63	0
4	CAP	V	1476	3	14,20,20	0.90	1 (7%)	15,31,31	0.77	0
5	EDO	V	1478	-	3,3,3	0.39	0	2,2,2	0.26	0
5	EDO	V	1479	-	3,3,3	0.33	0	2,2,2	0.52	0
5	EDO	V	1480	-	3,3,3	0.34	0	2,2,2	0.42	0
5	EDO	V	1481	-	3,3,3	0.38	0	2,2,2	0.16	0
5	EDO	V	1482	-	3,3,3	0.30	0	2,2,2	0.27	0
5	EDO	W	1141	-	3,3,3	0.34	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	W	1142	-	3,3,3	0.32	0	2,2,2	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	A	1477	3	-	0/23/29/29	0/0/0/0
5	EDO	A	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1483	-	-	0/1/1/1	0/0/0/0
4	CAP	B	1477	3	-	0/23/29/29	0/0/0/0
5	EDO	B	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1142	-	-	0/1/1/1	0/0/0/0
4	CAP	E	1477	3	-	0/23/29/29	0/0/0/0
5	EDO	E	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	E	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	H	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	I	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	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	1477	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	K	1481	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	M	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	M	1142	-	-	0/1/1/1	0/0/0/0
4	CAP	O	1476	3	-	0/23/29/29	0/0/0/0
4	CAP	O	1478	3	-	0/23/29/29	0/0/0/0
5	EDO	O	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1483	-	-	0/1/1/1	0/0/0/0
5	EDO	O	1484	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	P	1142	-	-	0/1/1/1	0/0/0/0
4	CAP	R	1476	3	-	0/23/29/29	0/0/0/0
4	CAP	R	1478	3	-	0/23/29/29	0/0/0/0
5	EDO	R	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	R	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	T	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	T	1142	-	-	0/1/1/1	0/0/0/0
4	CAP	V	1476	3	-	0/23/29/29	0/0/0/0
5	EDO	V	1478	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1479	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1480	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1481	-	-	0/1/1/1	0/0/0/0
5	EDO	V	1482	-	-	0/1/1/1	0/0/0/0
5	EDO	W	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	W	1142	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1477	CAP	O2-C2	2.11	1.46	1.43
4	V	1476	CAP	O2-C2	2.41	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1477	CAP	O3-C3-C4	2.08	113.37	108.91
4	E	1477	CAP	O5-P2-O4P	2.56	113.67	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1483	EDO	4	0
5	E	1482	EDO	3	0
5	H	1477	EDO	1	0
5	H	1479	EDO	1	0
5	I	1141	EDO	1	0
5	J	1141	EDO	1	0
5	K	1477	EDO	1	0
5	R	1482	EDO	1	0
5	T	1141	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	460/475 (96%)	-0.61	6 (1%)	79	83	12, 15, 28, 43	0
1	B	462/475 (97%)	-0.57	7 (1%)	76	81	12, 15, 28, 43	0
1	E	460/475 (96%)	-0.58	8 (1%)	73	78	12, 15, 28, 43	0
1	H	464/475 (97%)	-0.55	11 (2%)	62	68	12, 15, 29, 52	0
1	K	464/475 (97%)	-0.55	10 (2%)	65	71	12, 15, 29, 52	0
1	O	464/475 (97%)	-0.55	8 (1%)	73	78	12, 15, 29, 51	0
1	R	460/475 (96%)	-0.56	7 (1%)	76	81	12, 15, 28, 43	0
1	V	461/475 (97%)	-0.58	3 (0%)	89	91	12, 15, 28, 43	0
2	C	140/140 (100%)	-0.17	5 (3%)	46	53	13, 20, 33, 41	0
2	F	140/140 (100%)	-0.21	4 (2%)	55	62	13, 20, 33, 41	0
2	I	140/140 (100%)	-0.18	3 (2%)	67	72	13, 20, 33, 41	0
2	J	140/140 (100%)	-0.23	5 (3%)	46	53	13, 20, 33, 41	0
2	M	140/140 (100%)	-0.28	2 (1%)	78	82	13, 20, 33, 41	0
2	P	140/140 (100%)	-0.28	4 (2%)	55	62	13, 20, 33, 41	0
2	T	140/140 (100%)	-0.08	6 (4%)	39	44	13, 20, 33, 41	0
2	W	140/140 (100%)	-0.20	2 (1%)	78	82	13, 20, 33, 41	0
All	All	4815/4920 (97%)	-0.48	91 (1%)	70	75	12, 16, 30, 52	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	10	GLY	11.3
1	O	7	THR	5.7
2	T	130	ARG	5.4
1	E	92	GLY	5.0
1	E	11	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	O	8	LYS	4.5
1	K	8	LYS	4.5
1	E	91	PRO	4.3
1	H	94	ASP	4.3
1	O	94	ASP	4.2
1	H	10	GLY	4.2
2	J	130	ARG	4.2
1	K	7	THR	4.1
1	H	8	LYS	4.0
1	H	439	ARG	4.0
1	B	10	GLY	3.8
1	H	92	GLY	3.8
1	R	439	ARG	3.7
2	C	130	ARG	3.7
2	F	130	ARG	3.6
1	B	91	PRO	3.6
1	R	11	ALA	3.6
1	A	11	ALA	3.5
1	K	94	ASP	3.4
1	E	89	PRO	3.4
1	A	439	ARG	3.4
1	B	439	ARG	3.3
1	E	94	ASP	3.3
1	O	439	ARG	3.3
2	C	84	ARG	3.2
1	V	11	ALA	3.1
2	T	132	TRP	3.1
2	P	130	ARG	3.1
2	T	84	ARG	3.1
1	K	9	ALA	3.0
1	R	92	GLY	3.0
2	C	127	LYS	3.0
1	H	9	ALA	2.9
1	H	91	PRO	2.9
2	I	22	THR	2.9
1	B	9	ALA	2.9
1	H	464	GLU	2.8
1	O	9	ALA	2.8
1	K	439	ARG	2.8
1	H	7	THR	2.7
1	R	94	ASP	2.7
2	M	130	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	V	439	ARG	2.6
1	B	464	GLU	2.6
2	F	84	ARG	2.6
1	K	91	PRO	2.6
2	J	84	ARG	2.6
2	P	84	ARG	2.5
2	P	132	TRP	2.5
1	K	89	PRO	2.5
2	F	136	ASN	2.4
1	O	91	PRO	2.3
1	A	94	ASP	2.3
2	M	84	ARG	2.3
1	E	30	VAL	2.3
1	E	12	GLY	2.3
1	O	10	GLY	2.3
2	T	136	ASN	2.3
1	E	439	ARG	2.3
2	W	127	LYS	2.3
1	K	464	GLU	2.3
2	W	22	THR	2.3
1	B	450	LYS	2.2
1	R	89	PRO	2.2
2	C	136	ASN	2.2
1	A	89	PRO	2.2
2	J	132	TRP	2.2
2	F	113	GLN	2.1
2	T	23	ASP	2.1
1	A	464	GLU	2.1
1	R	450	LYS	2.1
1	K	10	GLY	2.1
1	B	94	ASP	2.1
2	C	132	TRP	2.1
2	J	136	ASN	2.1
1	R	91	PRO	2.1
2	T	127	LYS	2.1
1	A	91	PRO	2.1
1	H	438	ALA	2.1
2	I	130	ARG	2.1
1	O	464	GLU	2.0
1	H	12	GLY	2.0
2	P	134	PRO	2.0
2	I	113	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	92	GLY	2.0
2	J	127	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	H	104	8/9	0.95	0.09	-	14,14,14,14	0
1	HYP	K	151	8/9	0.97	0.07	-	12,13,13,13	0
1	SMC	A	256	7/8	0.98	0.06	-	11,13,13,13	0
1	HYP	A	104	8/9	0.95	0.08	-	13,14,14,14	0
1	SMC	O	369	7/8	0.98	0.07	-	15,16,16,17	0
1	SMC	K	256	7/8	0.99	0.05	-	11,13,13,13	0
1	KCX	R	201	12/13	0.96	0.08	-	11,12,13,14	0
1	HYP	V	151	8/9	0.94	0.08	-	12,13,13,13	0
1	HYP	H	151	8/9	0.96	0.09	-	12,13,13,13	0
1	SMC	H	369	7/8	0.97	0.07	-	15,16,16,17	0
1	HYP	V	104	8/9	0.96	0.08	-	14,14,14,14	0
1	HYP	E	104	8/9	0.97	0.07	-	14,14,14,14	0
1	SMC	R	369	7/8	0.98	0.06	-	15,16,16,17	0
1	KCX	E	201	12/13	0.98	0.07	-	11,12,13,14	0
1	HYP	O	151	8/9	0.97	0.07	-	12,13,13,13	0
1	KCX	K	201	12/13	0.98	0.08	-	11,12,13,14	0
1	HYP	A	151	8/9	0.95	0.07	-	12,13,13,13	0
1	SMC	V	256	7/8	0.97	0.07	-	11,12,13,13	0
1	HYP	R	151	8/9	0.95	0.09	-	12,13,13,13	0
1	KCX	H	201	12/13	0.97	0.08	-	11,12,13,14	0
1	KCX	B	201	12/13	0.97	0.08	-	11,12,13,14	0
1	HYP	K	104	8/9	0.93	0.10	-	14,14,14,15	0
1	KCX	O	201	12/13	0.97	0.08	-	11,12,13,14	0
1	KCX	A	201	12/13	0.97	0.07	-	11,12,13,14	0
1	KCX	V	201	12/13	0.98	0.07	-	11,12,13,14	0
1	HYP	B	104	8/9	0.95	0.10	-	13,14,14,15	0
1	SMC	V	369	7/8	0.98	0.08	-	15,16,16,18	0
1	SMC	R	256	7/8	0.99	0.06	-	11,12,13,13	0
1	SMC	B	256	7/8	0.99	0.08	-	11,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	O	104	8/9	0.96	0.07	-	14,14,14,15	0
1	HYP	E	151	8/9	0.96	0.08	-	12,13,13,13	0
1	SMC	H	256	7/8	0.98	0.06	-	11,13,13,13	0
1	SMC	E	256	7/8	0.98	0.06	-	11,13,13,13	0
1	SMC	A	369	7/8	0.98	0.10	-	15,16,16,17	0
1	HYP	B	151	8/9	0.97	0.06	-	12,13,13,13	0
1	SMC	E	369	7/8	0.98	0.06	-	15,16,16,18	0
1	SMC	K	369	7/8	0.97	0.07	-	15,16,16,18	0
1	SMC	B	369	7/8	0.98	0.07	-	15,16,16,17	0
1	SMC	O	256	7/8	0.98	0.07	-	11,13,13,13	0
1	HYP	R	104	8/9	0.97	0.06	-	14,14,14,14	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, 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	H	1482	4/4	0.96	0.16	8.10	30,30,30,31	0
5	EDO	B	1482	4/4	0.94	0.13	6.02	28,29,29,29	0
5	EDO	O	1483	4/4	0.94	0.14	5.58	27,30,31,31	0
5	EDO	K	1481	4/4	0.91	0.17	5.56	28,29,30,30	0
5	EDO	E	1479	4/4	0.93	0.12	4.80	25,27,27,27	0
5	EDO	T	1141	4/4	0.96	0.14	4.28	26,26,27,28	0
5	EDO	A	1480	4/4	0.89	0.13	3.95	31,31,31,32	0
5	EDO	E	1482	4/4	0.95	0.14	3.64	21,21,21,21	0
5	EDO	O	1484	4/4	0.94	0.13	3.64	24,24,25,26	0
5	EDO	H	1480	4/4	0.85	0.15	3.55	33,33,33,33	0
5	EDO	W	1141	4/4	0.92	0.15	3.54	30,32,32,33	0
5	EDO	V	1480	4/4	0.87	0.15	3.38	25,28,29,30	0
5	EDO	K	1479	4/4	0.88	0.15	3.16	29,29,29,29	0
5	EDO	H	1479	4/4	0.94	0.11	3.08	26,28,29,30	0
5	EDO	K	1477	4/4	0.90	0.15	2.84	19,19,20,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	A	1482	4/4	0.96	0.11	2.83	25,25,27,28	0
5	EDO	A	1483	4/4	0.93	0.13	2.47	18,18,18,20	0
5	EDO	I	1141	4/4	0.91	0.15	2.20	39,42,43,45	0
5	EDO	M	1141	4/4	0.82	0.17	2.09	42,42,43,43	0
5	EDO	R	1481	4/4	0.90	0.12	2.03	22,23,25,26	0
5	EDO	O	1481	4/4	0.90	0.12	1.95	23,25,25,26	0
5	EDO	B	1478	4/4	0.95	0.11	1.76	13,13,14,15	0
5	EDO	B	1480	4/4	0.86	0.13	1.69	26,27,27,27	0
5	EDO	H	1477	4/4	0.96	0.10	1.54	17,18,18,19	0
5	EDO	W	1142	4/4	0.87	0.18	1.45	36,38,39,39	0
5	EDO	H	1478	4/4	0.94	0.12	1.36	20,21,21,21	0
5	EDO	C	1141	4/4	0.94	0.12	1.29	25,28,28,33	0
5	EDO	V	1482	4/4	0.97	0.10	1.16	25,25,26,27	0
5	EDO	E	1478	4/4	0.97	0.09	1.15	15,16,17,18	0
5	EDO	V	1478	4/4	0.96	0.09	0.65	14,15,15,17	0
5	EDO	R	1480	4/4	0.96	0.09	0.63	18,19,20,21	0
5	EDO	A	1478	4/4	0.95	0.10	0.59	15,15,16,17	0
5	EDO	J	1141	4/4	0.91	0.09	0.45	32,33,33,34	0
5	EDO	J	1142	4/4	0.94	0.13	0.29	31,33,35,37	0
5	EDO	E	1480	4/4	0.95	0.10	0.22	26,27,27,28	0
5	EDO	A	1479	4/4	0.96	0.09	0.04	21,21,22,23	0
5	EDO	M	1142	4/4	0.78	0.18	-0.00	48,50,50,50	0
5	EDO	P	1142	4/4	0.96	0.10	-0.12	28,30,32,34	0
5	EDO	T	1142	4/4	0.96	0.11	-0.25	25,28,29,31	0
5	EDO	O	1479	4/4	0.97	0.08	-0.25	15,16,16,17	0
5	EDO	V	1479	4/4	0.97	0.08	-0.34	20,21,22,23	0
5	EDO	B	1479	4/4	0.97	0.08	-0.42	21,21,21,22	0
5	EDO	C	1142	4/4	0.96	0.08	-0.46	25,25,26,27	0
5	EDO	O	1480	4/4	0.96	0.08	-0.65	22,23,24,24	0
3	MG	B	1476	1/1	1.00	0.07	-0.68	12,12,12,12	0
5	EDO	P	1141	4/4	0.96	0.07	-0.92	27,29,30,32	0
4	CAP	R	1476	21/21	0.98	0.07	-1.09	14,16,16,17	0
4	CAP	A	1477	21/21	0.99	0.06	-1.15	11,14,15,16	0
5	EDO	R	1479	4/4	0.98	0.07	-1.18	13,14,14,15	0
4	CAP	R	1478	21/21	0.98	0.06	-1.35	14,16,16,17	0
4	CAP	E	1477	21/21	0.98	0.06	-1.35	13,15,16,16	0
4	CAP	V	1476	21/21	0.98	0.06	-1.39	10,13,14,15	0
5	EDO	K	1478	4/4	0.97	0.07	-1.47	25,25,25,26	0
3	MG	V	1477	1/1	0.98	0.04	-1.61	13,13,13,13	0
4	CAP	B	1477	21/21	0.99	0.05	-1.91	12,13,14,15	0
4	CAP	O	1478	21/21	0.99	0.05	-1.97	12,14,16,19	0
4	CAP	O	1476	21/21	0.99	0.05	-2.06	10,13,13,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	H	1476	1/1	0.96	0.04	-2.70	14,14,14,14	0
3	MG	R	1477	1/1	0.99	0.02	-3.20	12,12,12,12	0
3	MG	A	1476	1/1	0.99	0.03	-3.23	17,17,17,17	0
3	MG	E	1476	1/1	0.97	0.04	-3.26	14,14,14,14	0
3	MG	O	1477	1/1	0.99	0.03	-6.63	13,13,13,13	0
3	MG	K	1476	1/1	0.97	0.03	-8.15	13,13,13,13	0
5	EDO	K	1480	4/4	0.95	0.14	-	23,26,26,28	0
5	EDO	V	1481	4/4	0.95	0.11	-	17,21,23,23	0
5	EDO	A	1481	4/4	0.93	0.15	-	20,22,23,23	0
5	EDO	R	1482	4/4	0.94	0.23	-	23,24,24,26	0
5	EDO	B	1481	4/4	0.94	0.11	-	26,27,27,28	0
5	EDO	H	1481	4/4	0.97	0.14	-	21,23,23,24	0
5	EDO	O	1482	4/4	0.94	0.13	-	22,24,25,26	0
5	EDO	E	1481	4/4	0.96	0.17	-	26,27,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.