



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:53 PM GMT

PDB ID : 1IR2
Title : Crystal Structure of Activated Ribulose-1,5-bisphosphateCarboxylase/oxygenase(Rubisco) from Green alga, Chlamydomonas reinhardtii Complexed with 2-Carboxyarabinitol-1,5-bisphosphate(2-CABP)
Authors : Mizohata, E.; Matsumura, H.; Okano, Y.; Kumei, M.; Takuma, H.; Onodera, J.; Kato, K.; Shibata, N.; Inoue, T.; Yokota, A.; Kai, Y.
Deposited on : 2001-09-03
Resolution : 1.84 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

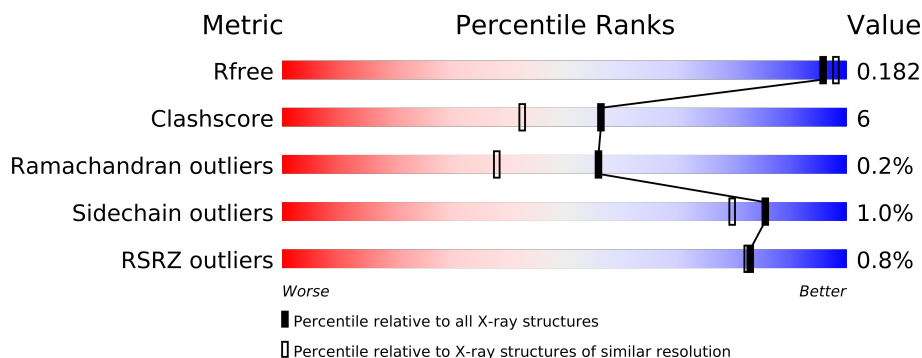
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 1.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1857 (1.86-1.82)
Clashscore	79885	2149 (1.86-1.82)
Ramachandran outliers	78287	2124 (1.86-1.82)
Sidechain outliers	78261	2125 (1.86-1.82)
RSRZ outliers	66119	1857 (1.86-1.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	
1	C	475	
1	D	475	
1	E	475	
1	F	475	
1	G	475	
1	H	475	
1	S	475	
1	T	475	
1	U	475	
1	V	475	
1	W	475	
1	X	475	

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Mol	Chain	Length	Quality of chain
1	Y	475	
1	Z	475	
2	1	140	
2	2	140	
2	3	140	
2	4	140	
2	5	140	
2	6	140	
2	7	140	
2	8	140	
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	605	-	X
5	GOL	A	613	-	X
5	GOL	B	606	-	X
5	GOL	B	614	-	X
5	GOL	C	615	-	X
5	GOL	D	608	-	X
5	GOL	D	616	-	X
5	GOL	E	601	-	X
5	GOL	E	609	-	X
5	GOL	E	620	-	X
5	GOL	F	617	-	X
5	GOL	G	611	-	X
5	GOL	G	618	-	X
5	GOL	H	604	-	X
5	GOL	H	612	-	X
5	GOL	H	619	-	X
5	GOL	S	609	-	X
5	GOL	S	613	-	X
5	GOL	T	614	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	U	607	-	X
5	GOL	V	608	-	X
5	GOL	V	616	-	X
5	GOL	W	620	-	X
5	GOL	X	610	-	X
5	GOL	X	617	-	X
5	GOL	Y	611	-	X
5	GOL	Y	618	-	X
5	GOL	Z	604	-	X
5	GOL	Z	612	-	X
5	GOL	Z	619	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 87087 atoms, of which 0 are hydrogen and 0 are deuterium.

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

^ Molecule 1 is a protein called Large subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	B	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	C	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	D	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	E	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	F	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	G	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	H	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	S	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	T	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	U	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	V	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	W	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	X	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	Y	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	Z	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	SEE REMARK 999	UNP P00877
A	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
A	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
A	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
A	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
A	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
B	46	PRO	LEU	SEE REMARK 999	UNP P00877
B	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
B	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
B	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
B	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
B	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
C	46	PRO	LEU	SEE REMARK 999	UNP P00877
C	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
C	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
C	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
C	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
C	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
D	46	PRO	LEU	SEE REMARK 999	UNP P00877
D	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
D	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
D	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
D	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
D	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
E	46	PRO	LEU	SEE REMARK 999	UNP P00877
E	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
E	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
E	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
E	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
E	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
F	46	PRO	LEU	SEE REMARK 999	UNP P00877
F	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
F	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
F	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
F	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
F	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
G	46	PRO	LEU	SEE REMARK 999	UNP P00877
G	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
G	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
G	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
G	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
G	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
H	46	PRO	LEU	SEE REMARK 999	UNP P00877
H	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
H	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
H	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
H	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
H	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
S	46	PRO	LEU	SEE REMARK 999	UNP P00877
S	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
S	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
S	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
S	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
S	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
T	46	PRO	LEU	SEE REMARK 999	UNP P00877
T	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
T	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
T	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
T	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
T	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
U	46	PRO	LEU	SEE REMARK 999	UNP P00877
U	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
U	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
U	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
U	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
U	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
V	46	PRO	LEU	SEE REMARK 999	UNP P00877
V	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
V	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
V	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
V	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
V	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
W	46	PRO	LEU	SEE REMARK 999	UNP P00877
W	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
W	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
W	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
W	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
W	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
X	46	PRO	LEU	SEE REMARK 999	UNP P00877
X	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
X	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
X	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
X	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
X	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	46	PRO	LEU	SEE REMARK 999	UNP P00877
Y	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Y	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Y	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
Y	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Y	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Z	46	PRO	LEU	SEE REMARK 999	UNP P00877
Z	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Z	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Z	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
Z	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Z	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

^ Molecule 2 is a protein called Small subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	J	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	K	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	L	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	M	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	N	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	O	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	P	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	1	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	2	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	3	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	4	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	5	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	6	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	7	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	8	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MME	MET	MODIFIED RESIDUE	UNP P08475
J	1	MME	MET	MODIFIED RESIDUE	UNP P08475
K	1	MME	MET	MODIFIED RESIDUE	UNP P08475
L	1	MME	MET	MODIFIED RESIDUE	UNP P08475
M	1	MME	MET	MODIFIED RESIDUE	UNP P08475
N	1	MME	MET	MODIFIED RESIDUE	UNP P08475
O	1	MME	MET	MODIFIED RESIDUE	UNP P08475
P	1	MME	MET	MODIFIED RESIDUE	UNP P08475
1	1	MME	MET	MODIFIED RESIDUE	UNP P08475
2	1	MME	MET	MODIFIED RESIDUE	UNP P08475
3	1	MME	MET	MODIFIED RESIDUE	UNP P08475
4	1	MME	MET	MODIFIED RESIDUE	UNP P08475
5	1	MME	MET	MODIFIED RESIDUE	UNP P08475
6	1	MME	MET	MODIFIED RESIDUE	UNP P08475
7	1	MME	MET	MODIFIED RESIDUE	UNP P08475
8	1	MME	MET	MODIFIED RESIDUE	UNP P08475

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

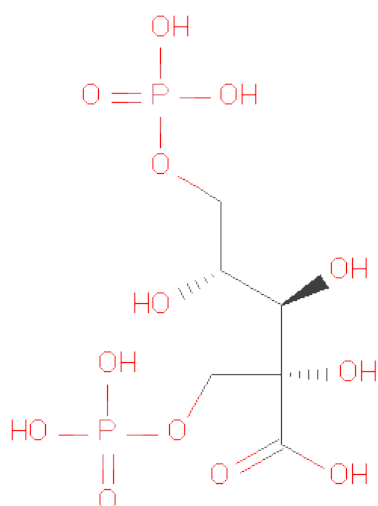
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	Z	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	T	1	Total	Mg	0	0
			1	1		
3	U	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	Y	1	Total	Mg	0	0
			1	1		
3	S	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

^ Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C₆H₁₄O₁₃P₂).



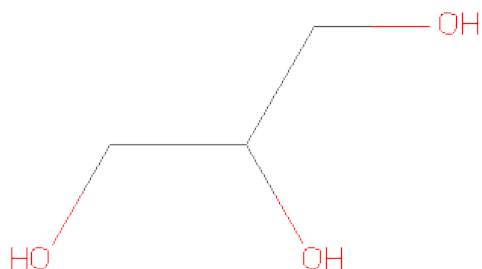
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	S	1	Total	C	O	P	0	0
			21	6	13	2		
4	T	1	Total	C	O	P	0	0
			21	6	13	2		
4	U	1	Total	C	O	P	0	0
			21	6	13	2		
4	V	1	Total	C	O	P	0	0
			21	6	13	2		
4	W	1	Total	C	O	P	0	0
			21	6	13	2		
4	X	1	Total	C	O	P	0	0
			21	6	13	2		
4	Y	1	Total	C	O	P	0	0
			21	6	13	2		
4	Z	1	Total	C	O	P	0	0
			21	6	13	2		

^ Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	F	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	W	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	Y	1	Total 6	C 3	O 3	0	0
5	Z	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0
5	V	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	Y	1	Total 6	C 3	O 3	0	0
5	Z	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	V	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		
5	Y	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		

^ Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	173	Total	O	0	0
			173	173		
6	2	173	Total	O	0	0
			173	173		
6	3	170	Total	O	0	0
			170	170		
6	4	174	Total	O	0	0
			174	174		
6	5	174	Total	O	0	0
			174	174		
6	6	146	Total	O	0	0
			146	146		
6	7	184	Total	O	0	0
			184	184		
6	8	185	Total	O	0	0
			185	185		
6	A	459	Total	O	0	0
			459	459		
6	B	406	Total	O	0	0
			406	406		
6	C	478	Total	O	0	0
			478	478		
6	D	480	Total	O	0	0
			480	480		
6	E	463	Total	O	0	0
			463	463		
6	F	450	Total	O	0	0
			450	450		

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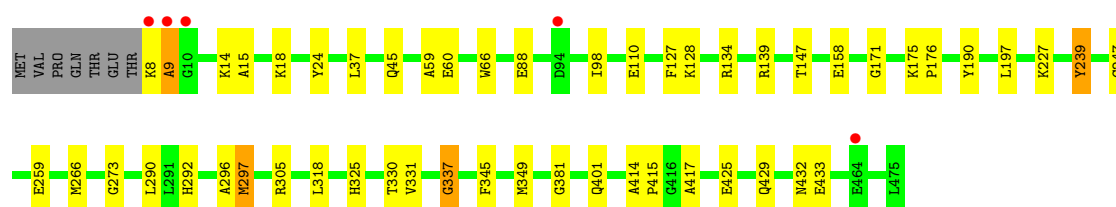
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	466	Total 466	O 466	0	0
6	H	452	Total 452	O 452	0	0
6	I	172	Total 172	O 172	0	0
6	J	170	Total 170	O 170	0	0
6	K	187	Total 187	O 187	0	0
6	L	186	Total 186	O 186	0	0
6	M	181	Total 181	O 181	0	0
6	N	186	Total 186	O 186	0	0
6	O	179	Total 179	O 179	0	0
6	P	200	Total 200	O 200	0	0
6	S	425	Total 425	O 425	0	0
6	T	426	Total 426	O 426	0	0
6	U	427	Total 427	O 427	0	0
6	V	456	Total 456	O 456	0	0
6	W	421	Total 421	O 421	0	0
6	X	450	Total 450	O 450	0	0
6	Y	426	Total 426	O 426	0	0
6	Z	474	Total 474	O 474	0	0

3 Residue-property plots

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

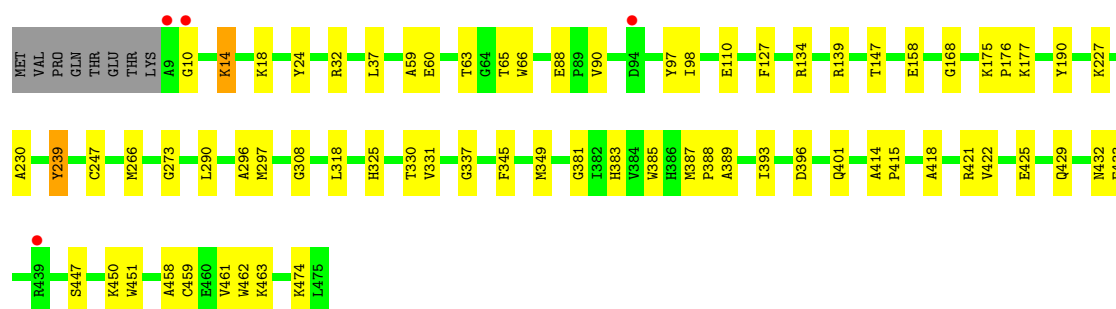
- Molecule 1: Large subunit of Rubisco

Chain A: 



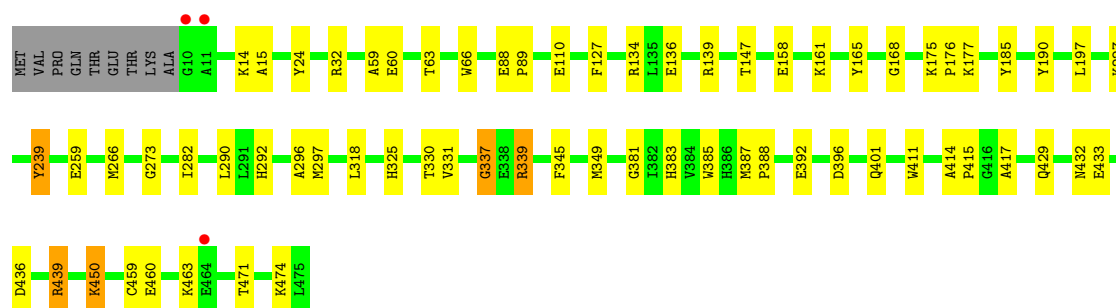
- Molecule 1: Large subunit of Rubisco

Chain B: 



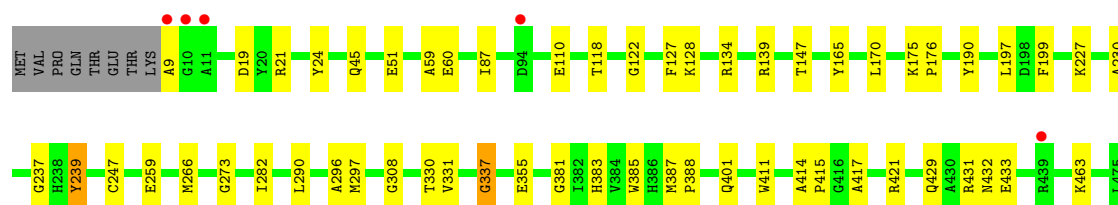
- Molecule 1: Large subunit of Rubisco

Chain C: 



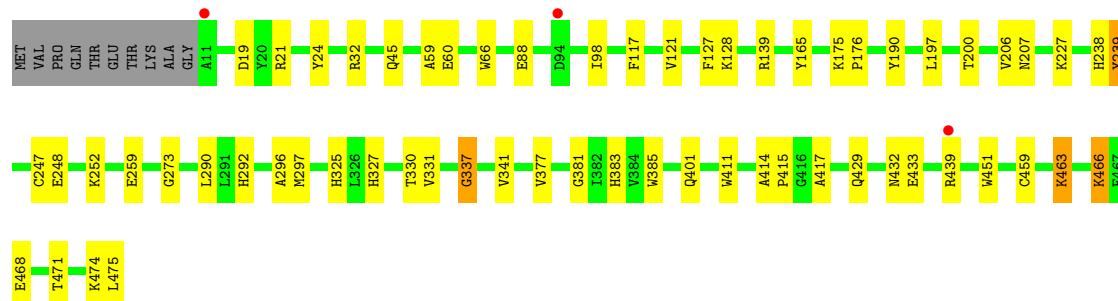
- Molecule 1: Large subunit of Rubisco

Chain D: 



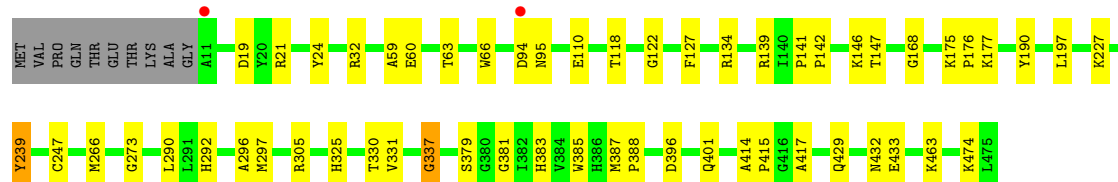
- Molecule 1: Large subunit of Rubisco

Chain E:



- Molecule 1: Large subunit of Rubisco

Chain F:



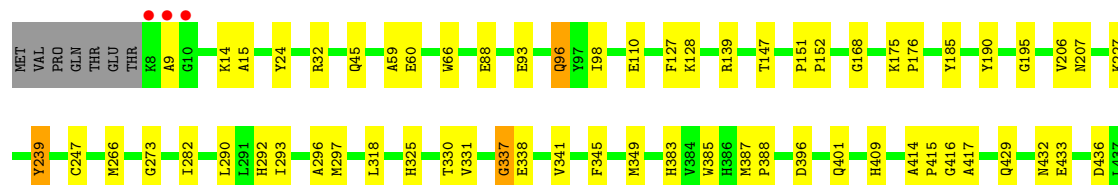
- Molecule 1: Large subunit of Rubisco

Chain G:



- Molecule 1: Large subunit of Rubisco

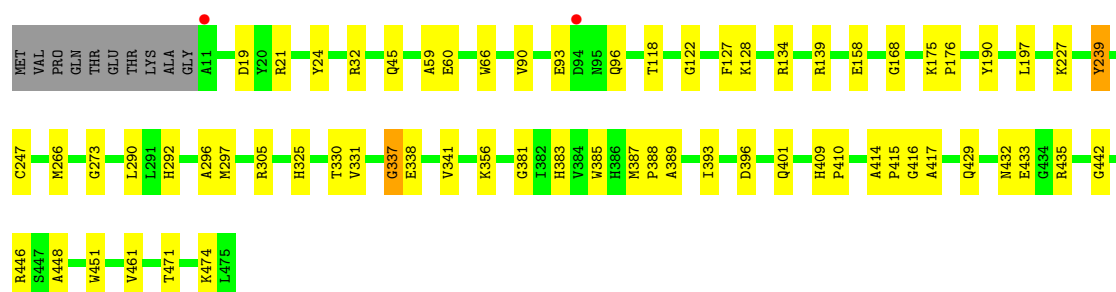
Chain H:





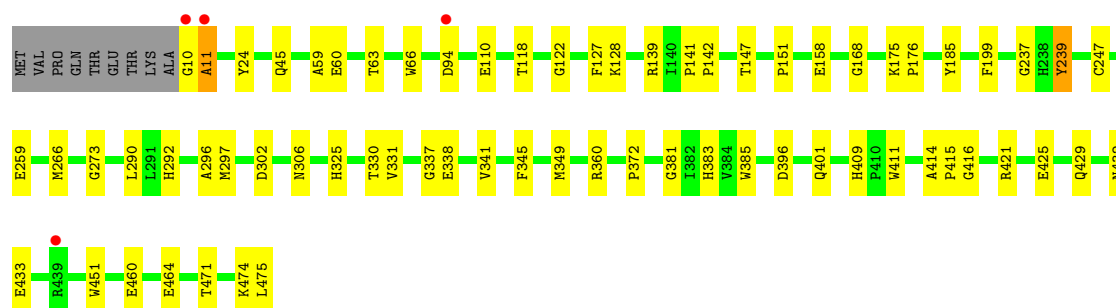
- Molecule 1: Large subunit of Rubisco

Chain S:



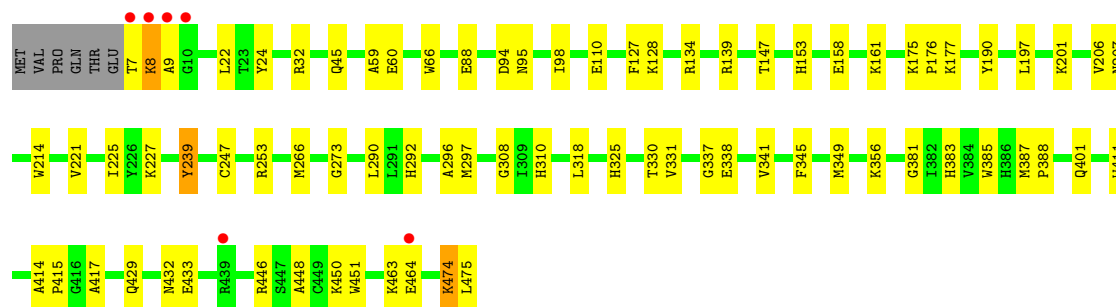
- Molecule 1: Large subunit of Rubisco

Chain T:



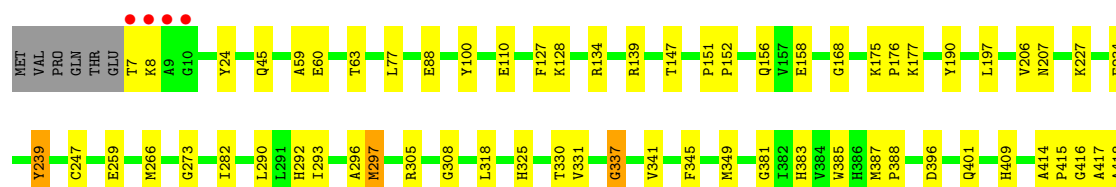
- Molecule 1: Large subunit of Rubisco

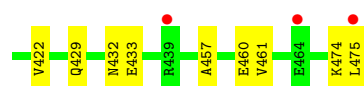
Chain U:



- Molecule 1: Large subunit of Rubisco

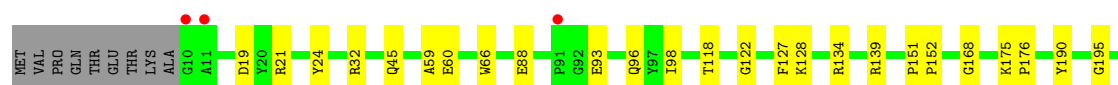
Chain V:





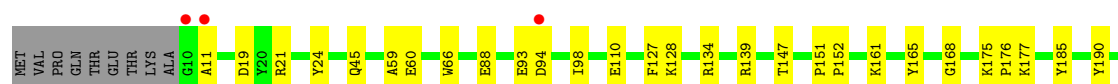
- Molecule 1: Large subunit of Rubisco

Chain W:



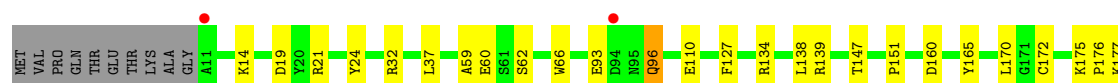
- Molecule 1: Large subunit of Rubisco

Chain X:



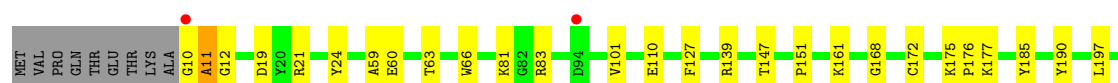
- Molecule 1: Large subunit of Rubisco

Chain Y:



- Molecule 1: Large subunit of Rubisco

Chain Z:





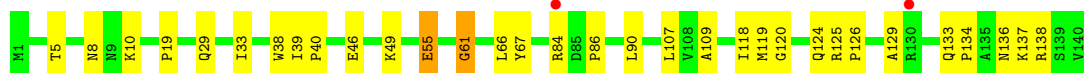
- Molecule 2: Small subunit of Rubisco

Chain I:



- Molecule 2: Small subunit of Rubisco

Chain J:



- Molecule 2: Small subunit of Rubisco

Chain K:



- Molecule 2: Small subunit of Rubisco

Chain L:



- Molecule 2: Small subunit of Rubisco

Chain M:



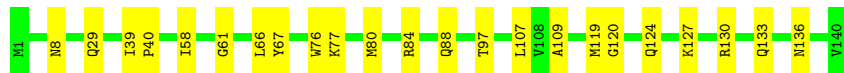
- Molecule 2: Small subunit of Rubisco

Chain N:



- Molecule 2: Small subunit of Rubisco

Chain O:



- Molecule 2: Small subunit of Rubisco

Chain P:



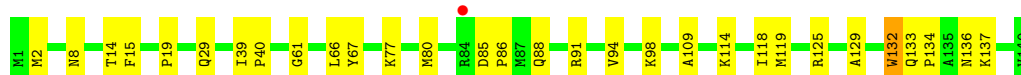
- Molecule 2: Small subunit of Rubisco

Chain 1:



- Molecule 2: Small subunit of Rubisco

Chain 2:



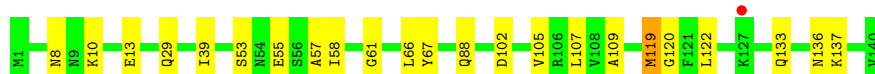
- Molecule 2: Small subunit of Rubisco

Chain 3:



- Molecule 2: Small subunit of Rubisco

Chain 4:



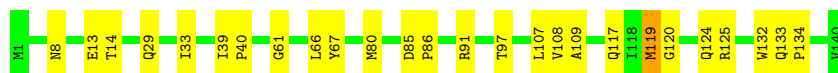
- Molecule 2: Small subunit of Rubisco

Chain 5:



- Molecule 2: Small subunit of Rubisco

Chain 6:



- Molecule 2: Small subunit of Rubisco

Chain 7:



- Molecule 2: Small subunit of Rubisco

Chain 8: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.17Å 174.75Å 222.27Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	39.89 – 1.84 40.02 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.89-1.84) 90.7 (40.02-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.84Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.152 , 0.181 0.153 , 0.182	Depositor DCC
R_{free} test set	37921 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 763081 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	87087	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CAP, 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	0.31	0/3684	0.60	0/4978
1	B	0.30	0/3675	0.61	0/4967
1	C	0.31	0/3670	0.61	0/4960
1	D	0.31	0/3675	0.61	0/4967
1	E	0.31	0/3666	0.62	0/4955
1	F	0.30	0/3666	0.60	0/4955
1	G	0.31	0/3670	0.61	0/4960
1	H	0.31	0/3684	0.62	0/4978
1	S	0.30	0/3666	0.61	0/4955
1	T	0.31	0/3670	0.61	0/4960
1	U	0.31	0/3691	0.61	0/4988
1	V	0.31	0/3691	0.62	0/4988
1	W	0.30	0/3670	0.60	0/4960
1	X	0.31	0/3670	0.60	0/4960
1	Y	0.31	0/3666	0.61	0/4955
1	Z	0.31	0/3670	0.61	0/4960
2	1	0.31	0/1169	0.60	1/1588 (0.1%)
2	2	0.30	0/1169	0.59	1/1588 (0.1%)
2	3	0.32	0/1169	0.60	1/1588 (0.1%)
2	4	0.32	0/1169	0.59	1/1588 (0.1%)
2	5	0.31	0/1169	0.61	1/1588 (0.1%)
2	6	0.31	0/1169	0.59	1/1588 (0.1%)
2	7	0.32	0/1169	0.60	1/1588 (0.1%)
2	8	0.32	0/1169	0.61	1/1588 (0.1%)
2	I	0.31	0/1169	0.59	1/1588 (0.1%)
2	J	0.30	0/1169	0.59	1/1588 (0.1%)
2	K	0.31	0/1169	0.60	1/1588 (0.1%)
2	L	0.32	0/1169	0.60	1/1588 (0.1%)
2	M	0.31	0/1169	0.60	1/1588 (0.1%)
2	N	0.31	0/1169	0.59	1/1588 (0.1%)
2	O	0.32	0/1169	0.60	1/1588 (0.1%)
2	P	0.32	0/1169	0.60	1/1588 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.31	0/77488	0.61	16/104854 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	61	GLY	N-CA-C	-6.03	98.03	113.10
2	M	61	GLY	N-CA-C	-6.02	98.05	113.10
2	J	61	GLY	N-CA-C	-5.99	98.13	113.10
2	6	61	GLY	N-CA-C	-5.97	98.17	113.10
2	L	61	GLY	N-CA-C	-5.96	98.19	113.10
2	1	61	GLY	N-CA-C	-5.96	98.20	113.10
2	8	61	GLY	N-CA-C	-5.96	98.20	113.10
2	P	61	GLY	N-CA-C	-5.93	98.26	113.10
2	N	61	GLY	N-CA-C	-5.93	98.28	113.10
2	7	61	GLY	N-CA-C	-5.86	98.45	113.10
2	I	61	GLY	N-CA-C	-5.82	98.56	113.10
2	K	61	GLY	N-CA-C	-5.78	98.65	113.10
2	4	61	GLY	N-CA-C	-5.78	98.65	113.10
2	2	61	GLY	N-CA-C	-5.58	99.15	113.10
2	5	61	GLY	N-CA-C	-5.56	99.20	113.10
2	O	61	GLY	N-CA-C	-5.25	99.98	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3646	0	3559	36	0
1	B	3637	0	3546	50	0
1	C	3632	0	3541	48	0
1	D	3637	0	3546	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3628	0	3538	41	0
1	F	3628	0	3538	39	0
1	G	3632	0	3541	37	0
1	H	3646	0	3559	42	0
1	S	3628	0	3538	47	0
1	T	3632	0	3541	44	0
1	U	3653	0	3566	65	0
1	V	3653	0	3566	47	0
1	W	3632	0	3541	46	0
1	X	3632	0	3541	39	0
1	Y	3628	0	3538	57	0
1	Z	3632	0	3541	44	0
2	1	1145	0	1119	23	0
2	2	1145	0	1119	22	0
2	3	1145	0	1119	33	0
2	4	1145	0	1119	19	0
2	5	1145	0	1119	15	0
2	6	1145	0	1119	23	0
2	7	1145	0	1119	18	0
2	8	1145	0	1119	27	0
2	I	1145	0	1119	19	0
2	J	1145	0	1119	25	0
2	K	1145	0	1119	30	0
2	L	1145	0	1119	25	0
2	M	1145	0	1119	30	0
2	N	1145	0	1119	23	0
2	O	1145	0	1119	16	0
2	P	1145	0	1119	20	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
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	8	0	0
4	C	21	0	8	0	0
4	D	21	0	7	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	8	0	0
4	H	21	0	7	0	0
4	S	21	0	7	0	0
4	T	21	0	7	0	0
4	U	21	0	8	0	0
4	V	21	0	7	0	0
4	W	21	0	8	0	0
4	X	21	0	8	0	0
4	Y	21	0	8	0	0
4	Z	21	0	8	0	0
5	A	12	0	16	1	0
5	B	18	0	24	2	0
5	C	12	0	16	1	0
5	D	12	0	16	1	0
5	E	18	0	24	0	0
5	F	12	0	16	1	0
5	G	18	0	24	0	0
5	H	18	0	24	1	0
5	S	18	0	24	0	0
5	T	12	0	16	0	0
5	U	12	0	16	0	0
5	V	12	0	16	1	0
5	W	12	0	16	1	0
5	X	18	0	24	0	0
5	Y	18	0	24	1	0
5	Z	18	0	24	0	0
6	1	173	0	0	2	0
6	2	173	0	0	1	0
6	3	170	0	0	3	0
6	4	174	0	0	2	0
6	5	174	0	0	0	0
6	6	146	0	0	2	0
6	7	184	0	0	3	0
6	8	185	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	459	0	0	1	0
6	B	406	0	0	4	0
6	C	478	0	0	2	0
6	D	480	0	0	6	0
6	E	463	0	0	3	0
6	F	450	0	0	5	0
6	G	466	0	0	3	0
6	H	452	0	0	3	0
6	I	172	0	0	3	0
6	J	170	0	0	3	0
6	K	187	0	0	3	0
6	L	186	0	0	5	0
6	M	181	0	0	5	0
6	N	186	0	0	2	0
6	O	179	0	0	0	0
6	P	200	0	0	3	0
6	S	425	0	0	5	0
6	T	426	0	0	5	0
6	U	427	0	0	7	0
6	V	456	0	0	3	0
6	W	421	0	0	6	0
6	X	450	0	0	2	0
6	Y	426	0	0	7	0
6	Z	474	0	0	5	0
All	All	87087	0	75085	975	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (975) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:8:LYS:HD2	2:8:84:ARG:HH11	1.07	1.10
1:U:8:LYS:HG2	1:U:9:ALA:H	1.00	1.08
1:A:247:CYS:HG	1:E:247:CYS:HG	1.07	0.96
1:U:8:LYS:HG2	1:U:9:ALA:N	1.84	0.92
1:D:247:CYS:HG	1:H:247:CYS:HG	1.11	0.92
1:T:306:ASN:HB3	6:T:1024:HOH:O	1.72	0.90
1:U:247:CYS:HG	1:Y:247:CYS:HG	0.90	0.89
2:3:133:GLN:OE1	2:3:137:LYS:HE2	1.73	0.89
1:U:8:LYS:HD2	2:8:84:ARG:NH1	1.87	0.88
1:D:9:ALA:HA	2:M:84:ARG:NH1	1.90	0.86
1:U:8:LYS:CG	1:U:9:ALA:H	1.83	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:247:CYS:HG	1:F:247:CYS:HG	0.83	0.83
1:S:247:CYS:HG	1:W:247:CYS:HG	0.96	0.82
2:J:126:PRO:HG2	2:J:129:ALA:HB2	1.62	0.81
2:I:130:ARG:HE	2:I:130:ARG:HA	1.45	0.80
1:T:432:ASN:HD22	2:2:29:GLN:HE22	1.28	0.80
1:U:8:LYS:CD	2:8:84:ARG:HH11	1.91	0.80
2:2:40:PRO:HG2	2:2:80:MET:HB2	1.64	0.79
1:S:338:GLU:OE1	1:S:341:VAL:HG23	1.82	0.78
1:F:432:ASN:HD22	2:N:29:GLN:HE22	1.31	0.77
1:Y:432:ASN:HD22	2:7:29:GLN:HE22	1.31	0.77
2:1:40:PRO:HG2	2:1:80:MET:HB2	1.66	0.77
1:U:474:LYS:HD3	1:U:475:LEU:O	1.84	0.77
1:C:432:ASN:HD22	2:K:29:GLN:HE22	1.33	0.77
1:A:432:ASN:HD22	2:I:29:GLN:HE22	1.32	0.77
1:V:432:ASN:HD22	2:4:29:GLN:HE22	1.32	0.76
1:S:432:ASN:HD22	2:1:29:GLN:HE22	1.33	0.76
2:3:53:SER:HB2	2:3:55:GLU:OE2	1.84	0.76
1:T:247:CYS:HG	1:X:247:CYS:HG	1.23	0.76
2:I:130:ARG:HD2	6:I:259:HOH:O	1.86	0.76
1:D:9:ALA:HA	2:M:84:ARG:HH11	1.51	0.75
2:M:137:LYS:HA	2:M:137:LYS:HE2	1.67	0.75
1:E:432:ASN:HD22	2:M:29:GLN:HE22	1.34	0.75
1:W:471:THR:O	1:W:474:LYS:HE3	1.88	0.74
1:G:432:ASN:HD22	2:O:29:GLN:HE22	1.33	0.74
2:5:40:PRO:HG2	2:5:80:MET:HB2	1.69	0.74
2:3:40:PRO:HG2	2:3:80:MET:HB2	1.70	0.74
1:U:8:LYS:HB3	2:8:84:ARG:HD3	1.69	0.73
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.70	0.73
6:D:1076:HOH:O	1:E:32:ARG:HD2	1.89	0.73
1:X:88:GLU:HG2	1:X:98:ILE:HB	1.69	0.73
2:I:130:ARG:NE	2:I:130:ARG:HA	2.03	0.73
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.71	0.73
1:D:9:ALA:HB2	6:M:197:HOH:O	1.88	0.73
2:M:109:ALA:HB3	2:M:119:MET:HG3	1.70	0.73
1:Z:151:HYP:HD22	1:Z:372:PRO:HG2	1.70	0.72
2:1:109:ALA:HB3	2:1:119:MET:HG3	1.71	0.72
1:C:471:THR:HB	1:C:474:LYS:HE3	1.72	0.72
1:Z:414:ALA:HB3	1:Z:415:PRO:HD3	1.70	0.72
1:S:414:ALA:HB3	1:S:415:PRO:HD3	1.71	0.72
2:6:119:MET:HG2	6:6:286:HOH:O	1.90	0.71
1:V:247:CYS:HG	1:Z:247:CYS:HG	0.72	0.71
1:W:334:LYS:HG3	1:W:335:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:136:ASN:OD1	2:L:137:LYS:HE3	1.90	0.71
1:H:438:ALA:HB3	1:H:439:ARG:HH11	1.55	0.71
1:X:432:ASN:HD22	2:6:29:GLN:HE22	1.38	0.71
1:U:88:GLU:HG2	1:U:98:ILE:HB	1.72	0.71
1:B:432:ASN:HD22	2:J:29:GLN:HE22	1.38	0.71
2:2:125:ARG:HD3	2:2:132:TRP:CE3	2.26	0.70
2:3:134:PRO:HD2	2:3:137:LYS:HD3	1.72	0.70
1:B:296:ALA:O	1:B:297:MET:HB3	1.89	0.70
1:U:432:ASN:HD22	2:3:29:GLN:HE22	1.37	0.70
1:D:9:ALA:HA	2:M:84:ARG:CZ	2.21	0.70
1:W:414:ALA:HB3	1:W:415:PRO:HD3	1.73	0.70
1:D:9:ALA:HB1	2:M:82:GLY:O	1.92	0.70
2:6:33:ILE:HD11	2:6:119:MET:HE2	1.74	0.69
2:7:53:SER:HB2	2:7:55:GLU:OE2	1.90	0.69
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.72	0.69
1:A:296:ALA:O	1:A:297:MET:HB3	1.92	0.69
1:T:471:THR:HB	1:T:474:LYS:HE3	1.72	0.69
1:Z:296:ALA:O	1:Z:297:MET:HB3	1.93	0.68
2:J:10:LYS:HE3	6:J:204:HOH:O	1.91	0.68
1:H:432:ASN:HD22	2:P:29:GLN:HE22	1.41	0.68
2:L:40:PRO:HG2	2:L:80:MET:HB2	1.76	0.68
1:U:296:ALA:O	1:U:297:MET:HB3	1.93	0.68
1:D:21:ARG:NH2	1:D:51:GLU:HG3	2.08	0.68
2:K:134:PRO:HG2	2:K:137:LYS:HD3	1.74	0.68
1:E:471:THR:O	1:E:474:LYS:HE3	1.94	0.67
1:D:432:ASN:HD22	2:L:29:GLN:HE22	1.40	0.67
1:D:9:ALA:HB3	6:D:1066:HOH:O	1.94	0.67
1:T:414:ALA:HB3	1:T:415:PRO:HD3	1.77	0.67
1:C:296:ALA:O	1:C:297:MET:HB3	1.95	0.67
1:V:414:ALA:HB3	1:V:415:PRO:HD3	1.76	0.67
1:T:151:HYP:HD22	1:T:372:PRO:HG2	1.75	0.67
2:L:137:LYS:HA	2:L:137:LYS:HE2	1.77	0.66
1:T:474:LYS:HE2	6:T:1034:HOH:O	1.94	0.66
1:G:436:ASP:OD1	1:G:439:ARG:HD3	1.95	0.66
2:2:109:ALA:HB3	2:2:119:MET:HG3	1.76	0.66
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.75	0.66
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.77	0.66
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.76	0.66
1:Y:414:ALA:HB3	1:Y:415:PRO:HD3	1.77	0.66
2:3:134:PRO:HG2	2:3:137:LYS:HG2	1.77	0.66
2:5:109:ALA:HB3	2:5:119:MET:HG3	1.77	0.66
1:Y:60:GLU:HG3	1:Y:127:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10:GLY:HA3	2:O:84:ARG:NH1	2.10	0.65
1:Y:296:ALA:O	1:Y:297:MET:HB3	1.96	0.65
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.78	0.65
1:T:296:ALA:O	1:T:297:MET:HB3	1.94	0.65
6:U:912:HOH:O	2:3:10:LYS:HE3	1.95	0.65
1:Y:151:HYP:HD22	1:Y:372:PRO:HG2	1.77	0.65
2:P:80:MET:HE1	2:P:88:GLN:HG3	1.78	0.65
1:D:429:GLN:O	1:D:433:GLU:HG3	1.97	0.65
1:W:432:ASN:HD22	2:5:29:GLN:HE22	1.44	0.65
2:N:130:ARG:HH21	2:N:130:ARG:HG3	1.62	0.64
1:X:60:GLU:HG3	1:X:127:PHE:CZ	2.32	0.64
1:X:414:ALA:HB3	1:X:415:PRO:HD3	1.78	0.64
1:W:306:ASN:HB3	6:W:1026:HOH:O	1.98	0.64
1:X:296:ALA:O	1:X:297:MET:HB3	1.96	0.64
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.79	0.64
2:3:109:ALA:HB3	2:3:119:MET:HG3	1.78	0.64
1:E:296:ALA:O	1:E:297:MET:HB3	1.97	0.64
2:J:109:ALA:HB3	2:J:119:MET:HG3	1.80	0.63
1:U:474:LYS:HD3	1:U:475:LEU:N	2.14	0.63
1:D:296:ALA:O	1:D:297:MET:HB3	1.97	0.63
2:6:33:ILE:CD1	2:6:119:MET:HE2	2.29	0.63
1:H:93:GLU:HB3	1:H:96:GLN:HB2	1.80	0.63
1:X:292:HIS:HA	1:X:325:HIS:HB2	1.81	0.63
1:S:197:LEU:HG	1:S:417:ALA:HB1	1.80	0.62
1:A:8:LYS:O	1:A:9:ALA:HB2	1.99	0.62
1:S:341:VAL:HG22	6:S:1033:HOH:O	1.98	0.62
2:I:109:ALA:HB3	2:I:119:MET:HG3	1.81	0.62
2:I:8:ASN:O	2:I:133:GLN:HG2	1.99	0.62
2:P:80:MET:CE	2:P:88:GLN:HG3	2.30	0.62
2:3:53:SER:CB	2:3:55:GLU:OE2	2.46	0.62
2:7:33:ILE:HD11	2:7:119:MET:SD	2.39	0.62
2:6:108:VAL:C	2:6:119:MET:HE3	2.19	0.62
1:V:296:ALA:O	1:V:297:MET:HB3	1.99	0.62
2:O:40:PRO:HG2	2:O:80:MET:HB2	1.82	0.62
1:C:14:LYS:HE3	1:C:15:ALA:O	2.00	0.62
2:P:109:ALA:HB3	2:P:119:MET:HG3	1.82	0.61
1:U:338:GLU:HB3	1:U:341:VAL:HG12	1.81	0.61
1:E:290:LEU:HG	2:M:66:LEU:HD11	1.81	0.61
1:U:414:ALA:HB3	1:U:415:PRO:HD3	1.81	0.61
2:6:109:ALA:N	2:6:119:MET:HE3	2.14	0.61
1:B:290:LEU:HG	2:J:66:LEU:HD11	1.82	0.61
1:X:429:GLN:O	1:X:433:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:LYS:HG2	5:B:606:GOL:H32	1.82	0.60
1:W:60:GLU:HG3	1:W:127:PHE:CZ	2.36	0.60
6:N:321:HOH:O	2:O:58:ILE:HD11	2.00	0.60
1:Y:341:VAL:HG22	1:Y:475:LEU:HD13	1.84	0.60
1:H:296:ALA:O	1:H:297:MET:HB3	2.00	0.60
1:G:296:ALA:O	1:G:297:MET:HB3	2.01	0.60
6:G:655:HOH:O	2:P:49:LYS:HE2	2.00	0.60
1:Z:11:ALA:HB3	6:Z:1061:HOH:O	2.02	0.60
2:J:134:PRO:HG2	2:J:137:LYS:HG3	1.84	0.60
1:X:341:VAL:HG23	1:X:475:LEU:HD21	1.84	0.60
1:S:60:GLU:HG3	1:S:127:PHE:CZ	2.37	0.59
1:U:411:TRP:CZ3	2:3:2:MET:HG3	2.38	0.59
2:3:58:ILE:HD12	2:4:57:ALA:HB3	1.83	0.59
2:6:133:GLN:HE21	2:6:134:PRO:HD2	1.67	0.59
1:Z:432:ASN:HD22	2:8:29:GLN:HE22	1.47	0.59
2:7:125:ARG:NH1	6:7:143:HOH:O	2.35	0.59
2:6:40:PRO:HG2	2:6:80:MET:HB2	1.85	0.59
1:E:463:LYS:HB2	1:E:463:LYS:NZ	2.18	0.59
2:8:109:ALA:HB3	2:8:119:MET:HG3	1.84	0.58
2:8:38:TRP:CD2	2:8:118:ILE:HG21	2.38	0.58
1:S:296:ALA:O	1:S:297:MET:HB3	2.02	0.58
1:W:292:HIS:HA	1:W:325:HIS:HB2	1.83	0.58
1:D:9:ALA:HA	2:M:84:ARG:NE	2.19	0.58
1:T:60:GLU:HG3	1:T:127:PHE:CZ	2.38	0.58
1:D:51:GLU:HA	1:D:87:ILE:HD11	1.86	0.57
1:Y:338:GLU:OE1	1:Y:341:VAL:HG23	2.04	0.57
2:3:58:ILE:HD13	2:3:58:ILE:O	2.04	0.57
1:G:60:GLU:HG3	1:G:127:PHE:CZ	2.39	0.57
1:U:446:ARG:O	1:U:450:LYS:HD3	2.05	0.57
2:4:136:ASN:OD1	2:4:137:LYS:HG3	2.04	0.57
1:F:296:ALA:O	1:F:297:MET:HB3	2.04	0.57
1:E:88:GLU:HG2	1:E:98:ILE:HB	1.87	0.57
1:E:429:GLN:O	1:E:433:GLU:HG3	2.05	0.57
1:Y:93:GLU:HG3	6:Y:803:HOH:O	2.04	0.57
6:D:1073:HOH:O	2:L:114:LYS:HD2	2.04	0.57
1:B:32:ARG:HD3	6:G:1064:HOH:O	2.02	0.57
2:3:87:MET:O	2:3:91:ARG:HG3	2.04	0.57
1:C:471:THR:HB	1:C:474:LYS:CE	2.34	0.57
2:I:130:ARG:CA	2:I:130:ARG:HE	2.10	0.57
1:S:290:LEU:HG	2:1:66:LEU:HD11	1.86	0.57
2:M:38:TRP:CD2	2:M:118:ILE:HG21	2.39	0.57
1:Y:330:THR:O	1:Y:331:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:1:53:SER:CB	2:1:55:GLU:OE2	2.53	0.57
2:J:55:GLU:N	2:J:55:GLU:OE1	2.35	0.57
2:8:136:ASN:ND2	2:8:137:LYS:HG2	2.20	0.56
1:U:239:TYR:HE2	1:U:401:GLN:HE22	1.53	0.56
1:W:93:GLU:HG3	6:W:892:HOH:O	2.04	0.56
1:Y:93:GLU:CG	1:Y:96:GLN:HB2	2.36	0.56
2:P:125:ARG:HD2	6:P:7352:HOH:O	2.05	0.56
1:E:411:TRP:CH2	2:M:2:MET:HE3	2.40	0.56
1:V:475:LEU:HD22	6:V:1039:HOH:O	2.05	0.56
1:E:60:GLU:HG3	1:E:127:PHE:CZ	2.41	0.56
1:Z:60:GLU:HG3	1:Z:127:PHE:CZ	2.40	0.56
1:X:290:LEU:HG	2:6:66:LEU:HD11	1.86	0.56
1:U:474:LYS:HD3	1:U:474:LYS:C	2.25	0.56
2:1:55:GLU:HG2	6:1:9716:HOH:O	2.06	0.55
1:U:60:GLU:HG3	1:U:127:PHE:CZ	2.40	0.55
1:H:436:ASP:OD1	1:H:439:ARG:HD3	2.07	0.55
1:F:463:LYS:HE2	6:F:1034:HOH:O	2.05	0.55
2:N:114:LYS:HE3	2:N:118:ILE:CG2	2.37	0.55
2:P:20:PRO:HD3	6:P:9682:HOH:O	2.05	0.55
2:1:53:SER:OG	2:1:55:GLU:OE2	2.23	0.55
1:A:429:GLN:O	1:A:433:GLU:HG3	2.06	0.55
2:1:38:TRP:CD2	2:1:118:ILE:HG21	2.41	0.55
1:V:292:HIS:HA	1:V:325:HIS:HB2	1.88	0.55
2:P:85:ASP:O	2:P:88:GLN:HB3	2.07	0.55
1:U:338:GLU:HB3	1:U:341:VAL:CG1	2.36	0.55
1:F:292:HIS:HA	1:F:325:HIS:HB2	1.89	0.55
1:C:429:GLN:O	1:C:433:GLU:HG3	2.07	0.55
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.42	0.55
1:Y:93:GLU:HG2	1:Y:96:GLN:HB2	1.89	0.55
2:1:136:ASN:C	2:1:137:LYS:HD2	2.26	0.55
2:1:134:PRO:HG2	2:1:137:LYS:HB2	1.89	0.55
2:I:1:MME:HE3	6:L:325:HOH:O	2.07	0.55
2:I:85:ASP:OD2	2:I:88:GLN:HG3	2.07	0.54
1:W:190:TYR:CZ	1:W:227:LYS:HE3	2.42	0.54
6:E:687:HOH:O	2:N:49:LYS:HE2	2.07	0.54
1:A:239:TYR:HB3	1:A:266:MET:HB3	1.89	0.54
2:6:109:ALA:HB3	2:6:119:MET:HG3	1.89	0.54
2:7:40:PRO:HG2	2:7:80:MET:HB2	1.88	0.54
1:T:290:LEU:HG	2:2:66:LEU:HD11	1.89	0.54
1:C:290:LEU:HG	2:K:66:LEU:HD11	1.88	0.54
1:S:158:GLU:CD	1:S:325:HIS:HE2	2.11	0.54
1:Y:290:LEU:HG	2:7:66:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:3:119:MET:HG2	6:3:291:HOH:O	2.06	0.54
2:I:118:ILE:HD12	2:I:119:MET:HG3	1.89	0.54
2:1:53:SER:HB2	2:1:55:GLU:OE2	2.08	0.54
1:X:442:GLY:O	1:X:446:ARG:HG3	2.08	0.54
1:B:177:LYS:HB2	1:F:63:THR:HA	1.89	0.54
1:C:345:PHE:O	1:C:349:MET:HG3	2.08	0.54
2:6:97:THR:HB	2:6:124:GLN:NE2	2.22	0.54
1:E:292:HIS:HA	1:E:325:HIS:HB2	1.89	0.54
2:P:33:ILE:HG21	2:P:40:PRO:HG3	1.89	0.54
2:2:125:ARG:HD3	2:2:132:TRP:CZ3	2.42	0.54
2:K:118:ILE:HD11	6:K:319:HOH:O	2.06	0.54
2:N:118:ILE:HD12	2:N:119:MET:HG3	1.90	0.54
2:4:10:LYS:NZ	6:4:235:HOH:O	2.40	0.54
1:A:292:HIS:HA	1:A:325:HIS:HB2	1.89	0.54
2:5:55:GLU:OE2	2:5:69:ASP:HB2	2.08	0.54
6:S:991:HOH:O	2:1:119:MET:HG2	2.06	0.54
1:F:474:LYS:HE2	6:F:976:HOH:O	2.08	0.54
1:D:282:ILE:HG23	5:D:616:GOL:H31	1.90	0.53
1:T:292:HIS:HA	1:T:325:HIS:HB2	1.90	0.53
1:B:60:GLU:HG3	1:B:127:PHE:CZ	2.44	0.53
2:7:1:MME:HE3	6:8:9896:HOH:O	2.08	0.53
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.44	0.53
1:V:60:GLU:HG3	1:V:127:PHE:CZ	2.43	0.53
1:B:330:THR:O	1:B:331:VAL:HB	2.09	0.53
1:S:24:TYR:CD2	1:S:59:ALA:HB2	2.44	0.53
1:U:448:ALA:HA	1:U:451:TRP:NE1	2.24	0.53
2:M:85:ASP:HB3	2:M:88:GLN:HE21	1.73	0.53
2:L:33:ILE:HD13	2:L:109:ALA:HB2	1.91	0.53
1:V:156:GLN:NE2	6:V:1069:HOH:O	2.41	0.53
2:N:111:ASP:OD2	2:N:114:LYS:HE2	2.09	0.53
1:Y:248:GLU:O	1:Y:252:LYS:HG3	2.09	0.53
1:Z:429:GLN:O	1:Z:433:GLU:HG3	2.09	0.53
2:7:107:LEU:O	2:7:120:GLY:HA2	2.09	0.53
1:B:273:GLY:HA3	1:F:273:GLY:HA3	1.91	0.53
1:B:14:LYS:HE3	6:B:975:HOH:O	2.09	0.53
1:U:22:LEU:HD21	6:U:1015:HOH:O	2.08	0.53
2:L:91:ARG:HG2	6:L:263:HOH:O	2.08	0.53
1:W:334:LYS:CG	1:W:335:LEU:HD22	2.37	0.52
1:Z:292:HIS:HA	1:Z:325:HIS:HB2	1.91	0.52
1:H:345:PHE:O	1:H:349:MET:HG3	2.09	0.52
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.56	0.52
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.55	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:GLU:CG	1:A:98:ILE:HB	2.39	0.52
1:V:7:THR:HG21	2:5:84:ARG:O	2.09	0.52
1:W:460:GLU:HG3	6:W:1041:HOH:O	2.07	0.52
1:Y:19:ASP:HB3	1:Y:21:ARG:HG2	1.90	0.52
6:F:941:HOH:O	2:N:10:LYS:HE3	2.09	0.52
6:Y:757:HOH:O	1:Z:372:PRO:HD3	2.09	0.52
2:K:136:ASN:HD22	2:K:136:ASN:N	2.06	0.52
1:S:442:GLY:O	1:S:446:ARG:HG3	2.09	0.52
1:U:197:LEU:HG	1:U:417:ALA:HB1	1.91	0.52
1:D:230:ALA:O	2:L:10:LYS:HE2	2.10	0.52
2:M:102:ASP:HB2	6:M:291:HOH:O	2.10	0.52
1:C:273:GLY:HA3	1:G:273:GLY:HA3	1.92	0.52
1:U:7:THR:OG1	1:U:8:LYS:N	2.41	0.52
1:B:10:GLY:HA3	2:O:84:ARG:HH12	1.75	0.52
1:Z:290:LEU:HG	2:8:66:LEU:HD11	1.91	0.52
2:1:61:GLY:HA3	1:T:259:GLU:OE1	2.09	0.52
1:F:190:TYR:CZ	1:F:227:LYS:HE3	2.45	0.52
1:Z:475:LEU:HD11	6:Z:778:HOH:O	2.09	0.52
2:M:84:ARG:NH2	2:M:84:ARG:HB2	2.25	0.52
1:Y:429:GLN:O	1:Y:433:GLU:HG3	2.10	0.52
1:H:429:GLN:O	1:H:433:GLU:HG3	2.09	0.52
1:D:290:LEU:HG	2:L:66:LEU:HD11	1.92	0.52
1:Y:282:ILE:HG23	5:Y:618:GOL:H31	1.92	0.52
2:3:88:GLN:HA	2:3:91:ARG:NH1	2.25	0.52
2:8:40:PRO:HG2	2:8:80:MET:HB2	1.91	0.52
1:A:66:TRP:CD1	1:E:381:GLY:HA2	2.45	0.52
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.58	0.52
1:F:290:LEU:HG	2:N:66:LEU:HD11	1.92	0.52
1:T:475:LEU:HD22	6:T:1037:HOH:O	2.09	0.52
2:8:53:SER:HG	2:8:55:GLU:CD	2.14	0.52
2:N:109:ALA:HB3	2:N:119:MET:HG3	1.92	0.51
1:F:197:LEU:HG	1:F:417:ALA:HB1	1.91	0.51
1:H:14:LYS:HE3	6:H:1038:HOH:O	2.10	0.51
1:S:32:ARG:HG2	1:S:32:ARG:HH11	1.75	0.51
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.58	0.51
1:Z:24:TYR:CD2	1:Z:59:ALA:HB2	2.45	0.51
1:G:292:HIS:HA	1:G:325:HIS:HB2	1.92	0.51
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.45	0.51
1:W:297:MET:HG3	1:W:297:MET:O	2.11	0.51
1:C:411:TRP:CZ3	2:K:2:MET:HG3	2.43	0.51
1:F:60:GLU:HG3	1:F:127:PHE:CZ	2.45	0.51
2:N:114:LYS:HE3	2:N:118:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:290:LEU:HG	2:4:66:LEU:HD11	1.91	0.51
1:V:273:GLY:HA3	1:Z:273:GLY:HA3	1.93	0.51
1:S:383:HIS:CE1	1:S:385:TRP:HB2	2.45	0.51
2:M:55:GLU:HG2	2:M:69:ASP:OD2	2.10	0.51
1:B:474:LYS:HE3	6:B:993:HOH:O	2.11	0.51
2:K:29:GLN:O	2:K:32:TYR:HB3	2.10	0.51
2:3:8:ASN:O	2:3:133:GLN:HG2	2.11	0.51
1:U:411:TRP:CH2	2:3:2:MET:HG3	2.45	0.51
1:A:330:THR:O	1:A:331:VAL:HB	2.11	0.51
1:F:32:ARG:NH1	6:F:801:HOH:O	2.44	0.51
1:X:190:TYR:CZ	1:X:227:LYS:HE3	2.45	0.51
2:N:130:ARG:HH21	2:N:130:ARG:CG	2.23	0.51
1:Y:197:LEU:HG	1:Y:417:ALA:HB1	1.93	0.51
1:H:14:LYS:NZ	1:H:15:ALA:O	2.43	0.51
1:H:60:GLU:HG3	1:H:127:PHE:CZ	2.45	0.51
1:U:429:GLN:O	1:U:433:GLU:HG3	2.10	0.51
1:B:168:GLY:HA2	1:B:396:ASP:O	2.10	0.51
2:4:119:MET:HE3	2:4:120:GLY:HA2	1.92	0.51
1:Y:432:ASN:HD22	2:7:29:GLN:NE2	2.05	0.51
2:J:8:ASN:O	2:J:133:GLN:HG2	2.10	0.51
1:W:286:ASP:OD1	5:W:620:GOL:H11	2.11	0.51
1:W:440:GLU:O	1:W:444:VAL:HG23	2.11	0.51
1:D:197:LEU:HG	1:D:417:ALA:HB1	1.93	0.51
1:C:460:GLU:OE2	1:C:463:LYS:HE3	2.11	0.50
1:V:239:TYR:HE2	1:V:401:GLN:HE22	1.59	0.50
1:Y:383:HIS:CE1	1:Y:385:TRP:HB2	2.46	0.50
2:N:8:ASN:O	2:N:133:GLN:HG2	2.12	0.50
1:Y:239:TYR:HB3	1:Y:266:MET:HB3	1.92	0.50
1:T:10:GLY:O	1:T:11:ALA:O	2.29	0.50
1:H:338:GLU:OE1	1:H:341:VAL:HG23	2.10	0.50
1:G:139:ARG:HD2	1:G:139:ARG:C	2.31	0.50
2:J:33:ILE:HG21	2:J:40:PRO:HG3	1.94	0.50
1:A:88:GLU:HG2	1:A:98:ILE:HB	1.93	0.50
1:T:330:THR:O	1:T:331:VAL:HB	2.10	0.50
1:U:330:THR:O	1:U:331:VAL:HB	2.11	0.50
6:C:1009:HOH:O	2:K:10:LYS:HE3	2.12	0.50
1:S:66:TRP:CD1	1:W:381:GLY:HA2	2.45	0.50
2:O:127:LYS:O	2:O:130:ARG:NH2	2.43	0.50
1:U:94:ASP:O	1:U:95:ASN:HB3	2.12	0.50
1:U:290:LEU:HG	2:3:66:LEU:HD11	1.94	0.50
1:Z:330:THR:O	1:Z:331:VAL:HB	2.11	0.50
2:7:91:ARG:NH1	6:7:2823:HOH:O	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:3:58:ILE:HD11	2:4:58:ILE:CA	2.42	0.50
2:8:136:ASN:HD22	2:8:137:LYS:N	2.10	0.50
1:T:239:TYR:HE2	1:T:401:GLN:HE22	1.60	0.50
1:C:282:ILE:HG23	5:C:615:GOL:H31	1.94	0.50
1:D:110:GLU:HB3	1:D:147:THR:HB	1.93	0.50
6:Y:638:HOH:O	1:Z:161:LYS:HE2	2.11	0.50
1:B:239:TYR:HB3	1:B:266:MET:HB3	1.93	0.50
2:1:87:MET:HB3	2:1:91:ARG:HH11	1.77	0.50
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.46	0.50
1:G:239:TYR:HB3	1:G:266:MET:HB3	1.94	0.50
2:1:49:LYS:NZ	6:1:9153:HOH:O	2.45	0.50
1:Z:239:TYR:HE2	1:Z:401:GLN:HE22	1.60	0.49
1:A:60:GLU:HG3	1:A:127:PHE:CZ	2.47	0.49
2:J:118:ILE:HD12	2:J:119:MET:HG3	1.93	0.49
1:X:341:VAL:HG23	1:X:475:LEU:CD2	2.42	0.49
2:4:8:ASN:O	2:4:133:GLN:HG2	2.12	0.49
1:H:290:LEU:HG	2:P:66:LEU:HD11	1.94	0.49
1:V:381:GLY:HA2	1:Z:66:TRP:CD1	2.47	0.49
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.47	0.49
2:J:5:THR:HG22	2:J:138:ARG:O	2.12	0.49
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.47	0.49
1:H:330:THR:O	1:H:331:VAL:HB	2.13	0.49
2:J:107:LEU:O	2:J:120:GLY:HA2	2.12	0.49
1:V:139:ARG:C	1:V:139:ARG:HD2	2.32	0.49
2:5:39:ILE:O	2:5:109:ALA:HA	2.12	0.49
2:7:33:ILE:HD11	2:7:119:MET:CE	2.42	0.49
2:N:39:ILE:O	2:N:109:ALA:HA	2.12	0.49
1:Y:32:ARG:CZ	6:Y:784:HOH:O	2.59	0.49
1:S:471:THR:O	1:S:474:LYS:HE3	2.12	0.49
1:Y:292:HIS:HA	1:Y:325:HIS:HB2	1.95	0.49
2:L:10:LYS:HE3	6:L:294:HOH:O	2.12	0.49
2:3:107:LEU:O	2:3:120:GLY:HA2	2.12	0.49
1:W:139:ARG:C	1:W:139:ARG:HD2	2.32	0.49
2:2:129:ALA:O	2:2:132:TRP:HZ3	1.96	0.49
1:D:51:GLU:H	1:D:51:GLU:CD	2.15	0.49
2:L:8:ASN:O	2:L:133:GLN:HG2	2.12	0.49
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.60	0.49
1:W:341:VAL:HG11	6:W:994:HOH:O	2.12	0.49
2:4:107:LEU:O	2:4:120:GLY:HA2	2.12	0.49
1:V:330:THR:O	1:V:331:VAL:HB	2.11	0.49
1:G:330:THR:O	1:G:331:VAL:HB	2.13	0.49
1:H:292:HIS:HA	1:H:325:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:474:LYS:HD2	6:U:968:HOH:O	2.11	0.49
1:Z:439:ARG:NH1	6:Z:851:HOH:O	2.46	0.49
1:S:389:ALA:O	1:S:393:ILE:HG13	2.12	0.49
1:B:139:ARG:C	1:B:139:ARG:HD2	2.33	0.49
1:D:431:ARG:NH2	6:D:1087:HOH:O	2.46	0.49
2:J:46:GLU:HG2	2:J:49:LYS:HG3	1.95	0.49
1:S:168:GLY:HA2	1:S:396:ASP:O	2.13	0.49
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.95	0.48
1:D:381:GLY:HA2	1:H:66:TRP:CD1	2.48	0.48
1:W:239:TYR:HB3	1:W:266:MET:HB3	1.95	0.48
1:T:168:GLY:HA2	1:T:396:ASP:O	2.13	0.48
2:K:136:ASN:ND2	2:K:137:LYS:HD2	2.28	0.48
1:W:296:ALA:O	1:W:297:MET:HB3	2.13	0.48
1:X:440:GLU:O	1:X:444:VAL:HG23	2.14	0.48
1:S:356:LYS:HE3	6:S:741:HOH:O	2.13	0.48
1:C:161:LYS:HE2	6:D:803:HOH:O	2.14	0.48
1:V:168:GLY:HA2	1:V:396:ASP:O	2.13	0.48
2:6:67:TYR:C	2:6:67:TYR:CD1	2.86	0.48
1:Z:168:GLY:HA2	1:Z:396:ASP:O	2.14	0.48
1:U:310:HIS:HE2	1:U:341:VAL:HG21	1.78	0.48
2:2:8:ASN:O	2:2:133:GLN:HG2	2.14	0.48
1:S:381:GLY:HA2	1:W:66:TRP:CD1	2.48	0.48
1:C:168:GLY:HA2	1:C:396:ASP:O	2.14	0.48
1:S:93:GLU:HG3	1:S:96:GLN:OE1	2.13	0.48
2:O:107:LEU:O	2:O:120:GLY:HA2	2.13	0.48
1:H:438:ALA:HB3	1:H:439:ARG:NH1	2.25	0.48
1:A:8:LYS:O	1:A:9:ALA:CB	2.61	0.48
1:X:134:ARG:HA	1:X:308:GLY:O	2.13	0.48
1:T:139:ARG:HD2	1:T:139:ARG:C	2.34	0.48
1:U:88:GLU:CG	1:U:98:ILE:HB	2.43	0.48
1:C:197:LEU:HG	1:C:417:ALA:HB1	1.94	0.48
1:D:411:TRP:CD1	2:L:1:MME:HB2	2.49	0.48
2:K:80:MET:HE2	6:K:281:HOH:O	2.13	0.48
1:Z:139:ARG:C	1:Z:139:ARG:HD2	2.33	0.48
2:M:10:LYS:NZ	6:M:235:HOH:O	2.46	0.48
1:A:290:LEU:HG	2:I:66:LEU:HD11	1.95	0.48
1:G:24:TYR:CD2	1:G:59:ALA:HB2	2.48	0.48
1:U:134:ARG:HA	1:U:308:GLY:O	2.14	0.48
1:S:239:TYR:HB3	1:S:266:MET:HB3	1.95	0.48
2:L:136:ASN:O	2:L:137:LYS:HE2	2.14	0.48
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.62	0.48
1:U:474:LYS:CD	1:U:475:LEU:O	2.58	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:136:ASN:ND2	2:K:137:LYS:CD	2.76	0.48
1:V:297:MET:O	1:V:297:MET:HG3	2.13	0.48
1:W:239:TYR:HE2	1:W:401:GLN:HE22	1.62	0.48
1:U:66:TRP:CD1	1:Y:381:GLY:HA2	2.49	0.48
2:I:127:LYS:HG2	6:I:214:HOH:O	2.13	0.48
1:S:273:GLY:HA3	1:W:273:GLY:HA3	1.95	0.48
1:C:32:ARG:HD3	6:C:748:HOH:O	2.13	0.48
1:D:330:THR:O	1:D:331:VAL:HB	2.13	0.47
1:W:330:THR:O	1:W:331:VAL:HB	2.14	0.47
1:Y:139:ARG:HD2	1:Y:139:ARG:C	2.35	0.47
1:S:139:ARG:C	1:S:139:ARG:HD2	2.34	0.47
1:C:330:THR:O	1:C:331:VAL:HB	2.13	0.47
1:C:66:TRP:CD1	1:G:381:GLY:HA2	2.49	0.47
1:F:330:THR:O	1:F:331:VAL:HB	2.13	0.47
2:2:129:ALA:O	2:2:132:TRP:CZ3	2.67	0.47
2:O:80:MET:CE	2:O:88:GLN:HG2	2.44	0.47
1:W:19:ASP:HB3	1:W:21:ARG:HG2	1.95	0.47
1:X:330:THR:O	1:X:331:VAL:HB	2.14	0.47
1:Y:474:LYS:HG2	6:Y:993:HOH:O	2.13	0.47
2:K:61:GLY:HA3	1:D:259:GLU:OE1	2.14	0.47
1:W:318:LEU:C	1:W:318:LEU:HD13	2.34	0.47
1:F:94:ASP:O	1:F:95:ASN:HB3	2.14	0.47
2:P:42:LEU:HD21	2:P:93:ILE:HG12	1.96	0.47
1:G:387:MET:HB3	1:G:388:PRO:HD3	1.96	0.47
1:E:139:ARG:HD2	1:E:139:ARG:C	2.34	0.47
2:M:85:ASP:HB3	2:M:88:GLN:NE2	2.29	0.47
1:A:139:ARG:C	1:A:139:ARG:HD2	2.34	0.47
1:B:134:ARG:HA	1:B:308:GLY:O	2.14	0.47
1:S:330:THR:O	1:S:331:VAL:HB	2.15	0.47
1:H:88:GLU:CG	1:H:98:ILE:HB	2.45	0.47
2:I:107:LEU:O	2:I:120:GLY:HA2	2.14	0.47
1:X:45:GLN:HG3	1:X:128:LYS:O	2.15	0.47
2:1:8:ASN:O	2:1:133:GLN:HG2	2.14	0.47
1:C:387:MET:HB3	1:C:388:PRO:HD3	1.97	0.47
1:V:197:LEU:HG	1:V:417:ALA:HB1	1.97	0.47
1:W:429:GLN:O	1:W:433:GLU:HG3	2.14	0.47
1:H:436:ASP:CG	1:H:439:ARG:HD3	2.35	0.47
1:D:51:GLU:HA	1:D:87:ILE:CD1	2.45	0.47
1:T:372:PRO:HD3	6:U:784:HOH:O	2.15	0.47
1:S:197:LEU:HG	1:S:417:ALA:CB	2.45	0.47
2:3:58:ILE:HD11	2:4:58:ILE:HA	1.97	0.47
2:3:58:ILE:HD11	2:4:58:ILE:N	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:6:8:ASN:O	2:6:133:GLN:HG2	2.15	0.47
1:U:239:TYR:HB3	1:U:266:MET:HB3	1.97	0.47
6:V:873:HOH:O	2:4:10:LYS:HE3	2.13	0.47
1:S:239:TYR:HE2	1:S:401:GLN:HE22	1.61	0.47
1:D:24:TYR:CD2	1:D:59:ALA:HB2	2.49	0.47
2:3:61:GLY:HA3	1:V:259:GLU:OE1	2.14	0.47
1:T:460:GLU:HA	1:T:460:GLU:OE2	2.14	0.47
1:T:429:GLN:O	1:T:433:GLU:HG3	2.15	0.47
2:J:84:ARG:HG2	6:J:168:HOH:O	2.13	0.47
1:T:24:TYR:CD2	1:T:59:ALA:HB2	2.50	0.47
6:X:701:HOH:O	1:Y:372:PRO:HD3	2.14	0.47
1:Y:385:TRP:CD1	1:Y:463:LYS:HA	2.49	0.47
2:J:61:GLY:HA3	1:C:259:GLU:OE1	2.15	0.47
1:B:63:THR:HA	1:F:177:LYS:HB2	1.97	0.47
1:T:383:HIS:CE1	1:T:385:TRP:HB2	2.50	0.47
2:6:107:LEU:O	2:6:120:GLY:HA2	2.15	0.47
2:8:134:PRO:HG2	2:8:136:ASN:ND2	2.30	0.47
1:B:158:GLU:CD	1:B:325:HIS:HE2	2.16	0.47
1:V:134:ARG:HA	1:V:308:GLY:O	2.14	0.47
1:V:429:GLN:O	1:V:433:GLU:HG3	2.15	0.47
1:C:24:TYR:CD2	1:C:59:ALA:HB2	2.50	0.47
2:4:39:ILE:O	2:4:109:ALA:HA	2.15	0.47
1:Y:239:TYR:HE2	1:Y:401:GLN:HE22	1.62	0.47
1:H:45:GLN:HG3	1:H:128:LYS:O	2.14	0.47
1:C:339:ARG:NH2	1:C:392:GLU:OE1	2.48	0.47
2:I:97:THR:HB	2:I:124:GLN:NE2	2.30	0.47
1:T:273:GLY:HA3	1:X:273:GLY:HA3	1.96	0.47
1:Y:259:GLU:OE1	2:8:61:GLY:HA3	2.14	0.47
2:K:107:LEU:O	2:K:120:GLY:HA2	2.15	0.47
1:C:165:TYR:CD1	2:K:117:GLN:HB3	2.50	0.47
1:B:463:LYS:HD2	6:B:972:HOH:O	2.14	0.47
1:U:32:ARG:CZ	6:U:1040:HOH:O	2.63	0.47
1:E:330:THR:O	1:E:331:VAL:HB	2.15	0.47
1:U:292:HIS:HA	1:U:325:HIS:HB2	1.96	0.46
2:K:127:LYS:NZ	6:K:302:HOH:O	2.47	0.46
2:P:10:LYS:HE3	6:P:5344:HOH:O	2.15	0.46
2:3:5:THR:HG22	2:3:138:ARG:O	2.16	0.46
1:F:139:ARG:HD2	1:F:139:ARG:C	2.36	0.46
1:A:37:LEU:HB2	1:A:139:ARG:HB3	1.97	0.46
1:A:273:GLY:HA3	1:E:273:GLY:HA3	1.97	0.46
1:X:383:HIS:CE1	1:X:385:TRP:HB2	2.49	0.46
2:7:97:THR:HB	2:7:124:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:290:LEU:HG	2:O:66:LEU:HD11	1.96	0.46
1:V:24:TYR:CD2	1:V:59:ALA:HB2	2.50	0.46
1:S:305:ARG:CZ	6:S:1003:HOH:O	2.63	0.46
1:W:464:GLU:OE1	1:W:464:GLU:HA	2.16	0.46
1:S:297:MET:O	1:S:297:MET:HG2	2.16	0.46
2:J:55:GLU:CD	2:J:55:GLU:H	2.18	0.46
1:Y:411:TRP:CD1	2:7:1:MME:HG3	2.50	0.46
2:K:119:MET:HG2	2:K:120:GLY:N	2.30	0.46
1:D:383:HIS:CE1	1:D:385:TRP:HB2	2.51	0.46
1:E:466:LYS:HD3	1:E:468:GLU:CD	2.35	0.46
2:O:67:TYR:CD1	2:O:67:TYR:C	2.89	0.46
1:W:168:GLY:HA2	1:W:396:ASP:O	2.15	0.46
1:V:190:TYR:CZ	1:V:227:LYS:HE3	2.50	0.46
2:M:82:GLY:O	2:M:84:ARG:HG3	2.16	0.46
2:3:39:ILE:O	2:3:109:ALA:HA	2.16	0.46
1:S:429:GLN:O	1:S:433:GLU:HG3	2.15	0.46
1:B:110:GLU:HB3	1:B:147:THR:HB	1.97	0.46
1:G:19:ASP:HB3	1:G:21:ARG:HG2	1.96	0.46
1:Z:10:GLY:O	1:Z:12:GLY:N	2.49	0.46
1:U:345:PHE:O	1:U:349:MET:HG3	2.15	0.46
1:D:273:GLY:HA3	1:H:273:GLY:HA3	1.98	0.46
2:L:91:ARG:CD	6:L:220:HOH:O	2.63	0.46
2:J:49:LYS:NZ	6:J:292:HOH:O	2.48	0.46
1:D:60:GLU:HG3	1:D:127:PHE:CZ	2.51	0.46
1:W:24:TYR:CD2	1:W:59:ALA:HB2	2.50	0.46
1:X:110:GLU:HB3	1:X:147:THR:HB	1.97	0.46
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.51	0.46
1:H:32:ARG:NE	6:H:711:HOH:O	2.48	0.46
2:K:125:ARG:HD3	2:K:132:TRP:NE1	2.31	0.46
2:K:97:THR:HB	2:K:124:GLN:NE2	2.31	0.46
2:L:67:TYR:CD1	2:L:67:TYR:C	2.89	0.46
1:X:19:ASP:HB3	1:X:21:ARG:HG2	1.97	0.46
1:W:383:HIS:CE1	1:W:385:TRP:HB2	2.51	0.46
1:V:305:ARG:HD2	1:V:474:LYS:O	2.16	0.46
2:K:69:ASP:O	2:K:70:ASN:HB2	2.16	0.46
1:Y:392:GLU:OE1	1:Y:438:ALA:HB2	2.16	0.46
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.50	0.46
1:V:331:VAL:HA	1:V:337:GLY:O	2.16	0.46
1:X:24:TYR:CD2	1:X:59:ALA:HB2	2.50	0.46
1:E:341:VAL:HG12	1:E:475:LEU:HD21	1.97	0.46
2:2:67:TYR:CD1	2:2:67:TYR:C	2.89	0.46
1:V:158:GLU:CD	1:V:325:HIS:HE2	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:114:LYS:NZ	6:2:303:HOH:O	2.45	0.46
1:W:206:VAL:C	1:W:207:ASN:HD22	2.19	0.46
1:U:474:LYS:HB2	6:U:1027:HOH:O	2.16	0.46
1:U:94:ASP:O	1:U:95:ASN:CB	2.64	0.46
1:G:197:LEU:HG	1:G:417:ALA:HB1	1.97	0.46
1:U:383:HIS:CE1	1:U:385:TRP:HB2	2.51	0.46
2:J:86:PRO:O	2:J:90:LEU:HD23	2.16	0.46
1:C:436:ASP:OD1	1:C:439:ARG:HG3	2.15	0.46
1:X:379:SER:HB2	1:X:401:GLN:HB2	1.98	0.46
1:B:387:MET:HB3	1:B:388:PRO:HD3	1.97	0.46
2:N:67:TYR:C	2:N:67:TYR:CD1	2.89	0.46
1:B:318:LEU:C	1:B:318:LEU:HD13	2.37	0.46
1:V:418:ALA:O	1:V:422:VAL:HG23	2.17	0.45
1:H:24:TYR:CD2	1:H:59:ALA:HB2	2.50	0.45
2:5:67:TYR:C	2:5:67:TYR:CD1	2.89	0.45
1:S:292:HIS:HA	1:S:325:HIS:HB2	1.98	0.45
2:K:38:TRP:CD2	2:K:118:ILE:HG21	2.51	0.45
2:1:107:LEU:O	2:1:120:GLY:HA2	2.16	0.45
1:B:389:ALA:O	1:B:393:ILE:HG13	2.16	0.45
2:I:39:ILE:O	2:I:109:ALA:HA	2.16	0.45
6:N:321:HOH:O	2:O:58:ILE:CD1	2.61	0.45
1:S:383:HIS:HE1	1:S:385:TRP:HB2	1.81	0.45
6:A:1064:HOH:O	2:N:81:PHE:HB3	2.16	0.45
1:V:318:LEU:C	1:V:318:LEU:HD13	2.37	0.45
1:F:175:LYS:HA	1:F:176:PRO:C	2.36	0.45
1:D:134:ARG:HA	1:D:308:GLY:O	2.16	0.45
1:B:66:TRP:CD1	1:F:381:GLY:HA2	2.51	0.45
1:H:206:VAL:C	1:H:207:ASN:HD22	2.20	0.45
1:C:381:GLY:HA2	1:G:66:TRP:CD1	2.52	0.45
1:Y:383:HIS:HE1	1:Y:385:TRP:HB2	1.81	0.45
1:B:90:VAL:HG23	1:B:97:TYR:HA	1.99	0.45
1:T:345:PHE:O	1:T:349:MET:HG3	2.16	0.45
2:P:118:ILE:HD12	2:P:119:MET:HG3	1.99	0.45
1:B:459:CYS:O	1:B:463:LYS:HB3	2.16	0.45
1:H:168:GLY:HA2	1:H:396:ASP:O	2.17	0.45
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.62	0.45
1:X:197:LEU:HG	1:X:417:ALA:HB1	1.97	0.45
1:W:290:LEU:HG	2:5:66:LEU:HD11	1.97	0.45
2:J:67:TYR:CD1	2:J:67:TYR:C	2.89	0.45
1:E:383:HIS:HE1	1:E:385:TRP:HB2	1.81	0.45
1:Y:170:LEU:HD11	1:Y:421:ARG:HA	1.99	0.45
1:Z:197:LEU:HG	1:Z:417:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:435:ARG:NH1	6:S:1018:HOH:O	2.47	0.45
1:C:177:LYS:HB2	1:G:63:THR:HA	1.98	0.45
1:D:139:ARG:HD2	1:D:139:ARG:C	2.37	0.45
1:H:331:VAL:HA	1:H:337:GLY:O	2.16	0.45
1:T:409:HIS:CD2	1:T:416:GLY:HA2	2.52	0.45
1:F:118:THR:O	1:F:122:GLY:HA3	2.17	0.45
2:3:67:TYR:C	2:3:67:TYR:CD1	2.90	0.45
1:X:139:ARG:HD2	1:X:139:ARG:C	2.36	0.45
1:Y:190:TYR:CZ	1:Y:227:LYS:HE3	2.51	0.45
1:G:471:THR:O	1:G:474:LYS:HE3	2.17	0.45
2:I:67:TYR:C	2:I:67:TYR:CD1	2.90	0.45
1:T:158:GLU:CD	1:T:325:HIS:HE2	2.20	0.45
2:J:33:ILE:HD11	2:J:119:MET:CE	2.47	0.45
1:X:331:VAL:HA	1:X:337:GLY:O	2.17	0.45
2:5:22:SER:OG	2:5:25:GLN:HG3	2.17	0.45
1:S:387:MET:HB3	1:S:388:PRO:HD3	1.99	0.45
1:Y:299:ALA:HA	1:Y:302:ASP:OD1	2.17	0.45
1:C:450:LYS:N	1:C:450:LYS:HE3	2.32	0.45
1:E:32:ARG:NH1	6:E:819:HOH:O	2.49	0.44
1:S:32:ARG:HG2	1:S:32:ARG:NH1	2.31	0.44
1:T:421:ARG:O	1:T:425:GLU:HG3	2.17	0.44
1:A:175:LYS:HA	1:A:176:PRO:C	2.38	0.44
1:V:282:ILE:HG23	5:V:616:GOL:H31	1.99	0.44
2:6:39:ILE:O	2:6:109:ALA:HA	2.18	0.44
2:N:118:ILE:CD1	2:N:119:MET:HG3	2.46	0.44
1:A:331:VAL:HA	1:A:337:GLY:O	2.17	0.44
1:B:463:LYS:HE3	1:B:463:LYS:HB2	1.76	0.44
1:W:385:TRP:CD1	1:W:463:LYS:HA	2.53	0.44
1:E:175:LYS:HA	1:E:176:PRO:C	2.37	0.44
1:V:383:HIS:CE1	1:V:385:TRP:HB2	2.53	0.44
1:U:45:GLN:HG3	1:U:128:LYS:O	2.17	0.44
1:Y:450:LYS:HE2	6:Y:975:HOH:O	2.16	0.44
1:C:63:THR:HA	1:G:177:LYS:HB2	1.99	0.44
1:E:45:GLN:HG3	1:E:128:LYS:O	2.17	0.44
2:4:105:VAL:O	2:4:122:LEU:HD12	2.17	0.44
1:D:463:LYS:HD3	1:D:463:LYS:O	2.17	0.44
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.52	0.44
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.99	0.44
2:P:107:LEU:O	2:P:120:GLY:HA2	2.18	0.44
2:6:91:ARG:NH2	6:6:260:HOH:O	2.50	0.44
2:O:97:THR:HB	2:O:124:GLN:NE2	2.32	0.44
1:B:429:GLN:O	1:B:433:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.52	0.44
2:4:109:ALA:HB3	2:4:119:MET:HG3	1.99	0.44
1:T:239:TYR:HB3	1:T:266:MET:HB3	2.00	0.44
2:L:24:GLU:HG3	6:L:245:HOH:O	2.17	0.44
1:G:168:GLY:HA2	1:G:396:ASP:O	2.17	0.44
1:W:118:THR:O	1:W:122:GLY:HA3	2.18	0.44
1:G:318:LEU:C	1:G:318:LEU:HD13	2.38	0.44
2:8:67:TYR:CD1	2:8:67:TYR:C	2.90	0.44
1:F:379:SER:HB2	1:F:401:GLN:HB2	1.99	0.44
1:X:302:ASP:HB2	6:X:623:HOH:O	2.17	0.44
1:Y:110:GLU:HB3	1:Y:147:THR:HB	1.99	0.44
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.99	0.44
1:U:190:TYR:CZ	1:U:227:LYS:HE3	2.52	0.44
1:U:139:ARG:C	1:U:139:ARG:HD2	2.37	0.44
1:W:93:GLU:CG	1:W:96:GLN:HB2	2.48	0.44
1:H:32:ARG:NH2	6:H:711:HOH:O	2.51	0.44
1:X:239:TYR:HE2	1:X:401:GLN:HE22	1.65	0.44
1:X:387:MET:HB3	1:X:388:PRO:HD3	1.99	0.44
1:V:175:LYS:HA	1:V:176:PRO:C	2.38	0.44
2:5:118:ILE:HD12	2:5:119:MET:HG3	2.00	0.44
2:N:130:ARG:CG	2:N:130:ARG:NH2	2.80	0.44
1:G:379:SER:HB2	1:G:401:GLN:HB2	1.99	0.44
1:S:175:LYS:HA	1:S:176:PRO:C	2.38	0.44
1:E:200:THR:O	1:E:238:HIS:HA	2.18	0.44
1:E:385:TRP:CZ2	1:E:459:CYS:HB3	2.53	0.44
1:F:19:ASP:HB3	1:F:21:ARG:HG2	1.98	0.44
1:G:175:LYS:HA	1:G:176:PRO:C	2.38	0.44
1:W:134:ARG:HA	1:W:308:GLY:O	2.18	0.44
2:8:8:ASN:O	2:8:133:GLN:HG2	2.18	0.44
1:Y:387:MET:HB3	1:Y:388:PRO:HD3	2.00	0.44
1:D:170:LEU:HD11	1:D:421:ARG:HA	2.00	0.44
2:O:109:ALA:HB3	2:O:119:MET:HG3	1.99	0.44
1:A:110:GLU:HB3	1:A:147:THR:HB	2.00	0.44
1:G:297:MET:HG2	1:G:297:MET:O	2.18	0.44
1:Z:475:LEU:OXT	1:Z:475:LEU:HD13	2.18	0.44
1:Z:331:VAL:HA	1:Z:337:GLY:O	2.17	0.44
1:D:175:LYS:HA	1:D:176:PRO:C	2.38	0.44
1:S:19:ASP:HB3	1:S:21:ARG:HG2	2.00	0.44
2:O:8:ASN:O	2:O:133:GLN:HG2	2.17	0.44
2:4:53:SER:OG	2:4:55:GLU:OE1	2.33	0.44
1:E:248:GLU:O	1:E:252:LYS:HG3	2.18	0.44
1:U:8:LYS:HB2	2:8:84:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:175:LYS:HA	1:C:176:PRO:C	2.38	0.43
2:1:39:ILE:O	2:1:109:ALA:HA	2.17	0.43
1:U:450:LYS:HD2	1:U:450:LYS:N	2.32	0.43
1:T:66:TRP:CD1	1:X:381:GLY:HA2	2.53	0.43
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.53	0.43
2:3:97:THR:HB	2:3:124:GLN:NE2	2.33	0.43
2:J:38:TRP:O	2:J:40:PRO:HD3	2.17	0.43
1:C:331:VAL:HA	1:C:337:GLY:O	2.18	0.43
1:H:88:GLU:HG2	1:H:98:ILE:HB	2.00	0.43
1:Z:411:TRP:CD1	2:8:1:MME:HG3	2.53	0.43
1:Z:19:ASP:HB3	1:Z:21:ARG:HG2	2.00	0.43
1:F:142:PRO:O	1:F:146:LYS:HG2	2.18	0.43
1:B:175:LYS:HA	1:B:176:PRO:C	2.38	0.43
1:Y:206:VAL:C	1:Y:207:ASN:HD22	2.22	0.43
1:B:461:VAL:HG23	1:B:462:TRP:CD2	2.53	0.43
1:E:411:TRP:HH2	2:M:2:MET:HE3	1.81	0.43
1:C:239:TYR:HB3	1:C:266:MET:HB3	2.01	0.43
1:C:411:TRP:CD1	2:K:1:MME:HG3	2.53	0.43
2:M:97:THR:HB	2:M:124:GLN:NE2	2.34	0.43
1:U:8:LYS:CB	2:8:84:ARG:HD3	2.43	0.43
2:3:13:GLU:HB3	2:3:14:THR:H	1.67	0.43
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.53	0.43
1:E:327:HIS:HA	1:E:377:VAL:HB	2.00	0.43
1:Y:175:LYS:HA	1:Y:176:PRO:C	2.39	0.43
2:4:102:ASP:HB3	6:4:312:HOH:O	2.18	0.43
1:W:175:LYS:HA	1:W:176:PRO:C	2.39	0.43
2:7:67:TYR:C	2:7:67:TYR:CD1	2.91	0.43
2:1:67:TYR:CD1	2:1:67:TYR:C	2.92	0.43
2:3:134:PRO:HD2	2:3:137:LYS:CD	2.46	0.43
2:5:8:ASN:O	2:5:133:GLN:HG2	2.19	0.43
1:V:206:VAL:C	1:V:207:ASN:HD22	2.22	0.43
1:A:18:LYS:O	5:A:605:GOL:H11	2.19	0.43
1:U:273:GLY:HA3	1:Y:273:GLY:HA3	2.01	0.43
1:A:45:GLN:HG3	1:A:128:LYS:O	2.19	0.43
1:W:45:GLN:HG3	1:W:128:LYS:O	2.18	0.43
2:2:94:VAL:O	2:2:98:LYS:HG3	2.18	0.43
1:A:24:TYR:CD2	1:A:59:ALA:HB2	2.53	0.43
1:D:165:TYR:CD1	2:L:117:GLN:HB3	2.54	0.43
1:Z:110:GLU:HB3	1:Z:147:THR:HB	2.00	0.43
1:A:134:ARG:HD2	1:A:305:ARG:O	2.19	0.43
1:B:230:ALA:O	2:J:10:LYS:HE2	2.18	0.43
6:W:664:HOH:O	1:X:161:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:87:MET:HE3	6:I:269:HOH:O	2.17	0.43
1:E:24:TYR:CD2	1:E:59:ALA:HB2	2.53	0.43
1:H:282:ILE:HG23	5:H:619:GOL:C3	2.49	0.43
1:E:165:TYR:CD1	2:M:117:GLN:HB3	2.53	0.43
1:B:381:GLY:HA2	1:F:66:TRP:CD1	2.53	0.43
2:M:67:TYR:C	2:M:67:TYR:CD1	2.92	0.43
1:B:18:LYS:CG	5:B:606:GOL:H32	2.49	0.43
1:F:383:HIS:HE1	1:F:385:TRP:HB2	1.83	0.43
1:F:24:TYR:CD2	1:F:59:ALA:HB2	2.54	0.43
1:B:345:PHE:O	1:B:349:MET:HG3	2.19	0.43
1:Z:175:LYS:HA	1:Z:176:PRO:C	2.39	0.43
1:U:153:HIS:CD2	1:U:161:LYS:HE3	2.53	0.43
1:U:175:LYS:HA	1:U:176:PRO:C	2.38	0.43
2:2:118:ILE:HD12	2:2:119:MET:HG3	2.01	0.43
1:F:297:MET:O	1:F:297:MET:HG2	2.18	0.43
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.21	0.43
1:U:385:TRP:NE1	1:U:463:LYS:HA	2.34	0.43
2:O:39:ILE:O	2:O:109:ALA:HA	2.19	0.43
1:Y:439:ARG:HD2	6:Y:942:HOH:O	2.19	0.43
1:E:206:VAL:C	1:E:207:ASN:HD22	2.22	0.43
2:7:119:MET:HB2	6:7:5747:HOH:O	2.19	0.43
1:X:175:LYS:HA	1:X:176:PRO:C	2.39	0.43
1:V:88:GLU:HG3	1:V:100:TYR:HE1	1.83	0.43
1:V:110:GLU:HB3	1:V:147:THR:HB	2.01	0.43
1:Y:185:TYR:O	1:Y:189:VAL:HG23	2.19	0.43
1:F:387:MET:HB3	1:F:388:PRO:HD3	2.00	0.43
1:V:457:ALA:O	1:V:461:VAL:HG23	2.19	0.43
2:P:67:TYR:CD1	2:P:67:TYR:C	2.92	0.43
2:M:39:ILE:O	2:M:109:ALA:HA	2.19	0.42
2:J:39:ILE:O	2:J:109:ALA:HA	2.19	0.42
1:Z:190:TYR:CZ	1:Z:227:LYS:HE3	2.54	0.42
1:Z:451:TRP:CH2	2:8:19:PRO:HD3	2.53	0.42
2:8:13:GLU:HB3	2:8:14:THR:H	1.70	0.42
1:H:139:ARG:C	1:H:139:ARG:HD2	2.39	0.42
2:4:67:TYR:CD1	2:4:67:TYR:C	2.92	0.42
1:D:239:TYR:HB3	1:D:266:MET:HB3	2.00	0.42
1:Z:451:TRP:CZ2	2:8:19:PRO:HD3	2.54	0.42
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.66	0.42
1:G:429:GLN:O	1:G:433:GLU:HG3	2.19	0.42
1:H:110:GLU:HB3	1:H:147:THR:HB	2.00	0.42
2:3:137:LYS:HB3	6:3:242:HOH:O	2.18	0.42
2:2:129:ALA:HB3	2:2:132:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:19:ASP:HB3	1:D:21:ARG:HG2	2.01	0.42
2:8:134:PRO:HG2	2:8:136:ASN:HD21	1.84	0.42
1:V:341:VAL:HG23	1:V:475:LEU:HD21	2.01	0.42
1:C:88:GLU:HA	1:C:89:PRO:HD3	1.92	0.42
1:T:175:LYS:HA	1:T:176:PRO:C	2.40	0.42
1:E:117:PHE:O	1:E:121:VAL:HG22	2.19	0.42
2:1:14:THR:O	2:1:15:PHE:HB2	2.20	0.42
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.54	0.42
1:T:381:GLY:HA2	1:X:66:TRP:CD1	2.54	0.42
1:S:432:ASN:HD22	2:1:29:GLN:NE2	2.10	0.42
1:C:14:LYS:HA	1:C:14:LYS:HD2	1.79	0.42
1:Z:24:TYR:CE1	1:Z:81:LYS:HB2	2.54	0.42
1:F:331:VAL:HA	1:F:337:GLY:O	2.19	0.42
1:E:259:GLU:OE1	2:N:61:GLY:HA3	2.20	0.42
1:T:199:PHE:HA	1:T:237:GLY:O	2.20	0.42
1:A:14:LYS:HE3	1:A:15:ALA:O	2.20	0.42
1:U:214:TRP:CD2	1:U:253:ARG:HG2	2.53	0.42
1:T:451:TRP:CH2	2:2:19:PRO:HD3	2.54	0.42
1:G:110:GLU:HB3	1:G:147:THR:HB	2.01	0.42
1:T:464:GLU:OE2	1:T:464:GLU:HA	2.20	0.42
1:T:45:GLN:HG3	1:T:128:LYS:O	2.19	0.42
1:V:239:TYR:HB3	1:V:266:MET:HB3	2.00	0.42
1:E:331:VAL:HA	1:E:337:GLY:O	2.19	0.42
1:S:134:ARG:HD2	1:S:305:ARG:O	2.19	0.42
2:L:13:GLU:HB3	2:L:14:THR:H	1.68	0.42
1:U:381:GLY:HA2	1:Y:66:TRP:CD1	2.54	0.42
1:S:45:GLN:HG3	1:S:128:LYS:O	2.19	0.42
1:F:429:GLN:O	1:F:433:GLU:HG3	2.18	0.42
1:V:45:GLN:HG3	1:V:128:LYS:O	2.19	0.42
1:D:387:MET:HB3	1:D:388:PRO:HD3	2.01	0.42
1:T:338:GLU:OE1	1:T:341:VAL:HG23	2.19	0.42
1:Y:24:TYR:CD2	1:Y:59:ALA:HB2	2.53	0.42
2:1:55:GLU:H	2:1:55:GLU:CD	2.17	0.42
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.21	0.42
1:G:331:VAL:HA	1:G:337:GLY:O	2.19	0.42
1:U:221:VAL:O	1:U:225:ILE:HG13	2.19	0.42
1:T:118:THR:O	1:T:122:GLY:HA3	2.20	0.42
1:Z:447:SER:O	1:Z:450:LYS:HB2	2.19	0.42
1:D:199:PHE:HA	1:D:237:GLY:O	2.19	0.42
1:U:356:LYS:HE3	6:U:832:HOH:O	2.20	0.42
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.55	0.42
1:G:49:PRO:HA	1:G:50:PRO:HD3	1.98	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:65:THR:HG22	6:B:662:HOH:O	2.20	0.42
1:Z:239:TYR:HB3	1:Z:266:MET:HB3	2.02	0.42
1:G:158:GLU:CD	1:G:325:HIS:HE2	2.20	0.42
1:D:331:VAL:HA	1:D:337:GLY:O	2.20	0.42
2:K:52:VAL:HA	2:K:69:ASP:O	2.19	0.42
2:N:102:ASP:O	2:N:126:PRO:HB3	2.20	0.42
1:F:168:GLY:HA2	1:F:396:ASP:O	2.20	0.42
1:B:88:GLU:HB3	1:B:98:ILE:HB	2.02	0.42
2:K:39:ILE:O	2:K:109:ALA:HA	2.20	0.42
2:M:32:TYR:HE1	6:M:313:HOH:O	2.02	0.42
2:K:67:TYR:CD1	2:K:67:TYR:C	2.93	0.42
2:6:133:GLN:NE2	2:6:134:PRO:HD2	2.34	0.42
1:W:93:GLU:HG2	1:W:96:GLN:HB2	2.02	0.42
1:A:171:GLY:HA3	1:A:401:GLN:HG2	2.02	0.42
1:Z:10:GLY:N	6:Z:1083:HOH:O	2.52	0.42
1:W:463:LYS:HB2	1:W:463:LYS:HE3	1.86	0.42
1:H:239:TYR:HB3	1:H:266:MET:HB3	2.01	0.42
2:K:39:ILE:HA	2:K:40:PRO:HD3	1.92	0.42
1:Y:214:TRP:CD2	1:Y:253:ARG:HG2	2.55	0.42
1:Y:318:LEU:C	1:Y:318:LEU:HD13	2.40	0.42
1:A:259:GLU:OE1	2:L:61:GLY:HA3	2.20	0.42
1:V:409:HIS:CD2	1:V:416:GLY:HA2	2.55	0.42
1:F:110:GLU:HB3	1:F:147:THR:HB	2.01	0.42
2:M:138:ARG:HD2	6:M:241:HOH:O	2.18	0.42
1:U:318:LEU:C	1:U:318:LEU:HD13	2.40	0.42
1:D:290:LEU:HG	2:L:66:LEU:CD1	2.48	0.41
1:B:418:ALA:O	1:B:422:VAL:HG23	2.19	0.41
1:X:206:VAL:C	1:X:207:ASN:HD22	2.23	0.41
2:7:57:ALA:HA	2:7:60:PHE:CD2	2.55	0.41
6:E:683:HOH:O	5:F:617:GOL:H31	2.19	0.41
1:T:110:GLU:HB3	1:T:147:THR:HB	2.02	0.41
1:H:409:HIS:CD2	1:H:416:GLY:HA2	2.55	0.41
2:1:69:ASP:O	2:1:70:ASN:HB2	2.20	0.41
2:N:14:THR:O	2:N:15:PHE:HB2	2.19	0.41
2:2:88:GLN:HG2	2:2:91:ARG:NH2	2.35	0.41
1:A:381:GLY:HA2	1:E:66:TRP:CD1	2.54	0.41
1:E:19:ASP:HB3	1:E:21:ARG:HG2	2.02	0.41
2:8:39:ILE:O	2:8:109:ALA:HA	2.20	0.41
1:Z:475:LEU:HD13	6:Z:702:HOH:O	2.19	0.41
1:Z:206:VAL:C	1:Z:207:ASN:HD22	2.23	0.41
1:H:195:GLY:HA3	1:H:417:ALA:HB3	2.02	0.41
2:6:13:GLU:HB3	2:6:14:THR:H	1.66	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:85:ASP:HA	2:2:86:PRO:HD2	1.93	0.41
1:U:24:TYR:CD2	1:U:59:ALA:HB2	2.55	0.41
1:E:190:TYR:CZ	1:E:227:LYS:HE3	2.55	0.41
1:V:77:LEU:HA	1:V:77:LEU:HD23	1.89	0.41
1:X:168:GLY:HA2	1:X:396:ASP:O	2.21	0.41
1:B:421:ARG:O	1:B:425:GLU:HG3	2.21	0.41
1:S:190:TYR:CZ	1:S:227:LYS:HE3	2.55	0.41
1:T:360:ARG:NH2	6:T:1026:HOH:O	2.53	0.41
1:V:177:LYS:HB2	1:Z:63:THR:HA	2.02	0.41
1:A:318:LEU:HD13	1:A:318:LEU:C	2.41	0.41
1:C:318:LEU:C	1:C:318:LEU:HD13	2.41	0.41
2:N:69:ASP:O	2:N:70:ASN:HB2	2.21	0.41
1:D:9:ALA:HA	2:M:84:ARG:HE	1.84	0.41
1:U:158:GLU:CD	1:U:325:HIS:HE2	2.19	0.41
1:V:293:ILE:HG13	1:V:318:LEU:HD21	2.02	0.41
1:B:458:ALA:O	1:B:461:VAL:HG22	2.20	0.41
1:X:165:TYR:CD1	2:6:117:GLN:HB3	2.55	0.41
2:L:97:THR:HB	2:L:124:GLN:NE2	2.36	0.41
1:W:32:ARG:NH1	6:W:862:HOH:O	2.52	0.41
2:L:15:PHE:CE2	2:L:119:MET:HE1	2.56	0.41
2:O:76:TRP:CZ2	2:O:77:LYS:HE3	2.56	0.41
2:P:38:TRP:O	2:P:40:PRO:HD3	2.20	0.41
2:L:119:MET:CG	2:L:120:GLY:N	2.84	0.41
2:2:134:PRO:HG2	2:2:137:LYS:HB2	2.02	0.41
1:C:139:ARG:HD2	1:C:139:ARG:C	2.41	0.41
2:L:118:ILE:HD12	2:L:118:ILE:C	2.40	0.41
2:5:85:ASP:HA	2:5:86:PRO:HD2	1.89	0.41
1:T:411:TRP:CZ3	2:2:2:MET:HG3	2.56	0.41
1:V:234:GLU:OE2	2:4:13:GLU:HA	2.21	0.41
1:U:387:MET:HB3	1:U:388:PRO:HD3	2.02	0.41
1:D:45:GLN:HG3	1:D:128:LYS:O	2.19	0.41
1:Z:83:ARG:O	1:Z:101:VAL:HA	2.21	0.41
2:K:134:PRO:HG2	2:K:137:LYS:HB2	2.03	0.41
1:F:474:LYS:HG2	6:F:976:HOH:O	2.20	0.41
1:S:90:VAL:O	1:S:93:GLU:HB2	2.20	0.41
1:S:331:VAL:HA	1:S:337:GLY:O	2.19	0.41
1:C:385:TRP:CZ2	1:C:459:CYS:HB3	2.55	0.41
1:S:448:ALA:HA	1:S:451:TRP:NE1	2.36	0.41
2:K:14:THR:O	2:K:15:PHE:HB2	2.21	0.41
1:B:447:SER:O	1:B:450:LYS:HB2	2.20	0.41
2:8:97:THR:HB	2:8:124:GLN:NE2	2.36	0.41
2:7:14:THR:O	2:7:15:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:ALA:O	1:B:297:MET:CB	2.64	0.41
2:2:39:ILE:O	2:2:109:ALA:HA	2.20	0.41
2:P:39:ILE:O	2:P:109:ALA:HA	2.20	0.41
2:M:85:ASP:HA	2:M:86:PRO:HD2	1.93	0.41
1:C:266:MET:HA	1:C:292:HIS:O	2.20	0.41
2:K:33:ILE:HG21	2:K:40:PRO:HG3	2.03	0.41
1:V:387:MET:HB3	1:V:388:PRO:HD3	2.03	0.41
1:E:451:TRP:CZ2	2:M:19:PRO:HD3	2.56	0.41
1:C:110:GLU:HB3	1:C:147:THR:HB	2.03	0.41
1:Y:160:ASP:HA	1:Y:165:TYR:OH	2.21	0.41
2:2:14:THR:O	2:2:15:PHE:HB2	2.20	0.41
1:X:151:HYP:HA	1:X:152:PRO:HD3	1.95	0.41
2:8:130:ARG:NH1	2:8:130:ARG:HB2	2.36	0.41
1:S:410:PRO:HD3	1:S:461:VAL:HG21	2.02	0.41
2:M:14:THR:O	2:M:15:PHE:HB2	2.20	0.41
1:W:151:HYP:HA	1:W:152:PRO:HD3	2.00	0.41
1:H:387:MET:HB3	1:H:388:PRO:HD3	2.01	0.41
2:6:107:LEU:HG	2:6:119:MET:HE1	2.03	0.41
1:Y:331:VAL:HA	1:Y:337:GLY:O	2.20	0.41
1:B:37:LEU:HB2	1:B:139:ARG:HB3	2.03	0.41
1:F:141:PRO:HA	1:F:142:PRO:HD3	1.99	0.41
1:H:293:ILE:HG13	1:H:318:LEU:HD21	2.03	0.41
2:6:85:ASP:HA	2:6:86:PRO:HD2	1.93	0.41
1:G:214:TRP:CD2	1:G:253:ARG:HG2	2.55	0.41
1:Y:177:LYS:HG2	1:Y:203:ASP:OD2	2.21	0.41
2:2:77:LYS:HB3	2:3:1:MME:HE3	2.03	0.41
1:G:32:ARG:NH2	6:G:939:HOH:O	2.54	0.41
1:V:345:PHE:O	1:V:349:MET:HG3	2.21	0.41
2:P:13:GLU:HB3	2:P:14:THR:H	1.68	0.41
2:P:14:THR:O	2:P:15:PHE:HB2	2.20	0.41
2:6:33:ILE:HD11	2:6:119:MET:CE	2.47	0.40
1:D:170:LEU:CD1	1:D:421:ARG:HA	2.52	0.40
1:G:151:HYP:HA	1:G:152:PRO:HD3	1.97	0.40
1:T:141:PRO:HA	1:T:142:PRO:HD3	1.98	0.40
2:8:107:LEU:O	2:8:120:GLY:HA2	2.21	0.40
1:D:118:THR:O	1:D:122:GLY:HA3	2.21	0.40
1:C:134:ARG:HD3	1:C:136:GLU:OE2	2.21	0.40
1:Z:387:MET:HB3	1:Z:388:PRO:HD3	2.03	0.40
1:Y:134:ARG:HA	1:Y:308:GLY:O	2.21	0.40
1:Y:290:LEU:HG	2:7:66:LEU:CD1	2.51	0.40
2:M:13:GLU:HB3	2:M:14:THR:H	1.68	0.40
1:Y:37:LEU:O	1:Y:138:LEU:HA	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:8:ASN:O	2:P:133:GLN:HG2	2.21	0.40
1:W:411:TRP:CD1	2:5:1:MME:HG3	2.56	0.40
2:K:136:ASN:ND2	2:K:136:ASN:N	2.69	0.40
2:N:118:ILE:HD12	2:N:119:MET:N	2.36	0.40
1:Z:266:MET:HA	1:Z:292:HIS:O	2.21	0.40
1:W:195:GLY:HA3	1:W:417:ALA:HB3	2.04	0.40
1:A:345:PHE:O	1:A:349:MET:HG3	2.22	0.40
1:U:110:GLU:HB3	1:U:147:THR:HB	2.03	0.40
1:H:175:LYS:HA	1:H:176:PRO:C	2.41	0.40
2:I:14:THR:O	2:I:15:PHE:HB2	2.20	0.40
1:V:151:HYP:HA	1:V:152:PRO:HD3	1.94	0.40
1:Z:383:HIS:CE1	1:Z:385:TRP:HB2	2.56	0.40
1:S:118:THR:O	1:S:122:GLY:HA3	2.21	0.40
1:C:24:TYR:CG	1:C:59:ALA:HB2	2.57	0.40
2:3:14:THR:O	2:3:15:PHE:HB2	2.21	0.40
2:K:13:GLU:HB3	2:K:14:THR:H	1.67	0.40
2:6:125:ARG:HD3	2:6:132:TRP:CD1	2.55	0.40
1:T:63:THR:HA	1:X:177:LYS:HB2	2.04	0.40
1:H:151:HYP:HA	1:H:152:PRO:HD3	1.99	0.40
2:5:13:GLU:HB3	2:5:14:THR:H	1.68	0.40
2:J:124:GLN:HG2	2:J:125:ARG:N	2.37	0.40
1:B:451:TRP:CH2	2:J:19:PRO:HD3	2.56	0.40
1:U:177:LYS:HB2	1:Y:62:SER:O	2.21	0.40
1:F:134:ARG:HD2	1:F:305:ARG:O	2.22	0.40
2:3:130:ARG:NH2	6:3:283:HOH:O	2.53	0.40
2:5:107:LEU:O	2:5:120:GLY:HA2	2.21	0.40
1:T:302:ASP:HB2	6:T:816:HOH:O	2.20	0.40
1:U:201:KCX:HB2	1:U:239:TYR:CD2	2.56	0.40
1:F:239:TYR:HB3	1:F:266:MET:HB3	2.03	0.40
1:G:293:ILE:HG13	1:G:318:LEU:HD21	2.04	0.40
1:Y:269:TYR:CD2	1:Y:318:LEU:HD23	2.57	0.40
6:D:1017:HOH:O	2:L:119:MET:CE	2.70	0.40
2:N:107:LEU:O	2:N:120:GLY:HA2	2.21	0.40
1:U:206:VAL:C	1:U:207:ASN:HD22	2.25	0.40
1:A:425:GLU:OE1	2:I:17:TYR:HB2	2.22	0.40
1:V:63:THR:HA	1:Z:177:LYS:HB2	2.03	0.40
1:X:422:VAL:HG13	1:X:451:TRP:CH2	2.56	0.40
1:S:409:HIS:CD2	1:S:416:GLY:HA2	2.56	0.40
1:Y:284:CYS:HB3	1:Y:289:LEU:O	2.21	0.40
1:W:88:GLU:CG	1:W:98:ILE:HB	2.51	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	461/475 (97%)	444 (96%)	15 (3%)	2 (0%)	43	25
1	B	460/475 (97%)	443 (96%)	16 (4%)	1 (0%)	56	38
1	C	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	56	38
1	D	460/475 (97%)	445 (97%)	14 (3%)	1 (0%)	56	38
1	E	458/475 (96%)	442 (96%)	15 (3%)	1 (0%)	56	38
1	F	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	56	38
1	G	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	56	38
1	H	461/475 (97%)	448 (97%)	11 (2%)	2 (0%)	43	25
1	S	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	56	38
1	T	459/475 (97%)	445 (97%)	12 (3%)	2 (0%)	43	25
1	U	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	43	25
1	V	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	43	25
1	W	459/475 (97%)	443 (96%)	15 (3%)	1 (0%)	56	38
1	X	459/475 (97%)	444 (97%)	13 (3%)	2 (0%)	43	25
1	Y	458/475 (96%)	444 (97%)	13 (3%)	1 (0%)	56	38
1	Z	459/475 (97%)	442 (96%)	15 (3%)	2 (0%)	43	25
2	1	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	2	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	3	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	4	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	5	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	6	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	7	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	8	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	I	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	J	138/140 (99%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
2	L	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	M	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	O	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	P	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
All	All	9560/9840 (97%)	9177 (96%)	360 (4%)	23 (0%)	56	38

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	T	11	ALA
1	U	8	LYS
1	Z	11	ALA
1	X	11	ALA
1	H	9	ALA
1	V	8	LYS
1	C	337	GLY
1	T	337	GLY
1	U	337	GLY
1	Z	337	GLY
1	D	337	GLY
1	F	337	GLY
1	G	337	GLY
1	H	337	GLY
1	S	337	GLY
1	V	337	GLY
1	W	337	GLY
1	X	337	GLY
1	Y	337	GLY
1	A	337	GLY
1	B	337	GLY
1	E	337	GLY

5.3.2 Protein sidechains

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

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/376 (98%)	367 (100%)	2 (0%)	94	91
1	B	368/376 (98%)	366 (100%)	2 (0%)	94	91
1	C	368/376 (98%)	363 (99%)	5 (1%)	78	68
1	D	368/376 (98%)	366 (100%)	2 (0%)	94	91
1	E	368/376 (98%)	364 (99%)	4 (1%)	84	77
1	F	368/376 (98%)	367 (100%)	1 (0%)	96	94
1	G	368/376 (98%)	363 (99%)	5 (1%)	78	68
1	H	369/376 (98%)	366 (99%)	3 (1%)	89	85
1	S	368/376 (98%)	367 (100%)	1 (0%)	96	94
1	T	368/376 (98%)	365 (99%)	3 (1%)	89	85
1	U	370/376 (98%)	367 (99%)	3 (1%)	89	85
1	V	370/376 (98%)	367 (99%)	3 (1%)	89	85
1	W	368/376 (98%)	364 (99%)	4 (1%)	84	77
1	X	368/376 (98%)	364 (99%)	4 (1%)	84	77
1	Y	368/376 (98%)	364 (99%)	4 (1%)	84	77
1	Z	368/376 (98%)	363 (99%)	5 (1%)	78	68
2	1	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	2	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	3	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	4	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	5	123/123 (100%)	122 (99%)	1 (1%)	89	85
2	6	123/123 (100%)	122 (99%)	1 (1%)	89	85
2	7	123/123 (100%)	122 (99%)	1 (1%)	89	85
2	8	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	I	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	J	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	K	123/123 (100%)	120 (98%)	3 (2%)	61	44
2	L	123/123 (100%)	120 (98%)	3 (2%)	61	44
2	M	123/123 (100%)	121 (98%)	2 (2%)	75	62
2	N	123/123 (100%)	122 (99%)	1 (1%)	89	85
2	O	123/123 (100%)	122 (99%)	1 (1%)	89	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	123/123 (100%)	121 (98%)	2 (2%)	75	62
All	All	7862/7984 (98%)	7782 (99%)	80 (1%)	85	80

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	TYR
1	A	297	MET
2	I	12	PHE
2	I	130	ARG
1	B	14	LYS
1	B	239	TYR
2	J	55	GLU
2	J	136	ASN
1	C	185	TYR
1	C	239	TYR
1	C	339	ARG
1	C	439	ARG
1	C	450	LYS
2	K	84	ARG
2	K	119	MET
2	K	136	ASN
1	D	239	TYR
1	D	355	GLU
2	L	12	PHE
2	L	55	GLU
2	L	91	ARG
1	E	239	TYR
1	E	439	ARG
1	E	463	LYS
1	E	466	LYS
2	M	12	PHE
2	M	23	ASP
1	F	239	TYR
2	N	130	ARG
1	G	96	GLN
1	G	172	CYS
1	G	185	TYR
1	G	239	TYR
1	G	475	LEU
2	O	136	ASN
1	H	96	GLN

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Mol	Chain	Res	Type
1	H	185	TYR
1	H	239	TYR
2	P	12	PHE
2	P	88	GLN
1	S	239	TYR
2	1	55	GLU
2	1	137	LYS
1	T	94	ASP
1	T	185	TYR
1	T	239	TYR
2	2	132	TRP
2	2	136	ASN
1	U	239	TYR
1	U	464	GLU
1	U	474	LYS
2	3	12	PHE
2	3	58	ILE
1	V	239	TYR
1	V	297	MET
1	V	460	GLU
2	4	88	GLN
2	4	119	MET
1	W	239	TYR
1	W	297	MET
1	W	463	LYS
1	W	475	LEU
2	5	55	GLU
1	X	93	GLU
1	X	94	ASP
1	X	185	TYR
1	X	239	TYR
2	6	119	MET
1	Y	14	LYS
1	Y	96	GLN
1	Y	172	CYS
1	Y	239	TYR
2	7	12	PHE
1	Z	172	CYS
1	Z	185	TYR
1	Z	203	ASP
1	Z	239	TYR
1	Z	475	LEU

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Mol	Chain	Res	Type
2	8	12	PHE
2	8	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	401	GLN
2	I	8	ASN
2	I	29	GLN
2	I	124	GLN
2	I	133	GLN
1	B	207	ASN
1	B	401	GLN
2	J	8	ASN
2	J	29	GLN
2	J	124	GLN
2	J	133	GLN
2	J	136	ASN
1	C	401	GLN
2	K	8	ASN
2	K	29	GLN
2	K	124	GLN
2	K	136	ASN
1	D	401	GLN
2	L	8	ASN
2	L	29	GLN
2	L	113	GLN
2	L	124	GLN
1	E	207	ASN
1	E	401	GLN
2	M	8	ASN
2	M	29	GLN
2	M	88	GLN
2	M	124	GLN
1	F	401	GLN
2	N	8	ASN
2	N	29	GLN
2	N	124	GLN
1	G	207	ASN
1	G	401	GLN
2	O	8	ASN

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Mol	Chain	Res	Type
2	O	29	GLN
2	O	88	GLN
2	O	113	GLN
2	O	124	GLN
2	O	136	ASN
1	H	401	GLN
2	P	8	ASN
2	P	29	GLN
2	P	88	GLN
2	P	113	GLN
2	P	124	GLN
2	P	133	GLN
1	S	207	ASN
1	S	401	GLN
2	1	8	ASN
2	1	29	GLN
2	1	88	GLN
2	1	117	GLN
2	1	124	GLN
2	1	133	GLN
1	T	401	GLN
2	2	8	ASN
2	2	29	GLN
2	2	88	GLN
2	2	124	GLN
2	2	136	ASN
1	U	207	ASN
1	U	401	GLN
2	3	8	ASN
2	3	29	GLN
2	3	88	GLN
2	3	124	GLN
1	V	207	ASN
1	V	401	GLN
2	4	8	ASN
2	4	29	GLN
2	4	113	GLN
2	4	124	GLN
2	4	133	GLN
1	W	207	ASN
1	W	401	GLN
2	5	8	ASN

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Mol	Chain	Res	Type
2	5	29	GLN
2	5	113	GLN
2	5	124	GLN
1	X	401	GLN
2	6	8	ASN
2	6	29	GLN
2	6	88	GLN
2	6	124	GLN
2	6	133	GLN
1	Y	207	ASN
1	Y	401	GLN
2	7	8	ASN
2	7	29	GLN
2	7	88	GLN
2	7	124	GLN
1	Z	401	GLN
2	8	8	ASN
2	8	29	GLN
2	8	88	GLN
2	8	124	GLN
2	8	136	ASN

5.3.3 RNA

There are no RNA chains in this entry.

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

96 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	$\# Z > 2$
2	MME	1	1	2	8,8,9	6.50	3 (37%)	5,8,10	1.26	1 (20%)
2	MME	2	1	2	8,8,9	6.33	3 (37%)	5,8,10	1.31	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MME	3	1	2	8,8,9	6.43	3 (37%)	5,8,10	1.32	1 (20%)
2	MME	4	1	2	8,8,9	6.52	3 (37%)	5,8,10	1.33	1 (20%)
2	MME	5	1	2	8,8,9	6.44	3 (37%)	5,8,10	1.36	1 (20%)
2	MME	6	1	2	8,8,9	6.47	3 (37%)	5,8,10	1.31	1 (20%)
2	MME	7	1	2	8,8,9	6.46	3 (37%)	5,8,10	1.28	1 (20%)
2	MME	8	1	2	8,8,9	6.39	3 (37%)	5,8,10	1.32	1 (20%)
1	HYP	A	104	1	8,8,9	8.51	2 (25%)	8,10,12	1.14	0
1	HYP	A	151	1	8,8,9	8.24	1 (12%)	8,10,12	1.29	1 (12%)
1	KCX	A	201	1,3	11,11,12	6.07	2 (18%)	10,12,14	2.22	3 (30%)
1	SMC	A	256	1	6,6,7	7.53	2 (33%)	4,6,8	2.20	1 (25%)
1	SMC	A	369	1	6,6,7	8.37	2 (33%)	4,6,8	0.70	0
1	HYP	B	104	1	8,8,9	8.58	2 (25%)	8,10,12	1.04	0
1	HYP	B	151	1	8,8,9	8.32	1 (12%)	8,10,12	1.31	1 (12%)
1	KCX	B	201	1,3	11,11,12	5.74	1 (9%)	10,12,14	2.16	3 (30%)
1	SMC	B	256	1	6,6,7	7.64	2 (33%)	4,6,8	2.38	1 (25%)
1	SMC	B	369	1	6,6,7	8.14	2 (33%)	4,6,8	0.82	0
1	HYP	C	104	1	8,8,9	8.52	1 (12%)	8,10,12	1.05	1 (12%)
1	HYP	C	151	1	8,8,9	8.37	1 (12%)	8,10,12	1.32	1 (12%)
1	KCX	C	201	1,3	11,11,12	6.06	2 (18%)	10,12,14	2.19	3 (30%)
1	SMC	C	256	1	6,6,7	7.61	2 (33%)	4,6,8	2.03	1 (25%)
1	SMC	C	369	1	6,6,7	7.71	2 (33%)	4,6,8	0.93	0
1	HYP	D	104	1	8,8,9	8.48	2 (25%)	8,10,12	1.10	1 (12%)
1	HYP	D	151	1	8,8,9	8.43	2 (25%)	8,10,12	1.33	1 (12%)
1	KCX	D	201	1,3	11,11,12	5.76	1 (9%)	10,12,14	2.11	3 (30%)
1	SMC	D	256	1	6,6,7	7.66	2 (33%)	4,6,8	2.11	1 (25%)
1	SMC	D	369	1	6,6,7	7.92	2 (33%)	4,6,8	0.68	0
1	HYP	E	104	1	8,8,9	8.36	2 (25%)	8,10,12	1.02	1 (12%)
1	HYP	E	151	1	8,8,9	8.60	1 (12%)	8,10,12	1.36	1 (12%)
1	KCX	E	201	1,3	11,11,12	5.81	2 (18%)	10,12,14	2.20	3 (30%)
1	SMC	E	256	1	6,6,7	7.78	2 (33%)	4,6,8	2.07	1 (25%)
1	SMC	E	369	1	6,6,7	8.01	2 (33%)	4,6,8	0.68	0
1	HYP	F	104	1	8,8,9	8.36	2 (25%)	8,10,12	1.07	0
1	HYP	F	151	1	8,8,9	8.23	2 (25%)	8,10,12	1.33	1 (12%)
1	KCX	F	201	1,3	11,11,12	5.92	2 (18%)	10,12,14	2.17	3 (30%)
1	SMC	F	256	1	6,6,7	7.56	2 (33%)	4,6,8	2.10	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SMC	F	369	1	6,6,7	8.11	2 (33%)	4,6,8	0.68	0
1	HYP	G	104	1	8,8,9	8.49	2 (25%)	8,10,12	1.04	0
1	HYP	G	151	1	8,8,9	8.45	1 (12%)	8,10,12	1.35	1 (12%)
1	KCX	G	201	1,3	11,11,12	5.68	2 (18%)	10,12,14	2.17	3 (30%)
1	SMC	G	256	1	6,6,7	7.73	2 (33%)	4,6,8	2.21	1 (25%)
1	SMC	G	369	1	6,6,7	7.79	2 (33%)	4,6,8	0.72	0
1	HYP	H	104	1	8,8,9	8.21	1 (12%)	8,10,12	1.09	0
1	HYP	H	151	1	8,8,9	8.33	2 (25%)	8,10,12	1.23	1 (12%)
1	KCX	H	201	1,3	11,11,12	5.98	2 (18%)	10,12,14	2.27	4 (40%)
1	SMC	H	256	1	6,6,7	7.63	2 (33%)	4,6,8	2.10	1 (25%)
1	SMC	H	369	1	6,6,7	8.02	2 (33%)	4,6,8	0.88	0
2	MME	I	1	2	8,8,9	6.40	3 (37%)	5,8,10	1.31	1 (20%)
2	MME	J	1	2	8,8,9	6.44	3 (37%)	5,8,10	1.33	1 (20%)
2	MME	K	1	2	8,8,9	6.55	3 (37%)	5,8,10	1.32	1 (20%)
2	MME	L	1	2	8,8,9	6.48	3 (37%)	5,8,10	1.28	1 (20%)
2	MME	M	1	2	8,8,9	6.44	3 (37%)	5,8,10	1.30	1 (20%)
2	MME	N	1	2	8,8,9	6.31	3 (37%)	5,8,10	1.33	1 (20%)
2	MME	O	1	2	8,8,9	6.38	3 (37%)	5,8,10	1.31	1 (20%)
2	MME	P	1	2	8,8,9	6.36	3 (37%)	5,8,10	1.39	1 (20%)
1	HYP	S	104	1	8,8,9	8.21	2 (25%)	8,10,12	1.14	1 (12%)
1	HYP	S	151	1	8,8,9	8.27	1 (12%)	8,10,12	1.35	1 (12%)
1	KCX	S	201	1,3	11,11,12	5.93	2 (18%)	10,12,14	2.18	3 (30%)
1	SMC	S	256	1	6,6,7	7.56	2 (33%)	4,6,8	2.15	1 (25%)
1	SMC	S	369	1	6,6,7	7.92	2 (33%)	4,6,8	0.67	0
1	HYP	T	104	1	8,8,9	8.30	2 (25%)	8,10,12	1.07	1 (12%)
1	HYP	T	151	1	8,8,9	8.18	1 (12%)	8,10,12	1.32	1 (12%)
1	KCX	T	201	1,3	11,11,12	5.79	2 (18%)	10,12,14	2.18	3 (30%)
1	SMC	T	256	1	6,6,7	7.42	2 (33%)	4,6,8	2.26	1 (25%)
1	SMC	T	369	1	6,6,7	8.34	2 (33%)	4,6,8	0.77	0
1	HYP	U	104	1	8,8,9	8.26	2 (25%)	8,10,12	1.04	1 (12%)
1	HYP	U	151	1	8,8,9	8.23	1 (12%)	8,10,12	1.23	1 (12%)
1	KCX	U	201	1,3	11,11,12	6.03	2 (18%)	10,12,14	2.30	3 (30%)
1	SMC	U	256	1	6,6,7	7.55	2 (33%)	4,6,8	2.28	1 (25%)
1	SMC	U	369	1	6,6,7	8.04	2 (33%)	4,6,8	0.67	0
1	HYP	V	104	1	8,8,9	8.57	2 (25%)	8,10,12	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	V	151	1	8,8,9	8.21	1 (12%)	8,10,12	1.36	1 (12%)
1	KCX	V	201	1,3	11,11,12	5.95	1 (9%)	10,12,14	2.07	3 (30%)
1	SMC	V	256	1	6,6,7	7.49	2 (33%)	4,6,8	2.16	1 (25%)
1	SMC	V	369	1	6,6,7	7.89	2 (33%)	4,6,8	0.71	0
1	HYP	W	104	1	8,8,9	8.40	2 (25%)	8,10,12	1.07	0
1	HYP	W	151	1	8,8,9	8.26	2 (25%)	8,10,12	1.29	1 (12%)
1	KCX	W	201	1,3	11,11,12	5.85	2 (18%)	10,12,14	2.23	4 (40%)
1	SMC	W	256	1	6,6,7	7.94	2 (33%)	4,6,8	2.08	1 (25%)
1	SMC	W	369	1	6,6,7	8.02	2 (33%)	4,6,8	0.87	0
1	HYP	X	104	1	8,8,9	8.76	2 (25%)	8,10,12	1.07	0
1	HYP	X	151	1	8,8,9	8.19	2 (25%)	8,10,12	1.41	2 (25%)
1	KCX	X	201	1,3	11,11,12	5.84	2 (18%)	10,12,14	2.20	3 (30%)
1	SMC	X	256	1	6,6,7	7.67	2 (33%)	4,6,8	2.02	1 (25%)
1	SMC	X	369	1	6,6,7	7.89	2 (33%)	4,6,8	0.85	0
1	HYP	Y	104	1	8,8,9	8.17	2 (25%)	8,10,12	1.08	0
1	HYP	Y	151	1	8,8,9	8.19	1 (12%)	8,10,12	1.30	1 (12%)
1	KCX	Y	201	1,3	11,11,12	5.93	2 (18%)	10,12,14	2.18	3 (30%)
1	SMC	Y	256	1	6,6,7	7.62	2 (33%)	4,6,8	2.50	1 (25%)
1	SMC	Y	369	1	6,6,7	8.16	2 (33%)	4,6,8	0.54	0
1	HYP	Z	104	1	8,8,9	8.27	2 (25%)	8,10,12	1.08	1 (12%)
1	HYP	Z	151	1	8,8,9	8.57	1 (12%)	8,10,12	1.24	1 (12%)
1	KCX	Z	201	1,3	11,11,12	5.88	2 (18%)	10,12,14	2.11	3 (30%)
1	SMC	Z	256	1	6,6,7	7.75	2 (33%)	4,6,8	2.10	1 (25%)
1	SMC	Z	369	1	6,6,7	7.93	2 (33%)	4,6,8	0.50	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
2	MME	1	1	2	-	0/6/8/10	0/0/0/0
2	MME	2	1	2	-	0/6/8/10	0/0/0/0
2	MME	3	1	2	-	0/6/8/10	0/0/0/0
2	MME	4	1	2	-	0/6/8/10	0/0/0/0
2	MME	5	1	2	-	0/6/8/10	0/0/0/0
2	MME	6	1	2	-	0/6/8/10	0/0/0/0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MME	I	1	2	-	0/6/8/10	0/0/0/0
2	MME	J	1	2	-	0/6/8/10	0/0/0/0
2	MME	K	1	2	-	0/6/8/10	0/0/0/0
2	MME	L	1	2	-	0/6/8/10	0/0/0/0
2	MME	M	1	2	-	0/6/8/10	0/0/0/0
2	MME	N	1	2	-	0/6/8/10	0/0/0/0
2	MME	O	1	2	-	0/6/8/10	0/0/0/0
2	MME	P	1	2	-	0/6/8/10	0/0/0/0
1	HYP	S	104	1	-	0/0/11/13	0/1/1/1
1	HYP	S	151	1	-	0/0/11/13	0/1/1/1
1	KCX	S	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	S	256	1	-	0/3/5/7	0/0/0/0
1	SMC	S	369	1	-	0/3/5/7	0/0/0/0
1	HYP	T	104	1	-	0/0/11/13	0/1/1/1
1	HYP	T	151	1	-	0/0/11/13	0/1/1/1
1	KCX	T	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	T	256	1	-	0/3/5/7	0/0/0/0
1	SMC	T	369	1	-	0/3/5/7	0/0/0/0
1	HYP	U	104	1	-	0/0/11/13	0/1/1/1
1	HYP	U	151	1	-	0/0/11/13	0/1/1/1
1	KCX	U	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	U	256	1	-	0/3/5/7	0/0/0/0
1	SMC	U	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	-	0/8/10/12	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
1	HYP	W	104	1	-	0/0/11/13	0/1/1/1
1	HYP	W	151	1	-	0/0/11/13	0/1/1/1
1	KCX	W	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	W	256	1	-	0/3/5/7	0/0/0/0
1	SMC	W	369	1	-	0/3/5/7	0/0/0/0
1	HYP	X	104	1	-	0/0/11/13	0/1/1/1
1	HYP	X	151	1	-	0/0/11/13	0/1/1/1
1	KCX	X	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	X	256	1	-	0/3/5/7	0/0/0/0
1	SMC	X	369	1	-	0/3/5/7	0/0/0/0
1	HYP	Y	104	1	-	0/0/11/13	0/1/1/1
1	HYP	Y	151	1	-	0/0/11/13	0/1/1/1
1	KCX	Y	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	Y	256	1	-	0/3/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	Y	369	1	-	0/3/5/7	0/0/0/0
1	HYP	Z	104	1	-	0/0/11/13	0/1/1/1
1	HYP	Z	151	1	-	0/0/11/13	0/1/1/1
1	KCX	Z	201	1,3	-	0/8/10/12	0/0/0/0
1	SMC	Z	256	1	-	0/3/5/7	0/0/0/0
1	SMC	Z	369	1	-	0/3/5/7	0/0/0/0

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	104	HYP	O-C	24.62	1.28	1.11
1	E	151	HYP	O-C	24.19	1.28	1.11
1	B	104	HYP	O-C	24.12	1.28	1.11
1	Z	151	HYP	O-C	24.12	1.28	1.11
1	V	104	HYP	O-C	24.09	1.28	1.11
1	C	104	HYP	O-C	23.97	1.28	1.11
1	A	104	HYP	O-C	23.93	1.28	1.11
1	G	104	HYP	O-C	23.86	1.27	1.11
1	D	104	HYP	O-C	23.84	1.27	1.11
1	G	151	HYP	O-C	23.78	1.27	1.11
1	D	151	HYP	O-C	23.70	1.27	1.11
1	W	104	HYP	O-C	23.60	1.27	1.11
1	C	151	HYP	O-C	23.54	1.27	1.11
1	F	104	HYP	O-C	23.49	1.27	1.11
1	E	104	HYP	O-C	23.48	1.27	1.11
1	H	151	HYP	O-C	23.42	1.27	1.11
1	B	151	HYP	O-C	23.41	1.27	1.11
1	T	104	HYP	O-C	23.31	1.27	1.11
1	S	151	HYP	O-C	23.25	1.27	1.11
1	Z	104	HYP	O-C	23.25	1.27	1.11
1	W	151	HYP	O-C	23.20	1.27	1.11
1	A	151	HYP	O-C	23.20	1.27	1.11
1	U	104	HYP	O-C	23.19	1.27	1.11
1	U	151	HYP	O-C	23.14	1.27	1.11
1	F	151	HYP	O-C	23.13	1.27	1.11
1	V	151	HYP	O-C	23.09	1.27	1.11
1	H	104	HYP	O-C	23.07	1.27	1.11
1	Y	151	HYP	O-C	23.05	1.27	1.11
1	S	104	HYP	O-C	23.04	1.27	1.11
1	T	151	HYP	O-C	23.03	1.27	1.11
1	X	151	HYP	O-C	23.02	1.27	1.11
1	Y	104	HYP	O-C	22.94	1.27	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	SMC	O-C	20.13	1.25	1.11
1	T	369	SMC	O-C	20.04	1.25	1.11
1	A	201	KCX	O-C	19.77	1.25	1.11
1	C	201	KCX	O-C	19.75	1.25	1.11
1	U	201	KCX	O-C	19.61	1.24	1.11
1	B	369	SMC	O-C	19.57	1.24	1.11
1	Y	369	SMC	O-C	19.55	1.24	1.11
1	F	369	SMC	O-C	19.50	1.24	1.11
1	H	201	KCX	O-C	19.45	1.24	1.11
1	V	201	KCX	O-C	19.45	1.24	1.11
1	U	369	SMC	O-C	19.33	1.24	1.11
1	Y	201	KCX	O-C	19.32	1.24	1.11
1	F	201	KCX	O-C	19.30	1.24	1.11
1	H	369	SMC	O-C	19.27	1.24	1.11
1	S	201	KCX	O-C	19.27	1.24	1.11
1	W	369	SMC	O-C	19.24	1.24	1.11
1	E	369	SMC	O-C	19.22	1.24	1.11
1	W	256	SMC	O-C	19.16	1.24	1.11
1	Z	201	KCX	O-C	19.12	1.24	1.11
1	X	201	KCX	O-C	19.05	1.24	1.11
1	Z	369	SMC	O-C	19.05	1.24	1.11
1	D	369	SMC	O-C	19.04	1.24	1.11
1	S	369	SMC	O-C	18.99	1.24	1.11
1	X	369	SMC	O-C	18.98	1.24	1.11
1	W	201	KCX	O-C	18.97	1.24	1.11
1	V	369	SMC	O-C	18.96	1.24	1.11
1	E	201	KCX	O-C	18.85	1.24	1.11
1	T	201	KCX	O-C	18.77	1.24	1.11
1	D	201	KCX	O-C	18.74	1.24	1.11
1	E	256	SMC	O-C	18.74	1.24	1.11
1	B	201	KCX	O-C	18.73	1.24	1.11
1	Z	256	SMC	O-C	18.69	1.24	1.11
1	G	256	SMC	O-C	18.68	1.24	1.11
1	G	369	SMC	O-C	18.63	1.24	1.11
1	C	369	SMC	O-C	18.53	1.24	1.11
1	G	201	KCX	O-C	18.52	1.24	1.11
1	D	256	SMC	O-C	18.50	1.24	1.11
1	X	256	SMC	O-C	18.45	1.24	1.11
1	Y	256	SMC	O-C	18.44	1.24	1.11
1	B	256	SMC	O-C	18.44	1.24	1.11
1	H	256	SMC	O-C	18.41	1.24	1.11
1	C	256	SMC	O-C	18.36	1.24	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	256	SMC	O-C	18.27	1.24	1.11
1	S	256	SMC	O-C	18.25	1.24	1.11
1	F	256	SMC	O-C	18.24	1.24	1.11
1	A	256	SMC	O-C	18.15	1.23	1.11
1	V	256	SMC	O-C	18.06	1.23	1.11
1	T	256	SMC	O-C	17.93	1.23	1.11
2	K	1	MME	O-C	17.91	1.23	1.11
2	4	1	MME	O-C	17.70	1.23	1.11
2	1	1	MME	O-C	17.68	1.23	1.11
2	L	1	MME	O-C	17.66	1.23	1.11
2	7	1	MME	O-C	17.62	1.23	1.11
2	6	1	MME	O-C	17.58	1.23	1.11
2	5	1	MME	O-C	17.55	1.23	1.11
2	J	1	MME	O-C	17.54	1.23	1.11
2	3	1	MME	O-C	17.53	1.23	1.11
2	M	1	MME	O-C	17.51	1.23	1.11
2	I	1	MME	O-C	17.43	1.23	1.11
2	8	1	MME	O-C	17.38	1.23	1.11
2	O	1	MME	O-C	17.37	1.23	1.11
2	P	1	MME	O-C	17.32	1.23	1.11
2	2	1	MME	O-C	17.24	1.23	1.11
2	N	1	MME	O-C	17.18	1.23	1.11
2	4	1	MME	CM-N	-4.33	1.33	1.46
2	J	1	MME	CM-N	-4.31	1.33	1.46
2	6	1	MME	CM-N	-4.30	1.33	1.46
2	P	1	MME	CM-N	-4.29	1.33	1.46
2	3	1	MME	CM-N	-4.29	1.33	1.46
2	1	1	MME	CM-N	-4.29	1.33	1.46
2	8	1	MME	CM-N	-4.28	1.33	1.46
2	I	1	MME	CM-N	-4.28	1.33	1.46
2	7	1	MME	CM-N	-4.28	1.33	1.46
2	K	1	MME	CM-N	-4.27	1.33	1.46
2	N	1	MME	CM-N	-4.27	1.33	1.46
2	5	1	MME	CM-N	-4.27	1.33	1.46
2	M	1	MME	CM-N	-4.26	1.33	1.46
2	O	1	MME	CM-N	-4.26	1.33	1.46
2	2	1	MME	CM-N	-4.24	1.33	1.46
2	L	1	MME	CM-N	-4.24	1.33	1.46
1	Y	369	SMC	CA-C	4.04	1.56	1.48
1	G	369	SMC	CA-C	4.04	1.56	1.48
1	W	369	SMC	CA-C	3.93	1.55	1.48
1	S	369	SMC	CA-C	3.88	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	369	SMC	CA-C	3.84	1.55	1.48
1	E	369	SMC	CA-C	3.84	1.55	1.48
1	Z	369	SMC	CA-C	3.71	1.55	1.48
1	B	369	SMC	CA-C	3.71	1.55	1.48
1	F	369	SMC	CA-C	3.70	1.55	1.48
1	V	369	SMC	CA-C	3.68	1.55	1.48
1	A	369	SMC	CA-C	3.68	1.55	1.48
1	H	369	SMC	CA-C	3.65	1.55	1.48
1	D	369	SMC	CA-C	3.63	1.55	1.48
1	X	369	SMC	CA-C	3.59	1.55	1.48
1	C	369	SMC	CA-C	3.56	1.55	1.48
1	U	369	SMC	CA-C	3.56	1.55	1.48
1	X	256	SMC	CA-C	3.44	1.54	1.48
1	W	256	SMC	CA-C	3.33	1.54	1.48
1	E	256	SMC	CA-C	3.29	1.54	1.48
1	A	256	SMC	CA-C	3.23	1.54	1.48
1	F	256	SMC	CA-C	3.18	1.54	1.48
1	Z	256	SMC	CA-C	3.16	1.54	1.48
1	H	256	SMC	CA-C	3.10	1.54	1.48
1	G	256	SMC	CA-C	3.09	1.54	1.48
1	S	256	SMC	CA-C	3.08	1.54	1.48
1	C	256	SMC	CA-C	3.03	1.54	1.48
1	V	256	SMC	CA-C	3.01	1.54	1.48
1	B	256	SMC	CA-C	2.97	1.53	1.48
1	D	256	SMC	CA-C	2.93	1.53	1.48
1	T	256	SMC	CA-C	2.89	1.53	1.48
1	U	256	SMC	CA-C	2.83	1.53	1.48
1	E	201	KCX	CB-CA	2.76	1.55	1.53
1	Y	256	SMC	CA-C	2.76	1.53	1.48
2	6	1	MME	CA-C	2.73	1.53	1.48
1	H	201	KCX	CB-CA	2.73	1.55	1.53
2	4	1	MME	CA-C	2.71	1.53	1.48
1	T	201	KCX	CB-CA	2.70	1.55	1.53
2	M	1	MME	CA-C	2.60	1.53	1.48
1	W	201	KCX	CB-CA	2.59	1.55	1.53
2	1	1	MME	CA-C	2.50	1.53	1.48
1	A	201	KCX	CB-CA	2.47	1.55	1.53
1	U	201	KCX	CB-CA	2.47	1.55	1.53
2	5	1	MME	CA-C	2.42	1.52	1.48
2	I	1	MME	CA-C	2.40	1.52	1.48
2	2	1	MME	CA-C	2.35	1.52	1.48
2	8	1	MME	CA-C	2.35	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	MME	CA-C	2.33	1.52	1.48
1	F	201	KCX	CB-CA	2.32	1.55	1.53
1	Z	201	KCX	CB-CA	2.31	1.55	1.53
2	J	1	MME	CA-C	2.31	1.52	1.48
1	S	104	HYP	CA-C	2.30	1.52	1.48
2	O	1	MME	CA-C	2.28	1.52	1.48
1	Y	201	KCX	CB-CA	2.27	1.55	1.53
2	7	1	MME	CA-C	2.25	1.52	1.48
2	3	1	MME	CA-C	2.22	1.52	1.48
2	L	1	MME	CA-C	2.21	1.52	1.48
1	E	104	HYP	CA-C	2.21	1.52	1.48
1	Y	104	HYP	CA-C	2.19	1.52	1.48
1	H	151	HYP	CA-C	2.19	1.52	1.48
1	T	104	HYP	CA-C	2.19	1.52	1.48
1	Z	104	HYP	CA-C	2.19	1.52	1.48
1	C	201	KCX	CB-CA	2.19	1.55	1.53
1	F	104	HYP	CA-C	2.19	1.52	1.48
1	B	104	HYP	CA-C	2.18	1.52	1.48
2	K	1	MME	CA-C	2.17	1.52	1.48
1	D	104	HYP	CA-C	2.17	1.52	1.48
1	G	104	HYP	CA-C	2.15	1.52	1.48
2	N	1	MME	CA-C	2.14	1.52	1.48
1	A	104	HYP	CA-C	2.13	1.52	1.48
1	W	151	HYP	CA-C	2.13	1.52	1.48
1	U	104	HYP	CA-C	2.12	1.52	1.48
1	X	104	HYP	CA-C	2.12	1.52	1.48
1	S	201	KCX	CB-CA	2.09	1.55	1.53
1	D	151	HYP	CA-C	2.09	1.52	1.48
1	V	104	HYP	CA-C	2.08	1.52	1.48
1	G	201	KCX	CB-CA	2.05	1.55	1.53
1	X	151	HYP	CA-C	2.05	1.52	1.48
1	F	151	HYP	CA-C	2.04	1.52	1.48
1	W	104	HYP	CA-C	2.03	1.52	1.48
1	X	201	KCX	CB-CA	2.03	1.55	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	201	KCX	OQ2-CX-NZ	4.86	122.38	116.33
1	H	201	KCX	OQ2-CX-NZ	4.77	122.27	116.33
1	A	201	KCX	OQ2-CX-NZ	4.70	122.19	116.33
1	W	201	KCX	OQ2-CX-NZ	4.68	122.16	116.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	256	SMC	C-CA-N	-4.67	109.16	113.83
1	E	201	KCX	OQ2-CX-NZ	4.66	122.14	116.33
1	X	201	KCX	OQ2-CX-NZ	4.65	122.13	116.33
1	Y	201	KCX	OQ2-CX-NZ	4.62	122.08	116.33
1	C	201	KCX	OQ2-CX-NZ	4.58	122.03	116.33
1	F	201	KCX	OQ2-CX-NZ	4.56	122.01	116.33
1	S	201	KCX	OQ2-CX-NZ	4.55	121.99	116.33
1	G	201	KCX	OQ2-CX-NZ	4.53	121.97	116.33
1	T	201	KCX	OQ2-CX-NZ	4.53	121.97	116.33
1	B	201	KCX	OQ2-CX-NZ	4.52	121.96	116.33
1	D	201	KCX	OQ2-CX-NZ	4.38	121.78	116.33
1	Z	201	KCX	OQ2-CX-NZ	4.38	121.78	116.33
1	V	201	KCX	OQ2-CX-NZ	4.33	121.73	116.33
1	B	256	SMC	C-CA-N	-4.22	109.62	113.83
1	U	256	SMC	C-CA-N	-4.19	109.64	113.83
1	U	201	KCX	OQ2-CX-OQ1	-4.17	116.97	122.17
1	A	256	SMC	C-CA-N	-4.07	109.76	113.83
1	T	256	SMC	C-CA-N	-4.06	109.77	113.83
1	H	201	KCX	OQ2-CX-OQ1	-4.01	117.17	122.17
1	G	256	SMC	C-CA-N	-4.00	109.83	113.83
1	W	201	KCX	OQ2-CX-OQ1	-3.97	117.21	122.17
1	S	256	SMC	C-CA-N	-3.96	109.87	113.83
1	Y	201	KCX	OQ2-CX-OQ1	-3.96	117.22	122.17
1	C	201	KCX	OQ2-CX-OQ1	-3.95	117.23	122.17
1	S	201	KCX	OQ2-CX-OQ1	-3.90	117.31	122.17
1	F	256	SMC	C-CA-N	-3.88	109.95	113.83
1	G	201	KCX	OQ2-CX-OQ1	-3.88	117.33	122.17
1	B	201	KCX	OQ2-CX-OQ1	-3.86	117.35	122.17
1	E	201	KCX	OQ2-CX-OQ1	-3.85	117.36	122.17
1	H	256	SMC	C-CA-N	-3.85	109.99	113.83
1	T	201	KCX	OQ2-CX-OQ1	-3.84	117.37	122.17
1	X	201	KCX	OQ2-CX-OQ1	-3.84	117.38	122.17
1	A	201	KCX	OQ2-CX-OQ1	-3.83	117.38	122.17
1	F	201	KCX	OQ2-CX-OQ1	-3.83	117.39	122.17
1	D	201	KCX	OQ2-CX-OQ1	-3.82	117.40	122.17
1	D	256	SMC	C-CA-N	-3.81	110.02	113.83
1	V	256	SMC	C-CA-N	-3.78	110.06	113.83
1	C	256	SMC	C-CA-N	-3.78	110.06	113.83
1	E	256	SMC	C-CA-N	-3.75	110.08	113.83
1	Z	256	SMC	C-CA-N	-3.74	110.09	113.83
1	Z	201	KCX	OQ2-CX-OQ1	-3.71	117.54	122.17
1	W	256	SMC	C-CA-N	-3.68	110.15	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	256	SMC	C-CA-N	-3.63	110.20	113.83
1	V	201	KCX	OQ2-CX-OQ1	-3.59	117.69	122.17
1	S	151	HYP	CG-CD-N	-2.91	100.79	105.47
2	4	1	MME	CM-N-CA	2.88	121.89	113.11
2	5	1	MME	CM-N-CA	2.86	121.83	113.11
2	6	1	MME	CM-N-CA	2.85	121.79	113.11
2	P	1	MME	CM-N-CA	2.84	121.77	113.11
2	K	1	MME	CM-N-CA	2.84	121.77	113.11
2	I	1	MME	CM-N-CA	2.84	121.77	113.11
2	M	1	MME	CM-N-CA	2.82	121.72	113.11
2	J	1	MME	CM-N-CA	2.82	121.71	113.11
2	2	1	MME	CM-N-CA	2.81	121.68	113.11
2	O	1	MME	CM-N-CA	2.79	121.64	113.11
2	3	1	MME	CM-N-CA	2.79	121.63	113.11
2	N	1	MME	CM-N-CA	2.78	121.60	113.11
2	8	1	MME	CM-N-CA	2.77	121.56	113.11
1	G	151	HYP	CG-CD-N	-2.76	101.02	105.47
1	V	151	HYP	CG-CD-N	-2.76	101.02	105.47
1	D	151	HYP	CG-CD-N	-2.75	101.03	105.47
2	1	1	MME	CM-N-CA	2.75	121.49	113.11
2	7	1	MME	CM-N-CA	2.74	121.48	113.11
1	E	151	HYP	CG-CD-N	-2.73	101.07	105.47
1	A	201	KCX	OQ1-CX-NZ	-2.71	120.43	124.94
1	Y	151	HYP	CG-CD-N	-2.70	101.13	105.47
1	X	151	HYP	CG-CD-N	-2.69	101.14	105.47
1	X	201	KCX	OQ1-CX-NZ	-2.67	120.50	124.94
1	E	201	KCX	OQ1-CX-NZ	-2.67	120.50	124.94
1	B	151	HYP	CG-CD-N	-2.66	101.18	105.47
1	A	151	HYP	CG-CD-N	-2.65	101.21	105.47
1	W	151	HYP	CG-CD-N	-2.64	101.22	105.47
1	C	151	HYP	CG-CD-N	-2.63	101.23	105.47
1	H	201	KCX	OQ1-CX-NZ	-2.63	120.56	124.94
1	T	151	HYP	CG-CD-N	-2.63	101.24	105.47
1	V	201	KCX	OQ1-CX-NZ	-2.62	120.59	124.94
1	F	201	KCX	OQ1-CX-NZ	-2.60	120.61	124.94
1	W	201	KCX	OQ1-CX-NZ	-2.59	120.63	124.94
1	U	201	KCX	OQ1-CX-NZ	-2.58	120.65	124.94
1	T	201	KCX	OQ1-CX-NZ	-2.57	120.66	124.94
2	L	1	MME	CM-N-CA	2.57	120.95	113.11
1	Z	201	KCX	OQ1-CX-NZ	-2.56	120.68	124.94
1	B	201	KCX	OQ1-CX-NZ	-2.56	120.69	124.94
1	G	201	KCX	OQ1-CX-NZ	-2.55	120.69	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	201	KCX	OQ1-CX-NZ	-2.55	120.70	124.94
1	S	201	KCX	OQ1-CX-NZ	-2.55	120.70	124.94
1	F	151	HYP	CG-CD-N	-2.54	101.37	105.47
1	C	201	KCX	OQ1-CX-NZ	-2.53	120.73	124.94
1	U	151	HYP	CG-CD-N	-2.52	101.40	105.47
1	D	201	KCX	OQ1-CX-NZ	-2.48	120.82	124.94
1	H	151	HYP	CG-CD-N	-2.29	101.79	105.47
1	Z	151	HYP	CG-CD-N	-2.28	101.80	105.47
1	X	151	HYP	C-CA-N	2.21	114.95	110.86
1	Z	104	HYP	CG-CD-N	-2.13	102.03	105.47
1	T	104	HYP	CG-CD-N	-2.12	102.06	105.47
1	C	104	HYP	CG-CD-N	-2.11	102.07	105.47
1	H	201	KCX	CE-NZ-CX	2.06	125.74	121.99
1	E	104	HYP	CG-CD-N	-2.05	102.17	105.47
1	D	104	HYP	CG-CD-N	-2.03	102.21	105.47
1	W	201	KCX	CE-NZ-CX	2.02	125.68	121.99
1	S	104	HYP	CG-CD-N	-2.01	102.23	105.47
1	U	104	HYP	CG-CD-N	-2.00	102.25	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 72 ligands modelled in this entry, 16 are monoatomic - leaving 56 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	501	3	20,20,20	1.35	2 (10%)	31,31,31	1.51	6 (19%)
5	GOL	A	605	-	5,5,5	0.99	0	5,5,5	0.36	0
5	GOL	A	613	-	5,5,5	0.93	0	5,5,5	0.32	0
4	CAP	B	501	3	20,20,20	1.33	2 (10%)	31,31,31	1.45	5 (16%)
5	GOL	B	606	-	5,5,5	1.01	0	5,5,5	0.42	0
5	GOL	B	610	-	5,5,5	0.97	0	5,5,5	0.35	0
5	GOL	B	614	-	5,5,5	0.91	0	5,5,5	0.29	0
4	CAP	C	501	3	20,20,20	1.40	3 (15%)	31,31,31	1.53	5 (16%)
5	GOL	C	607	-	5,5,5	0.95	0	5,5,5	0.34	0
5	GOL	C	615	-	5,5,5	0.93	0	5,5,5	0.36	0
4	CAP	D	501	3	20,20,20	1.35	2 (10%)	31,31,31	1.44	5 (16%)
5	GOL	D	608	-	5,5,5	0.99	0	5,5,5	0.31	0
5	GOL	D	616	-	5,5,5	0.96	0	5,5,5	0.48	0
4	CAP	E	501	3	20,20,20	1.34	2 (10%)	31,31,31	1.48	4 (12%)
5	GOL	E	601	-	5,5,5	0.94	0	5,5,5	0.33	0
5	GOL	E	609	-	5,5,5	0.97	0	5,5,5	0.38	0
5	GOL	E	620	-	5,5,5	0.93	0	5,5,5	0.32	0
4	CAP	F	501	3	20,20,20	1.33	2 (10%)	31,31,31	1.43	5 (16%)
5	GOL	F	602	-	5,5,5	0.95	0	5,5,5	0.31	0
5	GOL	F	617	-	5,5,5	0.94	0	5,5,5	0.27	0
4	CAP	G	501	3	20,20,20	1.26	2 (10%)	31,31,31	1.47	5 (16%)
5	GOL	G	603	-	5,5,5	0.96	0	5,5,5	0.30	0
5	GOL	G	611	-	5,5,5	1.01	0	5,5,5	0.37	0
5	GOL	G	618	-	5,5,5	0.91	0	5,5,5	0.33	0
4	CAP	H	501	3	20,20,20	1.29	2 (10%)	31,31,31	1.46	5 (16%)
5	GOL	H	604	-	5,5,5	0.99	0	5,5,5	0.31	0
5	GOL	H	612	-	5,5,5	0.98	0	5,5,5	0.36	0
5	GOL	H	619	-	5,5,5	0.96	0	5,5,5	0.31	0
4	CAP	S	501	3	20,20,20	1.40	3 (15%)	31,31,31	1.44	5 (16%)
5	GOL	S	605	-	5,5,5	0.96	0	5,5,5	0.30	0
5	GOL	S	609	-	5,5,5	0.92	0	5,5,5	0.33	0
5	GOL	S	613	-	5,5,5	0.93	0	5,5,5	0.33	0
4	CAP	T	501	3	20,20,20	1.35	2 (10%)	31,31,31	1.52	6 (19%)
5	GOL	T	606	-	5,5,5	0.96	0	5,5,5	0.32	0
5	GOL	T	614	-	5,5,5	0.96	0	5,5,5	0.31	0
4	CAP	U	501	3	20,20,20	1.39	2 (10%)	31,31,31	1.46	4 (12%)
5	GOL	U	607	-	5,5,5	0.97	0	5,5,5	0.31	0
5	GOL	U	615	-	5,5,5	0.92	0	5,5,5	0.33	0
4	CAP	V	501	3	20,20,20	1.37	2 (10%)	31,31,31	1.47	5 (16%)
5	GOL	V	608	-	5,5,5	0.97	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	V	616	-	5,5,5	0.96	0	5,5,5	0.33	0
4	CAP	W	501	3	20,20,20	1.37	2 (10%)	31,31,31	1.48	5 (16%)
5	GOL	W	601	-	5,5,5	0.95	0	5,5,5	0.33	0
5	GOL	W	620	-	5,5,5	0.94	0	5,5,5	0.43	0
4	CAP	X	501	3	20,20,20	1.34	2 (10%)	31,31,31	1.52	4 (12%)
5	GOL	X	602	-	5,5,5	0.94	0	5,5,5	0.32	0
5	GOL	X	610	-	5,5,5	0.97	0	5,5,5	0.35	0
5	GOL	X	617	-	5,5,5	0.94	0	5,5,5	0.30	0
4	CAP	Y	501	3	20,20,20	1.35	2 (10%)	31,31,31	1.50	5 (16%)
5	GOL	Y	603	-	5,5,5	0.96	0	5,5,5	0.33	0
5	GOL	Y	611	-	5,5,5	0.99	0	5,5,5	0.35	0
5	GOL	Y	618	-	5,5,5	0.96	0	5,5,5	0.33	0
4	CAP	Z	501	3	20,20,20	1.27	2 (10%)	31,31,31	1.42	5 (16%)
5	GOL	Z	604	-	5,5,5	0.93	0	5,5,5	0.32	0
5	GOL	Z	612	-	5,5,5	0.99	0	5,5,5	0.34	0
5	GOL	Z	619	-	5,5,5	0.93	0	5,5,5	0.32	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	501	3	-	0/29/29/29	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
5	GOL	A	613	-	-	0/4/4/4	0/0/0/0
4	CAP	B	501	3	-	0/29/29/29	0/0/0/0
5	GOL	B	606	-	-	0/4/4/4	0/0/0/0
5	GOL	B	610	-	-	0/4/4/4	0/0/0/0
5	GOL	B	614	-	-	0/4/4/4	0/0/0/0
4	CAP	C	501	3	-	0/29/29/29	0/0/0/0
5	GOL	C	607	-	-	0/4/4/4	0/0/0/0
5	GOL	C	615	-	-	0/4/4/4	0/0/0/0
4	CAP	D	501	3	-	0/29/29/29	0/0/0/0
5	GOL	D	608	-	-	0/4/4/4	0/0/0/0
5	GOL	D	616	-	-	0/4/4/4	0/0/0/0
4	CAP	E	501	3	-	0/29/29/29	0/0/0/0
5	GOL	E	601	-	-	0/4/4/4	0/0/0/0
5	GOL	E	609	-	-	0/4/4/4	0/0/0/0
5	GOL	E	620	-	-	0/4/4/4	0/0/0/0
4	CAP	F	501	3	-	0/29/29/29	0/0/0/0
5	GOL	F	602	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	617	-	-	0/4/4/4	0/0/0/0
4	CAP	G	501	3	-	0/29/29/29	0/0/0/0
5	GOL	G	603	-	-	0/4/4/4	0/0/0/0
5	GOL	G	611	-	-	0/4/4/4	0/0/0/0
5	GOL	G	618	-	-	0/4/4/4	0/0/0/0
4	CAP	H	501	3	-	0/29/29/29	0/0/0/0
5	GOL	H	604	-	-	0/4/4/4	0/0/0/0
5	GOL	H	612	-	-	0/4/4/4	0/0/0/0
5	GOL	H	619	-	-	0/4/4/4	0/0/0/0
4	CAP	S	501	3	-	0/29/29/29	0/0/0/0
5	GOL	S	605	-	-	0/4/4/4	0/0/0/0
5	GOL	S	609	-	-	0/4/4/4	0/0/0/0
5	GOL	S	613	-	-	0/4/4/4	0/0/0/0
4	CAP	T	501	3	-	0/29/29/29	0/0/0/0
5	GOL	T	606	-	-	0/4/4/4	0/0/0/0
5	GOL	T	614	-	-	0/4/4/4	0/0/0/0
4	CAP	U	501	3	-	0/29/29/29	0/0/0/0
5	GOL	U	607	-	-	0/4/4/4	0/0/0/0
5	GOL	U	615	-	-	0/4/4/4	0/0/0/0
4	CAP	V	501	3	-	0/29/29/29	0/0/0/0
5	GOL	V	608	-	-	0/4/4/4	0/0/0/0
5	GOL	V	616	-	-	0/4/4/4	0/0/0/0
4	CAP	W	501	3	-	0/29/29/29	0/0/0/0
5	GOL	W	601	-	-	0/4/4/4	0/0/0/0
5	GOL	W	620	-	-	0/4/4/4	0/0/0/0
4	CAP	X	501	3	-	0/29/29/29	0/0/0/0
5	GOL	X	602	-	-	0/4/4/4	0/0/0/0
5	GOL	X	610	-	-	0/4/4/4	0/0/0/0
5	GOL	X	617	-	-	0/4/4/4	0/0/0/0
4	CAP	Y	501	3	-	0/29/29/29	0/0/0/0
5	GOL	Y	603	-	-	0/4/4/4	0/0/0/0
5	GOL	Y	611	-	-	0/4/4/4	0/0/0/0
5	GOL	Y	618	-	-	0/4/4/4	0/0/0/0
4	CAP	Z	501	3	-	0/29/29/29	0/0/0/0
5	GOL	Z	604	-	-	0/4/4/4	0/0/0/0
5	GOL	Z	612	-	-	0/4/4/4	0/0/0/0
5	GOL	Z	619	-	-	0/4/4/4	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	501	CAP	C2-C	3.66	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	501	CAP	C2-C	3.65	1.58	1.53
4	A	501	CAP	C2-C	3.53	1.58	1.53
4	E	501	CAP	C2-C	3.53	1.58	1.53
4	U	501	CAP	C2-C	3.50	1.58	1.53
4	V	501	CAP	C2-C	3.42	1.58	1.53
4	C	501	CAP	C2-C	3.39	1.58	1.53
4	S	501	CAP	C2-C	3.39	1.58	1.53
4	B	501	CAP	C2-C	3.37	1.58	1.53
4	Y	501	CAP	C2-C	3.36	1.58	1.53
4	T	501	CAP	C2-C	3.35	1.58	1.53
4	F	501	CAP	C2-C	3.33	1.58	1.53
4	H	501	CAP	C2-C	3.22	1.58	1.53
4	D	501	CAP	C2-C	3.20	1.58	1.53
4	Z	501	CAP	C2-C	3.12	1.57	1.53
4	G	501	CAP	C2-C	2.93	1.57	1.53
4	G	501	CAP	C5-C4	2.78	1.56	1.51
4	V	501	CAP	C5-C4	2.76	1.56	1.51
4	S	501	CAP	C5-C4	2.74	1.56	1.51
4	C	501	CAP	C5-C4	2.74	1.56	1.51
4	U	501	CAP	C5-C4	2.68	1.55	1.51
4	Y	501	CAP	C5-C4	2.53	1.55	1.51
4	D	501	CAP	C5-C4	2.49	1.55	1.51
4	Z	501	CAP	C5-C4	2.47	1.55	1.51
4	B	501	CAP	C5-C4	2.46	1.55	1.51
4	T	501	CAP	C5-C4	2.45	1.55	1.51
4	A	501	CAP	C5-C4	2.43	1.55	1.51
4	E	501	CAP	C5-C4	2.34	1.55	1.51
4	F	501	CAP	C5-C4	2.32	1.55	1.51
4	W	501	CAP	C5-C4	2.28	1.55	1.51
4	X	501	CAP	C5-C4	2.20	1.55	1.51
4	H	501	CAP	C5-C4	2.20	1.55	1.51
4	S	501	CAP	C2-C3	2.03	1.57	1.54
4	C	501	CAP	C2-C3	2.01	1.57	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	501	CAP	O1-C1-C2	4.05	113.06	108.34
4	A	501	CAP	O1-C1-C2	4.01	113.02	108.34
4	T	501	CAP	O1-C1-C2	3.98	112.99	108.34
4	Y	501	CAP	O1-C1-C2	3.89	112.88	108.34
4	C	501	CAP	O1-C1-C2	3.89	112.88	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	CAP	O1-C1-C2	3.85	112.83	108.34
4	C	501	CAP	O7-C-C2	3.76	121.78	113.58
4	W	501	CAP	O7-C-C2	3.71	121.67	113.58
4	T	501	CAP	O7-C-C2	3.69	121.62	113.58
4	V	501	CAP	O7-C-C2	3.68	121.60	113.58
4	D	501	CAP	O1-C1-C2	3.67	112.63	108.34
4	H	501	CAP	O1-C1-C2	3.65	112.60	108.34
4	X	501	CAP	O7-C-C2	3.64	121.52	113.58
4	A	501	CAP	O7-C-C2	3.64	121.51	113.58
4	E	501	CAP	O7-C-C2	3.63	121.50	113.58
4	Y	501	CAP	O7-C-C2	3.62	121.47	113.58
4	G	501	CAP	O7-C-C2	3.61	121.44	113.58
4	U	501	CAP	O1-C1-C2	3.59	112.54	108.34
4	F	501	CAP	O7-C-C2	3.57	121.37	113.58
4	Z	501	CAP	O7-C-C2	3.57	121.36	113.58
4	U	501	CAP	O7-C-C2	3.56	121.34	113.58
4	B	501	CAP	O7-C-C2	3.56	121.34	113.58
4	H	501	CAP	O7-C-C2	3.55	121.31	113.58
4	S	501	CAP	O7-C-C2	3.50	121.21	113.58
4	V	501	CAP	O1-C1-C2	3.48	112.41	108.34
4	W	501	CAP	O1-C1-C2	3.46	112.38	108.34
4	S	501	CAP	O1-C1-C2	3.46	112.39	108.34
4	D	501	CAP	O7-C-C2	3.46	121.12	113.58
4	G	501	CAP	O1-C1-C2	3.45	112.37	108.34
4	B	501	CAP	O1-C1-C2	3.39	112.30	108.34
4	F	501	CAP	O1-C1-C2	3.32	112.22	108.34
4	C	501	CAP	C2-C3-C4	3.03	119.74	113.28
4	Z	501	CAP	O1-C1-C2	2.98	111.82	108.34
4	S	501	CAP	C2-C3-C4	2.98	119.62	113.28
4	W	501	CAP	C2-C3-C4	2.91	119.49	113.28
4	G	501	CAP	C2-C3-C4	2.85	119.35	113.28
4	A	501	CAP	C2-C3-C4	2.82	119.28	113.28
4	Y	501	CAP	C2-C3-C4	2.81	119.25	113.28
4	B	501	CAP	C2-C3-C4	2.80	119.25	113.28
4	H	501	CAP	C2-C3-C4	2.80	119.24	113.28
4	V	501	CAP	C2-C3-C4	2.79	119.23	113.28
4	F	501	CAP	C2-C3-C4	2.79	119.22	113.28
4	E	501	CAP	C2-C3-C4	2.78	119.19	113.28
4	X	501	CAP	C2-C3-C4	2.77	119.19	113.28
4	Z	501	CAP	C2-C3-C4	2.74	119.12	113.28
4	D	501	CAP	C2-C3-C4	2.73	119.10	113.28
4	T	501	CAP	C2-C3-C4	2.72	119.08	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	501	CAP	C2-C3-C4	2.69	119.01	113.28
4	V	501	CAP	O2P-P1-O1P	2.35	118.13	110.44
4	W	501	CAP	O2P-P1-O1P	2.34	118.08	110.44
4	X	501	CAP	O2P-P1-O1P	2.34	118.08	110.44
4	B	501	CAP	O2P-P1-O1P	2.33	118.07	110.44
4	F	501	CAP	O2P-P1-O1P	2.32	118.03	110.44
4	D	501	CAP	O2P-P1-O1P	2.32	118.04	110.44
4	T	501	CAP	O2P-P1-O1P	2.32	118.03	110.44
4	U	501	CAP	O2P-P1-O1P	2.30	117.97	110.44
4	G	501	CAP	O2P-P1-O1P	2.30	117.97	110.44
4	H	501	CAP	O2P-P1-O1P	2.28	117.90	110.44
4	Z	501	CAP	O2P-P1-O1P	2.28	117.89	110.44
4	C	501	CAP	O2P-P1-O1P	2.25	117.81	110.44
4	A	501	CAP	O2P-P1-O1P	2.24	117.75	110.44
4	S	501	CAP	O2P-P1-O1P	2.23	117.73	110.44
4	A	501	CAP	C1-C2-C	2.21	113.21	109.17
4	S	501	CAP	O5P-P2-O4P	2.18	117.58	110.44
4	E	501	CAP	O2P-P1-O1P	2.18	117.56	110.44
4	Y	501	CAP	O2P-P1-O1P	2.18	117.55	110.44
4	Y	501	CAP	C1-C2-C	2.16	113.12	109.17
4	G	501	CAP	O5P-P2-O4P	2.15	117.46	110.44
4	Z	501	CAP	O5P-P2-O4P	2.14	117.43	110.44
4	W	501	CAP	O5P-P2-O4P	2.12	117.37	110.44
4	F	501	CAP	O5P-P2-O4P	2.09	117.28	110.44
4	D	501	CAP	O5P-P2-O4P	2.09	117.27	110.44
4	V	501	CAP	O5P-P2-O4P	2.08	117.23	110.44
4	H	501	CAP	O5P-P2-O4P	2.07	117.21	110.44
4	B	501	CAP	O5P-P2-O4P	2.04	117.11	110.44
4	T	501	CAP	C1-C2-C	2.03	112.88	109.17
4	A	501	CAP	O5P-P2-O4P	2.03	117.07	110.44
4	T	501	CAP	O5P-P2-O4P	2.03	117.06	110.44
4	C	501	CAP	O5P-P2-O4P	2.01	117.00	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	468/475 (98%)	-0.34	5 (1%) 77 76	5, 12, 27, 61	0
1	B	467/475 (98%)	-0.39	4 (0%) 81 80	7, 13, 28, 43	0
1	C	466/475 (98%)	-0.46	3 (0%) 86 87	6, 11, 24, 49	0
1	D	467/475 (98%)	-0.48	5 (1%) 77 76	6, 10, 23, 46	0
1	E	465/475 (97%)	-0.50	3 (0%) 86 87	6, 11, 24, 40	0
1	F	465/475 (97%)	-0.44	2 (0%) 90 91	7, 12, 24, 43	0
1	G	466/475 (98%)	-0.45	3 (0%) 86 87	6, 10, 24, 39	0
1	H	468/475 (98%)	-0.53	4 (0%) 81 80	4, 9, 22, 57	0
1	S	465/475 (97%)	-0.41	2 (0%) 90 91	6, 12, 27, 49	0
1	T	466/475 (98%)	-0.40	4 (0%) 81 80	6, 12, 27, 48	0
1	U	469/475 (98%)	-0.41	6 (1%) 74 72	6, 12, 27, 62	0
1	V	469/475 (98%)	-0.37	7 (1%) 70 69	5, 11, 26, 66	0
1	W	466/475 (98%)	-0.38	4 (0%) 81 80	6, 13, 29, 43	0
1	X	466/475 (98%)	-0.35	5 (1%) 77 76	6, 12, 27, 48	0
1	Y	465/475 (97%)	-0.42	4 (0%) 81 80	6, 11, 27, 45	0
1	Z	466/475 (98%)	-0.52	2 (0%) 90 91	5, 10, 23, 54	0
2	1	140/140 (100%)	-0.21	1 (0%) 84 85	8, 17, 30, 39	0
2	2	140/140 (100%)	-0.24	1 (0%) 84 85	9, 18, 31, 43	0
2	3	140/140 (100%)	-0.16	1 (0%) 84 85	9, 19, 34, 44	0
2	4	140/140 (100%)	-0.25	1 (0%) 84 85	9, 16, 30, 37	0
2	5	140/140 (100%)	-0.34	0 100 100	9, 16, 29, 38	0
2	6	140/140 (100%)	-0.23	0 100 100	9, 19, 33, 40	0
2	7	140/140 (100%)	-0.32	1 (0%) 84 85	8, 15, 28, 34	0
2	8	140/140 (100%)	-0.42	0 100 100	7, 14, 28, 34	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	I	140/140 (100%)	-0.21	2 (1%) 72 71	10, 18, 34, 45	0
2	J	140/140 (100%)	-0.17	2 (1%) 72 71	10, 20, 34, 42	0
2	K	140/140 (100%)	-0.23	0 100 100	8, 17, 31, 39	0
2	L	140/140 (100%)	-0.30	1 (0%) 84 85	9, 16, 30, 39	0
2	M	140/140 (100%)	-0.31	1 (0%) 84 85	8, 15, 31, 39	0
2	N	140/140 (100%)	-0.27	1 (0%) 84 85	8, 17, 29, 39	0
2	O	140/140 (100%)	-0.34	0 100 100	8, 14, 28, 36	0
2	P	140/140 (100%)	-0.36	1 (0%) 84 85	8, 14, 27, 37	0
All	All	9704/9840 (98%)	-0.39	76 (0%) 83 82	4, 12, 28, 66	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	10	GLY	8.5
1	T	10	GLY	8.3
1	D	9	ALA	7.3
1	U	9	ALA	6.8
1	X	10	GLY	6.8
1	V	7	THR	6.3
1	V	8	LYS	5.4
1	C	10	GLY	5.3
1	U	8	LYS	5.2
1	A	8	LYS	4.9
1	V	9	ALA	4.7
1	A	94	ASP	4.5
1	G	11	ALA	4.3
1	Y	11	ALA	4.2
1	W	10	GLY	4.1
1	F	11	ALA	4.0
1	S	94	ASP	3.9
1	D	10	GLY	3.9
1	D	94	ASP	3.9
1	A	10	GLY	3.8
1	B	9	ALA	3.8
1	Y	94	ASP	3.8
1	D	11	ALA	3.6
1	H	9	ALA	3.6
1	B	94	ASP	3.6
1	H	10	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	11	ALA	3.5
1	U	10	GLY	3.5
1	A	9	ALA	3.3
1	V	10	GLY	3.3
1	X	11	ALA	3.2
1	G	10	GLY	3.2
1	A	464	GLU	3.2
1	S	11	ALA	3.0
1	W	11	ALA	3.0
2	3	84	ARG	3.0
2	2	84	ARG	2.9
1	V	475	LEU	2.9
1	B	439	ARG	2.9
2	I	84	ARG	2.9
1	E	439	ARG	2.9
1	W	439	ARG	2.8
1	T	11	ALA	2.8
1	T	94	ASP	2.7
1	U	7	THR	2.7
1	D	439	ARG	2.6
1	V	439	ARG	2.6
1	B	10	GLY	2.6
1	H	8	LYS	2.5
1	F	94	ASP	2.5
1	X	439	ARG	2.5
1	U	439	ARG	2.4
2	J	84	ARG	2.4
2	N	130	ARG	2.4
1	T	439	ARG	2.4
1	Y	475	LEU	2.4
1	U	464	GLU	2.3
2	L	84	ARG	2.3
2	7	127	LYS	2.3
2	M	84	ARG	2.3
1	X	464	GLU	2.3
2	P	127	LYS	2.2
1	H	439	ARG	2.2
1	Y	439	ARG	2.2
2	1	127	LYS	2.2
2	I	127	LYS	2.2
1	V	464	GLU	2.1
1	W	91	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	94	ASP	2.1
1	Z	94	ASP	2.1
1	E	94	ASP	2.1
1	E	11	ALA	2.1
1	G	439	ARG	2.0
1	C	464	GLU	2.0
2	J	130	ARG	2.0
2	4	127	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MME	8	1	9/10	0.14	3.86	21,24,27,30	0
2	MME	N	1	9/10	0.12	3.23	18,20,28,31	0
2	MME	3	1	9/10	0.13	2.68	24,26,34,34	0
1	KCX	U	201	12/13	0.12	2.40	8,10,11,11	0
2	MME	L	1	9/10	0.13	2.27	18,24,30,30	0
2	MME	4	1	9/10	0.12	2.21	24,25,30,30	0
2	MME	O	1	9/10	0.12	2.14	18,21,28,31	0
2	MME	J	1	9/10	0.11	1.73	20,23,31,31	0
1	KCX	D	201	12/13	0.11	1.69	6,7,7,8	0
2	MME	6	1	9/10	0.10	1.68	20,21,26,27	0
2	MME	K	1	9/10	0.11	1.57	22,24,28,29	0
1	KCX	G	201	12/13	0.13	1.55	5,7,8,9	0
2	MME	M	1	9/10	0.13	1.53	21,22,30,31	0
1	KCX	H	201	12/13	0.11	1.52	5,6,7,9	0
1	KCX	V	201	12/13	0.14	1.51	8,9,11,11	0
1	KCX	B	201	12/13	0.10	1.37	7,10,11,12	0
1	KCX	S	201	12/13	0.13	1.25	5,8,8,11	0
1	HYP	E	151	8/9	0.08	1.19	8,9,10,10	0
1	KCX	Z	201	12/13	0.10	1.18	4,7,8,9	0
1	KCX	Y	201	12/13	0.11	1.14	6,7,8,8	0
1	KCX	C	201	12/13	0.10	1.09	7,9,11,11	0
1	KCX	A	201	12/13	0.14	1.08	7,9,10,11	0
2	MME	7	1	9/10	0.10	1.02	16,18,27,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MME	P	1	9/10	0.09	0.92	17,21,25,25	0
1	HYP	F	151	8/9	0.08	0.89	11,11,12,12	0
2	MME	5	1	9/10	0.09	0.72	18,21,30,31	0
2	MME	1	1	9/10	0.10	0.70	21,23,24,25	0
1	KCX	W	201	12/13	0.10	0.70	9,10,12,12	0
1	HYP	D	151	8/9	0.07	0.63	4,7,8,8	0
2	MME	2	1	9/10	0.09	0.45	21,23,27,27	0
1	KCX	F	201	12/13	0.11	0.40	5,8,10,10	0
1	HYP	V	151	8/9	0.07	0.38	7,7,9,9	0
1	HYP	C	151	8/9	0.07	0.32	7,8,9,9	0
1	SMC	W	369	7/8	0.07	0.32	9,10,11,11	0
2	MME	I	1	9/10	0.08	0.12	20,21,28,28	0
1	HYP	S	151	8/9	0.07	-0.02	7,8,9,9	0
1	HYP	A	104	8/9	0.07	-0.12	10,11,12,14	0
1	HYP	G	151	8/9	0.06	-0.13	9,9,10,11	0
1	HYP	H	151	8/9	0.07	-0.25	5,5,6,6	0
1	KCX	E	201	12/13	0.08	-0.29	6,8,10,11	0
1	KCX	T	201	12/13	0.08	-0.35	4,8,9,9	0
1	HYP	X	104	8/9	0.07	-0.35	10,10,11,11	0
1	HYP	V	104	8/9	0.07	-0.47	8,9,10,10	0
1	KCX	X	201	12/13	0.10	-0.49	7,8,10,10	0
1	HYP	D	104	8/9	0.07	-0.50	6,7,9,9	0
1	HYP	E	104	8/9	0.06	-0.52	7,9,10,10	0
1	HYP	T	151	8/9	0.07	-0.52	6,7,8,9	0
1	HYP	T	104	8/9	0.07	-0.60	9,11,12,14	0
1	HYP	U	151	8/9	0.07	-0.62	7,9,9,9	0
1	HYP	W	104	8/9	0.07	-0.63	10,11,11,12	0
1	SMC	S	256	7/8	0.05	-0.66	4,6,7,7	0
1	HYP	W	151	8/9	0.07	-0.68	5,8,9,9	0
1	HYP	X	151	8/9	0.06	-0.71	7,9,10,10	0
1	SMC	X	256	7/8	0.06	-0.71	7,7,9,11	0
1	HYP	A	151	8/9	0.07	-0.73	8,8,9,11	0
1	SMC	W	256	7/8	0.05	-0.74	8,9,9,10	0
1	SMC	E	256	7/8	0.05	-0.75	6,7,8,8	0
1	SMC	H	256	7/8	0.05	-0.76	6,6,7,8	0
1	HYP	S	104	8/9	0.06	-0.79	11,12,13,14	0
1	HYP	H	104	8/9	0.06	-0.79	6,7,8,9	0
1	HYP	B	151	8/9	0.07	-0.82	9,10,11,12	0
1	SMC	G	256	7/8	0.05	-0.85	5,6,8,8	0
1	SMC	A	369	7/8	0.06	-0.88	13,13,15,16	0
1	HYP	B	104	8/9	0.06	-0.92	8,11,11,13	0
1	HYP	F	104	8/9	0.06	-0.92	8,10,12,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SMC	B	256	7/8	0.05	-0.93	7,8,9,9	0
1	HYP	C	104	8/9	0.06	-0.94	6,8,9,9	0
1	SMC	A	256	7/8	0.05	-1.00	7,8,8,8	0
1	SMC	F	256	7/8	0.05	-1.01	8,9,9,9	0
1	HYP	Y	104	8/9	0.06	-1.05	10,11,11,12	0
1	HYP	G	104	8/9	0.06	-1.07	9,11,11,12	0
1	HYP	Z	104	8/9	0.06	-1.09	8,9,10,12	0
1	HYP	U	104	8/9	0.06	-1.09	9,9,9,9	0
1	SMC	Y	256	7/8	0.05	-1.15	6,7,8,8	0
1	SMC	C	256	7/8	0.05	-1.16	7,8,9,10	0
1	SMC	Z	256	7/8	0.04	-1.18	6,7,7,8	0
1	SMC	T	256	7/8	0.05	-1.20	6,6,7,8	0
1	HYP	Z	151	8/9	0.06	-1.26	6,7,8,9	0
1	SMC	D	256	7/8	0.04	-1.51	5,7,8,10	0
1	SMC	B	369	7/8	0.06	-1.53	12,13,13,14	0
1	SMC	U	256	7/8	0.04	-1.61	5,7,7,7	0
1	HYP	Y	151	8/9	0.06	-1.64	8,9,9,9	0
1	SMC	T	369	7/8	0.05	-1.83	11,12,13,15	0
1	SMC	X	369	7/8	0.05	-1.84	11,12,13,14	0
1	SMC	V	369	7/8	0.05	-1.86	10,10,12,14	0
1	SMC	G	369	7/8	0.06	-1.95	11,11,13,13	0
1	SMC	D	369	7/8	0.05	-1.97	8,9,10,10	0
1	SMC	V	256	7/8	0.04	-1.98	6,6,7,8	0
1	SMC	U	369	7/8	0.05	-2.07	8,9,10,11	0
1	SMC	C	369	7/8	0.05	-2.28	8,10,12,12	0
1	SMC	Y	369	7/8	0.05	-2.62	11,12,13,14	0
1	SMC	S	369	7/8	0.04	-2.75	10,10,12,12	0
1	SMC	F	369	7/8	0.04	-3.10	10,11,12,13	0
1	SMC	E	369	7/8	0.04	-3.38	8,9,10,11	0
1	SMC	H	369	7/8	0.04	-3.43	6,9,10,10	0
1	SMC	Z	369	7/8	0.04	-3.98	8,9,11,12	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	Y	618	6/6	0.19	17.09	37,40,41,41	0
5	GOL	D	616	6/6	0.17	13.99	22,26,30,32	0
5	GOL	C	615	6/6	0.15	12.12	26,28,31,32	0
5	GOL	W	620	6/6	0.15	11.66	34,36,36,37	0
5	GOL	H	619	6/6	0.17	11.17	29,32,34,34	0
5	GOL	V	616	6/6	0.14	10.66	25,27,29,30	0
5	GOL	F	617	6/6	0.18	8.31	32,32,33,34	0
5	GOL	H	604	6/6	0.20	8.07	25,30,33,34	0
5	GOL	B	614	6/6	0.15	7.41	25,31,33,34	0
5	GOL	S	609	6/6	0.18	5.98	23,25,28,32	0
5	GOL	E	620	6/6	0.14	5.89	22,26,28,28	0
5	GOL	X	617	6/6	0.12	5.65	21,27,29,30	0
5	GOL	S	613	6/6	0.12	5.48	23,25,25,26	0
5	GOL	H	612	6/6	0.14	5.47	14,18,21,21	0
5	GOL	G	611	6/6	0.18	5.28	16,18,23,26	0
5	GOL	E	609	6/6	0.14	4.47	14,17,20,22	0
5	GOL	Z	612	6/6	0.16	4.18	17,19,22,23	0
5	GOL	Y	611	6/6	0.15	4.09	19,21,22,23	0
5	GOL	Z	619	6/6	0.10	3.42	19,24,25,26	0
5	GOL	D	608	6/6	0.13	3.38	23,26,27,27	0
5	GOL	E	601	6/6	0.12	3.33	29,30,30,31	0
5	GOL	G	618	6/6	0.09	3.16	26,30,31,31	0
5	GOL	A	605	6/6	0.14	3.11	26,27,29,30	0
5	GOL	A	613	6/6	0.10	2.97	25,29,30,30	0
5	GOL	V	608	6/6	0.13	2.83	17,19,20,21	0
5	GOL	B	606	6/6	0.13	2.48	22,22,24,24	0
5	GOL	X	610	6/6	0.13	2.44	16,19,22,26	0
5	GOL	U	607	6/6	0.12	2.20	23,27,28,28	0
5	GOL	Z	604	6/6	0.11	2.15	24,26,26,28	0
5	GOL	T	614	6/6	0.08	2.10	22,27,29,29	0
5	GOL	B	610	6/6	0.13	1.98	18,20,21,23	0
5	GOL	Y	603	6/6	0.13	1.96	29,31,32,32	0
5	GOL	W	601	6/6	0.12	1.84	23,25,25,25	0
5	GOL	X	602	6/6	0.09	1.78	19,20,22,22	0
3	MG	X	476	1/1	0.11	1.68	13,13,13,13	0
5	GOL	T	606	6/6	0.12	1.58	21,22,24,25	0
5	GOL	C	607	6/6	0.09	1.15	23,24,26,27	0
5	GOL	G	603	6/6	0.10	0.91	20,22,25,27	0
5	GOL	S	605	6/6	0.10	0.86	26,28,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	U	615	6/6	0.08	0.76	20,23,25,27	0
3	MG	V	476	1/1	0.11	0.59	12,12,12,12	0
3	MG	A	476	1/1	0.12	0.55	9,9,9,9	0
3	MG	H	476	1/1	0.10	0.38	10,10,10,10	0
3	MG	G	476	1/1	0.10	0.33	11,11,11,11	0
4	CAP	S	501	21/21	0.10	0.25	10,12,12,13	0
3	MG	Z	476	1/1	0.09	0.11	9,9,9,9	0
3	MG	B	476	1/1	0.08	0.08	11,11,11,11	0
4	CAP	C	501	21/21	0.08	-0.17	8,10,11,13	0
3	MG	S	476	1/1	0.10	-0.17	11,11,11,11	0
4	CAP	A	501	21/21	0.10	-0.23	7,10,11,14	0
3	MG	Y	476	1/1	0.08	-0.26	11,11,11,11	0
4	CAP	F	501	21/21	0.09	-0.28	9,11,13,15	0
4	CAP	X	501	21/21	0.10	-0.28	8,11,13,14	0
3	MG	E	476	1/1	0.07	-0.31	11,11,11,11	0
4	CAP	V	501	21/21	0.09	-0.33	8,10,11,12	0
3	MG	W	476	1/1	0.09	-0.36	12,12,12,12	0
4	CAP	G	501	21/21	0.08	-0.46	6,8,10,11	0
4	CAP	Z	501	21/21	0.07	-0.55	7,9,10,11	0
4	CAP	U	501	21/21	0.09	-0.57	11,13,14,16	0
5	GOL	F	602	6/6	0.07	-0.60	22,24,25,27	0
3	MG	C	476	1/1	0.09	-0.60	13,13,13,13	0
4	CAP	W	501	21/21	0.08	-0.65	9,11,15,17	0
4	CAP	T	501	21/21	0.07	-0.68	6,10,11,12	0
4	CAP	B	501	21/21	0.07	-0.72	10,12,15,17	0
4	CAP	E	501	21/21	0.07	-0.82	8,11,11,12	0
4	CAP	D	501	21/21	0.07	-0.83	6,9,10,12	0
4	CAP	Y	501	21/21	0.08	-0.84	6,8,10,11	0
4	CAP	H	501	21/21	0.07	-1.03	6,8,9,11	0
3	MG	U	476	1/1	0.09	-1.03	11,11,11,11	0
3	MG	D	476	1/1	0.07	-1.52	9,9,9,9	0
3	MG	T	476	1/1	0.05	-1.63	12,12,12,12	0
3	MG	F	476	1/1	0.06	-3.17	11,11,11,11	0

6.5 Other polymers

There are no such residues in this entry.