



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:59 AM GMT

PDB ID : 3KDN  
Title : Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP  
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2009-10-23  
Resolution : 2.09 Å(reported)

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

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

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

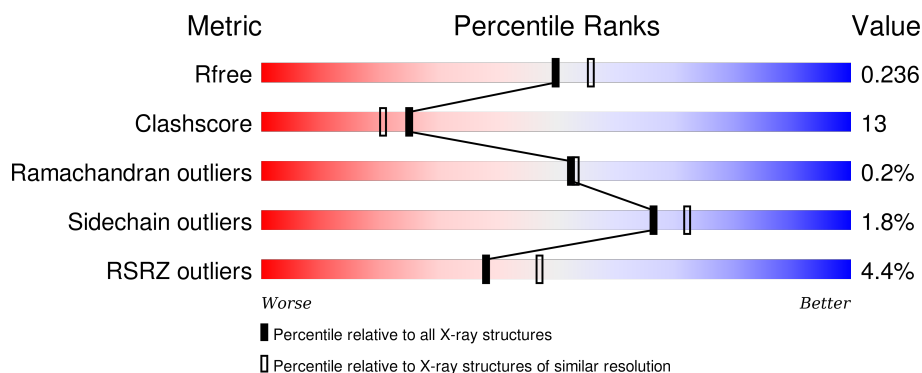
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	<div> <div>17%</div> <div>58%</div> <div>39%</div> <div>..</div> </div>
1	B	444	<div> <div>%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	C	444	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	D	444	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	E	444	<div> <div>3%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	444	<div><div></div><div>4%</div><div>78%</div><div>19%</div><div>..</div></div>
1	G	444	<div><div></div><div>%</div><div>82%</div><div>16%</div><div>.</div></div>
1	H	444	<div><div></div><div>10%</div><div>70%</div><div>27%</div><div>..</div></div>
1	I	444	<div><div></div><div>%</div><div>83%</div><div>15%</div><div>.</div></div>
1	J	444	<div><div></div><div>2%</div><div>81%</div><div>16%</div><div>..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3349	2145	577	617	10			
1	B	437	Total	C	N	O	S	0	0	0
			3430	2201	588	631	10			
1	C	437	Total	C	N	O	S	0	0	0
			3417	2195	585	627	10			
1	D	437	Total	C	N	O	S	0	0	0
			3421	2196	586	629	10			
1	E	438	Total	C	N	O	S	0	0	0
			3428	2197	586	635	10			
1	F	437	Total	C	N	O	S	0	0	0
			3404	2185	586	623	10			
1	G	437	Total	C	N	O	S	0	0	0
			3433	2204	588	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3396	2182	584	620	10			
1	I	436	Total	C	N	O	S	0	0	0
			3421	2195	586	630	10			
1	J	437	Total	C	N	O	S	0	0	0
			3428	2199	586	633	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	ENGINEERED	UNP O93627
A	327	ARG	LYS	ENGINEERED	UNP O93627
A	328	ASP	TRP	ENGINEERED	UNP O93627
A	329	ILE	ASP	ENGINEERED	UNP O93627
A	330	THR	VAL	ENGINEERED	UNP O93627
B	326	GLU	GLY	ENGINEERED	UNP O93627
B	327	ARG	LYS	ENGINEERED	UNP O93627
B	328	ASP	TRP	ENGINEERED	UNP O93627
B	329	ILE	ASP	ENGINEERED	UNP O93627

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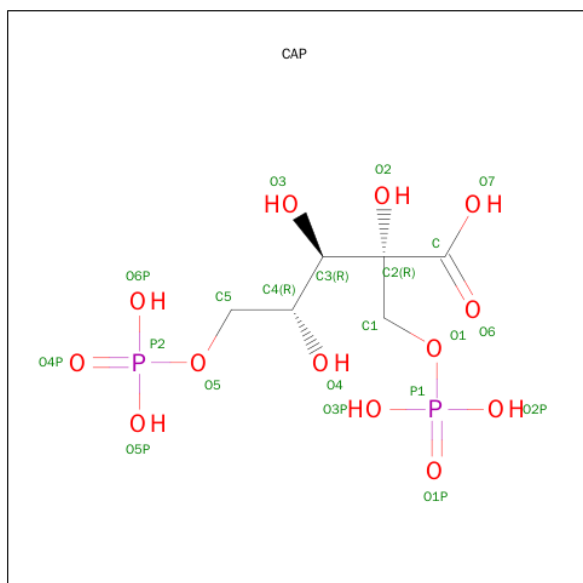
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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	ENGINEERED	UNP 093627
C	326	GLU	GLY	ENGINEERED	UNP 093627
C	327	ARG	LYS	ENGINEERED	UNP 093627
C	328	ASP	TRP	ENGINEERED	UNP 093627
C	329	ILE	ASP	ENGINEERED	UNP 093627
C	330	THR	VAL	ENGINEERED	UNP 093627
D	326	GLU	GLY	ENGINEERED	UNP 093627
D	327	ARG	LYS	ENGINEERED	UNP 093627
D	328	ASP	TRP	ENGINEERED	UNP 093627
D	329	ILE	ASP	ENGINEERED	UNP 093627
D	330	THR	VAL	ENGINEERED	UNP 093627
E	326	GLU	GLY	ENGINEERED	UNP 093627
E	327	ARG	LYS	ENGINEERED	UNP 093627
E	328	ASP	TRP	ENGINEERED	UNP 093627
E	329	ILE	ASP	ENGINEERED	UNP 093627
E	330	THR	VAL	ENGINEERED	UNP 093627
F	326	GLU	GLY	ENGINEERED	UNP 093627
F	327	ARG	LYS	ENGINEERED	UNP 093627
F	328	ASP	TRP	ENGINEERED	UNP 093627
F	329	ILE	ASP	ENGINEERED	UNP 093627
F	330	THR	VAL	ENGINEERED	UNP 093627
G	326	GLU	GLY	ENGINEERED	UNP 093627
G	327	ARG	LYS	ENGINEERED	UNP 093627
G	328	ASP	TRP	ENGINEERED	UNP 093627
G	329	ILE	ASP	ENGINEERED	UNP 093627
G	330	THR	VAL	ENGINEERED	UNP 093627
H	326	GLU	GLY	ENGINEERED	UNP 093627
H	327	ARG	LYS	ENGINEERED	UNP 093627
H	328	ASP	TRP	ENGINEERED	UNP 093627
H	329	ILE	ASP	ENGINEERED	UNP 093627
H	330	THR	VAL	ENGINEERED	UNP 093627
I	326	GLU	GLY	ENGINEERED	UNP 093627
I	327	ARG	LYS	ENGINEERED	UNP 093627
I	328	ASP	TRP	ENGINEERED	UNP 093627
I	329	ILE	ASP	ENGINEERED	UNP 093627
I	330	THR	VAL	ENGINEERED	UNP 093627
J	326	GLU	GLY	ENGINEERED	UNP 093627
J	327	ARG	LYS	ENGINEERED	UNP 093627
J	328	ASP	TRP	ENGINEERED	UNP 093627
J	329	ILE	ASP	ENGINEERED	UNP 093627
J	330	THR	VAL	ENGINEERED	UNP 093627

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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



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

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

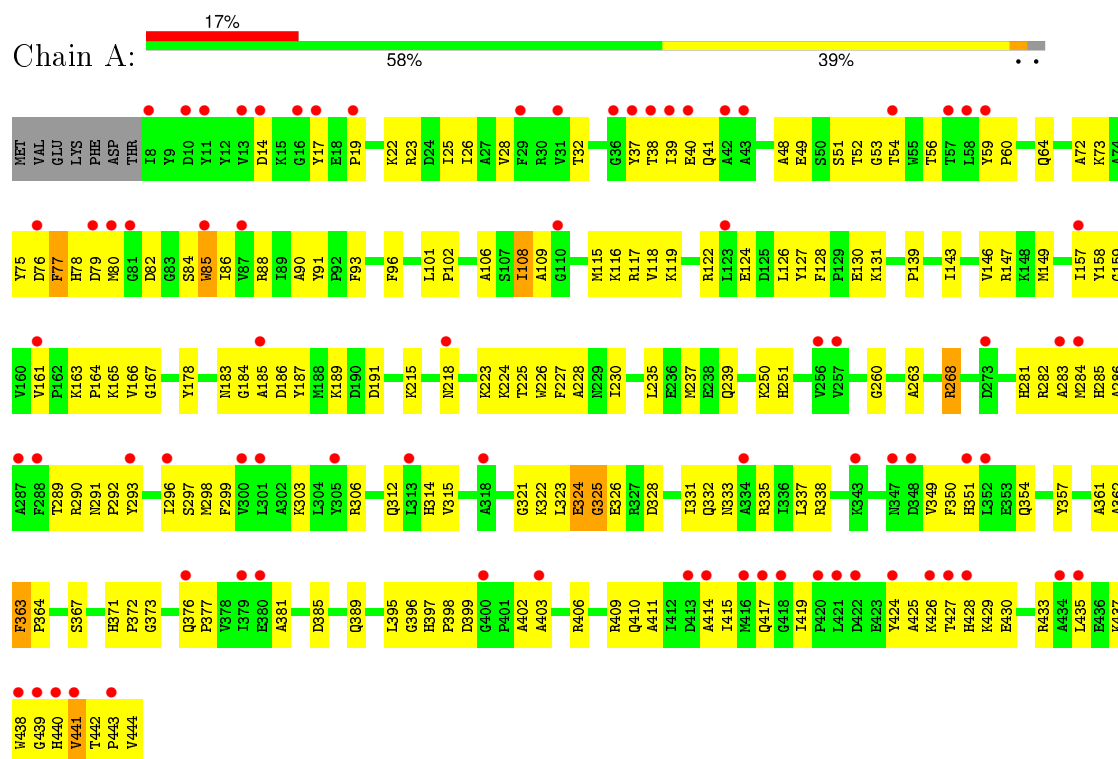
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	290	Total	O	0	0
			290	290		
4	C	311	Total	O	0	0
			311	311		
4	D	308	Total	O	0	0
			308	308		
4	E	258	Total	O	0	0
			258	258		
4	F	268	Total	O	0	0
			268	268		
4	G	267	Total	O	0	0
			267	267		
4	H	185	Total	O	0	0
			185	185		
4	I	291	Total	O	0	0
			291	291		
4	J	301	Total	O	0	0
			301	301		

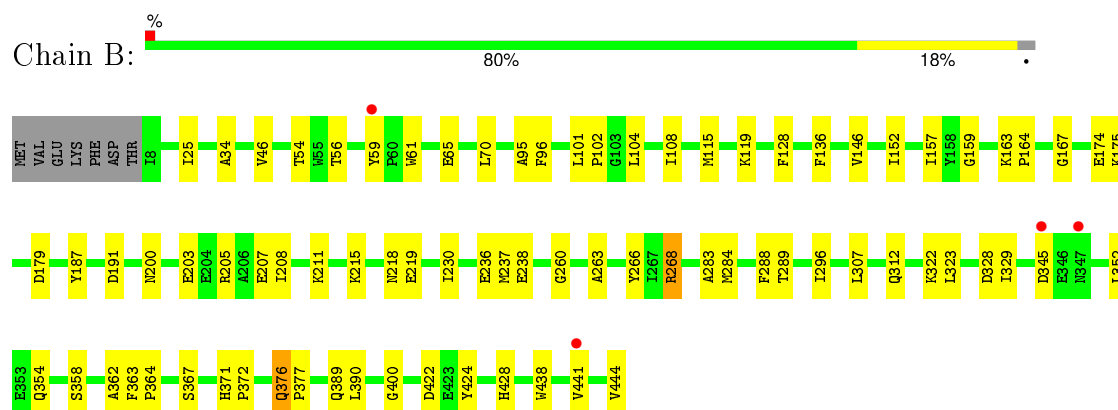
### 3 Residue-property plots [i](#)

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

- Molecule 1: Ribulose biphosphate carboxylase

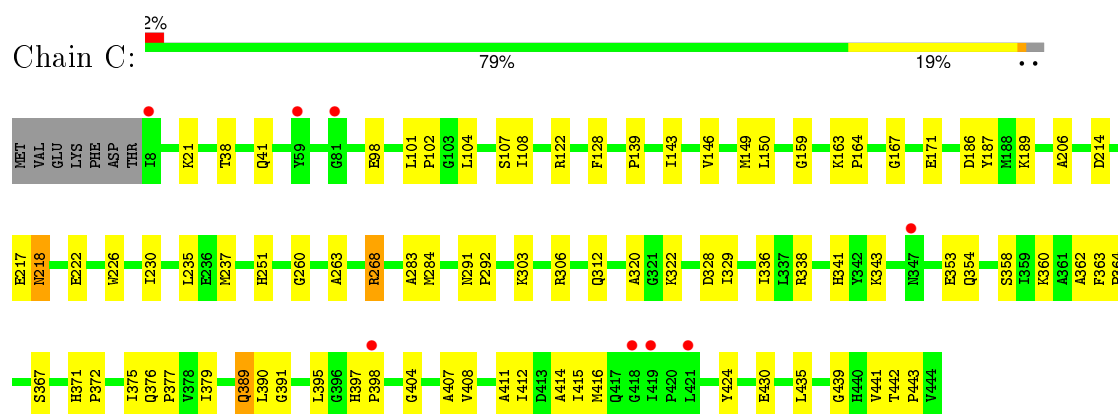


- Molecule 1: Ribulose biphosphate carboxylase

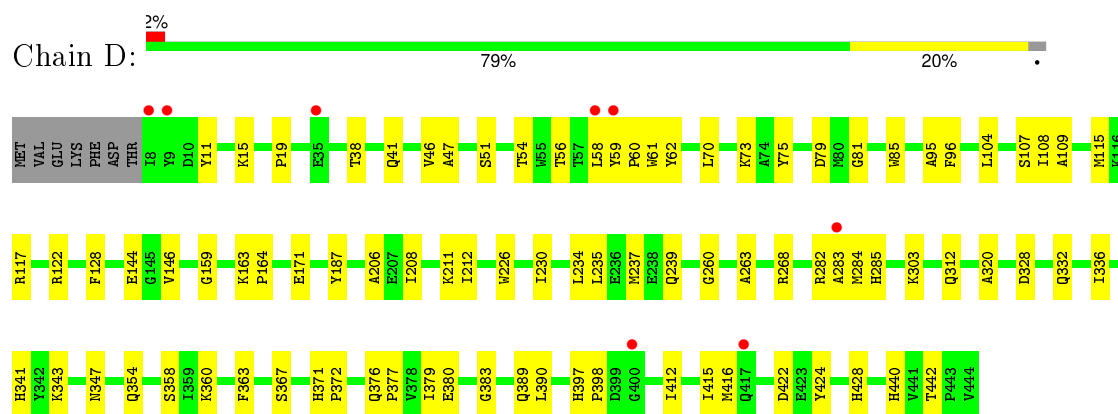


- Molecule 1: Ribulose biphosphate carboxylase

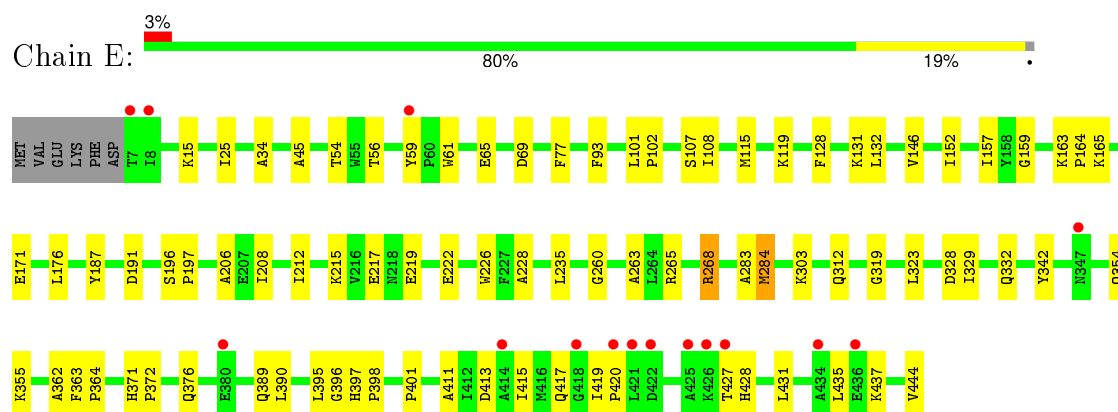




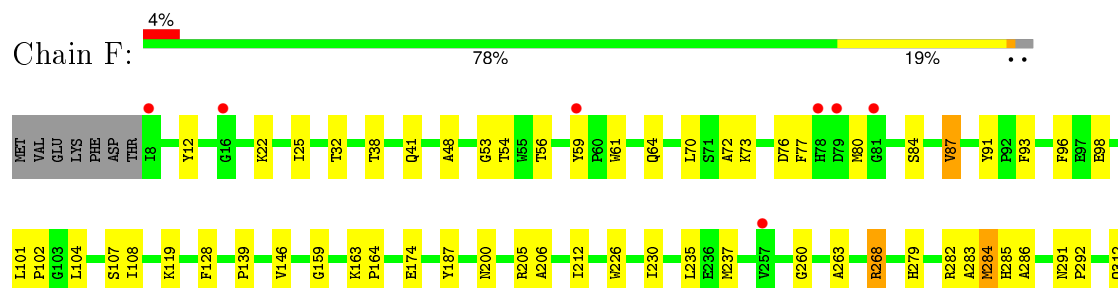
• Molecule 1: Ribulose biphosphate carboxylase

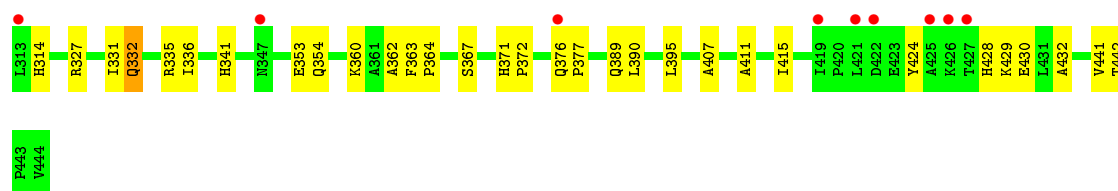


• Molecule 1: Ribulose biphosphate carboxylase

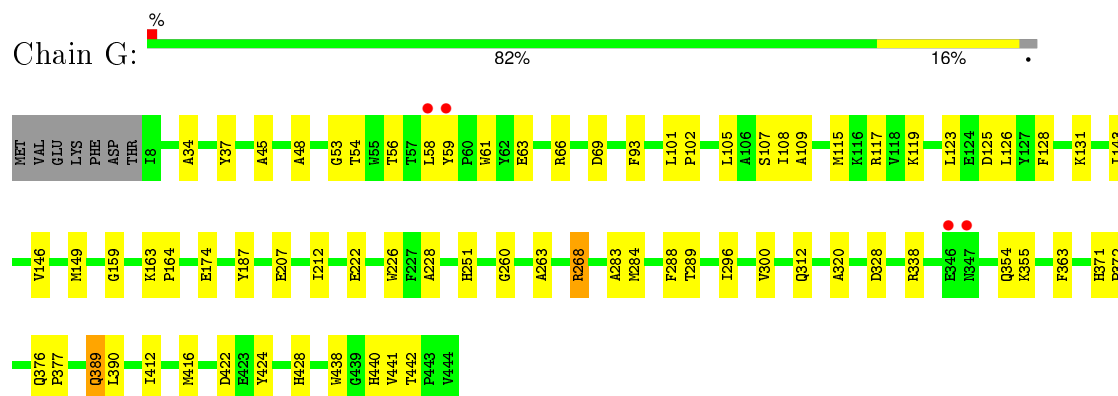


• Molecule 1: Ribulose biphosphate carboxylase

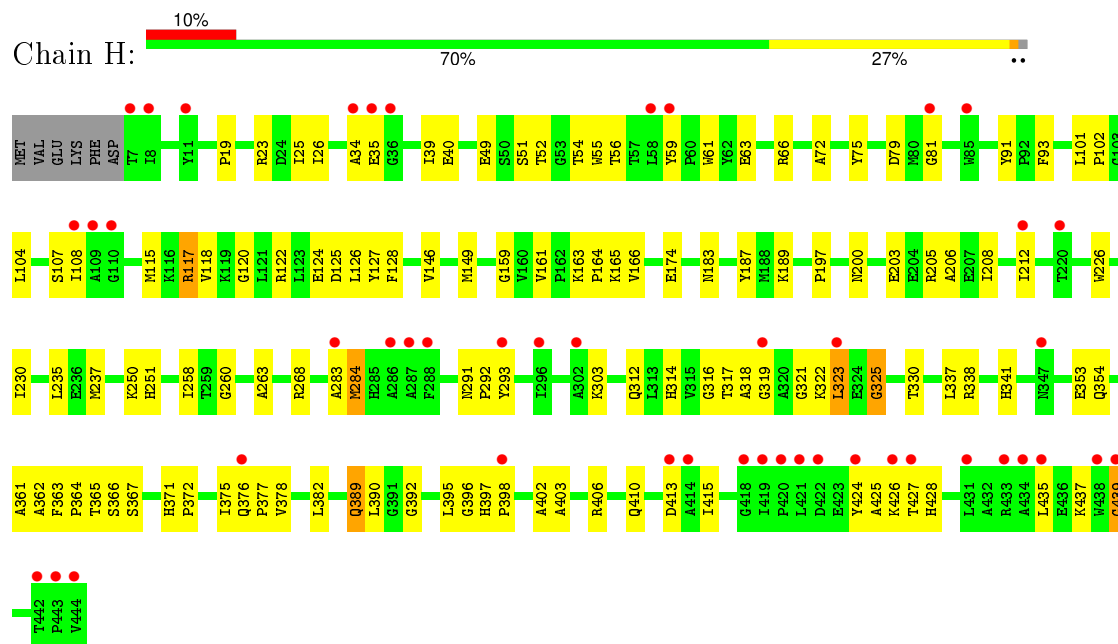




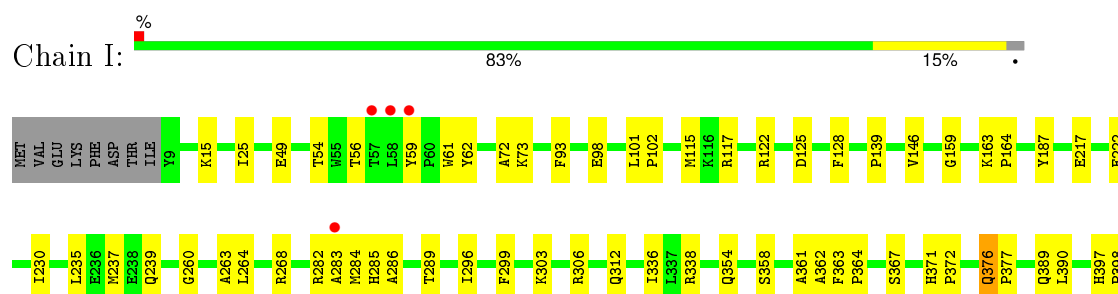
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase

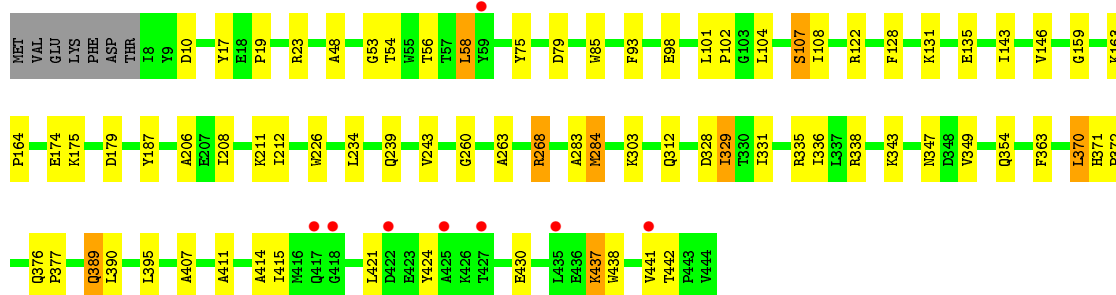
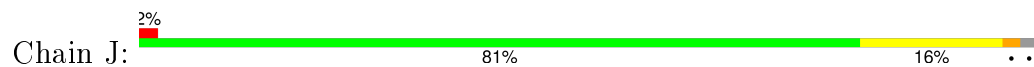


- Molecule 1: Ribulose biphosphate carboxylase





• Molecule 1: Ribulose biphosphate carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.47Å 246.24Å 133.08Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	42.86 – 2.09 42.86 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.86-2.09) 96.5 (42.86-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.213 , 0.253 0.202 , 0.236	Depositor DCC
$R_{free}$ test set	17388 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 345090 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	36999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, 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	0.23	0/3421	0.40	0/4652
1	B	0.26	0/3505	0.42	0/4753
1	C	0.26	0/3492	0.42	0/4740
1	D	0.27	0/3496	0.44	0/4744
1	E	0.25	0/3503	0.42	0/4753
1	F	0.26	0/3478	0.43	0/4719
1	G	0.25	0/3508	0.43	0/4757
1	H	0.24	0/3471	0.41	0/4713
1	I	0.25	0/3496	0.42	0/4742
1	J	0.26	0/3503	0.43	0/4753
All	All	0.25	0/34873	0.42	0/47326

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3204	204	0
1	B	3430	0	3346	68	0
1	C	3417	0	3325	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3421	0	3329	75	0
1	E	3428	0	3319	78	0
1	F	3404	0	3312	70	0
1	G	3433	0	3355	60	0
1	H	3396	0	3282	118	0
1	I	3421	0	3333	56	0
1	J	3428	0	3335	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	21	0	7	3	0
3	B	21	0	7	0	0
3	C	21	0	8	1	0
3	D	21	0	8	0	0
3	E	21	0	7	0	0
3	F	21	0	8	0	0
3	G	21	0	8	0	0
3	H	21	0	8	1	0
3	I	21	0	7	0	0
3	J	21	0	7	0	0
4	A	173	0	0	9	0
4	B	290	0	0	5	0
4	C	311	0	0	7	0
4	D	308	0	0	6	0
4	E	258	0	0	9	0
4	F	268	0	0	10	0
4	G	267	0	0	4	0
4	H	185	0	0	9	0
4	I	291	0	0	8	0
4	J	301	0	0	9	0
All	All	36999	0	33215	856	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (856) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HE3	1:A:250:LYS:CD	1.57	1.31
1:A:38:THR:HG23	1:A:41:GLN:OE1	1.53	1.07
1:A:149:MET:HE3	1:A:250:LYS:HD2	1.07	1.04
1:A:438:TRP:O	1:A:441:VAL:HG12	1.58	1.03
1:A:424:TYR:CE2	1:A:428:HIS:CE1	2.46	1.03
1:G:174:GLU:HG3	1:G:212:ILE:HD11	1.37	1.03
1:J:328:ASP:OD1	1:J:329:ILE:CD1	2.08	1.02
1:F:376:GLN:HG3	4:F:2817:HOH:O	1.61	1.00
1:J:347:ASN:HB2	4:J:2614:HOH:O	1.59	0.99
1:A:149:MET:HE3	1:A:250:LYS:CE	1.92	0.98
1:A:149:MET:CE	1:A:250:LYS:HD2	1.94	0.98
1:A:108:ILE:HD12	1:A:109:ALA:N	1.80	0.97
1:E:159:GLY:HA3	1:E:187:TYR:CZ	1.99	0.97
1:H:159:GLY:HA3	1:H:187:TYR:CZ	1.98	0.96
1:B:328:ASP:OD2	1:B:329:ILE:HD12	1.64	0.96
1:A:338:ARG:HA	1:A:361:ALA:HB1	1.47	0.94
1:A:424:TYR:CZ	1:A:428:HIS:CE1	2.55	0.94
1:D:15:LYS:HD2	4:D:2868:HOH:O	1.67	0.94
1:J:175:LYS:HE2	4:J:2582:HOH:O	1.68	0.91
1:A:290:ARG:HE	1:A:324:GLU:HG3	1.34	0.91
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.06	0.90
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.07	0.88
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.07	0.88
1:J:54:THR:HG21	1:J:58:LEU:CD1	2.05	0.87
1:J:329:ILE:N	1:J:329:ILE:HD12	1.89	0.86
1:D:263:ALA:HB2	1:J:263:ALA:HB2	1.56	0.86
1:D:128:PHE:H	1:D:354:GLN:HE22	1.22	0.86
1:G:128:PHE:H	1:G:354:GLN:HE22	1.22	0.85
1:G:45:ALA:HB1	1:G:115:MET:HE3	1.58	0.84
1:A:178:TYR:CE1	1:A:215:LYS:NZ	2.45	0.84
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.13	0.84
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.12	0.84
1:E:376:GLN:CB	4:E:2871:HOH:O	2.25	0.84
1:A:39:ILE:HD13	1:A:85:TRP:CE3	2.13	0.83
1:A:332:GLN:OE1	1:A:351:HIS:CE1	2.32	0.82
1:A:389:GLN:NE2	3:A:600:CAP:H11	1.95	0.82
1:H:317:THR:HG21	4:H:2909:HOH:O	1.79	0.82
1:B:328:ASP:OD2	1:B:329:ILE:CD1	2.28	0.81
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.15	0.81
1:B:203:GLU:O	1:B:207:GLU:HG2	1.81	0.81
1:C:263:ALA:HB2	1:F:263:ALA:HB2	1.61	0.81
1:J:328:ASP:OD1	1:J:329:ILE:HD12	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:THR:CG2	4:H:2909:HOH:O	2.30	0.80
1:B:263:ALA:HB2	1:G:263:ALA:HB2	1.63	0.79
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.18	0.78
1:A:324:GLU:OE2	1:A:325:GLY:N	2.16	0.78
1:F:98:GLU:CD	4:F:2195:HOH:O	2.21	0.78
1:H:322:LYS:HG2	1:H:323:LEU:HD12	1.65	0.77
1:J:328:ASP:CG	1:J:329:ILE:HD12	2.05	0.77
1:B:128:PHE:H	1:B:354:GLN:HE22	1.31	0.77
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.20	0.77
1:C:358:SER:HB2	4:C:2464:HOH:O	1.85	0.77
1:A:149:MET:CE	1:A:250:LYS:CE	2.62	0.76
1:H:128:PHE:H	1:H:354:GLN:HE22	1.31	0.76
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.68	0.76
1:A:38:THR:CG2	1:A:41:GLN:OE1	2.32	0.76
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.20	0.76
1:H:397:HIS:CG	1:H:398:PRO:HD2	2.21	0.76
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.21	0.75
1:A:376:GLN:HA	1:A:415:ILE:HD13	1.69	0.75
1:A:32:THR:HG21	1:A:119:LYS:HE2	1.69	0.74
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.22	0.74
1:D:341:HIS:CE1	1:D:343:LYS:HZ2	2.04	0.74
1:F:332:GLN:HA	1:F:332:GLN:HE21	1.50	0.74
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.21	0.74
1:B:215:LYS:NZ	1:B:219:GLU:OE2	2.21	0.74
1:I:358:SER:HB2	4:I:2433:HOH:O	1.87	0.73
1:H:293:TYR:CE2	4:H:2342:HOH:O	2.39	0.73
1:A:376:GLN:CB	4:A:2304:HOH:O	2.35	0.73
1:J:411:ALA:O	1:J:415:ILE:HG13	1.89	0.73
1:E:427:THR:HG23	1:E:428:HIS:ND1	2.03	0.73
1:J:174:GLU:OE1	1:J:211:LYS:NZ	2.22	0.73
1:D:341:HIS:CD2	1:D:343:LYS:HZ2	2.07	0.73
1:J:329:ILE:N	1:J:329:ILE:CD1	2.52	0.72
1:J:329:ILE:H	1:J:329:ILE:CD1	2.02	0.72
1:H:376:GLN:HB3	4:H:2840:HOH:O	1.89	0.72
1:B:59:TYR:O	1:B:61:TRP:HD1	1.71	0.72
1:A:376:GLN:HA	1:A:415:ILE:CD1	2.20	0.71
1:G:54:THR:HG21	1:G:58:LEU:HG	1.70	0.71
1:A:39:ILE:CD1	1:A:85:TRP:HB2	2.20	0.71
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.54	0.71
1:A:54:THR:CG2	1:A:56:THR:O	2.39	0.71
1:G:45:ALA:HB1	1:G:115:MET:CE	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:CE1	1:A:283:ALA:HB2	2.25	0.71
1:G:54:THR:HG21	1:G:58:LEU:CG	2.21	0.70
1:H:403:ALA:HA	1:H:406:ARG:NH2	2.06	0.70
1:I:15:LYS:HD2	4:I:1867:HOH:O	1.89	0.70
1:C:128:PHE:H	1:C:354:GLN:HE22	1.39	0.70
1:C:214:ASP:O	1:C:218:ASN:HB2	1.90	0.70
1:F:200:ASN:OD1	1:F:205:ARG:HG3	1.91	0.70
1:H:108:ILE:HG22	1:H:108:ILE:O	1.91	0.70
1:A:108:ILE:HD12	1:A:108:ILE:C	2.12	0.69
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.27	0.69
1:H:367:SER:HB2	1:H:389:GLN:HB3	1.75	0.69
1:E:263:ALA:HB2	1:I:263:ALA:HB2	1.73	0.69
1:A:39:ILE:HD13	1:A:85:TRP:HE3	1.58	0.69
1:A:54:THR:HG23	1:A:56:THR:O	1.92	0.69
1:E:431:LEU:O	1:E:435:LEU:HD23	1.93	0.69
1:A:389:GLN:HE22	3:A:600:CAP:H11	1.58	0.68
1:C:376:GLN:HB3	1:C:377:PRO:HD3	1.74	0.68
1:H:283:ALA:O	1:H:284:MET:HB3	1.93	0.68
1:E:428:HIS:NE2	4:E:2782:HOH:O	2.26	0.68
1:A:37:TYR:HA	1:A:41:GLN:NE2	2.07	0.68
1:E:65:GLU:N	1:E:65:GLU:OE1	2.25	0.68
1:D:58:LEU:HD12	1:D:58:LEU:N	2.09	0.68
1:E:427:THR:HG23	1:E:428:HIS:CE1	2.28	0.68
1:A:331:ILE:O	1:A:335:ARG:HG3	1.94	0.68
1:I:128:PHE:H	1:I:354:GLN:HE22	1.41	0.68
1:A:86:ILE:HG21	1:A:349:VAL:O	1.94	0.68
1:A:367:SER:HB2	1:A:389:GLN:HB3	1.75	0.67
1:E:119:LYS:HE2	4:E:777:HOH:O	1.94	0.67
1:H:396:GLY:O	1:H:437:LYS:NZ	2.25	0.67
1:A:108:ILE:C	1:A:108:ILE:CD1	2.63	0.67
1:J:389:GLN:C	1:J:390:LEU:HD12	2.14	0.67
1:I:235:LEU:O	1:I:239:GLN:HG3	1.94	0.67
1:C:303:LYS:NZ	1:C:354:GLN:HE21	1.93	0.67
1:G:93:PHE:CE1	1:G:131:LYS:HD3	2.30	0.67
1:A:49:GLU:HG3	1:A:115:MET:SD	2.35	0.67
1:A:115:MET:O	1:A:118:VAL:HG12	1.94	0.67
1:A:396:GLY:O	1:A:437:LYS:NZ	2.20	0.67
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.30	0.66
1:A:332:GLN:OE1	1:A:351:HIS:ND1	2.28	0.66
1:G:149:MET:CE	1:G:251:HIS:CE1	2.79	0.66
1:E:165:LYS:HE2	1:I:49:GLU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:A:41:GLN:HG3	1.95	0.66
1:F:32:THR:HG21	1:F:119:LYS:HE3	1.77	0.66
1:J:163:LYS:H	1:J:395:LEU:HD12	1.61	0.66
1:E:303:LYS:NZ	1:E:354:GLN:HE21	1.92	0.66
1:J:54:THR:HG21	1:J:58:LEU:HD11	1.78	0.66
1:H:183:ASN:OD1	1:H:406:ARG:NH1	2.29	0.66
1:B:358:SER:HB2	4:B:2811:HOH:O	1.95	0.66
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.31	0.66
1:G:207:GLU:HG3	4:G:1811:HOH:O	1.95	0.66
1:A:72:ALA:HA	1:A:90:ALA:O	1.96	0.65
1:A:165:LYS:HB3	1:A:191:ASP:OD2	1.96	0.65
1:D:422:ASP:OD1	1:D:440:HIS:HE1	1.79	0.65
1:H:125:ASP:OD1	1:H:126:LEU:N	2.30	0.65
1:H:366:SER:HA	4:H:2657:HOH:O	1.95	0.65
1:A:424:TYR:CD2	1:A:428:HIS:ND1	2.65	0.65
1:A:37:TYR:HA	1:A:41:GLN:HE22	1.61	0.65
1:A:424:TYR:CD2	1:A:428:HIS:CE1	2.85	0.65
1:C:328:ASP:OD1	1:C:329:ILE:CD1	2.44	0.65
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.32	0.65
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.32	0.65
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.78	0.65
1:F:376:GLN:CG	4:F:2817:HOH:O	2.32	0.65
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.62	0.65
1:J:54:THR:HG21	1:J:58:LEU:HD13	1.77	0.64
1:A:178:TYR:CZ	1:A:215:LYS:NZ	2.65	0.64
1:A:362:ALA:O	1:A:364:PRO:HD3	1.97	0.64
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.32	0.64
1:A:149:MET:CE	1:A:250:LYS:CB	2.75	0.64
1:A:39:ILE:HD13	1:A:85:TRP:HB2	1.79	0.64
1:H:376:GLN:HG2	1:H:415:ILE:CD1	2.27	0.64
1:G:149:MET:HE2	1:G:251:HIS:HE1	1.62	0.64
1:H:330:THR:HG22	1:H:382:LEU:HD21	1.79	0.64
1:A:282:ARG:HD3	1:A:298:MET:HE1	1.79	0.64
1:H:338:ARG:HH11	1:H:364:PRO:HG2	1.63	0.64
1:E:45:ALA:HB1	1:E:115:MET:CE	2.28	0.64
1:H:79:ASP:OD1	1:H:81:GLY:N	2.31	0.64
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.32	0.63
1:A:331:ILE:HG12	1:A:381:ALA:O	1.96	0.63
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.63	0.63
1:C:149:MET:HE2	1:C:251:HIS:HE1	1.63	0.63
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:THR:O	1:A:444:VAL:HG23	1.98	0.63
1:A:22:LYS:CE	1:G:63:GLU:OE1	2.46	0.63
1:B:329:ILE:N	1:B:329:ILE:HD12	2.13	0.63
1:D:341:HIS:CE1	1:D:343:LYS:NZ	2.67	0.63
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.34	0.63
1:F:54:THR:HG23	1:F:56:THR:O	1.99	0.63
1:E:128:PHE:H	1:E:354:GLN:HE22	1.46	0.62
1:C:149:MET:CE	1:C:251:HIS:CE1	2.82	0.62
1:E:260:GLY:HA3	1:I:260:GLY:HA3	1.81	0.62
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.81	0.62
1:A:23:ARG:NE	1:G:69:ASP:OD1	2.30	0.62
1:E:152:ILE:HD12	1:E:157:ILE:HD12	1.81	0.62
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.34	0.62
1:G:34:ALA:HA	1:G:119:LYS:HG3	1.82	0.62
1:B:389:GLN:C	1:B:390:LEU:HD12	2.20	0.62
1:H:284:MET:O	1:H:284:MET:HG2	1.98	0.62
1:H:389:GLN:C	1:H:390:LEU:HD12	2.19	0.62
1:J:343:LYS:HD2	4:J:2757:HOH:O	1.98	0.62
1:H:322:LYS:HG2	1:H:323:LEU:CD1	2.29	0.62
1:F:128:PHE:H	1:F:354:GLN:HE22	1.47	0.62
1:A:38:THR:H	1:A:41:GLN:CD	2.02	0.61
1:E:45:ALA:HB1	1:E:115:MET:HE1	1.82	0.61
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.36	0.61
1:A:26:ILE:HB	1:A:127:TYR:HB3	1.83	0.61
1:H:341:HIS:NE2	1:H:353:GLU:OE2	2.32	0.61
1:I:438:TRP:O	1:I:441:VAL:HG22	2.01	0.61
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.47	0.61
1:F:163:LYS:HA	1:F:164:PRO:C	2.21	0.61
1:A:424:TYR:CE2	1:A:428:HIS:ND1	2.68	0.61
1:H:159:GLY:CA	1:H:187:TYR:CZ	2.80	0.61
1:A:25:ILE:HD12	1:A:96:PHE:CE2	2.35	0.61
1:F:362:ALA:O	1:F:364:PRO:HD3	2.01	0.60
1:A:157:ILE:N	1:A:157:ILE:HD12	2.15	0.60
1:H:371:HIS:HB2	1:H:372:PRO:HD2	1.83	0.60
1:E:159:GLY:CA	1:E:187:TYR:CZ	2.80	0.60
1:F:327:ARG:NH2	4:F:2580:HOH:O	2.31	0.60
1:J:79:ASP:HB2	1:J:85:TRP:CH2	2.37	0.60
1:B:376:GLN:N	1:B:377:PRO:HD2	2.16	0.60
1:B:438:TRP:O	1:B:441:VAL:HG22	2.02	0.60
1:A:263:ALA:HB2	1:H:263:ALA:HB2	1.82	0.60
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:376:GLN:HB3	1:I:377:PRO:HD3	1.83	0.60
1:H:371:HIS:HB2	1:H:372:PRO:CD	2.32	0.60
1:A:430:GLU:N	1:A:430:GLU:OE1	2.22	0.60
1:H:283:ALA:O	1:H:284:MET:CB	2.50	0.60
1:A:235:LEU:O	1:A:239:GLN:HG3	2.01	0.60
1:J:79:ASP:HB2	1:J:85:TRP:CZ3	2.37	0.59
1:C:98:GLU:HG3	4:C:1235:HOH:O	2.02	0.59
1:C:322:LYS:HA	1:C:443:PRO:O	2.02	0.59
1:A:332:GLN:HA	1:A:332:GLN:NE2	2.17	0.59
1:H:403:ALA:HA	1:H:406:ARG:CZ	2.33	0.59
1:B:59:TYR:O	1:B:61:TRP:CD1	2.55	0.59
1:A:40:GLU:HB2	4:A:2245:HOH:O	2.03	0.59
1:J:328:ASP:OD1	1:J:329:ILE:HD13	1.98	0.59
1:D:59:TYR:O	1:D:61:TRP:HD1	1.85	0.59
1:E:59:TYR:O	1:E:61:TRP:HD1	1.84	0.59
1:H:338:ARG:NH1	1:H:364:PRO:HG2	2.17	0.59
1:C:328:ASP:OD1	1:C:329:ILE:HD12	2.02	0.59
1:C:441:VAL:HG12	1:C:442:THR:N	2.16	0.59
1:E:215:LYS:O	1:E:219:GLU:HG3	2.03	0.59
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.37	0.59
1:A:230:ILE:O	1:A:237:MET:HG2	2.03	0.59
1:F:38:THR:OG1	1:F:41:GLN:HG3	2.03	0.59
1:C:397:HIS:CG	1:C:398:PRO:HD2	2.38	0.59
1:D:108:ILE:HD12	1:D:108:ILE:C	2.23	0.59
1:A:218:ASN:HB2	4:A:1583:HOH:O	2.03	0.59
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.38	0.59
1:A:93:PHE:CE1	1:A:131:LYS:HE3	2.38	0.59
1:F:268:ARG:HD3	1:F:268:ARG:C	2.24	0.58
1:J:54:THR:HG21	1:J:58:LEU:CD2	2.34	0.58
1:A:268:ARG:HD3	1:A:268:ARG:C	2.23	0.58
1:F:59:TYR:O	1:F:61:TRP:HD1	1.85	0.58
1:A:126:LEU:O	1:A:303:LYS:NZ	2.36	0.58
1:G:389:GLN:C	1:G:390:LEU:HD12	2.24	0.58
1:E:444:VAL:O	1:I:117:ARG:HG3	2.04	0.58
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.39	0.58
1:J:128:PHE:H	1:J:354:GLN:HE22	1.50	0.58
1:H:120:GLY:C	4:H:2182:HOH:O	2.43	0.58
1:A:183:ASN:ND2	1:A:402:ALA:HB1	2.19	0.57
1:C:329:ILE:N	1:C:329:ILE:HD12	2.19	0.57
1:H:59:TYR:O	1:H:61:TRP:HD1	1.87	0.57
1:A:298:MET:HE2	1:A:314:HIS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:N	1:A:77:PHE:CD2	2.72	0.57
1:F:389:GLN:C	1:F:390:LEU:HD12	2.25	0.57
1:J:329:ILE:H	1:J:329:ILE:HD12	1.59	0.57
1:A:282:ARG:HD3	1:A:298:MET:CE	2.35	0.56
1:A:149:MET:CE	1:A:250:LYS:HB3	2.35	0.56
1:I:282:ARG:HG3	1:I:285:HIS:CD2	2.40	0.56
1:G:149:MET:HE2	1:G:251:HIS:CE1	2.39	0.56
1:D:376:GLN:NE2	1:D:380:GLU:OE1	2.34	0.56
1:D:54:THR:HG23	1:D:56:THR:O	2.04	0.56
1:B:163:LYS:HA	1:B:164:PRO:C	2.25	0.56
1:C:441:VAL:CG1	1:C:442:THR:N	2.68	0.56
1:A:163:LYS:HA	1:A:164:PRO:C	2.25	0.56
1:B:152:ILE:HD12	1:B:157:ILE:HD12	1.87	0.56
1:E:427:THR:HG23	1:E:428:HIS:HD1	1.68	0.56
1:A:39:ILE:HD11	1:A:85:TRP:HB2	1.87	0.56
1:C:341:HIS:NE2	1:C:353:GLU:OE2	2.31	0.56
1:H:39:ILE:HG23	1:H:40:GLU:N	2.21	0.56
1:C:328:ASP:CG	1:C:329:ILE:HD12	2.25	0.56
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.71	0.56
1:H:323:LEU:N	1:H:323:LEU:HD12	2.20	0.56
1:J:437:LYS:HG3	1:J:438:TRP:CG	2.41	0.56
1:A:149:MET:HE1	1:A:250:LYS:CB	2.36	0.56
1:A:425:ALA:C	1:A:427:THR:H	2.10	0.56
1:A:130:GLU:HG3	1:A:357:TYR:CE2	2.41	0.55
1:C:362:ALA:O	1:C:364:PRO:HD3	2.06	0.55
1:A:293:TYR:CE1	4:A:2523:HOH:O	2.59	0.55
1:B:260:GLY:HA3	1:G:260:GLY:HA3	1.88	0.55
1:E:332:GLN:NE2	1:E:342:TYR:OH	2.40	0.55
1:A:442:THR:HG22	1:A:442:THR:O	2.07	0.55
1:H:163:LYS:H	1:H:395:LEU:CD2	2.20	0.55
1:F:230:ILE:O	1:F:237:MET:HG2	2.07	0.55
1:H:208:ILE:O	1:H:212:ILE:HG13	2.06	0.55
1:J:56:THR:O	1:J:58:LEU:HD13	2.07	0.55
1:C:411:ALA:O	1:C:415:ILE:HG13	2.05	0.55
1:A:64:GLN:HG2	4:A:1148:HOH:O	2.05	0.55
1:B:167:GLY:O	1:G:66:ARG:HD2	2.07	0.55
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.41	0.55
1:E:431:LEU:O	1:E:435:LEU:CD2	2.55	0.55
1:A:131:LYS:NZ	4:A:1992:HOH:O	2.35	0.55
1:D:230:ILE:O	1:D:237:MET:HG2	2.06	0.55
1:A:149:MET:HE3	1:A:250:LYS:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:LYS:HA	1:J:164:PRO:C	2.27	0.55
1:I:424:TYR:CZ	1:I:428:HIS:CE1	2.93	0.55
1:I:303:LYS:HZ3	1:I:354:GLN:HE21	1.55	0.55
1:C:412:ILE:O	1:C:416:MET:HG2	2.07	0.55
1:F:80:MET:HE3	4:F:2035:HOH:O	2.06	0.55
1:F:376:GLN:NE2	4:F:2525:HOH:O	2.28	0.54
1:F:72:ALA:HB2	1:F:91:TYR:CD1	2.41	0.54
1:G:108:ILE:HD12	1:G:108:ILE:C	2.28	0.54
1:A:108:ILE:CD1	1:A:109:ALA:N	2.64	0.54
1:E:427:THR:HG21	4:E:2735:HOH:O	2.08	0.54
1:H:316:GLY:O	1:H:366:SER:CB	2.56	0.54
1:G:105:LEU:HD23	1:G:108:ILE:HD11	1.89	0.54
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.37	0.54
1:F:73:LYS:HG3	4:F:2809:HOH:O	2.07	0.54
1:D:260:GLY:HA3	1:J:260:GLY:HA3	1.89	0.54
1:J:54:THR:HG23	1:J:56:THR:O	2.08	0.54
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.06	0.54
1:A:328:ASP:N	1:A:328:ASP:OD1	2.37	0.54
1:J:108:ILE:O	1:J:108:ILE:CG2	2.55	0.54
1:A:260:GLY:HA3	1:H:260:GLY:HA3	1.89	0.54
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.89	0.54
1:A:78:HIS:C	1:A:85:TRP:HD1	2.10	0.54
1:B:25:ILE:HD12	1:B:96:PHE:CE2	2.43	0.54
1:J:104:LEU:HD23	1:J:104:LEU:C	2.28	0.54
1:A:149:MET:HE1	1:A:250:LYS:HB2	1.89	0.54
1:E:389:GLN:C	1:E:390:LEU:HD12	2.28	0.54
1:C:341:HIS:CE1	1:C:343:LYS:HZ2	2.25	0.53
1:G:163:LYS:HA	1:G:164:PRO:C	2.28	0.53
1:E:163:LYS:HA	1:E:164:PRO:C	2.28	0.53
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.89	0.53
1:E:15:LYS:NZ	4:E:1178:HOH:O	2.40	0.53
1:H:375:ILE:O	1:H:378:VAL:N	2.39	0.53
1:J:407:ALA:HB2	1:J:430:GLU:HB3	1.90	0.53
1:A:376:GLN:N	1:A:377:PRO:HD2	2.24	0.53
1:H:403:ALA:CA	1:H:406:ARG:NH2	2.71	0.53
1:J:19:PRO:HG3	1:J:75:TYR:CZ	2.44	0.53
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.73	0.53
1:B:329:ILE:HD12	1:B:329:ILE:H	1.72	0.53
1:A:165:LYS:CB	1:A:191:ASP:OD2	2.56	0.53
1:D:376:GLN:HB3	1:D:377:PRO:HD3	1.90	0.53
1:C:21:LYS:HE3	4:C:892:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LYS:HE3	4:D:508:HOH:O	2.07	0.53
1:E:159:GLY:HA3	1:E:187:TYR:CD1	2.43	0.53
1:H:435:LEU:O	1:H:439:GLY:N	2.41	0.53
1:J:268:ARG:C	1:J:268:ARG:HD3	2.29	0.53
1:J:376:GLN:HB3	1:J:377:PRO:HD3	1.91	0.53
1:E:165:LYS:HG2	1:E:191:ASP:OD2	2.09	0.53
1:H:338:ARG:HA	1:H:361:ALA:HB1	1.91	0.53
1:B:175:LYS:HE3	1:B:179:ASP:OD2	2.09	0.53
1:A:143:ILE:CD1	1:A:338:ARG:HG2	2.38	0.52
1:H:406:ARG:O	1:H:410:GLN:HG3	2.09	0.52
1:D:208:ILE:O	1:D:212:ILE:HG12	2.09	0.52
1:B:46:VAL:HG22	1:B:115:MET:HE1	1.91	0.52
1:A:324:GLU:C	1:A:324:GLU:OE2	2.48	0.52
1:C:149:MET:CE	1:C:251:HIS:HE1	2.21	0.52
1:A:76:ASP:OD1	1:A:77:PHE:N	2.42	0.52
1:D:424:TYR:CE1	1:D:428:HIS:CE1	2.97	0.52
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.40	0.52
1:E:159:GLY:CA	1:E:187:TYR:CE2	2.92	0.52
1:A:78:HIS:O	1:A:85:TRP:CD1	2.62	0.52
1:F:206:ALA:HA	1:F:226:TRP:CZ3	2.45	0.52
1:A:52:THR:HG22	1:H:166:VAL:O	2.10	0.52
1:A:424:TYR:CZ	1:A:428:HIS:HE1	2.22	0.52
1:F:32:THR:CG2	1:F:119:LYS:HE3	2.39	0.52
1:J:23:ARG:HD3	4:J:485:HOH:O	2.09	0.52
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.73	0.52
1:E:176:LEU:HD11	1:E:395:LEU:HD11	1.91	0.52
1:A:338:ARG:HA	1:A:361:ALA:CB	2.30	0.52
1:A:185:ALA:O	1:A:224:LYS:NZ	2.27	0.52
1:G:371:HIS:HB2	1:G:372:PRO:HD2	1.92	0.52
1:A:290:ARG:NE	1:A:324:GLU:HG3	2.14	0.52
1:D:422:ASP:OD1	1:D:440:HIS:CE1	2.60	0.52
1:I:283:ALA:O	1:I:284:MET:HB3	2.10	0.52
1:G:54:THR:HG23	1:G:56:THR:O	2.10	0.52
1:J:163:LYS:H	1:J:395:LEU:CD1	2.23	0.52
1:A:163:LYS:H	1:A:395:LEU:HD22	1.75	0.52
1:G:376:GLN:HB3	1:G:377:PRO:HD3	1.92	0.52
1:A:285:HIS:CG	1:A:286:ALA:N	2.78	0.52
1:H:159:GLY:HA3	1:H:187:TYR:CD1	2.45	0.51
1:H:93:PHE:CD1	1:H:93:PHE:C	2.84	0.51
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.92	0.51
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:ILE:HD12	1:F:108:ILE:C	2.30	0.51
1:C:389:GLN:C	1:C:390:LEU:HD12	2.30	0.51
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.92	0.51
1:I:230:ILE:O	1:I:237:MET:HG2	2.11	0.51
1:J:328:ASP:CG	1:J:329:ILE:CD1	2.70	0.51
1:A:282:ARG:O	1:A:283:ALA:C	2.49	0.51
1:A:283:ALA:O	1:A:284:MET:HB3	2.10	0.51
1:D:59:TYR:O	1:D:61:TRP:CD1	2.63	0.51
1:J:108:ILE:O	1:J:108:ILE:HG22	2.09	0.51
1:B:108:ILE:C	1:B:108:ILE:HD12	2.30	0.51
1:B:34:ALA:HA	1:B:119:LYS:HG3	1.91	0.51
1:J:343:LYS:CD	4:J:2757:HOH:O	2.57	0.51
1:A:424:TYR:CE1	1:A:428:HIS:HE1	2.28	0.51
1:H:397:HIS:ND1	1:H:398:PRO:HD2	2.25	0.51
1:G:54:THR:HA	4:G:466:HOH:O	2.11	0.51
1:D:282:ARG:HG3	1:D:285:HIS:CD2	2.46	0.51
1:A:78:HIS:O	1:A:85:TRP:HD1	1.93	0.51
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.93	0.51
1:A:76:ASP:C	1:A:77:PHE:CD2	2.84	0.51
1:E:108:ILE:O	1:E:108:ILE:CG2	2.58	0.51
1:A:406:ARG:O	1:A:410:GLN:HG3	2.11	0.50
1:A:289:THR:HA	1:A:296:ILE:O	2.10	0.50
1:I:424:TYR:CE1	1:I:428:HIS:CE1	2.99	0.50
1:J:414:ALA:HB2	1:J:424:TYR:CD2	2.46	0.50
1:D:96:PHE:CE1	1:D:104:LEU:CD1	2.94	0.50
1:D:96:PHE:CE1	1:D:104:LEU:HD13	2.46	0.50
1:A:178:TYR:HE1	1:A:215:LYS:HZ2	1.43	0.50
1:H:403:ALA:CB	1:H:406:ARG:NH2	2.75	0.50
1:D:58:LEU:CD1	1:D:58:LEU:N	2.75	0.50
1:E:283:ALA:O	1:E:284:MET:HB3	2.11	0.50
1:G:59:TYR:O	1:G:61:TRP:HD1	1.95	0.50
1:A:157:ILE:HD13	1:A:363:PHE:CZ	2.46	0.50
1:J:107:SER:HB3	1:J:108:ILE:HD12	1.93	0.50
1:D:412:ILE:O	1:D:416:MET:HG2	2.12	0.50
1:B:236:GLU:N	1:B:236:GLU:OE1	2.43	0.50
1:G:424:TYR:CE2	1:G:428:HIS:CE1	3.00	0.50
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.94	0.50
1:D:341:HIS:CG	1:D:343:LYS:NZ	2.80	0.50
1:C:376:GLN:N	1:C:377:PRO:CD	2.74	0.50
1:H:25:ILE:HD13	1:H:93:PHE:HA	1.94	0.50
1:H:149:MET:CE	1:H:251:HIS:CE1	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:SER:OG	1:H:52:THR:N	2.45	0.50
1:E:131:LYS:NZ	4:E:1899:HOH:O	2.27	0.50
1:H:316:GLY:O	1:H:366:SER:HB2	2.12	0.50
1:H:337:LEU:HD22	1:H:362:ALA:HB3	1.94	0.50
1:D:46:VAL:HG22	1:D:115:MET:HE1	1.94	0.50
1:I:25:ILE:CD1	1:I:93:PHE:HA	2.41	0.50
1:C:397:HIS:ND1	1:C:398:PRO:HD2	2.27	0.50
1:F:59:TYR:O	1:F:61:TRP:CD1	2.65	0.50
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.47	0.50
1:H:292:PRO:O	4:H:2255:HOH:O	2.20	0.50
1:E:265:ARG:HD3	4:I:2459:HOH:O	2.11	0.50
1:A:56:THR:HG21	1:H:392:GLY:O	2.12	0.49
1:F:73:LYS:CG	4:F:2809:HOH:O	2.60	0.49
1:D:96:PHE:CD1	1:D:104:LEU:HD13	2.47	0.49
1:A:86:ILE:HD11	1:A:350:PHE:CE1	2.47	0.49
1:C:303:LYS:HZ3	1:C:354:GLN:HE21	1.58	0.49
1:F:441:VAL:HG22	1:F:442:THR:N	2.28	0.49
1:D:19:PRO:HG3	1:D:75:TYR:CZ	2.47	0.49
1:J:206:ALA:HA	1:J:226:TRP:CZ3	2.48	0.49
1:H:203:GLU:N	1:H:203:GLU:OE1	2.31	0.49
1:J:159:GLY:CA	1:J:187:TYR:CZ	2.89	0.49
1:H:403:ALA:HB2	1:H:406:ARG:NH2	2.28	0.49
1:A:72:ALA:CA	1:A:90:ALA:O	2.60	0.49
1:B:367:SER:HB2	1:B:389:GLN:HB3	1.93	0.49
1:J:349:VAL:HG22	4:J:461:HOH:O	2.12	0.49
1:A:22:LYS:NZ	1:A:130:GLU:OE1	2.44	0.49
1:C:397:HIS:CE1	1:C:398:PRO:HD2	2.47	0.49
1:A:411:ALA:O	1:A:414:ALA:HB3	2.13	0.49
1:H:319:GLY:N	1:H:325:GLY:O	2.44	0.49
1:H:26:ILE:HB	1:H:127:TYR:HB3	1.93	0.49
1:G:48:ALA:HB1	1:G:53:GLY:HA3	1.93	0.49
1:D:159:GLY:CA	1:D:187:TYR:CZ	2.90	0.49
1:C:328:ASP:OD1	1:C:329:ILE:HD13	2.12	0.49
1:D:108:ILE:CD1	1:D:108:ILE:C	2.80	0.49
1:B:322:LYS:HG3	1:B:323:LEU:HG	1.94	0.49
1:D:389:GLN:C	1:D:390:LEU:HD12	2.33	0.49
1:E:25:ILE:HD11	1:E:132:LEU:HD21	1.94	0.49
1:A:32:THR:CG2	1:A:119:LYS:HE2	2.38	0.49
1:J:208:ILE:O	1:J:212:ILE:HG12	2.13	0.49
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.47	0.49
1:H:108:ILE:O	1:H:108:ILE:CG2	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:ILE:HD13	1:I:93:PHE:HA	1.93	0.49
1:B:54:THR:HG23	1:B:56:THR:O	2.12	0.49
1:I:72:ALA:O	1:I:73:LYS:HD3	2.13	0.49
1:C:407:ALA:HB2	1:C:430:GLU:HB3	1.95	0.49
1:C:149:MET:HE3	1:C:150:LEU:HD21	1.95	0.49
1:H:376:GLN:N	1:H:377:PRO:CD	2.75	0.49
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.47	0.49
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.42	0.49
1:J:414:ALA:HB2	1:J:424:TYR:CG	2.48	0.49
1:I:25:ILE:N	1:I:25:ILE:HD12	2.28	0.49
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.78	0.49
1:A:184:GLY:HA3	1:A:409:ARG:HG3	1.95	0.48
1:J:175:LYS:NZ	1:J:179:ASP:OD2	2.31	0.48
1:C:303:LYS:HZ2	1:C:354:GLN:HE21	1.61	0.48
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.11	0.48
1:A:299:PHE:CE2	1:A:351:HIS:CD2	3.00	0.48
1:A:22:LYS:NZ	1:G:63:GLU:OE1	2.45	0.48
1:D:397:HIS:CG	1:D:398:PRO:HD2	2.48	0.48
1:G:412:ILE:O	1:G:416:MET:HG2	2.13	0.48
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.95	0.48
1:H:117:ARG:HB2	4:H:1642:HOH:O	2.11	0.48
1:D:283:ALA:O	1:D:284:MET:HB3	2.13	0.48
1:H:149:MET:HE2	1:H:251:HIS:HE1	1.78	0.48
1:I:268:ARG:C	1:I:268:ARG:HD3	2.33	0.48
1:A:149:MET:CE	1:A:250:LYS:HE2	2.43	0.48
1:J:98:GLU:HG3	1:J:135:GLU:OE2	2.13	0.48
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.43	0.48
1:C:159:GLY:CA	1:C:187:TYR:CE2	2.95	0.48
1:C:283:ALA:O	1:C:284:MET:HB3	2.13	0.48
1:C:375:ILE:O	1:C:379:ILE:HG13	2.13	0.48
1:H:101:LEU:N	1:H:102:PRO:CD	2.75	0.48
1:A:51:SER:OG	1:A:52:THR:N	2.45	0.48
1:E:208:ILE:O	1:E:212:ILE:HG12	2.14	0.48
1:I:163:LYS:HA	1:I:164:PRO:C	2.34	0.48
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.95	0.48
1:C:38:THR:OG1	1:C:41:GLN:HG3	2.14	0.48
1:H:376:GLN:HG2	1:H:415:ILE:HD13	1.96	0.48
1:I:235:LEU:HB3	4:I:2572:HOH:O	2.13	0.48
1:J:159:GLY:CA	1:J:187:TYR:CE2	2.94	0.47
1:I:122:ARG:HD2	4:I:455:HOH:O	2.13	0.47
1:G:438:TRP:O	1:G:441:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:VAL:CG2	1:H:189:KCX:HD2	2.43	0.47
1:A:106:ALA:HA	1:H:258:ILE:CD1	2.44	0.47
1:B:65:GLU:CG	1:F:22:LYS:HD3	2.44	0.47
1:A:78:HIS:C	1:A:85:TRP:CD1	2.87	0.47
1:A:283:ALA:O	1:A:284:MET:CB	2.62	0.47
1:D:303:LYS:HZ3	1:D:354:GLN:HE21	1.62	0.47
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.94	0.47
1:D:376:GLN:N	1:D:377:PRO:CD	2.77	0.47
1:H:163:LYS:HE3	3:H:600:CAP:O2P	2.13	0.47
1:C:139:PRO:HD3	1:C:306:ARG:O	2.15	0.47
1:E:54:THR:HG23	1:E:56:THR:O	2.14	0.47
1:E:226:TRP:CZ3	1:E:228:ALA:HB2	2.50	0.47
1:C:341:HIS:CD2	1:C:343:LYS:HZ2	2.33	0.47
1:A:328:ASP:HB2	4:A:445:HOH:O	2.13	0.47
1:H:149:MET:HE2	1:H:251:HIS:CE1	2.50	0.47
1:E:108:ILE:HG22	1:E:108:ILE:O	2.14	0.47
1:F:283:ALA:O	1:F:284:MET:HB3	2.14	0.47
1:J:331:ILE:O	1:J:335:ARG:HG3	2.14	0.47
1:A:128:PHE:H	1:A:354:GLN:HE22	1.61	0.47
1:G:268:ARG:C	1:G:268:ARG:HD3	2.34	0.47
1:J:283:ALA:O	1:J:284:MET:HB3	2.15	0.47
1:I:93:PHE:C	1:I:93:PHE:CD1	2.87	0.47
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.95	0.47
1:J:441:VAL:HG13	4:J:677:HOH:O	2.13	0.47
1:D:397:HIS:CE1	1:D:398:PRO:HD2	2.50	0.47
1:C:230:ILE:O	1:C:237:MET:HG2	2.13	0.47
1:D:163:LYS:HA	1:D:164:PRO:C	2.34	0.47
1:J:143:ILE:HD11	1:J:338:ARG:HG2	1.97	0.47
1:A:147:ARG:HH21	1:A:385:ASP:HA	1.79	0.47
1:A:116:LYS:O	1:A:118:VAL:N	2.47	0.47
1:G:422:ASP:OD1	1:G:440:HIS:HE1	1.97	0.47
1:A:72:ALA:O	1:A:73:LYS:HD3	2.15	0.47
1:A:425:ALA:O	1:A:427:THR:N	2.48	0.47
1:B:329:ILE:H	1:B:329:ILE:CD1	2.28	0.47
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.13	0.47
1:B:444:VAL:HB	1:G:37:TYR:OH	2.15	0.47
1:A:80:MET:HB2	1:A:84:SER:O	2.15	0.47
1:B:400:GLY:HA2	1:G:59:TYR:CD1	2.50	0.46
1:F:96:PHE:CE1	1:F:104:LEU:HD13	2.50	0.46
1:B:70:LEU:HD22	1:B:95:ALA:HA	1.98	0.46
1:C:149:MET:HE2	1:C:251:HIS:CE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASN:OD1	1:H:292:PRO:HD2	2.15	0.46
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.97	0.46
1:A:116:LYS:C	1:A:118:VAL:N	2.69	0.46
1:B:175:LYS:CE	4:B:2916:HOH:O	2.63	0.46
1:E:159:GLY:HA3	1:E:187:TYR:CD2	2.50	0.46
1:E:413:ASP:O	1:E:417:GLN:HG2	2.16	0.46
1:B:283:ALA:O	1:B:284:MET:HB3	2.15	0.46
1:G:320:ALA:O	1:G:442:THR:HG23	2.15	0.46
1:H:34:ALA:O	1:H:35:GLU:C	2.54	0.46
1:C:260:GLY:HA3	1:F:260:GLY:HA3	1.97	0.46
1:B:211:LYS:HE3	1:B:211:LYS:HB2	1.81	0.46
1:A:263:ALA:HB2	1:H:263:ALA:CB	2.46	0.46
1:E:59:TYR:O	1:E:61:TRP:CD1	2.66	0.46
1:C:404:GLY:O	1:C:408:VAL:HG23	2.16	0.46
1:C:108:ILE:O	1:C:108:ILE:HG22	2.15	0.46
1:A:79:ASP:HA	1:A:85:TRP:CD1	2.50	0.46
1:G:149:MET:HE1	1:G:251:HIS:CE1	2.51	0.46
1:J:441:VAL:HG12	1:J:442:THR:N	2.30	0.46
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.51	0.46
1:A:326:GLU:HG2	4:A:2331:HOH:O	2.14	0.46
1:D:234:LEU:HD21	1:J:234:LEU:HD21	1.98	0.46
1:E:319:GLY:HA2	4:E:995:HOH:O	2.14	0.46
1:B:191:ASP:HB2	4:B:473:HOH:O	2.15	0.46
1:A:82:ASP:OD1	1:A:82:ASP:C	2.53	0.46
1:F:376:GLN:CB	1:F:377:PRO:CD	2.93	0.46
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.46	0.46
1:J:370:LEU:HB2	4:J:1892:HOH:O	2.15	0.46
1:J:303:LYS:HZ3	1:J:354:GLN:HE21	1.63	0.46
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.98	0.46
1:D:47:ALA:O	1:D:51:SER:HB2	2.16	0.46
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.81	0.46
1:F:336:ILE:HD12	1:F:336:ILE:HA	1.83	0.46
1:H:410:GLN:O	1:H:413:ASP:HB2	2.16	0.45
1:C:320:ALA:O	1:C:442:THR:HG23	2.15	0.45
1:D:397:HIS:ND1	1:D:398:PRO:HD2	2.30	0.45
1:B:283:ALA:O	1:B:284:MET:CB	2.65	0.45
1:D:108:ILE:HD12	1:D:109:ALA:N	2.30	0.45
1:G:283:ALA:O	1:G:284:MET:HB3	2.16	0.45
1:I:125:ASP:OD1	1:I:299:PHE:HE2	1.99	0.45
1:F:424:TYR:CZ	1:F:428:HIS:CE1	3.04	0.45
1:I:101:LEU:N	1:I:102:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:O	1:A:443:PRO:HD3	2.15	0.45
1:A:116:LYS:C	1:A:118:VAL:H	2.19	0.45
1:A:166:VAL:HG23	1:H:52:THR:HG22	1.98	0.45
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.97	0.45
1:I:289:THR:HG22	1:I:296:ILE:O	2.16	0.45
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.97	0.45
1:E:355:LYS:NZ	1:H:63:GLU:OE1	2.38	0.45
1:E:419:ILE:O	1:E:420:PRO:C	2.54	0.45
1:H:376:GLN:HB2	1:H:377:PRO:HD3	1.99	0.45
1:I:283:ALA:O	1:I:284:MET:CB	2.64	0.45
1:F:360:LYS:CE	4:F:452:HOH:O	2.65	0.45
1:I:338:ARG:HA	1:I:361:ALA:HB1	1.98	0.45
1:F:283:ALA:O	1:F:284:MET:CB	2.65	0.45
1:H:314:HIS:HA	1:H:365:THR:O	2.15	0.45
1:A:122:ARG:HG2	1:A:124:GLU:OE2	2.16	0.45
1:C:397:HIS:CG	1:C:398:PRO:CD	2.99	0.45
1:H:163:LYS:HA	1:H:164:PRO:C	2.36	0.45
1:D:383:GLY:HA3	4:D:872:HOH:O	2.15	0.45
1:H:424:TYR:CZ	1:H:428:HIS:CE1	3.04	0.45
1:C:189:KCX:OQ1	3:C:600:CAP:O3	2.35	0.45
1:A:165:LYS:NZ	1:A:191:ASP:OD2	2.38	0.45
1:A:337:LEU:HD22	1:A:362:ALA:HB3	1.98	0.45
1:G:143:ILE:HD11	1:G:338:ARG:HG2	1.98	0.45
1:A:429:LYS:O	1:A:433:ARG:HG2	2.16	0.45
1:B:362:ALA:O	1:B:364:PRO:HD3	2.17	0.45
1:A:59:TYR:CG	1:A:60:PRO:HD2	2.51	0.45
1:H:104:LEU:C	1:H:104:LEU:HD23	2.37	0.45
1:B:174:GLU:HB2	1:B:208:ILE:HD13	1.98	0.45
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.61	0.45
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.82	0.45
1:B:424:TYR:CZ	1:B:428:HIS:CE1	3.05	0.45
1:E:217:GLU:HG2	1:E:222:GLU:O	2.15	0.45
1:F:76:ASP:O	1:F:87:VAL:HA	2.17	0.45
1:H:200:ASN:OD1	1:H:205:ARG:HD3	2.16	0.45
1:H:321:GLY:HA3	4:H:2909:HOH:O	2.15	0.45
1:G:149:MET:HE1	1:G:251:HIS:ND1	2.31	0.45
1:J:283:ALA:O	1:J:284:MET:CB	2.65	0.45
1:F:139:PRO:O	1:F:360:LYS:HD3	2.17	0.45
1:I:62:TYR:OH	4:I:1237:HOH:O	2.21	0.45
1:B:230:ILE:O	1:B:237:MET:HG2	2.16	0.45
1:D:79:ASP:HB2	1:D:85:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HD11	1:C:338:ARG:HG2	1.98	0.45
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.52	0.45
1:D:320:ALA:O	1:D:442:THR:HG23	2.17	0.45
1:C:360:LYS:HE3	4:C:2743:HOH:O	2.17	0.45
1:F:331:ILE:O	1:F:335:ARG:HG3	2.16	0.45
1:A:149:MET:HE3	1:A:250:LYS:CG	2.37	0.44
1:B:329:ILE:N	1:B:329:ILE:CD1	2.79	0.44
1:H:323:LEU:HD12	1:H:323:LEU:H	1.82	0.44
1:A:158:TYR:O	1:A:186:ASP:HB2	2.18	0.44
1:I:101:LEU:HB3	1:I:102:PRO:HD3	1.99	0.44
1:A:417:GLN:C	1:A:419:ILE:H	2.21	0.44
1:A:14:ASP:OD1	1:A:17:TYR:N	2.44	0.44
1:A:226:TRP:CZ3	1:A:228:ALA:HB2	2.51	0.44
1:J:159:GLY:HA3	1:J:187:TYR:CD2	2.50	0.44
1:J:376:GLN:N	1:J:377:PRO:CD	2.80	0.44
1:H:149:MET:HE1	1:H:251:HIS:HD1	1.83	0.44
1:B:101:LEU:N	1:B:102:PRO:CD	2.80	0.44
1:H:425:ALA:O	1:H:427:THR:N	2.50	0.44
1:G:355:LYS:HB3	4:G:788:HOH:O	2.16	0.44
1:I:367:SER:HB2	1:I:389:GLN:HB3	1.99	0.44
1:A:424:TYR:O	1:A:428:HIS:ND1	2.48	0.44
1:D:59:TYR:HA	1:D:60:PRO:HD3	1.80	0.44
1:G:376:GLN:N	1:G:377:PRO:CD	2.80	0.44
1:A:184:GLY:O	1:A:409:ARG:HD3	2.17	0.44
1:I:59:TYR:O	1:I:61:TRP:HD1	2.00	0.44
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.44
1:J:347:ASN:CB	4:J:2614:HOH:O	2.39	0.44
1:A:165:LYS:HZ2	1:A:191:ASP:CG	2.18	0.44
1:C:186:ASP:OD1	4:C:1387:HOH:O	2.21	0.44
1:D:159:GLY:CA	1:D:187:TYR:CE2	2.95	0.44
1:D:341:HIS:CD2	1:D:343:LYS:NZ	2.80	0.44
1:C:329:ILE:N	1:C:329:ILE:CD1	2.81	0.44
1:G:108:ILE:HD12	1:G:109:ALA:N	2.33	0.44
1:H:19:PRO:HG3	1:H:75:TYR:CZ	2.52	0.44
1:E:283:ALA:O	1:E:284:MET:CB	2.65	0.44
1:D:79:ASP:HB2	1:D:85:TRP:CZ3	2.52	0.44
1:C:360:LYS:CE	4:C:2743:HOH:O	2.66	0.44
1:A:322:LYS:HG2	1:A:323:LEU:HG	2.00	0.44
1:E:69:ASP:OD1	1:H:23:ARG:NE	2.36	0.44
1:J:93:PHE:CD1	1:J:93:PHE:C	2.91	0.44
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:PHE:CD2	1:F:77:PHE:N	2.85	0.44
1:G:45:ALA:CB	1:G:117:ARG:HD2	2.48	0.44
1:E:376:GLN:HA	1:E:415:ILE:HD13	1.99	0.44
1:A:72:ALA:HB2	1:A:91:TYR:CD1	2.52	0.44
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.52	0.44
1:D:336:ILE:HA	1:D:336:ILE:HD12	1.83	0.44
1:A:149:MET:CE	1:A:250:LYS:HB2	2.47	0.44
1:B:159:GLY:CA	1:B:187:TYR:CZ	2.97	0.44
1:H:183:ASN:OD1	1:H:402:ALA:HB1	2.18	0.44
1:C:149:MET:HE1	1:C:251:HIS:CE1	2.52	0.44
1:G:424:TYR:CZ	1:G:428:HIS:CE1	3.06	0.44
1:C:122:ARG:HD2	4:C:475:HOH:O	2.18	0.44
1:J:239:GLN:O	1:J:243:VAL:HG23	2.18	0.44
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.48	0.43
1:H:230:ILE:O	1:H:237:MET:HG2	2.18	0.43
1:A:297:SER:C	1:A:299:PHE:N	2.72	0.43
1:A:115:MET:O	1:A:118:VAL:CG1	2.65	0.43
1:D:347:ASN:HA	4:D:2652:HOH:O	2.18	0.43
1:F:73:LYS:HD3	1:F:73:LYS:HA	1.85	0.43
1:A:19:PRO:HG3	1:A:75:TYR:CZ	2.53	0.43
1:G:125:ASP:OD1	1:G:126:LEU:N	2.51	0.43
1:B:288:PHE:HB3	1:G:288:PHE:HB3	2.00	0.43
1:A:38:THR:H	1:A:41:GLN:NE2	2.16	0.43
1:H:317:THR:O	1:H:318:ALA:HB3	2.18	0.43
1:A:282:ARG:HD3	1:A:314:HIS:O	2.19	0.43
1:H:203:GLU:CD	1:H:203:GLU:H	2.18	0.43
1:C:283:ALA:O	1:C:284:MET:CB	2.66	0.43
1:J:48:ALA:HB1	1:J:53:GLY:HA3	2.00	0.43
1:B:358:SER:OG	1:C:171:GLU:OE2	2.31	0.43
1:G:226:TRP:CZ3	1:G:228:ALA:HB2	2.53	0.43
1:D:38:THR:OG1	1:D:41:GLN:HG3	2.18	0.43
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.99	0.43
1:A:78:HIS:CE1	1:A:349:VAL:HG11	2.54	0.43
1:A:299:PHE:CZ	1:A:351:HIS:CD2	3.07	0.43
1:B:174:GLU:HB2	1:B:208:ILE:HG21	2.01	0.43
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.49	0.43
1:B:136:PHE:HB3	1:B:307:LEU:O	2.18	0.43
1:B:238:GLU:OE2	1:B:266:TYR:OH	2.24	0.43
1:A:161:VAL:CG2	1:A:189:KCX:HD2	2.48	0.43
1:D:206:ALA:HA	1:D:226:TRP:CZ3	2.54	0.43
1:F:282:ARG:O	1:F:285:HIS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.80	0.43
1:A:443:PRO:O	1:A:444:VAL:CG2	2.65	0.43
1:H:397:HIS:CD2	1:H:398:PRO:HD2	2.53	0.43
1:E:45:ALA:HB1	1:E:115:MET:HE2	2.00	0.43
1:I:54:THR:HG23	1:I:56:THR:O	2.18	0.43
1:C:149:MET:HE1	1:C:251:HIS:HD1	1.83	0.43
1:E:34:ALA:HA	1:E:119:LYS:HG3	2.01	0.43
1:B:358:SER:OG	1:C:171:GLU:HG2	2.19	0.43
1:H:59:TYR:O	1:H:61:TRP:CD1	2.70	0.43
1:E:390:LEU:N	1:E:390:LEU:HD12	2.33	0.43
1:H:54:THR:HG23	1:H:56:THR:H	1.84	0.43
1:H:49:GLU:HG3	1:H:115:MET:SD	2.59	0.43
1:A:225:THR:OG1	1:A:251:HIS:ND1	2.50	0.42
1:G:283:ALA:O	1:G:284:MET:CB	2.67	0.42
1:A:435:LEU:O	1:A:439:GLY:N	2.52	0.42
1:C:167:GLY:HA2	1:F:70:LEU:HD12	2.01	0.42
1:I:362:ALA:O	1:I:364:PRO:HD3	2.19	0.42
1:D:62:TYR:CD2	1:D:62:TYR:N	2.87	0.42
1:J:390:LEU:N	1:J:390:LEU:HD12	2.34	0.42
1:H:362:ALA:O	1:H:364:PRO:HD3	2.19	0.42
1:H:435:LEU:O	1:H:439:GLY:HA2	2.19	0.42
1:A:315:VAL:HG12	1:A:333:ASN:HB3	2.01	0.42
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.84	0.42
1:A:227:PHE:N	1:A:227:PHE:CD1	2.83	0.42
1:I:159:GLY:HA3	1:I:187:TYR:CD1	2.55	0.42
1:G:54:THR:HG21	1:G:58:LEU:CD2	2.49	0.42
1:C:149:MET:HE1	1:C:251:HIS:ND1	2.33	0.42
1:H:149:MET:CE	1:H:250:LYS:HD2	2.49	0.42
1:C:391:GLY:O	1:C:395:LEU:HD22	2.20	0.42
1:I:217:GLU:HG2	1:I:222:GLU:O	2.19	0.42
1:I:389:GLN:C	1:I:390:LEU:HD12	2.40	0.42
1:H:54:THR:HG23	1:H:55:TRP:N	2.35	0.42
1:A:49:GLU:O	1:H:165:LYS:HE2	2.18	0.42
1:H:25:ILE:N	1:H:25:ILE:HD12	2.35	0.42
1:E:319:GLY:CA	4:E:995:HOH:O	2.67	0.42
1:A:167:GLY:O	1:H:66:ARG:HD2	2.20	0.42
1:E:435:LEU:N	1:E:435:LEU:HD22	2.34	0.42
1:D:332:GLN:NE2	4:D:450:HOH:O	2.32	0.42
1:F:376:GLN:HB3	1:F:377:PRO:CD	2.48	0.42
1:F:80:MET:HB2	1:F:84:SER:O	2.19	0.42
1:D:211:LYS:HG3	1:D:212:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:TYR:CZ	1:D:428:HIS:CE1	3.07	0.42
1:F:407:ALA:HB2	1:F:430:GLU:HB3	2.01	0.42
1:F:279:HIS:NE2	1:F:314:HIS:NE2	2.61	0.42
1:C:217:GLU:HG2	1:C:222:GLU:O	2.19	0.42
1:C:268:ARG:HD3	1:C:268:ARG:C	2.40	0.42
1:A:299:PHE:CD2	1:A:351:HIS:HD2	2.38	0.42
1:F:12:TYR:CD2	1:F:48:ALA:HB2	2.54	0.42
1:F:101:LEU:HB3	1:F:102:PRO:HD3	2.01	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.94	0.42
1:F:101:LEU:N	1:F:102:PRO:CD	2.83	0.42
1:F:429:LYS:O	1:F:432:ALA:HB3	2.20	0.42
1:B:289:THR:HG22	1:B:296:ILE:O	2.20	0.42
1:D:11:TYR:CE2	1:D:73:LYS:NZ	2.87	0.42
1:E:77:PHE:N	1:E:77:PHE:CD2	2.87	0.42
1:A:443:PRO:C	1:A:444:VAL:HG23	2.40	0.42
1:A:425:ALA:C	1:A:427:THR:N	2.73	0.42
1:A:285:HIS:ND1	1:A:286:ALA:N	2.68	0.42
1:G:440:HIS:CD2	4:G:712:HOH:O	2.72	0.42
1:D:79:ASP:OD1	1:D:81:GLY:N	2.51	0.42
1:C:291:ASN:HA	1:C:292:PRO:HD3	1.81	0.42
1:C:367:SER:HB2	1:C:389:GLN:HB3	2.01	0.41
1:B:65:GLU:HG3	1:F:22:LYS:HD3	2.01	0.41
1:A:28:VAL:HG22	1:A:88:ARG:HG2	2.02	0.41
1:A:373:GLY:O	1:A:440:HIS:HA	2.20	0.41
1:F:327:ARG:HB3	4:F:1943:HOH:O	2.20	0.41
1:D:70:LEU:HD22	1:D:95:ALA:HA	2.01	0.41
1:C:159:GLY:CA	1:C:187:TYR:CZ	2.93	0.41
1:I:159:GLY:CA	1:I:187:TYR:CZ	3.00	0.41
1:F:163:LYS:O	1:F:395:LEU:HD22	2.21	0.41
1:I:376:GLN:N	1:I:377:PRO:CD	2.83	0.41
1:E:362:ALA:O	1:E:364:PRO:HD3	2.19	0.41
1:F:291:ASN:HA	1:F:292:PRO:HD3	1.87	0.41
1:E:268:ARG:HD3	1:E:268:ARG:C	2.41	0.41
1:F:424:TYR:CE2	1:F:428:HIS:CE1	3.08	0.41
1:D:235:LEU:O	1:D:239:GLN:HG3	2.20	0.41
1:A:139:PRO:HD3	1:A:306:ARG:O	2.21	0.41
1:H:303:LYS:HZ3	1:H:354:GLN:HE21	1.68	0.41
1:D:58:LEU:HD12	1:D:58:LEU:H	1.85	0.41
1:A:25:ILE:HD12	1:A:96:PHE:HE2	1.84	0.41
1:B:376:GLN:N	1:B:377:PRO:CD	2.83	0.41
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:PRO:HD2	1:H:200:ASN:O	2.20	0.41
1:D:144:GLU:CD	4:D:1914:HOH:O	2.58	0.41
1:A:149:MET:HE2	1:A:225:THR:HB	2.03	0.41
1:J:175:LYS:HD3	1:J:179:ASP:OD2	2.20	0.41
1:A:417:GLN:O	1:A:419:ILE:N	2.46	0.41
1:F:411:ALA:O	1:F:415:ILE:HG13	2.20	0.41
1:I:417:GLN:HG3	4:I:686:HOH:O	2.21	0.41
1:E:396:GLY:O	1:E:437:LYS:NZ	2.34	0.41
1:A:149:MET:CE	1:A:250:LYS:HE3	2.49	0.41
1:A:39:ILE:HB	1:A:85:TRP:CE3	2.56	0.41
1:A:298:MET:CE	1:A:314:HIS:O	2.69	0.41
1:A:77:PHE:N	1:A:77:PHE:HD2	2.16	0.41
1:D:283:ALA:O	1:D:284:MET:CB	2.69	0.41
1:E:101:LEU:HB3	1:E:102:PRO:HD3	2.01	0.41
1:J:336:ILE:HD12	1:J:336:ILE:HA	1.96	0.41
1:J:54:THR:CG2	1:J:58:LEU:CD2	2.98	0.41
1:J:437:LYS:HG3	1:J:438:TRP:N	2.33	0.41
1:J:414:ALA:HB3	1:J:421:LEU:CD2	2.50	0.41
1:A:433:ARG:HG2	1:A:433:ARG:H	1.72	0.41
1:E:323:LEU:HD23	1:I:115:MET:HA	2.02	0.41
1:F:341:HIS:NE2	1:F:353:GLU:OE2	2.37	0.41
1:E:196:SER:N	1:E:197:PRO:CD	2.84	0.41
1:B:345:ASP:OD2	4:B:1444:HOH:O	2.21	0.41
1:E:329:ILE:HG23	4:E:827:HOH:O	2.20	0.41
1:E:93:PHE:C	1:E:93:PHE:CD1	2.94	0.41
1:H:122:ARG:HG2	1:H:124:GLU:OE2	2.21	0.41
1:A:399:ASP:HB2	1:A:403:ALA:HB3	2.03	0.41
1:G:101:LEU:N	1:G:102:PRO:CD	2.83	0.41
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.51	0.41
1:J:93:PHE:CE1	1:J:131:LYS:HE3	2.55	0.41
1:A:321:GLY:HA3	4:A:573:HOH:O	2.21	0.41
1:F:25:ILE:CD1	1:F:93:PHE:HA	2.51	0.41
1:I:98:GLU:HG3	4:I:2591:HOH:O	2.21	0.41
1:G:289:THR:HG22	1:G:296:ILE:O	2.21	0.41
1:B:422:ASP:O	4:B:2564:HOH:O	2.21	0.41
1:E:159:GLY:N	1:E:187:TYR:CE2	2.89	0.41
1:E:411:ALA:O	1:E:415:ILE:HG13	2.20	0.41
1:H:322:LYS:HE2	1:H:323:LEU:HD11	2.03	0.41
1:E:395:LEU:HD13	1:E:401:PRO:HB3	2.02	0.41
1:A:223:LYS:O	1:A:224:LYS:HD3	2.21	0.41
1:H:115:MET:O	1:H:118:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:C	1:B:104:LEU:HD23	2.41	0.41
1:C:104:LEU:C	1:C:104:LEU:HD23	2.41	0.41
1:D:379:ILE:HD12	1:D:415:ILE:HD13	2.03	0.41
1:J:159:GLY:HA3	1:J:187:TYR:CD1	2.56	0.40
1:B:34:ALA:HA	1:B:119:LYS:CG	2.50	0.40
1:C:336:ILE:HD12	1:C:336:ILE:HA	1.89	0.40
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.56	0.40
1:C:101:LEU:HB3	1:C:102:PRO:HD3	2.03	0.40
1:D:159:GLY:HA3	1:D:187:TYR:CD2	2.56	0.40
1:A:76:ASP:C	1:A:76:ASP:OD1	2.57	0.40
1:E:176:LEU:HD11	1:E:395:LEU:CD1	2.51	0.40
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.57	0.40
1:F:285:HIS:CG	1:F:286:ALA:N	2.89	0.40
1:J:101:LEU:N	1:J:102:PRO:CD	2.84	0.40
1:C:435:LEU:O	1:C:439:GLY:N	2.53	0.40
1:D:358:SER:HB2	1:E:171:GLU:OE2	2.21	0.40
1:H:403:ALA:HB2	1:H:406:ARG:HH22	1.87	0.40
1:E:34:ALA:HA	1:E:119:LYS:CG	2.51	0.40
1:A:72:ALA:CB	1:A:90:ALA:O	2.70	0.40
1:I:285:HIS:CG	1:I:286:ALA:N	2.89	0.40
1:F:174:GLU:HG3	1:F:212:ILE:HD11	2.02	0.40
1:C:358:SER:OG	1:D:171:GLU:OE2	2.23	0.40
1:H:390:LEU:HD12	1:H:390:LEU:N	2.36	0.40
1:J:437:LYS:HG2	1:J:438:TRP:CE2	2.56	0.40
1:B:25:ILE:HD12	1:B:96:PHE:HE2	1.86	0.40
1:B:200:ASN:OD1	1:B:205:ARG:HD3	2.22	0.40
3:A:600:CAP:H12	3:A:600:CAP:O4	2.22	0.40
1:D:341:HIS:CG	1:D:343:LYS:HZ2	2.35	0.40
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.56	0.40
1:I:139:PRO:HD3	1:I:306:ARG:O	2.22	0.40
1:G:123:LEU:HG	1:G:300:VAL:HG21	2.04	0.40
1:C:414:ALA:HB2	1:C:424:TYR:CG	2.56	0.40
1:I:336:ILE:HD12	1:I:336:ILE:HA	1.86	0.40
1:B:268:ARG:C	1:B:268:ARG:HD3	2.42	0.40
1:I:264:LEU:HA	1:I:264:LEU:HD12	1.95	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	434/444 (98%)	394 (91%)	37 (8%)	3 (1%)	26	21
1	B	434/444 (98%)	418 (96%)	16 (4%)	0	100	100
1	C	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	D	434/444 (98%)	422 (97%)	12 (3%)	0	100	100
1	E	435/444 (98%)	418 (96%)	16 (4%)	1 (0%)	52	53
1	F	434/444 (98%)	419 (96%)	14 (3%)	1 (0%)	52	53
1	G	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	H	435/444 (98%)	399 (92%)	32 (7%)	4 (1%)	21	15
1	I	433/444 (98%)	418 (96%)	15 (4%)	0	100	100
1	J	434/444 (98%)	420 (97%)	13 (3%)	1 (0%)	52	53
All	All	4341/4440 (98%)	4146 (96%)	185 (4%)	10 (0%)	52	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	LYS
1	E	284	MET
1	J	284	MET
1	A	117	ARG
1	A	325	GLY
1	F	284	MET
1	H	284	MET
1	H	426	LYS
1	H	325	GLY
1	H	439	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	323/356 (91%)	316 (98%)	7 (2%)	60	64
1	B	341/356 (96%)	336 (98%)	5 (2%)	72	78
1	C	338/356 (95%)	332 (98%)	6 (2%)	66	72
1	D	339/356 (95%)	333 (98%)	6 (2%)	66	72
1	E	339/356 (95%)	334 (98%)	5 (2%)	72	78
1	F	335/356 (94%)	328 (98%)	7 (2%)	61	66
1	G	342/356 (96%)	336 (98%)	6 (2%)	66	72
1	H	330/356 (93%)	323 (98%)	7 (2%)	61	66
1	I	340/356 (96%)	338 (99%)	2 (1%)	90	94
1	J	341/356 (96%)	331 (97%)	10 (3%)	50	53
All	All	3368/3560 (95%)	3307 (98%)	61 (2%)	66	72

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	PHE
1	A	85	TRP
1	A	108	ILE
1	A	268	ARG
1	A	324	GLU
1	A	363	PHE
1	A	441	VAL
1	B	218	ASN
1	B	268	ARG
1	B	352	LEU
1	B	363	PHE
1	B	376	GLN
1	C	107	SER
1	C	218	ASN
1	C	235	LEU
1	C	268	ARG

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Mol	Chain	Res	Type
1	C	363	PHE
1	C	389	GLN
1	D	107	SER
1	D	117	ARG
1	D	122	ARG
1	D	268	ARG
1	D	328	ASP
1	D	363	PHE
1	E	107	SER
1	E	235	LEU
1	E	268	ARG
1	E	328	ASP
1	E	363	PHE
1	F	64	GLN
1	F	87	VAL
1	F	107	SER
1	F	235	LEU
1	F	268	ARG
1	F	332	GLN
1	F	363	PHE
1	G	107	SER
1	G	222	GLU
1	G	268	ARG
1	G	328	ASP
1	G	363	PHE
1	G	389	GLN
1	H	107	SER
1	H	117	ARG
1	H	235	LEU
1	H	268	ARG
1	H	323	LEU
1	H	363	PHE
1	H	389	GLN
1	I	363	PHE
1	I	376	GLN
1	J	10	ASP
1	J	58	LEU
1	J	107	SER
1	J	122	ARG
1	J	268	ARG
1	J	329	ILE
1	J	363	PHE

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Mol	Chain	Res	Type
1	J	370	LEU
1	J	389	GLN
1	J	437	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	78	HIS
1	A	183	ASN
1	A	312	GLN
1	A	354	GLN
1	B	64	GLN
1	B	312	GLN
1	B	347	ASN
1	B	354	GLN
1	B	376	GLN
1	C	312	GLN
1	C	354	GLN
1	C	376	GLN
1	C	440	HIS
1	D	312	GLN
1	D	354	GLN
1	D	440	HIS
1	E	312	GLN
1	E	332	GLN
1	E	354	GLN
1	E	417	GLN
1	F	312	GLN
1	F	332	GLN
1	F	354	GLN
1	G	312	GLN
1	G	354	GLN
1	G	440	HIS
1	H	64	GLN
1	H	312	GLN
1	H	354	GLN
1	I	312	GLN
1	I	354	GLN
1	I	376	GLN
1	J	312	GLN
1	J	354	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	A	189	1,2	7,11,12	0.71	0	7,12,14	1.21	1 (14%)
1	KCX	B	189	1,2	7,11,12	0.76	0	7,12,14	0.98	0
1	KCX	C	189	1,2	7,11,12	0.70	0	7,12,14	1.04	0
1	KCX	D	189	1,2	7,11,12	0.69	0	7,12,14	1.07	1 (14%)
1	KCX	E	189	1,2	7,11,12	0.67	0	7,12,14	1.29	1 (14%)
1	KCX	F	189	1,2	7,11,12	0.76	0	7,12,14	1.14	1 (14%)
1	KCX	G	189	1,2	7,11,12	0.79	0	7,12,14	0.96	0
1	KCX	H	189	1,2	7,11,12	0.64	0	7,12,14	1.10	0
1	KCX	I	189	1,2	7,11,12	0.74	0	7,12,14	1.15	1 (14%)
1	KCX	J	189	1,2	7,11,12	0.66	0	7,12,14	1.12	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	D	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	E	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	F	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	G	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	H	189	1,2	-	0/6/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	I	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	J	189	1,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	KCX	CE-NZ-CX	-2.77	120.35	123.49
1	A	189	KCX	CE-NZ-CX	-2.38	120.80	123.49
1	F	189	KCX	CE-NZ-CX	-2.20	121.00	123.49
1	I	189	KCX	CE-NZ-CX	-2.18	121.03	123.49
1	J	189	KCX	CE-NZ-CX	-2.14	121.06	123.49
1	D	189	KCX	CE-NZ-CX	-2.01	121.22	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	189	KCX	1	0
1	C	189	KCX	1	0
1	H	189	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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
3	CAP	A	600	2	14,20,20	0.82	0	15,31,31	0.74	0
3	CAP	B	600	2	14,20,20	0.80	0	15,31,31	0.72	0
3	CAP	C	600	2	14,20,20	0.84	0	15,31,31	0.69	0
3	CAP	D	600	2	14,20,20	0.85	0	15,31,31	0.74	0
3	CAP	E	600	2	14,20,20	0.80	0	15,31,31	0.64	0
3	CAP	F	600	2	14,20,20	0.75	0	15,31,31	0.70	0
3	CAP	G	600	2	14,20,20	0.78	0	15,31,31	0.67	0
3	CAP	H	600	2	14,20,20	0.77	0	15,31,31	0.65	0
3	CAP	I	600	2	14,20,20	0.78	0	15,31,31	0.67	0
3	CAP	J	600	2	14,20,20	0.85	0	15,31,31	0.60	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
3	CAP	A	600	2	-	0/23/29/29	0/0/0/0
3	CAP	B	600	2	-	0/23/29/29	0/0/0/0
3	CAP	C	600	2	-	0/23/29/29	0/0/0/0
3	CAP	D	600	2	-	0/23/29/29	0/0/0/0
3	CAP	E	600	2	-	0/23/29/29	0/0/0/0
3	CAP	F	600	2	-	0/23/29/29	0/0/0/0
3	CAP	G	600	2	-	0/23/29/29	0/0/0/0
3	CAP	H	600	2	-	0/23/29/29	0/0/0/0
3	CAP	I	600	2	-	0/23/29/29	0/0/0/0
3	CAP	J	600	2	-	0/23/29/29	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	CAP	3	0
3	C	600	CAP	1	0
3	H	600	CAP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	436/444 (98%)	1.02	77 (17%) 2 3	22, 36, 52, 58	0
1	B	436/444 (98%)	-0.10	4 (0%) 85 88	13, 22, 34, 37	0
1	C	436/444 (98%)	0.01	8 (1%) 71 76	12, 21, 40, 45	0
1	D	436/444 (98%)	-0.03	8 (1%) 71 76	11, 20, 32, 39	0
1	E	437/444 (98%)	0.04	15 (3%) 49 58	15, 24, 47, 51	0
1	F	436/444 (98%)	0.20	16 (3%) 45 54	12, 24, 38, 46	0
1	G	436/444 (98%)	0.00	4 (0%) 85 88	13, 24, 36, 41	0
1	H	437/444 (98%)	0.64	46 (10%) 8 11	22, 32, 57, 61	0
1	I	435/444 (97%)	-0.07	4 (0%) 85 88	15, 23, 34, 40	0
1	J	436/444 (98%)	-0.02	8 (1%) 71 76	11, 20, 41, 47	0
All	All	4361/4440 (98%)	0.17	190 (4%) 38 47	11, 24, 42, 61	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	59	TYR	5.9
1	A	59	TYR	5.6
1	E	7	THR	5.0
1	D	59	TYR	4.9
1	H	7	THR	4.7
1	A	414	ALA	4.7
1	H	414	ALA	4.5
1	F	59	TYR	4.5
1	A	16	GLY	4.4
1	E	59	TYR	4.3
1	J	427	THR	4.3
1	B	59	TYR	4.2
1	J	59	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLU	4.0
1	A	87	VAL	4.0
1	H	439	GLY	3.9
1	H	85	TRP	3.9
1	H	435	LEU	3.9
1	H	8	ILE	3.9
1	A	85	TRP	3.9
1	A	347	ASN	3.8
1	H	421	LEU	3.8
1	F	347	ASN	3.8
1	A	8	ILE	3.8
1	H	59	TYR	3.7
1	A	421	LEU	3.7
1	H	426	LYS	3.6
1	A	435	LEU	3.6
1	H	419	ILE	3.6
1	A	38	THR	3.5
1	H	443	PRO	3.5
1	H	424	TYR	3.5
1	A	427	THR	3.4
1	A	36	GLY	3.4
1	E	8	ILE	3.4
1	H	398	PRO	3.4
1	A	441	VAL	3.4
1	A	426	LYS	3.4
1	A	417	GLN	3.4
1	E	427	THR	3.3
1	A	257	VAL	3.3
1	A	293	TYR	3.3
1	A	29	PHE	3.3
1	A	422	ASP	3.3
1	G	59	TYR	3.3
1	B	347	ASN	3.3
1	A	54	THR	3.3
1	E	418	GLY	3.2
1	A	13	VAL	3.2
1	A	420	PRO	3.2
1	D	58	LEU	3.2
1	H	81	GLY	3.2
1	H	444	VAL	3.2
1	F	421	LEU	3.2
1	A	443	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	296	ILE	3.2
1	H	34	ALA	3.1
1	H	420	PRO	3.1
1	F	16	GLY	3.1
1	A	424	TYR	3.1
1	H	286	ALA	3.1
1	C	419	ILE	3.0
1	A	413	ASP	3.0
1	J	418	GLY	3.0
1	F	8	ILE	2.9
1	A	351	HIS	2.9
1	H	287	ALA	2.9
1	J	425	ALA	2.9
1	D	8	ILE	2.9
1	B	441	VAL	2.9
1	H	36	GLY	2.9
1	G	347	ASN	2.9
1	E	421	LEU	2.8
1	C	421	LEU	2.8
1	A	80	MET	2.8
1	E	426	LYS	2.8
1	A	296	ILE	2.8
1	F	426	LYS	2.8
1	H	433	ARG	2.8
1	H	376	GLN	2.8
1	A	283	ALA	2.7
1	F	78	HIS	2.7
1	A	157	ILE	2.7
1	H	427	THR	2.7
1	A	110	GLY	2.7
1	H	434	ALA	2.6
1	A	288	PHE	2.6
1	A	39	ILE	2.6
1	A	376	GLN	2.6
1	A	284	MET	2.6
1	H	418	GLY	2.6
1	A	17	TYR	2.6
1	A	379	ILE	2.6
1	A	434	ALA	2.6
1	E	420	PRO	2.6
1	A	352	LEU	2.6
1	A	403	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	81	GLY	2.6
1	H	293	TYR	2.6
1	H	422	ASP	2.6
1	A	313	LEU	2.6
1	E	434	ALA	2.6
1	A	14	ASP	2.6
1	D	9	TYR	2.5
1	H	11	TYR	2.5
1	C	418	GLY	2.5
1	A	57	THR	2.5
1	A	11	TYR	2.5
1	F	422	ASP	2.5
1	E	347	ASN	2.5
1	H	58	LEU	2.5
1	A	79	ASP	2.5
1	A	287	ALA	2.4
1	H	438	TRP	2.4
1	H	212	ILE	2.4
1	A	40	GLU	2.4
1	A	10	ASP	2.4
1	A	273	ASP	2.4
1	B	345	ASP	2.4
1	E	414	ALA	2.3
1	H	283	ALA	2.3
1	I	58	LEU	2.3
1	D	283	ALA	2.3
1	D	35	GLU	2.3
1	A	318	ALA	2.3
1	A	428	HIS	2.3
1	A	218	ASN	2.3
1	G	346	GLU	2.3
1	H	442	THR	2.3
1	C	347	ASN	2.3
1	E	422	ASP	2.3
1	A	43	ALA	2.3
1	A	81	GLY	2.2
1	D	400	GLY	2.2
1	C	59	TYR	2.2
1	F	257	VAL	2.2
1	I	57	THR	2.2
1	A	301	LEU	2.2
1	E	436	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	440	HIS	2.2
1	A	343	LYS	2.2
1	A	123	LEU	2.2
1	D	417	GLN	2.2
1	J	441	VAL	2.2
1	A	439	GLY	2.2
1	A	334	ALA	2.2
1	F	425	ALA	2.2
1	A	76	ASP	2.2
1	A	19	PRO	2.2
1	A	418	GLY	2.2
1	H	319	GLY	2.2
1	A	348	ASP	2.2
1	F	419	ILE	2.2
1	F	427	THR	2.2
1	H	35	GLU	2.2
1	E	425	ALA	2.2
1	C	8	ILE	2.2
1	H	220	THR	2.1
1	A	31	VAL	2.1
1	A	42	ALA	2.1
1	A	300	VAL	2.1
1	A	416	MET	2.1
1	C	81	GLY	2.1
1	H	110	GLY	2.1
1	A	256	VAL	2.1
1	H	108	ILE	2.1
1	H	323	LEU	2.1
1	J	435	LEU	2.1
1	H	302	ALA	2.1
1	A	37	TYR	2.1
1	A	305	TYR	2.1
1	E	380	GLU	2.1
1	F	313	LEU	2.1
1	H	431	LEU	2.1
1	A	185	ALA	2.1
1	H	109	ALA	2.1
1	F	376	GLN	2.1
1	J	417	GLN	2.1
1	H	413	ASP	2.1
1	J	422	ASP	2.1
1	G	58	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	398	PRO	2.1
1	I	283	ALA	2.1
1	H	288	PHE	2.1
1	A	161	VAL	2.1
1	A	438	TRP	2.0
1	A	400	GLY	2.0
1	H	347	ASN	2.0
1	A	58	LEU	2.0
1	F	79	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	189	12/13	0.93	0.20	-	29,30,31,31	0
1	KCX	G	189	12/13	0.98	0.13	-	16,17,17,17	0
1	KCX	E	189	12/13	0.96	0.12	-	21,22,23,23	0
1	KCX	I	189	12/13	0.97	0.12	-	17,18,18,18	0
1	KCX	D	189	12/13	0.97	0.14	-	11,14,15,15	0
1	KCX	B	189	12/13	0.98	0.11	-	18,19,19,20	0
1	KCX	H	189	12/13	0.93	0.13	-	30,30,31,31	0
1	KCX	F	189	12/13	0.96	0.20	-	17,18,20,20	0
1	KCX	J	189	12/13	0.98	0.14	-	18,18,19,20	0
1	KCX	C	189	12/13	0.96	0.11	-	14,16,17,17	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CAP	H	600	21/21	0.90	0.16	-0.11	31,34,36,37	0
3	CAP	J	600	21/21	0.96	0.12	-0.38	17,21,22,22	0
3	CAP	G	600	21/21	0.97	0.11	-0.48	17,17,18,18	0
3	CAP	I	600	21/21	0.98	0.11	-0.51	16,18,18,19	0
3	CAP	A	600	21/21	0.93	0.15	-0.58	27,33,34,35	0
3	CAP	B	600	21/21	0.97	0.09	-0.64	17,20,21,22	0
3	CAP	E	600	21/21	0.97	0.11	-0.70	21,24,26,26	0
3	CAP	D	600	21/21	0.98	0.10	-0.72	13,14,15,16	0
3	CAP	F	600	21/21	0.99	0.12	-0.75	15,17,17,18	0
3	CAP	C	600	21/21	0.98	0.10	-1.03	19,21,22,23	0
2	MG	H	500	1/1	0.96	0.10	-1.69	29,29,29,29	0
2	MG	J	500	1/1	0.99	0.10	-1.92	16,16,16,16	0
2	MG	B	500	1/1	0.98	0.07	-2.46	18,18,18,18	0
2	MG	I	500	1/1	0.99	0.07	-2.92	13,13,13,13	0
2	MG	F	500	1/1	1.00	0.08	-2.93	19,19,19,19	0
2	MG	C	500	1/1	0.97	0.07	-3.46	16,16,16,16	0
2	MG	D	500	1/1	1.00	0.06	-4.12	11,11,11,11	0
2	MG	A	500	1/1	0.94	0.12	-4.15	29,29,29,29	0
2	MG	G	500	1/1	0.97	0.05	-4.55	16,16,16,16	0
2	MG	E	500	1/1	0.99	0.07	-4.98	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.