Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:16 AM GMT

PDB ID	:	3A13
Title	:	Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP and activated with Ca
Authors	:	Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2009-03-25
Resolution	:	2.34 Å(reported)

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

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

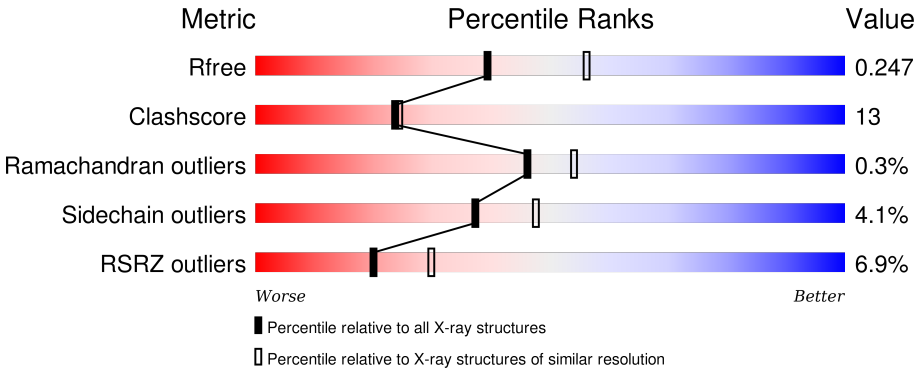
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	5% 74% 23%
1	B	444	7% 77% 20%
1	C	444	9% 76% 20%
1	D	444	8% 77% 20%
1	E	444	5% 79% 17%

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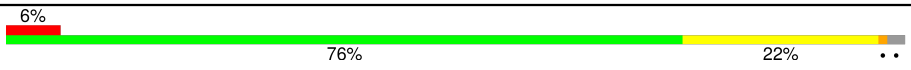
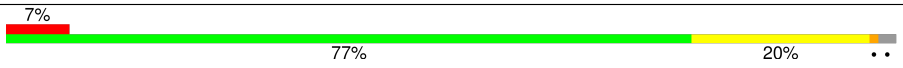
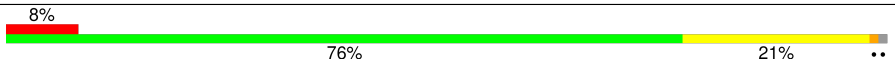
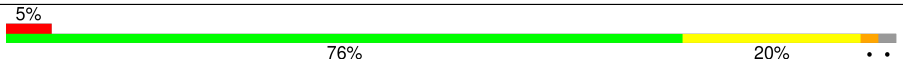
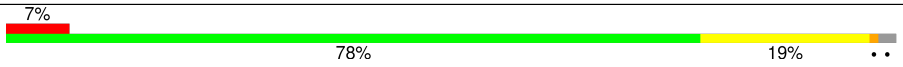
Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36193 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribulose bisphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3408	2186	586	626	10			
1	B	437	Total	C	N	O	S	0	0	0
			3412	2187	586	629	10			
1	C	437	Total	C	N	O	S	0	0	0
			3399	2181	584	624	10			
1	D	437	Total	C	N	O	S	0	0	0
			3392	2170	584	628	10			
1	E	432	Total	C	N	O	S	0	0	0
			3379	2163	581	625	10			
1	F	437	Total	C	N	O	S	0	0	0
			3405	2184	586	625	10			
1	G	437	Total	C	N	O	S	0	0	0
			3413	2190	585	628	10			
1	H	438	Total	C	N	O	S	0	0	0
			3412	2189	588	625	10			
1	I	437	Total	C	N	O	S	0	0	0
			3423	2195	587	631	10			
1	J	434	Total	C	N	O	S	0	0	0
			3379	2161	583	625	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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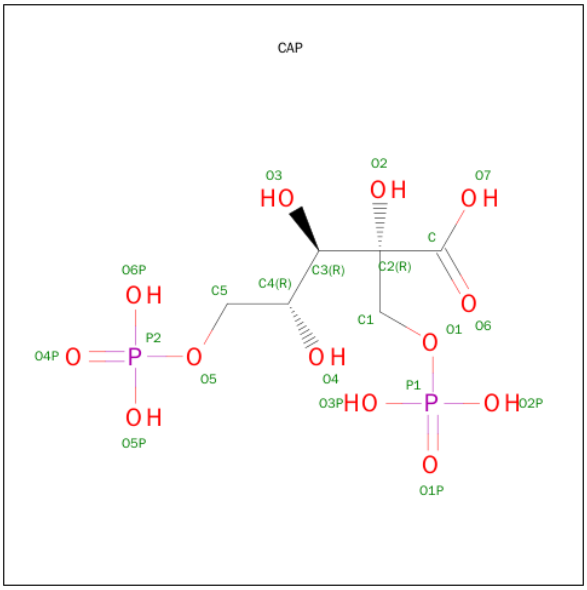
Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	ENGINEERED	UNP O93627
C	326	GLU	GLY	ENGINEERED	UNP O93627
C	327	ARG	LYS	ENGINEERED	UNP O93627
C	328	ASP	TRP	ENGINEERED	UNP O93627
C	329	ILE	ASP	ENGINEERED	UNP O93627
C	330	THR	VAL	ENGINEERED	UNP O93627
D	326	GLU	GLY	ENGINEERED	UNP O93627
D	327	ARG	LYS	ENGINEERED	UNP O93627
D	328	ASP	TRP	ENGINEERED	UNP O93627
D	329	ILE	ASP	ENGINEERED	UNP O93627
D	330	THR	VAL	ENGINEERED	UNP O93627
E	326	GLU	GLY	ENGINEERED	UNP O93627
E	327	ARG	LYS	ENGINEERED	UNP O93627
E	328	ASP	TRP	ENGINEERED	UNP O93627
E	329	ILE	ASP	ENGINEERED	UNP O93627
E	330	THR	VAL	ENGINEERED	UNP O93627
F	326	GLU	GLY	ENGINEERED	UNP O93627
F	327	ARG	LYS	ENGINEERED	UNP O93627
F	328	ASP	TRP	ENGINEERED	UNP O93627
F	329	ILE	ASP	ENGINEERED	UNP O93627
F	330	THR	VAL	ENGINEERED	UNP O93627
G	326	GLU	GLY	ENGINEERED	UNP O93627
G	327	ARG	LYS	ENGINEERED	UNP O93627
G	328	ASP	TRP	ENGINEERED	UNP O93627
G	329	ILE	ASP	ENGINEERED	UNP O93627
G	330	THR	VAL	ENGINEERED	UNP O93627
H	326	GLU	GLY	ENGINEERED	UNP O93627
H	327	ARG	LYS	ENGINEERED	UNP O93627
H	328	ASP	TRP	ENGINEERED	UNP O93627
H	329	ILE	ASP	ENGINEERED	UNP O93627
H	330	THR	VAL	ENGINEERED	UNP O93627
I	326	GLU	GLY	ENGINEERED	UNP O93627
I	327	ARG	LYS	ENGINEERED	UNP O93627
I	328	ASP	TRP	ENGINEERED	UNP O93627
I	329	ILE	ASP	ENGINEERED	UNP O93627
I	330	THR	VAL	ENGINEERED	UNP O93627
J	326	GLU	GLY	ENGINEERED	UNP O93627
J	327	ARG	LYS	ENGINEERED	UNP O93627
J	328	ASP	TRP	ENGINEERED	UNP O93627
J	329	ILE	ASP	ENGINEERED	UNP O93627
J	330	THR	VAL	ENGINEERED	UNP O93627

- 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	D	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
3	B	1	Total C O P 21 6 13 2	0	0
3	C	1	Total C O P 21 6 13 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	204	Total	O	0	0
			204	204		
5	C	186	Total	O	0	0
			186	186		
5	D	210	Total	O	0	0
			210	210		
5	E	193	Total	O	0	0
			193	193		
5	F	176	Total	O	0	0
			176	176		
5	G	203	Total	O	0	0
			203	203		
5	H	180	Total	O	0	0
			180	180		

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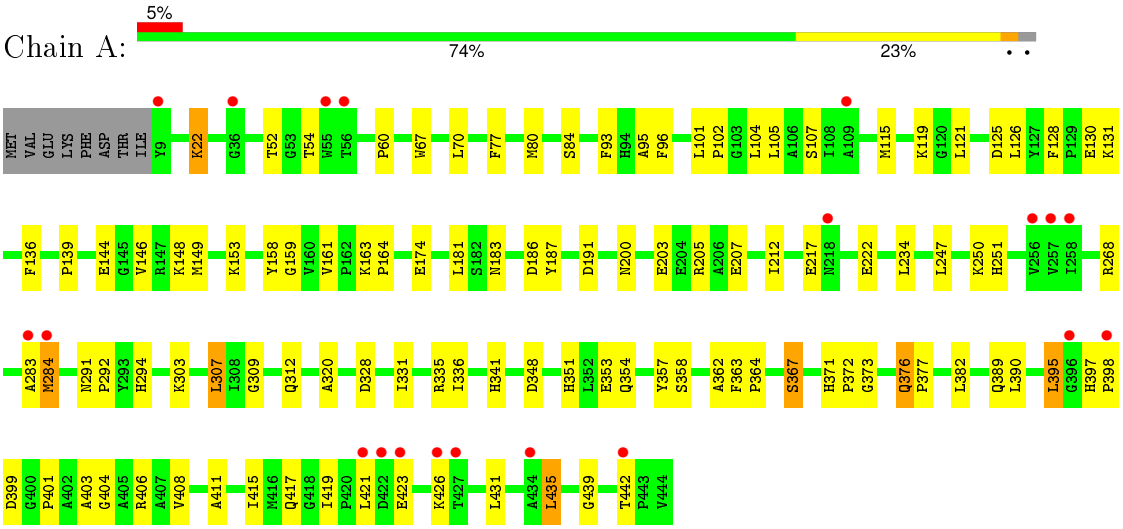
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	212	Total O 212 212	0	0
5	J	194	Total O 194 194	0	0

3 Residue-property plots (i)

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

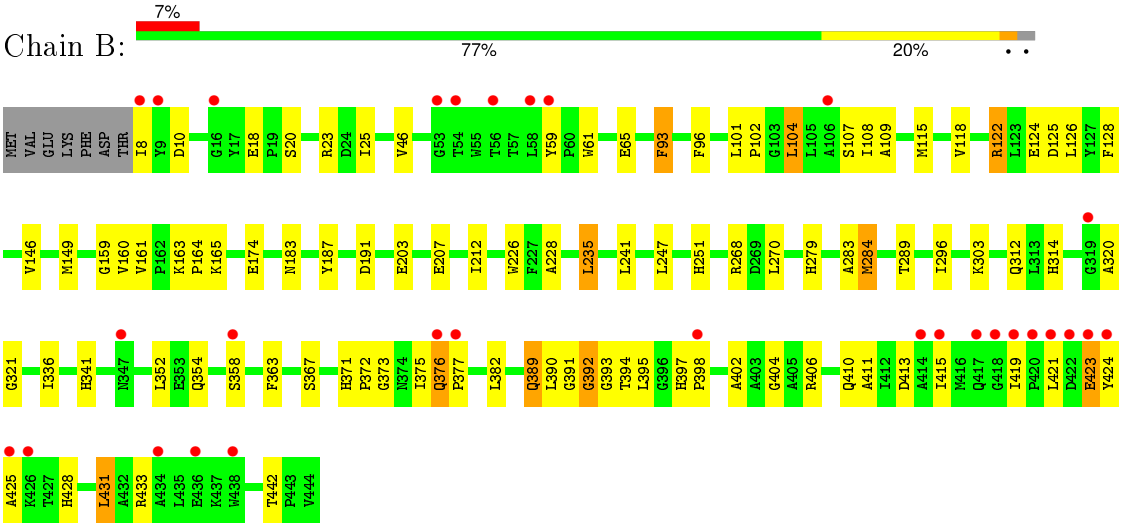
- Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



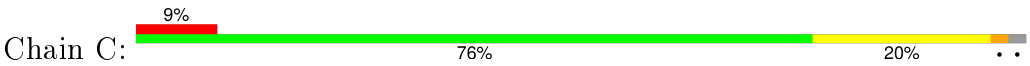
- Molecule 1: Ribulose bisphosphate carboxylase

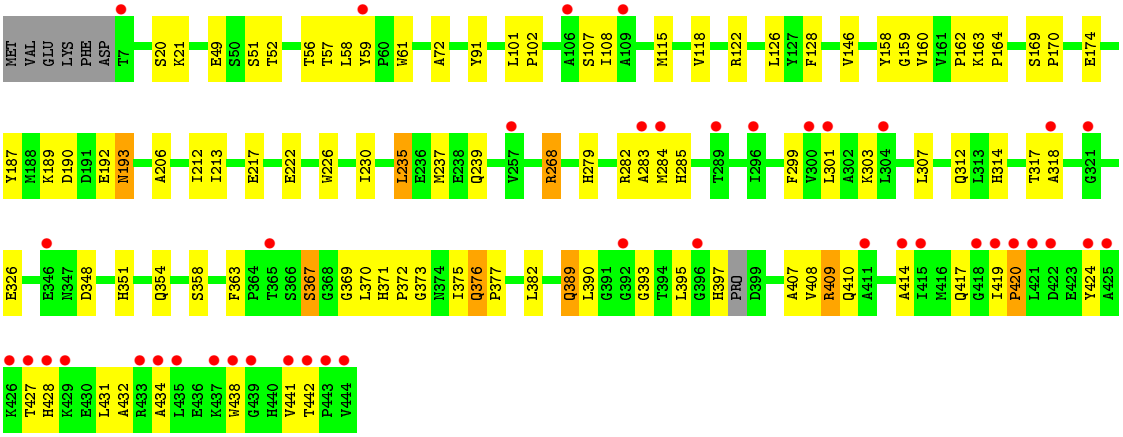
Chain B:



- Molecule 1: Ribulose bisphosphate carboxylase

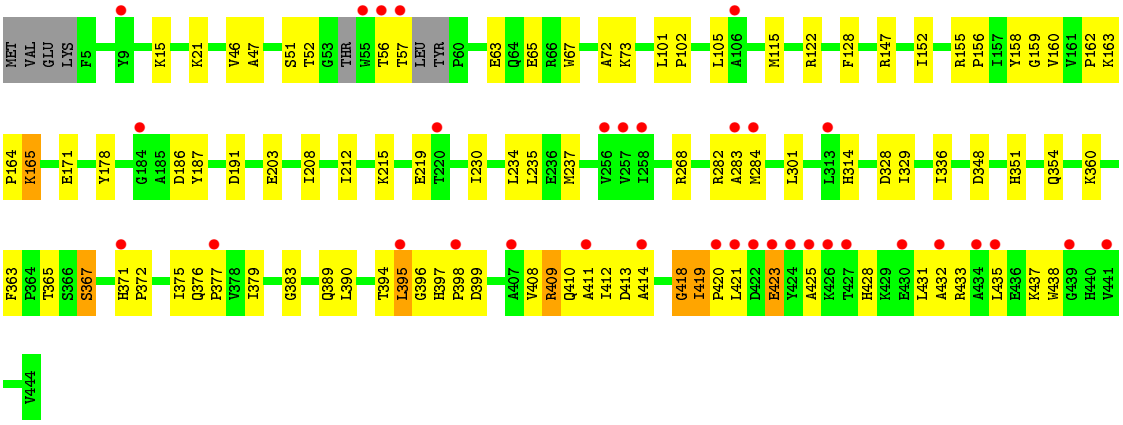
Chain C:





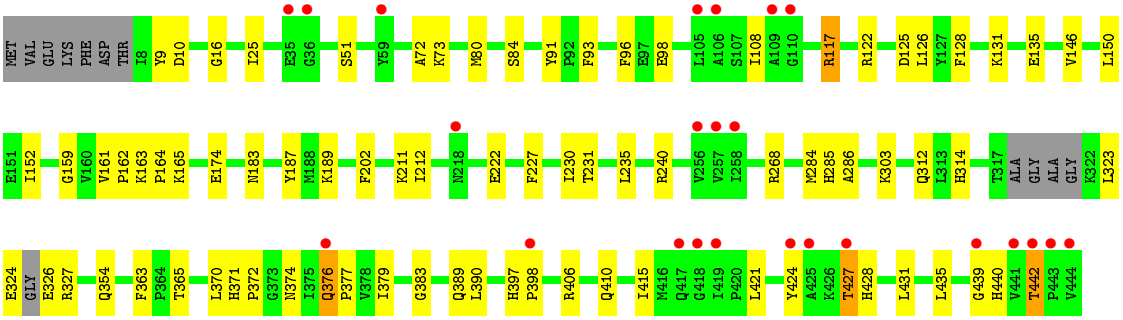
• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



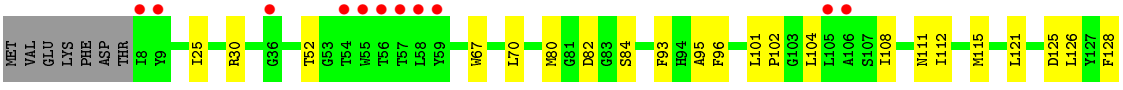
• Molecule 1: Ribulose bisphosphate carboxylase

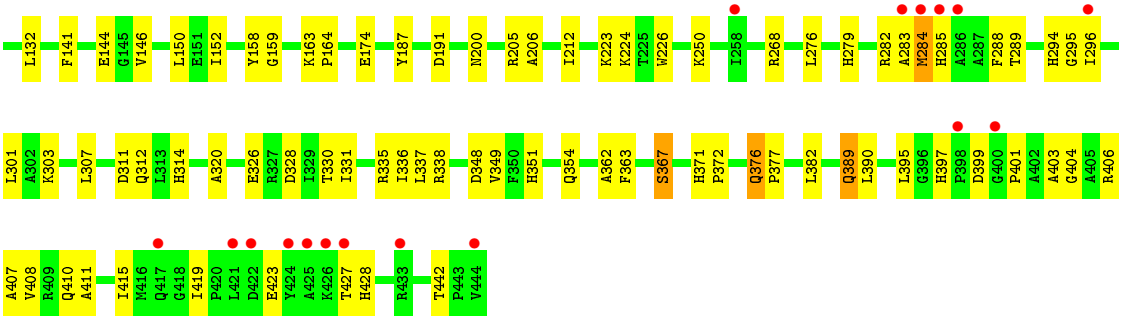
Chain E:



• Molecule 1: Ribulose bisphosphate carboxylase

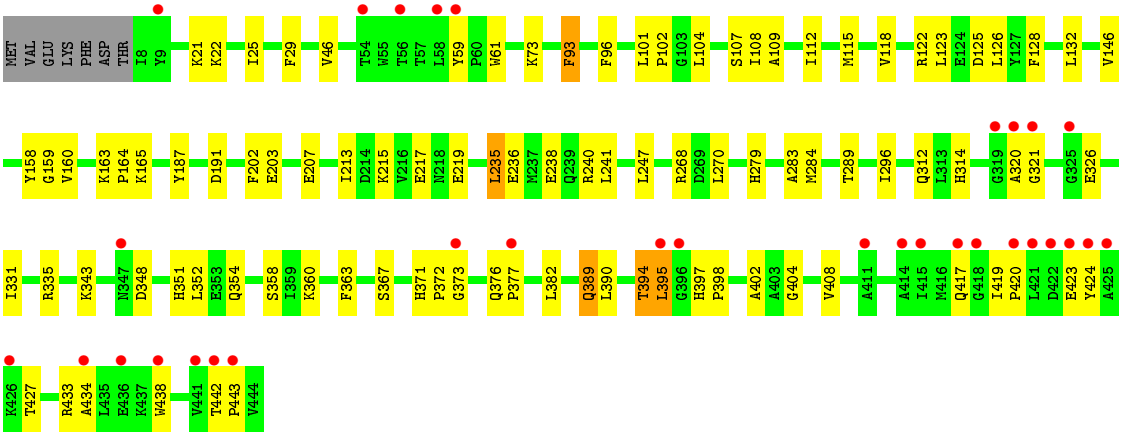
Chain F:





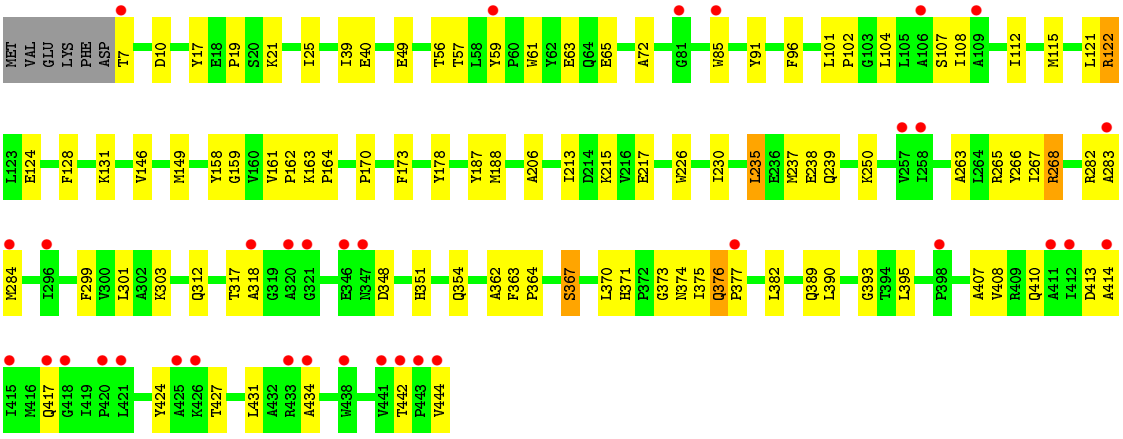
• Molecule 1: Ribulose bisphosphate carboxylase

Chain G:



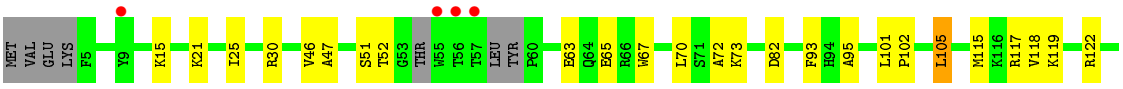
• Molecule 1: Ribulose bisphosphate carboxylase

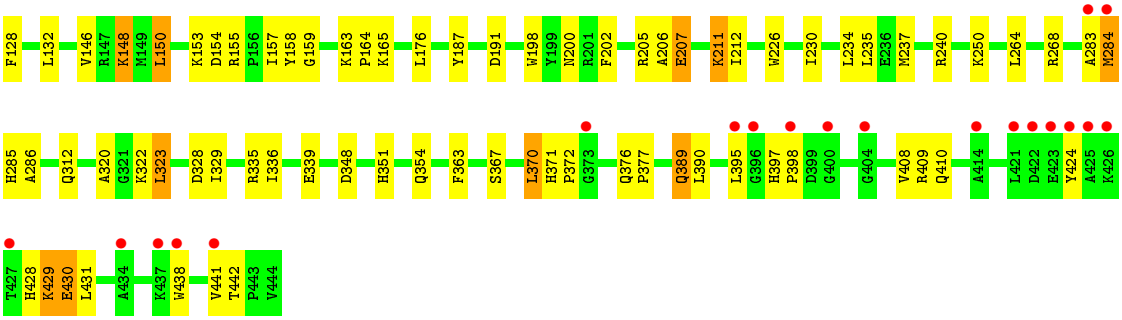
Chain H:



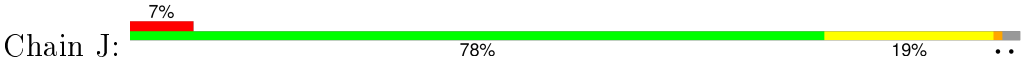
• Molecule 1: Ribulose bisphosphate carboxylase

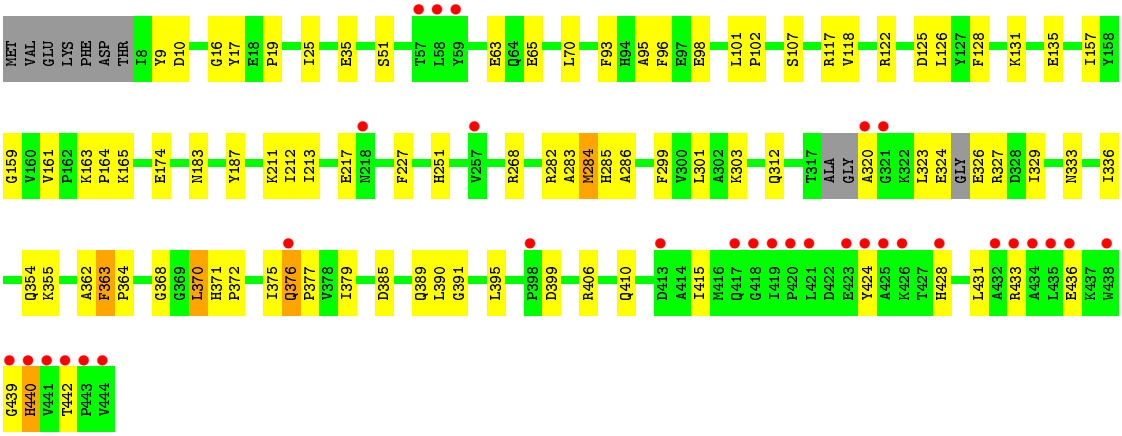
Chain I:





- Molecule 1: Ribulose bisphosphate carboxylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.68Å 247.09Å 144.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.22 – 2.34 42.22 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.22-2.34) 99.4 (42.22-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.250 0.206 , 0.247	Depositor DCC
R_{free} test set	13104 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	4 of 261352 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36193	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.31 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5974e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CAP, MG, 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	0.36	0/3482	0.51	0/4722
1	B	0.37	0/3486	0.52	0/4729
1	C	0.35	0/3472	0.50	0/4711
1	D	0.38	0/3463	0.51	0/4695
1	E	0.37	0/3451	0.51	0/4680
1	F	0.35	0/3479	0.50	0/4719
1	G	0.37	0/3488	0.51	0/4732
1	H	0.37	0/3486	0.51	0/4729
1	I	0.39	0/3495	0.53	0/4735
1	J	0.38	0/3451	0.51	0/4679
All	All	0.37	0/34753	0.51	0/47131

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	3408	0	3311	86	0
1	B	3412	0	3307	119	0
1	C	3399	0	3284	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3392	0	3267	91	0
1	E	3379	0	3253	74	0
1	F	3405	0	3301	73	0
1	G	3413	0	3303	86	0
1	H	3412	0	3315	95	0
1	I	3423	0	3330	83	0
1	J	3379	0	3235	81	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	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
3	A	21	0	7	1	0
3	B	21	0	7	1	0
3	C	21	0	7	3	0
3	D	21	0	7	0	0
3	E	21	0	9	1	0
3	F	21	0	8	2	0
3	G	21	0	7	1	0
3	H	21	0	8	2	0
3	I	21	0	7	0	0
3	J	21	0	9	1	0
4	E	1	0	0	0	0
4	J	1	0	0	0	0
5	A	193	0	0	15	0
5	B	204	0	0	14	0
5	C	186	0	0	9	0
5	D	210	0	0	16	0
5	E	193	0	0	12	0
5	F	176	0	0	9	0
5	G	203	0	0	14	0
5	H	180	0	0	6	0
5	I	212	0	0	14	0
5	J	194	0	0	10	0
All	All	36193	0	32982	885	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 (885) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLU:HG2	5:F:602:HOH:O	1.45	1.16
1:J:174:GLU:HG3	1:J:212:ILE:HD11	1.29	1.13
1:J:391:GLY:O	1:J:395:LEU:HD12	1.49	1.12
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.28	1.11
1:I:429:LYS:H	1:I:429:LYS:HD3	0.98	1.09
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.15	1.09
3:C:446:CAP:H4	3:C:446:CAP:O6	1.50	1.09
1:B:104:LEU:C	1:B:104:LEU:HD23	1.72	1.09
1:A:358:SER:HB2	5:A:678:HOH:O	1.48	1.08
1:H:235:LEU:HD12	5:H:602:HOH:O	1.54	1.05
1:D:203:GLU:HG3	5:D:551:HOH:O	1.58	1.03
3:H:446:CAP:O6	3:H:446:CAP:H4	1.59	1.02
1:I:335:ARG:HD2	1:I:339:GLU:OE2	1.59	1.02
1:B:104:LEU:O	1:B:104:LEU:HD23	1.57	1.02
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.39	1.02
1:C:417:GLN:HA	5:C:601:HOH:O	1.60	1.01
1:D:165:LYS:HB3	1:D:191:ASP:OD2	1.64	0.97
1:C:371:HIS:CE1	1:C:373:GLY:HA3	2.00	0.97
1:B:371:HIS:CE1	1:B:373:GLY:HA3	1.99	0.96
1:I:429:LYS:N	1:I:429:LYS:HD3	1.76	0.96
1:D:419:ILE:HD12	1:D:419:ILE:N	1.78	0.95
1:A:367:SER:HB2	1:A:389:GLN:HB3	1.51	0.93
1:H:371:HIS:CE1	1:H:373:GLY:HA3	2.03	0.92
1:C:235:LEU:HD12	5:C:666:HOH:O	1.69	0.91
1:H:149:MET:CE	1:H:250:LYS:HD2	2.00	0.90
1:E:431:LEU:O	1:E:435:LEU:HD13	1.69	0.90
1:B:398:PRO:HG3	1:B:433:ARG:O	1.71	0.90
1:D:438:TRP:HB2	5:D:587:HOH:O	1.71	0.90
1:C:163:LYS:H	1:C:395:LEU:CD2	1.85	0.89
1:J:440:HIS:CE1	5:J:694:HOH:O	2.25	0.88
1:D:383:GLY:HA3	5:D:609:HOH:O	1.73	0.88
1:I:429:LYS:H	1:I:429:LYS:CD	1.81	0.88
1:B:371:HIS:HE1	1:B:373:GLY:HA3	1.38	0.88
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.56	0.87
1:F:174:GLU:HG3	1:F:212:ILE:HD11	1.58	0.86
1:C:49:GLU:HG3	1:C:115:MET:HE3	1.56	0.86
1:C:193:ASN:HD22	1:C:193:ASN:H	1.23	0.86
1:G:397:HIS:ND1	1:G:398:PRO:HD2	1.91	0.86
1:H:149:MET:HE3	1:H:250:LYS:CD	2.04	0.85
1:B:425:ALA:HB2	1:B:431:LEU:HG	1.58	0.85
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.58	0.85
1:I:329:ILE:HD11	5:I:679:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:C	1:B:104:LEU:CD2	2.46	0.84
1:C:174:GLU:HG3	1:C:212:ILE:HD11	1.57	0.84
1:C:371:HIS:HE1	1:C:373:GLY:HA3	1.42	0.84
1:B:371:HIS:CE1	1:B:373:GLY:CA	2.61	0.84
1:E:128:PHE:H	1:E:354:GLN:HE22	1.25	0.84
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.43	0.83
1:H:348:ASP:OD2	1:H:351:HIS:HD2	1.61	0.83
1:G:104:LEU:C	1:G:104:LEU:HD23	1.98	0.83
1:I:21:LYS:HD3	5:I:689:HOH:O	1.78	0.83
1:C:49:GLU:HG3	1:C:115:MET:CE	2.08	0.82
1:H:163:LYS:H	1:H:395:LEU:CD2	1.93	0.82
1:D:155:ARG:CZ	1:D:409:ARG:NH2	2.43	0.82
1:J:128:PHE:H	1:J:354:GLN:HE22	1.27	0.81
1:D:419:ILE:CD1	1:D:419:ILE:N	2.43	0.80
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.17	0.80
1:G:398:PRO:HG2	1:G:433:ARG:O	1.81	0.79
1:F:163:LYS:H	1:F:395:LEU:HD22	1.47	0.79
1:D:413:ASP:HA	5:D:594:HOH:O	1.82	0.79
1:D:395:LEU:N	1:D:395:LEU:CD1	2.45	0.79
1:I:410:GLN:HE22	1:I:430:GLU:CG	1.97	0.77
1:J:174:GLU:CG	1:J:212:ILE:HD11	2.14	0.77
1:G:417:GLN:C	5:G:564:HOH:O	2.23	0.77
1:C:367:SER:HB2	1:C:389:GLN:HB3	1.66	0.76
1:I:348:ASP:OD2	1:I:351:HIS:HD2	1.68	0.76
1:A:121:LEU:H	1:A:294:HIS:HD2	1.31	0.76
1:A:331:ILE:O	1:A:335:ARG:HG3	1.85	0.76
1:F:338:ARG:HD2	5:F:574:HOH:O	1.86	0.76
1:J:410:GLN:NE2	1:J:431:LEU:H	1.83	0.76
1:E:440:HIS:CD2	5:E:691:HOH:O	2.38	0.76
1:A:411:ALA:O	1:A:415:ILE:HG13	1.85	0.76
1:B:371:HIS:ND1	1:B:373:GLY:N	2.33	0.76
1:D:397:HIS:ND1	1:D:398:PRO:HD2	2.00	0.76
1:H:161:VAL:H	1:H:389:GLN:NE2	1.83	0.76
1:D:428:HIS:CE1	5:D:583:HOH:O	2.37	0.76
1:D:21:LYS:HD3	5:D:709:HOH:O	1.84	0.76
1:H:371:HIS:HE1	1:H:373:GLY:HA3	1.49	0.75
1:B:423:GLU:HG3	1:B:424:TYR:N	2.02	0.75
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.22	0.75
1:D:395:LEU:N	1:D:395:LEU:HD12	2.00	0.75
1:I:128:PHE:H	1:I:354:GLN:HE22	1.33	0.75
1:H:128:PHE:H	1:H:354:GLN:HE22	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ASP:OD2	1:C:351:HIS:HD2	1.70	0.74
1:E:9:TYR:HD2	1:E:117:ARG:NH1	1.84	0.74
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.22	0.74
1:E:163:LYS:HD2	5:E:630:HOH:O	1.87	0.74
1:H:367:SER:HB2	1:H:389:GLN:HB3	1.69	0.73
1:J:368:GLY:O	1:J:370:LEU:HD13	1.88	0.73
1:C:128:PHE:H	1:C:354:GLN:HE22	1.36	0.73
1:D:165:LYS:CB	1:D:191:ASP:OD2	2.36	0.73
1:E:376:GLN:N	1:E:377:PRO:HD2	2.03	0.73
1:B:423:GLU:HG3	1:B:424:TYR:H	1.52	0.73
1:E:174:GLU:CG	1:E:212:ILE:HD11	2.14	0.73
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.70	0.73
1:I:438:TRP:HB2	5:I:597:HOH:O	1.88	0.73
1:B:128:PHE:H	1:B:354:GLN:HE22	1.37	0.72
1:A:121:LEU:H	1:A:294:HIS:CD2	2.07	0.72
1:C:162:PRO:HA	1:C:395:LEU:HD21	1.71	0.71
1:D:128:PHE:H	1:D:354:GLN:HE22	1.38	0.71
1:E:440:HIS:HB3	5:E:692:HOH:O	1.91	0.71
1:B:410:GLN:CG	5:B:628:HOH:O	2.38	0.71
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.26	0.71
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.25	0.71
1:H:317:THR:O	1:H:318:ALA:HB3	1.91	0.71
1:G:427:THR:HB	5:G:614:HOH:O	1.91	0.70
1:D:63:GLU:HG2	1:D:65:GLU:HG2	1.73	0.70
1:B:419:ILE:HG23	1:B:423:GLU:CG	2.21	0.70
1:E:93:PHE:CE1	1:E:131:LYS:HE3	2.27	0.70
1:E:442:THR:HG23	5:E:693:HOH:O	1.92	0.70
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.27	0.70
1:E:326:GLU:HG2	1:E:327:ARG:H	1.57	0.70
1:F:423:GLU:CB	5:F:633:HOH:O	2.39	0.70
1:I:370:LEU:HB2	5:I:659:HOH:O	1.92	0.70
1:G:128:PHE:H	1:G:354:GLN:HE22	1.40	0.70
1:A:389:GLN:C	1:A:390:LEU:HD12	2.12	0.69
1:G:320:ALA:O	1:G:442:THR:HG23	1.92	0.69
1:G:360:LYS:HE2	5:G:645:HOH:O	1.91	0.69
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.56	0.69
1:I:389:GLN:C	1:I:390:LEU:HD12	2.13	0.69
1:A:320:ALA:O	1:A:442:THR:HG23	1.92	0.69
1:J:410:GLN:HE21	1:J:431:LEU:N	1.89	0.69
1:F:121:LEU:H	1:F:294:HIS:HD2	1.38	0.69
1:F:163:LYS:HE3	3:F:446:CAP:O2P	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:HIS:CE1	1:G:373:GLY:HA3	2.26	0.69
1:C:317:THR:O	1:C:318:ALA:HB3	1.92	0.69
1:F:320:ALA:O	1:F:442:THR:HG23	1.93	0.69
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.27	0.68
1:C:235:LEU:CD1	5:C:666:HOH:O	2.35	0.68
1:E:371:HIS:CE1	1:E:439:GLY:O	2.46	0.68
1:E:410:GLN:HE21	1:E:431:LEU:HB2	1.58	0.68
1:I:410:GLN:NE2	1:I:430:GLU:CG	2.56	0.68
1:G:104:LEU:O	1:G:104:LEU:HD23	1.92	0.68
1:J:326:GLU:HG2	1:J:327:ARG:N	2.08	0.68
1:B:397:HIS:CG	1:B:398:PRO:HD2	2.27	0.68
1:D:348:ASP:OD2	1:D:351:HIS:HD2	1.76	0.68
1:H:39:ILE:HD13	1:H:85:TRP:CD1	2.28	0.68
1:I:428:HIS:NE2	5:I:531:HOH:O	2.26	0.68
1:B:419:ILE:CG2	1:B:423:GLU:CG	2.72	0.68
1:E:16:GLY:HA3	5:E:657:HOH:O	1.93	0.68
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.29	0.67
1:A:163:LYS:H	1:A:395:LEU:HD11	1.58	0.67
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.30	0.67
1:H:376:GLN:N	1:H:377:PRO:HD2	2.09	0.67
1:B:397:HIS:ND1	1:B:398:PRO:HD2	2.10	0.67
1:J:410:GLN:HE21	1:J:431:LEU:H	1.40	0.67
1:G:25:ILE:HD13	1:G:96:PHE:CE2	2.30	0.67
1:J:326:GLU:HG2	1:J:327:ARG:H	1.60	0.67
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.30	0.66
1:D:395:LEU:CD1	1:D:395:LEU:H	2.07	0.66
1:I:431:LEU:HD12	1:I:431:LEU:O	1.94	0.66
1:F:389:GLN:C	1:F:390:LEU:HD12	2.16	0.66
1:B:241:LEU:HD12	1:B:270:LEU:HD23	1.78	0.66
1:A:341:HIS:HE1	1:A:353:GLU:OE2	1.78	0.66
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.31	0.66
1:D:155:ARG:CZ	1:D:409:ARG:HH22	2.09	0.66
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.30	0.66
1:H:63:GLU:HG2	1:H:65:GLU:HG2	1.78	0.66
1:I:410:GLN:HE22	1:I:430:GLU:HG2	1.59	0.65
1:G:348:ASP:OD2	1:G:351:HIS:HD2	1.77	0.65
1:C:193:ASN:N	1:C:193:ASN:HD22	1.88	0.65
1:D:155:ARG:NE	1:D:409:ARG:HH22	1.94	0.65
1:B:367:SER:HB2	1:B:389:GLN:HB3	1.79	0.65
1:B:149:MET:HE2	1:B:251:HIS:HE1	1.61	0.65
1:B:65:GLU:OE1	1:B:65:GLU:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:H	1:C:395:LEU:HD23	1.60	0.65
1:H:348:ASP:OD2	1:H:351:HIS:CD2	2.47	0.64
1:A:411:ALA:HA	1:A:421:LEU:HD11	1.79	0.64
1:C:371:HIS:CE1	1:C:373:GLY:CA	2.78	0.64
1:D:329:ILE:HD11	5:D:669:HOH:O	1.97	0.64
1:J:163:LYS:HA	1:J:164:PRO:C	2.17	0.64
1:D:360:LYS:HE2	5:D:612:HOH:O	1.96	0.64
1:C:427:THR:O	1:C:427:THR:HG22	1.97	0.64
1:E:25:ILE:HD12	1:E:96:PHE:CE2	2.33	0.64
1:H:427:THR:HG22	1:H:427:THR:O	1.96	0.64
1:D:163:LYS:H	1:D:395:LEU:CD2	2.10	0.64
1:I:410:GLN:NE2	1:I:430:GLU:HG3	2.13	0.64
1:B:149:MET:CE	1:B:251:HIS:CE1	2.81	0.64
1:J:163:LYS:HD2	5:J:553:HOH:O	1.96	0.64
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.32	0.64
1:C:376:GLN:N	1:C:377:PRO:CD	2.60	0.64
1:H:56:THR:OG1	1:H:57:THR:N	2.31	0.64
1:B:203:GLU:O	1:B:207:GLU:HG2	1.98	0.64
1:H:161:VAL:H	1:H:389:GLN:HE21	1.46	0.64
1:E:162:PRO:O	1:E:163:LYS:HD3	1.98	0.64
1:G:165:LYS:NZ	1:G:191:ASP:OD2	2.26	0.64
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.33	0.64
1:H:371:HIS:ND1	1:H:373:GLY:N	2.46	0.63
1:E:442:THR:N	5:E:693:HOH:O	2.31	0.63
1:F:128:PHE:H	1:F:354:GLN:HE22	1.45	0.63
1:H:371:HIS:CE1	1:H:373:GLY:CA	2.81	0.63
1:I:376:GLN:N	1:I:377:PRO:CD	2.61	0.63
1:E:410:GLN:HE22	1:E:431:LEU:H	1.46	0.63
1:H:159:GLY:HA3	1:H:187:TYR:CZ	2.33	0.63
1:A:128:PHE:H	1:A:354:GLN:HE22	1.44	0.63
1:G:427:THR:CB	5:G:614:HOH:O	2.45	0.63
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.34	0.63
1:H:158:TYR:CD1	1:H:408:VAL:HG11	2.33	0.63
1:A:54:THR:CB	5:A:568:HOH:O	2.46	0.63
1:D:414:ALA:HB1	1:D:419:ILE:O	1.98	0.63
1:J:385:ASP:HB2	5:J:619:HOH:O	1.99	0.63
1:H:213:ILE:O	1:H:217:GLU:HG3	1.99	0.63
1:D:412:ILE:HG22	5:D:594:HOH:O	1.99	0.62
1:J:391:GLY:O	1:J:395:LEU:CD1	2.38	0.62
1:C:371:HIS:ND1	1:C:373:GLY:N	2.44	0.62
1:I:63:GLU:HG2	1:I:65:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HE3	1:A:250:LYS:HE3	1.81	0.62
1:F:348:ASP:OD2	1:F:351:HIS:HD2	1.82	0.62
1:B:149:MET:CE	1:B:251:HIS:HE1	2.12	0.62
1:I:119:LYS:HE2	5:I:562:HOH:O	2.00	0.62
1:C:163:LYS:H	1:C:395:LEU:HD22	1.65	0.62
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.35	0.62
1:A:421:LEU:HD23	5:A:641:HOH:O	2.00	0.62
1:I:438:TRP:HE3	5:I:597:HOH:O	1.82	0.62
1:D:395:LEU:HD13	1:D:395:LEU:H	1.62	0.62
1:A:348:ASP:OD2	1:A:351:HIS:HD2	1.83	0.62
1:D:160:VAL:HG11	1:D:395:LEU:HD11	1.82	0.62
1:F:121:LEU:H	1:F:294:HIS:CD2	2.17	0.62
1:J:389:GLN:C	1:J:390:LEU:HD12	2.20	0.61
1:I:165:LYS:HG2	1:I:191:ASP:OD2	2.00	0.61
1:A:22:LYS:HE3	5:A:558:HOH:O	1.98	0.61
1:I:207:GLU:HG3	5:I:574:HOH:O	2.01	0.61
1:G:73:LYS:HG3	5:G:683:HOH:O	1.99	0.61
1:I:65:GLU:HG3	5:I:711:HOH:O	2.00	0.61
1:A:397:HIS:ND1	1:A:398:PRO:HD2	2.16	0.61
1:J:371:HIS:CE1	1:J:439:GLY:O	2.53	0.60
1:G:397:HIS:CE1	1:G:398:PRO:HD2	2.36	0.60
1:F:93:PHE:CE2	5:F:665:HOH:O	2.50	0.60
1:H:407:ALA:O	1:H:410:GLN:HB2	2.01	0.60
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.36	0.60
1:B:320:ALA:O	1:B:442:THR:HG23	2.01	0.60
1:F:125:ASP:OD1	1:F:126:LEU:N	2.33	0.60
1:F:404:GLY:O	1:F:408:VAL:HG23	2.02	0.60
1:A:54:THR:HA	5:A:568:HOH:O	2.00	0.60
1:B:46:VAL:HG22	1:B:115:MET:HE1	1.83	0.60
1:D:155:ARG:HB2	1:D:156:PRO:HD2	1.84	0.60
1:B:391:GLY:O	1:B:394:THR:N	2.22	0.60
1:F:163:LYS:H	1:F:395:LEU:CD2	2.12	0.60
1:B:149:MET:HE1	1:B:251:HIS:CE1	2.37	0.59
3:B:446:CAP:H4	3:B:446:CAP:O6	2.02	0.59
1:C:235:LEU:CG	5:C:666:HOH:O	2.50	0.59
1:D:155:ARG:NE	1:D:409:ARG:NH2	2.49	0.59
1:A:376:GLN:N	1:A:377:PRO:CD	2.64	0.59
1:H:158:TYR:CE1	1:H:408:VAL:HG11	2.38	0.59
1:F:399:ASP:HB2	1:F:403:ALA:CB	2.32	0.59
1:B:423:GLU:CG	1:B:424:TYR:N	2.64	0.59
1:A:423:GLU:OE2	1:A:426:LYS:NZ	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:GLN:NE2	1:C:431:LEU:H	2.01	0.59
1:C:371:HIS:O	1:C:375:ILE:HG23	2.02	0.59
1:H:39:ILE:HD13	1:H:85:TRP:CG	2.37	0.59
1:F:349:VAL:HG22	5:F:537:HOH:O	2.03	0.59
1:D:371:HIS:HA	1:D:390:LEU:HD23	1.85	0.58
1:H:149:MET:CE	1:H:250:LYS:HB3	2.33	0.58
1:E:326:GLU:HG2	1:E:327:ARG:N	2.18	0.58
1:A:119:LYS:HG3	5:A:691:HOH:O	2.02	0.58
1:B:411:ALA:O	1:B:415:ILE:HG13	2.04	0.58
1:B:372:PRO:O	1:B:421:LEU:HD21	2.02	0.58
1:B:341:HIS:ND1	5:B:604:HOH:O	2.32	0.58
1:D:147:ARG:NH1	1:D:155:ARG:O	2.27	0.58
1:C:348:ASP:OD2	1:C:351:HIS:CD2	2.55	0.58
1:G:163:LYS:HA	1:G:164:PRO:C	2.23	0.58
1:D:418:GLY:C	1:D:419:ILE:HD12	2.23	0.57
1:E:98:GLU:HG3	1:E:135:GLU:OE2	2.03	0.57
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.39	0.57
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.39	0.57
1:G:279:HIS:HE1	1:G:314:HIS:NE2	2.01	0.57
1:I:335:ARG:CD	1:I:339:GLU:OE2	2.46	0.57
1:G:59:TYR:O	1:G:61:TRP:HD1	1.87	0.57
1:G:397:HIS:ND1	1:G:398:PRO:CD	2.66	0.57
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.39	0.57
1:F:158:TYR:CE1	1:F:408:VAL:HG11	2.39	0.57
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.39	0.57
1:D:371:HIS:HB2	1:D:372:PRO:CD	2.35	0.57
1:F:25:ILE:HD11	1:F:132:LEU:CD2	2.34	0.57
1:F:376:GLN:HB3	1:F:377:PRO:HD3	1.86	0.57
1:J:391:GLY:C	1:J:395:LEU:HD12	2.25	0.57
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.69	0.57
1:B:183:ASN:OD1	1:B:406:ARG:NH1	2.37	0.57
1:E:374:ASN:O	1:E:377:PRO:HG2	2.05	0.56
1:J:163:LYS:CD	5:J:553:HOH:O	2.52	0.56
1:D:158:TYR:CE1	1:D:408:VAL:HG11	2.40	0.56
1:B:373:GLY:C	5:B:608:HOH:O	2.43	0.56
1:F:25:ILE:HD11	1:F:132:LEU:HD21	1.86	0.56
1:F:223:LYS:O	1:F:224:LYS:HD3	2.05	0.56
1:C:193:ASN:ND2	1:C:193:ASN:H	2.00	0.56
1:D:394:THR:HB	1:D:395:LEU:CD1	2.35	0.56
1:A:54:THR:N	5:A:547:HOH:O	2.38	0.56
1:B:108:ILE:C	1:B:108:ILE:HD12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ILE:HD12	1:A:419:ILE:H	1.69	0.56
1:J:9:TYR:HD2	1:J:117:ARG:NH1	2.03	0.56
1:B:397:HIS:ND1	1:B:398:PRO:CD	2.69	0.56
1:G:417:GLN:HA	5:G:564:HOH:O	2.04	0.56
1:J:326:GLU:N	5:J:664:HOH:O	2.37	0.56
1:F:376:GLN:N	1:F:377:PRO:CD	2.69	0.56
1:H:230:ILE:O	1:H:237:MET:HG2	2.06	0.56
1:H:238:GLU:OE2	1:H:266:TYR:OH	2.21	0.56
1:B:10:ASP:CB	5:B:654:HOH:O	2.53	0.56
1:D:438:TRP:HE3	5:D:587:HOH:O	1.88	0.56
1:J:326:GLU:HB3	1:J:329:ILE:HD13	1.88	0.56
1:B:59:TYR:O	1:B:61:TRP:HD1	1.88	0.56
1:B:419:ILE:HG22	1:B:423:GLU:HG3	1.88	0.56
1:H:188:MET:HB3	5:H:597:HOH:O	2.06	0.56
1:J:375:ILE:O	1:J:379:ILE:HG13	2.05	0.56
1:B:104:LEU:HD21	1:B:108:ILE:CG1	2.35	0.56
1:J:174:GLU:HG3	1:J:212:ILE:CD1	2.20	0.56
1:H:163:LYS:H	1:H:395:LEU:HD22	1.67	0.56
1:H:235:LEU:HD23	1:H:239:GLN:NE2	2.21	0.55
1:D:163:LYS:HA	1:D:164:PRO:C	2.26	0.55
1:I:438:TRP:O	1:I:441:VAL:HG12	2.06	0.55
1:E:376:GLN:CG	1:E:415:ILE:HG12	2.37	0.55
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.36	0.55
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.89	0.55
1:G:417:GLN:O	1:G:419:ILE:HD12	2.06	0.55
1:E:427:THR:HB	1:E:428:HIS:CE1	2.41	0.55
3:J:446:CAP:C	3:J:446:CAP:O4	2.55	0.55
1:C:213:ILE:O	1:C:217:GLU:HG3	2.07	0.55
1:G:343:LYS:HE3	5:G:588:HOH:O	2.06	0.55
1:G:93:PHE:C	1:G:93:PHE:CD1	2.80	0.55
1:B:402:ALA:CB	5:B:550:HOH:O	2.54	0.55
1:E:323:LEU:O	1:E:324:GLU:C	2.45	0.55
1:C:56:THR:OG1	1:C:57:THR:N	2.40	0.55
1:E:376:GLN:HG2	1:E:415:ILE:HG12	1.88	0.55
1:F:150:LEU:O	1:F:152:ILE:HG13	2.07	0.55
1:B:419:ILE:HG23	1:B:423:GLU:HG2	1.88	0.54
1:G:376:GLN:N	1:G:377:PRO:HD2	2.23	0.54
1:B:371:HIS:ND1	1:B:373:GLY:CA	2.70	0.54
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.36	0.54
1:A:283:ALA:O	1:A:284:MET:CB	2.55	0.54
1:F:428:HIS:NE2	5:F:553:HOH:O	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG22	1:D:115:MET:HE1	1.90	0.54
1:J:376:GLN:N	1:J:377:PRO:HD2	2.23	0.54
1:B:372:PRO:O	1:B:421:LEU:CD2	2.56	0.54
1:A:149:MET:CE	1:A:251:HIS:CE1	2.90	0.54
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.38	0.54
1:C:21:LYS:HE2	5:C:682:HOH:O	2.07	0.54
1:A:200:ASN:OD1	1:A:205:ARG:HD3	2.07	0.54
1:A:104:LEU:HD13	1:A:104:LEU:C	2.28	0.54
1:B:398:PRO:CG	1:B:433:ARG:O	2.51	0.54
1:A:341:HIS:CE1	1:A:353:GLU:OE2	2.61	0.54
1:J:424:TYR:CZ	1:J:428:HIS:CE1	2.96	0.54
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.06	0.54
1:B:241:LEU:CD1	1:B:270:LEU:HD23	2.38	0.54
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.38	0.54
1:D:419:ILE:CD1	1:D:419:ILE:H	2.17	0.54
1:A:389:GLN:O	1:A:390:LEU:HD12	2.08	0.54
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.90	0.54
1:B:163:LYS:HA	1:B:164:PRO:C	2.29	0.54
1:B:25:ILE:HD12	1:B:96:PHE:CE2	2.43	0.54
1:G:108:ILE:HD12	1:G:108:ILE:C	2.27	0.54
1:G:389:GLN:C	1:G:390:LEU:HD12	2.29	0.54
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.43	0.54
1:E:25:ILE:HD12	1:E:96:PHE:HE2	1.73	0.54
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.42	0.54
1:C:59:TYR:O	1:C:61:TRP:HD1	1.91	0.54
1:H:178:TYR:CE1	1:H:215:LYS:HD3	2.42	0.54
1:G:46:VAL:HG22	1:G:115:MET:HE1	1.90	0.54
1:E:376:GLN:N	1:E:377:PRO:CD	2.72	0.53
1:I:320:ALA:O	1:I:442:THR:HG23	2.09	0.53
1:H:39:ILE:CD1	1:H:85:TRP:HB2	2.38	0.53
1:E:427:THR:HB	1:E:428:HIS:ND1	2.23	0.53
1:C:230:ILE:O	1:C:237:MET:HG2	2.08	0.53
1:H:263:ALA:O	1:H:267:ILE:HG12	2.08	0.53
1:A:191:ASP:HB2	5:A:567:HOH:O	2.08	0.53
1:F:331:ILE:O	1:F:335:ARG:HG3	2.08	0.53
1:E:410:GLN:HE21	1:E:431:LEU:CB	2.21	0.53
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.44	0.53
1:A:121:LEU:N	1:A:294:HIS:HD2	2.05	0.53
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.39	0.53
1:B:391:GLY:O	1:B:392:GLY:C	2.44	0.53
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:202:PHE:CD2	1:I:240:ARG:HG2	2.43	0.53
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.43	0.53
1:J:183:ASN:OD1	1:J:406:ARG:NH1	2.41	0.53
1:B:419:ILE:CG2	1:B:423:GLU:HG3	2.38	0.53
1:F:250:LYS:NZ	5:F:651:HOH:O	2.41	0.53
1:G:25:ILE:HD13	1:G:96:PHE:HE2	1.73	0.53
1:G:22:LYS:HG2	5:G:521:HOH:O	2.08	0.53
1:B:421:LEU:HD22	5:B:692:HOH:O	2.08	0.53
1:H:161:VAL:N	1:H:389:GLN:HE21	2.05	0.53
1:C:158:TYR:CE1	1:C:408:VAL:HG11	2.44	0.53
1:H:162:PRO:O	1:H:163:LYS:HD3	2.09	0.52
1:H:159:GLY:HA3	1:H:187:TYR:CD2	2.44	0.52
1:B:283:ALA:O	1:B:284:MET:HB3	2.08	0.52
1:H:122:ARG:HD2	1:H:124:GLU:OE2	2.08	0.52
1:I:47:ALA:O	1:I:51:SER:HB2	2.10	0.52
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.39	0.52
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.40	0.52
1:B:423:GLU:OE1	1:B:424:TYR:HA	2.10	0.52
1:F:348:ASP:OD2	1:F:351:HIS:CD2	2.62	0.52
1:G:279:HIS:CE1	1:G:314:HIS:NE2	2.76	0.52
1:J:376:GLN:N	1:J:377:PRO:CD	2.73	0.52
1:G:236:GLU:HG3	5:G:523:HOH:O	2.09	0.52
1:B:419:ILE:CG2	1:B:423:GLU:CD	2.78	0.52
1:B:163:LYS:H	1:B:395:LEU:HD22	1.73	0.52
1:G:235:LEU:HD12	1:G:238:GLU:OE1	2.10	0.52
1:I:250:LYS:HD3	5:I:667:HOH:O	2.08	0.52
1:I:163:LYS:HA	1:I:164:PRO:C	2.30	0.52
1:B:104:LEU:HD21	1:B:108:ILE:HG12	1.92	0.52
1:A:163:LYS:HA	1:A:164:PRO:C	2.30	0.52
1:C:397:HIS:HA	1:C:438:TRP:CH2	2.45	0.52
1:E:440:HIS:CD2	1:E:440:HIS:N	2.78	0.52
1:A:158:TYR:O	1:A:186:ASP:HB2	2.09	0.52
1:D:72:ALA:O	1:D:73:LYS:HD3	2.09	0.52
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.75	0.52
1:H:371:HIS:O	1:H:375:ILE:HG23	2.09	0.52
1:H:389:GLN:C	1:H:390:LEU:HD12	2.30	0.52
1:E:163:LYS:HA	1:E:164:PRO:C	2.30	0.52
1:B:8:ILE:N	5:B:654:HOH:O	2.43	0.52
1:D:163:LYS:H	1:D:395:LEU:HD23	1.74	0.52
1:B:279:HIS:HE1	1:B:314:HIS:NE2	2.08	0.52
1:B:376:GLN:N	1:B:377:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ASP:OD1	1:G:126:LEU:N	2.42	0.51
1:A:54:THR:CA	5:A:568:HOH:O	2.56	0.51
1:A:283:ALA:O	1:A:284:MET:HB3	2.10	0.51
1:E:72:ALA:O	1:E:73:LYS:HD3	2.10	0.51
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.76	0.51
1:A:161:VAL:HG23	1:A:389:GLN:CD	2.30	0.51
1:I:348:ASP:OD2	1:I:351:HIS:CD2	2.56	0.51
1:H:376:GLN:N	1:H:377:PRO:CD	2.73	0.51
1:I:117:ARG:HH11	1:I:117:ARG:HG3	1.74	0.51
1:F:303:LYS:NZ	1:F:354:GLN:HE21	2.08	0.51
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.93	0.51
1:J:282:ARG:HG3	1:J:285:HIS:CD2	2.46	0.51
1:D:397:HIS:HE1	1:D:399:ASP:OD2	1.94	0.51
1:I:206:ALA:HA	1:I:226:TRP:CZ3	2.46	0.51
1:H:65:GLU:H	1:H:65:GLU:CD	2.11	0.51
1:F:163:LYS:HA	1:F:164:PRO:C	2.30	0.51
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.45	0.51
1:F:283:ALA:O	1:F:284:MET:CB	2.58	0.51
1:B:375:ILE:HG13	1:B:415:ILE:CD1	2.41	0.50
1:C:160:VAL:HG11	1:C:395:LEU:HD11	1.93	0.50
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.76	0.50
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.93	0.50
1:G:397:HIS:CD2	1:G:404:GLY:HA2	2.47	0.50
1:C:235:LEU:HD23	1:C:239:GLN:NE2	2.26	0.50
1:D:419:ILE:HG22	1:D:423:GLU:CB	2.41	0.50
1:G:104:LEU:CD2	1:G:104:LEU:C	2.73	0.50
1:F:80:MET:HB2	1:F:84:SER:O	2.11	0.50
1:G:395:LEU:C	1:G:395:LEU:HD12	2.32	0.50
1:I:431:LEU:HD12	1:I:431:LEU:C	2.31	0.50
1:F:330:THR:HG22	1:F:382:LEU:HD21	1.92	0.50
1:B:104:LEU:HD23	1:B:108:ILE:HG13	1.93	0.50
1:A:303:LYS:NZ	1:A:354:GLN:HE21	2.10	0.50
1:I:46:VAL:HG22	1:I:115:MET:HE1	1.94	0.50
1:D:162:PRO:HA	1:D:395:LEU:HD21	1.93	0.50
1:G:371:HIS:CE1	1:G:373:GLY:CA	2.94	0.50
1:C:317:THR:O	1:C:318:ALA:CB	2.59	0.50
1:I:65:GLU:CG	5:I:711:HOH:O	2.59	0.50
1:C:158:TYR:CD1	1:C:408:VAL:HG11	2.47	0.50
1:B:93:PHE:C	1:B:93:PHE:CD1	2.84	0.50
1:G:402:ALA:CB	5:G:599:HOH:O	2.59	0.50
1:F:337:LEU:HD22	1:F:362:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:HIS:HE1	1:G:373:GLY:HA3	1.71	0.50
1:A:431:LEU:HD12	1:A:435:LEU:HD13	1.94	0.50
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.10	0.50
1:F:283:ALA:O	1:F:284:MET:HB3	2.12	0.50
1:I:72:ALA:O	1:I:73:LYS:HD3	2.11	0.50
1:J:65:GLU:H	1:J:65:GLU:CD	2.14	0.50
3:E:446:CAP:C	3:E:446:CAP:O4	2.59	0.50
1:H:371:HIS:ND1	1:H:373:GLY:CA	2.75	0.49
1:G:417:GLN:HB3	1:G:419:ILE:HD13	1.93	0.49
1:C:159:GLY:CA	1:C:187:TYR:CE2	2.94	0.49
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.47	0.49
1:A:52:THR:HB	1:A:67:TRP:NE1	2.27	0.49
1:A:125:ASP:OD1	1:A:126:LEU:N	2.44	0.49
1:H:149:MET:CE	1:H:250:LYS:CB	2.91	0.49
1:F:411:ALA:O	1:F:415:ILE:HG13	2.12	0.49
1:F:419:ILE:N	1:F:419:ILE:HD13	2.27	0.49
1:A:70:LEU:HD22	1:A:95:ALA:HA	1.93	0.49
1:B:419:ILE:HG23	1:B:423:GLU:CD	2.33	0.49
1:D:152:ILE:HD13	1:D:155:ARG:NH2	2.27	0.49
1:B:25:ILE:HD12	1:B:96:PHE:HE2	1.77	0.49
1:B:283:ALA:O	1:B:284:MET:CB	2.60	0.49
1:B:104:LEU:CD2	1:B:108:ILE:HG13	2.42	0.49
1:J:161:VAL:HG12	1:J:163:LYS:HE2	1.95	0.49
1:B:25:ILE:CD1	1:B:96:PHE:CE2	2.95	0.49
1:B:20:SER:OG	1:B:23:ARG:HG3	2.12	0.49
1:I:335:ARG:NH2	5:I:549:HOH:O	2.40	0.49
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.47	0.49
1:J:329:ILE:N	1:J:329:ILE:HD12	2.28	0.49
1:E:410:GLN:NE2	1:E:431:LEU:H	2.09	0.49
1:E:9:TYR:CD2	1:E:117:ARG:NH1	2.74	0.49
1:H:442:THR:O	1:H:444:VAL:HG23	2.11	0.49
1:F:141:PHE:HB2	1:F:311:ASP:OD1	2.12	0.49
1:E:439:GLY:C	1:E:440:HIS:CD2	2.86	0.49
1:I:65:GLU:H	1:I:65:GLU:CD	2.16	0.49
1:F:289:THR:HG22	1:F:296:ILE:O	2.12	0.49
1:J:93:PHE:CD1	1:J:93:PHE:C	2.86	0.49
1:D:397:HIS:ND1	1:D:398:PRO:CD	2.74	0.48
1:B:160:VAL:HG21	1:B:394:THR:HG21	1.95	0.48
1:B:289:THR:HG22	1:B:296:ILE:O	2.13	0.48
1:B:389:GLN:C	1:B:390:LEU:HD12	2.33	0.48
1:J:440:HIS:ND1	5:J:694:HOH:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:ILE:O	1:G:420:PRO:C	2.51	0.48
1:D:65:GLU:HG3	5:D:648:HOH:O	2.13	0.48
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.49	0.48
1:J:93:PHE:CE1	1:J:131:LYS:HE3	2.48	0.48
1:J:101:LEU:HB3	1:J:102:PRO:HD3	1.96	0.48
1:C:432:ALA:C	1:C:434:ALA:H	2.15	0.48
1:B:165:LYS:NZ	1:B:191:ASP:OD2	2.33	0.48
1:D:65:GLU:H	1:D:65:GLU:CD	2.16	0.48
1:C:414:ALA:HB2	1:C:424:TYR:CD2	2.48	0.48
1:I:424:TYR:CE2	1:I:428:HIS:CE1	3.01	0.48
1:C:424:TYR:HA	5:C:577:HOH:O	2.14	0.48
1:A:397:HIS:ND1	1:A:398:PRO:CD	2.77	0.48
1:G:367:SER:HB2	1:G:389:GLN:HB3	1.95	0.48
1:C:441:VAL:CG1	1:C:442:THR:N	2.76	0.48
1:D:348:ASP:OD2	1:D:351:HIS:CD2	2.63	0.48
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.49	0.48
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.94	0.48
1:C:389:GLN:C	1:C:390:LEU:HD12	2.33	0.48
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.95	0.48
1:A:411:ALA:HA	1:A:421:LEU:CD1	2.43	0.48
1:B:161:VAL:HG12	1:B:163:LYS:HE2	1.95	0.48
1:A:207:GLU:O	5:A:675:HOH:O	2.20	0.48
1:F:108:ILE:HD12	1:F:108:ILE:C	2.34	0.48
1:G:397:HIS:CD2	1:G:434:ALA:HB2	2.49	0.48
1:D:397:HIS:CG	1:D:398:PRO:HD2	2.49	0.48
1:G:390:LEU:O	1:G:394:THR:HB	2.14	0.48
1:B:279:HIS:CE1	1:B:314:HIS:NE2	2.82	0.48
1:H:21:LYS:HG3	5:H:578:HOH:O	2.12	0.48
1:G:159:GLY:HA3	1:G:187:TYR:CD1	2.49	0.47
1:H:265:ARG:CD	5:H:564:HOH:O	2.62	0.47
1:I:118:VAL:O	1:I:118:VAL:HG23	2.14	0.47
1:E:303:LYS:NZ	1:E:354:GLN:HE21	2.12	0.47
1:B:174:GLU:HG3	1:B:212:ILE:CD1	2.43	0.47
1:H:131:LYS:HG2	1:I:198:TRP:CD2	2.49	0.47
1:I:211:LYS:HG3	1:I:212:ILE:N	2.29	0.47
1:C:222:GLU:OE2	1:C:409:ARG:NH1	2.47	0.47
1:J:25:ILE:HD12	1:J:96:PHE:CE2	2.49	0.47
1:H:149:MET:HE1	1:H:250:LYS:HB3	1.97	0.47
1:B:108:ILE:HD12	1:B:109:ALA:N	2.30	0.47
1:H:389:GLN:O	1:H:390:LEU:HD12	2.14	0.47
1:B:46:VAL:CG2	1:B:115:MET:HE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ALA:O	1:D:51:SER:CB	2.62	0.47
1:I:101:LEU:N	1:I:102:PRO:CD	2.76	0.47
1:B:174:GLU:CG	1:B:212:ILE:HD11	2.41	0.47
1:I:390:LEU:HD12	1:I:390:LEU:N	2.29	0.47
1:B:410:GLN:HG2	5:B:628:HOH:O	2.09	0.47
1:B:410:GLN:NE2	5:B:628:HOH:O	2.47	0.47
1:G:351:HIS:HE1	5:G:526:HOH:O	1.97	0.47
1:B:376:GLN:HG3	1:B:377:PRO:N	2.30	0.47
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.44	0.47
1:J:395:LEU:H	1:J:395:LEU:HD12	1.80	0.47
1:G:371:HIS:ND1	1:G:373:GLY:N	2.59	0.47
1:A:93:PHE:CD1	1:A:93:PHE:C	2.88	0.47
1:B:371:HIS:HE1	1:B:373:GLY:CA	2.09	0.47
1:J:410:GLN:NE2	1:J:431:LEU:N	2.51	0.47
1:E:439:GLY:C	5:E:691:HOH:O	2.53	0.47
1:D:399:ASP:OD2	1:D:433:ARG:HG3	2.14	0.47
1:D:47:ALA:O	1:D:51:SER:HB2	2.13	0.47
1:E:285:HIS:CG	1:E:286:ALA:N	2.83	0.47
1:J:323:LEU:O	1:J:324:GLU:C	2.52	0.47
1:C:282:ARG:HD2	1:C:285:HIS:CD2	2.49	0.47
1:D:376:GLN:N	1:D:377:PRO:CD	2.77	0.47
1:J:371:HIS:O	1:J:375:ILE:HG23	2.15	0.47
1:I:47:ALA:O	1:I:51:SER:CB	2.63	0.47
1:D:215:LYS:O	1:D:219:GLU:HG3	2.15	0.47
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.97	0.47
1:H:104:LEU:C	1:H:104:LEU:HD23	2.35	0.47
1:D:282:ARG:O	1:D:283:ALA:C	2.53	0.47
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.50	0.47
1:B:410:GLN:O	1:B:413:ASP:HB2	2.15	0.47
1:G:93:PHE:HB2	1:G:132:LEU:HD11	1.97	0.47
1:I:117:ARG:HG3	1:I:117:ARG:NH1	2.30	0.47
1:G:331:ILE:O	1:G:335:ARG:HG3	2.15	0.47
1:H:282:ARG:O	1:H:283:ALA:C	2.53	0.47
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.97	0.46
1:E:150:LEU:O	1:E:152:ILE:HG13	2.15	0.46
1:C:371:HIS:ND1	1:C:373:GLY:CA	2.77	0.46
1:D:420:PRO:O	1:D:423:GLU:CB	2.63	0.46
1:E:431:LEU:O	1:E:435:LEU:CD1	2.54	0.46
1:A:149:MET:HE2	1:A:251:HIS:CE1	2.50	0.46
1:H:413:ASP:O	1:H:417:GLN:HG3	2.16	0.46
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:TYR:O	1:H:61:TRP:HD1	1.98	0.46
1:J:16:GLY:HA3	5:J:645:HOH:O	2.14	0.46
1:E:431:LEU:HD11	1:E:435:LEU:HD11	1.98	0.46
1:D:412:ILE:C	5:D:594:HOH:O	2.53	0.46
1:A:149:MET:HE1	1:A:251:HIS:ND1	2.29	0.46
1:E:370:LEU:HB2	1:E:390:LEU:HG	1.97	0.46
1:C:369:GLY:N	3:C:446:CAP:O3P	2.41	0.46
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.50	0.46
1:I:93:PHE:C	1:I:93:PHE:CD1	2.89	0.46
1:H:303:LYS:HZ3	1:H:354:GLN:HE21	1.63	0.46
1:D:396:GLY:O	1:D:437:LYS:NZ	2.38	0.46
1:J:433:ARG:O	1:J:436:GLU:HG2	2.15	0.46
1:A:203:GLU:CB	5:A:633:HOH:O	2.62	0.46
1:C:358:SER:HB3	1:D:171:GLU:OE2	2.16	0.46
1:G:417:GLN:HB3	1:G:419:ILE:CD1	2.46	0.46
1:A:96:PHE:HE1	1:A:107:SER:OG	1.97	0.46
1:J:355:LYS:HE3	5:J:558:HOH:O	2.15	0.46
1:C:235:LEU:HG	5:C:666:HOH:O	2.12	0.46
1:A:158:TYR:CE1	1:A:408:VAL:HG11	2.50	0.46
1:J:320:ALA:O	1:J:442:THR:CB	2.64	0.46
1:A:348:ASP:OD2	1:A:351:HIS:CD2	2.67	0.46
1:D:314:HIS:HA	1:D:365:THR:O	2.15	0.46
1:J:440:HIS:N	1:J:440:HIS:ND1	2.64	0.46
1:D:282:ARG:HG2	5:D:532:HOH:O	2.15	0.46
1:H:414:ALA:HB2	1:H:424:TYR:CD2	2.51	0.46
1:E:314:HIS:HA	1:E:365:THR:O	2.15	0.46
1:J:157:ILE:HD13	1:J:363:PHE:CZ	2.51	0.46
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.46	0.45
1:D:420:PRO:O	1:D:423:GLU:N	2.48	0.45
1:G:326:GLU:HB3	5:G:674:HOH:O	2.16	0.45
1:I:155:ARG:NH2	1:I:409:ARG:NH1	2.63	0.45
1:I:410:GLN:NE2	1:I:430:GLU:HG2	2.27	0.45
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.14	0.45
1:I:159:GLY:HA3	1:I:187:TYR:CD2	2.50	0.45
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.51	0.45
1:B:371:HIS:O	1:B:375:ILE:HG23	2.16	0.45
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.96	0.45
1:G:419:ILE:CG2	1:G:423:GLU:HG2	2.46	0.45
1:H:161:VAL:N	1:H:389:GLN:NE2	2.57	0.45
1:C:419:ILE:O	1:C:420:PRO:C	2.54	0.45
1:F:206:ALA:HA	1:F:226:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:446:CAP:H11	3:F:446:CAP:O4	2.16	0.45
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.81	0.45
1:F:112:ILE:O	1:F:115:MET:HE2	2.16	0.45
1:C:162:PRO:HA	1:C:395:LEU:CD2	2.43	0.45
1:C:193:ASN:N	1:C:193:ASN:ND2	2.59	0.45
1:B:425:ALA:CB	1:B:431:LEU:HG	2.38	0.45
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.97	0.45
1:D:208:ILE:O	1:D:212:ILE:HG12	2.16	0.45
1:A:362:ALA:O	1:A:364:PRO:HD3	2.15	0.45
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.51	0.45
1:C:427:THR:O	1:C:428:HIS:CG	2.70	0.45
1:A:130:GLU:HG3	1:A:357:TYR:CE2	2.51	0.45
1:A:115:MET:HE2	1:A:115:MET:HB2	1.72	0.45
1:B:428:HIS:CE1	5:B:596:HOH:O	2.70	0.45
1:F:250:LYS:HA	1:F:276:LEU:HD23	1.99	0.45
1:E:202:PHE:CD2	1:E:240:ARG:HG2	2.52	0.45
1:E:80:MET:HB2	1:E:84:SER:O	2.17	0.45
1:J:326:GLU:OE1	1:J:329:ILE:CD1	2.64	0.45
1:G:46:VAL:HG22	1:G:115:MET:CE	2.46	0.45
1:F:205:ARG:HH11	1:F:205:ARG:HG3	1.81	0.45
1:G:423:GLU:HG2	1:G:424:TYR:N	2.32	0.45
1:C:159:GLY:CA	1:C:187:TYR:CZ	2.98	0.45
1:E:131:LYS:NZ	5:E:642:HOH:O	2.37	0.45
1:A:149:MET:HE1	1:A:251:HIS:CE1	2.52	0.45
1:H:131:LYS:HD3	5:H:522:HOH:O	2.15	0.45
1:G:101:LEU:N	1:G:102:PRO:CD	2.80	0.45
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.99	0.45
1:I:322:LYS:HG3	1:I:323:LEU:HD13	1.99	0.45
1:J:391:GLY:C	1:J:395:LEU:CD1	2.84	0.44
1:H:149:MET:HE1	1:H:250:LYS:CB	2.46	0.44
1:J:370:LEU:N	1:J:370:LEU:CD1	2.79	0.44
1:C:283:ALA:O	1:C:284:MET:HB3	2.17	0.44
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.99	0.44
1:B:104:LEU:CD2	1:B:108:ILE:CG1	2.94	0.44
1:E:159:GLY:HA3	1:E:187:TYR:CD2	2.52	0.44
1:C:410:GLN:NE2	1:C:428:HIS:HB3	2.32	0.44
1:I:155:ARG:HH21	1:I:409:ARG:NH1	2.15	0.44
1:C:283:ALA:O	1:C:284:MET:CB	2.65	0.44
1:F:191:ASP:HB2	5:F:536:HOH:O	2.17	0.44
1:H:370:LEU:O	1:H:393:GLY:HA3	2.17	0.44
1:B:118:VAL:O	1:B:118:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:446:CAP:H11	3:A:446:CAP:O4	2.17	0.44
3:C:446:CAP:O6	3:C:446:CAP:C4	2.40	0.44
1:B:410:GLN:HG3	5:B:628:HOH:O	2.12	0.44
1:H:39:ILE:HD13	1:H:85:TRP:HB2	2.00	0.44
1:H:39:ILE:HG23	1:H:40:GLU:N	2.32	0.44
1:C:410:GLN:HE21	1:C:431:LEU:H	1.63	0.44
1:G:158:TYR:CE1	1:G:408:VAL:HG11	2.52	0.44
1:G:202:PHE:CD2	1:G:240:ARG:HG2	2.52	0.44
1:A:136:PHE:HB3	1:A:307:LEU:O	2.17	0.44
1:B:397:HIS:CE1	1:B:398:PRO:HG2	2.53	0.44
1:A:419:ILE:N	1:A:419:ILE:HD12	2.32	0.44
1:G:215:LYS:HE2	1:G:219:GLU:OE2	2.16	0.44
1:J:98:GLU:HG3	1:J:135:GLU:OE2	2.17	0.44
1:C:108:ILE:O	1:C:108:ILE:HG22	2.16	0.44
1:H:268:ARG:C	1:H:268:ARG:HD3	2.38	0.44
1:B:431:LEU:O	1:B:431:LEU:HD12	2.17	0.44
1:G:159:GLY:CA	1:G:187:TYR:CZ	2.96	0.44
1:D:394:THR:HB	1:D:395:LEU:HD13	1.99	0.44
1:A:351:HIS:HE1	5:A:526:HOH:O	2.00	0.44
1:I:101:LEU:HG	1:I:105:LEU:HD22	1.99	0.44
1:I:52:THR:HB	1:I:67:TRP:NE1	2.33	0.44
1:J:125:ASP:OD1	1:J:126:LEU:N	2.50	0.44
1:H:101:LEU:HB3	1:H:102:PRO:HD3	1.99	0.44
1:H:362:ALA:O	1:H:364:PRO:HD3	2.18	0.44
1:C:351:HIS:HE1	5:C:570:HOH:O	2.01	0.44
1:J:63:GLU:HG2	1:J:65:GLU:HG2	1.98	0.44
1:E:183:ASN:OD1	1:E:406:ARG:HD3	2.18	0.44
1:I:70:LEU:HD22	1:I:95:ALA:HA	1.99	0.44
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.44
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.66	0.44
1:J:399:ASP:OD1	1:J:433:ARG:NH2	2.45	0.44
1:F:96:PHE:CE1	1:F:104:LEU:HD12	2.53	0.44
1:H:17:TYR:CE2	1:H:19:PRO:HA	2.53	0.44
1:C:279:HIS:NE2	1:C:314:HIS:NE2	2.59	0.44
1:F:390:LEU:N	1:F:390:LEU:HD12	2.33	0.43
1:C:160:VAL:HG11	1:C:395:LEU:CD1	2.48	0.43
1:F:126:LEU:HA	1:F:126:LEU:HD12	1.82	0.43
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.18	0.43
1:J:70:LEU:HD22	1:J:95:ALA:HA	1.99	0.43
1:I:283:ALA:O	1:I:284:MET:HB3	2.18	0.43
1:B:410:GLN:O	1:B:413:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ALA:HB3	5:B:550:HOH:O	2.16	0.43
1:B:125:ASP:OD1	1:B:126:LEU:N	2.50	0.43
1:D:56:THR:OG1	1:D:57:THR:N	2.50	0.43
1:H:112:ILE:HD12	1:H:121:LEU:HD21	2.00	0.43
1:C:174:GLU:O	1:C:212:ILE:CD1	2.66	0.43
1:F:101:LEU:HB3	1:F:102:PRO:HD3	2.00	0.43
1:J:251:HIS:NE2	1:J:312:GLN:NE2	2.66	0.43
1:I:264:LEU:HA	1:I:264:LEU:HD23	1.89	0.43
1:E:161:VAL:HG22	1:E:189:KCX:HB2	1.99	0.43
1:J:326:GLU:OE1	1:J:329:ILE:HD13	2.19	0.43
1:C:424:TYR:CZ	1:C:428:HIS:CE1	3.07	0.43
5:A:655:HOH:O	1:H:427:THR:HG21	2.18	0.43
1:I:30:ARG:NH2	1:I:82:ASP:OD2	2.51	0.43
1:H:108:ILE:O	1:H:108:ILE:CG2	2.66	0.43
1:C:299:PHE:HB2	5:C:574:HOH:O	2.19	0.43
1:A:417:GLN:O	1:A:419:ILE:HD12	2.19	0.43
1:D:178:TYR:CE1	1:D:215:LYS:HE3	2.53	0.43
1:A:183:ASN:OD1	1:A:406:ARG:NH1	2.50	0.43
1:C:51:SER:OG	1:C:52:THR:N	2.52	0.43
1:H:371:HIS:ND1	1:H:373:GLY:HA3	2.29	0.43
1:G:160:VAL:HG21	1:G:394:THR:HG21	2.00	0.43
1:I:150:LEU:HD23	1:I:157:ILE:HD13	1.99	0.43
1:E:91:TYR:CZ	1:E:108:ILE:HG22	2.54	0.43
1:A:77:PHE:N	1:A:77:PHE:CD2	2.87	0.43
1:A:336:ILE:HA	1:A:336:ILE:HD12	1.80	0.43
1:B:336:ILE:HA	1:B:336:ILE:HD12	1.89	0.43
1:J:157:ILE:CD1	1:J:363:PHE:CZ	3.02	0.43
1:D:425:ALA:O	1:D:432:ALA:HB2	2.18	0.43
1:A:161:VAL:HG23	1:A:389:GLN:OE1	2.19	0.43
1:G:397:HIS:CG	1:G:398:PRO:HD2	2.53	0.43
1:B:251:HIS:NE2	1:B:312:GLN:NE2	2.66	0.43
1:H:410:GLN:HE22	1:H:431:LEU:H	1.66	0.43
1:C:72:ALA:HB2	1:C:91:TYR:CD1	2.54	0.43
1:A:217:GLU:HG2	1:A:222:GLU:O	2.19	0.43
1:E:431:LEU:CD1	1:E:435:LEU:HD11	2.49	0.43
1:G:434:ALA:HB1	1:G:438:TRP:CZ3	2.54	0.43
1:A:376:GLN:HA	1:A:415:ILE:HD13	2.01	0.43
1:B:423:GLU:OE1	1:B:424:TYR:N	2.52	0.43
1:C:376:GLN:HB3	1:C:377:PRO:HD3	2.01	0.43
1:H:431:LEU:O	1:H:434:ALA:HB3	2.19	0.43
1:J:376:GLN:CG	1:J:415:ILE:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:NH1	5:B:679:HOH:O	2.51	0.43
1:E:379:ILE:O	1:E:383:GLY:CA	2.66	0.43
1:I:336:ILE:HD12	1:I:336:ILE:HA	1.87	0.43
1:H:163:LYS:HA	1:H:164:PRO:C	2.39	0.42
1:J:299:PHE:CE1	1:J:336:ILE:HB	2.54	0.42
1:C:189:KCX:HG3	1:C:190:ASP:O	2.19	0.42
1:E:227:PHE:CD1	1:E:227:PHE:N	2.87	0.42
1:J:362:ALA:O	1:J:364:PRO:HD3	2.19	0.42
1:A:80:MET:HB2	1:A:84:SER:O	2.19	0.42
1:D:351:HIS:HE1	5:D:548:HOH:O	2.02	0.42
1:A:149:MET:HE2	1:A:251:HIS:HE1	1.82	0.42
1:F:115:MET:HB2	1:F:115:MET:HE2	1.79	0.42
1:J:333:ASN:OD1	5:J:543:HOH:O	2.21	0.42
1:A:101:LEU:HB3	1:A:102:PRO:HD3	2.00	0.42
1:C:268:ARG:HD3	1:C:268:ARG:C	2.39	0.42
1:B:391:GLY:O	1:B:393:GLY:N	2.52	0.42
1:H:283:ALA:O	1:H:284:MET:HB3	2.18	0.42
1:D:397:HIS:CE1	1:D:398:PRO:HD2	2.55	0.42
1:J:336:ILE:HD12	1:J:336:ILE:HA	1.91	0.42
1:D:375:ILE:O	1:D:379:ILE:HG13	2.19	0.42
1:E:125:ASP:OD1	1:E:126:LEU:N	2.52	0.42
1:B:371:HIS:CE1	1:B:373:GLY:C	2.92	0.42
1:D:419:ILE:CG2	1:D:423:GLU:CB	2.97	0.42
1:J:157:ILE:N	1:J:157:ILE:HD12	2.34	0.42
1:H:25:ILE:HD12	1:H:96:PHE:CE2	2.55	0.42
1:F:282:ARG:HD2	1:F:285:HIS:CD2	2.55	0.42
1:G:283:ALA:O	1:G:284:MET:HB3	2.20	0.42
1:J:285:HIS:CG	1:J:286:ALA:N	2.87	0.42
1:E:389:GLN:C	1:E:390:LEU:HD12	2.40	0.42
1:F:52:THR:HB	1:F:67:TRP:NE1	2.35	0.42
1:H:371:HIS:CE1	1:H:374:ASN:H	2.37	0.42
1:J:439:GLY:C	1:J:440:HIS:ND1	2.73	0.42
1:H:63:GLU:CG	1:H:65:GLU:HG2	2.47	0.42
1:A:284:MET:HG2	1:A:284:MET:O	2.20	0.42
1:D:421:LEU:O	1:D:425:ALA:HB2	2.19	0.42
1:I:285:HIS:CG	1:I:286:ALA:N	2.88	0.42
1:C:370:LEU:O	1:C:393:GLY:HA3	2.19	0.42
1:G:289:THR:HG22	1:G:296:ILE:O	2.20	0.42
1:F:30:ARG:NH2	1:F:82:ASP:OD2	2.51	0.42
1:G:203:GLU:O	1:G:207:GLU:HG2	2.20	0.42
1:G:118:VAL:HG23	1:G:118:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:GLY:CA	5:D:609:HOH:O	2.48	0.42
1:D:410:GLN:O	1:D:413:ASP:N	2.52	0.42
1:G:442:THR:HA	1:G:443:PRO:HD3	1.85	0.42
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.54	0.42
1:E:25:ILE:CD1	1:E:96:PHE:CE2	3.01	0.42
1:B:321:GLY:HA3	5:B:660:HOH:O	2.19	0.42
1:D:63:GLU:CG	1:D:65:GLU:HG2	2.44	0.42
1:H:39:ILE:HD11	1:H:85:TRP:HB2	2.02	0.42
1:I:101:LEU:HB3	1:I:102:PRO:HD3	2.01	0.42
1:J:51:SER:HA	5:J:597:HOH:O	2.19	0.42
1:F:288:PHE:O	1:F:295:GLY:HA3	2.20	0.42
1:G:241:LEU:HD12	1:G:270:LEU:HD23	2.01	0.42
1:J:368:GLY:O	1:J:370:LEU:CD1	2.64	0.42
1:E:51:SER:HA	5:E:519:HOH:O	2.18	0.42
1:H:49:GLU:HG3	1:H:115:MET:SD	2.60	0.42
1:B:108:ILE:C	1:B:108:ILE:CD1	2.88	0.41
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.01	0.41
1:J:159:GLY:CA	1:J:187:TYR:CZ	3.02	0.41
1:G:112:ILE:HG23	5:G:635:HOH:O	2.20	0.41
1:F:336:ILE:HD12	1:F:336:ILE:HA	1.78	0.41
1:J:118:VAL:HG23	1:J:118:VAL:O	2.20	0.41
1:A:131:LYS:HE3	5:A:543:HOH:O	2.19	0.41
1:E:376:GLN:HG3	1:E:415:ILE:HG12	2.03	0.41
1:I:441:VAL:HG22	1:I:442:THR:N	2.36	0.41
1:H:317:THR:O	1:H:318:ALA:CB	2.58	0.41
1:C:192:GLU:HG3	1:C:283:ALA:HB2	2.01	0.41
1:G:283:ALA:O	1:G:284:MET:CB	2.68	0.41
1:E:230:ILE:O	1:E:231:THR:C	2.59	0.41
1:H:7:THR:N	1:H:10:ASP:CB	2.83	0.41
1:J:227:PHE:CD1	1:J:227:PHE:N	2.87	0.41
1:I:176:LEU:HD21	1:I:395:LEU:HD11	2.01	0.41
3:H:446:CAP:C4	3:H:446:CAP:O6	2.46	0.41
1:D:152:ILE:HD11	1:D:186:ASP:OD1	2.19	0.41
1:J:389:GLN:O	1:J:390:LEU:HD12	2.20	0.41
1:F:397:HIS:CD2	1:F:404:GLY:HA2	2.55	0.41
1:H:178:TYR:HE1	1:H:215:LYS:HD3	1.86	0.41
1:D:178:TYR:OH	1:D:219:GLU:OE1	2.32	0.41
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.21	0.41
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.95	0.41
1:F:279:HIS:NE2	1:F:314:HIS:NE2	2.67	0.41
1:B:235:LEU:HA	1:B:235:LEU:HD12	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:GLN:HE21	1:C:431:LEU:N	2.19	0.41
1:H:427:THR:CG2	1:H:427:THR:O	2.67	0.41
1:I:119:LYS:CE	5:I:562:HOH:O	2.65	0.41
1:E:73:LYS:HA	1:E:73:LYS:HD3	1.70	0.41
1:D:230:ILE:O	1:D:237:MET:HG2	2.21	0.41
1:E:421:LEU:N	5:E:551:HOH:O	2.53	0.41
1:H:149:MET:HE3	1:H:250:LYS:CB	2.51	0.41
1:D:147:ARG:HD3	1:D:152:ILE:O	2.20	0.41
1:C:432:ALA:C	1:C:434:ALA:N	2.74	0.41
1:D:52:THR:HB	1:D:67:TRP:NE1	2.36	0.41
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.55	0.41
1:G:29:PHE:CE1	1:G:123:LEU:HD13	2.56	0.41
1:F:406:ARG:O	1:F:410:GLN:HG3	2.21	0.41
1:I:230:ILE:O	1:I:237:MET:HG2	2.21	0.41
3:G:446:CAP:H4	3:G:446:CAP:O6	2.21	0.41
1:D:410:GLN:OE1	1:D:431:LEU:N	2.54	0.41
1:B:159:GLY:HA3	1:B:187:TYR:CD2	2.56	0.41
1:A:397:HIS:CD2	1:A:404:GLY:HA2	2.55	0.41
1:F:93:PHE:CD1	1:F:93:PHE:C	2.94	0.41
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.69	0.41
1:I:283:ALA:O	1:I:284:MET:CB	2.68	0.41
1:A:373:GLY:HA3	1:A:439:GLY:O	2.21	0.41
1:E:222:GLU:CD	5:E:586:HOH:O	2.59	0.41
1:G:213:ILE:O	1:G:217:GLU:HG3	2.21	0.41
1:F:111:ASN:HA	5:F:621:HOH:O	2.21	0.41
1:C:169:SER:HB2	1:C:170:PRO:HD2	2.02	0.41
1:G:397:HIS:HA	1:G:398:PRO:HD3	1.88	0.40
1:E:439:GLY:CA	5:E:691:HOH:O	2.69	0.40
1:A:411:ALA:CA	1:A:421:LEU:HD11	2.49	0.40
1:F:407:ALA:HA	1:F:410:GLN:HB2	2.02	0.40
1:B:226:TRP:CE3	1:B:228:ALA:HB2	2.56	0.40
1:A:153:LYS:HA	5:A:614:HOH:O	2.20	0.40
1:I:148:LYS:HG3	5:I:601:HOH:O	2.20	0.40
1:I:153:LYS:NZ	1:I:154:ASP:OD2	2.55	0.40
1:J:283:ALA:O	1:J:284:MET:HB3	2.21	0.40
1:E:163:LYS:HA	1:E:163:LYS:HD3	1.81	0.40
1:G:108:ILE:CD1	1:G:108:ILE:C	2.89	0.40
1:F:82:ASP:OD1	1:F:82:ASP:C	2.60	0.40
1:F:70:LEU:HD22	1:F:95:ALA:HA	2.04	0.40
1:I:25:ILE:HD11	1:I:132:LEU:HD21	2.03	0.40
1:H:162:PRO:HA	1:H:395:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:TYR:CE2	1:B:428:HIS:CE1	3.10	0.40
1:C:407:ALA:O	1:C:410:GLN:HG2	2.20	0.40
1:B:122:ARG:HG3	1:B:124:GLU:OE2	2.20	0.40
1:G:321:GLY:HA3	5:G:642:HOH:O	2.21	0.40
1:B:303:LYS:NZ	1:B:354:GLN:HE21	2.19	0.40
1:I:367:SER:HB2	1:I:389:GLN:HB3	2.04	0.40
1:I:390:LEU:CD1	1:I:390:LEU:N	2.85	0.40
1:G:371:HIS:HB2	1:G:372:PRO:HD2	2.03	0.40
1:G:348:ASP:OD2	1:G:351:HIS:CD2	2.66	0.40
1:G:108:ILE:HD12	1:G:109:ALA:N	2.35	0.40
1:J:213:ILE:O	1:J:217:GLU:HG3	2.21	0.40
1:H:299:PHE:HB2	5:H:659:HOH:O	2.21	0.40
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.90	0.40
1:D:336:ILE:HA	1:D:336:ILE:HD12	1.86	0.40
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.57	0.40
1:B:397:HIS:CD2	1:B:404:GLY:HA2	2.56	0.40
1:D:372:PRO:HB3	1:D:411:ALA:HB2	2.03	0.40
1:G:59:TYR:O	1:G:61:TRP:CD1	2.72	0.40
1:E:424:TYR:CZ	1:E:428:HIS:CE1	3.09	0.40
1:B:161:VAL:CG1	1:B:163:LYS:HE2	2.52	0.40
1:H:170:PRO:O	1:H:173:PHE:HB3	2.22	0.40
1:D:15:LYS:HG3	5:D:574:HOH:O	2.22	0.40
1:A:139:PRO:N	1:A:309:GLY:HA2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/444 (98%)	417 (96%)	13 (3%)	3 (1%)	26	28
1	B	434/444 (98%)	413 (95%)	19 (4%)	2 (0%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	432/444 (97%)	408 (94%)	23 (5%)	1 (0%)	52 61
1	D	430/444 (97%)	401 (93%)	26 (6%)	3 (1%)	26 28
1	E	425/444 (96%)	410 (96%)	14 (3%)	1 (0%)	52 61
1	F	434/444 (98%)	409 (94%)	23 (5%)	2 (0%)	34 37
1	G	434/444 (98%)	411 (95%)	23 (5%)	0	100 100
1	H	435/444 (98%)	415 (95%)	20 (5%)	0	100 100
1	I	430/444 (97%)	411 (96%)	18 (4%)	1 (0%)	52 61
1	J	427/444 (96%)	407 (95%)	19 (4%)	1 (0%)	52 61
All	All	4314/4440 (97%)	4102 (95%)	198 (5%)	14 (0%)	46 54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	MET
1	E	284	MET
1	F	284	MET
1	F	401	PRO
1	I	284	MET
1	A	60	PRO
1	C	420	PRO
1	D	284	MET
1	D	423	GLU
1	B	284	MET
1	B	392	GLY
1	J	284	MET
1	D	418	GLY
1	A	401	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/356 (94%)	320 (95%)	16 (5%)	31 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	336/356 (94%)	320 (95%)	16 (5%)	31	39
1	C	332/356 (93%)	315 (95%)	17 (5%)	29	36
1	D	332/356 (93%)	318 (96%)	14 (4%)	36	46
1	E	333/356 (94%)	322 (97%)	11 (3%)	45	57
1	F	334/356 (94%)	324 (97%)	10 (3%)	48	61
1	G	335/356 (94%)	321 (96%)	14 (4%)	36	46
1	H	335/356 (94%)	326 (97%)	9 (3%)	52	65
1	I	339/356 (95%)	322 (95%)	17 (5%)	30	37
1	J	329/356 (92%)	317 (96%)	12 (4%)	42	54
All	All	3341/3560 (94%)	3205 (96%)	136 (4%)	37	47

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	105	LEU
1	A	144	GLU
1	A	148	LYS
1	A	181	LEU
1	A	234	LEU
1	A	247	LEU
1	A	268	ARG
1	A	307	LEU
1	A	328	ASP
1	A	363	PHE
1	A	367	SER
1	A	376	GLN
1	A	382	LEU
1	A	395	LEU
1	A	435	LEU
1	B	18	GLU
1	B	93	PHE
1	B	104	LEU
1	B	107	SER
1	B	122	ARG
1	B	235	LEU
1	B	247	LEU
1	B	268	ARG
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	358	SER
1	B	363	PHE
1	B	376	GLN
1	B	382	LEU
1	B	389	GLN
1	B	423	GLU
1	B	431	LEU
1	C	20	SER
1	C	58	LEU
1	C	107	SER
1	C	118	VAL
1	C	122	ARG
1	C	193	ASN
1	C	235	LEU
1	C	268	ARG
1	C	301	LEU
1	C	307	LEU
1	C	326	GLU
1	C	363	PHE
1	C	367	SER
1	C	376	GLN
1	C	382	LEU
1	C	389	GLN
1	C	409	ARG
1	D	105	LEU
1	D	122	ARG
1	D	165	LYS
1	D	234	LEU
1	D	235	LEU
1	D	268	ARG
1	D	301	LEU
1	D	328	ASP
1	D	363	PHE
1	D	367	SER
1	D	395	LEU
1	D	409	ARG
1	D	419	ILE
1	D	435	LEU
1	E	10	ASP
1	E	117	ARG
1	E	122	ARG
1	E	165	LYS

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Mol	Chain	Res	Type
1	E	211	LYS
1	E	235	LEU
1	E	268	ARG
1	E	363	PHE
1	E	376	GLN
1	E	427	THR
1	E	442	THR
1	F	144	GLU
1	F	268	ARG
1	F	301	LEU
1	F	307	LEU
1	F	328	ASP
1	F	363	PHE
1	F	367	SER
1	F	376	GLN
1	F	389	GLN
1	F	427	THR
1	G	21	LYS
1	G	93	PHE
1	G	107	SER
1	G	122	ARG
1	G	235	LEU
1	G	247	LEU
1	G	268	ARG
1	G	352	LEU
1	G	358	SER
1	G	363	PHE
1	G	382	LEU
1	G	389	GLN
1	G	394	THR
1	G	395	LEU
1	H	107	SER
1	H	122	ARG
1	H	235	LEU
1	H	268	ARG
1	H	301	LEU
1	H	363	PHE
1	H	367	SER
1	H	376	GLN
1	H	382	LEU
1	I	15	LYS
1	I	105	LEU

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Mol	Chain	Res	Type
1	I	122	ARG
1	I	148	LYS
1	I	150	LEU
1	I	207	GLU
1	I	211	LYS
1	I	234	LEU
1	I	235	LEU
1	I	268	ARG
1	I	323	LEU
1	I	328	ASP
1	I	363	PHE
1	I	370	LEU
1	I	389	GLN
1	I	429	LYS
1	I	430	GLU
1	J	10	ASP
1	J	35	GLU
1	J	107	SER
1	J	122	ARG
1	J	165	LYS
1	J	211	LYS
1	J	268	ARG
1	J	301	LEU
1	J	363	PHE
1	J	370	LEU
1	J	376	GLN
1	J	440	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	294	HIS
1	A	312	GLN
1	A	341	HIS
1	A	351	HIS
1	A	354	GLN
1	A	376	GLN
1	B	239	GLN
1	B	279	HIS
1	B	312	GLN
1	B	354	GLN

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Mol	Chain	Res	Type
1	B	376	GLN
1	B	417	GLN
1	C	64	GLN
1	C	193	ASN
1	C	239	GLN
1	C	312	GLN
1	C	351	HIS
1	C	354	GLN
1	C	376	GLN
1	C	410	GLN
1	D	312	GLN
1	D	351	HIS
1	D	354	GLN
1	D	428	HIS
1	E	218	ASN
1	E	312	GLN
1	E	354	GLN
1	E	410	GLN
1	E	440	HIS
1	F	294	HIS
1	F	312	GLN
1	F	351	HIS
1	F	354	GLN
1	F	376	GLN
1	G	239	GLN
1	G	279	HIS
1	G	312	GLN
1	G	351	HIS
1	G	354	GLN
1	H	312	GLN
1	H	351	HIS
1	H	354	GLN
1	H	376	GLN
1	H	389	GLN
1	H	410	GLN
1	H	417	GLN
1	H	440	HIS
1	I	64	GLN
1	I	312	GLN
1	I	351	HIS
1	I	354	GLN
1	J	312	GLN

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Mol	Chain	Res	Type
1	J	354	GLN
1	J	410	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.61	0	7,12,14	1.39	2 (28%)
1	KCX	B	189	1,2	7,11,12	0.76	0	7,12,14	1.79	2 (28%)
1	KCX	C	189	1,2	7,11,12	0.71	0	7,12,14	2.09	1 (14%)
1	KCX	D	189	1,2	7,11,12	0.47	0	7,12,14	1.31	2 (28%)
1	KCX	E	189	1,4	7,11,12	0.67	0	7,12,14	1.41	2 (28%)
1	KCX	F	189	1,2	7,11,12	0.79	0	7,12,14	0.90	1 (14%)
1	KCX	G	189	1,2	7,11,12	0.76	0	7,12,14	1.62	1 (14%)
1	KCX	H	189	1,2	7,11,12	0.85	0	7,12,14	1.71	1 (14%)
1	KCX	I	189	1,2	7,11,12	0.60	0	7,12,14	1.38	2 (28%)
1	KCX	J	189	1,4	7,11,12	0.71	0	7,12,14	1.47	2 (28%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	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
1	KCX	I	189	1,2	-	0/6/10/12	0/0/0/0
1	KCX	J	189	1,4	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	189	KCX	CE-NZ-CX	-5.15	117.66	123.49
1	H	189	KCX	CE-NZ-CX	-4.08	118.87	123.49
1	B	189	KCX	CE-NZ-CX	-4.06	118.90	123.49
1	G	189	KCX	CE-NZ-CX	-3.74	119.26	123.49
1	J	189	KCX	CE-NZ-CX	-3.29	119.77	123.49
1	E	189	KCX	CE-NZ-CX	-3.05	120.03	123.49
1	A	189	KCX	CE-NZ-CX	-2.81	120.31	123.49
1	I	189	KCX	CE-NZ-CX	-2.76	120.37	123.49
1	D	189	KCX	CE-NZ-CX	-2.65	120.49	123.49
1	B	189	KCX	O-C-CA	-2.13	119.95	125.49
1	E	189	KCX	O-C-CA	-2.06	120.12	125.49
1	A	189	KCX	O-C-CA	-2.05	120.14	125.49
1	I	189	KCX	O-C-CA	-2.04	120.17	125.49
1	J	189	KCX	O-C-CA	-2.02	120.22	125.49
1	D	189	KCX	O-C-CA	-2.01	120.25	125.49
1	F	189	KCX	O-C-CA	-2.00	120.28	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	189	KCX	1	0
1	E	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	446	2	14,20,20	0.86	0	15,31,31	0.86	1 (6%)
3	CAP	B	446	2	14,20,20	0.85	0	15,31,31	0.95	0
3	CAP	C	446	2	14,20,20	0.77	0	15,31,31	0.98	1 (6%)
3	CAP	D	446	2	14,20,20	0.84	0	15,31,31	0.97	1 (6%)
3	CAP	E	446	4	14,20,20	0.67	0	15,31,31	0.85	0
3	CAP	F	446	2	14,20,20	0.83	0	15,31,31	0.82	0
3	CAP	G	446	2	14,20,20	0.88	0	15,31,31	0.89	0
3	CAP	H	446	2	14,20,20	0.77	0	15,31,31	0.89	0
3	CAP	I	446	2	14,20,20	0.83	0	15,31,31	1.04	1 (6%)
3	CAP	J	446	4	14,20,20	0.85	0	15,31,31	0.78	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	446	2	-	0/23/29/29	0/0/0/0
3	CAP	B	446	2	-	0/23/29/29	0/0/0/0
3	CAP	C	446	2	-	0/23/29/29	0/0/0/0
3	CAP	D	446	2	-	0/23/29/29	0/0/0/0
3	CAP	E	446	4	-	0/23/29/29	0/0/0/0
3	CAP	F	446	2	-	0/23/29/29	0/0/0/0
3	CAP	G	446	2	-	0/23/29/29	0/0/0/0
3	CAP	H	446	2	-	0/23/29/29	0/0/0/0
3	CAP	I	446	2	-	0/23/29/29	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	J	446	4	-	0/23/29/29	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	446	CAP	O1-P1-O1P	2.11	112.51	107.14
3	D	446	CAP	O6P-P2-O5	2.31	113.20	106.56
3	A	446	CAP	O6P-P2-O5	2.40	113.47	106.56
3	I	446	CAP	O6P-P2-O5	2.64	114.17	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	446	CAP	1	0
3	B	446	CAP	1	0
3	C	446	CAP	3	0
3	E	446	CAP	1	0
3	F	446	CAP	2	0
3	G	446	CAP	1	0
3	H	446	CAP	2	0
3	J	446	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	435/444 (97%)	0.09	20 (4%)	36	49	17, 28, 49, 58	0
1	B	436/444 (98%)	0.17	30 (6%)	20	30	14, 26, 56, 62	0
1	C	436/444 (98%)	0.32	42 (9%)	10	16	16, 27, 60, 66	0
1	D	436/444 (98%)	0.33	34 (7%)	16	24	15, 26, 58, 85	0
1	E	431/444 (97%)	0.10	24 (5%)	28	40	15, 25, 53, 70	0
1	F	436/444 (98%)	0.29	28 (6%)	23	33	17, 30, 57, 64	0
1	G	436/444 (98%)	0.19	32 (7%)	18	27	13, 25, 52, 58	0
1	H	437/444 (98%)	0.29	35 (8%)	15	23	16, 28, 58, 61	0
1	I	436/444 (98%)	0.05	24 (5%)	29	41	13, 24, 52, 70	0
1	J	433/444 (97%)	0.17	32 (7%)	17	26	14, 25, 57, 74	0
All	All	4352/4440 (98%)	0.20	301 (6%)	20	30	13, 27, 56, 85	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ALA	8.8
1	G	434	ALA	8.4
1	D	421	LEU	8.2
1	C	421	LEU	7.4
1	G	421	LEU	7.2
1	C	434	ALA	6.9
1	J	441	VAL	6.6
1	C	425	ALA	6.5
1	E	441	VAL	6.5
1	J	444	VAL	6.3
1	F	9	TYR	6.3
1	J	435	LEU	5.8
1	E	444	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	414	ALA	5.7
1	G	59	TYR	5.6
1	I	421	LEU	5.5
1	D	414	ALA	5.5
1	C	426	LYS	5.4
1	C	441	VAL	5.2
1	J	439	GLY	5.2
1	I	398	PRO	4.8
1	H	434	ALA	4.7
1	C	438	TRP	4.7
1	D	411	ALA	4.7
1	E	443	PRO	4.6
1	B	415	ILE	4.6
1	I	434	ALA	4.5
1	J	424	TYR	4.5
1	C	418	GLY	4.4
1	F	425	ALA	4.4
1	B	421	LEU	4.4
1	D	398	PRO	4.4
1	D	422	ASP	4.3
1	J	436	GLU	4.3
1	C	422	ASP	4.3
1	E	439	GLY	4.2
1	G	422	ASP	4.1
1	G	418	GLY	4.1
1	A	56	THR	4.0
1	H	414	ALA	4.0
1	C	427	THR	4.0
1	G	441	VAL	3.9
1	H	426	LYS	3.9
1	D	434	ALA	3.9
1	I	426	LYS	3.9
1	I	396	GLY	3.8
1	J	432	ALA	3.8
1	J	321	GLY	3.8
1	B	434	ALA	3.8
1	C	420	PRO	3.8
1	I	56	THR	3.8
1	J	419	ILE	3.8
1	H	443	PRO	3.8
1	E	419	ILE	3.7
1	G	420	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	3.7
1	B	426	LYS	3.7
1	D	56	THR	3.7
1	E	442	THR	3.6
1	I	55	TRP	3.6
1	E	417	GLN	3.5
1	H	441	VAL	3.5
1	H	442	THR	3.5
1	D	55	TRP	3.5
1	F	426	LYS	3.5
1	B	422	ASP	3.5
1	H	444	VAL	3.5
1	J	425	ALA	3.5
1	D	427	THR	3.4
1	C	414	ALA	3.4
1	F	427	THR	3.3
1	B	376	GLN	3.3
1	G	424	TYR	3.3
1	B	420	PRO	3.3
1	J	320	ALA	3.3
1	F	417	GLN	3.3
1	E	218	ASN	3.2
1	G	414	ALA	3.3
1	D	441	VAL	3.2
1	G	443	PRO	3.2
1	A	442	THR	3.2
1	D	420	PRO	3.2
1	F	56	THR	3.2
1	H	346	GLU	3.2
1	B	425	ALA	3.2
1	C	59	TYR	3.2
1	C	439	GLY	3.2
1	F	421	LEU	3.2
1	A	258	ILE	3.1
1	B	418	GLY	3.1
1	F	286	ALA	3.1
1	B	438	TRP	3.1
1	J	442	THR	3.1
1	D	258	ILE	3.1
1	B	59	TYR	3.1
1	G	321	GLY	3.1
1	D	57	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	184	GLY	3.0
1	A	421	LEU	3.0
1	D	423	GLU	3.0
1	J	417	GLN	3.0
1	B	398	PRO	3.0
1	C	433	ARG	3.0
1	H	398	PRO	2.9
1	G	425	ALA	2.9
1	B	424	TYR	2.9
1	C	419	ILE	2.9
1	I	422	ASP	2.9
1	G	442	THR	2.9
1	A	426	LYS	2.9
1	J	438	TRP	2.9
1	J	426	LYS	2.9
1	F	444	VAL	2.9
1	F	8	ILE	2.9
1	C	392	GLY	2.8
1	H	7	THR	2.8
1	A	422	ASP	2.8
1	C	283	ALA	2.8
1	C	442	THR	2.8
1	F	59	TYR	2.8
1	H	258	ILE	2.8
1	D	430	GLU	2.8
1	B	358	SER	2.8
1	C	296	ILE	2.8
1	F	58	LEU	2.8
1	H	415	ILE	2.8
1	G	9	TYR	2.8
1	A	55	TRP	2.8
1	C	411	ALA	2.8
1	H	421	LEU	2.8
1	H	377	PRO	2.8
1	C	435	LEU	2.7
1	J	443	PRO	2.7
1	I	400	GLY	2.7
1	G	415	ILE	2.7
1	B	9	TYR	2.7
1	F	424	TYR	2.7
1	C	257	VAL	2.7
1	F	283	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	347	ASN	2.7
1	H	257	VAL	2.7
1	F	422	ASP	2.7
1	A	423	GLU	2.7
1	D	283	ALA	2.7
1	H	109	ALA	2.7
1	F	54	THR	2.7
1	B	16	GLY	2.7
1	E	398	PRO	2.7
1	F	296	ILE	2.7
1	C	106	ALA	2.7
1	E	106	ALA	2.7
1	A	36	GLY	2.7
1	G	438	TRP	2.7
1	H	420	PRO	2.7
1	D	284	MET	2.6
1	B	8	ILE	2.6
1	I	425	ALA	2.6
1	G	319	GLY	2.6
1	E	427	THR	2.6
1	C	428	HIS	2.6
1	B	56	THR	2.6
1	H	433	ARG	2.6
1	E	110	GLY	2.6
1	F	105	LEU	2.6
1	H	321	GLY	2.6
1	J	398	PRO	2.6
1	J	420	PRO	2.6
1	G	411	ALA	2.6
1	I	427	THR	2.6
1	C	437	LYS	2.6
1	D	426	LYS	2.6
1	C	424	TYR	2.6
1	D	9	TYR	2.6
1	A	283	ALA	2.6
1	H	320	ALA	2.6
1	D	439	GLY	2.5
1	E	376	GLN	2.5
1	H	318	ALA	2.5
1	H	438	TRP	2.5
1	B	436	GLU	2.5
1	D	257	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	109	ALA	2.5
1	H	283	ALA	2.5
1	J	59	TYR	2.5
1	G	56	THR	2.5
1	C	346	GLU	2.5
1	E	105	LEU	2.5
1	F	284	MET	2.5
1	A	257	VAL	2.5
1	J	376	GLN	2.5
1	F	55	TRP	2.5
1	H	284	MET	2.5
1	C	443	PRO	2.5
1	H	296	ILE	2.5
1	H	106	ALA	2.4
1	A	398	PRO	2.4
1	C	396	GLY	2.4
1	I	57	THR	2.4
1	J	57	THR	2.4
1	C	284	MET	2.4
1	G	373	GLY	2.4
1	A	434	ALA	2.4
1	C	318	ALA	2.4
1	J	428	HIS	2.4
1	F	258	ILE	2.4
1	G	377	PRO	2.4
1	B	53	GLY	2.4
1	D	256	VAL	2.4
1	D	106	ALA	2.4
1	B	58	LEU	2.4
1	D	313	LEU	2.4
1	C	321	GLY	2.4
1	H	425	ALA	2.4
1	J	433	ARG	2.4
1	C	415	ILE	2.3
1	B	319	GLY	2.3
1	F	400	GLY	2.3
1	A	256	VAL	2.3
1	C	7	THR	2.3
1	D	220	THR	2.3
1	G	320	ALA	2.3
1	D	435	LEU	2.3
1	C	289	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	404	GLY	2.3
1	E	257	VAL	2.3
1	I	414	ALA	2.3
1	A	396	GLY	2.3
1	E	256	VAL	2.3
1	I	441	VAL	2.3
1	I	395	LEU	2.3
1	I	438	TRP	2.3
1	G	325	GLY	2.2
1	B	54	THR	2.2
1	B	417	GLN	2.2
1	I	423	GLU	2.2
1	D	395	LEU	2.2
1	H	81	GLY	2.2
1	B	423	GLU	2.2
1	F	106	ALA	2.2
1	H	411	ALA	2.2
1	C	300	VAL	2.2
1	H	417	GLN	2.2
1	I	9	TYR	2.2
1	E	35	GLU	2.2
1	J	423	GLU	2.2
1	D	432	ALA	2.2
1	J	440	HIS	2.2
1	E	424	TYR	2.2
1	I	424	TYR	2.2
1	E	418	GLY	2.2
1	H	418	GLY	2.2
1	G	423	GLU	2.2
1	I	373	GLY	2.2
1	G	426	LYS	2.2
1	B	377	PRO	2.2
1	G	58	LEU	2.2
1	G	347	ASN	2.1
1	H	59	TYR	2.1
1	C	301	LEU	2.1
1	I	284	MET	2.1
1	B	419	ILE	2.1
1	F	398	PRO	2.1
1	C	304	LEU	2.1
1	A	427	THR	2.1
1	C	365	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	2.1
1	A	218	ASN	2.1
1	E	258	ILE	2.1
1	D	377	PRO	2.1
1	J	257	VAL	2.1
1	F	433	ARG	2.1
1	C	109	ALA	2.1
1	E	36	GLY	2.1
1	J	434	ALA	2.1
1	B	347	ASN	2.1
1	G	417	GLN	2.1
1	E	59	TYR	2.1
1	G	395	LEU	2.1
1	C	429	LYS	2.1
1	J	218	ASN	2.1
1	G	436	GLU	2.1
1	J	413	ASP	2.1
1	C	444	VAL	2.1
1	F	57	THR	2.1
1	G	396	GLY	2.1
1	J	418	GLY	2.1
1	H	85	TRP	2.1
1	H	412	ILE	2.1
1	J	58	LEU	2.0
1	D	424	TYR	2.0
1	E	425	ALA	2.0
1	I	283	ALA	2.0
1	F	36	GLY	2.0
1	G	54	THR	2.0
1	I	437	LYS	2.0
1	F	285	HIS	2.0
1	A	284	MET	2.0
1	B	106	ALA	2.0
1	D	407	ALA	2.0
1	J	421	LEU	2.0
1	D	371	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	A	189	12/13	0.98	0.18	-	20,23,24,24	0
1	KCX	G	189	12/13	0.97	0.16	-	16,19,20,20	0
1	KCX	E	189	12/13	0.97	0.14	-	18,19,23,24	0
1	KCX	I	189	12/13	0.96	0.14	-	19,21,25,25	0
1	KCX	D	189	12/13	0.98	0.21	-	21,22,24,25	0
1	KCX	B	189	12/13	0.96	0.20	-	18,20,21,22	0
1	KCX	H	189	12/13	0.97	0.17	-	20,21,25,26	0
1	KCX	F	189	12/13	0.96	0.19	-	23,25,27,27	0
1	KCX	J	189	12/13	0.97	0.17	-	19,19,24,26	0
1	KCX	C	189	12/13	0.97	0.16	-	21,22,26,28	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	H	445	1/1	0.99	0.24	1.97	22,22,22,22	0
2	MG	C	445	1/1	0.95	0.24	1.32	23,23,23,23	0
4	CA	J	445	1/1	0.98	0.19	0.38	27,27,27,27	0
3	CAP	C	446	21/21	0.93	0.21	0.26	23,34,37,39	0
3	CAP	J	446	21/21	0.95	0.18	0.16	20,28,40,40	0
3	CAP	H	446	21/21	0.94	0.17	0.09	24,35,37,39	0
3	CAP	E	446	21/21	0.96	0.15	-0.12	16,27,37,38	0
2	MG	G	445	1/1	0.95	0.16	-0.34	22,22,22,22	0
3	CAP	G	446	21/21	0.95	0.15	-0.37	16,29,33,34	0
3	CAP	B	446	21/21	0.96	0.15	-0.54	18,29,35,36	0
2	MG	B	445	1/1	0.94	0.16	-0.62	19,19,19,19	0
3	CAP	D	446	21/21	0.96	0.15	-0.71	18,28,31,32	0
3	CAP	F	446	21/21	0.96	0.15	-1.07	24,33,34,35	0
3	CAP	I	446	21/21	0.96	0.12	-1.14	15,25,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CAP	A	446	21/21	0.98	0.12	-1.34	21,30,31,32	0
4	CA	E	445	1/1	0.97	0.13	-1.91	27,27,27,27	0
2	MG	D	445	1/1	0.99	0.13	-2.64	27,27,27,27	0
2	MG	I	445	1/1	0.97	0.08	-3.53	21,21,21,21	0
2	MG	A	445	1/1	0.97	0.09	-3.99	32,32,32,32	0
2	MG	F	445	1/1	0.97	0.05	-10.70	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.