Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:16 AM GMT

PDB ID	:	3A12
Title	:	Crystal structure of Type III Rubisco complexed with 2-CABP
Authors	:	Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2009-03-25
Resolution	:	2.30 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:

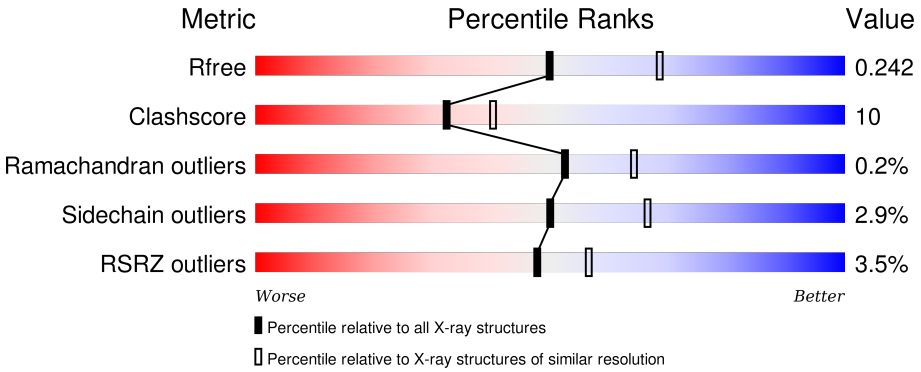
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	2% 80% 17%
1	B	444	2% 85% 14%
1	C	444	2% 79% 18%
1	D	444	2% 80% 17%
1	E	444	5% 80% 18%

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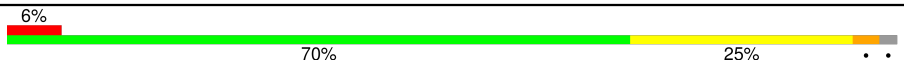
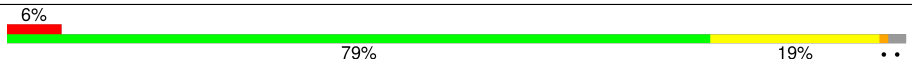
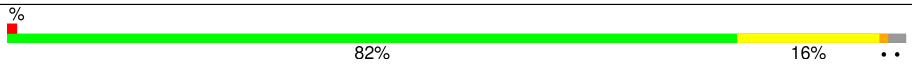
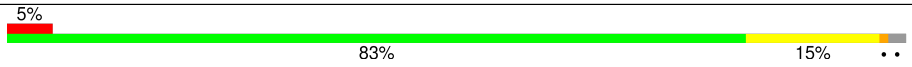
Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36651 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	437	Total	C	N	O	S	0	0	0
			3404	2186	584	624	10			
1	B	438	Total	C	N	O	S	0	0	0
			3432	2207	589	626	10			
1	C	438	Total	C	N	O	S	0	0	0
			3421	2202	586	623	10			
1	D	436	Total	C	N	O	S	0	0	0
			3424	2199	584	631	10			
1	E	436	Total	C	N	O	S	0	0	0
			3406	2189	583	624	10			
1	F	435	Total	C	N	O	S	0	0	0
			3367	2162	580	615	10			
1	G	436	Total	C	N	O	S	0	0	0
			3412	2193	584	625	10			
1	H	437	Total	C	N	O	S	0	0	0
			3421	2200	585	626	10			
1	I	436	Total	C	N	O	S	0	0	0
			3424	2199	585	630	10			
1	J	437	Total	C	N	O	S	0	0	0
			3414	2195	583	626	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	J	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

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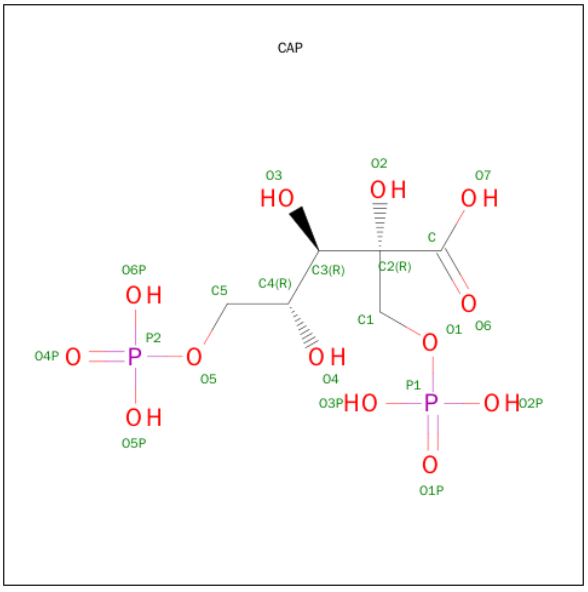
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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.

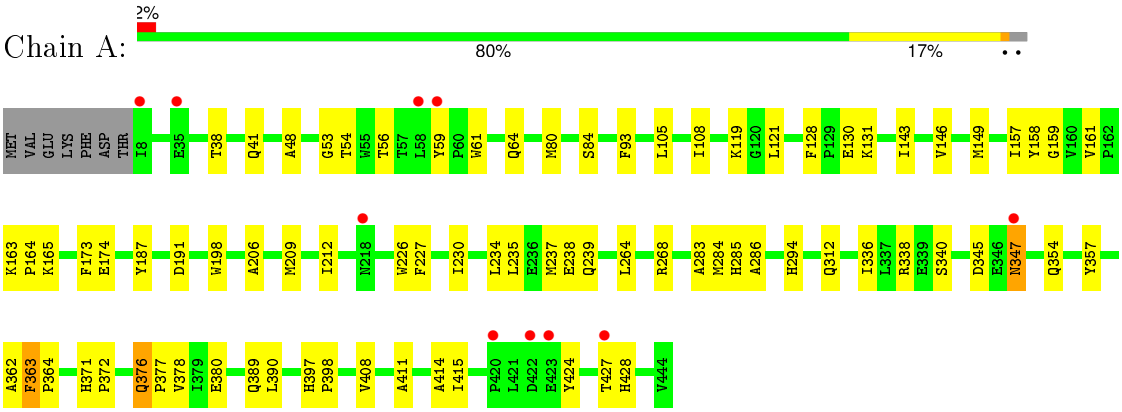
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	246	Total	O	0	0
			246	246		
4	C	260	Total	O	0	0
			260	260		
4	D	256	Total	O	0	0
			256	256		
4	E	224	Total	O	0	0
			224	224		
4	F	168	Total	O	0	0
			168	168		
4	G	195	Total	O	0	0
			195	195		
4	H	217	Total	O	0	0
			217	217		
4	I	266	Total	O	0	0
			266	266		
4	J	253	Total	O	0	0
			253	253		

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.

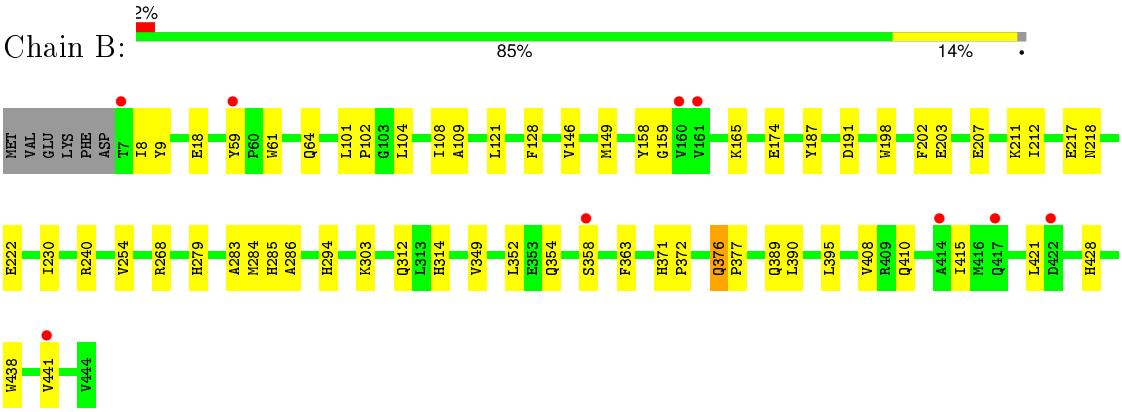
- Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



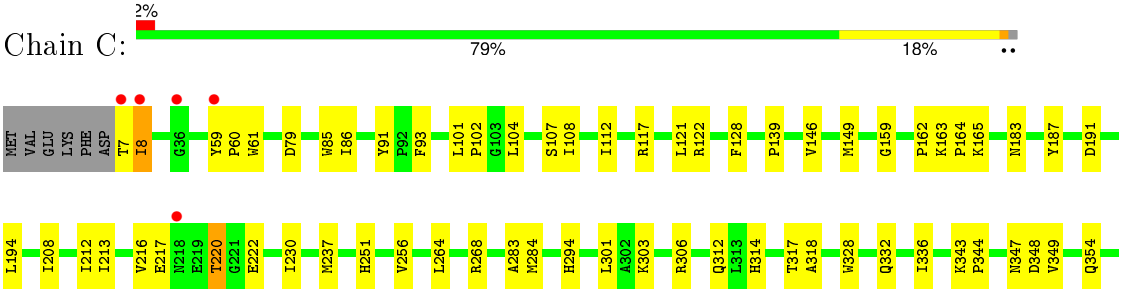
- Molecule 1: Ribulose bisphosphate carboxylase

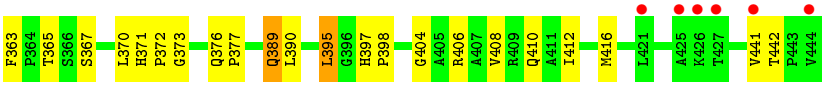
Chain B:



- Molecule 1: Ribulose bisphosphate carboxylase

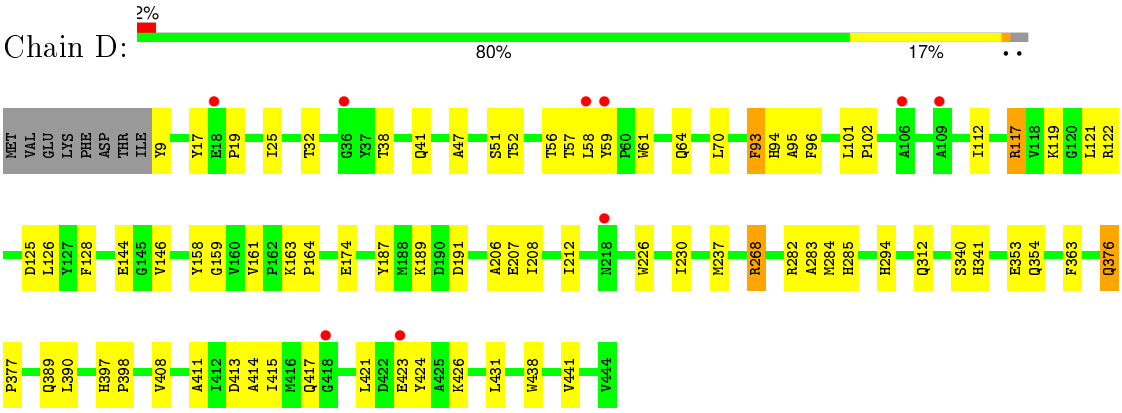
Chain C:





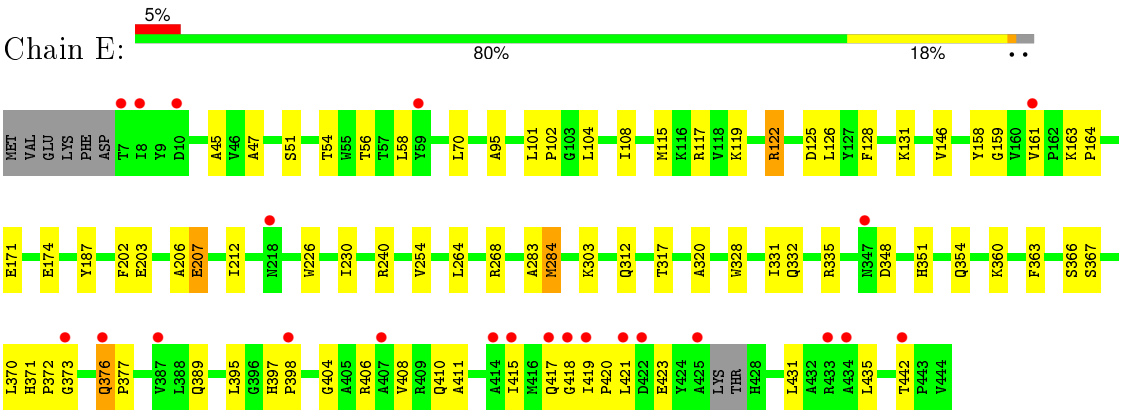
• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



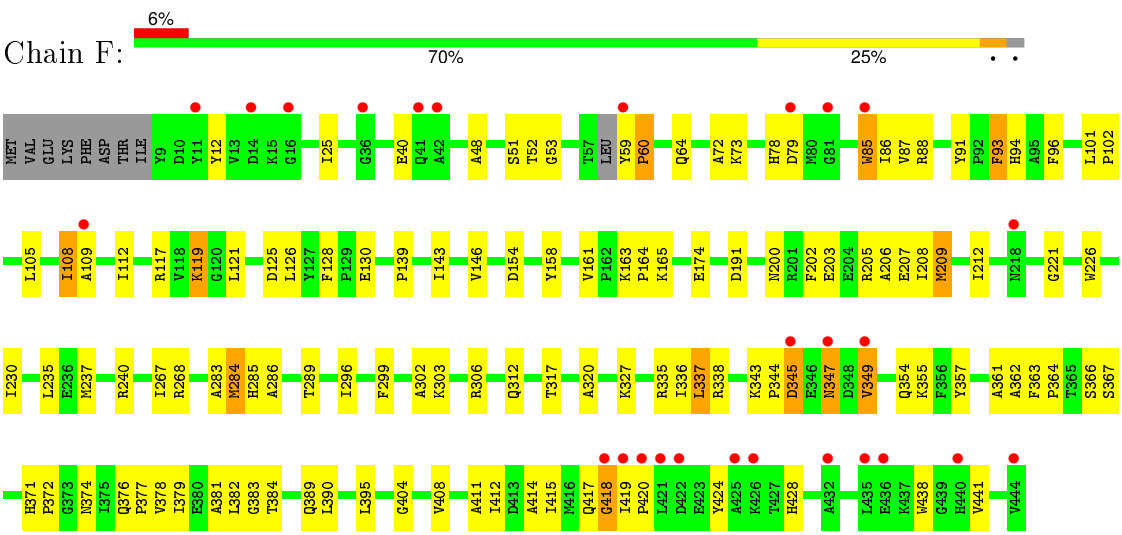
• Molecule 1: Ribulose bisphosphate carboxylase

Chain E:



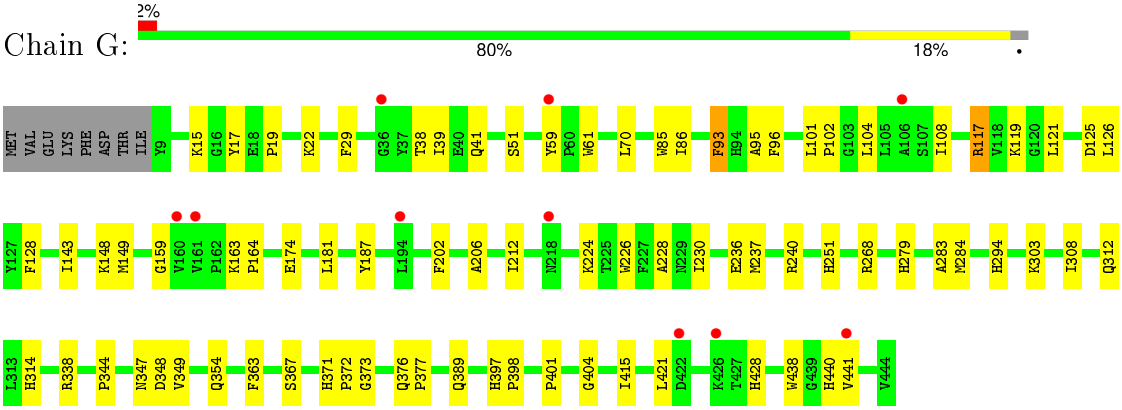
• Molecule 1: Ribulose bisphosphate carboxylase

Chain F:



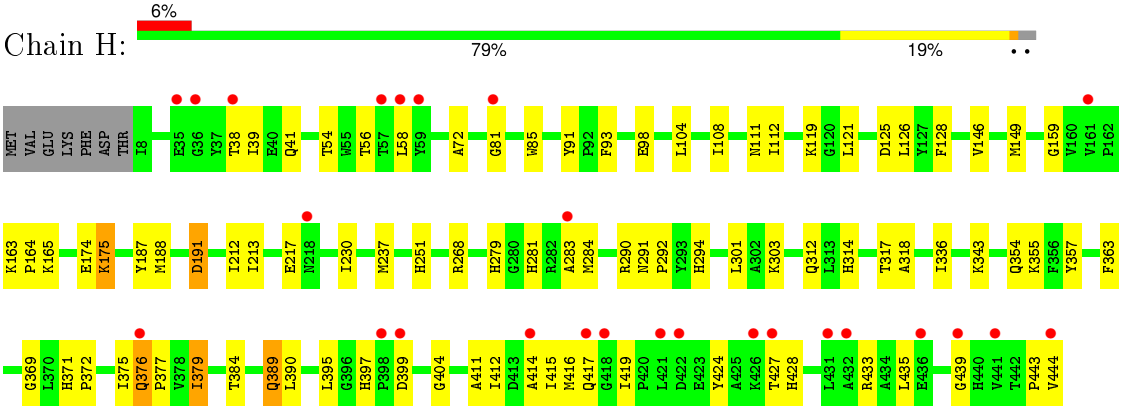
• Molecule 1: Ribulose bisphosphate carboxylase

Chain G:



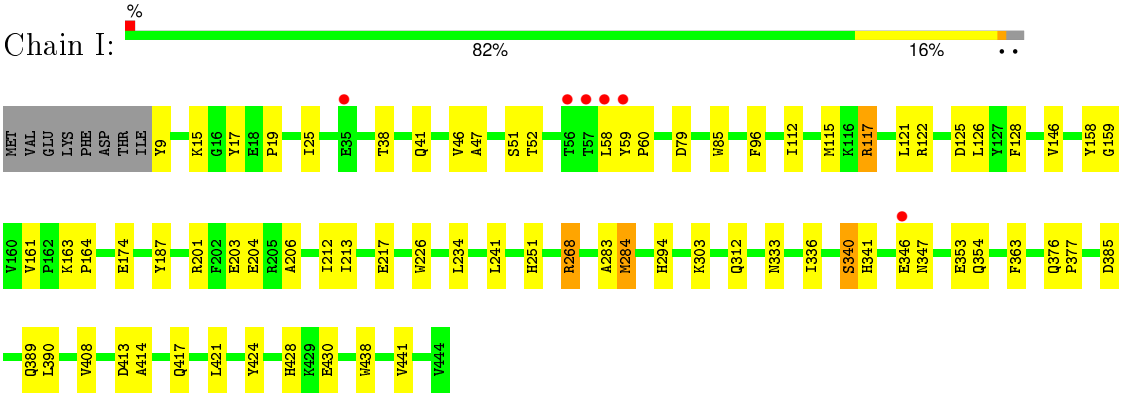
• Molecule 1: Ribulose bisphosphate carboxylase

Chain H:



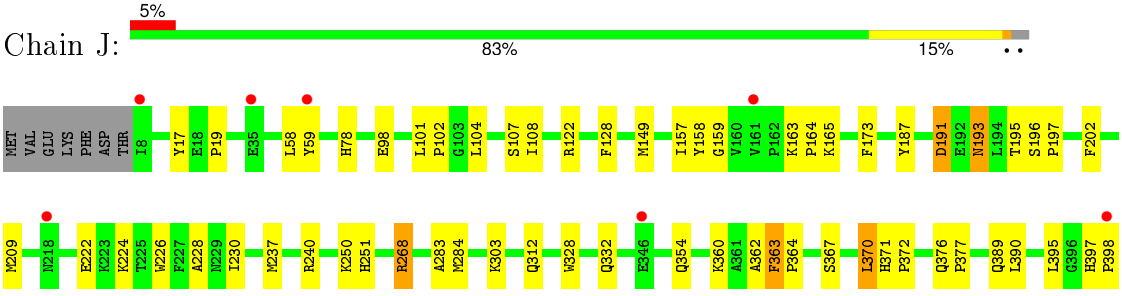
• Molecule 1: Ribulose bisphosphate carboxylase

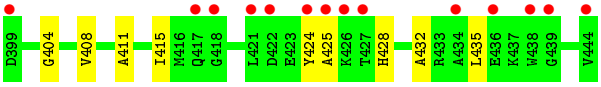
Chain I:



• Molecule 1: Ribulose bisphosphate carboxylase

Chain J:




D399
G404
V408
A411
I415
N416
Q417
G418
L421
D422
E423
Y424
A425
K426
T427
H428
A432
R433
A434
L435
E436
K437
W438
G439
V444

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.29Å 246.38Å 144.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.39 – 2.30 35.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.39-2.30) 99.6 (35.39-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.199 , 0.244 0.200 , 0.242	Depositor DCC
R_{free} test set	13629 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	2 of 271361 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36651	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 48.04 % 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 9.1080e-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: 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	0.35	0/3480	0.50	0/4724
1	B	0.37	0/3509	0.51	0/4758
1	C	0.36	0/3498	0.50	0/4748
1	D	0.37	0/3501	0.50	0/4750
1	E	0.36	0/3482	0.52	0/4725
1	F	0.34	0/3441	0.49	0/4673
1	G	0.33	0/3489	0.49	0/4735
1	H	0.34	0/3498	0.49	0/4747
1	I	0.36	0/3500	0.50	0/4747
1	J	0.36	0/3491	0.50	0/4738
All	All	0.35	0/34889	0.50	0/47345

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	3404	0	3295	64	0
1	B	3432	0	3348	39	0
1	C	3421	0	3332	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3424	0	3328	66	0
1	E	3406	0	3299	70	0
1	F	3367	0	3249	132	0
1	G	3412	0	3316	71	0
1	H	3421	0	3329	82	0
1	I	3424	0	3341	54	0
1	J	3414	0	3306	57	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	8	0	0
3	B	21	0	7	0	0
3	C	21	0	8	1	0
3	D	21	0	7	1	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	0	0
3	I	21	0	7	0	0
3	J	21	0	8	0	0
4	A	221	0	0	6	0
4	B	246	0	0	5	0
4	C	260	0	0	6	0
4	D	256	0	0	8	0
4	E	224	0	0	6	0
4	F	168	0	0	15	0
4	G	195	0	0	8	0
4	H	217	0	0	9	0
4	I	266	0	0	10	0
4	J	253	0	0	4	0
All	All	36651	0	33219	709	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 10.

All (709) 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:209:MET:HA	1:F:209:MET:CE	1.61	1.28
1:J:397:HIS:ND1	1:J:398:PRO:HD2	1.49	1.26
1:D:58:LEU:HA	4:D:738:HOH:O	1.44	1.17
1:D:64:GLN:HB3	4:D:631:HOH:O	1.47	1.12
1:H:376:GLN:HG3	1:H:377:PRO:HD3	1.31	1.09
1:F:209:MET:HA	1:F:209:MET:HE2	1.14	1.08
1:J:173:PHE:CE2	1:J:209:MET:CE	2.37	1.06
1:J:58:LEU:HD23	1:J:59:TYR:H	1.11	1.04
1:J:58:LEU:HD23	1:J:59:TYR:N	1.72	1.02
1:I:174:GLU:HG3	1:I:212:ILE:HD11	1.38	1.02
1:F:335:ARG:HA	4:F:602:HOH:O	1.62	1.00
1:E:417:GLN:HG3	1:E:419:ILE:CD1	1.92	1.00
1:C:347:ASN:HB3	4:C:737:HOH:O	1.59	0.99
1:J:397:HIS:CE1	1:J:398:PRO:HD2	1.96	0.99
1:A:347:ASN:N	1:A:347:ASN:HD22	1.60	0.98
1:J:397:HIS:ND1	1:J:398:PRO:CD	2.26	0.98
1:H:38:THR:H	1:H:41:GLN:NE2	1.61	0.98
1:J:173:PHE:HE2	1:J:209:MET:HE3	1.29	0.96
1:J:173:PHE:CE2	1:J:209:MET:HE3	2.01	0.96
1:H:163:LYS:H	1:H:395:LEU:CD2	1.80	0.95
1:A:347:ASN:H	1:A:347:ASN:ND2	1.59	0.95
1:H:38:THR:H	1:H:41:GLN:HE21	0.95	0.94
1:D:340:SER:HB3	4:D:745:HOH:O	1.68	0.94
1:H:376:GLN:HG3	1:H:377:PRO:CD	1.96	0.94
1:E:417:GLN:HG3	1:E:419:ILE:HD13	1.48	0.94
1:G:86:ILE:HG13	1:G:349:VAL:HG12	1.47	0.93
1:D:174:GLU:HG3	1:D:212:ILE:HD11	1.51	0.92
1:D:376:GLN:HG3	1:D:377:PRO:HD3	1.50	0.92
1:C:163:LYS:H	1:C:395:LEU:CD2	1.83	0.92
1:J:173:PHE:CE2	1:J:209:MET:HE1	2.05	0.89
1:C:8:ILE:HD12	1:C:8:ILE:H	1.37	0.89
1:H:163:LYS:H	1:H:395:LEU:HD21	1.38	0.88
1:E:360:LYS:HE2	4:E:639:HOH:O	1.71	0.88
1:G:376:GLN:HB3	1:G:377:PRO:HD3	1.55	0.88
1:C:8:ILE:HD12	1:C:8:ILE:N	1.89	0.87
1:G:149:MET:HE2	1:G:251:HIS:HE1	1.40	0.86
1:E:410:GLN:NE2	1:E:431:LEU:H	1.73	0.86
1:G:86:ILE:HG13	1:G:349:VAL:CG1	2.05	0.85
1:B:438:TRP:O	1:B:441:VAL:HG22	1.76	0.85
1:G:438:TRP:O	1:G:441:VAL:HG12	1.77	0.84
1:H:119:LYS:HB2	4:H:669:HOH:O	1.77	0.84
1:F:209:MET:CA	1:F:209:MET:CE	2.52	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.60	0.82
1:H:121:LEU:H	1:H:294:HIS:HD2	1.28	0.82
1:F:174:GLU:HG3	1:F:212:ILE:HD11	1.62	0.81
1:F:302:ALA:HB1	1:F:337:LEU:HD13	1.62	0.81
1:F:79:ASP:HA	1:F:85:TRP:CD1	2.15	0.81
1:F:345:ASP:HB3	4:F:583:HOH:O	1.80	0.81
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.16	0.80
1:C:149:MET:HE2	1:C:251:HIS:HE1	1.46	0.80
1:B:203:GLU:O	1:B:207:GLU:HG2	1.82	0.80
1:H:38:THR:N	1:H:41:GLN:HE21	1.79	0.79
1:C:220:THR:HG22	1:C:222:GLU:H	1.47	0.79
1:C:149:MET:CE	1:C:251:HIS:CE1	2.66	0.79
1:F:209:MET:HA	1:F:209:MET:HE3	1.63	0.79
1:E:45:ALA:HB1	1:E:115:MET:HE3	1.63	0.78
1:A:347:ASN:H	1:A:347:ASN:HD22	0.82	0.78
1:B:121:LEU:H	1:B:294:HIS:HD2	1.32	0.78
1:G:149:MET:HE2	1:G:251:HIS:CE1	2.18	0.78
1:G:174:GLU:HG3	1:G:212:ILE:HD11	1.66	0.77
1:F:128:PHE:H	1:F:354:GLN:HE22	1.31	0.77
1:J:163:LYS:H	1:J:395:LEU:CD1	1.97	0.77
1:F:79:ASP:CA	1:F:85:TRP:NE1	2.48	0.77
1:J:193:ASN:H	1:J:193:ASN:HD22	1.33	0.77
1:E:397:HIS:ND1	1:E:398:PRO:HD2	2.01	0.76
1:D:128:PHE:H	1:D:354:GLN:HE22	1.32	0.76
1:I:128:PHE:H	1:I:354:GLN:HE22	1.31	0.76
1:H:213:ILE:O	1:H:217:GLU:HG3	1.86	0.76
1:A:347:ASN:HB3	4:A:580:HOH:O	1.86	0.76
1:C:149:MET:CE	1:C:251:HIS:HE1	1.98	0.76
1:J:173:PHE:HE2	1:J:209:MET:CE	1.87	0.76
1:F:376:GLN:HG3	4:F:639:HOH:O	1.84	0.76
1:D:161:VAL:H	1:D:389:GLN:NE2	1.84	0.76
1:A:38:THR:OG1	1:A:41:GLN:HG3	1.86	0.75
1:F:108:ILE:HD12	1:F:108:ILE:C	2.07	0.75
1:C:163:LYS:H	1:C:395:LEU:HD23	1.50	0.75
1:C:149:MET:HE1	1:C:251:HIS:CE1	2.22	0.75
1:F:317:THR:O	1:F:378:VAL:HG22	1.87	0.75
1:E:320:ALA:O	1:E:442:THR:HB	1.86	0.75
1:D:9:TYR:HD2	1:D:117:ARG:NH2	1.85	0.74
1:I:38:THR:OG1	1:I:41:GLN:HG3	1.86	0.74
1:E:410:GLN:HE21	1:E:431:LEU:HB2	1.53	0.74
1:F:125:ASP:OD1	1:F:126:LEU:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PHE:H	1:C:354:GLN:HE22	1.36	0.73
1:G:149:MET:CE	1:G:251:HIS:CE1	2.72	0.73
1:H:417:GLN:CB	1:H:419:ILE:CD1	2.66	0.73
1:C:303:LYS:HZ3	1:C:354:GLN:HE21	1.35	0.73
1:D:64:GLN:CD	4:D:631:HOH:O	2.27	0.72
1:H:417:GLN:HB3	1:H:419:ILE:CD1	2.18	0.72
1:G:128:PHE:H	1:G:354:GLN:HE22	1.33	0.72
1:D:438:TRP:O	1:D:441:VAL:HG12	1.89	0.72
1:F:79:ASP:HA	1:F:85:TRP:NE1	2.03	0.72
1:F:414:ALA:HB2	1:F:424:TYR:CD2	2.25	0.72
1:F:108:ILE:HD12	1:F:109:ALA:N	2.04	0.71
1:F:112:ILE:HD12	1:F:121:LEU:HD21	1.72	0.71
1:F:86:ILE:HG13	1:F:349:VAL:CG2	2.20	0.71
1:E:45:ALA:HB1	1:E:115:MET:CE	2.19	0.71
1:C:8:ILE:CD1	1:C:8:ILE:H	2.04	0.71
1:E:203:GLU:O	1:E:207:GLU:HG2	1.90	0.71
1:H:121:LEU:H	1:H:294:HIS:CD2	2.08	0.71
1:H:284:MET:HG2	1:H:284:MET:O	1.89	0.71
1:C:121:LEU:H	1:C:294:HIS:HD2	1.38	0.70
1:D:161:VAL:H	1:D:389:GLN:HE21	1.36	0.70
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.72	0.70
1:F:376:GLN:CG	4:F:639:HOH:O	2.39	0.70
1:D:421:LEU:HD13	1:D:431:LEU:HD21	1.72	0.70
1:J:128:PHE:H	1:J:354:GLN:HE22	1.38	0.70
1:B:9:TYR:HB2	4:B:524:HOH:O	1.92	0.70
1:B:128:PHE:H	1:B:354:GLN:HE22	1.37	0.70
1:I:121:LEU:H	1:I:294:HIS:HD2	1.40	0.69
1:F:411:ALA:O	1:F:415:ILE:HG13	1.91	0.69
1:F:79:ASP:HB2	1:F:85:TRP:HE1	1.58	0.69
1:E:410:GLN:HE21	1:E:431:LEU:H	1.39	0.69
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.28	0.69
1:I:201:ARG:HB2	1:I:204:GLU:HG3	1.74	0.69
1:C:303:LYS:NZ	1:C:354:GLN:HE21	1.89	0.69
1:H:119:LYS:CB	4:H:669:HOH:O	2.36	0.68
1:J:108:ILE:CG2	1:J:108:ILE:O	2.41	0.68
1:I:340:SER:HB3	4:I:701:HOH:O	1.94	0.68
1:B:64:GLN:HG3	4:B:726:HOH:O	1.92	0.68
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.29	0.68
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.29	0.68
1:E:371:HIS:CE1	1:E:373:GLY:HA3	2.29	0.67
1:A:80:MET:HE3	4:A:662:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:VAL:O	1:F:349:VAL:CG2	2.42	0.67
1:J:78:HIS:ND1	4:J:687:HOH:O	2.26	0.67
1:F:209:MET:CA	1:F:209:MET:HE2	2.08	0.67
1:F:161:VAL:H	1:F:389:GLN:NE2	1.93	0.67
1:H:303:LYS:HZ3	1:H:354:GLN:HE21	1.42	0.67
1:H:281:HIS:CE1	1:H:283:ALA:HB2	2.30	0.67
1:J:163:LYS:H	1:J:395:LEU:HD12	1.59	0.67
1:A:128:PHE:H	1:A:354:GLN:HE22	1.42	0.67
1:F:79:ASP:CA	1:F:85:TRP:CD1	2.79	0.66
1:E:163:LYS:H	1:E:395:LEU:CD2	2.08	0.66
1:H:303:LYS:NZ	1:H:354:GLN:HE21	1.93	0.66
1:E:161:VAL:H	1:E:389:GLN:NE2	1.93	0.66
1:F:79:ASP:HB2	1:F:85:TRP:NE1	2.11	0.66
1:H:279:HIS:HE1	1:H:314:HIS:NE2	1.94	0.66
1:E:128:PHE:H	1:E:354:GLN:HE22	1.43	0.66
1:F:376:GLN:CB	1:F:377:PRO:CD	2.74	0.65
1:E:376:GLN:HB3	1:E:377:PRO:HD3	1.78	0.65
1:C:213:ILE:O	1:C:217:GLU:HG3	1.97	0.65
1:D:121:LEU:H	1:D:294:HIS:HD2	1.42	0.65
1:F:108:ILE:C	1:F:108:ILE:CD1	2.65	0.65
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.30	0.65
1:F:25:ILE:HD12	1:F:96:PHE:CE2	2.31	0.65
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.62	0.65
1:D:9:TYR:CD2	1:D:117:ARG:NH2	2.64	0.65
1:J:303:LYS:NZ	1:J:354:GLN:HE21	1.94	0.65
1:F:143:ILE:HD11	1:F:338:ARG:HG2	1.78	0.64
1:E:410:GLN:HE21	1:E:431:LEU:N	1.95	0.64
1:B:108:ILE:C	1:B:108:ILE:HD12	2.18	0.64
1:A:121:LEU:H	1:A:294:HIS:HD2	1.44	0.64
1:H:149:MET:CE	1:H:251:HIS:CE1	2.81	0.64
1:J:58:LEU:CD2	1:J:59:TYR:H	1.99	0.63
1:E:411:ALA:O	1:E:415:ILE:HG13	1.98	0.63
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.34	0.63
1:C:220:THR:CG2	1:C:222:GLU:HB2	2.29	0.63
1:I:161:VAL:H	1:I:389:GLN:NE2	1.97	0.63
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.33	0.62
1:G:104:LEU:C	1:G:104:LEU:HD23	2.20	0.62
1:F:143:ILE:HD12	1:F:361:ALA:HB1	1.81	0.62
1:H:417:GLN:HB2	1:H:419:ILE:CD1	2.29	0.62
1:A:234:LEU:HD11	1:A:238:GLU:OE2	1.99	0.62
1:F:88:ARG:NH2	4:F:641:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:GLU:CB	4:F:529:HOH:O	2.47	0.62
1:G:376:GLN:CB	1:G:377:PRO:HD3	2.27	0.62
1:F:78:HIS:C	1:F:85:TRP:CD1	2.73	0.62
1:C:121:LEU:H	1:C:294:HIS:CD2	2.16	0.62
1:E:410:GLN:HE21	1:E:431:LEU:CB	2.13	0.62
1:H:376:GLN:N	1:H:377:PRO:HD2	2.15	0.62
1:B:121:LEU:H	1:B:294:HIS:CD2	2.17	0.62
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.34	0.62
1:F:86:ILE:HG13	1:F:349:VAL:HG22	1.81	0.61
1:F:158:TYR:CE1	1:F:408:VAL:HG11	2.35	0.61
1:H:417:GLN:HB3	1:H:419:ILE:HD11	1.82	0.61
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.83	0.61
1:F:344:PRO:C	4:F:560:HOH:O	2.39	0.61
1:F:376:GLN:HB3	1:F:377:PRO:HD3	1.83	0.61
1:E:367:SER:HB2	1:E:389:GLN:HB3	1.83	0.61
1:F:79:ASP:CB	1:F:85:TRP:NE1	2.63	0.61
1:I:203:GLU:HG3	4:I:537:HOH:O	2.01	0.61
1:C:389:GLN:C	1:C:390:LEU:HD12	2.22	0.60
1:C:165:LYS:HG2	1:C:191:ASP:OD2	2.01	0.60
1:C:376:GLN:N	1:C:377:PRO:HD2	2.16	0.60
1:F:376:GLN:CB	1:F:377:PRO:HD3	2.32	0.60
1:F:143:ILE:CD1	1:F:338:ARG:HG2	2.30	0.60
1:A:235:LEU:O	1:A:239:GLN:HG3	2.01	0.60
1:J:370:LEU:HB2	4:J:546:HOH:O	2.01	0.60
1:C:86:ILE:HG13	1:C:349:VAL:HG13	1.83	0.60
1:B:104:LEU:C	1:B:104:LEU:HD23	2.22	0.60
1:E:351:HIS:HE1	4:E:586:HOH:O	1.84	0.60
1:A:234:LEU:HD13	1:A:234:LEU:C	2.22	0.59
1:G:397:HIS:CD2	1:G:404:GLY:HA2	2.37	0.59
1:E:397:HIS:ND1	1:E:398:PRO:CD	2.66	0.59
1:C:86:ILE:HG13	1:C:349:VAL:CG1	2.33	0.59
1:G:121:LEU:H	1:G:294:HIS:HD2	1.51	0.59
1:F:299:PHE:CE1	1:F:336:ILE:HB	2.37	0.59
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.36	0.59
1:H:159:GLY:HA3	1:H:187:TYR:CZ	2.38	0.59
1:D:426:LYS:HB3	1:F:221:GLY:HA3	1.84	0.59
1:C:397:HIS:CG	1:C:398:PRO:HD2	2.37	0.59
1:F:130:GLU:HG3	1:F:357:TYR:CE2	2.38	0.58
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.38	0.58
1:F:376:GLN:HA	1:F:415:ILE:HD13	1.84	0.58
1:C:220:THR:HG22	1:C:222:GLU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LYS:HA	1:F:164:PRO:C	2.23	0.58
1:F:79:ASP:N	1:F:85:TRP:CD1	2.72	0.58
1:F:376:GLN:HB3	1:F:377:PRO:CD	2.32	0.58
1:J:108:ILE:HG22	1:J:108:ILE:O	2.03	0.58
1:H:149:MET:HE2	1:H:251:HIS:CE1	2.38	0.58
1:C:216:VAL:O	1:C:220:THR:HB	2.04	0.58
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.38	0.58
1:F:174:GLU:CG	1:F:212:ILE:HD11	2.33	0.57
1:D:59:TYR:O	1:D:61:TRP:HD1	1.87	0.57
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.34	0.57
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.85	0.57
1:D:174:GLU:CG	1:D:212:ILE:HD11	2.29	0.57
1:A:389:GLN:C	1:A:390:LEU:HD12	2.23	0.57
1:F:209:MET:CE	1:F:212:ILE:HB	2.35	0.57
1:F:376:GLN:CG	1:F:377:PRO:HD3	2.34	0.57
1:I:121:LEU:H	1:I:294:HIS:CD2	2.21	0.57
1:E:161:VAL:H	1:E:389:GLN:HE21	1.52	0.57
1:H:149:MET:HE2	1:H:251:HIS:HE1	1.67	0.57
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.86	0.57
1:F:412:ILE:CG2	4:F:567:HOH:O	2.51	0.57
1:C:163:LYS:H	1:C:395:LEU:HD21	1.67	0.57
1:J:411:ALA:O	1:J:415:ILE:HG13	2.04	0.57
1:F:376:GLN:HG3	1:F:377:PRO:N	2.19	0.57
1:D:161:VAL:N	1:D:389:GLN:HE21	2.03	0.57
1:B:421:LEU:HD22	4:B:629:HOH:O	2.03	0.57
1:E:47:ALA:O	1:E:51:SER:HB3	2.04	0.57
1:E:397:HIS:CD2	1:E:404:GLY:HA2	2.40	0.56
1:H:279:HIS:CE1	1:H:314:HIS:NE2	2.72	0.56
1:C:397:HIS:ND1	1:C:398:PRO:HD2	2.21	0.56
1:G:22:LYS:HG2	4:G:588:HOH:O	2.06	0.56
1:C:60:PRO:CA	4:C:729:HOH:O	2.53	0.56
1:H:371:HIS:HB2	1:H:372:PRO:HD2	1.88	0.56
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.71	0.56
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.70	0.56
1:F:283:ALA:O	1:F:284:MET:HB3	2.05	0.56
1:D:51:SER:OG	1:D:52:THR:N	2.38	0.56
1:C:162:PRO:HA	1:C:395:LEU:HD21	1.87	0.56
1:E:410:GLN:NE2	1:E:431:LEU:N	2.48	0.55
1:E:421:LEU:HD22	4:E:686:HOH:O	2.05	0.55
1:I:9:TYR:HD2	1:I:117:ARG:NH2	2.04	0.55
1:A:121:LEU:H	1:A:294:HIS:CD2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:ARG:HH11	1:F:205:ARG:HG3	1.71	0.55
1:F:25:ILE:HD12	1:F:96:PHE:HE2	1.69	0.55
1:D:208:ILE:O	1:D:212:ILE:HG13	2.07	0.55
1:D:421:LEU:CD1	1:D:431:LEU:HD21	2.35	0.55
1:G:279:HIS:HD2	1:G:312:GLN:OE1	1.89	0.55
1:F:78:HIS:C	1:F:85:TRP:HD1	2.10	0.55
1:C:149:MET:HE1	1:C:251:HIS:ND1	2.21	0.55
1:E:163:LYS:HA	1:E:164:PRO:C	2.27	0.55
1:J:58:LEU:CD2	1:J:59:TYR:N	2.60	0.55
1:F:327:LYS:NZ	1:F:381:ALA:HB2	2.22	0.55
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.41	0.55
1:G:93:PHE:C	1:G:93:PHE:CD1	2.80	0.55
1:H:104:LEU:C	1:H:104:LEU:HD23	2.28	0.55
1:H:444:VAL:O	1:H:444:VAL:HG12	2.06	0.55
1:F:209:MET:HE2	1:F:212:ILE:HB	1.87	0.55
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.42	0.55
1:H:149:MET:HE1	1:H:251:HIS:ND1	2.21	0.54
1:C:59:TYR:O	1:C:61:TRP:HD1	1.90	0.54
1:F:327:LYS:HZ2	1:F:381:ALA:HB2	1.72	0.54
1:D:56:THR:OG1	1:D:57:THR:N	2.41	0.54
1:F:101:LEU:HB3	1:F:102:PRO:HD3	1.88	0.54
1:F:349:VAL:HG22	1:F:349:VAL:O	2.08	0.54
1:G:104:LEU:O	1:G:104:LEU:HD23	2.07	0.54
1:F:376:GLN:HG3	1:F:377:PRO:HD3	1.87	0.54
1:C:163:LYS:N	1:C:395:LEU:CD2	2.62	0.54
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.42	0.54
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.89	0.54
1:A:376:GLN:HA	1:A:415:ILE:HD13	1.90	0.54
1:G:230:ILE:HD11	1:G:237:MET:CE	2.38	0.54
1:C:108:ILE:O	1:C:108:ILE:HG22	2.08	0.54
1:H:188:MET:HB3	4:H:671:HOH:O	2.06	0.54
1:F:362:ALA:O	1:F:364:PRO:HD3	2.08	0.54
1:H:251:HIS:NE2	1:H:312:GLN:NE2	2.54	0.53
1:G:121:LEU:H	1:G:294:HIS:CD2	2.26	0.53
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.90	0.53
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.44	0.53
1:C:220:THR:HG22	1:C:222:GLU:HB2	1.89	0.53
1:D:341:HIS:NE2	1:D:353:GLU:OE2	2.30	0.53
1:F:93:PHE:CD1	1:F:93:PHE:C	2.81	0.53
1:G:163:LYS:HA	1:G:164:PRO:C	2.29	0.53
1:J:101:LEU:HB3	1:J:102:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:608:HOH:O	1:E:171:GLU:HG2	2.08	0.53
1:B:376:GLN:N	1:B:377:PRO:HD2	2.23	0.53
1:D:121:LEU:H	1:D:294:HIS:CD2	2.25	0.53
1:A:376:GLN:N	1:A:377:PRO:HD2	2.23	0.53
1:J:222:GLU:HG3	1:J:224:LYS:HE2	1.90	0.53
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.43	0.53
1:G:349:VAL:O	1:G:349:VAL:HG12	2.08	0.53
1:I:46:VAL:HG22	1:I:115:MET:HE1	1.91	0.53
1:D:59:TYR:O	1:D:61:TRP:CD1	2.62	0.52
1:D:125:ASP:OD1	1:D:126:LEU:N	2.37	0.52
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.73	0.52
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.40	0.52
1:H:417:GLN:HB2	1:H:419:ILE:HD13	1.90	0.52
1:E:348:ASP:OD2	1:E:351:HIS:HD2	1.93	0.52
1:H:399:ASP:OD1	1:H:433:ARG:NH2	2.40	0.52
1:E:371:HIS:ND1	1:E:373:GLY:N	2.52	0.52
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.45	0.52
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.75	0.52
1:A:347:ASN:N	1:A:347:ASN:ND2	2.33	0.52
1:E:371:HIS:CE1	1:E:373:GLY:CA	2.91	0.52
1:G:347:ASN:OD1	1:G:347:ASN:N	2.40	0.52
1:F:376:GLN:HG3	1:F:377:PRO:CD	2.39	0.52
1:H:371:HIS:HB2	1:H:372:PRO:CD	2.39	0.52
1:A:424:TYR:CZ	1:A:428:HIS:CE1	2.98	0.52
1:E:331:ILE:O	1:E:335:ARG:HG3	2.10	0.52
1:G:421:LEU:HD22	4:G:672:HOH:O	2.09	0.52
1:H:369:GLY:O	1:H:443:PRO:HG2	2.10	0.52
1:H:149:MET:HE1	1:H:251:HIS:HD1	1.75	0.52
1:F:93:PHE:CD1	1:F:94:HIS:N	2.78	0.52
1:J:328:TRP:O	1:J:332:GLN:HG2	2.10	0.52
1:F:347:ASN:OD1	1:F:347:ASN:N	2.42	0.52
1:J:397:HIS:CG	1:J:398:PRO:CD	2.93	0.51
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.39	0.51
1:I:303:LYS:HZ3	1:I:354:GLN:HE21	1.57	0.51
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.45	0.51
1:H:435:LEU:O	1:H:439:GLY:N	2.41	0.51
1:F:59:TYR:O	1:F:60:PRO:C	2.47	0.51
1:A:239:GLN:HB3	4:A:712:HOH:O	2.11	0.51
1:E:410:GLN:NE2	1:E:431:LEU:HB2	2.23	0.51
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.45	0.51
1:H:128:PHE:H	1:H:354:GLN:HE22	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:413:ASP:O	1:I:417:GLN:HG3	2.11	0.51
1:I:421:LEU:HD12	4:I:736:HOH:O	2.08	0.51
1:D:58:LEU:CA	4:D:738:HOH:O	2.25	0.51
1:J:303:LYS:HZ3	1:J:354:GLN:HE21	1.56	0.51
1:I:161:VAL:H	1:I:389:GLN:HE21	1.59	0.51
1:F:119:LYS:HE3	4:F:564:HOH:O	2.10	0.51
1:A:173:PHE:CE2	1:A:209:MET:CE	2.93	0.51
1:D:376:GLN:HA	1:D:415:ILE:HD13	1.92	0.51
1:C:139:PRO:HD3	1:C:306:ARG:O	2.11	0.51
1:G:59:TYR:O	1:G:61:TRP:HD1	1.94	0.51
1:H:376:GLN:NE2	4:H:704:HOH:O	2.34	0.50
1:J:209:MET:HG2	1:J:226:TRP:CG	2.44	0.50
1:F:283:ALA:O	1:F:284:MET:CB	2.58	0.50
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.77	0.50
1:B:389:GLN:C	1:B:390:LEU:HD12	2.30	0.50
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.92	0.50
1:G:230:ILE:HG13	1:G:237:MET:HE3	1.94	0.50
1:F:165:LYS:HE3	1:F:191:ASP:OD2	2.11	0.50
1:F:379:ILE:O	1:F:383:GLY:N	2.39	0.50
1:H:163:LYS:N	1:H:395:LEU:CD2	2.63	0.50
1:C:7:THR:CB	1:C:117:ARG:HH22	2.25	0.50
1:I:283:ALA:O	1:I:284:MET:HB3	2.11	0.50
1:F:158:TYR:CD1	1:F:408:VAL:HG11	2.47	0.50
1:G:349:VAL:HG13	4:G:670:HOH:O	2.10	0.50
1:I:389:GLN:C	1:I:390:LEU:HD12	2.32	0.50
1:F:139:PRO:HD3	1:F:306:ARG:O	2.11	0.50
1:I:341:HIS:NE2	1:I:353:GLU:OE2	2.40	0.49
1:H:108:ILE:HG22	1:H:108:ILE:O	2.11	0.49
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.41	0.49
1:G:96:PHE:HB3	4:G:546:HOH:O	2.11	0.49
1:G:230:ILE:CD1	1:G:237:MET:HE2	2.42	0.49
1:A:230:ILE:O	1:A:237:MET:HG2	2.11	0.49
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.42	0.49
1:D:25:ILE:CD1	1:D:96:PHE:CE2	2.95	0.49
1:F:208:ILE:HG22	1:F:209:MET:HE3	1.94	0.49
1:F:357:TYR:HA	4:F:577:HOH:O	2.12	0.49
1:C:371:HIS:CE1	1:C:373:GLY:HA3	2.47	0.49
1:I:159:GLY:CA	1:I:187:TYR:CZ	2.93	0.49
1:D:389:GLN:C	1:D:390:LEU:HD12	2.32	0.49
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.48	0.49
1:H:389:GLN:C	1:H:390:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LYS:HG3	4:I:634:HOH:O	2.12	0.49
1:F:417:GLN:O	1:F:419:ILE:HG13	2.11	0.49
1:B:303:LYS:NZ	1:B:354:GLN:HE21	2.10	0.49
1:I:251:HIS:NE2	1:I:312:GLN:NE2	2.61	0.49
1:D:206:ALA:HA	1:D:226:TRP:CZ3	2.48	0.49
1:C:441:VAL:CG1	1:C:442:THR:N	2.76	0.49
1:I:376:GLN:HB3	1:I:377:PRO:HD3	1.94	0.49
1:A:161:VAL:HG23	1:A:389:GLN:CD	2.33	0.49
1:C:112:ILE:HD12	1:C:121:LEU:HD21	1.95	0.49
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.95	0.49
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.78	0.49
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.48	0.48
1:C:208:ILE:O	1:C:212:ILE:HG12	2.13	0.48
1:A:163:LYS:HA	1:A:164:PRO:C	2.33	0.48
1:B:279:HIS:HD2	1:B:312:GLN:OE1	1.96	0.48
1:D:93:PHE:CD1	1:D:94:HIS:N	2.81	0.48
1:J:149:MET:HE3	1:J:250:LYS:HD2	1.94	0.48
1:I:163:LYS:HA	1:I:164:PRO:C	2.33	0.48
1:G:376:GLN:HA	1:G:415:ILE:HD13	1.96	0.48
1:H:317:THR:O	1:H:318:ALA:HB3	2.13	0.48
1:B:158:TYR:CE1	1:B:408:VAL:HG11	2.48	0.48
1:F:320:ALA:O	1:F:374:ASN:ND2	2.46	0.48
1:D:376:GLN:N	1:D:377:PRO:CD	2.77	0.48
1:E:108:ILE:HG22	1:E:108:ILE:O	2.13	0.48
1:F:119:LYS:O	1:F:119:LYS:HG3	2.12	0.48
1:G:367:SER:HB2	1:G:389:GLN:HB3	1.94	0.48
1:D:230:ILE:O	1:D:237:MET:HG2	2.14	0.48
1:A:93:PHE:CE2	4:A:576:HOH:O	2.65	0.48
1:D:414:ALA:HB2	1:D:424:TYR:CD2	2.48	0.48
1:F:335:ARG:HG2	4:F:602:HOH:O	2.13	0.48
1:E:371:HIS:HE1	1:E:373:GLY:HA3	1.76	0.48
1:D:93:PHE:C	1:D:93:PHE:CD1	2.87	0.48
1:C:79:ASP:HB2	1:C:85:TRP:CZ3	2.48	0.48
1:B:149:MET:HB3	4:B:654:HOH:O	2.13	0.48
1:G:236:GLU:OE1	1:G:236:GLU:N	2.45	0.48
1:G:349:VAL:O	1:G:349:VAL:CG1	2.62	0.48
1:H:417:GLN:CB	1:H:419:ILE:HD12	2.43	0.48
1:B:283:ALA:O	1:B:284:MET:CB	2.61	0.48
1:H:290:ARG:N	4:H:505:HOH:O	2.47	0.48
1:F:78:HIS:CD2	1:F:78:HIS:C	2.87	0.47
1:D:17:TYR:CE2	1:D:19:PRO:HA	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:ALA:O	1:H:415:ILE:HG13	2.15	0.47
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.50	0.47
1:F:51:SER:OG	1:F:52:THR:N	2.47	0.47
1:G:401:PRO:HD2	4:G:664:HOH:O	2.13	0.47
1:H:149:MET:HE1	1:H:251:HIS:CE1	2.49	0.47
1:G:371:HIS:HB2	1:G:372:PRO:HD2	1.96	0.47
1:F:417:GLN:O	1:F:419:ILE:N	2.48	0.47
1:C:283:ALA:O	1:C:284:MET:HB3	2.14	0.47
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.95	0.47
1:F:230:ILE:O	1:F:237:MET:HG2	2.14	0.47
1:H:165:LYS:NZ	1:H:191:ASP:OD1	2.32	0.47
1:D:163:LYS:HA	1:D:164:PRO:C	2.35	0.47
1:J:367:SER:HB2	1:J:389:GLN:HB3	1.96	0.47
1:D:283:ALA:O	1:D:284:MET:HB3	2.13	0.47
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.48	0.47
1:B:410:GLN:OE1	1:B:428:HIS:HB3	2.14	0.47
1:A:54:THR:HA	4:A:564:HOH:O	2.14	0.47
1:J:362:ALA:O	1:J:364:PRO:HD3	2.15	0.47
1:J:268:ARG:C	1:J:268:ARG:HD3	2.35	0.47
1:D:38:THR:OG1	1:D:41:GLN:HG3	2.14	0.47
1:C:149:MET:HE2	1:C:251:HIS:CE1	2.34	0.47
1:B:108:ILE:HD12	1:B:109:ALA:N	2.29	0.47
1:I:25:ILE:HD12	1:I:96:PHE:CE2	2.49	0.47
1:H:397:HIS:CD2	1:H:404:GLY:HA2	2.50	0.47
1:A:283:ALA:O	1:A:284:MET:HB3	2.14	0.47
1:A:59:TYR:O	1:A:61:TRP:HD1	1.98	0.47
1:F:389:GLN:C	1:F:390:LEU:HD12	2.35	0.47
1:B:283:ALA:O	1:B:284:MET:HB3	2.14	0.47
1:A:157:ILE:HD13	1:A:363:PHE:CZ	2.49	0.47
1:H:281:HIS:HE1	1:H:283:ALA:HB2	1.77	0.47
1:J:202:PHE:CD2	1:J:240:ARG:HG2	2.50	0.47
1:C:230:ILE:O	1:C:237:MET:HG2	2.15	0.47
1:I:268:ARG:C	1:I:268:ARG:HD3	2.36	0.47
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.51	0.47
1:H:81:GLY:C	4:H:590:HOH:O	2.53	0.47
1:C:60:PRO:HA	4:C:729:HOH:O	2.16	0.46
1:F:72:ALA:O	1:F:73:LYS:HD3	2.15	0.46
1:F:418:GLY:O	1:F:420:PRO:HD3	2.14	0.46
1:J:283:ALA:O	1:J:284:MET:HB3	2.14	0.46
1:F:165:LYS:HB3	1:F:191:ASP:OD2	2.14	0.46
1:J:251:HIS:NE2	1:J:312:GLN:NE2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:HA	1:C:164:PRO:C	2.36	0.46
1:C:390:LEU:HD12	1:C:390:LEU:N	2.29	0.46
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.80	0.46
1:A:93:PHE:C	1:A:93:PHE:CD1	2.88	0.46
1:A:165:LYS:HB3	1:A:191:ASP:OD2	2.15	0.46
1:G:303:LYS:HZ1	1:G:354:GLN:HE21	1.63	0.46
1:A:130:GLU:HG3	1:A:357:TYR:CE2	2.50	0.46
1:J:230:ILE:O	1:J:237:MET:HG2	2.16	0.46
1:C:349:VAL:O	1:C:349:VAL:HG13	2.15	0.46
1:C:122:ARG:HD2	4:C:546:HOH:O	2.15	0.46
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.98	0.46
1:E:423:GLU:O	4:E:637:HOH:O	2.20	0.46
1:G:226:TRP:CZ3	1:G:228:ALA:HB2	2.51	0.46
1:E:376:GLN:N	1:E:377:PRO:CD	2.79	0.46
1:C:108:ILE:O	1:C:108:ILE:CG2	2.64	0.46
1:I:213:ILE:O	1:I:217:GLU:HG3	2.16	0.46
1:F:203:GLU:O	1:F:207:GLU:HG2	2.15	0.46
1:C:183:ASN:OD1	1:C:406:ARG:NH1	2.39	0.46
1:C:60:PRO:HB3	4:C:729:HOH:O	2.15	0.46
1:C:104:LEU:HD23	1:C:104:LEU:C	2.36	0.46
1:J:163:LYS:HA	1:J:164:PRO:C	2.35	0.45
1:F:424:TYR:CZ	1:F:428:HIS:CE1	3.04	0.45
1:F:438:TRP:O	1:F:441:VAL:HG12	2.15	0.45
1:A:108:ILE:HD12	1:A:108:ILE:C	2.36	0.45
1:H:279:HIS:HD2	1:H:312:GLN:OE1	1.99	0.45
1:A:209:MET:HG3	1:A:226:TRP:CD2	2.50	0.45
1:D:413:ASP:O	1:D:417:GLN:HG3	2.16	0.45
1:D:144:GLU:CD	4:D:666:HOH:O	2.54	0.45
1:J:360:LYS:HE2	4:J:631:HOH:O	2.15	0.45
1:F:417:GLN:C	1:F:419:ILE:H	2.20	0.45
1:A:362:ALA:O	1:A:364:PRO:HD3	2.17	0.45
1:E:418:GLY:O	1:E:420:PRO:HD3	2.17	0.45
1:C:8:ILE:HG22	1:C:8:ILE:O	2.15	0.45
1:F:349:VAL:HG23	1:F:349:VAL:O	2.17	0.45
1:A:376:GLN:HB3	1:A:377:PRO:HD3	1.99	0.45
1:G:15:LYS:HG3	4:G:615:HOH:O	2.16	0.45
1:B:165:LYS:HG2	1:B:191:ASP:OD2	2.17	0.45
1:A:336:ILE:HA	1:A:336:ILE:HD12	1.78	0.45
1:G:237:MET:HE2	1:G:237:MET:HB3	1.75	0.45
1:H:376:GLN:HA	1:H:415:ILE:HD13	1.99	0.45
1:G:303:LYS:NZ	1:G:354:GLN:HE21	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HD22	1:E:95:ALA:HA	1.98	0.45
1:D:376:GLN:HG3	1:D:377:PRO:CD	2.35	0.45
1:D:47:ALA:O	1:D:51:SER:HB3	2.17	0.45
1:F:205:ARG:NH1	1:F:205:ARG:HG3	2.32	0.45
1:G:279:HIS:HE1	1:G:314:HIS:NE2	2.15	0.45
1:I:283:ALA:O	1:I:284:MET:CB	2.65	0.45
1:G:428:HIS:HA	4:G:689:HOH:O	2.16	0.45
1:E:158:TYR:CE1	1:E:408:VAL:HG11	2.51	0.45
1:A:376:GLN:OE1	1:A:380:GLU:OE1	2.35	0.45
1:F:303:LYS:NZ	1:F:354:GLN:HE21	2.15	0.44
1:D:159:GLY:HA3	1:D:187:TYR:CD2	2.53	0.44
1:C:406:ARG:O	1:C:410:GLN:HG3	2.18	0.44
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.98	0.44
1:G:149:MET:HE1	1:G:251:HIS:ND1	2.32	0.44
1:H:379:ILE:HD12	1:H:384:THR:HG22	1.98	0.44
1:J:191:ASP:HB2	4:J:577:HOH:O	2.17	0.44
1:B:158:TYR:CD1	1:B:408:VAL:HG11	2.52	0.44
1:E:125:ASP:OD1	1:E:126:LEU:N	2.48	0.44
1:F:349:VAL:HG12	4:F:563:HOH:O	2.16	0.44
1:F:25:ILE:CD1	1:F:96:PHE:CE2	2.98	0.44
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.46	0.44
1:D:397:HIS:CG	1:D:398:PRO:HD2	2.53	0.44
1:F:202:PHE:CD2	1:F:240:ARG:HG2	2.53	0.44
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.52	0.44
1:H:336:ILE:HD12	1:H:336:ILE:HA	1.89	0.44
1:B:108:ILE:C	1:B:108:ILE:CD1	2.85	0.44
1:G:29:PHE:CD1	1:G:121:LEU:HD11	2.52	0.44
1:I:430:GLU:HA	4:I:659:HOH:O	2.17	0.44
1:D:32:THR:O	1:D:119:LYS:N	2.44	0.44
1:A:165:LYS:CB	1:A:191:ASP:OD2	2.66	0.44
1:C:404:GLY:O	1:C:408:VAL:HG23	2.18	0.44
1:J:104:LEU:HD23	1:J:104:LEU:C	2.37	0.44
1:A:234:LEU:CD1	1:A:238:GLU:OE2	2.65	0.44
1:G:230:ILE:CD1	1:G:237:MET:CE	2.95	0.44
1:J:389:GLN:C	1:J:390:LEU:HD12	2.38	0.44
1:H:230:ILE:O	1:H:237:MET:HG2	2.18	0.44
1:H:376:GLN:CG	1:H:377:PRO:CD	2.83	0.44
1:D:414:ALA:HB2	1:D:424:TYR:CG	2.53	0.44
1:I:79:ASP:HB2	1:I:85:TRP:CZ3	2.53	0.44
1:H:93:PHE:CD1	1:H:93:PHE:C	2.90	0.44
1:D:423:GLU:OE2	1:D:423:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:LYS:HA	1:H:164:PRO:C	2.38	0.44
1:E:348:ASP:OD2	1:E:351:HIS:CD2	2.70	0.44
1:G:101:LEU:HD23	1:G:308:ILE:HD11	2.00	0.44
1:A:131:LYS:HD2	1:B:198:TRP:CG	2.53	0.44
1:C:370:LEU:HB2	4:C:562:HOH:O	2.18	0.44
1:G:149:MET:HE1	1:G:251:HIS:CE1	2.51	0.43
1:H:119:LYS:HA	4:H:669:HOH:O	2.17	0.43
1:F:376:GLN:NE2	4:F:639:HOH:O	2.39	0.43
1:I:96:PHE:HB3	4:I:681:HOH:O	2.18	0.43
1:G:51:SER:HB2	4:G:674:HOH:O	2.18	0.43
1:J:157:ILE:HD12	1:J:363:PHE:CE2	2.53	0.43
1:F:79:ASP:HA	1:F:85:TRP:CE2	2.53	0.43
1:A:157:ILE:HD12	1:A:157:ILE:N	2.32	0.43
1:I:125:ASP:OD1	1:I:126:LEU:N	2.51	0.43
1:F:285:HIS:CG	1:F:286:ALA:N	2.86	0.43
1:I:376:GLN:N	1:I:377:PRO:CD	2.81	0.43
1:C:412:ILE:O	1:C:416:MET:HG2	2.18	0.43
1:I:51:SER:OG	1:I:52:THR:N	2.50	0.43
1:D:411:ALA:O	1:D:415:ILE:HG13	2.17	0.43
1:I:159:GLY:CA	1:I:187:TYR:CE2	3.00	0.43
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.53	0.43
1:A:234:LEU:O	1:A:234:LEU:HD13	2.18	0.43
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.54	0.43
1:I:159:GLY:HA3	1:I:187:TYR:CD2	2.53	0.43
1:F:404:GLY:O	1:F:408:VAL:HG23	2.18	0.43
1:F:302:ALA:HB1	1:F:337:LEU:CD1	2.41	0.43
1:H:375:ILE:O	1:H:379:ILE:HG23	2.19	0.43
1:B:230:ILE:HD11	1:B:254:VAL:HG22	2.00	0.43
1:B:279:HIS:HE1	1:B:314:HIS:NE2	2.16	0.43
1:D:25:ILE:HD12	1:D:96:PHE:HE2	1.83	0.43
1:G:344:PRO:HB2	1:G:348:ASP:HB3	1.99	0.43
1:E:417:GLN:HG3	1:E:419:ILE:HD12	1.91	0.43
1:A:80:MET:HB2	1:A:84:SER:O	2.18	0.43
1:B:376:GLN:HA	1:B:415:ILE:HD13	2.01	0.43
1:A:93:PHE:CE1	1:A:131:LYS:HE3	2.54	0.43
1:G:125:ASP:OD1	1:G:126:LEU:N	2.51	0.43
1:F:289:THR:HG22	1:F:296:ILE:O	2.18	0.43
1:A:198:TRP:CG	1:E:131:LYS:HD2	2.53	0.43
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.54	0.43
1:F:237:MET:CE	1:F:267:ILE:HD11	2.49	0.43
1:E:283:ALA:O	1:E:284:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:414:ALA:HB2	1:H:424:TYR:CD2	2.54	0.43
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.54	0.43
1:C:256:VAL:HG12	1:C:264:LEU:HD11	2.01	0.43
1:I:38:THR:HA	4:I:720:HOH:O	2.19	0.43
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.49	0.43
1:I:117:ARG:HB2	4:I:554:HOH:O	2.18	0.42
1:H:111:ASN:HA	4:H:656:HOH:O	2.18	0.42
1:F:79:ASP:CG	1:F:85:TRP:CZ2	2.92	0.42
1:F:12:TYR:CD2	1:F:48:ALA:HB2	2.53	0.42
1:A:414:ALA:HB2	1:A:424:TYR:CD2	2.54	0.42
1:J:425:ALA:HB1	1:J:432:ALA:HA	2.01	0.42
1:F:86:ILE:HG21	1:F:349:VAL:O	2.20	0.42
1:F:86:ILE:HD13	1:F:86:ILE:N	2.34	0.42
1:F:161:VAL:H	1:F:389:GLN:HE21	1.63	0.42
1:F:25:ILE:HD12	1:F:96:PHE:CD2	2.55	0.42
1:F:163:LYS:H	1:F:395:LEU:HD22	1.85	0.42
1:A:173:PHE:CE2	1:A:209:MET:HE3	2.54	0.42
1:E:108:ILE:CG2	1:E:108:ILE:O	2.67	0.42
1:C:344:PRO:HB2	1:C:348:ASP:HB3	2.02	0.42
1:D:64:GLN:CB	4:D:631:HOH:O	2.27	0.42
1:G:206:ALA:HA	1:G:226:TRP:CZ3	2.55	0.42
1:E:283:ALA:O	1:E:284:MET:CB	2.67	0.42
1:I:206:ALA:HA	1:I:226:TRP:CZ3	2.55	0.42
1:B:217:GLU:HG2	1:B:222:GLU:O	2.19	0.42
1:B:349:VAL:HG22	4:B:585:HOH:O	2.19	0.42
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.54	0.42
1:H:291:ASN:HA	1:H:292:PRO:HD3	1.81	0.42
1:I:59:TYR:HA	1:I:60:PRO:HD3	1.91	0.42
1:I:15:LYS:NZ	4:I:610:HOH:O	2.53	0.42
1:C:441:VAL:HG12	1:C:442:THR:N	2.34	0.42
1:E:54:THR:HG23	1:E:56:THR:O	2.19	0.42
1:D:70:LEU:HD22	1:D:95:ALA:HA	2.02	0.42
1:E:317:THR:HA	1:E:366:SER:HG	1.85	0.42
1:H:54:THR:HG23	1:H:56:THR:H	1.84	0.42
1:F:105:LEU:HD23	1:F:108:ILE:HD11	2.01	0.42
1:C:91:TYR:N	1:C:91:TYR:CD2	2.87	0.42
1:H:112:ILE:HD12	1:H:121:LEU:HD21	2.01	0.42
1:C:149:MET:HE1	1:C:251:HIS:HD1	1.85	0.42
1:A:411:ALA:O	1:A:415:ILE:HG13	2.20	0.42
1:G:373:GLY:O	1:G:440:HIS:CD2	2.73	0.42
1:I:424:TYR:CZ	1:I:428:HIS:CE1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ILE:HG12	1:G:85:TRP:CG	2.55	0.42
1:I:17:TYR:CE2	1:I:19:PRO:HA	2.55	0.42
1:F:343:LYS:N	4:F:517:HOH:O	2.34	0.42
1:E:303:LYS:NZ	1:E:354:GLN:HE21	2.18	0.42
1:E:370:LEU:HB2	4:E:532:HOH:O	2.18	0.42
1:D:268:ARG:HD3	1:D:268:ARG:C	2.39	0.42
1:F:206:ALA:HA	1:F:226:TRP:CZ3	2.54	0.42
1:F:72:ALA:HB2	1:F:91:TYR:CD1	2.55	0.42
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.02	0.42
1:G:283:ALA:O	1:G:284:MET:CB	2.67	0.42
1:H:175:LYS:H	1:H:175:LYS:HG2	1.49	0.42
1:G:108:ILE:HD12	1:G:108:ILE:C	2.40	0.42
1:D:112:ILE:HD12	1:D:121:LEU:HD21	2.02	0.41
1:C:367:SER:HB2	1:C:389:GLN:HB3	2.01	0.41
1:F:119:LYS:CE	4:F:564:HOH:O	2.68	0.41
1:H:412:ILE:O	1:H:416:MET:HG2	2.19	0.41
1:C:317:THR:O	1:C:318:ALA:HB3	2.20	0.41
1:F:154:ASP:O	1:F:384:THR:OG1	2.32	0.41
1:G:70:LEU:HD22	1:G:95:ALA:HA	2.01	0.41
1:E:406:ARG:O	1:E:410:GLN:HG2	2.19	0.41
1:G:230:ILE:HG13	1:G:237:MET:CE	2.50	0.41
1:A:283:ALA:O	1:A:284:MET:CB	2.67	0.41
1:G:38:THR:OG1	1:G:41:GLN:HG3	2.20	0.41
1:G:119:LYS:HB2	1:G:119:LYS:HE3	1.47	0.41
1:H:174:GLU:HG3	1:H:212:ILE:HD11	2.01	0.41
1:I:112:ILE:HD12	1:I:121:LEU:HD21	2.02	0.41
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.20	0.41
1:A:54:THR:HG23	1:A:56:THR:O	2.20	0.41
1:A:158:TYR:CE1	1:A:408:VAL:HG11	2.55	0.41
1:A:227:PHE:N	1:A:227:PHE:CD1	2.88	0.41
1:E:104:LEU:C	1:E:104:LEU:HD23	2.41	0.41
1:D:282:ARG:HG3	1:D:285:HIS:CD2	2.55	0.41
1:G:149:MET:HE1	1:G:251:HIS:HD1	1.85	0.41
1:F:25:ILE:CD1	1:F:96:PHE:CD2	3.03	0.41
1:A:397:HIS:HA	1:A:398:PRO:HD3	1.87	0.41
1:D:25:ILE:HD13	1:D:96:PHE:CE2	2.55	0.41
1:J:165:LYS:HB3	1:J:191:ASP:OD2	2.21	0.41
1:H:98:GLU:CD	4:H:667:HOH:O	2.59	0.41
1:A:285:HIS:CG	1:A:286:ALA:N	2.88	0.41
1:I:438:TRP:O	1:I:441:VAL:HG22	2.20	0.41
1:J:158:TYR:CE1	1:J:408:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:HIS:CG	1:B:286:ALA:N	2.89	0.41
1:E:328:TRP:O	1:E:332:GLN:HG2	2.21	0.41
1:G:230:ILE:CG1	1:G:237:MET:HE3	2.50	0.41
1:F:119:LYS:HE3	1:F:119:LYS:HB2	1.85	0.41
1:H:39:ILE:CD1	1:H:85:TRP:HB2	2.50	0.41
1:G:17:TYR:CE2	1:G:19:PRO:HA	2.55	0.41
1:J:424:TYR:CZ	1:J:428:HIS:CE1	3.08	0.41
1:B:59:TYR:O	1:B:61:TRP:HD1	2.04	0.41
1:E:122:ARG:HD2	4:E:528:HOH:O	2.20	0.41
1:I:385:ASP:HB2	4:I:566:HOH:O	2.19	0.41
1:G:143:ILE:HD11	1:G:338:ARG:HG2	2.02	0.41
1:E:320:ALA:O	1:E:442:THR:CB	2.64	0.41
1:A:338:ARG:HD2	4:A:710:HOH:O	2.20	0.41
1:G:41:GLN:HB3	1:G:117:ARG:NH1	2.36	0.41
1:E:230:ILE:HD11	1:E:254:VAL:HG22	2.02	0.41
1:F:209:MET:CA	1:F:209:MET:HE3	2.36	0.41
1:I:47:ALA:O	1:I:51:SER:HB3	2.21	0.41
1:D:158:TYR:CE1	1:D:408:VAL:HG11	2.56	0.41
1:I:333:ASN:O	1:I:336:ILE:HG22	2.20	0.41
1:C:163:LYS:HE3	3:C:446:CAP:O2P	2.21	0.41
1:H:121:LEU:N	1:H:294:HIS:HD2	2.08	0.41
1:I:414:ALA:HB2	1:I:424:TYR:CD2	2.56	0.41
1:C:336:ILE:HA	1:C:336:ILE:HD12	1.80	0.41
1:I:347:ASN:N	1:I:347:ASN:OD1	2.42	0.41
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.87	0.41
1:E:202:PHE:CD2	1:E:240:ARG:HG2	2.56	0.41
1:G:202:PHE:CD2	1:G:240:ARG:HG2	2.56	0.41
1:D:189:KCX:OQ1	3:D:446:CAP:O3	2.39	0.41
1:J:376:GLN:N	1:J:377:PRO:CD	2.83	0.41
1:J:196:SER:N	1:J:197:PRO:CD	2.84	0.41
1:J:397:HIS:CD2	1:J:404:GLY:HA2	2.56	0.40
1:D:126:LEU:HA	1:D:126:LEU:HD12	1.97	0.40
1:J:195:THR:OG1	1:J:196:SER:N	2.53	0.40
1:C:314:HIS:HA	1:C:365:THR:HB	2.03	0.40
1:H:125:ASP:OD1	1:H:126:LEU:N	2.53	0.40
1:J:226:TRP:CD2	1:J:228:ALA:HB2	2.57	0.40
1:C:349:VAL:O	1:C:349:VAL:CG1	2.68	0.40
1:J:283:ALA:O	1:J:284:MET:CB	2.69	0.40
1:G:397:HIS:ND1	1:G:398:PRO:HD2	2.36	0.40
1:G:181:LEU:HD22	1:G:224:LYS:HD2	2.03	0.40
1:H:355:LYS:HE3	1:H:357:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:LYS:HE2	1:F:355:LYS:HB3	1.92	0.40
1:A:206:ALA:HA	1:A:226:TRP:CZ3	2.56	0.40
1:D:284:MET:HG2	1:D:284:MET:O	2.21	0.40
1:E:101:LEU:HB3	1:E:102:PRO:HD3	2.04	0.40
1:C:328:TRP:O	1:C:332:GLN:HG2	2.20	0.40
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.85	0.40
1:E:397:HIS:HD2	1:E:404:GLY:HA2	1.84	0.40
1:H:283:ALA:O	1:H:284:MET:HB3	2.22	0.40
1:F:336:ILE:HA	1:F:336:ILE:HD12	1.83	0.40
1:H:427:THR:HG23	1:H:428:HIS:ND1	2.36	0.40
1:B:202:PHE:CD2	1:B:240:ARG:HG2	2.57	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	434/444 (98%)	418 (96%)	16 (4%)	0	100	100
1	B	435/444 (98%)	418 (96%)	16 (4%)	1 (0%)	52	64
1	C	435/444 (98%)	420 (97%)	15 (3%)	0	100	100
1	D	433/444 (98%)	417 (96%)	16 (4%)	0	100	100
1	E	431/444 (97%)	415 (96%)	15 (4%)	1 (0%)	52	64
1	F	430/444 (97%)	405 (94%)	21 (5%)	4 (1%)	21	24
1	G	433/444 (98%)	415 (96%)	18 (4%)	0	100	100
1	H	434/444 (98%)	417 (96%)	17 (4%)	0	100	100
1	I	433/444 (98%)	417 (96%)	15 (4%)	1 (0%)	52	64
1	J	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
All	All	4332/4440 (98%)	4161 (96%)	164 (4%)	7 (0%)	52	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	345	ASP
1	F	418	GLY
1	F	60	PRO
1	I	284	MET
1	E	284	MET
1	F	284	MET
1	B	8	ILE

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	334/355 (94%)	322 (96%)	12 (4%)	42	57
1	B	339/355 (96%)	330 (97%)	9 (3%)	52	70
1	C	337/355 (95%)	326 (97%)	11 (3%)	45	61
1	D	340/355 (96%)	332 (98%)	8 (2%)	57	74
1	E	335/355 (94%)	326 (97%)	9 (3%)	52	70
1	F	328/355 (92%)	312 (95%)	16 (5%)	31	41
1	G	337/355 (95%)	332 (98%)	5 (2%)	72	85
1	H	338/355 (95%)	328 (97%)	10 (3%)	48	65
1	I	341/355 (96%)	332 (97%)	9 (3%)	54	71
1	J	335/355 (94%)	326 (97%)	9 (3%)	52	70
All	All	3364/3550 (95%)	3266 (97%)	98 (3%)	50	66

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	105	LEU
1	A	119	LYS
1	A	149	MET
1	A	268	ARG

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Mol	Chain	Res	Type
1	A	340	SER
1	A	345	ASP
1	A	347	ASN
1	A	363	PHE
1	A	376	GLN
1	A	378	VAL
1	A	427	THR
1	B	18	GLU
1	B	211	LYS
1	B	218	ASN
1	B	268	ARG
1	B	352	LEU
1	B	358	SER
1	B	363	PHE
1	B	376	GLN
1	B	395	LEU
1	C	8	ILE
1	C	93	PHE
1	C	107	SER
1	C	194	LEU
1	C	220	THR
1	C	268	ARG
1	C	301	LEU
1	C	343	LYS
1	C	363	PHE
1	C	389	GLN
1	C	395	LEU
1	D	93	PHE
1	D	117	ARG
1	D	122	ARG
1	D	191	ASP
1	D	207	GLU
1	D	268	ARG
1	D	363	PHE
1	D	376	GLN
1	E	58	LEU
1	E	117	ARG
1	E	119	LYS
1	E	122	ARG
1	E	207	GLU
1	E	268	ARG
1	E	363	PHE

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Mol	Chain	Res	Type
1	E	376	GLN
1	E	435	LEU
1	F	64	GLN
1	F	85	TRP
1	F	87	VAL
1	F	93	PHE
1	F	108	ILE
1	F	117	ARG
1	F	119	LYS
1	F	209	MET
1	F	235	LEU
1	F	268	ARG
1	F	337	LEU
1	F	347	ASN
1	F	349	VAL
1	F	363	PHE
1	F	366	SER
1	F	382	LEU
1	G	93	PHE
1	G	117	ARG
1	G	148	LYS
1	G	268	ARG
1	G	363	PHE
1	H	58	LEU
1	H	175	LYS
1	H	191	ASP
1	H	268	ARG
1	H	301	LEU
1	H	343	LYS
1	H	363	PHE
1	H	376	GLN
1	H	379	ILE
1	H	389	GLN
1	I	58	LEU
1	I	117	ARG
1	I	122	ARG
1	I	234	LEU
1	I	241	LEU
1	I	268	ARG
1	I	340	SER
1	I	346	GLU
1	I	363	PHE

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Mol	Chain	Res	Type
1	J	98	GLU
1	J	107	SER
1	J	122	ARG
1	J	191	ASP
1	J	193	ASN
1	J	268	ARG
1	J	363	PHE
1	J	370	LEU
1	J	435	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	312	GLN
1	A	347	ASN
1	A	354	GLN
1	A	376	GLN
1	B	279	HIS
1	B	294	HIS
1	B	312	GLN
1	B	354	GLN
1	B	376	GLN
1	C	294	HIS
1	C	312	GLN
1	C	354	GLN
1	C	417	GLN
1	D	294	HIS
1	D	312	GLN
1	D	354	GLN
1	D	376	GLN
1	D	389	GLN
1	D	417	GLN
1	D	440	HIS
1	E	312	GLN
1	E	351	HIS
1	E	354	GLN
1	E	376	GLN
1	E	389	GLN
1	E	410	GLN
1	E	417	GLN
1	F	78	HIS

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Mol	Chain	Res	Type
1	F	312	GLN
1	F	332	GLN
1	F	354	GLN
1	F	389	GLN
1	G	279	HIS
1	G	294	HIS
1	G	312	GLN
1	G	354	GLN
1	H	41	GLN
1	H	279	HIS
1	H	294	HIS
1	H	312	GLN
1	H	354	GLN
1	H	376	GLN
1	I	294	HIS
1	I	312	GLN
1	I	332	GLN
1	I	354	GLN
1	I	389	GLN
1	J	193	ASN
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	0.72	0	7,12,14	1.59	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KCX	B	189	1,2	7,11,12	0.85	0	7,12,14	0.90	0
1	KCX	C	189	1,2	7,11,12	0.75	0	7,12,14	1.04	0
1	KCX	D	189	1,2	7,11,12	0.80	0	7,12,14	1.14	2 (28%)
1	KCX	E	189	1,2	7,11,12	0.54	0	7,12,14	1.36	1 (14%)
1	KCX	F	189	1,2	7,11,12	0.83	1 (14%)	7,12,14	1.47	1 (14%)
1	KCX	G	189	1,2	7,11,12	0.72	0	7,12,14	0.98	0
1	KCX	H	189	1,2	7,11,12	0.69	0	7,12,14	1.18	1 (14%)
1	KCX	I	189	1,2	7,11,12	0.71	0	7,12,14	1.64	2 (28%)
1	KCX	J	189	1,2	7,11,12	0.74	0	7,12,14	1.39	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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	189	KCX	CE-NZ	2.01	1.50	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	KCX	CE-NZ-CX	-3.63	119.38	123.49
1	I	189	KCX	CE-NZ-CX	-3.58	119.44	123.49
1	F	189	KCX	CE-NZ-CX	-3.20	119.87	123.49
1	J	189	KCX	CE-NZ-CX	-3.02	120.08	123.49
1	E	189	KCX	CE-NZ-CX	-2.80	120.32	123.49
1	H	189	KCX	CE-NZ-CX	-2.14	121.06	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	189	KCX	CE-NZ-CX	-2.12	121.09	123.49
1	I	189	KCX	O-C-CA	-2.07	120.10	125.49
1	D	189	KCX	O-C-CA	-2.03	120.21	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	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	0.90	0	15,31,31	0.90	0
3	CAP	B	446	2	14,20,20	0.88	0	15,31,31	0.77	0
3	CAP	C	446	2	14,20,20	0.95	1 (7%)	15,31,31	0.80	0
3	CAP	D	446	2	14,20,20	0.87	0	15,31,31	0.76	0
3	CAP	E	446	2	14,20,20	0.90	0	15,31,31	0.74	0
3	CAP	F	446	2	14,20,20	0.88	0	15,31,31	0.94	1 (6%)
3	CAP	G	446	2	14,20,20	0.79	0	15,31,31	0.77	1 (6%)
3	CAP	H	446	2	14,20,20	0.83	0	15,31,31	0.80	0
3	CAP	I	446	2	14,20,20	0.85	0	15,31,31	0.79	0
3	CAP	J	446	2	14,20,20	0.88	1 (7%)	15,31,31	0.76	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	2	-	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
3	CAP	J	446	2	-	0/23/29/29	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	446	CAP	O2-C2	2.03	1.45	1.43
3	C	446	CAP	O2-C2	2.09	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	446	CAP	O6P-P2-O5	2.03	112.40	106.56
3	F	446	CAP	O6P-P2-O5P	2.06	115.23	107.38

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
3	C	446	CAP	1	0
3	D	446	CAP	1	0

5.7 Other polymers (i)

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	436/444 (98%)	-0.03	10 (2%) 64 72	12, 23, 39, 50	0
1	B	437/444 (98%)	-0.08	9 (2%) 67 74	10, 21, 34, 43	0
1	C	437/444 (98%)	-0.09	11 (2%) 61 70	9, 20, 40, 47	0
1	D	435/444 (97%)	-0.03	9 (2%) 67 74	10, 21, 37, 44	0
1	E	435/444 (97%)	0.04	23 (5%) 30 39	11, 21, 48, 56	0
1	F	434/444 (97%)	0.39	27 (6%) 24 32	14, 29, 46, 55	0
1	G	435/444 (97%)	0.11	10 (2%) 64 72	14, 26, 40, 46	0
1	H	436/444 (98%)	0.21	26 (5%) 25 33	14, 26, 48, 55	0
1	I	435/444 (97%)	-0.12	6 (1%) 78 83	11, 21, 34, 44	0
1	J	436/444 (98%)	0.03	21 (4%) 34 43	10, 21, 53, 58	0
All	All	4356/4440 (98%)	0.04	152 (3%) 48 56	9, 23, 41, 58	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	421	LEU	5.9
1	J	59	TYR	5.4
1	D	59	TYR	5.1
1	F	425	ALA	4.9
1	J	418	GLY	4.8
1	F	59	TYR	4.6
1	C	7	THR	4.2
1	H	427	THR	4.2
1	F	36	GLY	4.2
1	A	59	TYR	4.1
1	H	418	GLY	3.9
1	H	421	LEU	3.9
1	H	218	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	59	TYR	3.9
1	J	421	LEU	3.8
1	J	8	ILE	3.8
1	F	16	GLY	3.7
1	E	434	ALA	3.6
1	C	59	TYR	3.6
1	H	426	LYS	3.5
1	D	58	LEU	3.5
1	A	422	ASP	3.4
1	F	420	PRO	3.4
1	B	7	THR	3.4
1	H	422	ASP	3.4
1	E	8	ILE	3.4
1	E	422	ASP	3.3
1	E	418	GLY	3.3
1	H	35	GLU	3.3
1	J	426	LYS	3.2
1	E	414	ALA	3.2
1	E	425	ALA	3.2
1	H	36	GLY	3.2
1	E	7	THR	3.2
1	A	218	ASN	3.1
1	J	398	PRO	3.1
1	F	421	LEU	3.1
1	C	444	VAL	3.1
1	F	435	LEU	3.0
1	E	59	TYR	3.0
1	G	441	VAL	3.0
1	F	426	LYS	3.0
1	J	427	THR	3.0
1	G	218	ASN	3.0
1	I	58	LEU	3.0
1	J	434	ALA	3.0
1	J	346	GLU	3.0
1	B	59	TYR	2.9
1	F	347	ASN	2.9
1	E	398	PRO	2.9
1	J	425	ALA	2.8
1	H	161	VAL	2.8
1	J	424	TYR	2.8
1	J	436	GLU	2.8
1	B	358	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	427	THR	2.8
1	J	444	VAL	2.7
1	H	57	THR	2.7
1	E	161	VAL	2.7
1	J	161	VAL	2.7
1	H	414	ALA	2.7
1	E	419	ILE	2.7
1	F	79	ASP	2.7
1	G	161	VAL	2.7
1	H	81	GLY	2.7
1	F	81	GLY	2.6
1	G	36	GLY	2.6
1	F	422	ASP	2.6
1	H	444	VAL	2.6
1	F	436	GLU	2.6
1	I	57	THR	2.6
1	J	218	ASN	2.6
1	H	436	GLU	2.6
1	H	398	PRO	2.6
1	B	441	VAL	2.6
1	E	376	GLN	2.5
1	G	426	LYS	2.5
1	G	59	TYR	2.5
1	B	160	VAL	2.5
1	A	35	GLU	2.5
1	J	439	GLY	2.5
1	E	415	ILE	2.5
1	D	418	GLY	2.5
1	C	426	LYS	2.5
1	E	433	ARG	2.5
1	J	422	ASP	2.4
1	F	444	VAL	2.4
1	J	417	GLN	2.4
1	J	35	GLU	2.4
1	E	417	GLN	2.4
1	C	8	ILE	2.4
1	H	441	VAL	2.4
1	C	427	THR	2.4
1	H	432	ALA	2.4
1	G	194	LEU	2.4
1	H	283	ALA	2.4
1	I	56	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLN	2.4
1	E	218	ASN	2.3
1	C	441	VAL	2.3
1	C	421	LEU	2.3
1	A	8	ILE	2.3
1	G	106	ALA	2.3
1	A	420	PRO	2.3
1	J	399	ASP	2.3
1	F	419	ILE	2.3
1	F	85	TRP	2.3
1	G	422	ASP	2.3
1	C	36	GLY	2.3
1	D	423	GLU	2.3
1	H	376	GLN	2.2
1	E	373	GLY	2.2
1	E	407	ALA	2.2
1	I	346	GLU	2.2
1	C	425	ALA	2.2
1	F	109	ALA	2.2
1	E	387	VAL	2.2
1	B	414	ALA	2.2
1	D	106	ALA	2.2
1	D	109	ALA	2.2
1	F	418	GLY	2.2
1	A	347	ASN	2.2
1	F	41	GLN	2.2
1	H	417	GLN	2.2
1	A	423	GLU	2.2
1	I	35	GLU	2.2
1	F	345	ASP	2.2
1	E	442	THR	2.2
1	H	59	TYR	2.2
1	F	432	ALA	2.2
1	D	36	GLY	2.1
1	A	58	LEU	2.1
1	F	42	ALA	2.1
1	F	11	TYR	2.1
1	H	38	THR	2.1
1	F	440	HIS	2.1
1	H	439	GLY	2.1
1	H	58	LEU	2.1
1	B	422	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	160	VAL	2.1
1	C	218	ASN	2.1
1	D	18	GLU	2.1
1	E	347	ASN	2.1
1	F	14	ASP	2.1
1	H	399	ASP	2.1
1	B	161	VAL	2.1
1	F	349	VAL	2.1
1	F	218	ASN	2.0
1	E	10	ASP	2.0
1	J	438	TRP	2.0
1	H	431	LEU	2.0
1	D	218	ASN	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	E	189	12/13	0.97	0.24	-	15,17,18,19	0
1	KCX	A	189	12/13	0.98	0.18	-	15,17,18,18	0
1	KCX	G	189	12/13	0.98	0.26	-	20,21,22,23	0
1	KCX	C	189	12/13	0.97	0.17	-	14,15,18,18	0
1	KCX	J	189	12/13	0.97	0.21	-	18,19,20,22	0
1	KCX	H	189	12/13	0.98	0.19	-	20,22,22,23	0
1	KCX	F	189	12/13	0.94	0.20	-	22,22,26,28	0
1	KCX	D	189	12/13	0.98	0.22	-	10,12,14,14	0
1	KCX	B	189	12/13	0.98	0.22	-	12,13,14,15	0
1	KCX	I	189	12/13	0.98	0.19	-	10,12,13,13	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.96	0.20	0.08	27,27,27,27	0
3	CAP	E	446	21/21	0.95	0.17	0.03	19,28,30,31	0
3	CAP	G	446	21/21	0.97	0.15	-0.37	16,25,26,27	0
3	CAP	D	446	21/21	0.99	0.13	-0.55	14,14,16,17	0
3	CAP	J	446	21/21	0.97	0.14	-0.56	19,26,27,28	0
3	CAP	I	446	21/21	0.99	0.12	-0.66	11,14,16,18	0
3	CAP	C	446	21/21	0.98	0.13	-0.72	16,21,22,23	0
3	CAP	H	446	21/21	0.97	0.14	-0.79	26,28,31,32	0
3	CAP	B	446	21/21	0.98	0.13	-0.79	14,19,20,21	0
2	MG	G	445	1/1	0.99	0.19	-0.81	26,26,26,26	0
2	MG	E	445	1/1	0.99	0.18	-0.84	25,25,25,25	0
3	CAP	A	446	21/21	0.98	0.11	-1.10	13,18,19,20	0
3	CAP	F	446	21/21	0.97	0.11	-1.85	12,23,25,25	0
2	MG	D	445	1/1	0.99	0.12	-1.88	12,12,12,12	0
2	MG	J	445	1/1	0.96	0.09	-2.35	16,16,16,16	0
2	MG	I	445	1/1	0.99	0.11	-2.37	11,11,11,11	0
2	MG	B	445	1/1	0.99	0.12	-2.48	17,17,17,17	0
2	MG	C	445	1/1	0.99	0.09	-3.67	21,21,21,21	0
2	MG	A	445	1/1	0.98	0.08	-4.25	15,15,15,15	0
2	MG	F	445	1/1	0.97	0.09	-4.44	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.