



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:00 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 wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

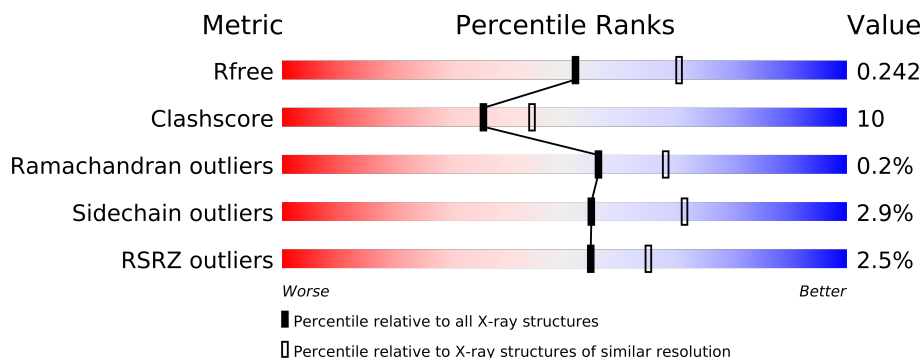
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
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 hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Ribulose biphosphate 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).

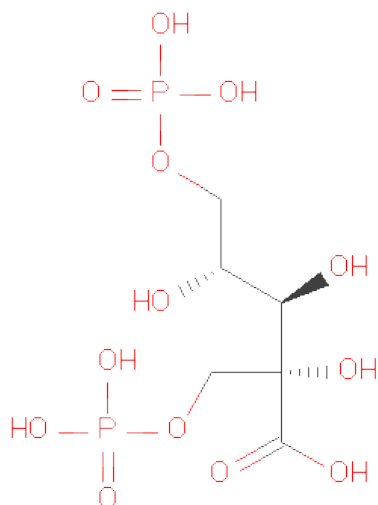
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	J	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

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

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

*Continued on next page...*

*Continued from previous page...*

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.

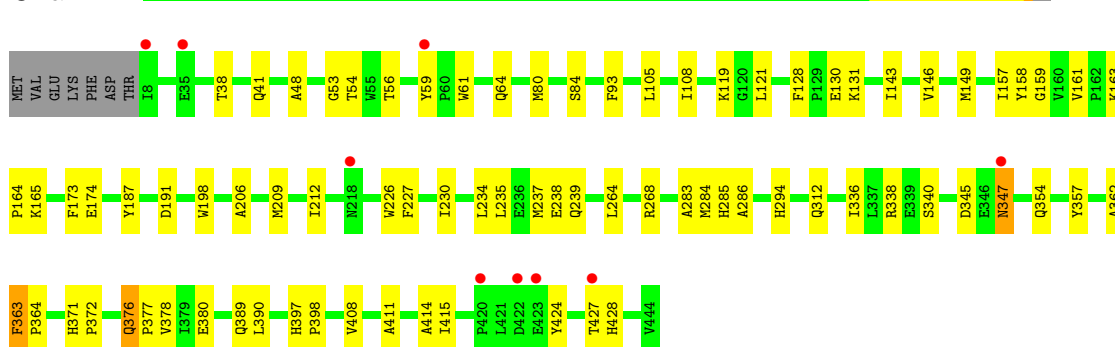
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	246	Total	O	0	0
			246	246		
4	C	260	Total	O	0	0
			260	260		
4	D	256	Total	O	0	0
			256	256		
4	E	224	Total	O	0	0
			224	224		
4	F	168	Total	O	0	0
			168	168		
4	G	195	Total	O	0	0
			195	195		
4	H	217	Total	O	0	0
			217	217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

### 3 Residue-property plots

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

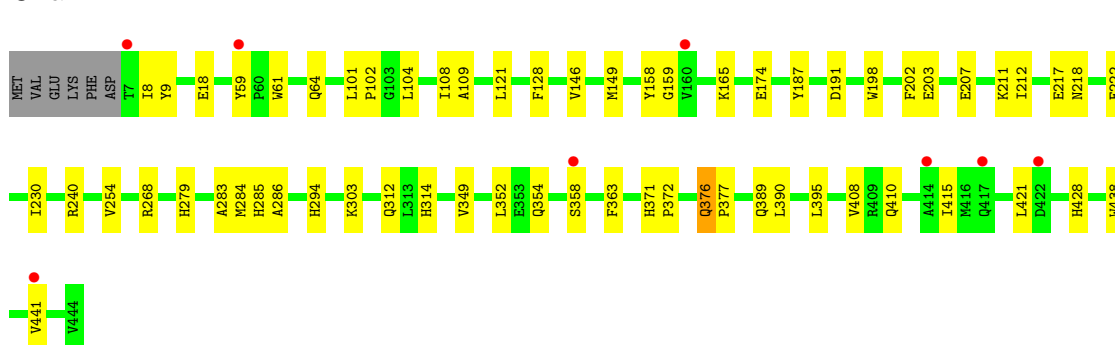
- Molecule 1: Ribulose biphosphate carboxylase

Chain A:



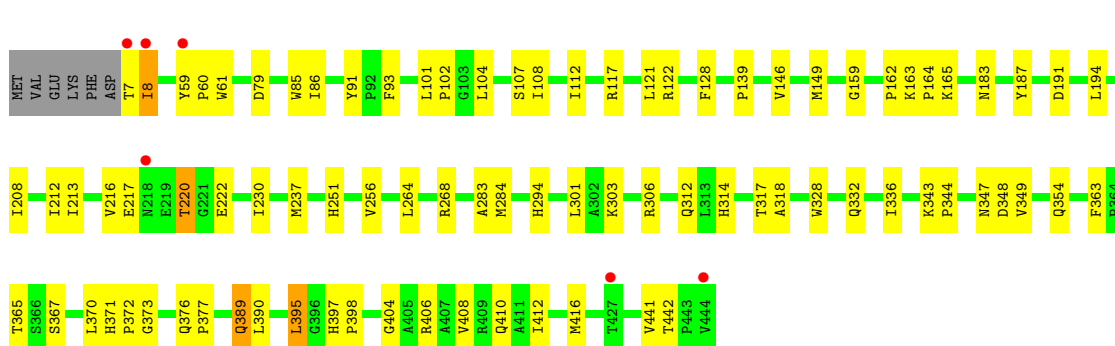
- Molecule 1: Ribulose biphosphate carboxylase

Chain B:



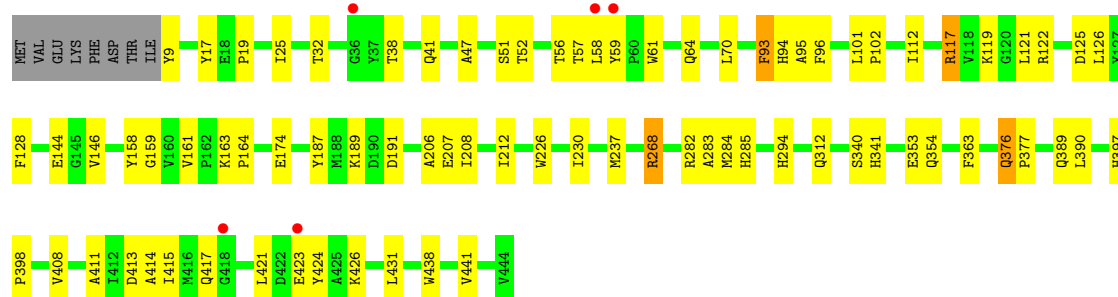
- Molecule 1: Ribulose biphosphate carboxylase

Chain C:



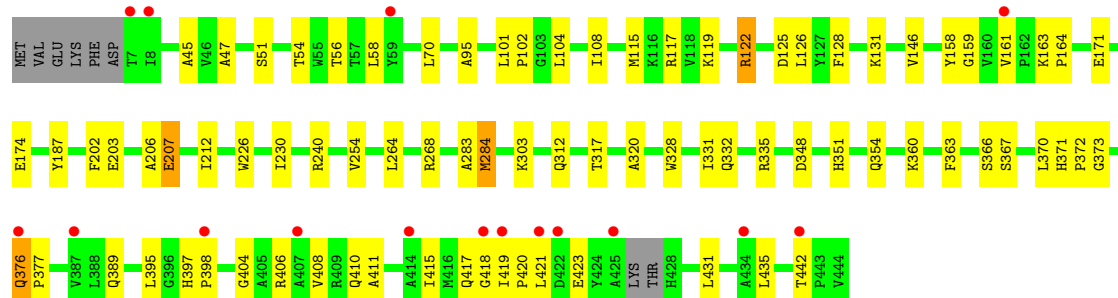
- Molecule 1: Ribulose biphosphate carboxylase

Chain D:



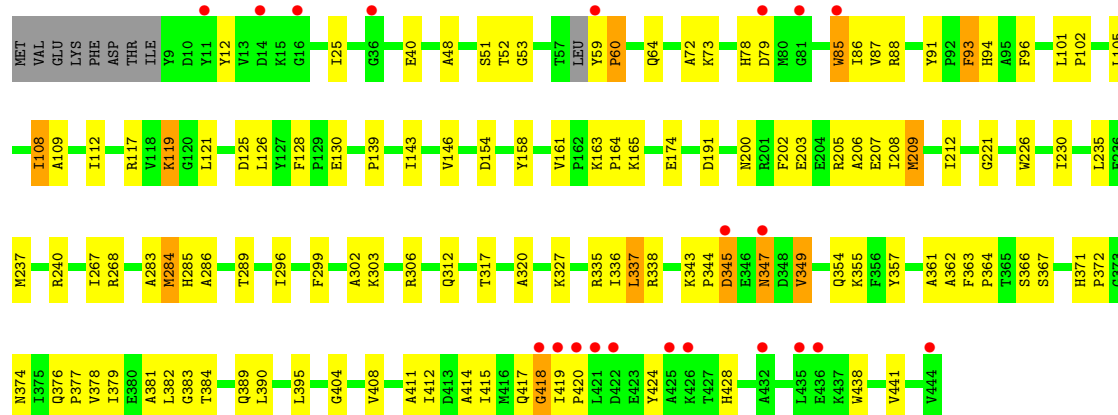
- Molecule 1: Ribulose biphosphate carboxylase

Chain E:



- Molecule 1: Ribulose biphosphate carboxylase

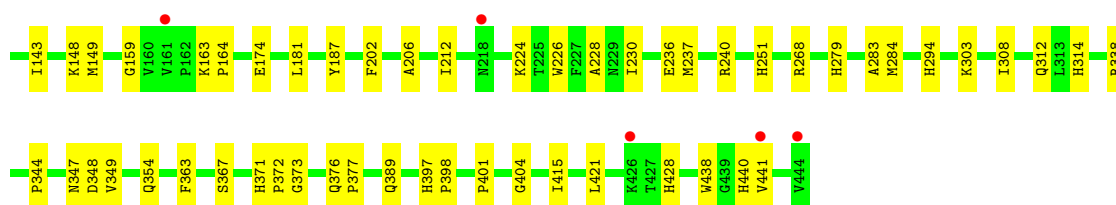
Chain F:



- Molecule 1: Ribulose biphosphate carboxylase

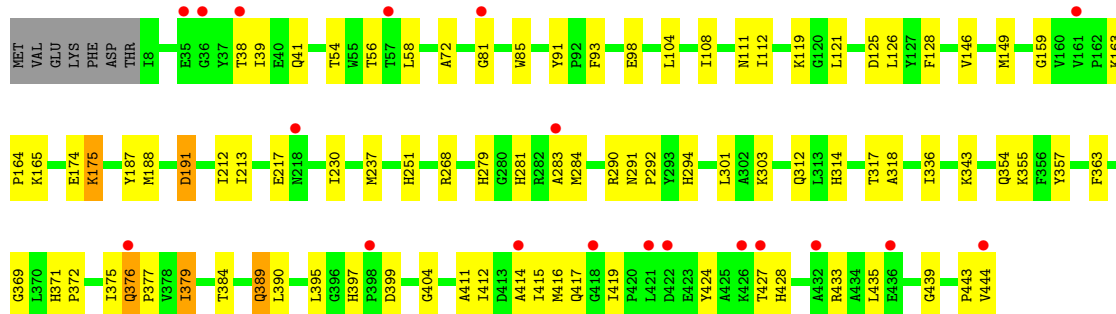
Chain G:





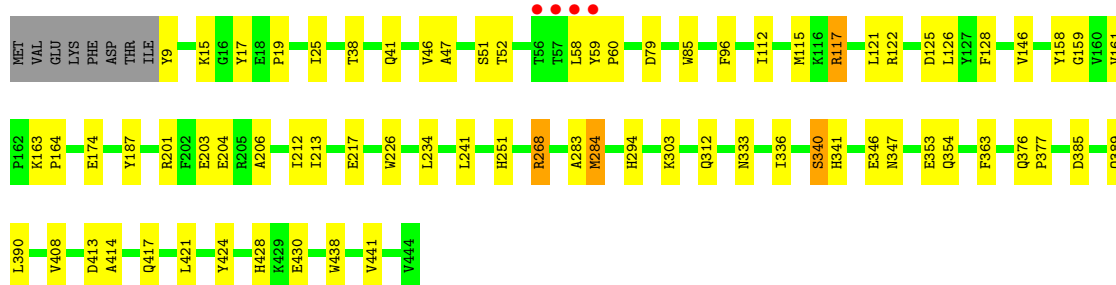
• Molecule 1: Ribulose biphosphate carboxylase

Chain H:



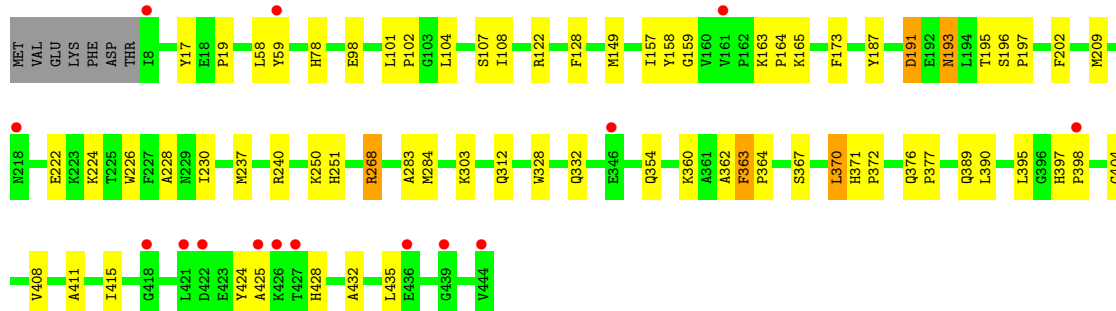
• Molecule 1: Ribulose biphosphate carboxylase

Chain I:



• Molecule 1: Ribulose biphosphate carboxylase

Chain J:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	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 <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3404	0	3295	64	0
1	B	3432	0	3348	39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3421	0	3332	77	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 709 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/444 (98%)	418 (96%)	16 (4%)	0	100	100
1	B	435/444 (98%)	418 (96%)	16 (4%)	1 (0%)	56	68
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%)	56	68
1	F	430/444 (97%)	405 (94%)	21 (5%)	4 (1%)	25	26
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%)	56	68
1	J	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
All	All	4332/4440 (98%)	4161 (96%)	164 (4%)	7 (0%)	56	68

5 of 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	284	MET

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/355 (94%)	322 (96%)	12 (4%)	47	61
1	B	339/355 (96%)	330 (97%)	9 (3%)	57	74
1	C	337/355 (95%)	326 (97%)	11 (3%)	50	66
1	D	340/355 (96%)	332 (98%)	8 (2%)	61	79
1	E	335/355 (94%)	326 (97%)	9 (3%)	57	74
1	F	328/355 (92%)	312 (95%)	16 (5%)	35	45
1	G	337/355 (95%)	332 (98%)	5 (2%)	76	89
1	H	338/355 (95%)	328 (97%)	10 (3%)	53	70
1	I	341/355 (96%)	332 (97%)	9 (3%)	59	76
1	J	335/355 (94%)	326 (97%)	9 (3%)	57	74
All	All	3364/3550 (95%)	3266 (97%)	98 (3%)	55	71

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	207	GLU
1	F	117	ARG
1	J	107	SER
1	E	268	ARG
1	F	64	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
1	F	78	HIS
1	I	389	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	389	GLN
1	F	312	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	11,11,12	5.32	2 (18%)	10,12,14	2.13	4 (40%)
1	KCX	B	189	1,2	11,11,12	5.40	2 (18%)	10,12,14	2.11	4 (40%)
1	KCX	C	189	1,2	11,11,12	5.46	2 (18%)	10,12,14	1.79	4 (40%)
1	KCX	D	189	1,2	11,11,12	5.48	2 (18%)	10,12,14	1.84	4 (40%)
1	KCX	E	189	1,2	11,11,12	5.09	1 (9%)	10,12,14	1.84	3 (30%)
1	KCX	F	189	1,2	11,11,12	5.38	2 (18%)	10,12,14	1.84	4 (40%)
1	KCX	G	189	1,2	11,11,12	5.32	2 (18%)	10,12,14	1.57	3 (30%)
1	KCX	H	189	1,2	11,11,12	5.35	2 (18%)	10,12,14	1.78	4 (40%)
1	KCX	I	189	1,2	11,11,12	5.36	2 (18%)	10,12,14	2.03	3 (30%)
1	KCX	J	189	1,2	11,11,12	5.09	2 (18%)	10,12,14	1.90	3 (30%)

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	-	0/8/10/12	0/0/0/0
1	KCX	B	189	1,2	-	0/8/10/12	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	D	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	E	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	F	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	G	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	H	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	I	189	1,2	-	0/8/10/12	0/0/0/0
1	KCX	J	189	1,2	-	0/8/10/12	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	KCX	O-C	17.86	1.23	1.11
1	C	189	KCX	O-C	17.68	1.23	1.11
1	B	189	KCX	O-C	17.58	1.23	1.11
1	H	189	KCX	O-C	17.41	1.23	1.11
1	I	189	KCX	O-C	17.39	1.23	1.11

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	KCX	OQ2-CX-NZ	4.05	121.38	116.33
1	B	189	KCX	OQ2-CX-NZ	3.88	121.16	116.33
1	I	189	KCX	C-CA-N	-3.75	110.08	113.83
1	F	189	KCX	OQ2-CX-NZ	3.58	120.78	116.33
1	C	189	KCX	OQ2-CX-NZ	3.54	120.74	116.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	20,20,20	0.79	0	31,31,31	0.91	1 (3%)
3	CAP	B	446	2	20,20,20	0.77	0	31,31,31	0.99	2 (6%)
3	CAP	C	446	2	20,20,20	0.79	0	31,31,31	0.91	1 (3%)
3	CAP	D	446	2	20,20,20	0.74	0	31,31,31	0.90	1 (3%)
3	CAP	E	446	2	20,20,20	0.77	0	31,31,31	1.01	2 (6%)
3	CAP	F	446	2	20,20,20	0.75	0	31,31,31	0.96	0
3	CAP	G	446	2	20,20,20	0.69	0	31,31,31	0.97	2 (6%)
3	CAP	H	446	2	20,20,20	0.75	0	31,31,31	1.22	2 (6%)
3	CAP	I	446	2	20,20,20	0.79	0	31,31,31	0.94	1 (3%)
3	CAP	J	446	2	20,20,20	0.74	0	31,31,31	0.99	1 (3%)

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	-	0/29/29/29	0/0/0/0
3	CAP	B	446	2	-	0/29/29/29	0/0/0/0
3	CAP	C	446	2	-	0/29/29/29	0/0/0/0
3	CAP	D	446	2	-	0/29/29/29	0/0/0/0
3	CAP	E	446	2	-	0/29/29/29	0/0/0/0
3	CAP	F	446	2	-	0/29/29/29	0/0/0/0
3	CAP	G	446	2	-	0/29/29/29	0/0/0/0
3	CAP	H	446	2	-	0/29/29/29	0/0/0/0
3	CAP	I	446	2	-	0/29/29/29	0/0/0/0
3	CAP	J	446	2	-	0/29/29/29	0/0/0/0

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	446	CAP	O1-C1-C2	4.17	113.21	108.34
3	E	446	CAP	O7-C-C2	3.17	120.49	113.58
3	G	446	CAP	O7-C-C2	3.05	120.22	113.58
3	J	446	CAP	O7-C-C2	3.04	120.21	113.58
3	D	446	CAP	O7-C-C2	2.94	119.99	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/444 (98%)	-0.13	9 (2%) 60 70	12, 23, 39, 50	0
1	B	438/444 (98%)	-0.18	8 (1%) 65 74	10, 21, 34, 43	0
1	C	438/444 (98%)	-0.19	6 (1%) 72 80	9, 20, 40, 47	0
1	D	436/444 (98%)	-0.13	5 (1%) 77 85	10, 21, 37, 44	0
1	E	436/444 (98%)	-0.07	16 (3%) 39 50	11, 21, 48, 56	0
1	F	435/444 (97%)	0.26	21 (4%) 29 39	14, 29, 46, 55	0
1	G	436/444 (98%)	0.01	7 (1%) 68 77	14, 26, 40, 46	0
1	H	437/444 (98%)	0.09	19 (4%) 34 44	14, 26, 48, 55	0
1	I	436/444 (98%)	-0.21	4 (0%) 81 88	11, 21, 34, 44	0
1	J	437/444 (98%)	-0.09	15 (3%) 43 53	10, 21, 53, 58	0
All	All	4366/4440 (98%)	-0.06	110 (2%) 54 65	9, 23, 41, 58	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	TYR	5.1
1	J	59	TYR	5.1
1	E	421	LEU	4.8
1	F	425	ALA	4.3
1	J	418	GLY	4.2

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

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

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	F	189	12/13	0.19	2.17	22,22,26,28	0
1	KCX	D	189	12/13	0.20	1.57	10,12,14,14	0
1	KCX	G	189	12/13	0.23	1.53	20,21,22,23	0
1	KCX	E	189	12/13	0.22	1.25	15,17,18,19	0
1	KCX	J	189	12/13	0.20	1.14	18,19,20,22	0
1	KCX	B	189	12/13	0.20	0.94	12,13,14,15	0
1	KCX	I	189	12/13	0.17	0.86	10,12,13,13	0
1	KCX	A	189	12/13	0.17	0.77	15,17,18,18	0
1	KCX	H	189	12/13	0.18	0.37	20,22,22,23	0
1	KCX	C	189	12/13	0.16	0.22	14,15,18,18	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	H	445	1/1	0.22	0.83	27,27,27,27	0
3	CAP	E	446	21/21	0.18	0.45	19,28,30,31	0
2	MG	E	445	1/1	0.19	-0.12	25,25,25,25	0
2	MG	G	445	1/1	0.19	-0.18	26,26,26,26	0
3	CAP	J	446	21/21	0.14	-0.23	19,26,27,28	0
3	CAP	D	446	21/21	0.13	-0.29	14,14,16,17	0
3	CAP	G	446	21/21	0.14	-0.35	16,25,26,27	0
3	CAP	H	446	21/21	0.15	-0.37	26,28,31,32	0
3	CAP	I	446	21/21	0.12	-0.42	11,14,16,18	0
3	CAP	C	446	21/21	0.13	-0.51	16,21,22,23	0
3	CAP	B	446	21/21	0.13	-0.58	14,19,20,21	0
2	MG	D	445	1/1	0.15	-0.74	12,12,12,12	0
3	CAP	A	446	21/21	0.11	-0.79	13,18,19,20	0
2	MG	B	445	1/1	0.13	-1.54	17,17,17,17	0
3	CAP	F	446	21/21	0.11	-1.79	12,23,25,25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	I	445	1/1	0.12	-1.87	11,11,11,11	0
2	MG	A	445	1/1	0.11	-2.14	15,15,15,15	0
2	MG	J	445	1/1	0.09	-2.26	16,16,16,16	0
2	MG	F	445	1/1	0.10	-2.53	21,21,21,21	0
2	MG	C	445	1/1	0.10	-3.54	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.