



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 03:19 AM GMT

PDB ID : 3MV3  
Title : Crystal Structure of  $\alpha$ -COP in Complex with e-COP  
Authors : Hoelz, A.; Hsia, K.C.  
Deposited on : 2010-05-03  
Resolution : 3.25 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>

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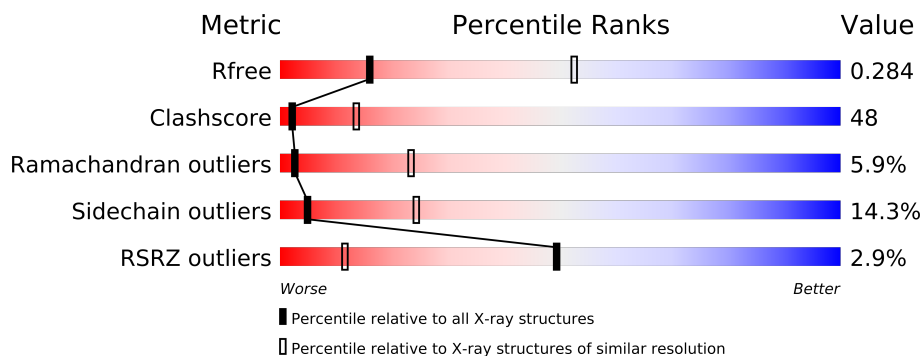
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 3.25 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	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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	325	
1	C	325	
1	E	325	
2	B	310	
2	D	310	
2	F	310	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14256 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP P53622
A	-21	GLY	-	EXPRESSION TAG	UNP P53622
A	-20	SER	-	EXPRESSION TAG	UNP P53622
A	-19	SER	-	EXPRESSION TAG	UNP P53622
A	-18	HIS	-	EXPRESSION TAG	UNP P53622
A	-17	HIS	-	EXPRESSION TAG	UNP P53622
A	-16	HIS	-	EXPRESSION TAG	UNP P53622
A	-15	HIS	-	EXPRESSION TAG	UNP P53622
A	-14	HIS	-	EXPRESSION TAG	UNP P53622
A	-13	HIS	-	EXPRESSION TAG	UNP P53622
A	-12	SER	-	EXPRESSION TAG	UNP P53622
A	-11	SER	-	EXPRESSION TAG	UNP P53622
A	-10	GLY	-	EXPRESSION TAG	UNP P53622
A	-9	LEU	-	EXPRESSION TAG	UNP P53622
A	-8	GLU	-	EXPRESSION TAG	UNP P53622
A	-7	VAL	-	EXPRESSION TAG	UNP P53622
A	-6	LEU	-	EXPRESSION TAG	UNP P53622
A	-5	PHE	-	EXPRESSION TAG	UNP P53622
A	-4	GLN	-	EXPRESSION TAG	UNP P53622
A	-3	GLY	-	EXPRESSION TAG	UNP P53622
A	-2	PRO	-	EXPRESSION TAG	UNP P53622
A	-1	HIS	-	EXPRESSION TAG	UNP P53622
A	0	MSE	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	EXPRESSION TAG	UNP P53622
C	-21	GLY	-	EXPRESSION TAG	UNP P53622
C	-20	SER	-	EXPRESSION TAG	UNP P53622
C	-19	SER	-	EXPRESSION TAG	UNP P53622
C	-18	HIS	-	EXPRESSION TAG	UNP P53622
C	-17	HIS	-	EXPRESSION TAG	UNP P53622
C	-16	HIS	-	EXPRESSION TAG	UNP P53622
C	-15	HIS	-	EXPRESSION TAG	UNP P53622
C	-14	HIS	-	EXPRESSION TAG	UNP P53622
C	-13	HIS	-	EXPRESSION TAG	UNP P53622
C	-12	SER	-	EXPRESSION TAG	UNP P53622
C	-11	SER	-	EXPRESSION TAG	UNP P53622
C	-10	GLY	-	EXPRESSION TAG	UNP P53622
C	-9	LEU	-	EXPRESSION TAG	UNP P53622
C	-8	GLU	-	EXPRESSION TAG	UNP P53622
C	-7	VAL	-	EXPRESSION TAG	UNP P53622
C	-6	LEU	-	EXPRESSION TAG	UNP P53622
C	-5	PHE	-	EXPRESSION TAG	UNP P53622
C	-4	GLN	-	EXPRESSION TAG	UNP P53622
C	-3	GLY	-	EXPRESSION TAG	UNP P53622
C	-2	PRO	-	EXPRESSION TAG	UNP P53622
C	-1	HIS	-	EXPRESSION TAG	UNP P53622
C	0	MSE	-	EXPRESSION TAG	UNP P53622
E	-22	MSE	-	EXPRESSION TAG	UNP P53622
E	-21	GLY	-	EXPRESSION TAG	UNP P53622
E	-20	SER	-	EXPRESSION TAG	UNP P53622
E	-19	SER	-	EXPRESSION TAG	UNP P53622
E	-18	HIS	-	EXPRESSION TAG	UNP P53622
E	-17	HIS	-	EXPRESSION TAG	UNP P53622
E	-16	HIS	-	EXPRESSION TAG	UNP P53622
E	-15	HIS	-	EXPRESSION TAG	UNP P53622
E	-14	HIS	-	EXPRESSION TAG	UNP P53622
E	-13	HIS	-	EXPRESSION TAG	UNP P53622
E	-12	SER	-	EXPRESSION TAG	UNP P53622
E	-11	SER	-	EXPRESSION TAG	UNP P53622
E	-10	GLY	-	EXPRESSION TAG	UNP P53622
E	-9	LEU	-	EXPRESSION TAG	UNP P53622
E	-8	GLU	-	EXPRESSION TAG	UNP P53622
E	-7	VAL	-	EXPRESSION TAG	UNP P53622
E	-6	LEU	-	EXPRESSION TAG	UNP P53622
E	-5	PHE	-	EXPRESSION TAG	UNP P53622
E	-4	GLN	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P53622
E	-2	PRO	-	EXPRESSION TAG	UNP P53622
E	-1	HIS	-	EXPRESSION TAG	UNP P53622
E	0	MSE	-	EXPRESSION TAG	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	D	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	F	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MSE	-	EXPRESSION TAG	UNP P40509
B	-12	GLY	-	EXPRESSION TAG	UNP P40509
B	-11	SER	-	EXPRESSION TAG	UNP P40509
B	-10	SER	-	EXPRESSION TAG	UNP P40509
B	-9	HIS	-	EXPRESSION TAG	UNP P40509
B	-8	HIS	-	EXPRESSION TAG	UNP P40509
B	-7	HIS	-	EXPRESSION TAG	UNP P40509
B	-6	HIS	-	EXPRESSION TAG	UNP P40509
B	-5	HIS	-	EXPRESSION TAG	UNP P40509
B	-4	HIS	-	EXPRESSION TAG	UNP P40509
B	-3	SER	-	EXPRESSION TAG	UNP P40509
B	-2	GLN	-	EXPRESSION TAG	UNP P40509
B	-1	ASP	-	EXPRESSION TAG	UNP P40509
B	0	PRO	-	EXPRESSION TAG	UNP P40509
D	-13	MSE	-	EXPRESSION TAG	UNP P40509
D	-12	GLY	-	EXPRESSION TAG	UNP P40509
D	-11	SER	-	EXPRESSION TAG	UNP P40509
D	-10	SER	-	EXPRESSION TAG	UNP P40509
D	-9	HIS	-	EXPRESSION TAG	UNP P40509
D	-8	HIS	-	EXPRESSION TAG	UNP P40509
D	-7	HIS	-	EXPRESSION TAG	UNP P40509
D	-6	HIS	-	EXPRESSION TAG	UNP P40509
D	-5	HIS	-	EXPRESSION TAG	UNP P40509
D	-4	HIS	-	EXPRESSION TAG	UNP P40509

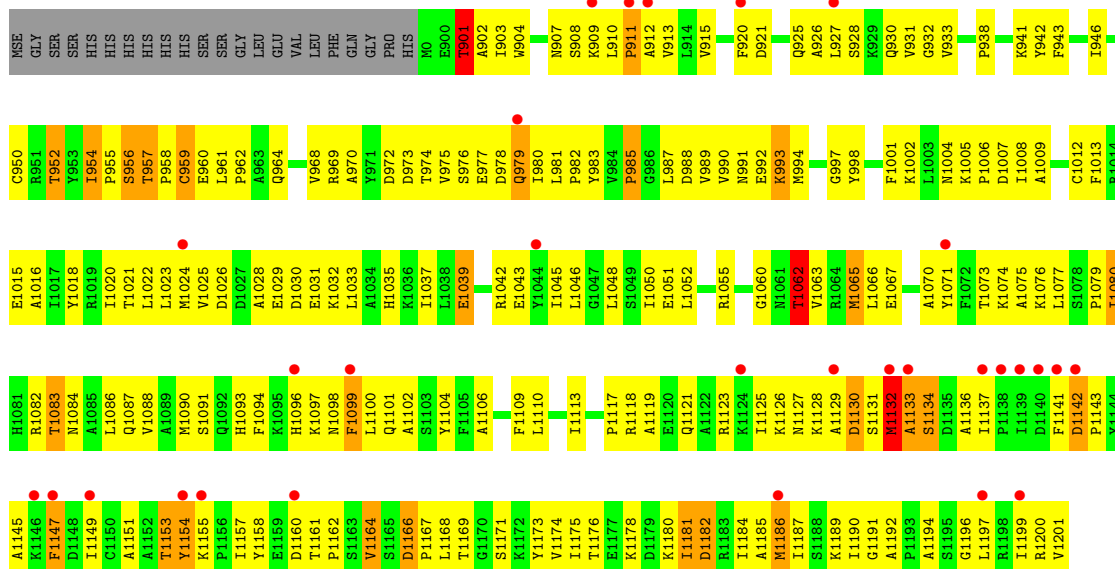
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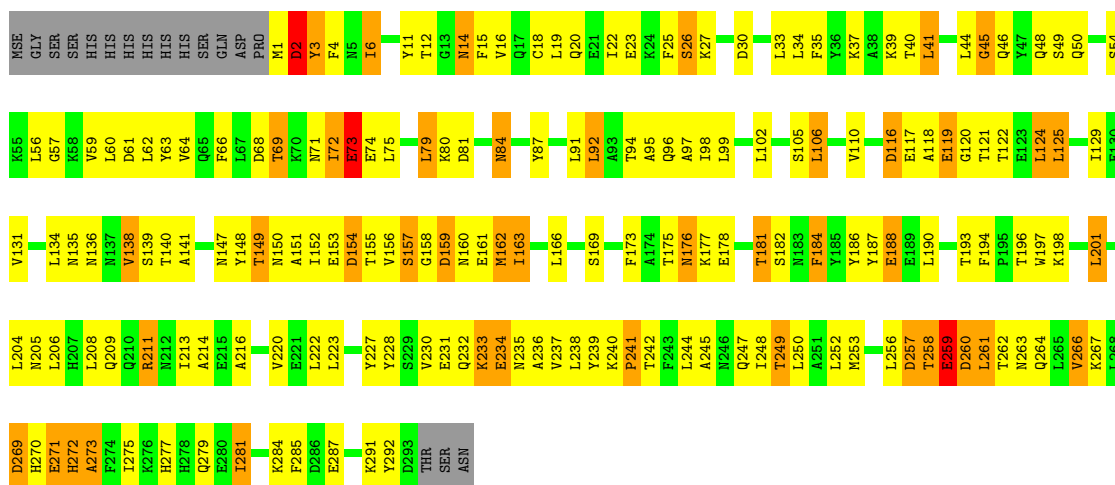
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MSE	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION TAG	UNP P40509
F	-11	SER	-	EXPRESSION TAG	UNP P40509
F	-10	SER	-	EXPRESSION TAG	UNP P40509
F	-9	HIS	-	EXPRESSION TAG	UNP P40509
F	-8	HIS	-	EXPRESSION TAG	UNP P40509
F	-7	HIS	-	EXPRESSION TAG	UNP P40509
F	-6	HIS	-	EXPRESSION TAG	UNP P40509
F	-5	HIS	-	EXPRESSION TAG	UNP P40509
F	-4	HIS	-	EXPRESSION TAG	UNP P40509
F	-3	SER	-	EXPRESSION TAG	UNP P40509
F	-2	GLN	-	EXPRESSION TAG	UNP P40509
F	-1	ASP	-	EXPRESSION TAG	UNP P40509
F	0	PRO	-	EXPRESSION TAG	UNP P40509



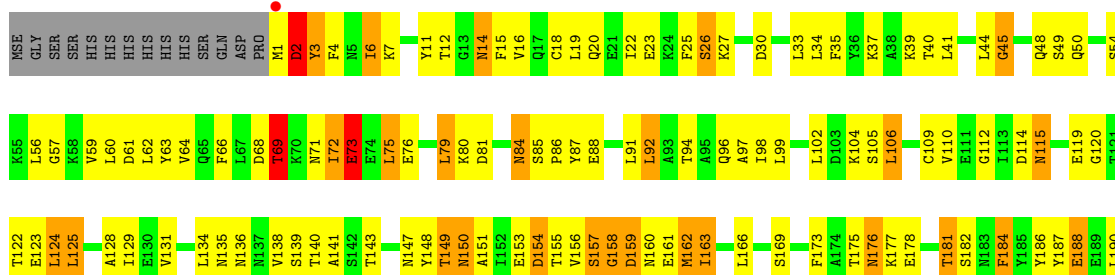
- Molecule 1: Coatomer subunit alpha

Chain E: 

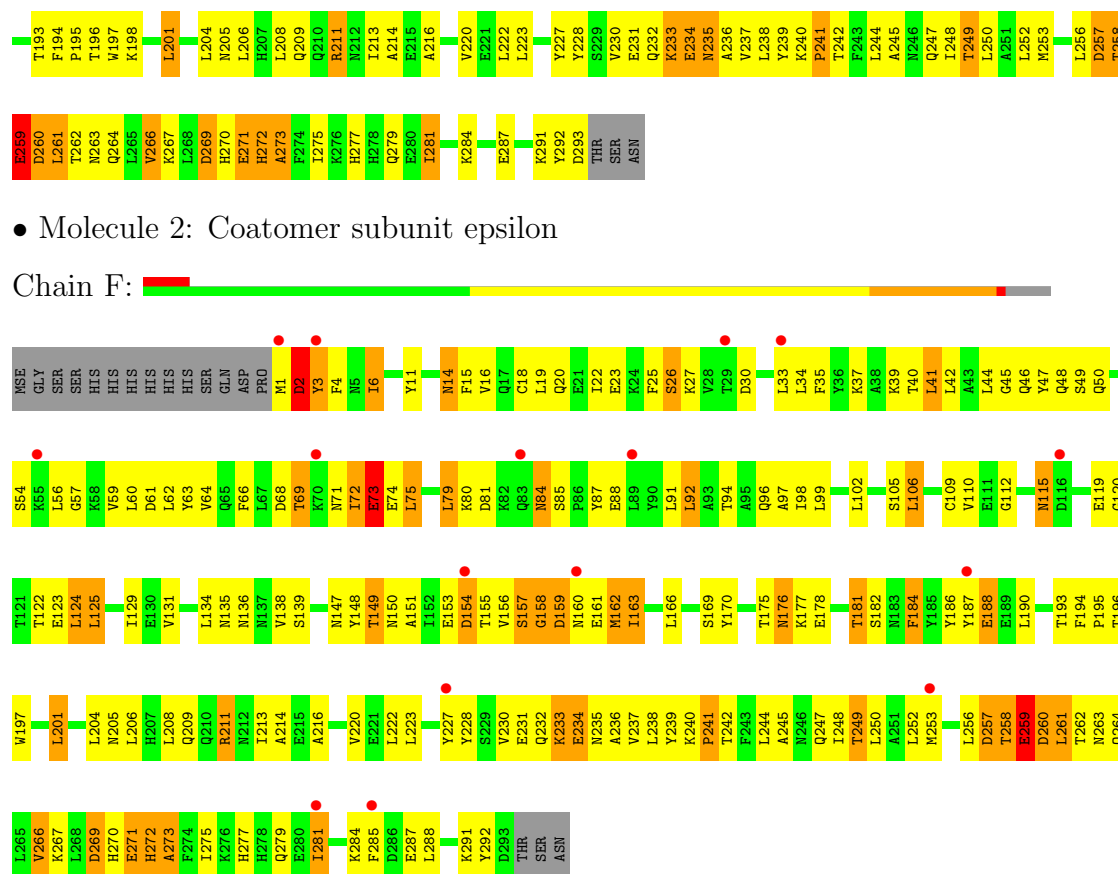
- Molecule 2: Coatomer subunit epsilon

Chain B: 

- Molecule 2: Coatomer subunit epsilon

Chain D: 





• Molecule 2: Coatomer subunit epsilon

Chain F:

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.13Å 74.31Å 96.40Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 48.68 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-3.25) 96.1 (48.68-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.287 0.249 , 0.284	Depositor DCC
$R_{free}$ test set	1705 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 90.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 68519 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.50	0/2429	0.79	1/3273 (0.0%)
1	C	0.49	0/2429	0.79	1/3273 (0.0%)
1	E	0.47	0/2429	0.78	1/3273 (0.0%)
2	B	0.51	0/2401	0.76	1/3255 (0.0%)
2	D	0.51	0/2401	0.76	1/3255 (0.0%)
2	F	0.49	0/2401	0.75	1/3255 (0.0%)
All	All	0.49	0/14490	0.77	6/19584 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1155	LYS	N-CA-C	-5.69	95.63	111.00
1	A	1155	LYS	N-CA-C	-5.69	95.65	111.00
1	E	1155	LYS	N-CA-C	-5.68	95.67	111.00
2	F	125	LEU	CA-CB-CG	-5.21	103.31	115.30
2	B	125	LEU	CA-CB-CG	-5.18	103.37	115.30

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	2388	0	2441	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2388	0	2441	246	0
1	E	2388	0	2441	249	0
2	B	2364	0	2319	214	0
2	D	2364	0	2319	239	0
2	F	2364	0	2319	215	0
All	All	14256	0	14280	1363	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 48.

The worst 5 of 1363 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1090:MSE:HE2	1:C:1106:ALA:HA	1.30	1.12
1:E:1090:MSE:HE2	1:E:1106:ALA:HA	1.29	1.12
1:C:1028:ALA:HB2	1:C:1200:ARG:CZ	1.80	1.10
2:B:211:ARG:HB2	2:B:211:ARG:HH11	1.11	1.10
1:A:1090:MSE:HE2	1:A:1106:ALA:HA	1.30	1.08

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	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	3	29
1	C	301/325 (93%)	232 (77%)	53 (18%)	16 (5%)	3	26
1	E	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	3	29
2	B	291/310 (94%)	211 (72%)	59 (20%)	21 (7%)	2	16
2	D	291/310 (94%)	215 (74%)	56 (19%)	20 (7%)	2	17
2	F	291/310 (94%)	212 (73%)	61 (21%)	18 (6%)	2	21
All	All	1776/1905 (93%)	1336 (75%)	335 (19%)	105 (6%)	2	23

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	957	THR
1	A	973	ASP
1	A	977	GLU
1	A	979	GLN
1	A	985	PRO

### 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	257/268 (96%)	226 (88%)	31 (12%)	7	34
1	C	257/268 (96%)	226 (88%)	31 (12%)	7	34
1	E	257/268 (96%)	226 (88%)	31 (12%)	7	34
2	B	263/275 (96%)	221 (84%)	42 (16%)	3	18
2	D	263/275 (96%)	218 (83%)	45 (17%)	3	16
2	F	263/275 (96%)	220 (84%)	43 (16%)	3	17
All	All	1560/1629 (96%)	1337 (86%)	223 (14%)	5	24

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1166	ASP
2	D	124	LEU
2	F	163	ILE
1	C	1182	ASP
2	D	69	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	GLN
1	C	1093	HIS
1	C	1101	GLN
2	D	50	GLN
2	F	50	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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	303/325 (93%)	-0.02	3 (0%) 79 32	47, 89, 149, 193	0
1	C	303/325 (93%)	0.03	2 (0%) 84 40	56, 111, 177, 201	0
1	E	303/325 (93%)	0.67	30 (9%) 8 2	113, 171, 201, 201	0
2	B	293/310 (94%)	-0.04	0 100 100	44, 96, 169, 188	0
2	D	293/310 (94%)	0.01	1 (0%) 91 60	59, 110, 174, 201	0
2	F	293/310 (94%)	0.41	16 (5%) 24 5	92, 177, 201, 201	0
All	All	1788/1905 (93%)	0.18	52 (2%) 49 11	44, 127, 196, 201	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1197	LEU	5.8
1	A	0	MSE	5.6
1	E	1141	PHE	5.5
2	D	1	MSE	4.4
1	E	1024	MSE	4.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.