



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 4, 2017 – 07:13 PM EDT

PDB ID : 5D98
Title : Influenza C Virus RNA-dependent RNA Polymerase - Space group P43212
Authors : Hengrung, N.; El Omari, K.; Serna Martin, I.; Vreede, F.T.; Cusack, S.; Rambo, R.P.; Vonrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor, E.
Deposited on : unknown
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

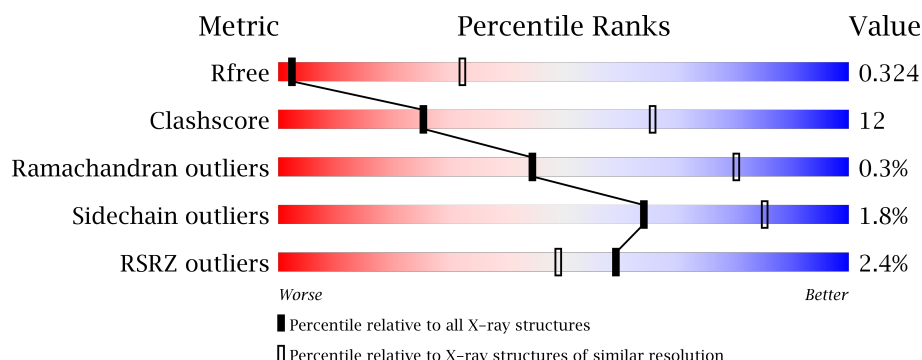
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	709	<div> <div>2%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>
1	D	709	<div> <div>%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
2	B	754	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>
2	E	754	<div> <div>3%</div> <div>73%</div> <div>20%</div> <div>6%</div> </div>
3	C	782	<div> <div>3%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	782	<div><div></div><div>3%</div><div>67%</div><div>29%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34720 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	D	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	E	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	F	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	ALA	-	expression tag	UNP Q9IMP3
C	776	ARG	-	expression tag	UNP Q9IMP3
C	777	GLU	-	expression tag	UNP Q9IMP3
C	778	ASN	-	expression tag	UNP Q9IMP3
C	779	LEU	-	expression tag	UNP Q9IMP3
C	780	TYR	-	expression tag	UNP Q9IMP3
C	781	PHE	-	expression tag	UNP Q9IMP3
C	782	GLN	-	expression tag	UNP Q9IMP3

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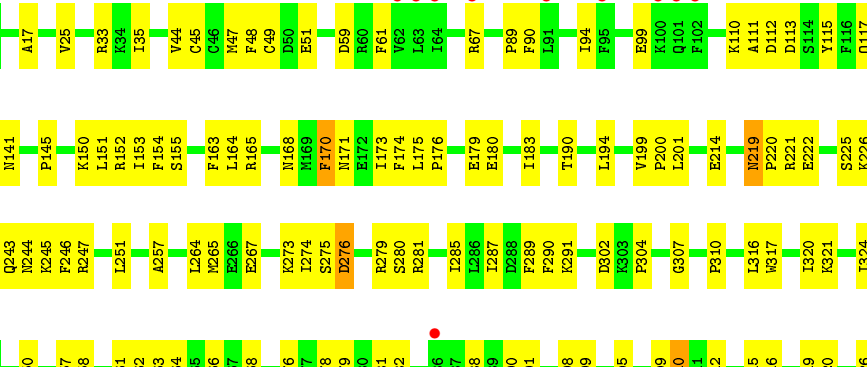
Chain	Residue	Modelled	Actual	Comment	Reference
F	775	ALA	-	expression tag	UNP Q9IMP3
F	776	ARG	-	expression tag	UNP Q9IMP3
F	777	GLU	-	expression tag	UNP Q9IMP3
F	778	ASN	-	expression tag	UNP Q9IMP3
F	779	LEU	-	expression tag	UNP Q9IMP3
F	780	TYR	-	expression tag	UNP Q9IMP3
F	781	PHE	-	expression tag	UNP Q9IMP3
F	782	GLN	-	expression tag	UNP Q9IMP3

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

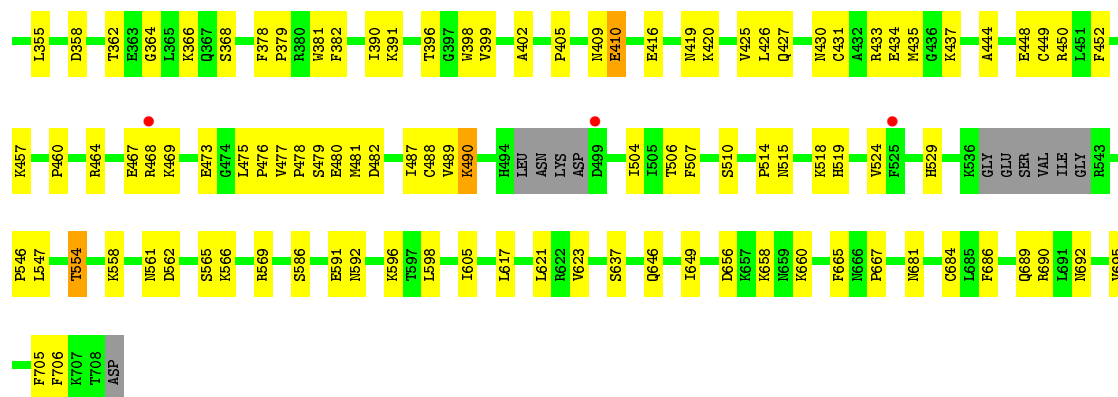
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain A: 

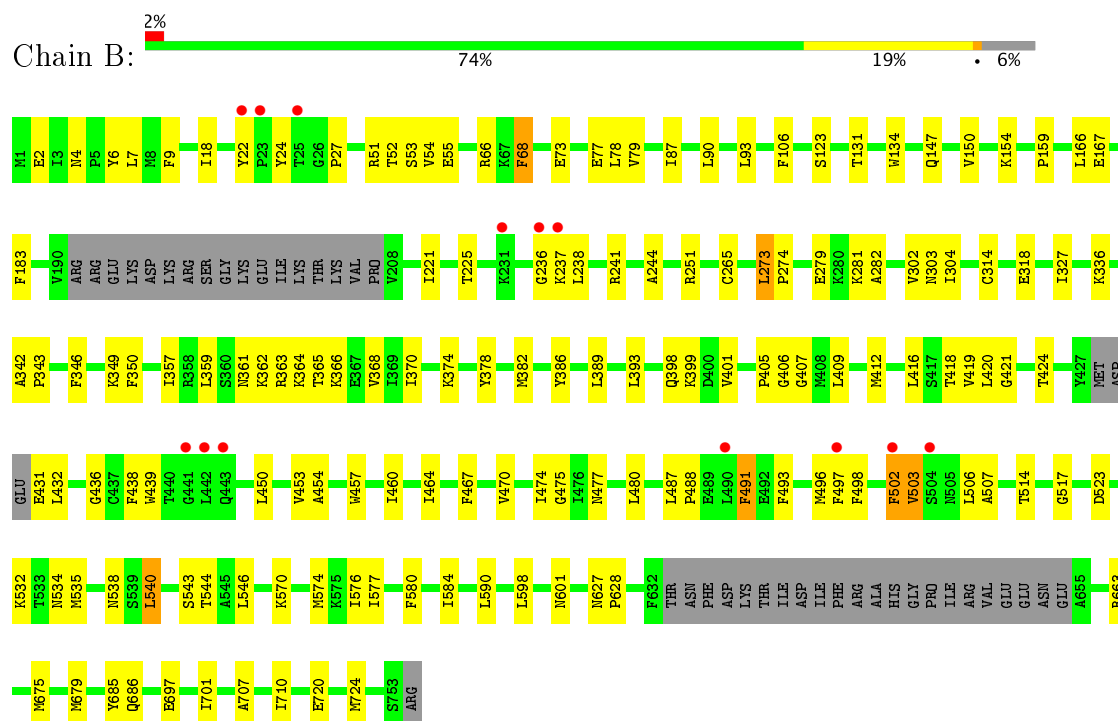


Position	Amino Acid	Frequency (bits)
1	Q620	0.01
2	N659	0.01
3	K680	0.01
4	Y522	0.01
5	T523	0.01
6	V524	0.01
7	P667	0.01
8	G536	0.01
9	GLY	0.01
10	L671	0.01
11	GLU	0.01
12	GLU	0.01
13	SER	0.01
14	VAL	0.01
15	ILE	0.01
16	ILE	0.01
17	R543	0.01
18	N681	0.01
19	L547	0.01
20	C684	0.01
21	L685	0.01
22	F686	0.01
23	T553	0.01
24	T554	0.01
25	R690	0.01
26	K558	0.01
27	L694	0.01
28	V695	0.01
29	N561	0.01
30	D562	0.01
31	S565	0.01
32	K706	0.01
33	K566	0.01
34	T708	0.01
35	ASP	0.01
36	R569	0.01
37	M575	0.01
38	S586	0.01
39	E591	0.01
40	N592	0.01
41	L593	0.01
42	I605	0.01
43	L621	0.01
44	R622	0.01
45	V623	0.01
46	V626	0.01
47	N635	0.01
48	N644	0.01
49	E645	0.01
50	Q646	0.01
51	T649	0.01
52	N651	0.01
53	D656	0.01
54	K657	0.01
55	T659	0.01
56	K437	0.01
57	T441	0.01
58	A444	0.01
59	L445	0.01
60	E448	0.01
61	C449	0.01
62	F452	0.01
63	K457	0.01
64	V458	0.01
65	V459	0.01
66	I461	0.01
67	R464	0.01
68	S465	0.01
69	K466	0.01
70	E467	0.01
71	R468	0.01
72	N471	0.01
73	L475	0.01
74	P476	0.01
75	V477	0.01
76	R478	0.01
77	S479	0.01
78	N481	0.01
79	D482	0.01
80	T487	0.01
81	C488	0.01
82	V489	0.01
83	K490	0.01
84	H494	0.01
85	L500	0.01
86	ASN	0.01
87	LVS	0.01
88	ASP	0.01
89	D499	0.01
90	T504	0.01
91	I505	0.01
92	T506	0.01
93	F507	0.01
94	F508	0.01
95	F509	0.01
96	S510	0.01
97	P514	0.01
98	K518	0.01
99	H519	0.01
100	F339	0.01
101	G342	0.01
102	ILE	0.01
103	GLY	0.01
104	R345	0.01
105	I350	0.01
106	Q357	0.01
107	D358	0.01
108	T361	0.01
109	T362	0.01
110	E363	0.01
111	G364	0.01
112	K366	0.01
113	Q367	0.01
114	S368	0.01
115	R376	0.01
116	S377	0.01
117	F378	0.01
118	P379	0.01
119	N381	0.01
120	F382	0.01
121	N386	0.01
122	P387	0.01
123	K388	0.01
124	A389	0.01
125	I390	0.01
126	K391	0.01
127	K398	0.01
128	V399	0.01
129	P405	0.01
130	M409	0.01
131	E410	0.01
132	L411	0.01
133		

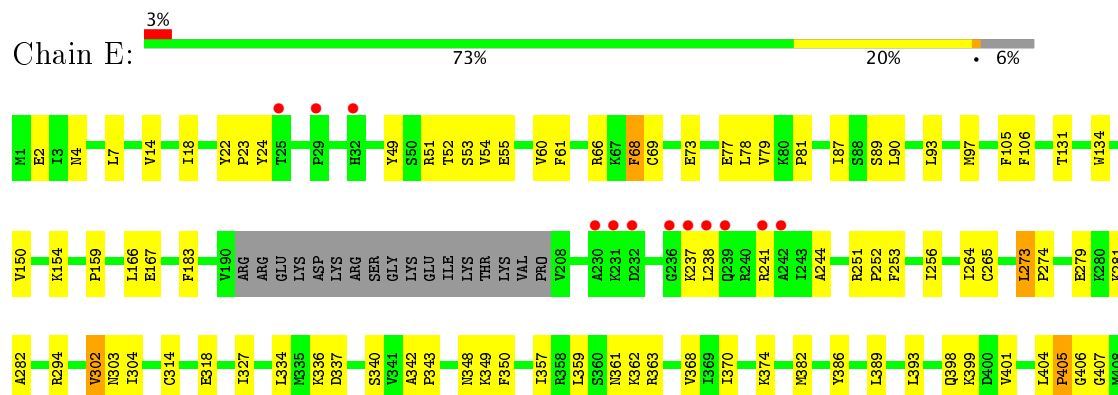
- Chain D: 

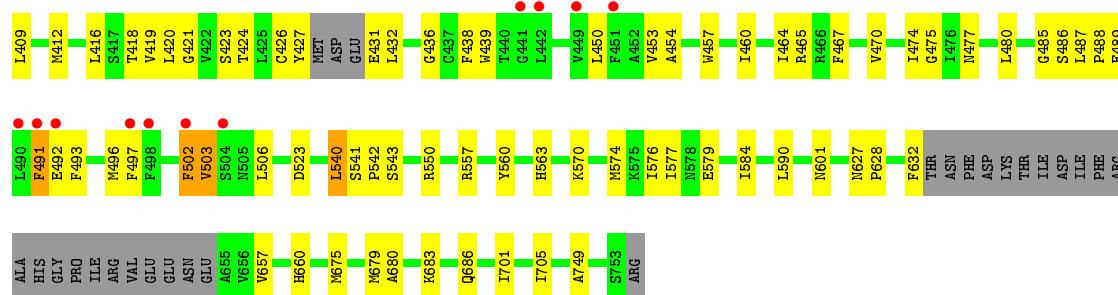


- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 2: RNA-directed RNA polymerase catalytic subunit







4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.66Å 185.66Å 598.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.90 100.57 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-3.90) 98.8 (100.57-3.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.286 , 0.326 0.286 , 0.324	Depositor DCC
R_{free} test set	4770 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	161.2	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 132.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34720	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/5746	0.57	1/7717 (0.0%)
1	D	0.43	0/5746	0.57	1/7717 (0.0%)
2	B	0.40	0/5749	0.56	0/7723
2	E	0.41	0/5749	0.57	0/7723
3	C	0.41	0/6185	0.59	0/8322
3	F	0.42	0/6185	0.59	0/8322
All	All	0.41	0/35360	0.58	2/47524 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASN	C-N-CD	5.11	139.14	128.40
1	D	219	ASN	C-N-CD	5.11	139.12	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5630	0	5632	147	0
1	D	5630	0	5632	167	0
2	B	5652	0	5749	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5652	0	5749	126	0
3	C	6076	0	6183	182	0
3	F	6076	0	6183	198	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
All	All	34720	0	35128	840	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 12.

The worst 5 of 840 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)
3:F:138:LYS:HE2	3:F:250:GLU:CG	1.22	1.59
3:F:138:LYS:CE	3:F:250:GLU:HG2	1.34	1.48
3:F:138:LYS:CE	3:F:250:GLU:CG	1.83	1.46
3:F:138:LYS:CE	3:F:250:GLU:CD	1.86	1.41
3:F:138:LYS:NZ	3:F:250:GLU:HG2	1.33	1.36

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	685/709 (97%)	643 (94%)	42 (6%)	0	100	100
1	D	685/709 (97%)	645 (94%)	40 (6%)	0	100	100
2	B	703/754 (93%)	666 (95%)	35 (5%)	2 (0%)	44	80
2	E	703/754 (93%)	673 (96%)	27 (4%)	3 (0%)	38	76
3	C	756/782 (97%)	688 (91%)	63 (8%)	5 (1%)	25	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	38	76
All	All	4288/4490 (96%)	4001 (93%)	274 (6%)	13 (0%)	44	80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	405	PRO
3	C	698	GLY
2	E	405	PRO
2	B	503	VAL
2	E	503	VAL

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	618/631 (98%)	603 (98%)	15 (2%)	54	79
1	D	618/631 (98%)	608 (98%)	10 (2%)	68	86
2	B	629/669 (94%)	620 (99%)	9 (1%)	71	87
2	E	629/669 (94%)	618 (98%)	11 (2%)	66	86
3	C	669/686 (98%)	660 (99%)	9 (1%)	73	88
3	F	669/686 (98%)	655 (98%)	14 (2%)	59	82
All	All	3832/3972 (96%)	3764 (98%)	68 (2%)	64	85

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	450	MET
1	D	366	LYS
3	F	445	TYR
3	C	594	LEU
1	D	48	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	550	GLN
1	D	141	ASN
3	F	717	ASN
3	C	717	ASN
1	D	31	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	693/709 (97%)	-0.05	17 (2%) 58 47	132, 195, 269, 299	0
1	D	693/709 (97%)	-0.11	4 (0%) 89 84	129, 191, 258, 295	0
2	B	711/754 (94%)	-0.03	13 (1%) 69 59	131, 192, 256, 317	0
2	E	711/754 (94%)	0.06	23 (3%) 48 38	130, 184, 266, 315	0
3	C	762/782 (97%)	0.02	23 (3%) 51 40	149, 222, 285, 358	0
3	F	762/782 (97%)	0.13	26 (3%) 46 36	134, 224, 287, 343	0
All	All	4332/4490 (96%)	0.00	106 (2%) 59 49	129, 202, 275, 358	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	242	ALA	6.1
3	F	631	HIS	5.3
2	E	237	LYS	5.1
3	C	1	MET	4.8
3	C	696	VAL	4.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
4	MG	A	801	1/1	0.93	0.10	-1.07	185,185,185,185	0
4	MG	D	800	1/1	0.94	0.09	-1.28	200,200,200,200	0
4	MG	A	800	1/1	0.89	0.07	-1.43	204,204,204,204	0
4	MG	D	801	1/1	0.90	0.16	-	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.